



## Full wwPDB EM Validation Report ⓘ

Mar 19, 2026 – 09:49 PM UTC

PDB ID : 7T64 / pdb\_00007t64  
EMDB ID : EMD-25709  
Title : Rabbit RyR1 disease mutant Y523S in complex with FKBP12.6 embedded in lipidic nanodisc in the closed state  
Authors : Iyer, K.A.; Hu, Y.; Murayama, T.; Samso, M.  
Deposited on : 2021-12-13  
Resolution : 4.00 Å(reported)  
Based on initial model : 6WOT

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

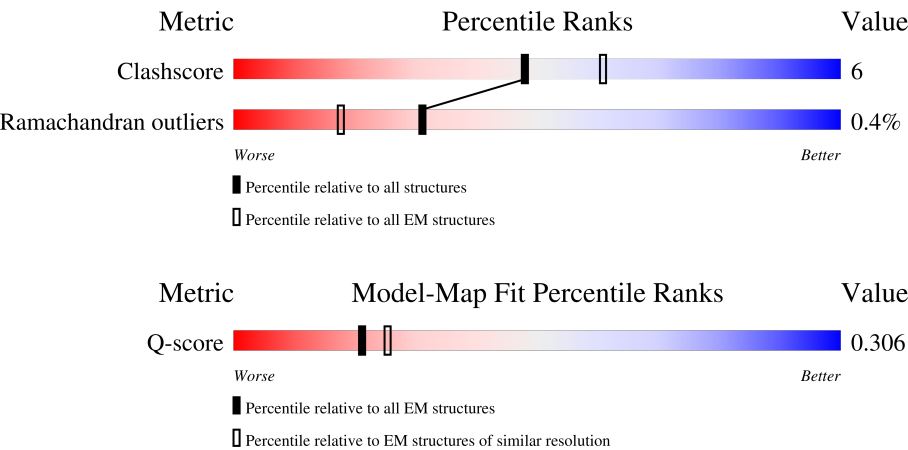
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins)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

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 4.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Q-score               | -                           | 25397                       | 7587 ( 3.50 - 4.50 )                                     |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain                                                    |
|-----|-------|--------|---------------------------------------------------------------------|
| 1   | A     | 5037   | <div><div>15%</div><div>72%</div><div>13%</div><div>16%</div></div> |
| 1   | B     | 5037   | <div><div>15%</div><div>72%</div><div>12%</div><div>16%</div></div> |
| 1   | C     | 5037   | <div><div>15%</div><div>72%</div><div>13%</div><div>16%</div></div> |
| 1   | D     | 5037   | <div><div>15%</div><div>72%</div><div>12%</div><div>16%</div></div> |
| 2   | E     | 107    | <div><div>7%</div><div>82%</div><div>18%</div></div>                |

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| Mol | Chain | Length | Quality of chain                                                                   |
|-----|-------|--------|------------------------------------------------------------------------------------|
| 2   | F     | 107    |  |
| 2   | G     | 107    |  |
| 2   | H     | 107    |  |

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 134196 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ryanodine receptor 1.

| Mol | Chain | Residues | Atoms |       |      |      |     | AltConf | Trace |
|-----|-------|----------|-------|-------|------|------|-----|---------|-------|
| 1   | A     | 4247     | Total | C     | N    | O    | S   | 0       | 0     |
|     |       |          | 32730 | 20849 | 5597 | 6079 | 205 |         |       |
| 1   | B     | 4247     | Total | C     | N    | O    | S   | 0       | 0     |
|     |       |          | 32730 | 20849 | 5597 | 6079 | 205 |         |       |
| 1   | C     | 4247     | Total | C     | N    | O    | S   | 0       | 0     |
|     |       |          | 32730 | 20849 | 5597 | 6079 | 205 |         |       |
| 1   | D     | 4247     | Total | C     | N    | O    | S   | 0       | 0     |
|     |       |          | 32730 | 20849 | 5597 | 6079 | 205 |         |       |

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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





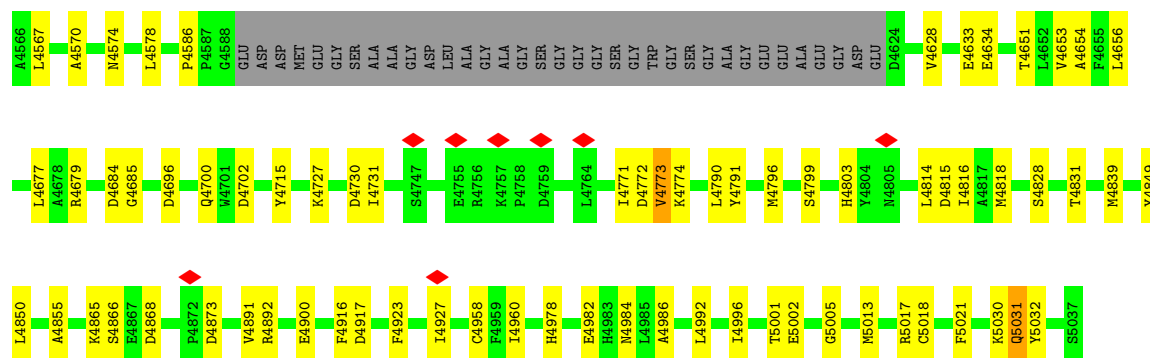




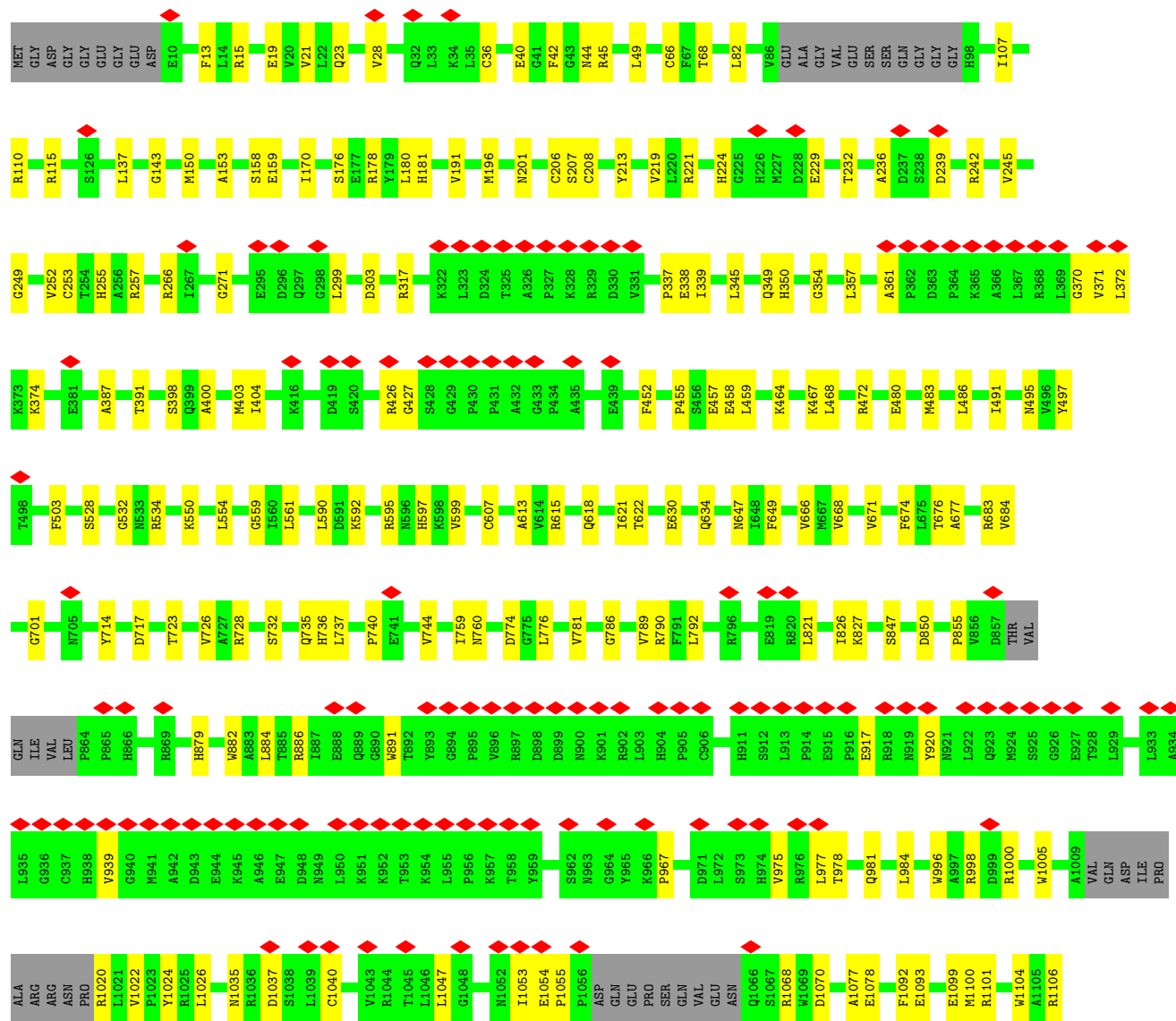


|       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| V3107 | E3108 | N3109 | L3110 | R3111 | LEU   | GLY   | LYS   | VAL   | K3023 | V3024 | L3025 | GLY   | THR   | GLN   | VAL   | L3029 | H3030 | A3031 | K3034 | T3040 | K3045 | H3052 | V3053 | S3055 | L3056 | F3057 | G3058 | T3059 | D3060 | A3061 | R3073 | A3077 | R3078 | T3079 | V3080 | M3081 | S3082 | G3084 | P3085 | E3086 | I3087 | V3088 | K3089 | A3090 | G3091 | S3094 | D3102 | I3103 | E3104 | K3105 | M3106 | K3178 | K3179 |       |       |       |       |       |
| Q2993 | I3001 | L3002 | P3021 | A3022 | K3023 | V3024 | L3025 | GLY   | THR   | GLN   | VAL   | L3029 | H3030 | A3031 | K3034 | T3040 | K3045 | H3052 | V3053 | S3055 | L3056 | F3057 | G3058 | T3059 | D3060 | A3061 | R3073 | A3077 | R3078 | T3079 | V3080 | M3081 | S3082 | G3084 | P3085 | E3086 | I3087 | V3088 | K3089 | A3090 | G3091 | S3094 | D3102 | I3103 | E3104 | K3105 | M3106 | K3178 | K3179 |       |       |       |       |       |       |       |       |       |
| E2917 | R2918 | D2919 | R2920 | E2921 | K2922 | A2923 | Q2924 | E2925 | L2926 | L2927 | K2928 | F2929 | L2930 | Q2931 | M2932 | M2933 | Q2934 | Y2935 | A2936 | V2937 | L2938 | R2939 | Q2940 | L2941 | K2942 | D2943 | M2944 | E2945 | L2946 | D2947 | T2948 | S2949 | K2953 | F2959 | V2966 | E2972 | F2973 | I2974 | A2975 | H2976 | L2977 | E2978 | ALA   | VAL   | VAL   | SER   | SER   | GLY   | ARG   | VAL   | GLU   | LYS   | SER   | PRO   | HIS   |       |       |       |
| Q2993 | I3001 | L3002 | P3021 | A3022 | K3023 | V3024 | L3025 | GLY   | THR   | GLN   | VAL   | L3029 | H3030 | A3031 | K3034 | T3040 | K3045 | H3052 | V3053 | S3055 | L3056 | F3057 | G3058 | T3059 | D3060 | A3061 | R3073 | A3077 | R3078 | T3079 | V3080 | M3081 | S3082 | G3084 | P3085 | E3086 | I3087 | V3088 | K3089 | A3090 | G3091 | S3094 | D3102 | I3103 | E3104 | K3105 | M3106 | K3178 | K3179 |       |       |       |       |       |       |       |       |       |
| E2917 | R2918 | D2919 | R2920 | E2921 | K2922 | A2923 | Q2924 | E2925 | L2926 | L2927 | K2928 | F2929 | L2930 | Q2931 | M2932 | M2933 | Q2934 | Y2935 | A2936 | V2937 | L2938 | R2939 | Q2940 | L2941 | K2942 | D2943 | M2944 | E2945 | L2946 | D2947 | T2948 | S2949 | K2953 | F2959 | V2966 | E2972 | F2973 | I2974 | A2975 | H2976 | L2977 | E2978 | ALA   | VAL   | VAL   | SER   | SER   | GLY   | ARG   | VAL   | GLU   | LYS   | SER   | PRO   | HIS   |       |       |       |
| E2670 | E2671 | L2672 | H2673 | L2674 | T2675 | R2676 | K2677 | L2678 | V2679 | W2680 | G2681 | K2690 | TYR   | ASP   | GLN   | GLU   | LEU   | TYR   | ARG   | MET   | ALA   | PRO   | CYS   | LEU   | CYS   | ALA   | ILE   | GLY   | ALA   | LEU   | PRO   | ASP   | TYR   | VAL   | ASP   | SER   | TYR   | SER   | SER   | SER   | LYS   | GLU   | ALA   | LYS   | LYS   | ALA   | THR   | VAL   | ASP   | ALA   | GLY   | N2734 | F2735 | D2736 |       |       |       |       |
| E2670 | E2671 | L2672 | H2673 | L2674 | T2675 | R2676 | K2677 | L2678 | V2679 | W2680 | G2681 | K2690 | TYR   | ASP   | GLN   | GLU   | LEU   | TYR   | ARG   | MET   | ALA   | PRO   | CYS   | LEU   | CYS   | ALA   | ILE   | GLY   | ALA   | LEU   | PRO   | ASP   | TYR   | VAL   | ASP   | SER   | TYR   | SER   | SER   | SER   | LYS   | GLU   | ALA   | LYS   | LYS   | ALA   | THR   | VAL   | ASP   | ALA   | GLY   | N2734 | F2735 | D2736 |       |       |       |       |
| F2737 | R2738 | F2739 | V2740 | E2741 | T2742 | L2743 | N2744 | V2745 | L2746 | L2747 | P2748 | E2749 | K2750 | L2751 | D2752 | S2753 | T2754 | L2755 | N2756 | L2757 | I2758 | A2759 | E2760 | V2761 | T2762 | H2763 | E2764 | K2765 | W2766 | A2767 | F2768 | Q2769 | K2770 | I2771 | Q2772 | N2773 | W2774 | W2775 | S2776 | V2777 | Q2778 | E2779 | N2780 | W2781 | D2782 | E2783 | E2784 | L2785 | T2786 | T2787 | H2788 | F2789 | L2791 | T2792 | F2793 | V2794 | K2795 | T2796 |
| F2797 | S2798 | E2799 | K2800 | D2801 | K2802 | E2803 | I2804 | Y2805 | R2806 | W2807 | P2808 | L2809 | K2810 | E2811 | S2812 | L2813 | K2814 | A2815 | M2816 | L2817 | L2818 | W2819 | E2820 | W2821 | T2822 | L2823 | N2824 | T2825 | A2826 | R2827 | E2828 | K2829 | E2830 | GLU   | GLU   | THR   | GLU   | LYS   | LYS   | THR   | ARG   | LYS   | ILE   | SER   | GLN   | THR   | ALA   | GLN   | THR   | TYR   | ASP   | PRO   | ARG   | GLU   | GLY   | Y2855 | N2856 |       |
| P2857 | Q2858 | P2859 | P2860 | D2861 | L2862 | S2863 | G2864 | V2865 | T2866 | L2867 | S2868 | R2869 | E2870 | L2871 | Q2872 | A2873 | A2874 | A2875 | E2876 | Q2877 | L2878 | A2879 | E2880 | N2881 | T2882 | H2883 | N2884 | T2885 | W2886 | G2887 | K2888 | K2889 | K2890 | K2891 | Q2892 | E2893 | L2894 | E2895 | A2896 | K2897 | E2898 | G2899 | Q2900 | T2901 | H2902 | P2903 | L2904 | L2905 | V2906 | P2907 | V2908 | D2909 | T2910 | L2911 | T2912 | A2913 | E2915 | K2916 |
| A2917 | R2918 | D2919 | R2920 | E2921 | K2922 | A2923 | Q2924 | E2925 | L2926 | L2927 | K2928 | F2929 | L2930 | Q2931 | M2932 | M2933 | Q2934 | Y2935 | A2936 | V2937 | L2938 | R2939 | Q2940 | L2941 | K2942 | D2943 | M2944 | E2945 | L2946 | D2947 | T2948 | S2949 | K2953 | F2959 | V2966 | E2972 | F2973 | I2974 | A2975 | H2976 | L2977 | E2978 | ALA   | VAL   | VAL   | SER   | SER   | GLY   | ARG   | VAL   | GLU   | LYS   | SER   | PRO   | HIS   |       |       |       |
| Q2993 | I3001 | L3002 | P3021 | A3022 | K3023 | V3024 | L3025 | GLY   | THR   | GLN   | VAL   | L3029 | H3030 | A3031 | K3034 | T3040 | K3045 | H3052 | V3053 | S3055 | L3056 | F3057 | G3058 | T3059 | D3060 | A3061 | R3073 | A3077 | R3078 | T3079 | V3080 | M3081 | S3082 | G3084 | P3085 | E3086 | I3087 | V3088 | K3089 | A3090 | G3091 | S3094 | D3102 | I3103 | E3104 | K3105 | M3106 | K3178 | K3179 |       |       |       |       |       |       |       |       |       |
| E3108 | N3109 | L3110 | R3111 | LEU   | GLY   | LYS   | VAL   | K3023 | V3024 | L3025 | GLY   | THR   | GLN   | VAL   | L3029 | H3030 | A3031 | K3034 | T3040 | K3045 | H3052 | V3053 | S3055 | L3056 | F3057 | G3058 | T3059 | D3060 | A3061 | R3073 | A3077 | R3078 | T3079 | V3080 | M3081 | S3082 | G3084 | P3085 | E3086 | I3087 | V3088 | K3089 | A3090 | G3091 | S3094 | D3102 | I3103 | E3104 | K3105 | M3106 | K3178 | K3179 |       |       |       |       |       |       |
| E3108 | N3109 | L3110 | R3111 | LEU   | GLY   | LYS   | VAL   | K3023 | V3024 | L3025 | GLY   | THR   | GLN   | VAL   | L3029 | H3030 | A3031 | K3034 | T3040 | K3045 | H3052 | V3053 | S3055 | L3056 | F3057 | G3058 | T3059 | D3060 | A3061 | R3073 | A3077 | R3078 | T3079 | V3080 | M3081 | S3082 | G3084 | P3085 | E3086 | I3087 | V3088 | K3089 | A3090 | G3091 | S3094 | D3102 | I3103 | E3104 | K3105 | M3106 | K3178 | K3179 |       |       |       |       |       |       |
| E3108 | N3109 | L3110 | R3111 | LEU   | GLY   | LYS   | VAL   | K3023 | V3024 | L3025 | GLY   | THR   | GLN   | VAL   | L3029 | H3030 | A3031 | K3034 | T3040 | K3045 | H3052 | V3053 | S3055 | L3056 | F3057 | G3058 | T3059 | D3060 | A3061 | R3073 | A3077 | R3078 | T3079 | V3080 | M3081 | S3082 | G3084 | P3085 | E3086 | I3087 | V3088 | K3089 | A3090 | G3091 | S3094 | D3102 | I3103 | E3104 | K3105 | M3106 | K3178 | K3179 |       |       |       |       |       |       |
| E3108 | N3109 | L3110 | R3111 | LEU   | GLY   | LYS   | VAL   | K3023 | V3024 | L3025 | GLY   | THR   | GLN   | VAL   | L3029 | H3030 | A3031 | K3034 | T3040 | K3045 | H3052 | V3053 | S3055 | L3056 | F3057 | G3058 | T3059 | D3060 | A3061 | R3073 | A3077 | R3078 | T3079 | V3080 | M3081 | S3082 | G3084 | P3085 | E3086 | I3087 | V3088 | K3089 | A3090 | G3091 | S3094 | D3102 | I3103 | E3104 | K3105 | M3106 | K3178 | K3179 |       |       |       |       |       |       |
| E3108 | N3109 | L3110 | R3111 | LEU   | GLY   | LYS   | VAL   | K3023 | V3024 | L3025 | GLY   | THR   | GLN   | VAL   | L3029 | H3030 | A3031 | K3034 | T3040 | K3045 | H3052 | V3053 | S3055 | L3056 | F3057 | G3058 | T3059 | D3060 | A3061 | R3073 | A3077 | R3078 | T3079 | V3080 | M3081 | S3082 | G3084 | P3085 | E3086 | I3087 | V3088 | K3089 | A3090 | G3091 | S3094 | D3102 | I3103 | E3104 | K3105 | M3106 | K3178 | K3179 |       |       |       |       |       |       |
| E3108 | N3109 | L3110 | R3111 | LEU   | GLY   | LYS   | VAL   | K3023 | V3024 | L3025 | GLY   | THR   | GLN   | VAL   | L3029 | H3030 | A3031 | K3034 | T3040 | K3045 | H3052 | V3053 | S3055 | L3056 | F3057 | G3058 | T3059 | D3060 | A3061 | R3073 | A3077 | R3078 | T3079 | V3080 | M3081 | S3082 | G3084 | P3085 | E3086 | I3087 | V3088 | K3089 | A3090 | G3091 | S3094 | D3102 | I3103 | E3104 | K3105 | M3106 | K3178 | K3179 |       |       |       |       |       |       |
| E3108 | N3109 | L3110 | R3111 | LEU   | GLY   | LYS   | VAL   | K3023 | V3024 | L3025 | GLY   | THR   | GLN   | VAL   | L3029 | H3030 | A3031 | K3034 | T3040 | K3045 | H3052 | V3053 | S3055 | L3056 | F3057 | G3058 | T3059 | D3060 | A3061 | R3073 | A3077 | R3078 | T3079 | V3080 | M3081 | S3082 | G3084 | P3085 | E3086 | I3087 | V3088 | K3089 | A3090 | G3091 | S3094 | D3102 | I3103 | E3104 | K3105 | M3106 | K3178 | K3179 |       |       |       |       |       |       |
| E3108 | N3109 | L3110 | R3111 | LEU   | GLY   | LYS   | VAL   | K3023 | V3024 | L3025 | GLY   | THR   | GLN   | VAL   | L3029 | H3030 | A3031 | K3034 | T3040 | K3045 | H3052 | V3053 | S3055 | L3056 | F3057 | G3058 | T3059 | D3060 | A3061 | R3073 | A3077 | R3078 | T3079 | V3080 | M3081 | S3082 | G3084 | P3085 | E3086 | I3087 | V3088 | K3089 | A3090 | G3091 | S3094 | D3102 | I3103 | E3104 | K3105 | M3106 | K3178 | K3179 |       |       |       |       |       |       |
| E3108 | N3109 | L3110 | R3111 | LEU   | GLY   | LYS   | VAL   | K3023 | V3024 | L3025 | GLY   | THR   | GLN   | VAL   | L3029 | H3030 | A3031 | K3034 | T3040 | K3045 | H3052 | V3053 | S3055 | L3056 | F3057 | G3058 | T3059 | D3060 | A3061 | R3073 | A3077 | R3078 | T3079 | V3080 | M3081 | S3082 | G3084 | P3085 | E3086 | I3087 | V3088 | K3089 | A3090 | G3091 | S3094 | D3102 | I3103 | E3104 | K3105 | M3106 | K3178 | K3179 |       |       |       |       |       |       |
| E3108 | N3109 | L3110 | R3111 | LEU   | GLY   | LYS   | VAL   | K3023 | V3024 | L3025 | GLY   | THR   | GLN   | VAL   | L3029 | H3030 | A3031 | K3034 | T3040 | K3045 | H3052 | V3053 | S3055 | L3056 | F3057 | G3058 | T3059 | D3060 | A3061 | R3073 | A3077 | R3078 | T3079 | V3080 | M3081 | S3082 | G3084 | P3085 | E3086 | I3087 | V3088 | K3089 | A3090 | G3091 | S3094 | D3102 | I3103 | E3104 | K3105 | M3106 | K3178 | K3179 |       |       |       |       |       |       |
| E3108 | N3109 | L3110 | R3111 | LEU   | GLY   | LYS   | VAL   | K3023 | V3024 | L3025 | GLY   | THR   | GLN   | VAL   | L3029 | H3030 | A3031 | K3034 | T3040 | K3045 | H3052 | V3053 | S3055 | L3056 | F3057 | G3058 | T3059 | D3060 | A3061 | R3073 | A3077 | R3078 | T3079 | V3080 | M3081 | S3082 | G3084 | P3085 | E3086 | I3087 | V3088 | K3089 | A3090 | G3091 | S3094 | D3102 | I3103 | E3104 | K3105 | M3106 | K3178 | K3179 |       |       |       |       |       |       |
| E3108 | N3109 | L3110 | R3111 | LEU   | GLY   | LYS   | VAL   | K3023 | V3024 | L3025 | GLY   | THR   | GLN   | VAL   | L3029 | H3030 | A3031 | K3034 | T3040 | K3045 | H3052 | V3053 | S3055 | L3056 | F3057 | G3058 | T3059 | D3060 | A3061 | R3073 | A3077 | R3078 | T3079 | V3080 | M3081 | S3082 | G3084 | P3085 | E3086 | I3087 | V3088 | K3089 | A3090 | G3091 | S3094 | D3102 | I3103 | E3104 | K3105 | M3106 | K3178 | K3179 |       |       |       |       |       |       |
| E3108 | N3109 | L3110 | R3111 | LEU   | GLY   | LYS   | VAL   | K3023 | V3024 | L3025 | GLY   | THR   | GLN   | VAL   | L3029 | H3030 | A3031 | K3034 | T3040 | K3045 | H3052 | V3053 | S3055 | L3056 | F3057 | G3058 | T3059 | D3060 | A3061 | R3073 | A3077 | R3078 | T3079 | V3080 | M3081 | S3082 | G3084 | P3085 | E3086 | I3087 | V3088 | K3089 | A3090 | G3091 | S3094 | D3102 | I3103 | E3104 | K3105 | M3106 | K3178 | K3179 |       |       |       |       |       |       |
| E3108 | N3109 | L3110 | R3111 | LEU   | GLY   | LYS   | VAL   | K3023 | V3024 | L3025 | GLY   | THR   | GLN   | VAL   | L3029 | H3030 | A3031 | K3034 | T3040 | K3045 | H3052 | V3053 | S3055 | L3056 | F3057 | G3058 | T3059 | D3060 | A3061 | R3073 | A3077 | R3078 | T3079 | V3080 | M3081 | S3082 | G3084 | P3085 | E3086 | I3087 | V3088 | K3089 | A3090 | G3091 | S3094 | D3102 | I3103 | E3104 | K3105 | M3106 | K3178 | K3179 |       |       |       |       |       |       |
| E3108 | N3109 | L3110 | R3111 | LEU   | GLY   | LYS   | VAL   | K3023 | V3024 | L3025 | GLY   | THR   | GLN   | VAL   | L3029 | H3030 | A3031 | K3034 | T     |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |

[illegible]

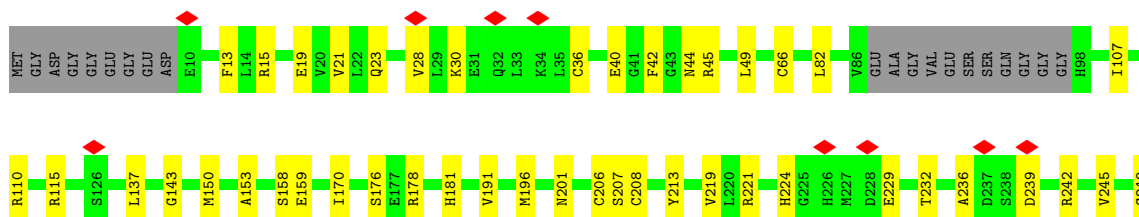


• Molecule 1: Ryanodine receptor 1





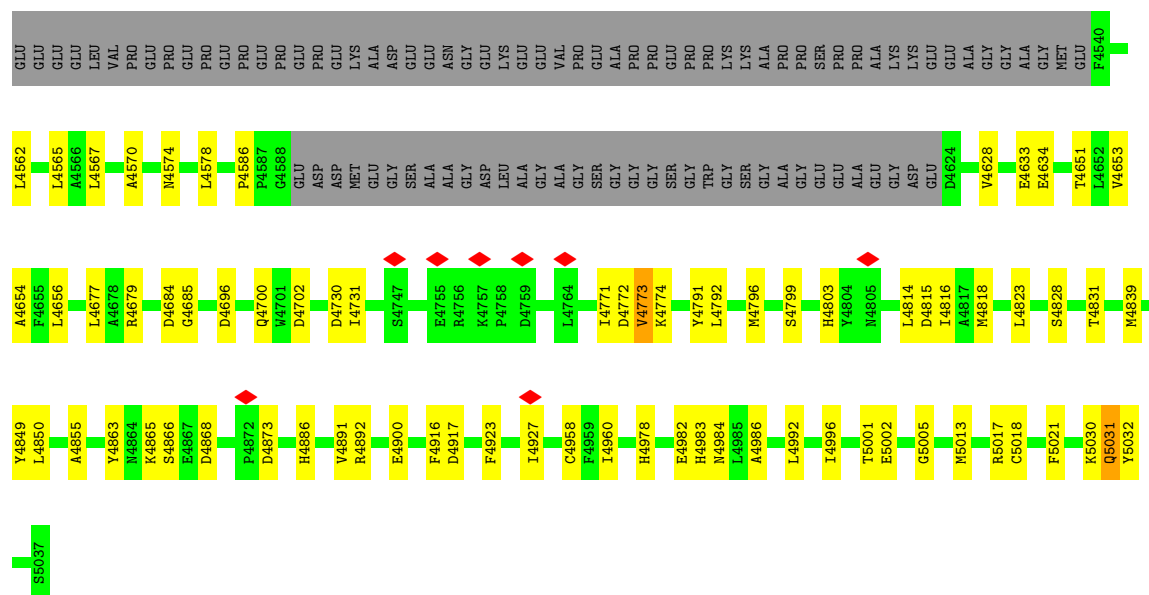




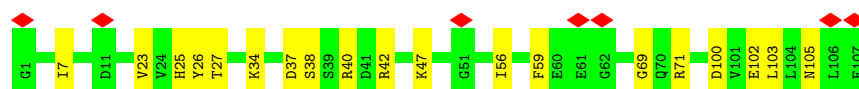
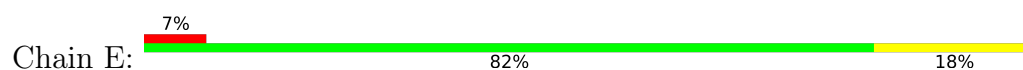




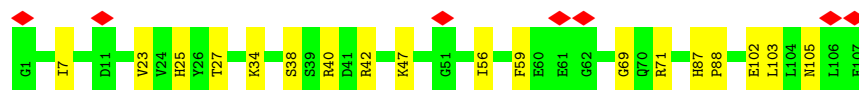
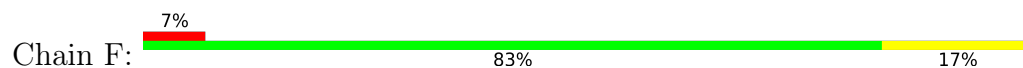




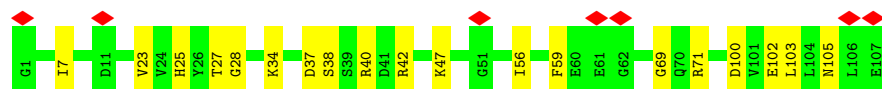
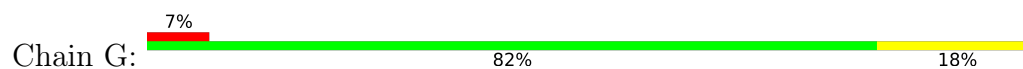
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



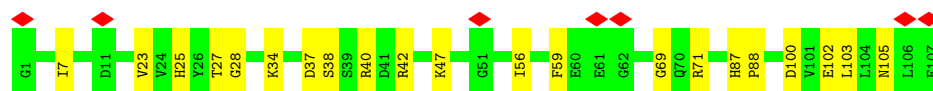
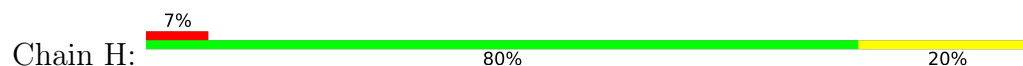
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



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



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



## 4 Experimental information

| Property                             | Value                           | Source    |
|--------------------------------------|---------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                 | Depositor |
| Imposed symmetry                     | POINT, C4                       | Depositor |
| Number of particles used             | 141098                          | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF               | Depositor |
| CTF correction method                | NONE                            | Depositor |
| Microscope                           | FEI TITAN KRIOS                 | Depositor |
| Voltage (kV)                         | 300                             | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 53.69                           | Depositor |
| Minimum defocus (nm)                 | 700                             | Depositor |
| Maximum defocus (nm)                 | 2500                            | Depositor |
| Magnification                        | 81000                           | Depositor |
| Image detector                       | GATAN K3 (6k x 4k)              | Depositor |
| Maximum map value                    | 1.247                           | Depositor |
| Minimum map value                    | -0.732                          | Depositor |
| Average map value                    | 0.006                           | Depositor |
| Map value standard deviation         | 0.038                           | Depositor |
| Recommended contour level            | 0.155                           | Depositor |
| Map size ( $\text{\AA}$ )            | 464.40002, 464.40002, 464.40002 | wwPDB     |
| Map dimensions                       | 430, 430, 430                   | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.08, 1.08, 1.08                | Depositor |

## 5 Model quality

### 5.1 Standard geometry

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

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     | 0.13         | 0/33461     | 0.34        | 1/45464 (0.0%)  |
| 1   | B     | 0.13         | 0/33461     | 0.33        | 1/45464 (0.0%)  |
| 1   | C     | 0.13         | 0/33461     | 0.33        | 1/45464 (0.0%)  |
| 1   | D     | 0.13         | 0/33461     | 0.33        | 1/45464 (0.0%)  |
| 2   | E     | 0.16         | 0/834       | 0.44        | 0/1123          |
| 2   | F     | 0.16         | 0/834       | 0.44        | 0/1123          |
| 2   | G     | 0.16         | 0/834       | 0.44        | 0/1123          |
| 2   | H     | 0.16         | 0/834       | 0.44        | 0/1123          |
| All | All   | 0.13         | 0/137180    | 0.34        | 4/186348 (0.0%) |

There are no bond length outliers.

All (4) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 28  | VAL  | N-CA-C | -5.59 | 108.40      | 113.71   |
| 1   | C     | 28  | VAL  | N-CA-C | -5.58 | 108.41      | 113.71   |
| 1   | D     | 28  | VAL  | N-CA-C | -5.58 | 108.41      | 113.71   |
| 1   | B     | 28  | VAL  | N-CA-C | -5.54 | 108.45      | 113.71   |

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 1   | A     | 32730  | 0        | 31483    | 387     | 0            |
| 1   | B     | 32730  | 0        | 31483    | 378     | 0            |
| 1   | C     | 32730  | 0        | 31483    | 387     | 0            |
| 1   | D     | 32730  | 0        | 31483    | 382     | 0            |
| 2   | E     | 818    | 0        | 824      | 14      | 0            |
| 2   | F     | 818    | 0        | 824      | 13      | 0            |
| 2   | G     | 818    | 0        | 824      | 14      | 0            |
| 2   | H     | 818    | 0        | 824      | 15      | 0            |
| 3   | A     | 1      | 0        | 0        | 0       | 0            |
| 3   | B     | 1      | 0        | 0        | 0       | 0            |
| 3   | C     | 1      | 0        | 0        | 0       | 0            |
| 3   | D     | 1      | 0        | 0        | 0       | 0            |
| All | All   | 134196 | 0        | 129228   | 1564    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (1564) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1476:MET:HE3  | 1:A:1477:GLY:H    | 1.48                     | 0.79              |
| 1:D:1476:MET:HE3  | 1:D:1477:GLY:H    | 1.47                     | 0.79              |
| 1:B:1476:MET:HE3  | 1:B:1477:GLY:H    | 1.47                     | 0.78              |
| 1:C:1476:MET:HE3  | 1:C:1477:GLY:H    | 1.48                     | 0.78              |
| 1:B:4045:VAL:HG22 | 1:B:4160:LEU:HD11 | 1.75                     | 0.69              |
| 1:D:4045:VAL:HG22 | 1:D:4160:LEU:HD11 | 1.75                     | 0.68              |
| 1:A:3144:PHE:HA   | 1:A:3196:ARG:HG3  | 1.75                     | 0.68              |
| 1:B:3144:PHE:HA   | 1:B:3196:ARG:HG3  | 1.75                     | 0.67              |
| 1:A:2248:ARG:HG2  | 1:A:2286:LEU:HD21 | 1.76                     | 0.67              |
| 1:C:2248:ARG:HG2  | 1:C:2286:LEU:HD21 | 1.76                     | 0.67              |
| 1:C:4045:VAL:HG22 | 1:C:4160:LEU:HD11 | 1.75                     | 0.67              |
| 1:D:3144:PHE:HA   | 1:D:3196:ARG:HG3  | 1.75                     | 0.67              |
| 1:D:82:LEU:HD11   | 1:D:143:GLY:HA3   | 1.77                     | 0.67              |
| 1:A:82:LEU:HD11   | 1:A:143:GLY:HA3   | 1.77                     | 0.67              |
| 1:C:3144:PHE:HA   | 1:C:3196:ARG:HG3  | 1.75                     | 0.67              |
| 1:B:2248:ARG:HG2  | 1:B:2286:LEU:HD21 | 1.76                     | 0.67              |
| 1:A:4045:VAL:HG22 | 1:A:4160:LEU:HD11 | 1.75                     | 0.66              |
| 1:A:886:ARG:HG3   | 1:A:891:TRP:HB2   | 1.78                     | 0.66              |
| 1:B:886:ARG:HG3   | 1:B:891:TRP:HB2   | 1.78                     | 0.66              |
| 1:C:886:ARG:HG3   | 1:C:891:TRP:HB2   | 1.78                     | 0.66              |
| 1:A:4892:ARG:NH1  | 1:D:4917:ASP:OD1  | 2.29                     | 0.66              |
| 1:D:886:ARG:HG3   | 1:D:891:TRP:HB2   | 1.78                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:2248:ARG:HG2  | 1:D:2286:LEU:HD21 | 1.76                     | 0.65              |
| 1:B:82:LEU:HD11   | 1:B:143:GLY:HA3   | 1.77                     | 0.65              |
| 1:C:82:LEU:HD11   | 1:C:143:GLY:HA3   | 1.77                     | 0.65              |
| 1:C:3770:LEU:HD22 | 1:C:3804:ILE:HD13 | 1.79                     | 0.65              |
| 1:A:5013:MET:HE1  | 1:A:5018:CYS:HB3  | 1.79                     | 0.65              |
| 1:C:5013:MET:HE1  | 1:C:5018:CYS:HB3  | 1.79                     | 0.65              |
| 1:B:2885:THR:HG22 | 1:B:2889:LYS:HZ3  | 1.61                     | 0.65              |
| 1:B:4917:ASP:OD1  | 1:C:4892:ARG:NH1  | 2.30                     | 0.64              |
| 1:D:3770:LEU:HD22 | 1:D:3804:ILE:HD13 | 1.79                     | 0.64              |
| 1:C:426:ARG:NH1   | 1:C:427:GLY:O     | 2.31                     | 0.64              |
| 1:B:224:HIS:HB3   | 1:B:229:GLU:HG3   | 1.80                     | 0.64              |
| 1:C:224:HIS:HB3   | 1:C:229:GLU:HG3   | 1.80                     | 0.64              |
| 1:A:224:HIS:HB3   | 1:A:229:GLU:HG3   | 1.80                     | 0.64              |
| 1:A:426:ARG:NH1   | 1:A:427:GLY:O     | 2.31                     | 0.64              |
| 1:C:4917:ASP:OD1  | 1:D:4892:ARG:NH1  | 2.31                     | 0.64              |
| 1:A:3770:LEU:HD22 | 1:A:3804:ILE:HD13 | 1.79                     | 0.64              |
| 1:B:3770:LEU:HD22 | 1:B:3804:ILE:HD13 | 1.79                     | 0.64              |
| 1:A:4917:ASP:OD1  | 1:B:4892:ARG:NH1  | 2.30                     | 0.63              |
| 1:B:426:ARG:NH1   | 1:B:427:GLY:O     | 2.31                     | 0.63              |
| 1:B:5013:MET:HE1  | 1:B:5018:CYS:HB3  | 1.79                     | 0.63              |
| 1:D:5013:MET:HE1  | 1:D:5018:CYS:HB3  | 1.79                     | 0.63              |
| 1:D:426:ARG:NH1   | 1:D:427:GLY:O     | 2.31                     | 0.63              |
| 1:B:452:PHE:O     | 1:B:528:SER:OG    | 2.17                     | 0.62              |
| 1:C:4772:ASP:O    | 1:C:4774:LYS:N    | 2.32                     | 0.62              |
| 1:D:224:HIS:HB3   | 1:D:229:GLU:HG3   | 1.80                     | 0.62              |
| 2:E:7:ILE:HD13    | 2:E:71:ARG:HG3    | 1.80                     | 0.62              |
| 2:F:7:ILE:HD13    | 2:F:71:ARG:HG3    | 1.80                     | 0.62              |
| 1:A:452:PHE:O     | 1:A:528:SER:OG    | 2.17                     | 0.62              |
| 1:B:4772:ASP:O    | 1:B:4774:LYS:N    | 2.32                     | 0.62              |
| 1:D:1738:LEU:HB2  | 1:D:2146:PRO:HD3  | 1.82                     | 0.62              |
| 2:G:7:ILE:HD13    | 2:G:71:ARG:HG3    | 1.80                     | 0.62              |
| 1:C:1935:VAL:HG12 | 1:C:1939:MET:HE2  | 1.81                     | 0.62              |
| 2:G:25:HIS:O      | 2:G:40:ARG:NH1    | 2.32                     | 0.62              |
| 1:D:4772:ASP:O    | 1:D:4774:LYS:N    | 2.32                     | 0.62              |
| 1:A:1738:LEU:HB2  | 1:A:2146:PRO:HD3  | 1.82                     | 0.62              |
| 1:A:4772:ASP:O    | 1:A:4774:LYS:N    | 2.32                     | 0.62              |
| 1:D:1106:ARG:NH2  | 1:D:1183:GLU:O    | 2.33                     | 0.62              |
| 1:C:452:PHE:O     | 1:C:528:SER:OG    | 2.18                     | 0.62              |
| 1:C:1106:ARG:NH2  | 1:C:1183:GLU:O    | 2.33                     | 0.62              |
| 2:E:25:HIS:O      | 2:E:40:ARG:NH1    | 2.32                     | 0.62              |
| 2:H:25:HIS:O      | 2:H:40:ARG:NH1    | 2.32                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:1935:VAL:HG12 | 1:D:1939:MET:HE2  | 1.81                     | 0.62              |
| 2:F:25:HIS:O      | 2:F:40:ARG:NH1    | 2.32                     | 0.62              |
| 1:A:1106:ARG:NH2  | 1:A:1183:GLU:O    | 2.33                     | 0.61              |
| 1:C:1077:ALA:H    | 1:C:1189:LEU:HD21 | 1.65                     | 0.61              |
| 1:C:491:ILE:HG22  | 1:C:550:LYS:HZ2   | 1.66                     | 0.61              |
| 1:D:2271:THR:HG22 | 1:D:2273:LEU:H    | 1.65                     | 0.61              |
| 2:H:7:ILE:HD13    | 2:H:71:ARG:HG3    | 1.80                     | 0.61              |
| 1:A:1935:VAL:HG12 | 1:A:1939:MET:HE2  | 1.81                     | 0.61              |
| 1:B:1106:ARG:NH2  | 1:B:1183:GLU:O    | 2.33                     | 0.61              |
| 1:B:1935:VAL:HG12 | 1:B:1939:MET:HE2  | 1.81                     | 0.61              |
| 1:B:1077:ALA:H    | 1:B:1189:LEU:HD21 | 1.65                     | 0.61              |
| 1:B:2271:THR:HG22 | 1:B:2273:LEU:H    | 1.65                     | 0.61              |
| 1:A:1077:ALA:H    | 1:A:1189:LEU:HD21 | 1.65                     | 0.61              |
| 1:B:1721:GLU:OE2  | 1:B:1725:ARG:NH1  | 2.34                     | 0.61              |
| 1:B:1653:LEU:HD22 | 1:B:1704:PRO:HB3  | 1.83                     | 0.60              |
| 1:D:1077:ALA:H    | 1:D:1189:LEU:HD21 | 1.65                     | 0.60              |
| 1:D:257:ARG:NH1   | 1:D:480:GLU:OE2   | 2.34                     | 0.60              |
| 1:A:2552:ARG:NH1  | 1:A:2590:SER:O    | 2.34                     | 0.60              |
| 1:B:1738:LEU:HB2  | 1:B:2146:PRO:HD3  | 1.82                     | 0.60              |
| 1:D:1141:ARG:H    | 1:D:1169:LEU:HD11 | 1.67                     | 0.60              |
| 1:D:2552:ARG:NH1  | 1:D:2590:SER:O    | 2.34                     | 0.60              |
| 1:C:1653:LEU:HD22 | 1:C:1704:PRO:HB3  | 1.84                     | 0.60              |
| 1:C:2552:ARG:NH1  | 1:C:2590:SER:O    | 2.34                     | 0.60              |
| 1:D:1721:GLU:OE2  | 1:D:1725:ARG:NH1  | 2.34                     | 0.60              |
| 1:B:2552:ARG:NH1  | 1:B:2590:SER:O    | 2.34                     | 0.60              |
| 1:C:1721:GLU:OE2  | 1:C:1725:ARG:NH1  | 2.34                     | 0.60              |
| 1:C:1738:LEU:HB2  | 1:C:2146:PRO:HD3  | 1.82                     | 0.60              |
| 1:C:1141:ARG:H    | 1:C:1169:LEU:HD11 | 1.67                     | 0.60              |
| 1:D:452:PHE:O     | 1:D:528:SER:OG    | 2.17                     | 0.60              |
| 1:C:2271:THR:HG22 | 1:C:2273:LEU:H    | 1.65                     | 0.60              |
| 1:D:107:ILE:HG13  | 1:D:150:MET:HE3   | 1.84                     | 0.60              |
| 1:A:2271:THR:HG22 | 1:A:2273:LEU:H    | 1.65                     | 0.59              |
| 1:A:1721:GLU:OE2  | 1:A:1725:ARG:NH1  | 2.34                     | 0.59              |
| 1:D:2458:ARG:NH2  | 1:D:2510:TYR:O    | 2.35                     | 0.59              |
| 1:B:257:ARG:NH1   | 1:B:480:GLU:OE2   | 2.34                     | 0.59              |
| 1:B:1141:ARG:H    | 1:B:1169:LEU:HD11 | 1.67                     | 0.59              |
| 1:D:2558:VAL:HG23 | 1:D:2560:PRO:HD3  | 1.85                     | 0.59              |
| 1:A:1653:LEU:HD22 | 1:A:1704:PRO:HB3  | 1.83                     | 0.59              |
| 1:A:2458:ARG:NH2  | 1:A:2510:TYR:O    | 2.35                     | 0.59              |
| 1:C:107:ILE:HG13  | 1:C:150:MET:HE3   | 1.84                     | 0.59              |
| 1:A:4866:SER:OG   | 1:A:4873:ASP:OD2  | 2.20                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:49:LEU:HD11   | 1:C:191:VAL:HG23  | 1.85                     | 0.59              |
| 1:C:257:ARG:NH1   | 1:C:480:GLU:OE2   | 2.34                     | 0.59              |
| 1:D:1653:LEU:HD22 | 1:D:1704:PRO:HB3  | 1.84                     | 0.59              |
| 1:D:4866:SER:OG   | 1:D:4873:ASP:OD2  | 2.21                     | 0.59              |
| 1:A:2558:VAL:HG23 | 1:A:2560:PRO:HD3  | 1.85                     | 0.59              |
| 1:B:107:ILE:HG13  | 1:B:150:MET:HE3   | 1.84                     | 0.59              |
| 1:B:2503:VAL:HG13 | 1:B:2554:LEU:HD22 | 1.85                     | 0.59              |
| 1:B:4866:SER:OG   | 1:B:4873:ASP:OD2  | 2.21                     | 0.59              |
| 1:D:2503:VAL:HG13 | 1:D:2554:LEU:HD22 | 1.85                     | 0.59              |
| 1:A:1141:ARG:H    | 1:A:1169:LEU:HD11 | 1.66                     | 0.59              |
| 1:A:2503:VAL:HG13 | 1:A:2554:LEU:HD22 | 1.85                     | 0.59              |
| 1:C:4866:SER:OG   | 1:C:4873:ASP:OD2  | 2.21                     | 0.59              |
| 1:D:3965:LEU:HA   | 1:D:3968:TYR:HD2  | 1.68                     | 0.59              |
| 1:B:49:LEU:HD11   | 1:B:191:VAL:HG23  | 1.85                     | 0.58              |
| 1:B:2458:ARG:NH2  | 1:B:2510:TYR:O    | 2.35                     | 0.58              |
| 1:B:3965:LEU:HA   | 1:B:3968:TYR:HD2  | 1.68                     | 0.58              |
| 1:C:2503:VAL:HG13 | 1:C:2554:LEU:HD22 | 1.85                     | 0.58              |
| 1:D:49:LEU:HD11   | 1:D:191:VAL:HG23  | 1.85                     | 0.58              |
| 1:B:726:VAL:HB    | 1:B:728:ARG:HH21  | 1.68                     | 0.58              |
| 1:C:3965:LEU:HA   | 1:C:3968:TYR:HD2  | 1.68                     | 0.58              |
| 1:A:400:ALA:O     | 1:A:404:ILE:HG12  | 2.04                     | 0.58              |
| 1:A:1495:VAL:HG21 | 1:A:1537:ASN:HA   | 1.86                     | 0.58              |
| 1:A:3142:THR:O    | 1:A:3196:ARG:NH1  | 2.36                     | 0.58              |
| 1:C:2885:THR:HG22 | 1:C:2889:LYS:HZ3  | 1.68                     | 0.58              |
| 1:D:3142:THR:O    | 1:D:3196:ARG:NH1  | 2.36                     | 0.58              |
| 2:H:23:VAL:HG12   | 2:H:47:LYS:HG2    | 1.86                     | 0.58              |
| 1:A:49:LEU:HD11   | 1:A:191:VAL:HG23  | 1.85                     | 0.58              |
| 1:B:2558:VAL:HG23 | 1:B:2560:PRO:HD3  | 1.84                     | 0.58              |
| 1:C:317:ARG:NH2   | 1:C:349:GLN:O     | 2.36                     | 0.58              |
| 1:C:400:ALA:O     | 1:C:404:ILE:HG12  | 2.04                     | 0.58              |
| 1:C:726:VAL:HB    | 1:C:728:ARG:HH21  | 1.68                     | 0.58              |
| 1:D:317:ARG:NH2   | 1:D:349:GLN:O     | 2.36                     | 0.58              |
| 1:D:726:VAL:HB    | 1:D:728:ARG:HH21  | 1.68                     | 0.58              |
| 1:A:107:ILE:HG13  | 1:A:150:MET:HE3   | 1.84                     | 0.58              |
| 1:C:2458:ARG:NH2  | 1:C:2510:TYR:O    | 2.35                     | 0.58              |
| 1:C:2558:VAL:HG23 | 1:C:2560:PRO:HD3  | 1.85                     | 0.58              |
| 2:E:23:VAL:HG12   | 2:E:47:LYS:HG2    | 1.86                     | 0.58              |
| 2:F:23:VAL:HG12   | 2:F:47:LYS:HG2    | 1.86                     | 0.58              |
| 1:B:491:ILE:HG22  | 1:B:550:LYS:HZ2   | 1.68                     | 0.57              |
| 1:B:1495:VAL:HG21 | 1:B:1537:ASN:HA   | 1.85                     | 0.57              |
| 2:G:23:VAL:HG12   | 2:G:47:LYS:HG2    | 1.86                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:726:VAL:HB    | 1:A:728:ARG:HH21  | 1.68                     | 0.57              |
| 1:A:917:GLU:HA    | 1:A:920:TYR:CE1   | 2.39                     | 0.57              |
| 1:B:826:ILE:HG22  | 1:B:827:LYS:HG2   | 1.87                     | 0.57              |
| 1:C:917:GLU:HA    | 1:C:920:TYR:CE1   | 2.39                     | 0.57              |
| 1:D:917:GLU:HA    | 1:D:920:TYR:CE1   | 2.39                     | 0.57              |
| 1:D:2885:THR:HG22 | 1:D:2889:LYS:HZ3  | 1.69                     | 0.57              |
| 1:A:826:ILE:HG22  | 1:A:827:LYS:HG2   | 1.87                     | 0.57              |
| 1:A:2974:ILE:O    | 1:A:3053:ARG:NH1  | 2.38                     | 0.57              |
| 1:C:1742:THR:HG22 | 1:C:1769:THR:HG21 | 1.87                     | 0.57              |
| 1:D:400:ALA:O     | 1:D:404:ILE:HG12  | 2.04                     | 0.57              |
| 1:D:1495:VAL:HG21 | 1:D:1537:ASN:HA   | 1.86                     | 0.57              |
| 1:B:917:GLU:HA    | 1:B:920:TYR:CE1   | 2.39                     | 0.57              |
| 1:B:1742:THR:HG22 | 1:B:1769:THR:HG21 | 1.87                     | 0.57              |
| 1:B:2974:ILE:O    | 1:B:3053:ARG:NH1  | 2.38                     | 0.57              |
| 1:B:3308:THR:OG1  | 1:B:3310:ASP:OD1  | 2.22                     | 0.57              |
| 1:C:2974:ILE:O    | 1:C:3053:ARG:NH1  | 2.38                     | 0.57              |
| 1:D:1724:CYS:SG   | 1:D:1728:ARG:NH1  | 2.78                     | 0.57              |
| 1:B:400:ALA:O     | 1:B:404:ILE:HG12  | 2.04                     | 0.57              |
| 1:C:1495:VAL:HG21 | 1:C:1537:ASN:HA   | 1.86                     | 0.57              |
| 1:C:3106:MET:O    | 1:C:3110:LEU:HB2  | 2.05                     | 0.57              |
| 1:A:3965:LEU:HA   | 1:A:3968:TYR:HD2  | 1.68                     | 0.57              |
| 1:C:1724:CYS:SG   | 1:C:1728:ARG:NH1  | 2.78                     | 0.57              |
| 1:C:826:ILE:HG22  | 1:C:827:LYS:HG2   | 1.87                     | 0.57              |
| 1:D:4696:ASP:O    | 1:D:4700:GLN:NE2  | 2.38                     | 0.57              |
| 1:A:483:MET:HG2   | 1:A:486:LEU:HD11  | 1.87                     | 0.57              |
| 1:A:1724:CYS:SG   | 1:A:1728:ARG:NH1  | 2.78                     | 0.57              |
| 1:B:2552:ARG:HH22 | 1:B:2590:SER:HA   | 1.70                     | 0.57              |
| 1:B:1261:ASP:HA   | 1:B:1268:PRO:HB3  | 1.87                     | 0.56              |
| 1:B:1724:CYS:SG   | 1:B:1728:ARG:NH1  | 2.78                     | 0.56              |
| 1:A:2552:ARG:HH22 | 1:A:2590:SER:HA   | 1.70                     | 0.56              |
| 1:A:3106:MET:O    | 1:A:3110:LEU:HB2  | 2.05                     | 0.56              |
| 1:A:4696:ASP:O    | 1:A:4700:GLN:NE2  | 2.38                     | 0.56              |
| 1:C:3675:ASP:OD2  | 1:C:3769:ARG:NH1  | 2.39                     | 0.56              |
| 1:D:2974:ILE:O    | 1:D:3053:ARG:NH1  | 2.38                     | 0.56              |
| 1:A:668:VAL:HG22  | 1:A:789:VAL:HG23  | 1.87                     | 0.56              |
| 1:B:668:VAL:HG22  | 1:B:789:VAL:HG23  | 1.87                     | 0.56              |
| 1:B:3106:MET:O    | 1:B:3110:LEU:HB2  | 2.05                     | 0.56              |
| 1:B:3353:LEU:HG   | 1:B:3356:SER:HB2  | 1.88                     | 0.56              |
| 1:B:4567:LEU:HD12 | 1:B:4816:ILE:HG22 | 1.88                     | 0.56              |
| 1:C:668:VAL:HG22  | 1:C:789:VAL:HG23  | 1.87                     | 0.56              |
| 1:C:4696:ASP:O    | 1:C:4700:GLN:NE2  | 2.38                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:668:VAL:HG22  | 1:D:789:VAL:HG23  | 1.87                     | 0.56              |
| 1:D:826:ILE:HG22  | 1:D:827:LYS:HG2   | 1.87                     | 0.56              |
| 1:D:3675:ASP:OD2  | 1:D:3769:ARG:NH1  | 2.39                     | 0.56              |
| 1:D:4567:LEU:HD12 | 1:D:4816:ILE:HG22 | 1.88                     | 0.56              |
| 1:A:4567:LEU:HD12 | 1:A:4816:ILE:HG22 | 1.88                     | 0.56              |
| 1:A:984:LEU:HD13  | 1:A:1055:PRO:HB3  | 1.87                     | 0.56              |
| 1:B:559:GLY:O     | 1:B:561:LEU:N     | 2.38                     | 0.56              |
| 1:C:2552:ARG:HH22 | 1:C:2590:SER:HA   | 1.70                     | 0.56              |
| 1:C:3142:THR:O    | 1:C:3196:ARG:NH1  | 2.35                     | 0.56              |
| 1:B:3471:THR:OG1  | 1:B:3472:ALA:N    | 2.39                     | 0.56              |
| 1:C:3353:LEU:HG   | 1:C:3356:SER:HB2  | 1.88                     | 0.56              |
| 1:D:483:MET:HG2   | 1:D:486:LEU:HD11  | 1.87                     | 0.56              |
| 1:D:1261:ASP:HA   | 1:D:1268:PRO:HB3  | 1.87                     | 0.56              |
| 1:A:3675:ASP:OD2  | 1:A:3769:ARG:NH1  | 2.39                     | 0.56              |
| 1:A:684:VAL:HG12  | 1:A:781:VAL:HG12  | 1.88                     | 0.56              |
| 1:B:984:LEU:HD13  | 1:B:1055:PRO:HB3  | 1.87                     | 0.56              |
| 1:D:684:VAL:HG12  | 1:D:781:VAL:HG12  | 1.88                     | 0.56              |
| 2:F:23:VAL:HG22   | 2:F:105:ASN:HB2   | 1.88                     | 0.56              |
| 1:D:3106:MET:O    | 1:D:3110:LEU:HB2  | 2.05                     | 0.56              |
| 1:A:1678:ASN:HB3  | 1:A:1681:VAL:HG22 | 1.88                     | 0.56              |
| 1:A:2977:LEU:H    | 1:A:3053:ARG:HH12 | 1.54                     | 0.56              |
| 1:B:676:THR:OG1   | 1:B:677:ALA:N     | 2.38                     | 0.56              |
| 1:B:4696:ASP:O    | 1:B:4700:GLN:NE2  | 2.38                     | 0.56              |
| 1:D:1437:VAL:HG12 | 1:D:1556:PRO:HB3  | 1.87                     | 0.56              |
| 1:D:1742:THR:HG22 | 1:D:1769:THR:HG21 | 1.87                     | 0.56              |
| 1:A:1742:THR:HG22 | 1:A:1769:THR:HG21 | 1.87                     | 0.55              |
| 1:A:3471:THR:OG1  | 1:A:3472:ALA:N    | 2.39                     | 0.55              |
| 1:B:1638:ALA:HA   | 1:B:1650:ILE:HG12 | 1.89                     | 0.55              |
| 1:B:3675:ASP:OD2  | 1:B:3769:ARG:NH1  | 2.39                     | 0.55              |
| 1:C:1078:GLU:OE2  | 1:C:1607:ARG:NH1  | 2.39                     | 0.55              |
| 1:D:3471:THR:OG1  | 1:D:3472:ALA:N    | 2.39                     | 0.55              |
| 2:H:23:VAL:HG22   | 2:H:105:ASN:HB2   | 1.88                     | 0.55              |
| 1:A:176:SER:HB3   | 1:A:178:ARG:HD3   | 1.88                     | 0.55              |
| 1:A:1261:ASP:HA   | 1:A:1268:PRO:HB3  | 1.87                     | 0.55              |
| 1:A:1638:ALA:HA   | 1:A:1650:ILE:HG12 | 1.89                     | 0.55              |
| 1:B:483:MET:HG2   | 1:B:486:LEU:HD11  | 1.87                     | 0.55              |
| 1:C:676:THR:OG1   | 1:C:677:ALA:N     | 2.38                     | 0.55              |
| 1:B:4651:THR:OG1  | 1:B:4803:HIS:NE2  | 2.34                     | 0.55              |
| 1:C:1437:VAL:HG12 | 1:C:1556:PRO:HB3  | 1.87                     | 0.55              |
| 1:D:1678:ASN:HB3  | 1:D:1681:VAL:HG22 | 1.88                     | 0.55              |
| 1:A:1078:GLU:OE2  | 1:A:1607:ARG:NH1  | 2.40                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:534:ARG:NH1   | 1:D:534:ARG:O     | 2.40                     | 0.55              |
| 1:D:559:GLY:O     | 1:D:561:LEU:N     | 2.38                     | 0.55              |
| 1:C:984:LEU:HD13  | 1:C:1055:PRO:HB3  | 1.87                     | 0.55              |
| 1:C:1261:ASP:HA   | 1:C:1268:PRO:HB3  | 1.87                     | 0.55              |
| 1:C:4567:LEU:HD12 | 1:C:4816:ILE:HG22 | 1.88                     | 0.55              |
| 1:D:176:SER:HB3   | 1:D:178:ARG:HD3   | 1.88                     | 0.55              |
| 1:D:2552:ARG:HH22 | 1:D:2590:SER:HA   | 1.71                     | 0.55              |
| 2:E:23:VAL:HG22   | 2:E:105:ASN:HB2   | 1.88                     | 0.55              |
| 1:A:2885:THR:HG22 | 1:A:2889:LYS:HZ3  | 1.72                     | 0.55              |
| 1:B:1678:ASN:HB3  | 1:B:1681:VAL:HG22 | 1.88                     | 0.55              |
| 1:D:1638:ALA:HA   | 1:D:1650:ILE:HG12 | 1.89                     | 0.55              |
| 1:D:2977:LEU:H    | 1:D:3053:ARG:HH12 | 1.54                     | 0.55              |
| 1:D:4651:THR:OG1  | 1:D:4803:HIS:NE2  | 2.34                     | 0.55              |
| 1:A:676:THR:OG1   | 1:A:677:ALA:N     | 2.38                     | 0.55              |
| 1:A:1000:ARG:O    | 1:A:1000:ARG:NH1  | 2.40                     | 0.55              |
| 1:C:483:MET:HG2   | 1:C:486:LEU:HD11  | 1.87                     | 0.55              |
| 1:D:984:LEU:HD13  | 1:D:1055:PRO:HB3  | 1.87                     | 0.55              |
| 1:D:1005:TRP:HA   | 1:D:1020:ARG:HH21 | 1.72                     | 0.55              |
| 1:D:3353:LEU:HG   | 1:D:3356:SER:HB2  | 1.88                     | 0.55              |
| 1:A:257:ARG:NH1   | 1:A:480:GLU:OE2   | 2.34                     | 0.55              |
| 1:A:559:GLY:O     | 1:A:561:LEU:N     | 2.38                     | 0.55              |
| 1:A:786:GLY:N     | 1:A:1630:CYS:SG   | 2.78                     | 0.55              |
| 1:B:1078:GLU:OE2  | 1:B:1607:ARG:NH1  | 2.39                     | 0.55              |
| 1:D:1000:ARG:O    | 1:D:1000:ARG:NH1  | 2.40                     | 0.55              |
| 1:B:1000:ARG:O    | 1:B:1000:ARG:NH1  | 2.40                     | 0.55              |
| 1:C:1005:TRP:HA   | 1:C:1020:ARG:HH21 | 1.72                     | 0.55              |
| 1:A:4978:HIS:ND1  | 1:A:4982:GLU:OE1  | 2.40                     | 0.55              |
| 1:B:176:SER:HB3   | 1:B:178:ARG:HD3   | 1.89                     | 0.55              |
| 1:B:1115:LEU:HB3  | 1:B:1123:VAL:HG21 | 1.89                     | 0.55              |
| 1:C:714:TYR:HE1   | 1:C:1514:LEU:HD13 | 1.72                     | 0.55              |
| 1:C:2977:LEU:H    | 1:C:3053:ARG:HH12 | 1.54                     | 0.55              |
| 1:B:684:VAL:HG12  | 1:B:781:VAL:HG12  | 1.88                     | 0.54              |
| 1:C:176:SER:HB3   | 1:C:178:ARG:HD3   | 1.88                     | 0.54              |
| 1:C:684:VAL:HG12  | 1:C:781:VAL:HG12  | 1.88                     | 0.54              |
| 1:C:1638:ALA:HA   | 1:C:1650:ILE:HG12 | 1.88                     | 0.54              |
| 1:C:1805:GLU:OE1  | 1:C:1808:ARG:NH2  | 2.39                     | 0.54              |
| 1:C:4654:ALA:HB1  | 1:C:4796:MET:HE1  | 1.88                     | 0.54              |
| 1:C:4978:HIS:ND1  | 1:C:4982:GLU:OE1  | 2.40                     | 0.54              |
| 1:D:4570:ALA:O    | 1:D:4574:ASN:ND2  | 2.36                     | 0.54              |
| 1:B:1805:GLU:OE1  | 1:B:1808:ARG:NH2  | 2.40                     | 0.54              |
| 1:C:534:ARG:O     | 1:C:534:ARG:NH1   | 2.40                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:317:ARG:NH2   | 1:A:349:GLN:O     | 2.36                     | 0.54              |
| 1:A:534:ARG:O     | 1:A:534:ARG:NH1   | 2.40                     | 0.54              |
| 1:A:4654:ALA:HB1  | 1:A:4796:MET:HE1  | 1.88                     | 0.54              |
| 1:B:1437:VAL:HG12 | 1:B:1556:PRO:HB3  | 1.87                     | 0.54              |
| 1:B:2977:LEU:H    | 1:B:3053:ARG:HH12 | 1.54                     | 0.54              |
| 1:B:4654:ALA:HB1  | 1:B:4796:MET:HE1  | 1.89                     | 0.54              |
| 1:C:1678:ASN:HB3  | 1:C:1681:VAL:HG22 | 1.88                     | 0.54              |
| 1:D:4654:ALA:HB1  | 1:D:4796:MET:HE1  | 1.88                     | 0.54              |
| 2:G:23:VAL:HG22   | 2:G:105:ASN:HB2   | 1.88                     | 0.54              |
| 1:B:714:TYR:HE1   | 1:B:1514:LEU:HD13 | 1.72                     | 0.54              |
| 1:B:4978:HIS:ND1  | 1:B:4982:GLU:OE1  | 2.40                     | 0.54              |
| 1:C:1000:ARG:O    | 1:C:1000:ARG:NH1  | 2.40                     | 0.54              |
| 1:D:4978:HIS:ND1  | 1:D:4982:GLU:OE1  | 2.40                     | 0.54              |
| 1:A:1005:TRP:HA   | 1:A:1020:ARG:HH21 | 1.72                     | 0.54              |
| 1:A:1437:VAL:HG12 | 1:A:1556:PRO:HB3  | 1.87                     | 0.54              |
| 1:C:4570:ALA:O    | 1:C:4574:ASN:ND2  | 2.36                     | 0.54              |
| 1:C:4800:LEU:HA   | 1:C:4803:HIS:HD1  | 1.73                     | 0.54              |
| 1:D:1115:LEU:HB3  | 1:D:1123:VAL:HG21 | 1.89                     | 0.54              |
| 1:B:1005:TRP:HA   | 1:B:1020:ARG:HH21 | 1.72                     | 0.54              |
| 1:C:2185:ILE:O    | 1:C:2188:ASN:ND2  | 2.40                     | 0.54              |
| 1:D:714:TYR:HE1   | 1:D:1514:LEU:HD13 | 1.72                     | 0.54              |
| 1:A:1437:VAL:HG22 | 1:A:1445:PRO:HG3  | 1.90                     | 0.54              |
| 1:A:3353:LEU:HG   | 1:A:3356:SER:HB2  | 1.88                     | 0.54              |
| 1:D:1078:GLU:OE2  | 1:D:1607:ARG:NH1  | 2.40                     | 0.54              |
| 1:A:1115:LEU:HB3  | 1:A:1123:VAL:HG21 | 1.89                     | 0.54              |
| 1:B:534:ARG:O     | 1:B:534:ARG:NH1   | 2.40                     | 0.54              |
| 1:A:491:ILE:HG22  | 1:A:550:LYS:HZ2   | 1.73                     | 0.54              |
| 1:A:3995:VAL:O    | 1:A:3999:MET:HG2  | 2.08                     | 0.54              |
| 1:B:317:ARG:NH2   | 1:B:349:GLN:O     | 2.36                     | 0.54              |
| 1:B:671:VAL:HG12  | 1:B:740:PRO:HG3   | 1.90                     | 0.54              |
| 1:B:3995:VAL:O    | 1:B:3999:MET:HG2  | 2.08                     | 0.54              |
| 1:D:2675:THR:HG23 | 1:D:2678:LEU:H    | 1.73                     | 0.54              |
| 1:A:3131:TYR:HA   | 1:A:3135:ALA:HB3  | 1.90                     | 0.54              |
| 1:B:1437:VAL:HG22 | 1:B:1445:PRO:HG3  | 1.90                     | 0.54              |
| 1:D:3977:GLN:NE2  | 1:D:4030:LEU:O    | 2.41                     | 0.54              |
| 1:B:2208:MET:HE3  | 1:B:2253:HIS:HB3  | 1.90                     | 0.53              |
| 1:C:2012:PHE:HA   | 1:C:2015:GLU:HG3  | 1.91                     | 0.53              |
| 1:A:714:TYR:HE1   | 1:A:1514:LEU:HD13 | 1.72                     | 0.53              |
| 1:A:2012:PHE:HA   | 1:A:2015:GLU:HG3  | 1.91                     | 0.53              |
| 1:B:4562:LEU:HD21 | 1:B:4656:LEU:HB3  | 1.90                     | 0.53              |
| 1:C:2208:MET:HE3  | 1:C:2253:HIS:HB3  | 1.90                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:3995:VAL:O    | 1:C:3999:MET:HG2  | 2.08                     | 0.53              |
| 1:A:671:VAL:HG12  | 1:A:740:PRO:HG3   | 1.90                     | 0.53              |
| 1:B:2274:ASP:OD2  | 1:B:2330:ARG:NH1  | 2.42                     | 0.53              |
| 1:C:1115:LEU:HB3  | 1:C:1123:VAL:HG21 | 1.89                     | 0.53              |
| 1:C:2274:ASP:OD2  | 1:C:2330:ARG:NH1  | 2.42                     | 0.53              |
| 1:D:2012:PHE:HA   | 1:D:2015:GLU:HG3  | 1.91                     | 0.53              |
| 1:D:2274:ASP:OD2  | 1:D:2330:ARG:NH1  | 2.42                     | 0.53              |
| 1:A:4562:LEU:HD21 | 1:A:4656:LEU:HB3  | 1.90                     | 0.53              |
| 1:B:3131:TYR:HA   | 1:B:3135:ALA:HB3  | 1.90                     | 0.53              |
| 1:D:221:ARG:O     | 1:D:391:THR:OG1   | 2.27                     | 0.53              |
| 1:D:1101:ARG:NH1  | 1:D:1115:LEU:O    | 2.42                     | 0.53              |
| 1:A:618:GLN:NE2   | 1:A:1673:VAL:O    | 2.42                     | 0.53              |
| 1:B:3142:THR:O    | 1:B:3196:ARG:NH1  | 2.36                     | 0.53              |
| 1:B:3977:GLN:NE2  | 1:B:4030:LEU:O    | 2.41                     | 0.53              |
| 1:B:4570:ALA:O    | 1:B:4574:ASN:ND2  | 2.36                     | 0.53              |
| 1:C:559:GLY:O     | 1:C:561:LEU:N     | 2.38                     | 0.53              |
| 1:C:1101:ARG:NH1  | 1:C:1115:LEU:O    | 2.42                     | 0.53              |
| 1:C:1499:ASP:OD1  | 1:C:1499:ASP:N    | 2.42                     | 0.53              |
| 1:C:2675:THR:HG23 | 1:C:2678:LEU:H    | 1.73                     | 0.53              |
| 1:C:4633:GLU:HG2  | 1:C:4634:GLU:H    | 1.74                     | 0.53              |
| 1:B:2012:PHE:HA   | 1:B:2015:GLU:HG3  | 1.91                     | 0.53              |
| 1:C:42:PHE:HB2    | 1:C:403:MET:HE1   | 1.91                     | 0.53              |
| 1:C:1708:ARG:NH1  | 1:C:1836:PHE:O    | 2.42                     | 0.53              |
| 1:D:618:GLN:NE2   | 1:D:1673:VAL:O    | 2.42                     | 0.53              |
| 1:D:671:VAL:HG12  | 1:D:740:PRO:HG3   | 1.90                     | 0.53              |
| 1:D:1499:ASP:N    | 1:D:1499:ASP:OD1  | 2.42                     | 0.53              |
| 1:D:3144:PHE:HD1  | 1:D:3196:ARG:HB2  | 1.73                     | 0.53              |
| 1:D:3995:VAL:O    | 1:D:3999:MET:HG2  | 2.08                     | 0.53              |
| 1:D:4633:GLU:HG2  | 1:D:4634:GLU:H    | 1.74                     | 0.53              |
| 1:A:674:PHE:HB3   | 2:E:40:ARG:HE     | 1.74                     | 0.53              |
| 1:B:618:GLN:NE2   | 1:B:1673:VAL:O    | 2.42                     | 0.53              |
| 1:B:4633:GLU:HG2  | 1:B:4634:GLU:H    | 1.74                     | 0.53              |
| 1:C:618:GLN:NE2   | 1:C:1673:VAL:O    | 2.42                     | 0.53              |
| 1:D:1708:ARG:NH1  | 1:D:1836:PHE:O    | 2.42                     | 0.53              |
| 1:D:3308:THR:OG1  | 1:D:3310:ASP:OD1  | 2.22                     | 0.53              |
| 1:D:4158:PRO:O    | 1:D:4162:ASN:ND2  | 2.42                     | 0.53              |
| 1:B:2185:ILE:O    | 1:B:2188:ASN:ND2  | 2.40                     | 0.53              |
| 1:A:595:ARG:HH22  | 1:A:1642:PRO:HD2  | 1.74                     | 0.53              |
| 1:A:4158:PRO:O    | 1:A:4162:ASN:ND2  | 2.42                     | 0.53              |
| 1:B:674:PHE:HB3   | 2:F:40:ARG:HE     | 1.74                     | 0.53              |
| 1:D:3131:TYR:HA   | 1:D:3135:ALA:HB3  | 1.90                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1101:ARG:NH1  | 1:A:1115:LEU:O    | 2.42                     | 0.53              |
| 1:B:42:PHE:HB2    | 1:B:403:MET:HE1   | 1.91                     | 0.53              |
| 1:B:595:ARG:HH22  | 1:B:1642:PRO:HD2  | 1.74                     | 0.53              |
| 1:C:1437:VAL:HG22 | 1:C:1445:PRO:HG3  | 1.90                     | 0.53              |
| 1:C:3131:TYR:HA   | 1:C:3135:ALA:HB3  | 1.90                     | 0.53              |
| 1:D:674:PHE:HB3   | 2:H:40:ARG:HE     | 1.74                     | 0.53              |
| 1:B:40:GLU:OE2    | 1:B:44:ASN:N      | 2.43                     | 0.52              |
| 1:C:221:ARG:O     | 1:C:391:THR:OG1   | 2.27                     | 0.52              |
| 1:C:671:VAL:HG12  | 1:C:740:PRO:HG3   | 1.90                     | 0.52              |
| 1:D:2513:GLU:CD   | 1:D:2514:ASN:H    | 2.17                     | 0.52              |
| 1:A:790:ARG:NH2   | 1:A:1624:LEU:O    | 2.43                     | 0.52              |
| 1:A:4633:GLU:HG2  | 1:A:4634:GLU:H    | 1.74                     | 0.52              |
| 1:B:1101:ARG:NH1  | 1:B:1115:LEU:O    | 2.42                     | 0.52              |
| 1:B:4158:PRO:O    | 1:B:4162:ASN:ND2  | 2.42                     | 0.52              |
| 1:C:790:ARG:NH2   | 1:C:1624:LEU:O    | 2.43                     | 0.52              |
| 1:A:2185:ILE:O    | 1:A:2188:ASN:ND2  | 2.40                     | 0.52              |
| 1:A:2208:MET:HE3  | 1:A:2253:HIS:HB3  | 1.90                     | 0.52              |
| 1:A:2274:ASP:OD2  | 1:A:2330:ARG:NH1  | 2.42                     | 0.52              |
| 1:A:2675:THR:HG23 | 1:A:2678:LEU:H    | 1.73                     | 0.52              |
| 1:B:464:LYS:HE2   | 1:B:468:LEU:HD21  | 1.92                     | 0.52              |
| 1:B:3144:PHE:HD1  | 1:B:3196:ARG:HB2  | 1.73                     | 0.52              |
| 1:C:786:GLY:N     | 1:C:1630:CYS:SG   | 2.78                     | 0.52              |
| 1:C:2513:GLU:CD   | 1:C:2514:ASN:H    | 2.17                     | 0.52              |
| 1:D:491:ILE:HG22  | 1:D:550:LYS:HZ2   | 1.74                     | 0.52              |
| 1:D:2208:MET:HE3  | 1:D:2253:HIS:HB3  | 1.90                     | 0.52              |
| 1:A:42:PHE:HB2    | 1:A:403:MET:HE1   | 1.91                     | 0.52              |
| 1:A:4984:ASN:O    | 1:A:4986:ALA:N    | 2.42                     | 0.52              |
| 1:B:221:ARG:O     | 1:B:391:THR:OG1   | 2.27                     | 0.52              |
| 1:C:4158:PRO:O    | 1:C:4162:ASN:ND2  | 2.42                     | 0.52              |
| 1:D:676:THR:OG1   | 1:D:677:ALA:N     | 2.38                     | 0.52              |
| 1:D:790:ARG:NH2   | 1:D:1624:LEU:O    | 2.43                     | 0.52              |
| 1:D:3376:GLU:HG3  | 1:D:3394:VAL:HG11 | 1.92                     | 0.52              |
| 1:B:774:ASP:OD1   | 1:B:774:ASP:N     | 2.43                     | 0.52              |
| 1:B:790:ARG:NH2   | 1:B:1624:LEU:O    | 2.43                     | 0.52              |
| 1:D:2185:ILE:O    | 1:D:2188:ASN:ND2  | 2.40                     | 0.52              |
| 1:A:40:GLU:OE2    | 1:A:44:ASN:N      | 2.43                     | 0.52              |
| 1:A:3717:ASP:N    | 1:A:3717:ASP:OD1  | 2.43                     | 0.52              |
| 1:C:674:PHE:HB3   | 2:G:40:ARG:HE     | 1.74                     | 0.52              |
| 1:C:3376:GLU:HG3  | 1:C:3394:VAL:HG11 | 1.92                     | 0.52              |
| 1:D:464:LYS:HE2   | 1:D:468:LEU:HD21  | 1.92                     | 0.52              |
| 1:D:1437:VAL:HG22 | 1:D:1445:PRO:HG3  | 1.90                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:1805:GLU:OE1  | 1:D:1808:ARG:NH2  | 2.40                     | 0.52              |
| 1:A:3376:GLU:HG3  | 1:A:3394:VAL:HG11 | 1.92                     | 0.52              |
| 1:B:2675:THR:HG23 | 1:B:2678:LEU:H    | 1.73                     | 0.52              |
| 1:D:42:PHE:HB2    | 1:D:403:MET:HE1   | 1.91                     | 0.52              |
| 1:A:1461:ASP:HB2  | 1:A:1493:TYR:HB2  | 1.92                     | 0.52              |
| 1:C:3144:PHE:HD1  | 1:C:3196:ARG:HB2  | 1.73                     | 0.52              |
| 1:D:774:ASP:N     | 1:D:774:ASP:OD1   | 2.43                     | 0.52              |
| 1:D:4562:LEU:HD21 | 1:D:4656:LEU:HB3  | 1.90                     | 0.52              |
| 1:D:4984:ASN:O    | 1:D:4986:ALA:N    | 2.42                     | 0.52              |
| 1:A:221:ARG:O     | 1:A:391:THR:OG1   | 2.27                     | 0.52              |
| 1:A:1499:ASP:OD1  | 1:A:1499:ASP:N    | 2.42                     | 0.52              |
| 1:B:1499:ASP:N    | 1:B:1499:ASP:OD1  | 2.42                     | 0.52              |
| 1:B:1708:ARG:NH1  | 1:B:1836:PHE:O    | 2.42                     | 0.52              |
| 1:A:3144:PHE:HD1  | 1:A:3196:ARG:HB2  | 1.73                     | 0.52              |
| 1:A:4570:ALA:O    | 1:A:4574:ASN:ND2  | 2.36                     | 0.52              |
| 1:B:3717:ASP:OD1  | 1:B:3717:ASP:N    | 2.43                     | 0.52              |
| 1:C:4562:LEU:HD21 | 1:C:4656:LEU:HB3  | 1.90                     | 0.52              |
| 1:A:1805:GLU:OE1  | 1:A:1808:ARG:NH2  | 2.39                     | 0.51              |
| 1:A:3977:GLN:NE2  | 1:A:4030:LEU:O    | 2.41                     | 0.51              |
| 1:B:3376:GLU:HG3  | 1:B:3394:VAL:HG11 | 1.92                     | 0.51              |
| 1:D:3242:ASP:OD1  | 1:D:3242:ASP:N    | 2.43                     | 0.51              |
| 1:B:4984:ASN:O    | 1:B:4986:ALA:N    | 2.42                     | 0.51              |
| 1:C:2347:GLU:O    | 1:C:2351:ASN:ND2  | 2.44                     | 0.51              |
| 1:D:40:GLU:OE2    | 1:D:44:ASN:N      | 2.43                     | 0.51              |
| 1:D:1644:GLU:OE1  | 1:D:1646:ARG:NH1  | 2.39                     | 0.51              |
| 1:D:3717:ASP:N    | 1:D:3717:ASP:OD1  | 2.43                     | 0.51              |
| 2:G:27:THR:HG23   | 2:G:40:ARG:HH11   | 1.76                     | 0.51              |
| 1:A:3242:ASP:OD1  | 1:A:3242:ASP:N    | 2.43                     | 0.51              |
| 1:A:3308:THR:OG1  | 1:A:3310:ASP:OD1  | 2.22                     | 0.51              |
| 1:B:1259:ARG:NH1  | 1:B:1596:GLU:OE2  | 2.44                     | 0.51              |
| 1:D:2347:GLU:O    | 1:D:2351:ASN:ND2  | 2.44                     | 0.51              |
| 1:A:2347:GLU:O    | 1:A:2351:ASN:ND2  | 2.44                     | 0.51              |
| 1:A:2513:GLU:CD   | 1:A:2514:ASN:H    | 2.17                     | 0.51              |
| 1:C:1644:GLU:OE1  | 1:C:1646:ARG:NH1  | 2.39                     | 0.51              |
| 1:C:1695:LEU:HD23 | 1:C:1810:LYS:HE3  | 1.92                     | 0.51              |
| 1:C:3290:GLU:HG2  | 1:C:3308:THR:HG22 | 1.93                     | 0.51              |
| 1:C:4001:MET:HE2  | 1:C:4001:MET:HA   | 1.92                     | 0.51              |
| 1:A:464:LYS:HE2   | 1:A:468:LEU:HD21  | 1.92                     | 0.51              |
| 1:A:1708:ARG:NH1  | 1:A:1836:PHE:O    | 2.42                     | 0.51              |
| 1:A:2196:ASN:OD1  | 1:A:2199:ARG:NH1  | 2.44                     | 0.51              |
| 1:A:3353:LEU:HB3  | 1:A:3357:HIS:CE1  | 2.46                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2513:GLU:CD   | 1:B:2514:ASN:H    | 2.17                     | 0.51              |
| 1:B:4891:VAL:HG23 | 1:B:4892:ARG:HG3  | 1.93                     | 0.51              |
| 1:C:350:HIS:HB3   | 1:C:354:GLY:H     | 1.76                     | 0.51              |
| 1:C:1461:ASP:HB2  | 1:C:1493:TYR:HB2  | 1.92                     | 0.51              |
| 1:D:350:HIS:HB3   | 1:D:354:GLY:H     | 1.76                     | 0.51              |
| 1:D:595:ARG:HH22  | 1:D:1642:PRO:HD2  | 1.74                     | 0.51              |
| 1:A:1022:VAL:HG21 | 1:A:1026:LEU:HB3  | 1.92                     | 0.51              |
| 1:A:4791:TYR:OH   | 1:A:4815:ASP:O    | 2.29                     | 0.51              |
| 1:B:786:GLY:N     | 1:B:1630:CYS:SG   | 2.78                     | 0.51              |
| 1:B:1649:ASP:HB3  | 1:B:1652:GLU:HG3  | 1.93                     | 0.51              |
| 1:B:3290:GLU:HG2  | 1:B:3308:THR:HG22 | 1.93                     | 0.51              |
| 1:C:736:HIS:ND1   | 1:C:737:LEU:O     | 2.44                     | 0.51              |
| 1:C:2196:ASN:OD1  | 1:C:2199:ARG:NH1  | 2.44                     | 0.51              |
| 1:C:4984:ASN:O    | 1:C:4986:ALA:N    | 2.42                     | 0.51              |
| 1:D:2196:ASN:OD1  | 1:D:2199:ARG:NH1  | 2.44                     | 0.51              |
| 1:D:4891:VAL:HG23 | 1:D:4892:ARG:HG3  | 1.93                     | 0.51              |
| 2:H:27:THR:HG23   | 2:H:40:ARG:HH11   | 1.75                     | 0.51              |
| 1:A:1695:LEU:HD23 | 1:A:1810:LYS:HE3  | 1.92                     | 0.51              |
| 1:B:1100:MET:O    | 1:B:1126:GLY:N    | 2.40                     | 0.51              |
| 1:C:255:HIS:CG    | 1:C:480:GLU:HG3   | 2.46                     | 0.51              |
| 1:D:1022:VAL:HG21 | 1:D:1026:LEU:HB3  | 1.92                     | 0.51              |
| 1:D:2013:LYS:HD3  | 1:D:2023:LEU:HD12 | 1.93                     | 0.51              |
| 2:H:40:ARG:NH2    | 2:H:102:GLU:OE1   | 2.44                     | 0.51              |
| 1:B:2211:MET:HA   | 1:B:2214:VAL:HG12 | 1.93                     | 0.51              |
| 1:C:1022:VAL:HG21 | 1:C:1026:LEU:HB3  | 1.92                     | 0.51              |
| 1:C:1259:ARG:NH1  | 1:C:1596:GLU:OE2  | 2.44                     | 0.51              |
| 1:C:2211:MET:HA   | 1:C:2214:VAL:HG12 | 1.93                     | 0.51              |
| 1:C:4891:VAL:HG23 | 1:C:4892:ARG:HG3  | 1.93                     | 0.51              |
| 1:D:2256:TYR:O    | 1:D:2260:ASN:ND2  | 2.44                     | 0.51              |
| 1:A:1259:ARG:NH1  | 1:A:1596:GLU:OE2  | 2.44                     | 0.51              |
| 1:A:5030:LYS:O    | 1:A:5032:TYR:N    | 2.44                     | 0.51              |
| 1:B:2196:ASN:OD1  | 1:B:2199:ARG:NH1  | 2.44                     | 0.51              |
| 1:B:3040:THR:HB   | 1:B:3088:VAL:HG21 | 1.93                     | 0.51              |
| 1:B:5030:LYS:O    | 1:B:5032:TYR:N    | 2.44                     | 0.51              |
| 1:C:3977:GLN:NE2  | 1:C:4030:LEU:O    | 2.41                     | 0.51              |
| 1:D:4001:MET:HE2  | 1:D:4001:MET:HA   | 1.92                     | 0.51              |
| 1:A:2013:LYS:HD3  | 1:A:2023:LEU:HD12 | 1.93                     | 0.51              |
| 1:A:4891:VAL:HG23 | 1:A:4892:ARG:HG3  | 1.93                     | 0.51              |
| 1:B:879:HIS:HA    | 1:B:882:TRP:CD1   | 2.46                     | 0.51              |
| 1:B:1022:VAL:HG21 | 1:B:1026:LEU:HB3  | 1.92                     | 0.51              |
| 1:B:2095:GLN:NE2  | 1:B:2127:GLN:O    | 2.43                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:4001:MET:HA   | 1:B:4001:MET:HE2  | 1.92                     | 0.51              |
| 1:D:723:THR:O     | 1:D:728:ARG:NH2   | 2.44                     | 0.51              |
| 1:A:3040:THR:HB   | 1:A:3088:VAL:HG21 | 1.93                     | 0.50              |
| 1:A:3817:LEU:HB2  | 1:A:3899:PHE:HE1  | 1.76                     | 0.50              |
| 1:B:1461:ASP:HB2  | 1:B:1493:TYR:HB2  | 1.92                     | 0.50              |
| 1:C:595:ARG:HH22  | 1:C:1642:PRO:HD2  | 1.74                     | 0.50              |
| 1:C:774:ASP:OD1   | 1:C:774:ASP:N     | 2.43                     | 0.50              |
| 1:C:1116:GLY:HA3  | 1:C:1132:TRP:HB3  | 1.93                     | 0.50              |
| 1:C:1649:ASP:HB3  | 1:C:1652:GLU:HG3  | 1.93                     | 0.50              |
| 1:D:1461:ASP:HB2  | 1:D:1493:TYR:HB2  | 1.92                     | 0.50              |
| 1:D:2547:ALA:O    | 1:D:2551:ASN:ND2  | 2.45                     | 0.50              |
| 1:D:3353:LEU:HB3  | 1:D:3357:HIS:CE1  | 2.46                     | 0.50              |
| 2:G:40:ARG:NH2    | 2:G:102:GLU:OE1   | 2.44                     | 0.50              |
| 1:A:630:GLU:HA    | 1:A:1642:PRO:HB3  | 1.93                     | 0.50              |
| 1:A:3366:ARG:HD3  | 1:A:3437:MET:HA   | 1.94                     | 0.50              |
| 1:A:4001:MET:HE2  | 1:A:4001:MET:HA   | 1.92                     | 0.50              |
| 1:B:790:ARG:HH21  | 1:B:792:LEU:HD13  | 1.77                     | 0.50              |
| 1:B:2347:GLU:O    | 1:B:2351:ASN:ND2  | 2.44                     | 0.50              |
| 1:C:464:LYS:HE2   | 1:C:468:LEU:HD21  | 1.92                     | 0.50              |
| 1:C:790:ARG:HH21  | 1:C:792:LEU:HD13  | 1.76                     | 0.50              |
| 1:C:879:HIS:HA    | 1:C:882:TRP:CD1   | 2.46                     | 0.50              |
| 1:C:3366:ARG:HD3  | 1:C:3437:MET:HA   | 1.93                     | 0.50              |
| 1:D:786:GLY:N     | 1:D:1630:CYS:SG   | 2.78                     | 0.50              |
| 1:D:3817:LEU:HB2  | 1:D:3899:PHE:HE1  | 1.76                     | 0.50              |
| 1:A:774:ASP:N     | 1:A:774:ASP:OD1   | 2.43                     | 0.50              |
| 1:A:1245:PHE:CD1  | 1:A:1288:PHE:HE1  | 2.29                     | 0.50              |
| 1:B:255:HIS:CG    | 1:B:480:GLU:HG3   | 2.46                     | 0.50              |
| 1:B:1093:GLU:HB3  | 1:B:1201:HIS:HB3  | 1.94                     | 0.50              |
| 1:B:1245:PHE:CD1  | 1:B:1288:PHE:HE1  | 2.29                     | 0.50              |
| 1:B:3353:LEU:HB3  | 1:B:3357:HIS:CE1  | 2.46                     | 0.50              |
| 1:D:790:ARG:HH21  | 1:D:792:LEU:HD13  | 1.76                     | 0.50              |
| 1:D:1245:PHE:CD1  | 1:D:1288:PHE:HE1  | 2.29                     | 0.50              |
| 1:D:1259:ARG:NH1  | 1:D:1596:GLU:OE2  | 2.44                     | 0.50              |
| 1:D:3290:GLU:HG2  | 1:D:3308:THR:HG22 | 1.93                     | 0.50              |
| 1:D:4090:LYS:NZ   | 1:D:4115:SER:OG   | 2.41                     | 0.50              |
| 2:E:40:ARG:NH2    | 2:E:102:GLU:OE1   | 2.44                     | 0.50              |
| 1:A:1649:ASP:HB3  | 1:A:1652:GLU:HG3  | 1.93                     | 0.50              |
| 1:B:1116:GLY:HA3  | 1:B:1132:TRP:HB3  | 1.93                     | 0.50              |
| 1:C:1093:GLU:HB3  | 1:C:1201:HIS:HB3  | 1.94                     | 0.50              |
| 1:D:255:HIS:CG    | 1:D:480:GLU:HG3   | 2.46                     | 0.50              |
| 1:B:1695:LEU:HD23 | 1:B:1810:LYS:HE3  | 1.92                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2611:CYS:HA   | 1:B:2614:ILE:HG22 | 1.93                     | 0.50              |
| 1:C:3971:GLY:HA2  | 1:C:5005:GLY:HA3  | 1.94                     | 0.50              |
| 1:C:5030:LYS:O    | 1:C:5032:TYR:N    | 2.44                     | 0.50              |
| 1:D:630:GLU:HA    | 1:D:1642:PRO:HB3  | 1.93                     | 0.50              |
| 1:D:1695:LEU:HD23 | 1:D:1810:LYS:HE3  | 1.92                     | 0.50              |
| 1:D:3889:GLN:HG3  | 1:D:3967:GLU:HG3  | 1.94                     | 0.50              |
| 1:D:4791:TYR:OH   | 1:D:4815:ASP:O    | 2.29                     | 0.50              |
| 1:A:723:THR:O     | 1:A:728:ARG:NH2   | 2.44                     | 0.50              |
| 1:A:4651:THR:OG1  | 1:A:4803:HIS:NE2  | 2.34                     | 0.50              |
| 1:C:1245:PHE:CD1  | 1:C:1288:PHE:HE1  | 2.29                     | 0.50              |
| 1:C:3817:LEU:HB2  | 1:C:3899:PHE:HE1  | 1.76                     | 0.50              |
| 1:D:3040:THR:HB   | 1:D:3088:VAL:HG21 | 1.93                     | 0.50              |
| 1:D:5030:LYS:O    | 1:D:5032:TYR:N    | 2.44                     | 0.50              |
| 2:F:27:THR:HG23   | 2:F:40:ARG:HH11   | 1.75                     | 0.50              |
| 2:F:40:ARG:NH2    | 2:F:102:GLU:OE1   | 2.44                     | 0.50              |
| 1:A:879:HIS:HA    | 1:A:882:TRP:CD1   | 2.46                     | 0.50              |
| 1:A:1093:GLU:HB3  | 1:A:1201:HIS:HB3  | 1.94                     | 0.50              |
| 1:B:350:HIS:HB3   | 1:B:354:GLY:H     | 1.76                     | 0.50              |
| 1:B:1126:GLY:HA2  | 1:B:1143:TRP:CZ3  | 2.47                     | 0.50              |
| 1:C:2013:LYS:HD3  | 1:C:2023:LEU:HD12 | 1.93                     | 0.50              |
| 1:C:2095:GLN:NE2  | 1:C:2127:GLN:O    | 2.43                     | 0.50              |
| 1:D:1126:GLY:HA2  | 1:D:1143:TRP:CZ3  | 2.47                     | 0.50              |
| 1:A:2547:ALA:O    | 1:A:2551:ASN:ND2  | 2.45                     | 0.50              |
| 1:A:3290:GLU:HG2  | 1:A:3308:THR:HG22 | 1.93                     | 0.50              |
| 1:B:3242:ASP:OD1  | 1:B:3242:ASP:N    | 2.43                     | 0.50              |
| 1:C:239:ASP:N     | 1:C:239:ASP:OD1   | 2.43                     | 0.50              |
| 1:C:1100:MET:O    | 1:C:1126:GLY:N    | 2.40                     | 0.50              |
| 1:C:3040:THR:HB   | 1:C:3088:VAL:HG21 | 1.94                     | 0.50              |
| 1:A:255:HIS:CG    | 1:A:480:GLU:HG3   | 2.46                     | 0.50              |
| 1:B:2547:ALA:O    | 1:B:2551:ASN:ND2  | 2.45                     | 0.50              |
| 1:B:4090:LYS:NZ   | 1:B:4115:SER:OG   | 2.41                     | 0.50              |
| 1:C:2547:ALA:O    | 1:C:2551:ASN:ND2  | 2.45                     | 0.50              |
| 1:C:3353:LEU:HB3  | 1:C:3357:HIS:CE1  | 2.46                     | 0.50              |
| 1:C:4850:LEU:HD13 | 1:D:4814:LEU:HD23 | 1.93                     | 0.50              |
| 1:A:592:LYS:HA    | 1:A:1580:PHE:HE2  | 1.77                     | 0.49              |
| 1:A:1126:GLY:HA2  | 1:A:1143:TRP:CZ3  | 2.47                     | 0.49              |
| 1:A:2611:CYS:HA   | 1:A:2614:ILE:HG22 | 1.93                     | 0.49              |
| 1:B:458:GLU:HG2   | 1:B:459:LEU:HD12  | 1.94                     | 0.49              |
| 1:C:458:GLU:HG2   | 1:C:459:LEU:HD12  | 1.94                     | 0.49              |
| 1:C:592:LYS:HA    | 1:C:1580:PHE:HE2  | 1.77                     | 0.49              |
| 1:C:723:THR:O     | 1:C:728:ARG:NH2   | 2.44                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:879:HIS:HA    | 1:D:882:TRP:CD1   | 2.46                     | 0.49              |
| 1:D:1116:GLY:HA3  | 1:D:1132:TRP:HB3  | 1.93                     | 0.49              |
| 1:D:2495:VAL:HG12 | 1:D:2497:ASP:H    | 1.77                     | 0.49              |
| 1:A:790:ARG:HH21  | 1:A:792:LEU:HD13  | 1.76                     | 0.49              |
| 1:A:2095:GLN:NE2  | 1:A:2127:GLN:O    | 2.43                     | 0.49              |
| 1:B:592:LYS:HA    | 1:B:1580:PHE:HE2  | 1.77                     | 0.49              |
| 1:B:723:THR:O     | 1:B:728:ARG:NH2   | 2.44                     | 0.49              |
| 1:B:4791:TYR:OH   | 1:B:4815:ASP:O    | 2.29                     | 0.49              |
| 1:C:2495:VAL:HG12 | 1:C:2497:ASP:H    | 1.77                     | 0.49              |
| 1:C:3471:THR:OG1  | 1:C:3472:ALA:N    | 2.39                     | 0.49              |
| 1:D:458:GLU:HG2   | 1:D:459:LEU:HD12  | 1.94                     | 0.49              |
| 1:D:1093:GLU:HB3  | 1:D:1201:HIS:HB3  | 1.94                     | 0.49              |
| 1:D:2611:CYS:HA   | 1:D:2614:ILE:HG22 | 1.93                     | 0.49              |
| 1:B:2013:LYS:HD3  | 1:B:2023:LEU:HD12 | 1.93                     | 0.49              |
| 1:C:4791:TYR:OH   | 1:C:4815:ASP:O    | 2.29                     | 0.49              |
| 1:D:221:ARG:NH1   | 1:D:253:CYS:O     | 2.46                     | 0.49              |
| 1:D:3366:ARG:HD3  | 1:D:3437:MET:HA   | 1.94                     | 0.49              |
| 1:A:2211:MET:HA   | 1:A:2214:VAL:HG12 | 1.93                     | 0.49              |
| 1:B:630:GLU:HA    | 1:B:1642:PRO:HB3  | 1.93                     | 0.49              |
| 1:B:2430:ILE:HD13 | 1:B:2502:MET:HE1  | 1.94                     | 0.49              |
| 1:C:2611:CYS:HA   | 1:C:2614:ILE:HG22 | 1.93                     | 0.49              |
| 1:D:592:LYS:HA    | 1:D:1580:PHE:HE2  | 1.77                     | 0.49              |
| 1:D:1649:ASP:HB3  | 1:D:1652:GLU:HG3  | 1.93                     | 0.49              |
| 1:A:221:ARG:NH1   | 1:A:253:CYS:O     | 2.46                     | 0.49              |
| 1:A:458:GLU:HG2   | 1:A:459:LEU:HD12  | 1.94                     | 0.49              |
| 1:A:2430:ILE:HD13 | 1:A:2502:MET:HE1  | 1.95                     | 0.49              |
| 1:A:4090:LYS:NZ   | 1:A:4115:SER:OG   | 2.41                     | 0.49              |
| 1:B:2256:TYR:O    | 1:B:2260:ASN:ND2  | 2.44                     | 0.49              |
| 1:B:3366:ARG:HD3  | 1:B:3437:MET:HA   | 1.94                     | 0.49              |
| 1:B:3503:TYR:HA   | 1:B:3507:THR:HG21 | 1.95                     | 0.49              |
| 1:B:3971:GLY:HA2  | 1:B:5005:GLY:HA3  | 1.94                     | 0.49              |
| 1:C:40:GLU:OE2    | 1:C:44:ASN:N      | 2.43                     | 0.49              |
| 1:C:1973:GLN:OE1  | 1:C:1976:ARG:NH2  | 2.44                     | 0.49              |
| 1:C:3717:ASP:OD1  | 1:C:3717:ASP:N    | 2.43                     | 0.49              |
| 1:C:3889:GLN:HG3  | 1:C:3967:GLU:HG3  | 1.94                     | 0.49              |
| 2:E:27:THR:HG23   | 2:E:40:ARG:HH11   | 1.75                     | 0.49              |
| 1:A:350:HIS:HB3   | 1:A:354:GLY:H     | 1.76                     | 0.49              |
| 1:A:1100:MET:O    | 1:A:1126:GLY:N    | 2.40                     | 0.49              |
| 1:A:4814:LEU:HD23 | 1:D:4850:LEU:HD13 | 1.93                     | 0.49              |
| 1:C:630:GLU:HA    | 1:C:1642:PRO:HB3  | 1.93                     | 0.49              |
| 1:C:1101:ARG:HB2  | 1:C:1193:SER:HB3  | 1.95                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:2564:LYS:HD2  | 1:C:2565:CYS:HB2  | 1.95                     | 0.49              |
| 1:D:736:HIS:ND1   | 1:D:737:LEU:O     | 2.44                     | 0.49              |
| 1:A:1101:ARG:HB2  | 1:A:1193:SER:HB3  | 1.95                     | 0.49              |
| 1:B:2495:VAL:HG12 | 1:B:2497:ASP:H    | 1.77                     | 0.49              |
| 1:D:2211:MET:HA   | 1:D:2214:VAL:HG12 | 1.93                     | 0.49              |
| 1:A:1116:GLY:HA3  | 1:A:1132:TRP:HB3  | 1.93                     | 0.49              |
| 1:B:221:ARG:NH1   | 1:B:253:CYS:O     | 2.46                     | 0.49              |
| 1:B:1644:GLU:OE1  | 1:B:1646:ARG:NH1  | 2.39                     | 0.49              |
| 1:B:4183:ILE:HG23 | 1:B:5021:PHE:HB2  | 1.95                     | 0.49              |
| 1:C:3503:TYR:HA   | 1:C:3507:THR:HG21 | 1.95                     | 0.49              |
| 1:B:1101:ARG:HB2  | 1:B:1193:SER:HB3  | 1.95                     | 0.49              |
| 1:B:3817:LEU:HB2  | 1:B:3899:PHE:HE1  | 1.76                     | 0.49              |
| 1:C:2430:ILE:HD13 | 1:C:2502:MET:HE1  | 1.95                     | 0.49              |
| 1:D:1100:MET:O    | 1:D:1126:GLY:N    | 2.40                     | 0.49              |
| 1:A:736:HIS:ND1   | 1:A:737:LEU:O     | 2.44                     | 0.49              |
| 1:B:847:SER:OG    | 1:B:850:ASP:OD2   | 2.31                     | 0.49              |
| 1:B:2660:GLY:HA2  | 1:B:2663:ASN:HD21 | 1.78                     | 0.49              |
| 1:B:3889:GLN:HG3  | 1:B:3967:GLU:HG3  | 1.94                     | 0.49              |
| 1:C:221:ARG:NH1   | 1:C:253:CYS:O     | 2.46                     | 0.49              |
| 1:C:4047:MET:HE3  | 1:C:4048:LEU:HD22 | 1.95                     | 0.49              |
| 1:D:3503:TYR:HA   | 1:D:3507:THR:HG21 | 1.95                     | 0.49              |
| 1:D:3781:GLN:OE1  | 1:D:3819:TYR:OH   | 2.28                     | 0.49              |
| 1:D:4183:ILE:HG23 | 1:D:5021:PHE:HB2  | 1.95                     | 0.49              |
| 1:B:736:HIS:ND1   | 1:B:737:LEU:O     | 2.44                     | 0.48              |
| 1:C:1126:GLY:HA2  | 1:C:1143:TRP:CZ3  | 2.47                     | 0.48              |
| 1:C:2256:TYR:O    | 1:C:2260:ASN:ND2  | 2.44                     | 0.48              |
| 1:D:3971:GLY:HA2  | 1:D:5005:GLY:HA3  | 1.94                     | 0.48              |
| 1:A:847:SER:OG    | 1:A:850:ASP:OD2   | 2.31                     | 0.48              |
| 1:A:3971:GLY:HA2  | 1:A:5005:GLY:HA3  | 1.94                     | 0.48              |
| 1:C:3308:THR:OG1  | 1:C:3310:ASP:OD1  | 2.22                     | 0.48              |
| 1:C:4183:ILE:HG23 | 1:C:5021:PHE:HB2  | 1.95                     | 0.48              |
| 1:A:1024:TYR:HE2  | 1:A:1035:ASN:HD22 | 1.60                     | 0.48              |
| 1:B:4850:LEU:HD13 | 1:C:4814:LEU:HD23 | 1.94                     | 0.48              |
| 1:C:847:SER:OG    | 1:C:850:ASP:OD2   | 2.31                     | 0.48              |
| 1:C:2289:ALA:HA   | 1:C:3849:ARG:HD3  | 1.96                     | 0.48              |
| 1:D:847:SER:OG    | 1:D:850:ASP:OD2   | 2.31                     | 0.48              |
| 1:A:2495:VAL:HG12 | 1:A:2497:ASP:H    | 1.77                     | 0.48              |
| 1:B:2564:LYS:HD2  | 1:B:2565:CYS:HB2  | 1.95                     | 0.48              |
| 1:D:1101:ARG:HB2  | 1:D:1193:SER:HB3  | 1.95                     | 0.48              |
| 1:D:2095:GLN:NE2  | 1:D:2127:GLN:O    | 2.43                     | 0.48              |
| 1:B:4047:MET:HE3  | 1:B:4048:LEU:HD22 | 1.95                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:855:PRO:HG3   | 1:D:998:ARG:HD3   | 1.96                     | 0.48              |
| 1:D:3566:SER:HB2  | 1:D:3569:LEU:HB2  | 1.95                     | 0.48              |
| 1:A:2289:ALA:HA   | 1:A:3849:ARG:HD3  | 1.96                     | 0.48              |
| 1:A:4047:MET:HE3  | 1:A:4048:LEU:HD22 | 1.95                     | 0.48              |
| 1:B:4865:LYS:HE3  | 1:B:4900:GLU:HB2  | 1.95                     | 0.48              |
| 1:C:1671:ARG:HH11 | 1:C:1713:ASP:HB3  | 1.79                     | 0.48              |
| 1:D:2289:ALA:HA   | 1:D:3849:ARG:HD3  | 1.96                     | 0.48              |
| 1:A:759:ILE:HG13  | 1:A:760:ASN:H     | 1.79                     | 0.48              |
| 1:B:2289:ALA:HA   | 1:B:3849:ARG:HD3  | 1.96                     | 0.48              |
| 1:C:2660:GLY:HA2  | 1:C:2663:ASN:HD21 | 1.78                     | 0.48              |
| 1:A:723:THR:OG1   | 1:A:728:ARG:NH1   | 2.47                     | 0.48              |
| 1:A:2660:GLY:HA2  | 1:A:2663:ASN:HD21 | 1.78                     | 0.48              |
| 1:A:3503:TYR:HA   | 1:A:3507:THR:HG21 | 1.95                     | 0.48              |
| 1:A:4865:LYS:HE3  | 1:A:4900:GLU:HB2  | 1.96                     | 0.48              |
| 1:B:5031:GLN:HG2  | 1:B:5032:TYR:H    | 1.79                     | 0.48              |
| 1:C:1024:TYR:HE2  | 1:C:1035:ASN:HD22 | 1.60                     | 0.48              |
| 1:C:3102:ASP:O    | 1:C:3106:MET:HG2  | 2.14                     | 0.48              |
| 1:D:232:THR:HG21  | 1:D:252:VAL:HG21  | 1.96                     | 0.48              |
| 1:D:1024:TYR:HE2  | 1:D:1035:ASN:HD22 | 1.60                     | 0.48              |
| 1:D:1973:GLN:OE1  | 1:D:1976:ARG:NH2  | 2.44                     | 0.48              |
| 1:D:2430:ILE:HD13 | 1:D:2502:MET:HE1  | 1.94                     | 0.48              |
| 1:A:3889:GLN:HG3  | 1:A:3967:GLU:HG3  | 1.94                     | 0.48              |
| 1:A:4183:ILE:HG23 | 1:A:5021:PHE:HB2  | 1.95                     | 0.48              |
| 1:B:723:THR:OG1   | 1:B:728:ARG:NH1   | 2.47                     | 0.48              |
| 1:B:855:PRO:HG3   | 1:B:998:ARG:HD3   | 1.96                     | 0.48              |
| 1:D:723:THR:OG1   | 1:D:728:ARG:NH1   | 2.47                     | 0.48              |
| 1:D:4047:MET:HE3  | 1:D:4048:LEU:HD22 | 1.95                     | 0.48              |
| 1:A:3566:SER:HB2  | 1:A:3569:LEU:HB2  | 1.95                     | 0.48              |
| 1:A:4850:LEU:HD13 | 1:B:4814:LEU:HD23 | 1.94                     | 0.48              |
| 1:B:759:ILE:HG13  | 1:B:760:ASN:H     | 1.79                     | 0.48              |
| 1:B:2003:GLN:HB2  | 1:B:3652:MET:HE1  | 1.96                     | 0.48              |
| 1:B:3102:ASP:O    | 1:B:3106:MET:HG2  | 2.14                     | 0.48              |
| 1:B:3566:SER:HB2  | 1:B:3569:LEU:HB2  | 1.95                     | 0.48              |
| 1:C:855:PRO:HG3   | 1:C:998:ARG:HD3   | 1.96                     | 0.48              |
| 1:A:855:PRO:HG3   | 1:A:998:ARG:HD3   | 1.96                     | 0.47              |
| 1:A:4868:ASP:OD1  | 1:A:4868:ASP:N    | 2.47                     | 0.47              |
| 1:C:5031:GLN:HG2  | 1:C:5032:TYR:H    | 1.79                     | 0.47              |
| 1:D:2660:GLY:HA2  | 1:D:2663:ASN:HD21 | 1.78                     | 0.47              |
| 1:A:239:ASP:OD1   | 1:A:239:ASP:N     | 2.43                     | 0.47              |
| 1:A:5031:GLN:HG2  | 1:A:5032:TYR:H    | 1.79                     | 0.47              |
| 1:C:759:ILE:HG13  | 1:C:760:ASN:H     | 1.79                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:3781:GLN:OE1  | 1:C:3819:TYR:OH   | 2.28                     | 0.47              |
| 1:A:2564:LYS:HD2  | 1:A:2565:CYS:HB2  | 1.95                     | 0.47              |
| 1:B:1671:ARG:HH11 | 1:B:1713:ASP:HB3  | 1.79                     | 0.47              |
| 1:D:3102:ASP:O    | 1:D:3106:MET:HG2  | 2.14                     | 0.47              |
| 1:A:3462:ASN:HB3  | 1:A:3464:ILE:HG12 | 1.97                     | 0.47              |
| 1:A:4032:GLU:HB3  | 1:A:4033:GLY:H    | 1.55                     | 0.47              |
| 1:B:2782:ASP:N    | 1:B:2782:ASP:OD1  | 2.48                     | 0.47              |
| 1:D:1671:ARG:HH11 | 1:D:1713:ASP:HB3  | 1.79                     | 0.47              |
| 1:D:2782:ASP:OD1  | 1:D:2782:ASP:N    | 2.48                     | 0.47              |
| 1:B:1024:TYR:HE2  | 1:B:1035:ASN:HD22 | 1.60                     | 0.47              |
| 1:B:3906:GLN:NE2  | 1:B:3911:THR:O    | 2.48                     | 0.47              |
| 1:C:3906:GLN:NE2  | 1:C:3911:THR:O    | 2.48                     | 0.47              |
| 1:C:4679:ARG:NH1  | 1:C:4715:TYR:OH   | 2.38                     | 0.47              |
| 1:D:759:ILE:HG13  | 1:D:760:ASN:H     | 1.79                     | 0.47              |
| 1:D:4865:LYS:HE3  | 1:D:4900:GLU:HB2  | 1.96                     | 0.47              |
| 1:A:2003:GLN:HB2  | 1:A:3652:MET:HE1  | 1.97                     | 0.47              |
| 1:A:2006:ILE:HD13 | 1:A:2009:LEU:HD21 | 1.97                     | 0.47              |
| 1:A:3504:SER:O    | 1:A:3507:THR:OG1  | 2.33                     | 0.47              |
| 1:B:884:LEU:HB3   | 1:B:967:PRO:HB2   | 1.97                     | 0.47              |
| 1:B:2007:ASN:O    | 1:B:2011:HIS:ND1  | 2.36                     | 0.47              |
| 1:B:5001:THR:OG1  | 1:B:5002:GLU:OE1  | 2.30                     | 0.47              |
| 1:C:723:THR:OG1   | 1:C:728:ARG:NH1   | 2.47                     | 0.47              |
| 1:C:2782:ASP:OD1  | 1:C:2782:ASP:N    | 2.48                     | 0.47              |
| 1:C:3504:SER:O    | 1:C:3507:THR:OG1  | 2.33                     | 0.47              |
| 1:C:4090:LYS:NZ   | 1:C:4115:SER:OG   | 2.41                     | 0.47              |
| 1:D:996:TRP:O     | 1:D:1000:ARG:HB3  | 2.15                     | 0.47              |
| 1:D:2006:ILE:HD13 | 1:D:2009:LEU:HD21 | 1.97                     | 0.47              |
| 1:D:3906:GLN:NE2  | 1:D:3911:THR:O    | 2.48                     | 0.47              |
| 1:D:5031:GLN:HG2  | 1:D:5032:TYR:H    | 1.79                     | 0.47              |
| 1:B:232:THR:HG21  | 1:B:252:VAL:HG21  | 1.96                     | 0.47              |
| 1:B:597:HIS:HB2   | 1:B:1665:HIS:ND1  | 2.30                     | 0.47              |
| 1:B:647:ASN:HB2   | 1:B:821:LEU:HD12  | 1.97                     | 0.47              |
| 1:B:710:ASP:OD1   | 1:B:710:ASP:N     | 2.44                     | 0.47              |
| 1:B:1746:THR:HG23 | 1:B:1748:PHE:H    | 1.80                     | 0.47              |
| 1:A:4679:ARG:NH1  | 1:A:4715:TYR:OH   | 2.38                     | 0.47              |
| 1:B:1973:GLN:OE1  | 1:B:1976:ARG:NH2  | 2.44                     | 0.47              |
| 1:C:1746:THR:HG23 | 1:C:1748:PHE:H    | 1.80                     | 0.47              |
| 1:C:4865:LYS:HE3  | 1:C:4900:GLU:HB2  | 1.95                     | 0.47              |
| 1:D:2564:LYS:HD2  | 1:D:2565:CYS:HB2  | 1.95                     | 0.47              |
| 1:A:1671:ARG:HH11 | 1:A:1713:ASP:HB3  | 1.79                     | 0.47              |
| 1:A:2256:TYR:O    | 1:A:2260:ASN:ND2  | 2.44                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:4565:LEU:HD22 | 1:A:4653:VAL:HG21 | 1.97                     | 0.47              |
| 1:C:597:HIS:HB2   | 1:C:1665:HIS:ND1  | 2.30                     | 0.47              |
| 1:A:884:LEU:HB3   | 1:A:967:PRO:HB2   | 1.97                     | 0.46              |
| 1:A:1973:GLN:OE1  | 1:A:1976:ARG:NH2  | 2.44                     | 0.46              |
| 1:A:3906:GLN:NE2  | 1:A:3911:THR:O    | 2.48                     | 0.46              |
| 1:B:2006:ILE:HD13 | 1:B:2009:LEU:HD21 | 1.97                     | 0.46              |
| 1:C:232:THR:HG21  | 1:C:252:VAL:HG21  | 1.96                     | 0.46              |
| 1:C:884:LEU:HB3   | 1:C:967:PRO:HB2   | 1.97                     | 0.46              |
| 1:C:2006:ILE:HD13 | 1:C:2009:LEU:HD21 | 1.97                     | 0.46              |
| 1:C:4868:ASP:OD1  | 1:C:4868:ASP:N    | 2.47                     | 0.46              |
| 1:D:1708:ARG:HH12 | 1:D:1837:GLN:HA   | 1.80                     | 0.46              |
| 1:D:2003:GLN:HB2  | 1:D:3652:MET:HE1  | 1.96                     | 0.46              |
| 1:D:3462:ASN:HB3  | 1:D:3464:ILE:HG12 | 1.97                     | 0.46              |
| 1:A:232:THR:HG21  | 1:A:252:VAL:HG21  | 1.96                     | 0.46              |
| 1:A:3102:ASP:O    | 1:A:3106:MET:HG2  | 2.14                     | 0.46              |
| 1:B:996:TRP:O     | 1:B:1000:ARG:HB3  | 2.15                     | 0.46              |
| 1:B:1106:ARG:HB2  | 1:B:1120:LEU:HB3  | 1.97                     | 0.46              |
| 1:C:1106:ARG:HB2  | 1:C:1120:LEU:HB3  | 1.97                     | 0.46              |
| 1:C:1125:ASN:HB2  | 1:C:1132:TRP:CD1  | 2.51                     | 0.46              |
| 1:C:3566:SER:HB2  | 1:C:3569:LEU:HB2  | 1.95                     | 0.46              |
| 1:D:4032:GLU:HB3  | 1:D:4033:GLY:H    | 1.55                     | 0.46              |
| 1:B:4565:LEU:HD22 | 1:B:4653:VAL:HG21 | 1.97                     | 0.46              |
| 1:C:647:ASN:HB2   | 1:C:821:LEU:HD12  | 1.97                     | 0.46              |
| 1:C:3462:ASN:HB3  | 1:C:3464:ILE:HG12 | 1.97                     | 0.46              |
| 1:D:884:LEU:HB3   | 1:D:967:PRO:HB2   | 1.97                     | 0.46              |
| 1:D:1476:MET:HE3  | 1:D:1477:GLY:N    | 2.25                     | 0.46              |
| 1:A:4202:ARG:HA   | 1:A:4202:ARG:HD3  | 1.84                     | 0.46              |
| 1:B:1708:ARG:HH12 | 1:B:1837:GLN:HA   | 1.80                     | 0.46              |
| 1:C:1708:ARG:HH12 | 1:C:1837:GLN:HA   | 1.80                     | 0.46              |
| 1:D:1269:CYS:HB3  | 1:D:1473:THR:HG23 | 1.98                     | 0.46              |
| 2:E:26:TYR:OH     | 2:E:37:ASP:OD2    | 2.28                     | 0.46              |
| 1:A:2238:TYR:O    | 1:A:2242:ILE:HG12 | 2.16                     | 0.46              |
| 1:A:5001:THR:OG1  | 1:A:5002:GLU:OE1  | 2.30                     | 0.46              |
| 1:B:2294:ASP:N    | 1:B:2294:ASP:OD1  | 2.49                     | 0.46              |
| 1:C:996:TRP:O     | 1:C:1000:ARG:HB3  | 2.15                     | 0.46              |
| 1:A:647:ASN:HB2   | 1:A:821:LEU:HD12  | 1.97                     | 0.46              |
| 1:A:996:TRP:O     | 1:A:1000:ARG:HB3  | 2.15                     | 0.46              |
| 1:A:1746:THR:HG23 | 1:A:1748:PHE:H    | 1.80                     | 0.46              |
| 1:B:2238:TYR:O    | 1:B:2242:ILE:HG12 | 2.16                     | 0.46              |
| 1:C:1099:GLU:OE2  | 1:C:1101:ARG:NE   | 2.47                     | 0.46              |
| 1:C:1287:LEU:O    | 1:C:1460:HIS:N    | 2.39                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:303:ASP:OD1   | 1:D:303:ASP:N     | 2.47                     | 0.46              |
| 1:D:4565:LEU:HD22 | 1:D:4653:VAL:HG21 | 1.97                     | 0.46              |
| 1:A:2007:ASN:O    | 1:A:2011:HIS:ND1  | 2.36                     | 0.46              |
| 1:B:622:THR:HG21  | 1:B:1681:VAL:HG12 | 1.98                     | 0.46              |
| 1:B:1478:ASP:CG   | 1:B:1479:GLU:H    | 2.24                     | 0.46              |
| 1:C:1116:GLY:O    | 1:C:1134:LEU:N    | 2.48                     | 0.46              |
| 1:C:1478:ASP:CG   | 1:C:1479:GLU:H    | 2.24                     | 0.46              |
| 1:D:1125:ASN:HB2  | 1:D:1132:TRP:CD1  | 2.51                     | 0.46              |
| 1:D:1287:LEU:O    | 1:D:1460:HIS:N    | 2.39                     | 0.46              |
| 1:A:2294:ASP:OD1  | 1:A:2294:ASP:N    | 2.49                     | 0.46              |
| 1:A:2325:PRO:HB3  | 1:A:2421:ALA:HB1  | 1.98                     | 0.46              |
| 1:A:3661:TRP:O    | 1:A:3664:THR:OG1  | 2.30                     | 0.46              |
| 1:C:4679:ARG:HE   | 1:C:5017:ARG:CZ   | 2.29                     | 0.46              |
| 1:A:1708:ARG:HH12 | 1:A:1837:GLN:HA   | 1.80                     | 0.46              |
| 1:A:2782:ASP:OD1  | 1:A:2782:ASP:N    | 2.48                     | 0.46              |
| 1:C:3447:LYS:HA   | 1:C:3447:LYS:HD2  | 1.77                     | 0.46              |
| 1:D:622:THR:HG21  | 1:D:1681:VAL:HG12 | 1.98                     | 0.46              |
| 1:B:1116:GLY:O    | 1:B:1134:LEU:N    | 2.48                     | 0.45              |
| 1:B:2200:ALA:O    | 1:B:2202:GLY:N    | 2.49                     | 0.45              |
| 1:C:2211:MET:HB3  | 1:C:2211:MET:HE2  | 1.67                     | 0.45              |
| 1:C:3242:ASP:OD1  | 1:C:3242:ASP:N    | 2.43                     | 0.45              |
| 1:D:1746:THR:HG23 | 1:D:1748:PHE:H    | 1.80                     | 0.45              |
| 1:D:2325:PRO:HB3  | 1:D:2421:ALA:HB1  | 1.98                     | 0.45              |
| 1:D:4868:ASP:N    | 1:D:4868:ASP:OD1  | 2.47                     | 0.45              |
| 1:A:597:HIS:HB2   | 1:A:1665:HIS:ND1  | 2.30                     | 0.45              |
| 1:A:622:THR:HG21  | 1:A:1681:VAL:HG12 | 1.98                     | 0.45              |
| 1:B:1125:ASN:HB2  | 1:B:1132:TRP:CD1  | 2.51                     | 0.45              |
| 1:B:1291:LEU:HB2  | 1:B:1579:MET:HE2  | 1.99                     | 0.45              |
| 1:B:3462:ASN:HB3  | 1:B:3464:ILE:HG12 | 1.97                     | 0.45              |
| 1:C:3159:ASP:OD1  | 1:C:3159:ASP:N    | 2.49                     | 0.45              |
| 1:C:4651:THR:OG1  | 1:C:4803:HIS:NE2  | 2.34                     | 0.45              |
| 1:D:597:HIS:HB2   | 1:D:1665:HIS:ND1  | 2.30                     | 0.45              |
| 1:D:2238:TYR:O    | 1:D:2242:ILE:HG12 | 2.16                     | 0.45              |
| 1:A:1125:ASN:HB2  | 1:A:1132:TRP:CD1  | 2.51                     | 0.45              |
| 1:A:1269:CYS:HB3  | 1:A:1473:THR:HG23 | 1.98                     | 0.45              |
| 1:A:2208:MET:CE   | 1:A:2253:HIS:HB3  | 2.47                     | 0.45              |
| 1:A:4057:MET:SD   | 1:A:4057:MET:N    | 2.90                     | 0.45              |
| 1:A:4958:CYS:O    | 1:A:4960:ILE:N    | 2.49                     | 0.45              |
| 1:B:239:ASP:OD1   | 1:B:239:ASP:N     | 2.43                     | 0.45              |
| 1:B:1870:VAL:HG11 | 1:B:2091:PRO:HD2  | 1.99                     | 0.45              |
| 1:C:1269:CYS:HB3  | 1:C:1473:THR:HG23 | 1.98                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:1115:LEU:HD23 | 1:D:1123:VAL:HG11 | 1.99                     | 0.45              |
| 1:D:2211:MET:HE1  | 1:D:2257:LEU:HD13 | 1.98                     | 0.45              |
| 1:A:3159:ASP:OD1  | 1:A:3159:ASP:N    | 2.49                     | 0.45              |
| 1:B:4727:LYS:HE3  | 1:B:4727:LYS:HB3  | 1.82                     | 0.45              |
| 1:B:4868:ASP:N    | 1:B:4868:ASP:OD1  | 2.47                     | 0.45              |
| 1:C:236:ALA:HA    | 1:C:242:ARG:HD2   | 1.99                     | 0.45              |
| 1:C:649:PHE:HB3   | 1:C:776:LEU:HD21  | 1.99                     | 0.45              |
| 1:C:1291:LEU:HB2  | 1:C:1579:MET:HE2  | 1.99                     | 0.45              |
| 1:C:2325:PRO:HB3  | 1:C:2421:ALA:HB1  | 1.98                     | 0.45              |
| 1:D:1106:ARG:HB2  | 1:D:1120:LEU:HB3  | 1.97                     | 0.45              |
| 1:D:4679:ARG:HE   | 1:D:5017:ARG:CZ   | 2.29                     | 0.45              |
| 1:A:649:PHE:HB3   | 1:A:776:LEU:HD21  | 1.99                     | 0.45              |
| 1:A:5031:GLN:HG2  | 1:A:5032:TYR:N    | 2.32                     | 0.45              |
| 1:C:2003:GLN:HB2  | 1:C:3652:MET:HE1  | 1.97                     | 0.45              |
| 1:D:647:ASN:HB2   | 1:D:821:LEU:HD12  | 1.97                     | 0.45              |
| 1:A:2155:LEU:HD12 | 1:A:2185:ILE:HD11 | 1.98                     | 0.45              |
| 1:B:4679:ARG:HE   | 1:B:5017:ARG:CZ   | 2.29                     | 0.45              |
| 1:C:303:ASP:OD1   | 1:C:303:ASP:N     | 2.47                     | 0.45              |
| 1:C:622:THR:HG21  | 1:C:1681:VAL:HG12 | 1.98                     | 0.45              |
| 1:C:4565:LEU:HD22 | 1:C:4653:VAL:HG21 | 1.97                     | 0.45              |
| 1:C:4958:CYS:O    | 1:C:4960:ILE:N    | 2.49                     | 0.45              |
| 1:D:649:PHE:HB3   | 1:D:776:LEU:HD21  | 1.99                     | 0.45              |
| 1:D:2015:GLU:H    | 1:D:3661:TRP:HZ2  | 1.65                     | 0.45              |
| 1:D:2109:ASP:N    | 1:D:2109:ASP:OD1  | 2.50                     | 0.45              |
| 1:A:1291:LEU:HB2  | 1:A:1579:MET:HE2  | 1.99                     | 0.45              |
| 1:A:1870:VAL:HG11 | 1:A:2091:PRO:HD2  | 1.99                     | 0.45              |
| 1:A:2211:MET:HB3  | 1:A:2211:MET:HE2  | 1.67                     | 0.45              |
| 1:B:472:ARG:NE    | 1:B:532:GLY:O     | 2.44                     | 0.45              |
| 1:B:2109:ASP:OD1  | 1:B:2109:ASP:N    | 2.50                     | 0.45              |
| 1:B:2155:LEU:HD12 | 1:B:2185:ILE:HD11 | 1.98                     | 0.45              |
| 1:B:2211:MET:HB3  | 1:B:2211:MET:HE2  | 1.67                     | 0.45              |
| 1:C:483:MET:HG2   | 1:C:486:LEU:HD21  | 1.99                     | 0.45              |
| 1:C:2211:MET:HE1  | 1:C:2257:LEU:HD13 | 1.99                     | 0.45              |
| 1:C:4202:ARG:HA   | 1:C:4202:ARG:HD3  | 1.84                     | 0.45              |
| 1:D:236:ALA:HA    | 1:D:242:ARG:HD2   | 1.99                     | 0.45              |
| 1:D:2294:ASP:OD1  | 1:D:2294:ASP:N    | 2.49                     | 0.45              |
| 1:D:3159:ASP:OD1  | 1:D:3159:ASP:N    | 2.49                     | 0.45              |
| 1:A:236:ALA:HA    | 1:A:242:ARG:HD2   | 1.99                     | 0.45              |
| 1:A:1644:GLU:OE1  | 1:A:1646:ARG:NH1  | 2.39                     | 0.45              |
| 1:A:1804:LEU:HB3  | 1:A:1853:ILE:HD13 | 1.99                     | 0.45              |
| 1:B:1287:LEU:O    | 1:B:1460:HIS:N    | 2.39                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2015:GLU:H    | 1:B:3661:TRP:HZ2  | 1.65                     | 0.45              |
| 1:B:3104:GLU:HA   | 1:B:3107:VAL:HG12 | 1.99                     | 0.45              |
| 1:B:4057:MET:SD   | 1:B:4057:MET:N    | 2.90                     | 0.45              |
| 1:C:1101:ARG:HD3  | 1:C:1115:LEU:HB2  | 1.98                     | 0.45              |
| 1:C:2155:LEU:HD12 | 1:C:2185:ILE:HD11 | 1.98                     | 0.45              |
| 1:C:2238:TYR:O    | 1:C:2242:ILE:HG12 | 2.16                     | 0.45              |
| 1:D:552:ASP:OD1   | 1:D:552:ASP:N     | 2.46                     | 0.45              |
| 1:D:3833:GLN:NE2  | 1:D:3837:GLN:OE1  | 2.50                     | 0.45              |
| 1:A:206:CYS:SG    | 1:A:207:SER:N     | 2.90                     | 0.45              |
| 1:A:1106:ARG:HB2  | 1:A:1120:LEU:HB3  | 1.97                     | 0.45              |
| 1:A:1478:ASP:CG   | 1:A:1479:GLU:H    | 2.24                     | 0.45              |
| 1:A:1594:ARG:NH2  | 1:A:1643:GLU:OE2  | 2.50                     | 0.45              |
| 1:A:3781:GLN:OE1  | 1:A:3819:TYR:OH   | 2.28                     | 0.45              |
| 1:B:649:PHE:HB3   | 1:B:776:LEU:HD21  | 1.99                     | 0.45              |
| 1:B:1115:LEU:HD23 | 1:B:1123:VAL:HG11 | 1.99                     | 0.45              |
| 1:B:1269:CYS:HB3  | 1:B:1473:THR:HG23 | 1.98                     | 0.45              |
| 1:B:1594:ARG:NH2  | 1:B:1643:GLU:OE2  | 2.50                     | 0.45              |
| 1:B:1804:LEU:HB3  | 1:B:1853:ILE:HD13 | 1.99                     | 0.45              |
| 1:B:2211:MET:HE1  | 1:B:2257:LEU:HD13 | 1.99                     | 0.45              |
| 1:B:4828:SER:HA   | 1:B:4831:THR:HG22 | 1.99                     | 0.45              |
| 1:C:206:CYS:SG    | 1:C:207:SER:N     | 2.90                     | 0.45              |
| 1:C:981:GLN:NE2   | 1:C:1054:GLU:OE2  | 2.47                     | 0.45              |
| 1:C:1115:LEU:HD23 | 1:C:1123:VAL:HG11 | 1.99                     | 0.45              |
| 1:C:3104:GLU:HA   | 1:C:3107:VAL:HG12 | 1.99                     | 0.45              |
| 1:D:1467:SER:O    | 1:D:1467:SER:OG   | 2.33                     | 0.45              |
| 1:D:1668:ARG:HA   | 1:D:1671:ARG:HE   | 1.82                     | 0.45              |
| 1:D:1804:LEU:HB3  | 1:D:1853:ILE:HD13 | 1.99                     | 0.45              |
| 1:D:2208:MET:CE   | 1:D:2253:HIS:HB3  | 2.47                     | 0.45              |
| 1:D:3504:SER:O    | 1:D:3507:THR:OG1  | 2.33                     | 0.45              |
| 1:A:981:GLN:NE2   | 1:A:1054:GLU:OE2  | 2.47                     | 0.45              |
| 1:A:1790:GLY:O    | 1:A:1792:ALA:N    | 2.50                     | 0.45              |
| 1:A:2109:ASP:N    | 1:A:2109:ASP:OD1  | 2.50                     | 0.45              |
| 1:A:3269:VAL:O    | 1:A:3273:THR:OG1  | 2.24                     | 0.45              |
| 1:B:1068:ARG:O    | 1:B:1070:ASP:N    | 2.50                     | 0.45              |
| 1:B:3781:GLN:OE1  | 1:B:3819:TYR:OH   | 2.28                     | 0.45              |
| 1:C:2015:GLU:H    | 1:C:3661:TRP:HZ2  | 1.65                     | 0.45              |
| 1:C:2200:ALA:O    | 1:C:2202:GLY:N    | 2.49                     | 0.45              |
| 1:C:2826:ALA:O    | 1:C:2827:ARG:NH1  | 2.43                     | 0.45              |
| 1:C:3871:GLY:O    | 1:C:3949:ARG:NH1  | 2.49                     | 0.45              |
| 1:D:634:GLN:NE2   | 2:H:34:LYS:HE3    | 2.32                     | 0.45              |
| 2:G:100:ASP:OD1   | 2:G:100:ASP:N     | 2.50                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1101:ARG:HD3  | 1:A:1115:LEU:HB2  | 1.98                     | 0.44              |
| 1:B:23:GLN:HG3    | 1:B:201:ASN:HB3   | 2.00                     | 0.44              |
| 1:B:236:ALA:HA    | 1:B:242:ARG:HD2   | 1.99                     | 0.44              |
| 1:B:3159:ASP:OD1  | 1:B:3159:ASP:N    | 2.49                     | 0.44              |
| 1:C:472:ARG:NE    | 1:C:532:GLY:O     | 2.44                     | 0.44              |
| 1:C:1220:GLN:HA   | 1:D:3522:LEU:HD22 | 1.99                     | 0.44              |
| 1:C:1870:VAL:HG11 | 1:C:2091:PRO:HD2  | 1.99                     | 0.44              |
| 1:D:23:GLN:HA     | 1:D:36:CYS:HA     | 2.00                     | 0.44              |
| 1:D:206:CYS:SG    | 1:D:207:SER:N     | 2.90                     | 0.44              |
| 1:D:1478:ASP:CG   | 1:D:1479:GLU:H    | 2.24                     | 0.44              |
| 1:D:3871:GLY:O    | 1:D:3949:ARG:NH1  | 2.49                     | 0.44              |
| 2:E:100:ASP:OD1   | 2:E:100:ASP:N     | 2.50                     | 0.44              |
| 1:A:977:LEU:HG    | 1:A:978:THR:H     | 1.83                     | 0.44              |
| 1:A:1076:ARG:O    | 1:A:1237:TRP:N    | 2.35                     | 0.44              |
| 1:A:1220:GLN:HA   | 1:B:3522:LEU:HD22 | 1.98                     | 0.44              |
| 1:A:1287:LEU:O    | 1:A:1460:HIS:N    | 2.39                     | 0.44              |
| 1:A:1668:ARG:HA   | 1:A:1671:ARG:HE   | 1.82                     | 0.44              |
| 1:A:3522:LEU:HD22 | 1:D:1220:GLN:HA   | 1.99                     | 0.44              |
| 1:A:4679:ARG:HE   | 1:A:5017:ARG:CZ   | 2.29                     | 0.44              |
| 1:B:2208:MET:CE   | 1:B:2253:HIS:HB3  | 2.47                     | 0.44              |
| 1:B:3871:GLY:O    | 1:B:3949:ARG:NH1  | 2.49                     | 0.44              |
| 1:B:5031:GLN:HG2  | 1:B:5032:TYR:N    | 2.32                     | 0.44              |
| 1:C:1790:GLY:O    | 1:C:1792:ALA:N    | 2.50                     | 0.44              |
| 1:C:1804:LEU:HB3  | 1:C:1853:ILE:HD13 | 1.99                     | 0.44              |
| 1:C:2305:CYS:HB3  | 1:C:2324:ASN:HD22 | 1.83                     | 0.44              |
| 1:C:3661:TRP:O    | 1:C:3664:THR:OG1  | 2.30                     | 0.44              |
| 1:C:5031:GLN:HG2  | 1:C:5032:TYR:N    | 2.32                     | 0.44              |
| 1:D:239:ASP:OD1   | 1:D:239:ASP:N     | 2.43                     | 0.44              |
| 1:D:3644:LEU:HD12 | 1:D:3645:PRO:HD2  | 2.00                     | 0.44              |
| 1:D:4828:SER:HA   | 1:D:4831:THR:HG22 | 1.99                     | 0.44              |
| 1:A:590:LEU:HB2   | 1:A:599:VAL:HG11  | 2.00                     | 0.44              |
| 1:A:683:ARG:HG2   | 1:A:717:ASP:HB3   | 2.00                     | 0.44              |
| 1:A:1116:GLY:O    | 1:A:1134:LEU:N    | 2.48                     | 0.44              |
| 1:A:2200:ALA:O    | 1:A:2202:GLY:N    | 2.49                     | 0.44              |
| 1:A:3104:GLU:HA   | 1:A:3107:VAL:HG12 | 1.99                     | 0.44              |
| 1:A:3871:GLY:O    | 1:A:3949:ARG:NH1  | 2.49                     | 0.44              |
| 1:B:483:MET:HG2   | 1:B:486:LEU:HD21  | 1.99                     | 0.44              |
| 1:C:1068:ARG:O    | 1:C:1070:ASP:N    | 2.50                     | 0.44              |
| 1:C:3833:GLN:NE2  | 1:C:3837:GLN:OE1  | 2.50                     | 0.44              |
| 1:D:219:VAL:HG21  | 1:D:398:SER:HB3   | 1.99                     | 0.44              |
| 1:D:1291:LEU:HB2  | 1:D:1579:MET:HE2  | 1.99                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:1594:ARG:NH2  | 1:D:1643:GLU:OE2  | 2.50                     | 0.44              |
| 1:D:2890:LYS:HD2  | 1:D:2890:LYS:HA   | 1.82                     | 0.44              |
| 1:D:3104:GLU:HA   | 1:D:3107:VAL:HG12 | 1.99                     | 0.44              |
| 1:D:4958:CYS:O    | 1:D:4960:ILE:N    | 2.49                     | 0.44              |
| 1:A:370:GLY:O     | 1:A:372:LEU:N     | 2.51                     | 0.44              |
| 1:A:1115:LEU:HD23 | 1:A:1123:VAL:HG11 | 1.99                     | 0.44              |
| 1:A:2015:GLU:H    | 1:A:3661:TRP:HZ2  | 1.65                     | 0.44              |
| 1:A:3644:LEU:HD12 | 1:A:3645:PRO:HD2  | 2.00                     | 0.44              |
| 1:A:4923:PHE:O    | 1:A:4927:ILE:HB   | 2.18                     | 0.44              |
| 1:B:206:CYS:SG    | 1:B:207:SER:N     | 2.90                     | 0.44              |
| 1:B:590:LEU:HB2   | 1:B:599:VAL:HG11  | 2.00                     | 0.44              |
| 1:B:2325:PRO:HB3  | 1:B:2421:ALA:HB1  | 1.98                     | 0.44              |
| 1:C:2208:MET:CE   | 1:C:2253:HIS:HB3  | 2.47                     | 0.44              |
| 1:D:361:ALA:HB2   | 1:D:374:LYS:HD2   | 2.00                     | 0.44              |
| 1:D:1639:LEU:HD13 | 1:D:1648:MET:HG3  | 2.00                     | 0.44              |
| 1:D:1870:VAL:HG11 | 1:D:2091:PRO:HD2  | 1.99                     | 0.44              |
| 1:A:23:GLN:HA     | 1:A:36:CYS:HA     | 2.00                     | 0.44              |
| 1:A:732:SER:OG    | 1:A:735:GLN:OE1   | 2.33                     | 0.44              |
| 1:A:2556:LEU:HD21 | 1:A:2597:LYS:HA   | 1.99                     | 0.44              |
| 1:B:361:ALA:HB2   | 1:B:374:LYS:HD2   | 2.00                     | 0.44              |
| 1:B:977:LEU:HG    | 1:B:978:THR:H     | 1.83                     | 0.44              |
| 1:B:1037:ASP:HA   | 1:B:1040:CYS:SG   | 2.58                     | 0.44              |
| 1:B:1101:ARG:HD3  | 1:B:1115:LEU:HB2  | 1.98                     | 0.44              |
| 1:B:2442:LEU:HD12 | 1:B:2443:ILE:HB   | 2.00                     | 0.44              |
| 1:B:2523:ASP:HA   | 1:B:2526:PHE:CE1  | 2.53                     | 0.44              |
| 1:B:3644:LEU:HD12 | 1:B:3645:PRO:HD2  | 2.00                     | 0.44              |
| 1:B:4684:ASP:OD1  | 1:B:4685:GLY:N    | 2.51                     | 0.44              |
| 1:C:23:GLN:HA     | 1:C:36:CYS:HA     | 2.00                     | 0.44              |
| 1:C:219:VAL:HG21  | 1:C:398:SER:HB3   | 1.99                     | 0.44              |
| 1:C:1245:PHE:CG   | 1:C:1288:PHE:HE1  | 2.36                     | 0.44              |
| 1:C:1594:ARG:NH2  | 1:C:1643:GLU:OE2  | 2.50                     | 0.44              |
| 1:C:2294:ASP:OD1  | 1:C:2294:ASP:N    | 2.49                     | 0.44              |
| 1:D:683:ARG:HG2   | 1:D:717:ASP:HB3   | 2.00                     | 0.44              |
| 1:D:1101:ARG:HD3  | 1:D:1115:LEU:HB2  | 1.98                     | 0.44              |
| 1:D:2305:CYS:HB3  | 1:D:2324:ASN:HD22 | 1.83                     | 0.44              |
| 1:D:5001:THR:OG1  | 1:D:5002:GLU:OE1  | 2.30                     | 0.44              |
| 1:D:5031:GLN:HG2  | 1:D:5032:TYR:N    | 2.32                     | 0.44              |
| 1:A:2523:ASP:HA   | 1:A:2526:PHE:CE1  | 2.53                     | 0.44              |
| 1:A:3833:GLN:NE2  | 1:A:3837:GLN:OE1  | 2.50                     | 0.44              |
| 1:B:2794:TYR:HA   | 1:B:2797:PHE:HD2  | 1.83                     | 0.44              |
| 1:B:3833:GLN:NE2  | 1:B:3837:GLN:OE1  | 2.50                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:732:SER:OG    | 1:C:735:GLN:OE1   | 2.33                     | 0.44              |
| 1:C:1092:PHE:O    | 1:C:1149:VAL:N    | 2.37                     | 0.44              |
| 1:A:23:GLN:HG3    | 1:A:201:ASN:HB3   | 2.00                     | 0.44              |
| 1:A:1068:ARG:O    | 1:A:1070:ASP:N    | 2.50                     | 0.44              |
| 1:A:3923:LEU:HD13 | 1:A:3961:VAL:HG11 | 2.00                     | 0.44              |
| 1:B:2826:ALA:O    | 1:B:2827:ARG:NH1  | 2.43                     | 0.44              |
| 1:C:634:GLN:NE2   | 2:G:34:LYS:HE3    | 2.32                     | 0.44              |
| 1:C:683:ARG:HG2   | 1:C:717:ASP:HB3   | 2.00                     | 0.44              |
| 1:C:2442:LEU:HD12 | 1:C:2443:ILE:HB   | 2.00                     | 0.44              |
| 1:D:483:MET:HG2   | 1:D:486:LEU:HD21  | 1.99                     | 0.44              |
| 1:D:1068:ARG:O    | 1:D:1070:ASP:N    | 2.50                     | 0.44              |
| 1:D:1116:GLY:O    | 1:D:1134:LEU:N    | 2.48                     | 0.44              |
| 1:A:361:ALA:HB2   | 1:A:374:LYS:HD2   | 2.00                     | 0.44              |
| 1:A:483:MET:HG2   | 1:A:486:LEU:HD21  | 1.99                     | 0.44              |
| 1:A:607:CYS:HB2   | 1:A:618:GLN:HG2   | 2.00                     | 0.44              |
| 1:A:2211:MET:HE1  | 1:A:2257:LEU:HD13 | 1.98                     | 0.44              |
| 1:A:2442:LEU:HD12 | 1:A:2443:ILE:HB   | 2.00                     | 0.44              |
| 1:B:219:VAL:HG21  | 1:B:398:SER:HB3   | 1.99                     | 0.44              |
| 1:B:3923:LEU:HD13 | 1:B:3961:VAL:HG11 | 2.00                     | 0.44              |
| 1:C:370:GLY:O     | 1:C:372:LEU:N     | 2.50                     | 0.44              |
| 1:C:977:LEU:HG    | 1:C:978:THR:H     | 1.82                     | 0.44              |
| 1:C:3644:LEU:HD12 | 1:C:3645:PRO:HD2  | 2.00                     | 0.44              |
| 1:C:4828:SER:HA   | 1:C:4831:THR:HG22 | 1.99                     | 0.44              |
| 1:D:666:VAL:HG23  | 1:D:744:VAL:HB    | 2.00                     | 0.44              |
| 1:D:3353:LEU:O    | 1:D:3357:HIS:ND1  | 2.51                     | 0.44              |
| 1:D:3923:LEU:HD13 | 1:D:3961:VAL:HG11 | 2.00                     | 0.44              |
| 1:A:1099:GLU:OE2  | 1:A:1101:ARG:NE   | 2.47                     | 0.44              |
| 1:B:607:CYS:HB2   | 1:B:618:GLN:HG2   | 2.00                     | 0.44              |
| 1:B:683:ARG:HG2   | 1:B:717:ASP:HB3   | 2.00                     | 0.44              |
| 1:B:1245:PHE:CG   | 1:B:1288:PHE:HE1  | 2.36                     | 0.44              |
| 1:B:1520:VAL:HG11 | 1:B:1526:LEU:HB2  | 2.00                     | 0.44              |
| 1:C:19:GLU:OE2    | 1:C:68:THR:OG1    | 2.33                     | 0.44              |
| 1:C:361:ALA:HB2   | 1:C:374:LYS:HD2   | 2.00                     | 0.44              |
| 1:C:2120:MET:HE3  | 1:C:2120:MET:HB2  | 1.92                     | 0.44              |
| 1:C:2794:TYR:HA   | 1:C:2797:PHE:HD2  | 1.83                     | 0.44              |
| 1:D:370:GLY:O     | 1:D:372:LEU:N     | 2.51                     | 0.44              |
| 1:D:472:ARG:NE    | 1:D:532:GLY:O     | 2.44                     | 0.44              |
| 1:D:1245:PHE:CG   | 1:D:1288:PHE:HE1  | 2.36                     | 0.44              |
| 1:D:1439:VAL:HG22 | 1:D:1554:VAL:HA   | 2.00                     | 0.44              |
| 1:D:2660:GLY:HA2  | 1:D:2663:ASN:ND2  | 2.33                     | 0.44              |
| 1:D:3169:LEU:HD21 | 1:D:3194:LEU:HD13 | 2.00                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:100:ASP:OD1   | 2:H:100:ASP:N     | 2.50                     | 0.44              |
| 1:A:219:VAL:HG21  | 1:A:398:SER:HB3   | 1.99                     | 0.43              |
| 1:A:634:GLN:NE2   | 2:E:34:LYS:HE3    | 2.32                     | 0.43              |
| 1:A:1237:TRP:CE2  | 1:A:1607:ARG:HB2  | 2.53                     | 0.43              |
| 1:A:1458:HIS:NE2  | 1:A:1483:VAL:HG21 | 2.33                     | 0.43              |
| 1:A:1520:VAL:HG11 | 1:A:1526:LEU:HB2  | 2.00                     | 0.43              |
| 1:A:2088:GLU:HB3  | 1:A:2089:LYS:H    | 1.67                     | 0.43              |
| 1:A:2305:CYS:HB3  | 1:A:2324:ASN:HD22 | 1.82                     | 0.43              |
| 1:B:13:PHE:HD2    | 1:B:15:ARG:HG2    | 1.84                     | 0.43              |
| 1:B:634:GLN:NE2   | 2:F:34:LYS:HE3    | 2.32                     | 0.43              |
| 1:B:1668:ARG:HA   | 1:B:1671:ARG:HE   | 1.82                     | 0.43              |
| 1:B:2556:LEU:HD21 | 1:B:2597:LYS:HA   | 1.99                     | 0.43              |
| 1:B:3169:LEU:HD21 | 1:B:3194:LEU:HD13 | 2.00                     | 0.43              |
| 1:B:3353:LEU:O    | 1:B:3357:HIS:ND1  | 2.51                     | 0.43              |
| 1:C:23:GLN:HG3    | 1:C:201:ASN:HB3   | 1.99                     | 0.43              |
| 1:C:1037:ASP:HA   | 1:C:1040:CYS:SG   | 2.58                     | 0.43              |
| 1:C:1668:ARG:HA   | 1:C:1671:ARG:HE   | 1.82                     | 0.43              |
| 1:D:1037:ASP:HA   | 1:D:1040:CYS:SG   | 2.58                     | 0.43              |
| 1:D:2523:ASP:HA   | 1:D:2526:PHE:CE1  | 2.53                     | 0.43              |
| 1:B:1104:TRP:CE2  | 1:B:1153:ILE:HB   | 2.53                     | 0.43              |
| 1:B:1458:HIS:NE2  | 1:B:1483:VAL:HG21 | 2.33                     | 0.43              |
| 1:B:2523:ASP:O    | 1:B:2527:LEU:HG   | 2.18                     | 0.43              |
| 1:B:4923:PHE:O    | 1:B:4927:ILE:HB   | 2.18                     | 0.43              |
| 1:C:1450:VAL:HG23 | 1:C:1454:THR:HG21 | 2.00                     | 0.43              |
| 1:C:2556:LEU:HD21 | 1:C:2597:LYS:HA   | 1.99                     | 0.43              |
| 1:D:1592:PRO:HA   | 1:D:1593:PRO:HD3  | 1.86                     | 0.43              |
| 1:D:2200:ALA:O    | 1:D:2202:GLY:N    | 2.49                     | 0.43              |
| 1:D:2355:ARG:O    | 1:D:2359:ARG:HB2  | 2.18                     | 0.43              |
| 1:D:2920:ARG:HA   | 1:D:2920:ARG:HD3  | 1.82                     | 0.43              |
| 1:D:3447:LYS:HD2  | 1:D:3447:LYS:HA   | 1.77                     | 0.43              |
| 1:D:4923:PHE:O    | 1:D:4927:ILE:HB   | 2.18                     | 0.43              |
| 1:A:1639:LEU:HD13 | 1:A:1648:MET:HG3  | 2.00                     | 0.43              |
| 1:A:2355:ARG:O    | 1:A:2359:ARG:HB2  | 2.18                     | 0.43              |
| 1:B:23:GLN:HA     | 1:B:36:CYS:HA     | 2.00                     | 0.43              |
| 1:B:370:GLY:O     | 1:B:372:LEU:N     | 2.50                     | 0.43              |
| 1:B:1099:GLU:OE2  | 1:B:1101:ARG:NE   | 2.47                     | 0.43              |
| 1:C:666:VAL:HG23  | 1:C:744:VAL:HB    | 2.00                     | 0.43              |
| 1:C:1439:VAL:HG22 | 1:C:1554:VAL:HA   | 2.00                     | 0.43              |
| 1:C:2523:ASP:O    | 1:C:2527:LEU:HG   | 2.18                     | 0.43              |
| 1:C:2660:GLY:HA2  | 1:C:2663:ASN:ND2  | 2.33                     | 0.43              |
| 1:C:4633:GLU:HG2  | 1:C:4634:GLU:N    | 2.34                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:13:PHE:HD2    | 1:D:15:ARG:HG2    | 1.83                     | 0.43              |
| 1:D:590:LEU:HB2   | 1:D:599:VAL:HG11  | 2.00                     | 0.43              |
| 1:D:1259:ARG:NH2  | 1:D:1591:CYS:SG   | 2.92                     | 0.43              |
| 1:D:4202:ARG:HA   | 1:D:4202:ARG:HD3  | 1.84                     | 0.43              |
| 2:G:28:GLY:N      | 2:G:37:ASP:O      | 2.50                     | 0.43              |
| 1:A:266:ARG:H     | 1:A:266:ARG:HG2   | 1.67                     | 0.43              |
| 1:A:457:GLU:HG3   | 1:A:464:LYS:NZ    | 2.34                     | 0.43              |
| 1:A:529:LEU:HA    | 1:A:529:LEU:HD23  | 1.80                     | 0.43              |
| 1:A:666:VAL:HG23  | 1:A:744:VAL:HB    | 2.00                     | 0.43              |
| 1:A:1104:TRP:NE1  | 1:A:1152:MET:O    | 2.50                     | 0.43              |
| 1:A:1439:VAL:HG22 | 1:A:1554:VAL:HA   | 2.00                     | 0.43              |
| 1:A:3353:LEU:O    | 1:A:3357:HIS:ND1  | 2.51                     | 0.43              |
| 1:B:110:ARG:HD3   | 1:B:115:ARG:HD2   | 2.00                     | 0.43              |
| 1:B:1237:TRP:CE2  | 1:B:1607:ARG:HB2  | 2.53                     | 0.43              |
| 1:B:1439:VAL:HG22 | 1:B:1554:VAL:HA   | 2.00                     | 0.43              |
| 1:B:1790:GLY:O    | 1:B:1792:ALA:N    | 2.50                     | 0.43              |
| 1:B:2305:CYS:HB3  | 1:B:2324:ASN:HD22 | 1.83                     | 0.43              |
| 1:B:3380:ARG:O    | 1:B:3382:GLU:N    | 2.52                     | 0.43              |
| 1:C:975:VAL:HB    | 1:C:1047:LEU:HD23 | 2.00                     | 0.43              |
| 1:C:1259:ARG:NH2  | 1:C:1591:CYS:SG   | 2.92                     | 0.43              |
| 1:C:4684:ASP:OD1  | 1:C:4685:GLY:N    | 2.51                     | 0.43              |
| 1:D:457:GLU:HG3   | 1:D:464:LYS:NZ    | 2.34                     | 0.43              |
| 1:D:2155:LEU:HD12 | 1:D:2185:ILE:HD11 | 1.98                     | 0.43              |
| 1:D:2556:LEU:HD21 | 1:D:2597:LYS:HA   | 1.99                     | 0.43              |
| 1:D:3466:ASN:HB3  | 1:D:3509:LEU:HD11 | 2.01                     | 0.43              |
| 2:E:38:SER:O      | 2:E:42:ARG:NH1    | 2.52                     | 0.43              |
| 1:A:303:ASP:OD1   | 1:A:303:ASP:N     | 2.46                     | 0.43              |
| 1:A:1245:PHE:CG   | 1:A:1288:PHE:HE1  | 2.36                     | 0.43              |
| 1:A:4849:TYR:HE1  | 1:B:4578:LEU:HD13 | 1.83                     | 0.43              |
| 1:B:2770:LYS:HA   | 1:B:2770:LYS:HD3  | 1.78                     | 0.43              |
| 1:B:3447:LYS:HD2  | 1:B:3447:LYS:HA   | 1.77                     | 0.43              |
| 1:C:497:TYR:CD1   | 1:C:503:PHE:HB3   | 2.54                     | 0.43              |
| 1:C:3169:LEU:HD21 | 1:C:3194:LEU:HD13 | 2.00                     | 0.43              |
| 1:C:3923:LEU:HD13 | 1:C:3961:VAL:HG11 | 2.00                     | 0.43              |
| 1:D:213:TYR:CZ    | 1:D:337:PRO:HB3   | 2.54                     | 0.43              |
| 1:D:497:TYR:CD1   | 1:D:503:PHE:HB3   | 2.54                     | 0.43              |
| 1:D:1671:ARG:HD2  | 1:D:1713:ASP:OD2  | 2.19                     | 0.43              |
| 1:D:2211:MET:HB3  | 1:D:2211:MET:HE2  | 1.67                     | 0.43              |
| 1:A:13:PHE:HD2    | 1:A:15:ARG:HG2    | 1.83                     | 0.43              |
| 1:A:1037:ASP:HA   | 1:A:1040:CYS:SG   | 2.58                     | 0.43              |
| 1:A:2523:ASP:O    | 1:A:2527:LEU:HG   | 2.18                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1259:ARG:NH2  | 1:B:1591:CYS:SG   | 2.92                     | 0.43              |
| 1:B:4633:GLU:HG2  | 1:B:4634:GLU:N    | 2.34                     | 0.43              |
| 1:C:213:TYR:CZ    | 1:C:337:PRO:HB3   | 2.54                     | 0.43              |
| 1:C:2890:LYS:HD2  | 1:C:2890:LYS:HA   | 1.82                     | 0.43              |
| 1:D:153:ALA:HB2   | 1:D:170:ILE:HG12  | 2.01                     | 0.43              |
| 1:D:1104:TRP:CE2  | 1:D:1153:ILE:HB   | 2.54                     | 0.43              |
| 1:D:2442:LEU:HD12 | 1:D:2443:ILE:HB   | 2.00                     | 0.43              |
| 1:A:2663:ASN:HA   | 1:A:2666:VAL:HG22 | 2.00                     | 0.43              |
| 1:B:457:GLU:HG3   | 1:B:464:LYS:NZ    | 2.34                     | 0.43              |
| 1:B:495:ASN:HB2   | 1:B:550:LYS:HZ3   | 1.83                     | 0.43              |
| 1:B:529:LEU:HA    | 1:B:529:LEU:HD23  | 1.80                     | 0.43              |
| 1:C:153:ALA:HB2   | 1:C:170:ILE:HG12  | 2.01                     | 0.43              |
| 1:C:158:SER:OG    | 1:C:159:GLU:N     | 2.52                     | 0.43              |
| 1:C:317:ARG:CZ    | 1:C:349:GLN:HB3   | 2.49                     | 0.43              |
| 1:C:457:GLU:HG3   | 1:C:464:LYS:NZ    | 2.34                     | 0.43              |
| 1:C:590:LEU:HB2   | 1:C:599:VAL:HG11  | 2.00                     | 0.43              |
| 1:C:607:CYS:HB2   | 1:C:618:GLN:HG2   | 2.00                     | 0.43              |
| 1:C:3466:ASN:HB3  | 1:C:3509:LEU:HD11 | 2.01                     | 0.43              |
| 1:D:621:ILE:HD13  | 1:D:621:ILE:HA    | 1.92                     | 0.43              |
| 1:D:1237:TRP:CE2  | 1:D:1607:ARG:HB2  | 2.53                     | 0.43              |
| 1:A:497:TYR:CD1   | 1:A:503:PHE:HB3   | 2.54                     | 0.43              |
| 1:A:1450:VAL:HG23 | 1:A:1454:THR:HG21 | 2.00                     | 0.43              |
| 1:A:2552:ARG:HG3  | 1:A:2597:LYS:HD3  | 2.01                     | 0.43              |
| 1:B:317:ARG:CZ    | 1:B:349:GLN:HB3   | 2.49                     | 0.43              |
| 1:C:4923:PHE:O    | 1:C:4927:ILE:HB   | 2.18                     | 0.43              |
| 1:D:299:LEU:HD11  | 1:D:357:LEU:HB2   | 2.01                     | 0.43              |
| 1:D:1790:GLY:O    | 1:D:1792:ALA:N    | 2.50                     | 0.43              |
| 1:D:4677:LEU:HD13 | 1:D:4702:ASP:OD2  | 2.19                     | 0.43              |
| 2:F:38:SER:O      | 2:F:42:ARG:NH1    | 2.52                     | 0.43              |
| 2:G:25:HIS:HB3    | 2:G:102:GLU:HB3   | 2.01                     | 0.43              |
| 1:A:158:SER:OG    | 1:A:159:GLU:N     | 2.52                     | 0.43              |
| 1:A:206:CYS:HA    | 1:A:271:GLY:HA3   | 2.01                     | 0.43              |
| 1:A:1476:MET:HE3  | 1:A:1477:GLY:N    | 2.25                     | 0.43              |
| 1:A:2592:GLY:O    | 1:A:2595:LEU:HG   | 2.19                     | 0.43              |
| 1:A:2653:LYS:O    | 1:A:2657:LEU:HB2  | 2.19                     | 0.43              |
| 1:A:2794:TYR:HA   | 1:A:2797:PHE:HD2  | 1.83                     | 0.43              |
| 1:A:4828:SER:HA   | 1:A:4831:THR:HG22 | 1.99                     | 0.43              |
| 1:B:666:VAL:HG23  | 1:B:744:VAL:HB    | 2.00                     | 0.43              |
| 1:B:1931:LEU:HD22 | 1:B:1935:VAL:HG11 | 2.01                     | 0.43              |
| 1:C:110:ARG:HD3   | 1:C:115:ARG:HD2   | 2.00                     | 0.43              |
| 1:C:299:LEU:HD11  | 1:C:357:LEU:HB2   | 2.01                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1104:TRP:CE2  | 1:C:1153:ILE:HB   | 2.54                     | 0.43              |
| 1:C:2007:ASN:O    | 1:C:2011:HIS:ND1  | 2.36                     | 0.43              |
| 1:C:4586:PRO:HB3  | 1:C:4628:VAL:HG21 | 2.01                     | 0.43              |
| 1:D:23:GLN:HG3    | 1:D:201:ASN:HB3   | 2.00                     | 0.43              |
| 1:D:710:ASP:OD1   | 1:D:710:ASP:N     | 2.44                     | 0.43              |
| 1:D:1458:HIS:NE2  | 1:D:1483:VAL:HG21 | 2.33                     | 0.43              |
| 1:D:2592:GLY:O    | 1:D:2595:LEU:HG   | 2.19                     | 0.43              |
| 1:D:4057:MET:SD   | 1:D:4057:MET:N    | 2.89                     | 0.43              |
| 1:D:4633:GLU:HG2  | 1:D:4634:GLU:N    | 2.34                     | 0.43              |
| 2:F:25:HIS:HB3    | 2:F:102:GLU:HB3   | 2.01                     | 0.43              |
| 2:F:69:GLY:H      | 2:F:103:LEU:HB2   | 1.84                     | 0.43              |
| 1:A:495:ASN:HB2   | 1:A:550:LYS:HZ3   | 1.84                     | 0.43              |
| 1:A:1104:TRP:CE2  | 1:A:1153:ILE:HB   | 2.54                     | 0.43              |
| 1:A:2660:GLY:HA2  | 1:A:2663:ASN:ND2  | 2.33                     | 0.43              |
| 1:B:299:LEU:HD11  | 1:B:357:LEU:HB2   | 2.01                     | 0.43              |
| 1:B:1671:ARG:HD2  | 1:B:1713:ASP:OD2  | 2.19                     | 0.43              |
| 1:B:2552:ARG:HG3  | 1:B:2597:LYS:HD3  | 2.01                     | 0.43              |
| 1:B:3350:ARG:HD2  | 1:B:3350:ARG:HA   | 1.91                     | 0.43              |
| 1:C:13:PHE:CD2    | 1:C:15:ARG:HG2    | 2.54                     | 0.43              |
| 1:C:1458:HIS:NE2  | 1:C:1483:VAL:HG21 | 2.33                     | 0.43              |
| 1:C:1639:LEU:HD13 | 1:C:1648:MET:HG3  | 2.00                     | 0.43              |
| 1:C:1931:LEU:HD22 | 1:C:1935:VAL:HG11 | 2.01                     | 0.43              |
| 1:C:2355:ARG:O    | 1:C:2359:ARG:HB2  | 2.19                     | 0.43              |
| 1:C:3353:LEU:O    | 1:C:3357:HIS:ND1  | 2.51                     | 0.43              |
| 1:C:4057:MET:SD   | 1:C:4057:MET:N    | 2.90                     | 0.43              |
| 1:D:110:ARG:HD3   | 1:D:115:ARG:HD2   | 2.00                     | 0.43              |
| 1:D:206:CYS:HA    | 1:D:271:GLY:HA3   | 2.01                     | 0.43              |
| 1:D:975:VAL:HB    | 1:D:1047:LEU:HD23 | 2.00                     | 0.43              |
| 1:D:1207:ASP:OD1  | 1:D:1208:VAL:N    | 2.50                     | 0.43              |
| 1:D:1450:VAL:HG23 | 1:D:1454:THR:HG21 | 2.00                     | 0.43              |
| 1:D:1931:LEU:HD22 | 1:D:1935:VAL:HG11 | 2.01                     | 0.43              |
| 1:D:2523:ASP:O    | 1:D:2527:LEU:HG   | 2.18                     | 0.43              |
| 1:D:2653:LYS:O    | 1:D:2657:LEU:HB2  | 2.19                     | 0.43              |
| 1:D:4586:PRO:HB3  | 1:D:4628:VAL:HG21 | 2.01                     | 0.43              |
| 2:H:25:HIS:HB3    | 2:H:102:GLU:HB3   | 2.01                     | 0.43              |
| 1:A:299:LEU:HD11  | 1:A:357:LEU:HB2   | 2.01                     | 0.42              |
| 1:A:1259:ARG:NH2  | 1:A:1591:CYS:SG   | 2.92                     | 0.42              |
| 1:A:1671:ARG:HD2  | 1:A:1713:ASP:OD2  | 2.19                     | 0.42              |
| 1:B:13:PHE:CD2    | 1:B:15:ARG:HG2    | 2.54                     | 0.42              |
| 1:B:732:SER:OG    | 1:B:735:GLN:OE1   | 2.33                     | 0.42              |
| 1:B:1639:LEU:HD13 | 1:B:1648:MET:HG3  | 2.00                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2660:GLY:HA2  | 1:B:2663:ASN:ND2  | 2.33                     | 0.42              |
| 1:B:4202:ARG:HA   | 1:B:4202:ARG:HD3  | 1.84                     | 0.42              |
| 1:C:1281:ASN:HA   | 1:C:1464:PHE:HZ   | 1.84                     | 0.42              |
| 1:C:1520:VAL:HG11 | 1:C:1526:LEU:HB2  | 2.00                     | 0.42              |
| 1:C:2523:ASP:HA   | 1:C:2526:PHE:CE1  | 2.53                     | 0.42              |
| 1:D:317:ARG:CZ    | 1:D:349:GLN:HB3   | 2.48                     | 0.42              |
| 1:D:607:CYS:HB2   | 1:D:618:GLN:HG2   | 2.00                     | 0.42              |
| 1:D:1289:LEU:HD23 | 1:D:1289:LEU:HA   | 1.85                     | 0.42              |
| 1:D:1520:VAL:HG11 | 1:D:1526:LEU:HB2  | 2.00                     | 0.42              |
| 1:D:2134:LEU:HD12 | 1:D:2134:LEU:HA   | 1.89                     | 0.42              |
| 1:D:2552:ARG:HG3  | 1:D:2597:LYS:HD3  | 2.01                     | 0.42              |
| 1:D:4684:ASP:OD1  | 1:D:4685:GLY:N    | 2.51                     | 0.42              |
| 1:A:13:PHE:CD2    | 1:A:15:ARG:HG2    | 2.54                     | 0.42              |
| 1:A:1249:PRO:HA   | 1:A:1250:PRO:HD3  | 1.95                     | 0.42              |
| 1:A:4586:PRO:HB3  | 1:A:4628:VAL:HG21 | 2.01                     | 0.42              |
| 1:A:4873:ASP:OD1  | 1:A:4873:ASP:N    | 2.52                     | 0.42              |
| 1:B:2663:ASN:HA   | 1:B:2666:VAL:HG22 | 2.00                     | 0.42              |
| 1:B:3466:ASN:HB3  | 1:B:3509:LEU:HD11 | 2.01                     | 0.42              |
| 1:B:4137:ARG:NH2  | 1:B:4199:GLU:OE2  | 2.52                     | 0.42              |
| 1:B:4839:MET:HB3  | 1:C:4823:LEU:HD21 | 2.01                     | 0.42              |
| 1:C:206:CYS:HA    | 1:C:271:GLY:HA3   | 2.01                     | 0.42              |
| 1:C:1671:ARG:HD2  | 1:C:1713:ASP:OD2  | 2.19                     | 0.42              |
| 1:C:1749:PRO:HA   | 1:C:1750:PRO:HD3  | 1.95                     | 0.42              |
| 1:C:2743:LEU:HD23 | 1:C:2743:LEU:H    | 1.84                     | 0.42              |
| 1:C:3380:ARG:O    | 1:C:3382:GLU:N    | 2.52                     | 0.42              |
| 1:D:2663:ASN:HA   | 1:D:2666:VAL:HG22 | 2.00                     | 0.42              |
| 2:G:38:SER:O      | 2:G:42:ARG:NH1    | 2.52                     | 0.42              |
| 1:A:1931:LEU:HD22 | 1:A:1935:VAL:HG11 | 2.01                     | 0.42              |
| 1:A:3086:GLU:O    | 1:A:3088:VAL:N    | 2.52                     | 0.42              |
| 1:A:3169:LEU:HD21 | 1:A:3194:LEU:HD13 | 2.00                     | 0.42              |
| 1:A:3466:ASN:HB3  | 1:A:3509:LEU:HD11 | 2.01                     | 0.42              |
| 1:B:158:SER:OG    | 1:B:159:GLU:N     | 2.52                     | 0.42              |
| 1:B:206:CYS:HA    | 1:B:271:GLY:HA3   | 2.01                     | 0.42              |
| 1:B:213:TYR:CZ    | 1:B:337:PRO:HB3   | 2.54                     | 0.42              |
| 1:B:975:VAL:HB    | 1:B:1047:LEU:HD23 | 2.00                     | 0.42              |
| 1:B:4586:PRO:HB3  | 1:B:4628:VAL:HG21 | 2.01                     | 0.42              |
| 1:B:4679:ARG:NH1  | 1:B:4715:TYR:OH   | 2.38                     | 0.42              |
| 1:C:1237:TRP:CE2  | 1:C:1607:ARG:HB2  | 2.53                     | 0.42              |
| 1:C:1694:LEU:HB3  | 1:C:1715:LEU:HD12 | 2.01                     | 0.42              |
| 1:C:1777:PHE:HB3  | 1:C:1801:ALA:HB2  | 2.01                     | 0.42              |
| 1:D:977:LEU:HG    | 1:D:978:THR:H     | 1.83                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:3405:LEU:HB3  | 1:A:3409:TYR:CE1  | 2.54                     | 0.42              |
| 1:A:4771:ILE:HG22 | 1:A:4773:VAL:H    | 1.84                     | 0.42              |
| 1:B:153:ALA:HB2   | 1:B:170:ILE:HG12  | 2.01                     | 0.42              |
| 1:B:497:TYR:CD1   | 1:B:503:PHE:HB3   | 2.54                     | 0.42              |
| 1:B:2134:LEU:HD12 | 1:B:2134:LEU:HA   | 1.89                     | 0.42              |
| 1:B:2232:CYS:O    | 1:B:2236:LEU:HG   | 2.19                     | 0.42              |
| 1:B:3045:LYS:HB2  | 1:B:3045:LYS:HE3  | 1.82                     | 0.42              |
| 1:C:13:PHE:HD2    | 1:C:15:ARG:HG2    | 1.83                     | 0.42              |
| 1:C:2592:GLY:O    | 1:C:2595:LEU:HG   | 2.19                     | 0.42              |
| 1:C:4152:GLU:OE2  | 1:C:4192:ARG:NH1  | 2.52                     | 0.42              |
| 1:D:1777:PHE:HB3  | 1:D:1801:ALA:HB2  | 2.01                     | 0.42              |
| 1:D:2743:LEU:HD23 | 1:D:2743:LEU:H    | 1.84                     | 0.42              |
| 1:D:3132:THR:HA   | 1:D:3136:LEU:HG   | 2.01                     | 0.42              |
| 2:E:25:HIS:HB3    | 2:E:102:GLU:HB3   | 2.01                     | 0.42              |
| 2:H:69:GLY:H      | 2:H:103:LEU:HB2   | 1.84                     | 0.42              |
| 1:A:110:ARG:HD3   | 1:A:115:ARG:HD2   | 2.00                     | 0.42              |
| 1:A:3986:TRP:HB3  | 1:A:4047:MET:HG2  | 2.02                     | 0.42              |
| 1:B:303:ASP:OD1   | 1:B:303:ASP:N     | 2.47                     | 0.42              |
| 1:B:4771:ILE:HG22 | 1:B:4773:VAL:H    | 1.84                     | 0.42              |
| 1:C:2088:GLU:HB3  | 1:C:2089:LYS:H    | 1.67                     | 0.42              |
| 1:C:2109:ASP:OD1  | 1:C:2109:ASP:N    | 2.50                     | 0.42              |
| 1:C:2232:CYS:O    | 1:C:2236:LEU:HG   | 2.19                     | 0.42              |
| 1:C:2552:ARG:HG3  | 1:C:2597:LYS:HD3  | 2.01                     | 0.42              |
| 1:C:3405:LEU:HB3  | 1:C:3409:TYR:CE1  | 2.54                     | 0.42              |
| 1:C:4677:LEU:HD13 | 1:C:4702:ASP:OD2  | 2.19                     | 0.42              |
| 1:D:357:LEU:H     | 1:D:357:LEU:HD23  | 1.85                     | 0.42              |
| 1:D:2107:GLN:NE2  | 1:D:3680:ALA:O    | 2.53                     | 0.42              |
| 2:H:38:SER:O      | 2:H:42:ARG:NH1    | 2.52                     | 0.42              |
| 1:A:107:ILE:HD13  | 1:A:107:ILE:HA    | 1.95                     | 0.42              |
| 1:A:153:ALA:HB2   | 1:A:170:ILE:HG12  | 2.01                     | 0.42              |
| 1:A:472:ARG:NE    | 1:A:532:GLY:O     | 2.44                     | 0.42              |
| 1:A:1289:LEU:HD23 | 1:A:1289:LEU:HA   | 1.85                     | 0.42              |
| 1:A:4677:LEU:HD13 | 1:A:4702:ASP:OD2  | 2.19                     | 0.42              |
| 1:B:1450:VAL:HG23 | 1:B:1454:THR:HG21 | 2.00                     | 0.42              |
| 1:B:2743:LEU:HD23 | 1:B:2743:LEU:H    | 1.84                     | 0.42              |
| 1:B:4958:CYS:O    | 1:B:4960:ILE:N    | 2.49                     | 0.42              |
| 1:C:495:ASN:HB2   | 1:C:550:LYS:HZ3   | 1.84                     | 0.42              |
| 1:C:2653:LYS:O    | 1:C:2657:LEU:HB2  | 2.19                     | 0.42              |
| 1:D:3106:MET:HE2  | 1:D:3132:THR:HB   | 2.02                     | 0.42              |
| 1:D:4137:ARG:NH2  | 1:D:4199:GLU:OE2  | 2.52                     | 0.42              |
| 2:E:69:GLY:H      | 2:E:103:LEU:HB2   | 1.84                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:45:ARG:HG3    | 1:A:137:LEU:HB2   | 2.01                     | 0.42              |
| 1:A:181:HIS:ND1   | 1:A:196:MET:SD    | 2.93                     | 0.42              |
| 1:A:317:ARG:CZ    | 1:A:349:GLN:HB3   | 2.49                     | 0.42              |
| 1:A:975:VAL:HB    | 1:A:1047:LEU:HD23 | 2.00                     | 0.42              |
| 1:A:1207:ASP:OD1  | 1:A:1208:VAL:N    | 2.50                     | 0.42              |
| 1:A:3380:ARG:O    | 1:A:3382:GLU:N    | 2.52                     | 0.42              |
| 1:A:4152:GLU:OE2  | 1:A:4192:ARG:NH1  | 2.52                     | 0.42              |
| 1:B:2592:GLY:O    | 1:B:2595:LEU:HG   | 2.19                     | 0.42              |
| 1:B:4790:LEU:HD23 | 1:B:4790:LEU:HA   | 1.89                     | 0.42              |
| 1:C:3132:THR:HA   | 1:C:3136:LEU:HG   | 2.01                     | 0.42              |
| 1:D:158:SER:OG    | 1:D:159:GLU:N     | 2.52                     | 0.42              |
| 1:D:2794:TYR:HA   | 1:D:2797:PHE:HD2  | 1.83                     | 0.42              |
| 1:D:2826:ALA:O    | 1:D:2827:ARG:NH1  | 2.43                     | 0.42              |
| 1:D:3405:LEU:HB3  | 1:D:3409:TYR:CE1  | 2.54                     | 0.42              |
| 1:A:1281:ASN:HA   | 1:A:1464:PHE:HZ   | 1.84                     | 0.42              |
| 1:A:3106:MET:HE2  | 1:A:3132:THR:HB   | 2.02                     | 0.42              |
| 1:A:4633:GLU:HG2  | 1:A:4634:GLU:N    | 2.34                     | 0.42              |
| 1:A:4863:TYR:HH   | 1:A:4886:HIS:HE2  | 1.65                     | 0.42              |
| 1:B:107:ILE:HD13  | 1:B:107:ILE:HA    | 1.95                     | 0.42              |
| 1:B:615:ARG:HH21  | 1:B:2168:VAL:HG21 | 1.84                     | 0.42              |
| 1:B:2355:ARG:O    | 1:B:2359:ARG:HB2  | 2.18                     | 0.42              |
| 1:B:2890:LYS:HA   | 1:B:2890:LYS:HD2  | 1.82                     | 0.42              |
| 1:C:207:SER:OG    | 1:C:208:CYS:N     | 2.53                     | 0.42              |
| 1:C:2203:MET:HE1  | 1:C:2235:PHE:CE2  | 2.55                     | 0.42              |
| 1:D:2007:ASN:O    | 1:D:2011:HIS:ND1  | 2.36                     | 0.42              |
| 1:D:3380:ARG:O    | 1:D:3382:GLU:N    | 2.52                     | 0.42              |
| 1:A:2107:GLN:NE2  | 1:A:3680:ALA:O    | 2.53                     | 0.42              |
| 1:A:2232:CYS:O    | 1:A:2236:LEU:HG   | 2.19                     | 0.42              |
| 1:A:2743:LEU:H    | 1:A:2743:LEU:HD23 | 1.84                     | 0.42              |
| 1:A:3350:ARG:HD2  | 1:A:3350:ARG:HA   | 1.91                     | 0.42              |
| 1:A:3514:LEU:HD23 | 1:A:3606:LEU:HD13 | 2.02                     | 0.42              |
| 1:B:45:ARG:HG3    | 1:B:137:LEU:HB2   | 2.01                     | 0.42              |
| 1:B:181:HIS:ND1   | 1:B:196:MET:SD    | 2.93                     | 0.42              |
| 1:B:357:LEU:H     | 1:B:357:LEU:HD23  | 1.85                     | 0.42              |
| 1:B:1777:PHE:HB3  | 1:B:1801:ALA:HB2  | 2.01                     | 0.42              |
| 1:B:2107:GLN:NE2  | 1:B:3680:ALA:O    | 2.53                     | 0.42              |
| 1:B:2552:ARG:HH11 | 1:B:2594:SER:HB3  | 1.85                     | 0.42              |
| 1:B:2653:LYS:O    | 1:B:2657:LEU:HB2  | 2.19                     | 0.42              |
| 1:B:3569:LEU:HD12 | 1:B:3569:LEU:HA   | 1.93                     | 0.42              |
| 1:C:181:HIS:ND1   | 1:C:196:MET:SD    | 2.93                     | 0.42              |
| 1:C:621:ILE:HD13  | 1:C:621:ILE:HA    | 1.92                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:3106:MET:HE2  | 1:C:3132:THR:HB   | 2.02                     | 0.42              |
| 1:C:4849:TYR:HE1  | 1:D:4578:LEU:HD13 | 1.84                     | 0.42              |
| 1:D:1648:MET:HE2  | 1:D:1648:MET:HA   | 2.02                     | 0.42              |
| 1:D:2203:MET:HE1  | 1:D:2235:PHE:CE2  | 2.55                     | 0.42              |
| 1:D:3661:TRP:O    | 1:D:3664:THR:OG1  | 2.30                     | 0.42              |
| 1:D:3986:TRP:HB3  | 1:D:4047:MET:HG2  | 2.02                     | 0.42              |
| 1:D:4799:SER:O    | 1:D:4803:HIS:ND1  | 2.53                     | 0.42              |
| 2:G:69:GLY:H      | 2:G:103:LEU:HB2   | 1.84                     | 0.42              |
| 1:A:1694:LEU:HB3  | 1:A:1715:LEU:HD12 | 2.01                     | 0.42              |
| 1:A:2203:MET:HE1  | 1:A:2235:PHE:CE2  | 2.55                     | 0.42              |
| 1:A:4137:ARG:NH2  | 1:A:4199:GLU:OE2  | 2.52                     | 0.42              |
| 1:C:1289:LEU:HD23 | 1:C:1289:LEU:HA   | 1.85                     | 0.42              |
| 1:C:2552:ARG:HH11 | 1:C:2594:SER:HB3  | 1.85                     | 0.42              |
| 1:C:4771:ILE:HG22 | 1:C:4773:VAL:H    | 1.84                     | 0.42              |
| 1:D:207:SER:OG    | 1:D:208:CYS:N     | 2.53                     | 0.42              |
| 1:D:939:VAL:HA    | 1:D:1053:ILE:HD13 | 2.01                     | 0.42              |
| 1:D:2232:CYS:O    | 1:D:2236:LEU:HG   | 2.19                     | 0.42              |
| 1:A:213:TYR:CZ    | 1:A:337:PRO:HB3   | 2.54                     | 0.41              |
| 1:A:2498:HIS:CE1  | 1:A:2502:MET:HE3  | 2.55                     | 0.41              |
| 1:A:4017:LEU:HD13 | 1:A:4135:PRO:HB2  | 2.02                     | 0.41              |
| 1:B:3086:GLU:O    | 1:B:3088:VAL:N    | 2.52                     | 0.41              |
| 1:C:1265:ASP:OD1  | 1:C:1265:ASP:N    | 2.47                     | 0.41              |
| 1:C:3177:THR:HG23 | 1:C:3178:THR:HG23 | 2.02                     | 0.41              |
| 1:C:4017:LEU:HD13 | 1:C:4135:PRO:HB2  | 2.02                     | 0.41              |
| 1:C:4873:ASP:N    | 1:C:4873:ASP:OD1  | 2.52                     | 0.41              |
| 1:D:21:VAL:HG22   | 1:D:66:CYS:HA     | 2.02                     | 0.41              |
| 1:D:615:ARG:HH21  | 1:D:2168:VAL:HG21 | 1.84                     | 0.41              |
| 1:D:1099:GLU:OE2  | 1:D:1101:ARG:NE   | 2.47                     | 0.41              |
| 1:D:1694:LEU:HB3  | 1:D:1715:LEU:HD12 | 2.01                     | 0.41              |
| 1:D:1728:ARG:HA   | 1:D:1731:LEU:HG   | 2.02                     | 0.41              |
| 1:D:2552:ARG:HH11 | 1:D:2594:SER:HB3  | 1.85                     | 0.41              |
| 1:D:3569:LEU:HD12 | 1:D:3569:LEU:HA   | 1.93                     | 0.41              |
| 1:D:4958:CYS:SG   | 1:D:4983:HIS:CD2  | 3.08                     | 0.41              |
| 1:A:1728:ARG:HA   | 1:A:1731:LEU:HG   | 2.03                     | 0.41              |
| 1:A:3319:ILE:O    | 1:A:3323:ILE:HG12 | 2.20                     | 0.41              |
| 1:A:4799:SER:O    | 1:A:4803:HIS:ND1  | 2.53                     | 0.41              |
| 1:B:1694:LEU:HB3  | 1:B:1715:LEU:HD12 | 2.01                     | 0.41              |
| 1:B:3106:MET:HE2  | 1:B:3132:THR:HB   | 2.02                     | 0.41              |
| 1:B:3319:ILE:O    | 1:B:3323:ILE:HG12 | 2.20                     | 0.41              |
| 1:B:3405:LEU:HB3  | 1:B:3409:TYR:CE1  | 2.54                     | 0.41              |
| 1:B:4677:LEU:HD13 | 1:B:4702:ASP:OD2  | 2.19                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:4849:TYR:HE1  | 1:C:4578:LEU:HD13 | 1.85                     | 0.41              |
| 1:C:615:ARG:HH21  | 1:C:2168:VAL:HG21 | 1.84                     | 0.41              |
| 1:C:2663:ASN:HA   | 1:C:2666:VAL:HG22 | 2.00                     | 0.41              |
| 1:C:2885:THR:HG22 | 1:C:2889:LYS:NZ   | 2.35                     | 0.41              |
| 1:C:3319:ILE:O    | 1:C:3323:ILE:HG12 | 2.20                     | 0.41              |
| 1:C:4992:LEU:O    | 1:C:4996:ILE:HG12 | 2.20                     | 0.41              |
| 1:D:13:PHE:CD2    | 1:D:15:ARG:HG2    | 2.54                     | 0.41              |
| 1:D:181:HIS:ND1   | 1:D:196:MET:SD    | 2.93                     | 0.41              |
| 1:D:701:GLY:HA2   | 1:D:1645:ASN:HB3  | 2.02                     | 0.41              |
| 1:D:1281:ASN:HA   | 1:D:1464:PHE:HZ   | 1.84                     | 0.41              |
| 1:D:2512:ILE:HD12 | 1:D:2512:ILE:HA   | 1.92                     | 0.41              |
| 1:D:3362:ILE:HG13 | 1:D:3366:ARG:HH12 | 1.85                     | 0.41              |
| 1:D:3514:LEU:HD23 | 1:D:3606:LEU:HD13 | 2.02                     | 0.41              |
| 1:A:21:VAL:HG22   | 1:A:66:CYS:HA     | 2.02                     | 0.41              |
| 1:A:259:LEU:HD23  | 1:A:259:LEU:HA    | 1.91                     | 0.41              |
| 1:A:939:VAL:HA    | 1:A:1053:ILE:HD13 | 2.01                     | 0.41              |
| 1:A:2552:ARG:HH11 | 1:A:2594:SER:HB3  | 1.85                     | 0.41              |
| 1:B:613:ALA:HB2   | 1:B:1676:LEU:HD12 | 2.03                     | 0.41              |
| 1:B:939:VAL:HA    | 1:B:1053:ILE:HD13 | 2.01                     | 0.41              |
| 1:B:2498:HIS:CE1  | 1:B:2502:MET:HE3  | 2.55                     | 0.41              |
| 1:C:338:GLU:HG2   | 1:C:339:ILE:H     | 1.85                     | 0.41              |
| 1:C:3514:LEU:HD23 | 1:C:3606:LEU:HD13 | 2.02                     | 0.41              |
| 1:D:229:GLU:HA    | 1:D:249:GLY:HA2   | 2.02                     | 0.41              |
| 1:D:1870:VAL:HG11 | 1:D:2092:GLN:H    | 1.85                     | 0.41              |
| 1:D:3878:ASP:OD1  | 1:D:3878:ASP:N    | 2.54                     | 0.41              |
| 1:A:338:GLU:HG2   | 1:A:339:ILE:H     | 1.85                     | 0.41              |
| 1:A:1648:MET:HE2  | 1:A:1648:MET:HA   | 2.02                     | 0.41              |
| 1:A:1777:PHE:HB3  | 1:A:1801:ALA:HB2  | 2.01                     | 0.41              |
| 1:A:2535:SER:HA   | 1:A:2583:LEU:HD22 | 2.03                     | 0.41              |
| 1:A:2890:LYS:HA   | 1:A:2890:LYS:HD2  | 1.82                     | 0.41              |
| 1:A:4684:ASP:OD1  | 1:A:4685:GLY:N    | 2.51                     | 0.41              |
| 1:A:4992:LEU:O    | 1:A:4996:ILE:HG12 | 2.20                     | 0.41              |
| 1:B:788:LYS:HG3   | 1:B:1629:GLN:HB3  | 2.03                     | 0.41              |
| 1:B:1076:ARG:O    | 1:B:1237:TRP:N    | 2.35                     | 0.41              |
| 1:B:3132:THR:HA   | 1:B:3136:LEU:HG   | 2.01                     | 0.41              |
| 1:B:3514:LEU:HD23 | 1:B:3606:LEU:HD13 | 2.02                     | 0.41              |
| 1:D:45:ARG:HG3    | 1:D:137:LEU:HB2   | 2.01                     | 0.41              |
| 1:D:495:ASN:HB2   | 1:D:550:LYS:HZ3   | 1.85                     | 0.41              |
| 1:D:4992:LEU:O    | 1:D:4996:ILE:HG12 | 2.20                     | 0.41              |
| 1:A:1870:VAL:HG11 | 1:A:2092:GLN:H    | 1.85                     | 0.41              |
| 1:A:3143:LEU:HD13 | 1:A:3147:ILE:HD13 | 2.03                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:338:GLU:HG2   | 1:B:339:ILE:H     | 1.85                     | 0.41              |
| 1:B:621:ILE:HD13  | 1:B:621:ILE:HA    | 1.92                     | 0.41              |
| 1:B:2120:MET:HE3  | 1:B:2120:MET:HB2  | 1.92                     | 0.41              |
| 1:B:2203:MET:HE1  | 1:B:2235:PHE:CE2  | 2.55                     | 0.41              |
| 1:B:3001:ILE:HG22 | 1:B:3002:LEU:HD22 | 2.02                     | 0.41              |
| 1:B:3177:THR:HG23 | 1:B:3178:THR:HG23 | 2.02                     | 0.41              |
| 1:B:4152:GLU:OE2  | 1:B:4192:ARG:NH1  | 2.52                     | 0.41              |
| 1:B:4958:CYS:SG   | 1:B:4978:HIS:CD2  | 3.13                     | 0.41              |
| 1:C:21:VAL:HG22   | 1:C:66:CYS:HA     | 2.02                     | 0.41              |
| 1:C:180:LEU:HD23  | 1:C:180:LEU:HA    | 1.92                     | 0.41              |
| 1:C:1648:MET:HE2  | 1:C:1648:MET:HA   | 2.02                     | 0.41              |
| 1:C:1671:ARG:HG2  | 1:C:1714:LEU:HA   | 2.03                     | 0.41              |
| 1:C:4727:LYS:HE3  | 1:C:4727:LYS:HB3  | 1.82                     | 0.41              |
| 1:D:732:SER:OG    | 1:D:735:GLN:OE1   | 2.33                     | 0.41              |
| 1:D:3319:ILE:O    | 1:D:3323:ILE:HG12 | 2.20                     | 0.41              |
| 1:D:4771:ILE:HG22 | 1:D:4773:VAL:H    | 1.84                     | 0.41              |
| 1:D:4873:ASP:OD1  | 1:D:4873:ASP:N    | 2.52                     | 0.41              |
| 2:G:56:ILE:HG22   | 2:G:59:PHE:H      | 1.86                     | 0.41              |
| 1:A:357:LEU:HD23  | 1:A:357:LEU:H     | 1.85                     | 0.41              |
| 1:A:1436:SER:HA   | 1:A:1445:PRO:HG2  | 2.03                     | 0.41              |
| 1:A:2023:LEU:HD23 | 1:A:2023:LEU:HA   | 1.91                     | 0.41              |
| 1:A:3132:THR:HA   | 1:A:3136:LEU:HG   | 2.01                     | 0.41              |
| 1:B:21:VAL:HG22   | 1:B:66:CYS:HA     | 2.02                     | 0.41              |
| 1:B:1870:VAL:HG11 | 1:B:2092:GLN:H    | 1.85                     | 0.41              |
| 1:B:2088:GLU:HB3  | 1:B:2089:LYS:H    | 1.67                     | 0.41              |
| 1:C:613:ALA:HB2   | 1:C:1676:LEU:HD12 | 2.03                     | 0.41              |
| 1:C:701:GLY:HA2   | 1:C:1645:ASN:HB3  | 2.03                     | 0.41              |
| 1:C:2107:GLN:NE2  | 1:C:3680:ALA:O    | 2.53                     | 0.41              |
| 1:C:4137:ARG:NH2  | 1:C:4199:GLU:OE2  | 2.52                     | 0.41              |
| 1:C:4799:SER:O    | 1:C:4803:HIS:ND1  | 2.53                     | 0.41              |
| 1:D:338:GLU:HG2   | 1:D:339:ILE:H     | 1.85                     | 0.41              |
| 1:D:4792:LEU:O    | 1:D:4796:MET:HG2  | 2.21                     | 0.41              |
| 1:D:4855:ALA:HB2  | 1:D:4916:PHE:CZ   | 2.56                     | 0.41              |
| 1:A:1676:LEU:HA   | 1:A:1725:ARG:NH1  | 2.36                     | 0.41              |
| 1:A:4792:LEU:O    | 1:A:4796:MET:HG2  | 2.21                     | 0.41              |
| 1:B:1281:ASN:HA   | 1:B:1464:PHE:HZ   | 1.84                     | 0.41              |
| 1:B:1592:PRO:HA   | 1:B:1593:PRO:HD3  | 1.86                     | 0.41              |
| 1:B:2920:ARG:HA   | 1:B:2920:ARG:HD3  | 1.82                     | 0.41              |
| 1:C:939:VAL:HA    | 1:C:1053:ILE:HD13 | 2.01                     | 0.41              |
| 1:D:2498:HIS:CE1  | 1:D:2502:MET:HE3  | 2.55                     | 0.41              |
| 1:D:3033:ASN:OD1  | 1:D:3033:ASN:N    | 2.53                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:4055:VAL:HA   | 1:D:4058:ILE:HD12 | 2.03                     | 0.41              |
| 2:H:56:ILE:HG22   | 2:H:59:PHE:H      | 1.86                     | 0.41              |
| 1:A:3878:ASP:OD1  | 1:A:3878:ASP:N    | 2.54                     | 0.41              |
| 1:A:4730:ASP:OD1  | 1:A:4731:ILE:N    | 2.54                     | 0.41              |
| 1:B:1863:LEU:HD12 | 1:B:1863:LEU:HA   | 1.94                     | 0.41              |
| 1:B:4855:ALA:HB2  | 1:B:4916:PHE:CZ   | 2.56                     | 0.41              |
| 1:B:4992:LEU:O    | 1:B:4996:ILE:HG12 | 2.20                     | 0.41              |
| 1:C:266:ARG:H     | 1:C:266:ARG:HG2   | 1.66                     | 0.41              |
| 1:C:3878:ASP:OD1  | 1:C:3878:ASP:N    | 2.54                     | 0.41              |
| 1:C:3986:TRP:HB3  | 1:C:4047:MET:HG2  | 2.02                     | 0.41              |
| 1:C:4730:ASP:OD1  | 1:C:4731:ILE:N    | 2.54                     | 0.41              |
| 1:D:1243:PRO:HB2  | 1:D:1600:LEU:HD21 | 2.03                     | 0.41              |
| 1:D:1671:ARG:HG2  | 1:D:1714:LEU:HA   | 2.03                     | 0.41              |
| 1:D:1676:LEU:HA   | 1:D:1725:ARG:NH1  | 2.36                     | 0.41              |
| 1:D:4730:ASP:OD1  | 1:D:4731:ILE:N    | 2.54                     | 0.41              |
| 2:F:56:ILE:HG22   | 2:F:59:PHE:H      | 1.86                     | 0.41              |
| 1:A:552:ASP:OD1   | 1:A:552:ASP:N     | 2.46                     | 0.41              |
| 1:A:613:ALA:HB2   | 1:A:1676:LEU:HD12 | 2.03                     | 0.41              |
| 1:A:615:ARG:HH21  | 1:A:2168:VAL:HG21 | 1.84                     | 0.41              |
| 1:A:1503:PRO:HB3  | 1:A:1508:ARG:HD2  | 2.03                     | 0.41              |
| 1:A:1505:GLN:HG2  | 1:A:1506:GLN:H    | 1.86                     | 0.41              |
| 1:A:3172:ILE:HD13 | 1:A:3172:ILE:HA   | 1.94                     | 0.41              |
| 1:A:3696:ASP:HB2  | 1:A:3697:PRO:HD3  | 2.02                     | 0.41              |
| 1:A:4958:CYS:SG   | 1:A:4978:HIS:CD2  | 3.14                     | 0.41              |
| 1:B:981:GLN:NE2   | 1:B:1054:GLU:OE2  | 2.47                     | 0.41              |
| 1:B:3674:ILE:HD13 | 1:B:3674:ILE:HA   | 1.96                     | 0.41              |
| 1:B:3712:GLU:HG2  | 1:B:3713:LYS:H    | 1.86                     | 0.41              |
| 1:B:3986:TRP:HB3  | 1:B:4047:MET:HG2  | 2.02                     | 0.41              |
| 1:B:4799:SER:O    | 1:B:4803:HIS:ND1  | 2.53                     | 0.41              |
| 1:B:4815:ASP:HA   | 1:B:4818:MET:HE2  | 2.03                     | 0.41              |
| 1:C:229:GLU:HA    | 1:C:249:GLY:HA2   | 2.02                     | 0.41              |
| 1:C:759:ILE:HD12  | 1:C:759:ILE:HA    | 1.98                     | 0.41              |
| 1:C:1022:VAL:HG21 | 1:C:1026:LEU:HD22 | 2.03                     | 0.41              |
| 1:C:1243:PRO:HB2  | 1:C:1600:LEU:HD21 | 2.03                     | 0.41              |
| 1:C:1728:ARG:HA   | 1:C:1731:LEU:HG   | 2.03                     | 0.41              |
| 1:C:2463:LEU:HD12 | 1:C:2463:LEU:HA   | 1.96                     | 0.41              |
| 1:C:3086:GLU:O    | 1:C:3088:VAL:N    | 2.52                     | 0.41              |
| 1:C:3696:ASP:HB2  | 1:C:3697:PRO:HD3  | 2.02                     | 0.41              |
| 1:C:4055:VAL:HA   | 1:C:4058:ILE:HD12 | 2.03                     | 0.41              |
| 1:C:4855:ALA:HB2  | 1:C:4916:PHE:CZ   | 2.56                     | 0.41              |
| 1:C:4958:CYS:SG   | 1:C:4978:HIS:CD2  | 3.14                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:1503:PRO:HB3  | 1:D:1508:ARG:HD2  | 2.03                     | 0.41              |
| 1:D:1815:LEU:HD12 | 1:D:1815:LEU:HA   | 1.89                     | 0.41              |
| 1:D:4958:CYS:SG   | 1:D:4978:HIS:CD2  | 3.13                     | 0.41              |
| 1:A:701:GLY:HA2   | 1:A:1645:ASN:HB3  | 2.02                     | 0.41              |
| 1:A:788:LYS:HG3   | 1:A:1629:GLN:HB3  | 2.03                     | 0.41              |
| 1:A:1092:PHE:O    | 1:A:1149:VAL:N    | 2.37                     | 0.41              |
| 1:A:1863:LEU:HD12 | 1:A:1863:LEU:HA   | 1.94                     | 0.41              |
| 1:A:3362:ILE:HG13 | 1:A:3366:ARG:HH12 | 1.85                     | 0.41              |
| 1:A:4823:LEU:HD21 | 1:D:4839:MET:HB3  | 2.01                     | 0.41              |
| 1:B:1436:SER:HA   | 1:B:1445:PRO:HG2  | 2.03                     | 0.41              |
| 1:B:1704:PRO:HG2  | 1:B:1707:LEU:HB2  | 2.03                     | 0.41              |
| 1:B:3772:THR:HG22 | 1:B:3804:ILE:HD11 | 2.03                     | 0.41              |
| 1:B:4730:ASP:OD1  | 1:B:4731:ILE:N    | 2.54                     | 0.41              |
| 1:C:19:GLU:HB2    | 1:C:206:CYS:HB3   | 2.03                     | 0.41              |
| 1:C:455:PRO:HG3   | 1:C:467:LYS:HB3   | 2.03                     | 0.41              |
| 1:C:2498:HIS:CE1  | 1:C:2502:MET:HE3  | 2.55                     | 0.41              |
| 1:C:4792:LEU:O    | 1:C:4796:MET:HG2  | 2.21                     | 0.41              |
| 1:C:4839:MET:HB3  | 1:D:4823:LEU:HD21 | 2.03                     | 0.41              |
| 1:D:1436:SER:HA   | 1:D:1445:PRO:HG2  | 2.03                     | 0.41              |
| 1:D:2885:THR:HG22 | 1:D:2889:LYS:NZ   | 2.35                     | 0.41              |
| 1:D:3829:PHE:HB3  | 1:D:3913:ILE:HG13 | 2.03                     | 0.41              |
| 1:D:4152:GLU:OE2  | 1:D:4192:ARG:NH1  | 2.52                     | 0.41              |
| 1:A:719:LEU:HD23  | 1:A:719:LEU:HA    | 1.94                     | 0.40              |
| 1:A:1704:PRO:HG2  | 1:A:1707:LEU:HB2  | 2.03                     | 0.40              |
| 1:A:1749:PRO:HA   | 1:A:1750:PRO:HD3  | 1.95                     | 0.40              |
| 1:B:19:GLU:HB2    | 1:B:206:CYS:HB3   | 2.04                     | 0.40              |
| 1:B:1728:ARG:HA   | 1:B:1731:LEU:HG   | 2.03                     | 0.40              |
| 1:B:3362:ILE:HG13 | 1:B:3366:ARG:HH12 | 1.86                     | 0.40              |
| 1:B:4017:LEU:HD13 | 1:B:4135:PRO:HB2  | 2.02                     | 0.40              |
| 1:C:45:ARG:HG3    | 1:C:137:LEU:HB2   | 2.01                     | 0.40              |
| 1:C:1476:MET:HE3  | 1:C:1477:GLY:N    | 2.25                     | 0.40              |
| 1:C:1676:LEU:HA   | 1:C:1725:ARG:NH1  | 2.36                     | 0.40              |
| 1:C:3001:ILE:HG22 | 1:C:3002:LEU:HD22 | 2.02                     | 0.40              |
| 1:C:3362:ILE:HG13 | 1:C:3366:ARG:HH12 | 1.85                     | 0.40              |
| 1:C:4815:ASP:HA   | 1:C:4818:MET:HE2  | 2.03                     | 0.40              |
| 1:D:266:ARG:H     | 1:D:266:ARG:HG2   | 1.66                     | 0.40              |
| 1:D:805:PRO:HA    | 1:D:806:PRO:HD3   | 1.98                     | 0.40              |
| 1:D:3001:ILE:HG22 | 1:D:3002:LEU:HD22 | 2.02                     | 0.40              |
| 1:A:345:LEU:HD13  | 1:A:387:ALA:HA    | 2.02                     | 0.40              |
| 1:A:1671:ARG:HG2  | 1:A:1714:LEU:HA   | 2.03                     | 0.40              |
| 1:A:2515:GLN:O    | 1:A:2518:LEU:HG   | 2.22                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2885:THR:HG22 | 1:A:2889:LYS:NZ   | 2.35                     | 0.40              |
| 1:A:4055:VAL:HA   | 1:A:4058:ILE:HD12 | 2.03                     | 0.40              |
| 1:B:229:GLU:HA    | 1:B:249:GLY:HA2   | 2.02                     | 0.40              |
| 1:B:1022:VAL:HG21 | 1:B:1026:LEU:HD22 | 2.03                     | 0.40              |
| 1:B:1503:PRO:HB3  | 1:B:1508:ARG:HD2  | 2.03                     | 0.40              |
| 1:B:1648:MET:HA   | 1:B:1648:MET:HE2  | 2.02                     | 0.40              |
| 1:B:3143:LEU:HD13 | 1:B:3147:ILE:HD13 | 2.03                     | 0.40              |
| 1:B:3930:ILE:HD12 | 1:B:3930:ILE:HA   | 1.93                     | 0.40              |
| 1:C:345:LEU:HD13  | 1:C:387:ALA:HA    | 2.02                     | 0.40              |
| 1:C:2512:ILE:HD12 | 1:C:2512:ILE:HA   | 1.92                     | 0.40              |
| 1:C:2535:SER:HA   | 1:C:2583:LEU:HD22 | 2.03                     | 0.40              |
| 1:C:3033:ASN:OD1  | 1:C:3033:ASN:N    | 2.53                     | 0.40              |
| 1:C:3712:GLU:HG2  | 1:C:3713:LYS:H    | 1.86                     | 0.40              |
| 1:D:19:GLU:HB2    | 1:D:206:CYS:HB3   | 2.04                     | 0.40              |
| 1:D:345:LEU:HD13  | 1:D:387:ALA:HA    | 2.02                     | 0.40              |
| 2:E:56:ILE:HG22   | 2:E:59:PHE:H      | 1.86                     | 0.40              |
| 2:F:87:HIS:ND1    | 2:F:88:PRO:HD2    | 2.37                     | 0.40              |
| 2:H:28:GLY:N      | 2:H:37:ASP:O      | 2.50                     | 0.40              |
| 1:A:229:GLU:HA    | 1:A:249:GLY:HA2   | 2.02                     | 0.40              |
| 1:A:2516:ASP:OD1  | 1:A:2517:PHE:N    | 2.55                     | 0.40              |
| 1:A:3033:ASN:OD1  | 1:A:3033:ASN:N    | 2.53                     | 0.40              |
| 1:A:3442:PHE:HE2  | 1:A:3514:LEU:HD13 | 1.87                     | 0.40              |
| 1:A:4578:LEU:HD13 | 1:D:4849:TYR:HE1  | 1.85                     | 0.40              |
| 1:A:4815:ASP:HA   | 1:A:4818:MET:HE2  | 2.03                     | 0.40              |
| 1:A:4855:ALA:HB2  | 1:A:4916:PHE:CZ   | 2.56                     | 0.40              |
| 1:B:4055:VAL:HA   | 1:B:4058:ILE:HD12 | 2.03                     | 0.40              |
| 1:C:357:LEU:HD23  | 1:C:357:LEU:H     | 1.85                     | 0.40              |
| 1:C:3772:THR:HG22 | 1:C:3804:ILE:HD11 | 2.03                     | 0.40              |
| 1:C:4911:LEU:HA   | 1:C:4914:VAL:HG12 | 2.04                     | 0.40              |
| 1:D:1092:PHE:O    | 1:D:1149:VAL:N    | 2.37                     | 0.40              |
| 1:D:1505:GLN:HG2  | 1:D:1506:GLN:H    | 1.86                     | 0.40              |
| 1:D:3177:THR:HG23 | 1:D:3178:THR:HG23 | 2.02                     | 0.40              |
| 1:D:4815:ASP:HA   | 1:D:4818:MET:HE2  | 2.03                     | 0.40              |
| 2:H:87:HIS:ND1    | 2:H:88:PRO:HD2    | 2.37                     | 0.40              |
| 1:A:19:GLU:HB2    | 1:A:206:CYS:HB3   | 2.03                     | 0.40              |
| 1:A:4911:LEU:HA   | 1:A:4914:VAL:HG12 | 2.04                     | 0.40              |
| 1:B:19:GLU:OE2    | 1:B:68:THR:OG1    | 2.33                     | 0.40              |
| 1:B:345:LEU:HD13  | 1:B:387:ALA:HA    | 2.02                     | 0.40              |
| 1:B:2535:SER:HA   | 1:B:2583:LEU:HD22 | 2.03                     | 0.40              |
| 1:B:2643:LEU:HB3  | 1:B:2648:TYR:HE1  | 1.87                     | 0.40              |
| 1:B:3842:LEU:O    | 1:B:3929:SER:OG   | 2.35                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1704:PRO:HG2  | 1:C:1707:LEU:HB2  | 2.03                     | 0.40              |
| 1:C:2515:GLN:O    | 1:C:2518:LEU:HG   | 2.22                     | 0.40              |
| 1:C:4032:GLU:HB3  | 1:C:4033:GLY:H    | 1.55                     | 0.40              |
| 1:C:4958:CYS:SG   | 1:C:4983:HIS:CD2  | 3.08                     | 0.40              |
| 1:D:30:LYS:HE2    | 1:D:30:LYS:HB2    | 1.94                     | 0.40              |
| 1:D:613:ALA:HB2   | 1:D:1676:LEU:HD12 | 2.03                     | 0.40              |
| 1:D:2023:LEU:HD23 | 1:D:2023:LEU:HA   | 1.91                     | 0.40              |
| 1:D:3301:PRO:HA   | 1:D:3302:PRO:HD3  | 1.97                     | 0.40              |
| 1:D:4863:TYR:OH   | 1:D:4886:HIS:NE2  | 2.55                     | 0.40              |
| 1:A:1243:PRO:HB2  | 1:A:1600:LEU:HD21 | 2.03                     | 0.40              |
| 1:A:3842:LEU:O    | 1:A:3929:SER:OG   | 2.35                     | 0.40              |
| 1:A:3930:ILE:HD12 | 1:A:3930:ILE:HA   | 1.93                     | 0.40              |
| 1:B:1496:TRP:CE2  | 1:B:1558:HIS:HD2  | 2.40                     | 0.40              |
| 1:B:1637:MET:SD   | 1:B:1650:ILE:HG13 | 2.62                     | 0.40              |
| 1:B:1671:ARG:HG2  | 1:B:1714:LEU:HA   | 2.03                     | 0.40              |
| 1:B:3442:PHE:HE2  | 1:B:3514:LEU:HD13 | 1.87                     | 0.40              |
| 1:C:1505:GLN:HG2  | 1:C:1506:GLN:H    | 1.86                     | 0.40              |
| 1:C:1870:VAL:HG11 | 1:C:2092:GLN:H    | 1.85                     | 0.40              |
| 1:C:1937:LEU:HG   | 1:C:2116:LEU:HD13 | 2.04                     | 0.40              |
| 1:C:2500:ALA:HB1  | 1:C:2550:LEU:HG   | 2.03                     | 0.40              |
| 1:C:2643:LEU:HB3  | 1:C:2648:TYR:HE1  | 1.87                     | 0.40              |
| 1:C:2770:LYS:HD3  | 1:C:2770:LYS:HA   | 1.78                     | 0.40              |
| 1:D:1704:PRO:HG2  | 1:D:1707:LEU:HB2  | 2.03                     | 0.40              |
| 1:D:3143:LEU:HD13 | 1:D:3147:ILE:HD13 | 2.03                     | 0.40              |
| 1:D:3772:THR:HG22 | 1:D:3804:ILE:HD11 | 2.03                     | 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 PDB entries followed by that with respect to all EM entries.

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

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles                 |
|-----|-------|-----------------|------------|----------|----------|-----------------------------|
| 1   | A     | 4197/5037 (83%) | 3926 (94%) | 254 (6%) | 17 (0%)  | <div>30</div> <div>65</div> |

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| Mol | Chain | Analysed          | Favoured    | Allowed   | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|-----------|----------|-------------|-----|
| 1   | B     | 4197/5037 (83%)   | 3927 (94%)  | 253 (6%)  | 17 (0%)  | 30          | 65  |
| 1   | C     | 4197/5037 (83%)   | 3924 (94%)  | 257 (6%)  | 16 (0%)  | 30          | 65  |
| 1   | D     | 4197/5037 (83%)   | 3922 (93%)  | 258 (6%)  | 17 (0%)  | 30          | 65  |
| 2   | E     | 105/107 (98%)     | 98 (93%)    | 7 (7%)    | 0        | 100         | 100 |
| 2   | F     | 105/107 (98%)     | 98 (93%)    | 7 (7%)    | 0        | 100         | 100 |
| 2   | G     | 105/107 (98%)     | 98 (93%)    | 7 (7%)    | 0        | 100         | 100 |
| 2   | H     | 105/107 (98%)     | 98 (93%)    | 7 (7%)    | 0        | 100         | 100 |
| All | All   | 17208/20576 (84%) | 16091 (94%) | 1050 (6%) | 67 (0%)  | 31          | 65  |

All (67) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 4773 | VAL  |
| 1   | A     | 5031 | GLN  |
| 1   | B     | 4773 | VAL  |
| 1   | B     | 5031 | GLN  |
| 1   | C     | 4773 | VAL  |
| 1   | C     | 5031 | GLN  |
| 1   | D     | 4773 | VAL  |
| 1   | D     | 5031 | GLN  |
| 1   | A     | 1469 | VAL  |
| 1   | A     | 2341 | VAL  |
| 1   | A     | 3381 | LEU  |
| 1   | B     | 1469 | VAL  |
| 1   | B     | 2341 | VAL  |
| 1   | B     | 3381 | LEU  |
| 1   | C     | 1469 | VAL  |
| 1   | C     | 2341 | VAL  |
| 1   | C     | 3381 | LEU  |
| 1   | D     | 1469 | VAL  |
| 1   | D     | 2341 | VAL  |
| 1   | D     | 3381 | LEU  |
| 1   | A     | 554  | LEU  |
| 1   | A     | 3187 | ARG  |
| 1   | B     | 554  | LEU  |
| 1   | B     | 3187 | ARG  |
| 1   | C     | 554  | LEU  |
| 1   | C     | 3187 | ARG  |
| 1   | D     | 554  | LEU  |
| 1   | D     | 3187 | ARG  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 3086 | GLU  |
| 1   | B     | 3086 | GLU  |
| 1   | C     | 3086 | GLU  |
| 1   | D     | 3086 | GLU  |
| 1   | A     | 3052 | HIS  |
| 1   | B     | 3052 | HIS  |
| 1   | C     | 3052 | HIS  |
| 1   | D     | 3052 | HIS  |
| 1   | A     | 2219 | GLU  |
| 1   | B     | 2219 | GLU  |
| 1   | D     | 2219 | GLU  |
| 1   | A     | 4081 | VAL  |
| 1   | B     | 4081 | VAL  |
| 1   | C     | 4081 | VAL  |
| 1   | D     | 4081 | VAL  |
| 1   | A     | 245  | VAL  |
| 1   | B     | 245  | VAL  |
| 1   | C     | 245  | VAL  |
| 1   | D     | 245  | VAL  |
| 1   | A     | 1767 | VAL  |
| 1   | A     | 1791 | VAL  |
| 1   | A     | 3087 | ILE  |
| 1   | A     | 3751 | VAL  |
| 1   | B     | 1767 | VAL  |
| 1   | B     | 1791 | VAL  |
| 1   | B     | 3087 | ILE  |
| 1   | B     | 3751 | VAL  |
| 1   | C     | 1767 | VAL  |
| 1   | C     | 1791 | VAL  |
| 1   | C     | 3087 | ILE  |
| 1   | C     | 3751 | VAL  |
| 1   | D     | 1767 | VAL  |
| 1   | D     | 1791 | VAL  |
| 1   | D     | 3087 | ILE  |
| 1   | D     | 3751 | VAL  |
| 1   | A     | 371  | VAL  |
| 1   | B     | 371  | VAL  |
| 1   | C     | 371  | VAL  |
| 1   | D     | 371  | VAL  |

### 5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

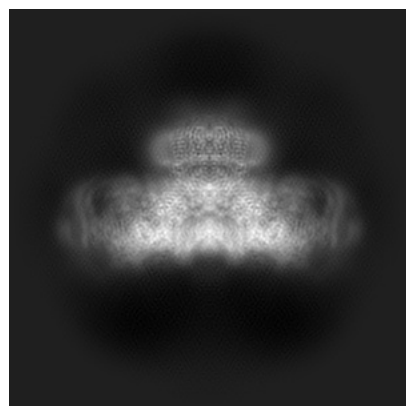
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25709. These allow visual inspection of the internal detail of the map and identification of artifacts.

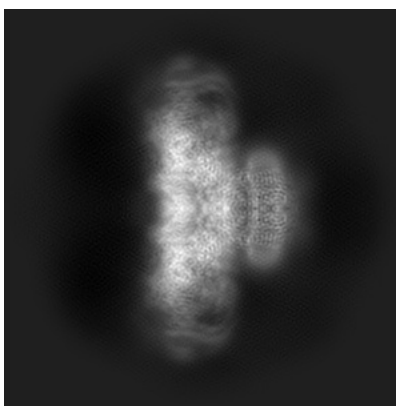
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

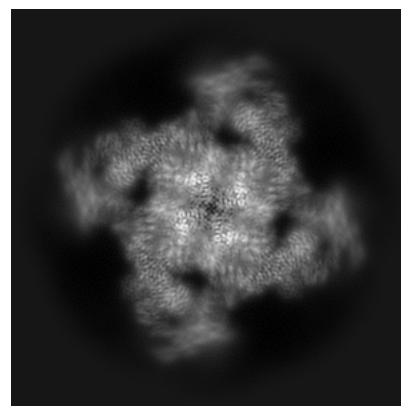
#### 6.1.1 Primary map



X

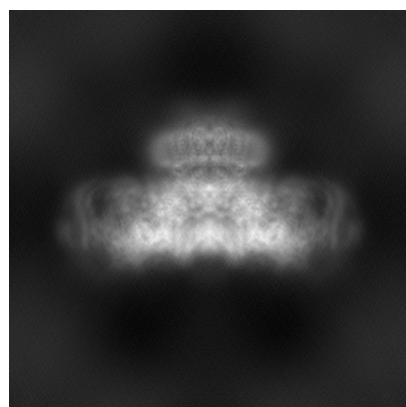


Y

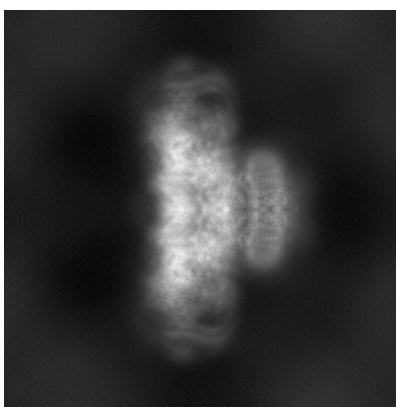


Z

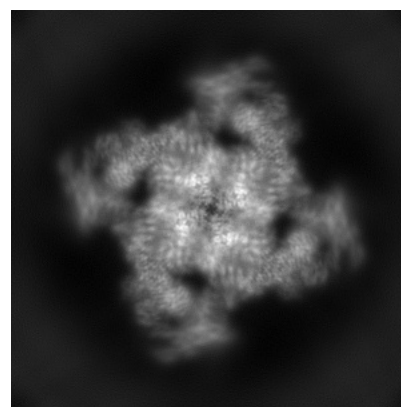
#### 6.1.2 Raw map



X



Y

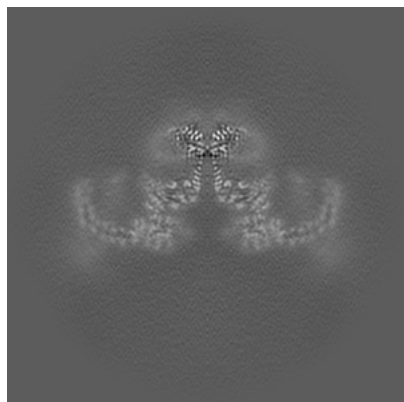


Z

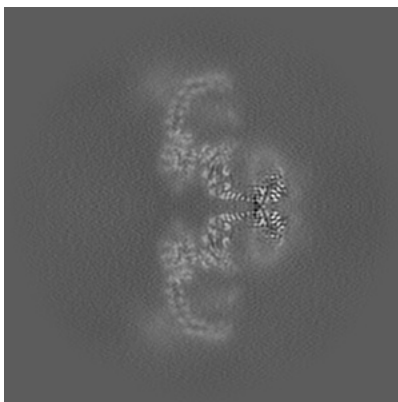
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

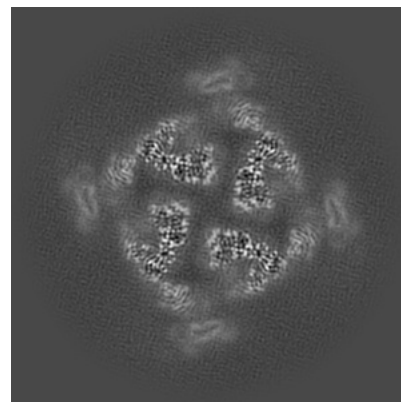
### 6.2.1 Primary map



X Index: 215

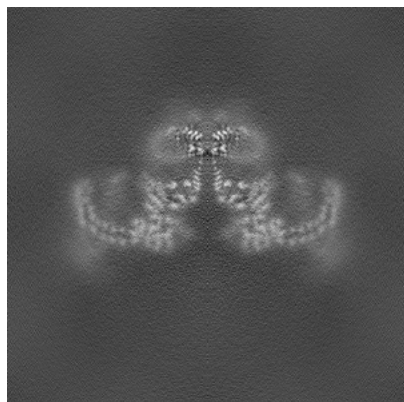


Y Index: 215

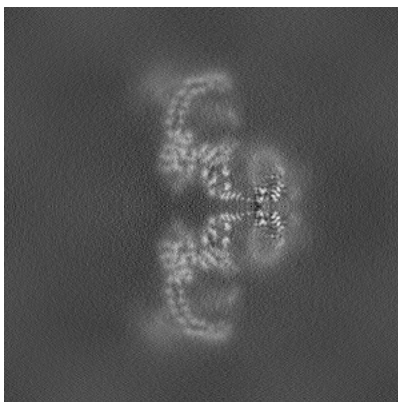


Z Index: 215

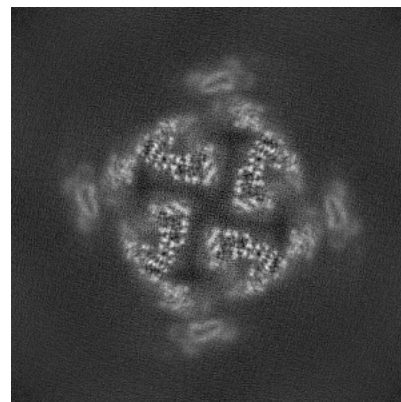
### 6.2.2 Raw map



X Index: 215



Y Index: 215

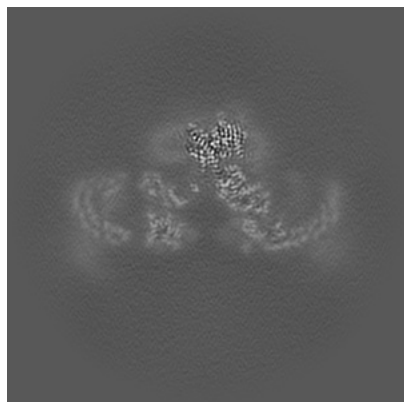


Z Index: 215

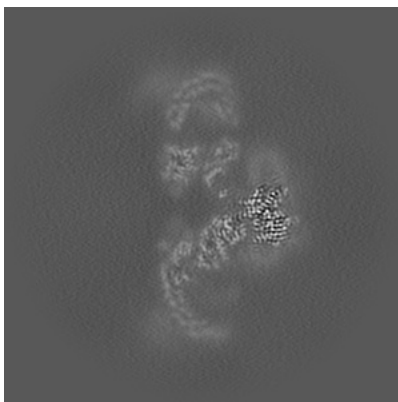
The images above show central slices of the map in three orthogonal directions.

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

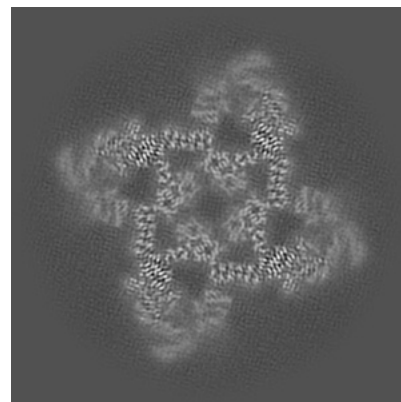
### 6.3.1 Primary map



X Index: 209

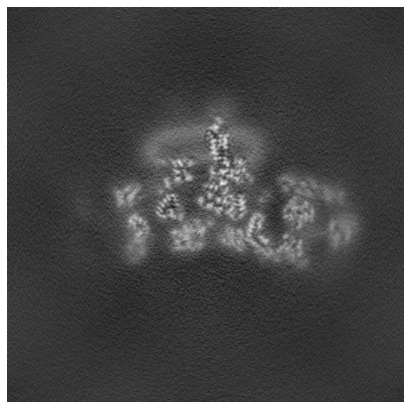


Y Index: 209

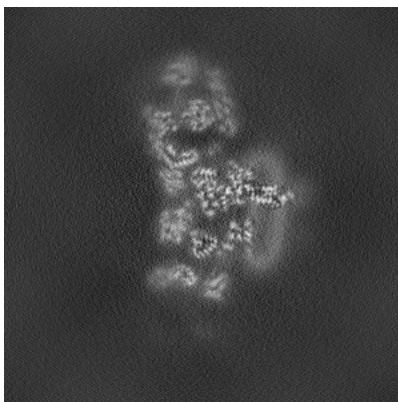


Z Index: 190

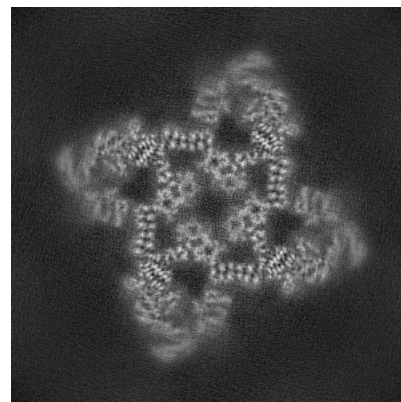
### 6.3.2 Raw map



X Index: 248



Y Index: 182

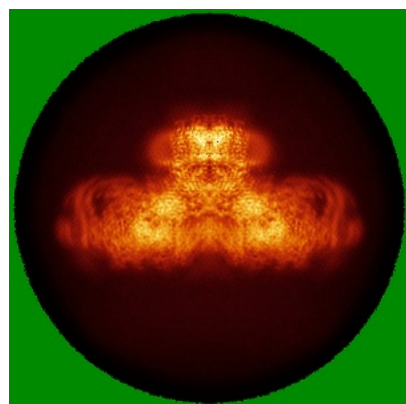


Z Index: 190

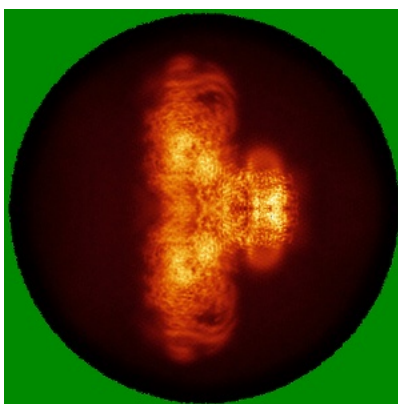
The images above show the largest variance slices of the map in three orthogonal directions.

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

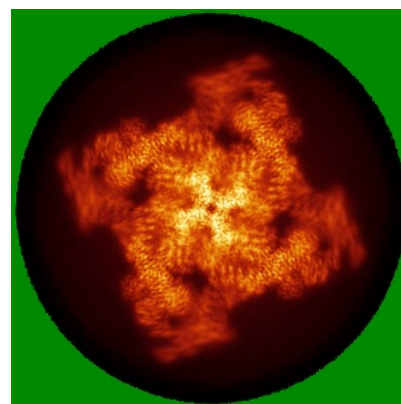
### 6.4.1 Primary map



X

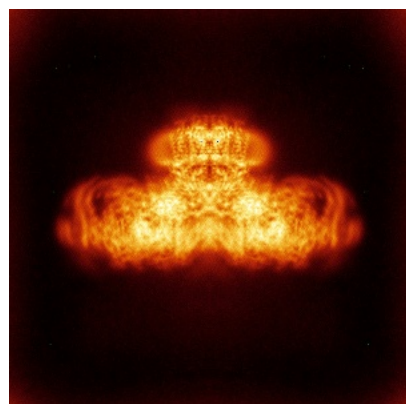


Y

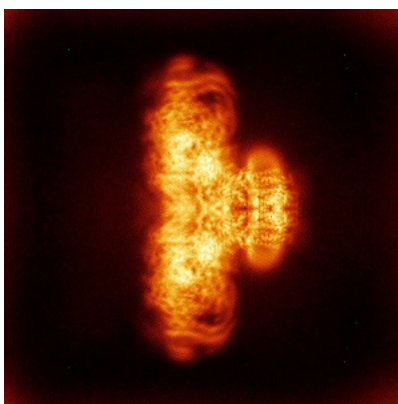


Z

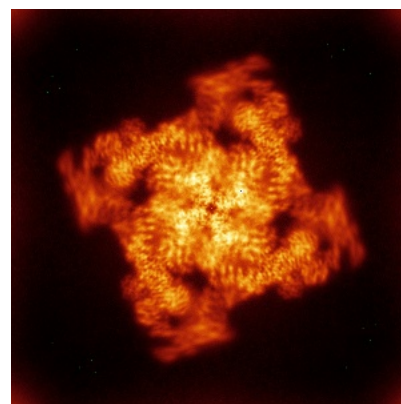
### 6.4.2 Raw map



X



Y

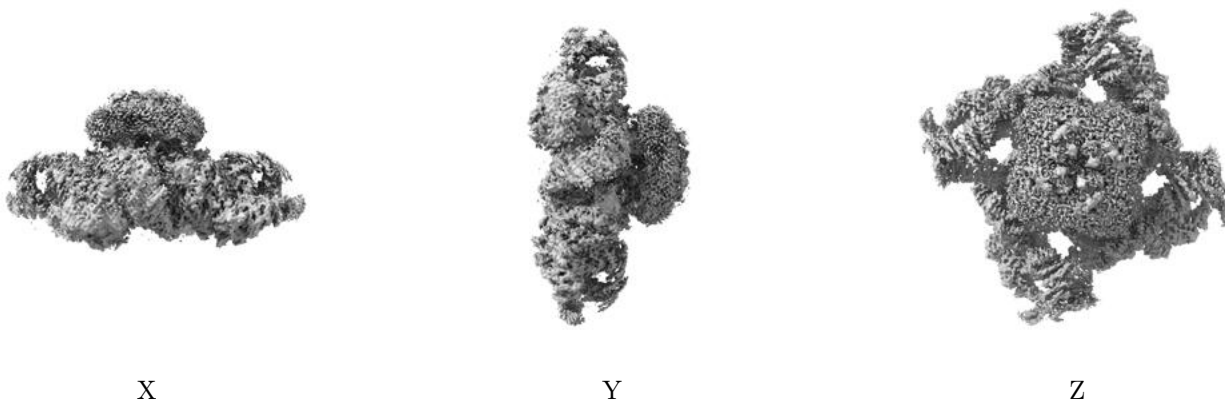


Z

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

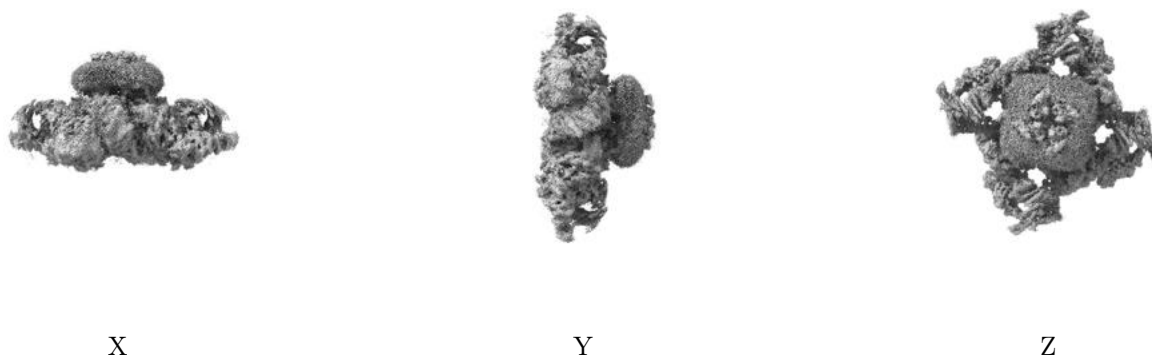
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.155. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

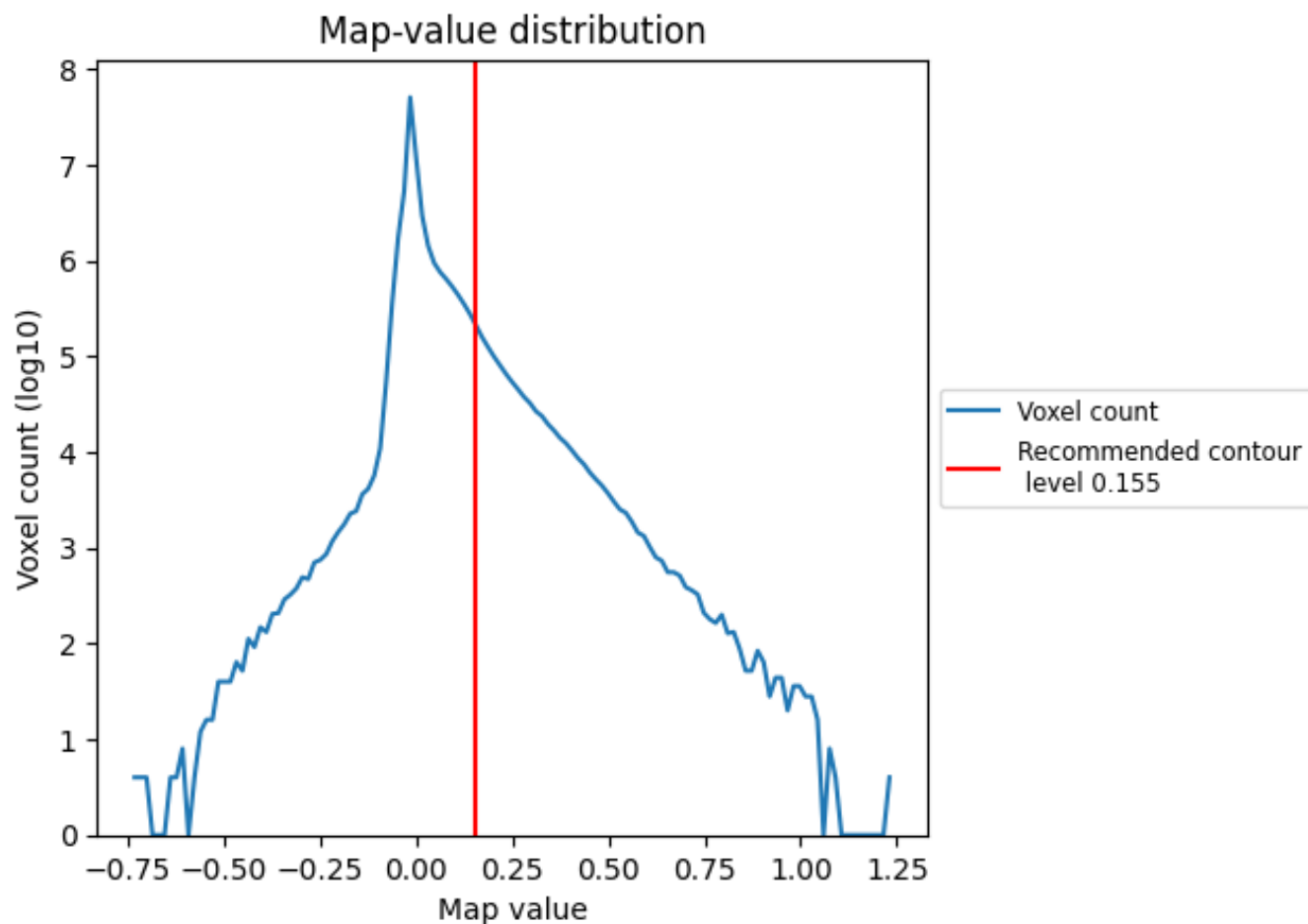
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

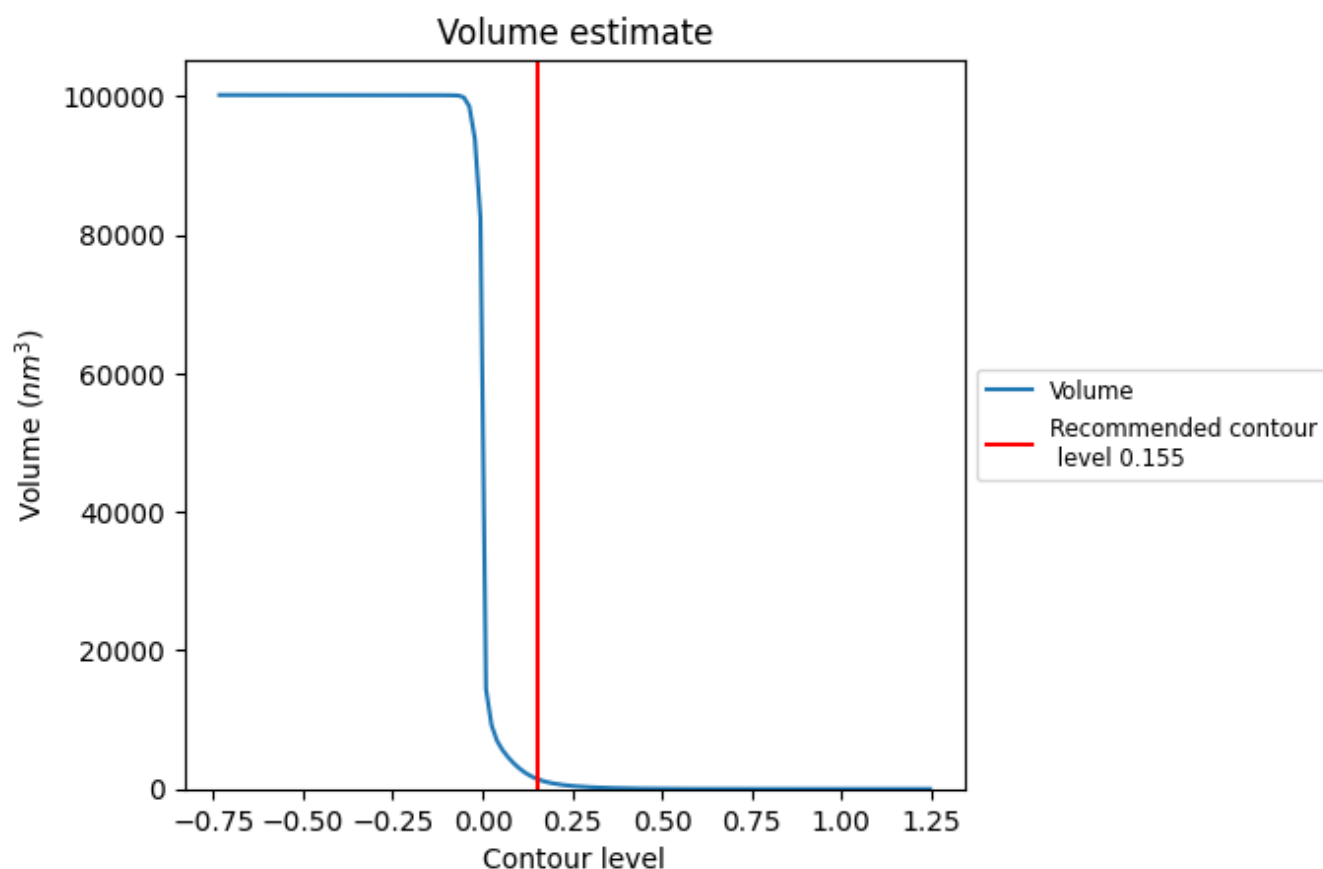
This section contains the results of statistical analysis of the map.

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



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

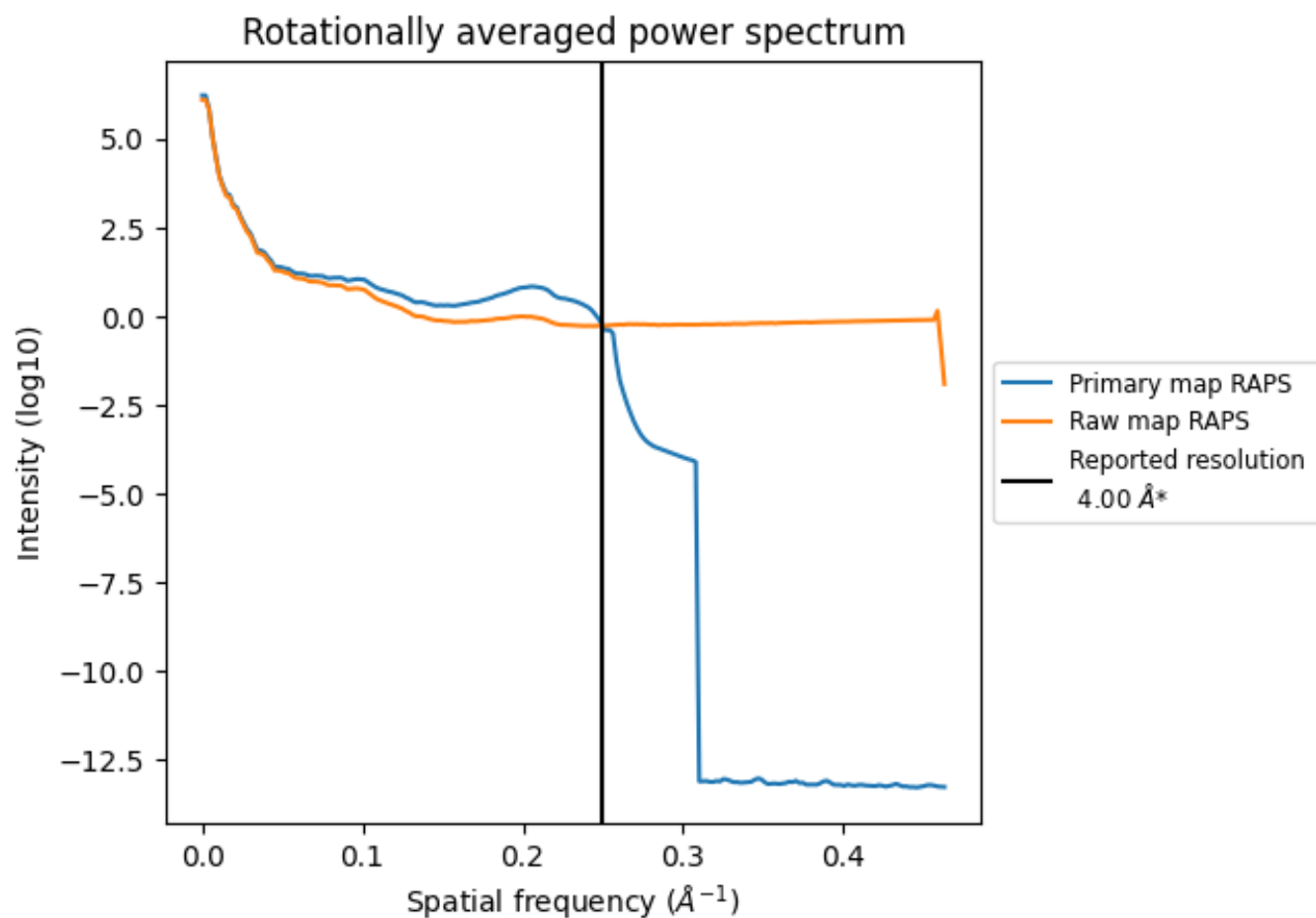
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1397 nm<sup>3</sup>; this corresponds to an approximate mass of 1262 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

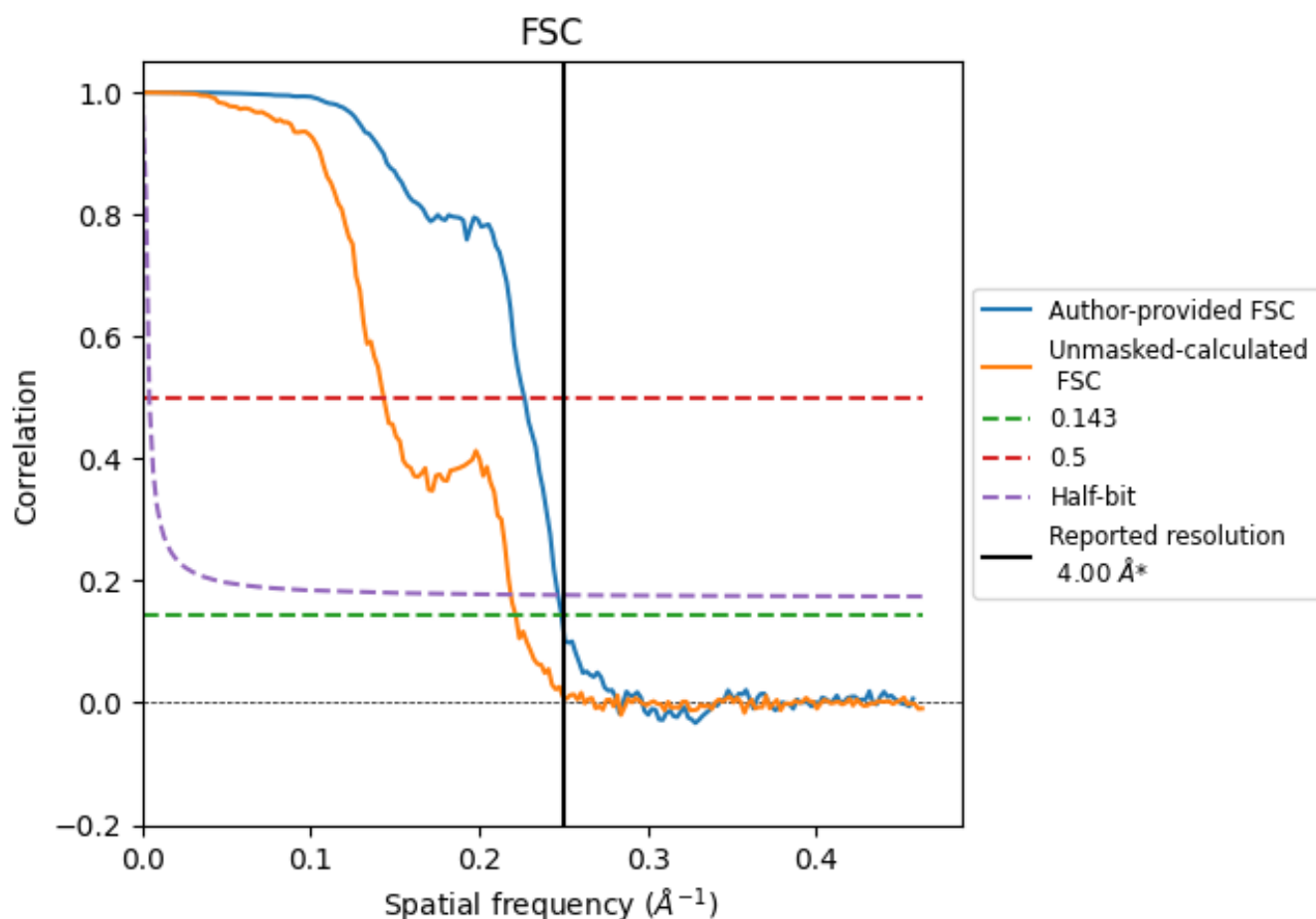


\*Reported resolution corresponds to spatial frequency of 0.250 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.250  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

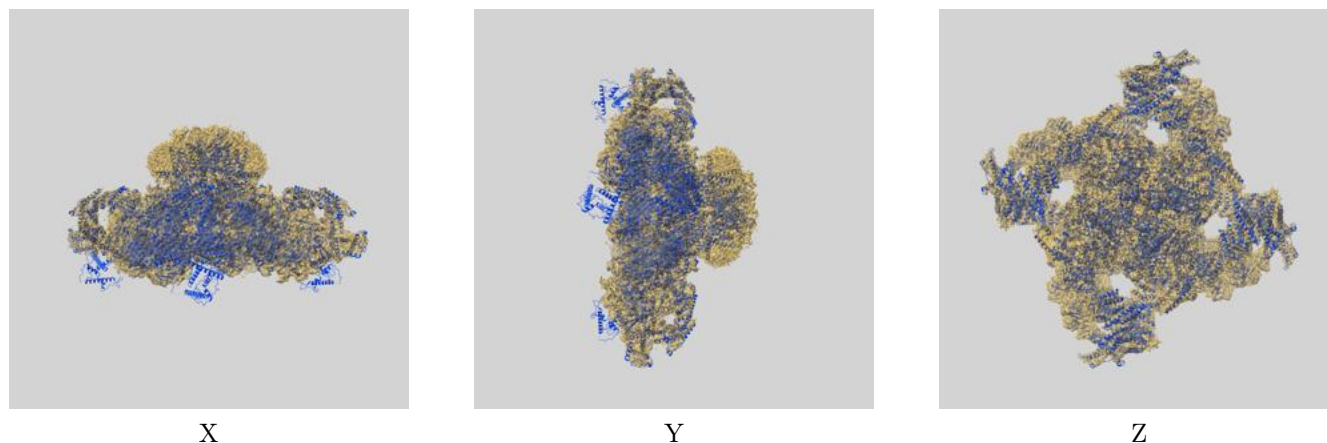
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 4.00                               | -    | -        |
| Author-provided FSC curve | 4.02                               | 4.41 | 4.05     |
| Unmasked-calculated*      | 4.51                               | 6.97 | 4.57     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.51 differs from the reported value 4.0 by more than 10 %

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

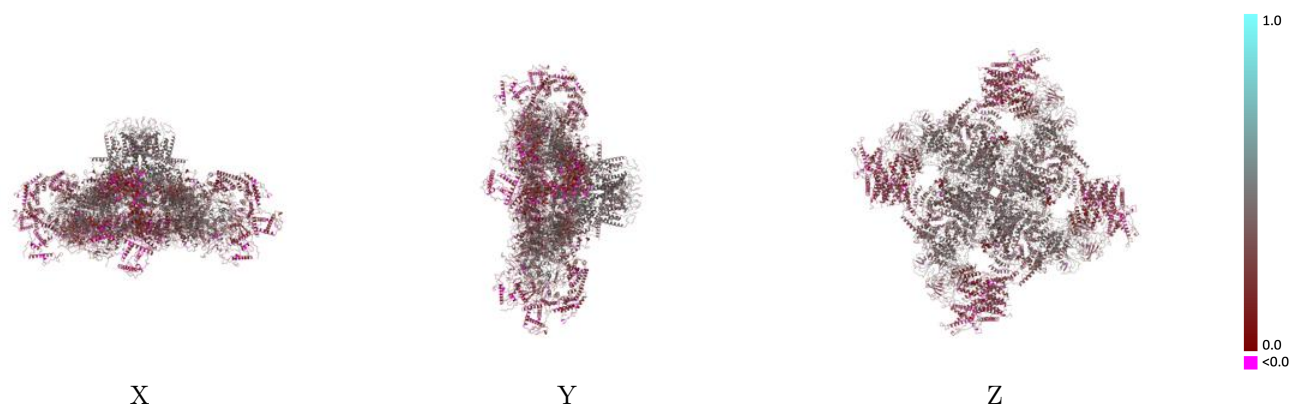
This section contains information regarding the fit between EMDB map EMD-25709 and PDB model 7T64. Per-residue inclusion information can be found in section [3](#) on page [6](#).

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



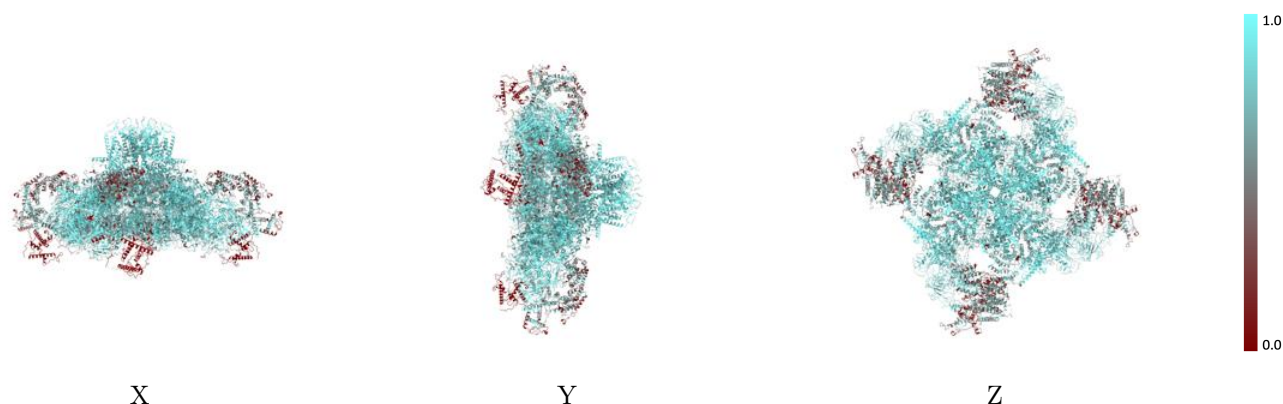
The images above show the 3D surface view of the map at the recommended contour level 0.155 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



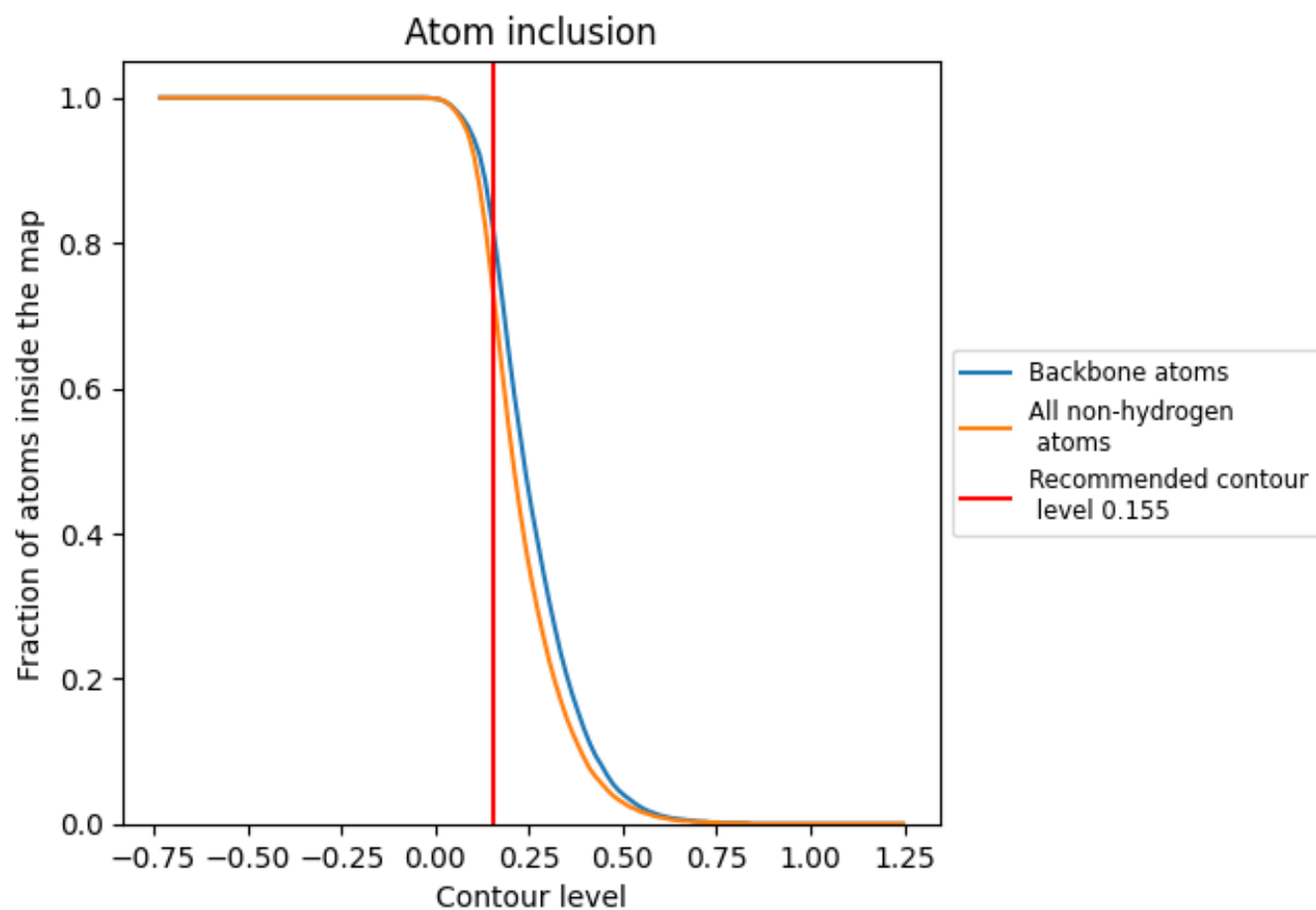
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.155).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 73% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.155) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion     | Q-score            |
|-------|--------------------|--------------------|
| All   | <div></div> 0.7310 | <div></div> 0.3060 |
| A     | <div></div> 0.7290 | <div></div> 0.3040 |
| B     | <div></div> 0.7290 | <div></div> 0.3040 |
| C     | <div></div> 0.7290 | <div></div> 0.3040 |
| D     | <div></div> 0.7290 | <div></div> 0.3040 |
| E     | <div></div> 0.8240 | <div></div> 0.3630 |
| F     | <div></div> 0.8240 | <div></div> 0.3670 |
| G     | <div></div> 0.8230 | <div></div> 0.3670 |
| H     | <div></div> 0.8250 | <div></div> 0.3660 |

1.0

0.0

<0.0