Full wwPDB EM Validation Report ⓘ

Nov 5, 2024 – 01:25 AM EST

PDB ID	:	9E18
EMDB ID	:	EMD-47385
Title	:	Structure of RyR1 in the primed state in the presence of pentoxifylline
Authors	:	Miotto, M.C.; Marks, A.R.
Deposited on	:	2024-10-21
Resolution	:	2.68 Å(reported)
Based on initial model	:	7TZC

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

We welcome your comments at *validation@mail.wwpdb.org*
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.

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

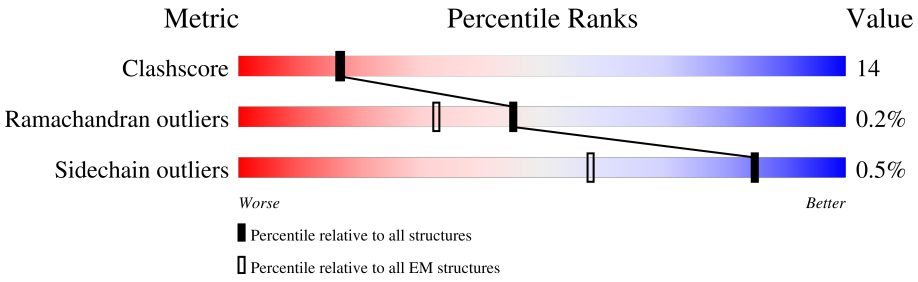
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance

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

The reported resolution of this entry is 2.68 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 (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 >=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 <=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	21% 64% 22% • 13%
1	B	5037	21% 64% 22% • 13%
1	C	5037	21% 65% 22% • 13%
1	D	5037	21% 64% 22% • 13%
2	E	108	5% 70% 24% • • •
2	F	108	6% 70% 24% • • •
2	G	108	5% 69% 25% • • •
2	H	108	• 69% 25% • • •

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 144144 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

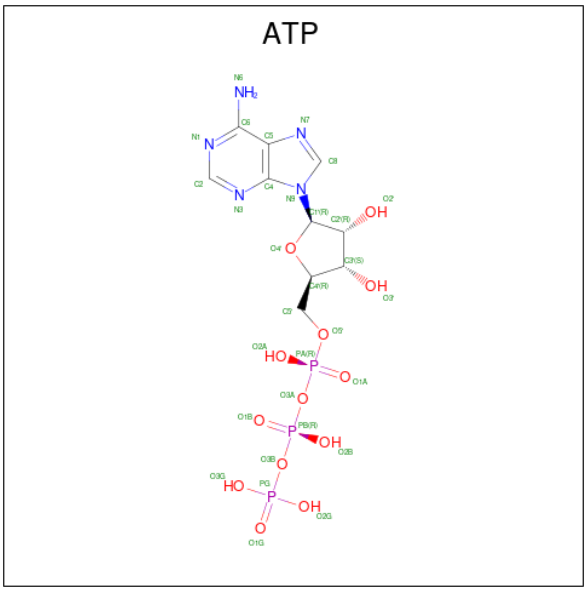
- Molecule 1 is a protein called Ryanodine receptor 1.

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

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

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

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Ca	0
			1	1	
4	B	1	Total	Ca	0
			1	1	
4	D	1	Total	Ca	0
			1	1	
4	C	1	Total	Ca	0
			1	1	

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Zn	0
			1	1	

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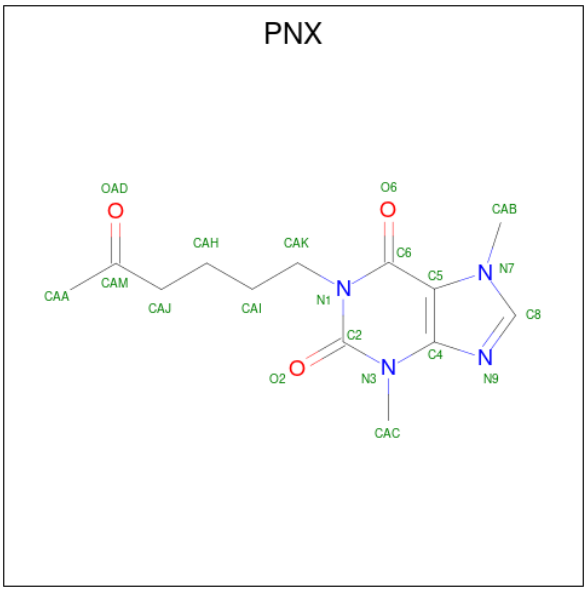
Mol	Chain	Residues	Atoms	AltConf
5	B	1	Total Zn 1 1	0
5	D	1	Total Zn 1 1	0
5	C	1	Total Zn 1 1	0

- Molecule 6 is 3,7-DIMETHYL-1-(5-OXOHEXYL)-3,7-DIHYDRO-1H-PURINE-2,6-DI ONE (three-letter code: PNX) (formula: $C_{13}H_{18}N_4O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
6	A	1	Total C N O 20 13 4 3	0
6	B	1	Total C N O 20 13 4 3	0
6	D	1	Total C N O 20 13 4 3	0
6	C	1	Total C N O 20 13 4 3	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	AltConf
7	A	2	Total O 2 2	0

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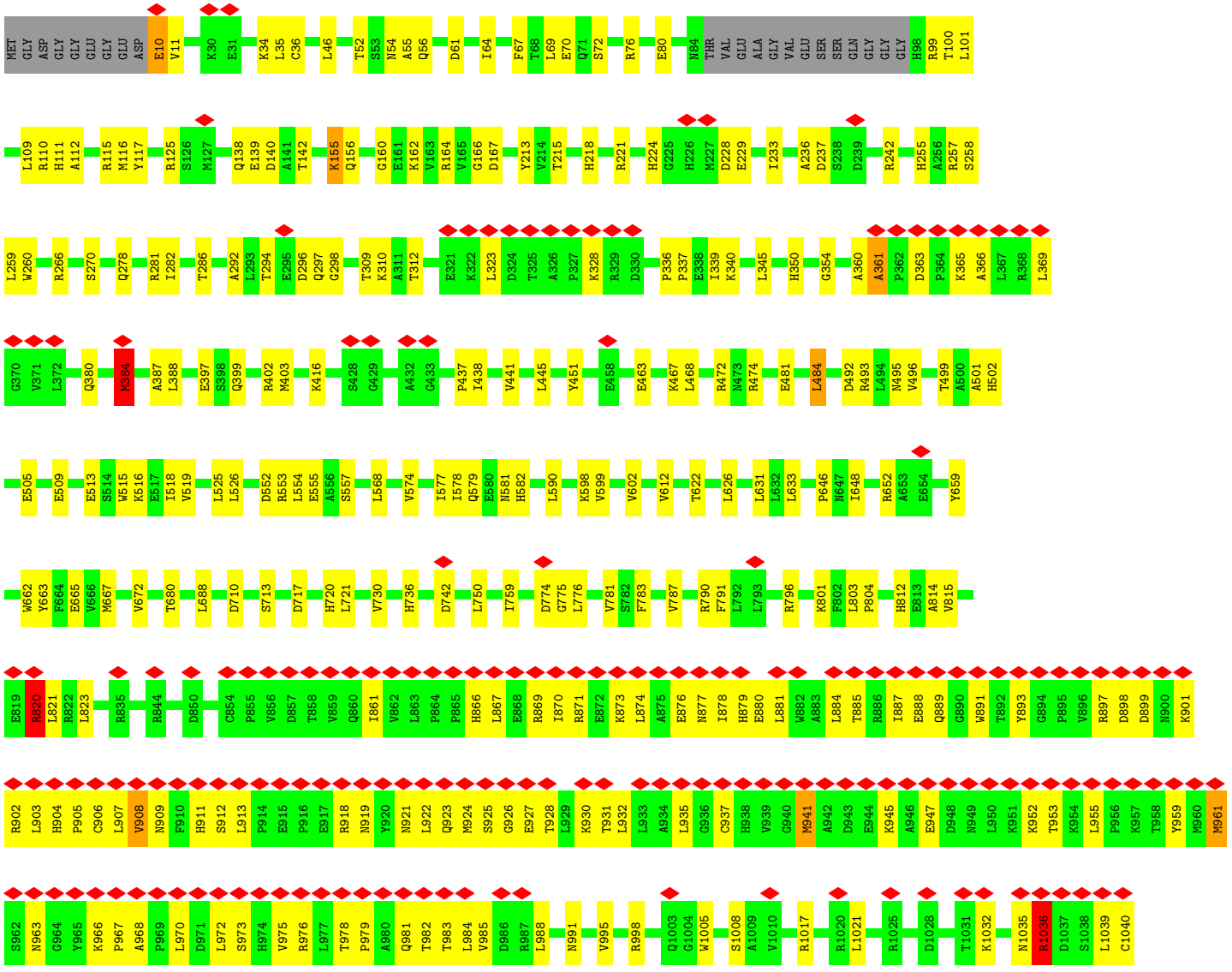
Mol	Chain	Residues	Atoms	AltConf
7	B	2	Total O 2 2	0
7	D	2	Total O 2 2	0
7	C	2	Total O 2 2	0

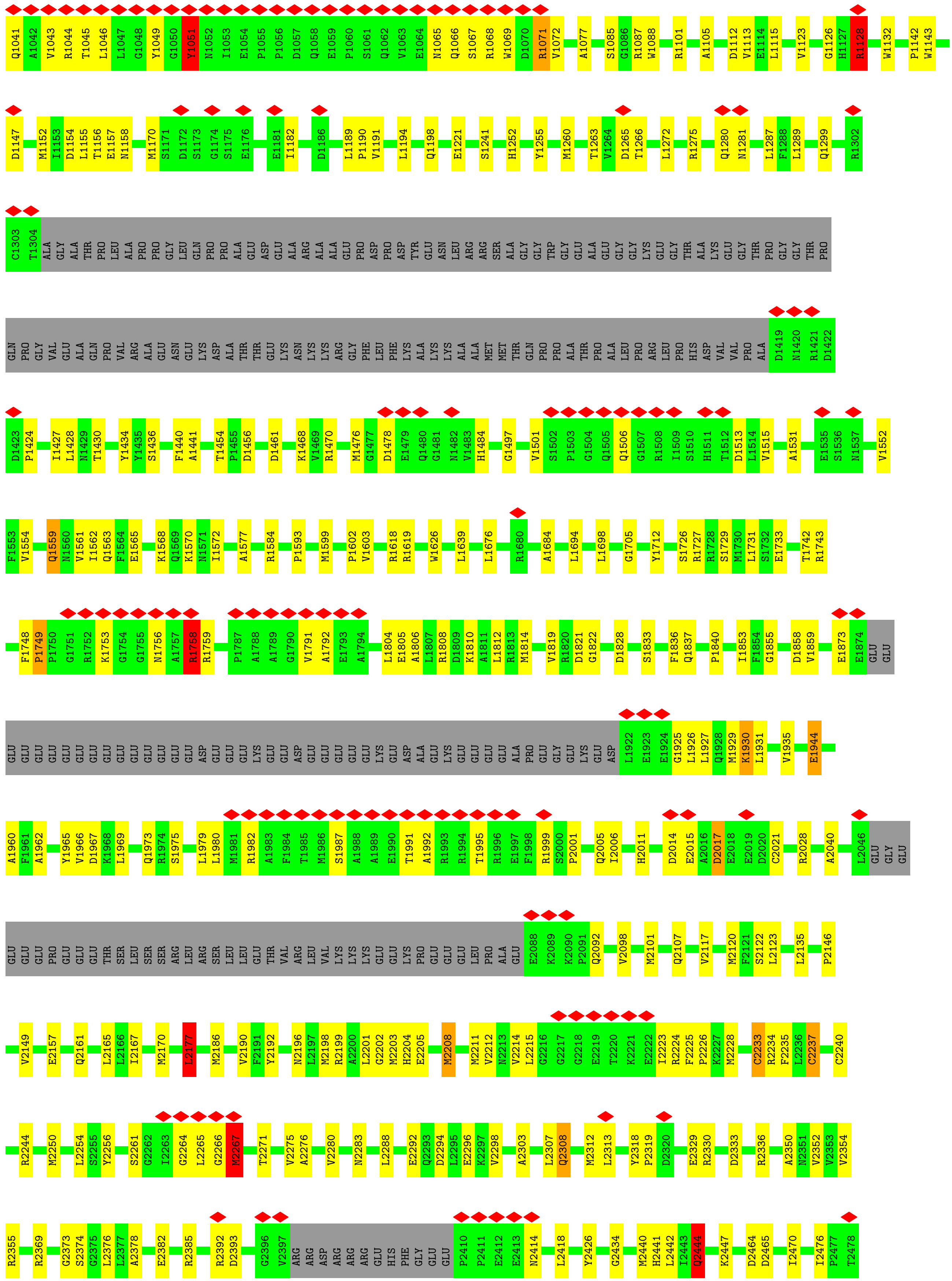
3 Residue-property plots (i)

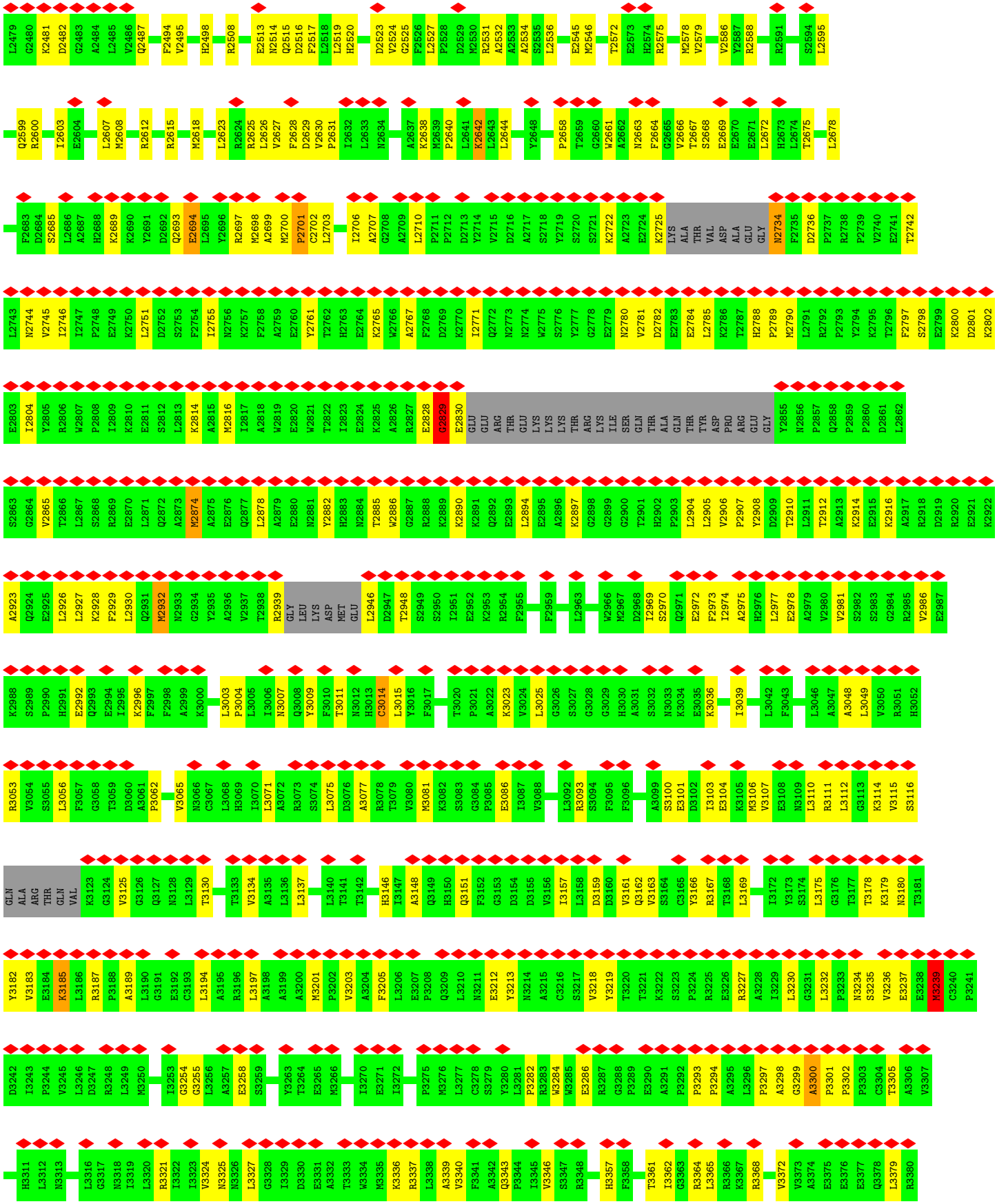
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Ryanodine receptor 1

Chain A:




Q1041 A1042 V1043 R1044 T1045 L1046 L1047 G1048 Y1049 G1050 Y1051 N1052 I1053 E1054 P1055 P1056 D1057 Q1058 E1059 P1060 S1061 Q1062 V1063 E1064 N1065 Q1066 S1067 R1068 W1069 D1070 R1071 V1072 A1077 S1085 G1086 R1087 W1088 R1101 A1105 D1112 V1113 E1114 L1115 V1123 G1126 H1127 R1128 W1132 P1142 W1143
D1147 M1152 I1153 D1154 L1155 T1156 E1157 N1158 M1170 S1171 D1172 S1173 G1174 S1175 E1176 E1181 I1182 D1186 L1189 P1190 V1191 L1194 Q1198 E1221 S1241 H1252 Y1255 M1260 T1263 V1264 D1265 T1266 L1272 R1275 Q1280 N1281 L1287 F1288 L1289 Q1299 R1302
C1303 T1304 ALA GLY ALA THR PRO LEU ALA PRO PRO GLY LEU GLN PRO PRO ALA GLU ASP GLU ALA ARG ALA ALA GLU PRO ASP PRO ASP TYR GLU ASN LEU ARG ARG SER ALA GLY GLY TRP GLY GLU ALA GLU GLY GLY LYS GLU GLY THR ALA LYS GLU GLY THR PRO GLY GLY THR PRO
GLN PRO GLY VAL GLU ALA GLN PRO VAL ARG ALA GLU ASN GLU LYS ASP ALA THR THR GLU LYS ASN LYS LYS ARG GLY PHE LEU PHE LYS ALA LYS LYS ALA ALA MET MET THR GLN PRO PRO ALA THR PRO ALA LEU PRO ARG LEU PRO HIS ASP VAL VAL PRO ALA D1419 N1420 R1421 D1422
D1423 P1424 I1427 L1428 N1429 T1430 Y1434 Y1435 S1436 F1440 A1441 T1454 P1455 D1456 D1461 K1468 V1469 R1470 M1476 G1477 D1478 E1479 Q1480 G1481 N1482 V1483 H1484 G1497 V1501 S1502 P1503 G1504 Q1505 Q1506 G1507 R1508 I1509 S1510 H1511 T1512 D1513 L1514 V1515 A1531 E1535 S1536 N1537 V1552
F1553 V1554 Q1559 N1560 V1561 I1562 Q1563 F1564 E1565 K1568 Q1569 K1570 N1571 I1572 A1577 R1584 P1593 M1599 P1602 V1603 R1618 R1619 W1626 L1639 L1676 R1680 A1684 L1694 L1698 G1705 Y1712 S1726 R1727 R1728 S1729 M1730 L1731 S1732 E1733 T1742 R1743
F1748 P1749 P1750 G1751 R1752 K1753 G1754 G1755 N1756 A1757 R1758 R1759 P1787 A1788 A1789 G1790 V1791 A1792 E1793 A1794 L1804 E1805 A1806 L1807 R1808 D1809 K1810 A1811 L1812 R1813 M1814 V1819 R1820 D1821 G1822 D1828 S1833 F1836 Q1837 P1840 I1853 F1854 G1855 D1858 V1859 E1873 E1874 GLU GLU
GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU ASP GLU GLU GLU LYS GLU GLU ASP GLU GLU GLU GLU GLU LYS GLU ASP ALA GLU LYS GLU GLU GLU GLU ALA PRO GLU GLY GLU LYS GLU ASP L1922 E1923 E1924 G1925 L1926 L1927 Q1928 M1929 K1930 L1931 V1935 E1944
A1960 F1961 A1962 Y1965 V1966 D1967 K1968 L1969 Q1973 R1974 S1975 L1979 L1980 M1981 R1982 A1983 F1984 T1985 M1986 S1987 A1988 A1989 E1990 T1991 A1992 R1993 R1994 T1995 R1996 E1997 F1998 R1999 S2000 P2001 Q2005 I2006 H2011 D2014 E2015 A2016 D2017 E2018 E2019 D2020 C2021 R2028 A2040 L2046 GLU GLY GLU
GLU GLU GLU PRO GLU GLU GLU THR SER LEU SER SER ARG LEU ARG SER LEU LEU GLU THR VAL ARG LEU VAL LYS LYS LYS GLU GLU LYS PRO GLU GLU GLU LEU PRO ALA GLU E2088 K2089 K2090 P2091 Q2092 V2098 M2101 Q2107 V2117 M2120 F2121 S2122 L2123 L2135 P2146
V2149 E2157 Q2161 L2165 L2166 I2167 M2170 L2177 M2186 V2190 F2191 Y2192 N2196 L2197 M2198 R2199 A2200 L2201 G2202 M2203 H2204 E2205 M2208 M2211 V2212 N2213 V2214 L2215 G2216 G2217 G2218 E2219 T2220 K2221 E2222 I2223 R2224 F2225 P2226 K2227 M2228 C2233 R2234 F2235 L2236 C2237 C2240
R2244 M2250 L2254 S2255 Y2256 S2261 G2262 I2263 G2264 L2265 G2266 M2267 T2271 V2275 A2276 V2280 N2283 L2288 E2292 Q2293 D2294 L2295 E2296 K2297 V2298 A2303 L2307 Q2308 M2312 L2313 Y2318 P2319 D2320 E2329 R2330 D2333 R2336 A2350 N2351 V2352 V2353 V2354
R2355 R2369 G2373 S2374 G2375 L2376 L2377 A2378 E2382 R2385 R2392 D2393 G2396 V2397 ARG ARG ASP ARG ARG ARG GLU HIS PHE GLY GLU GLU P2410 P2411 E2412 E2413 N2414 L2418 Y2426 G2434 M2440 H2441 L2442 I2443 Q2444 K2447 D2464 D2465 I2470 I2476 P2477 T2478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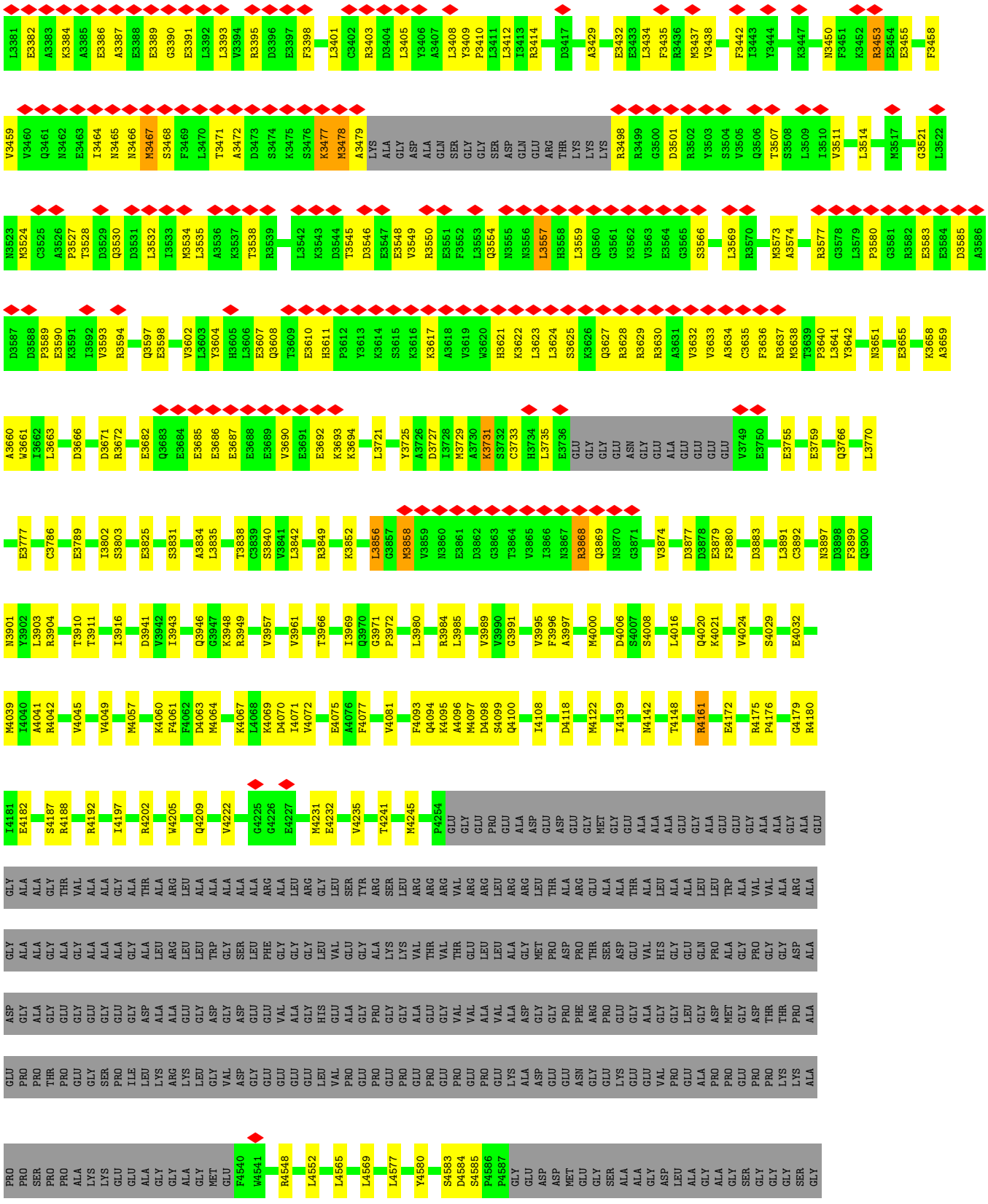
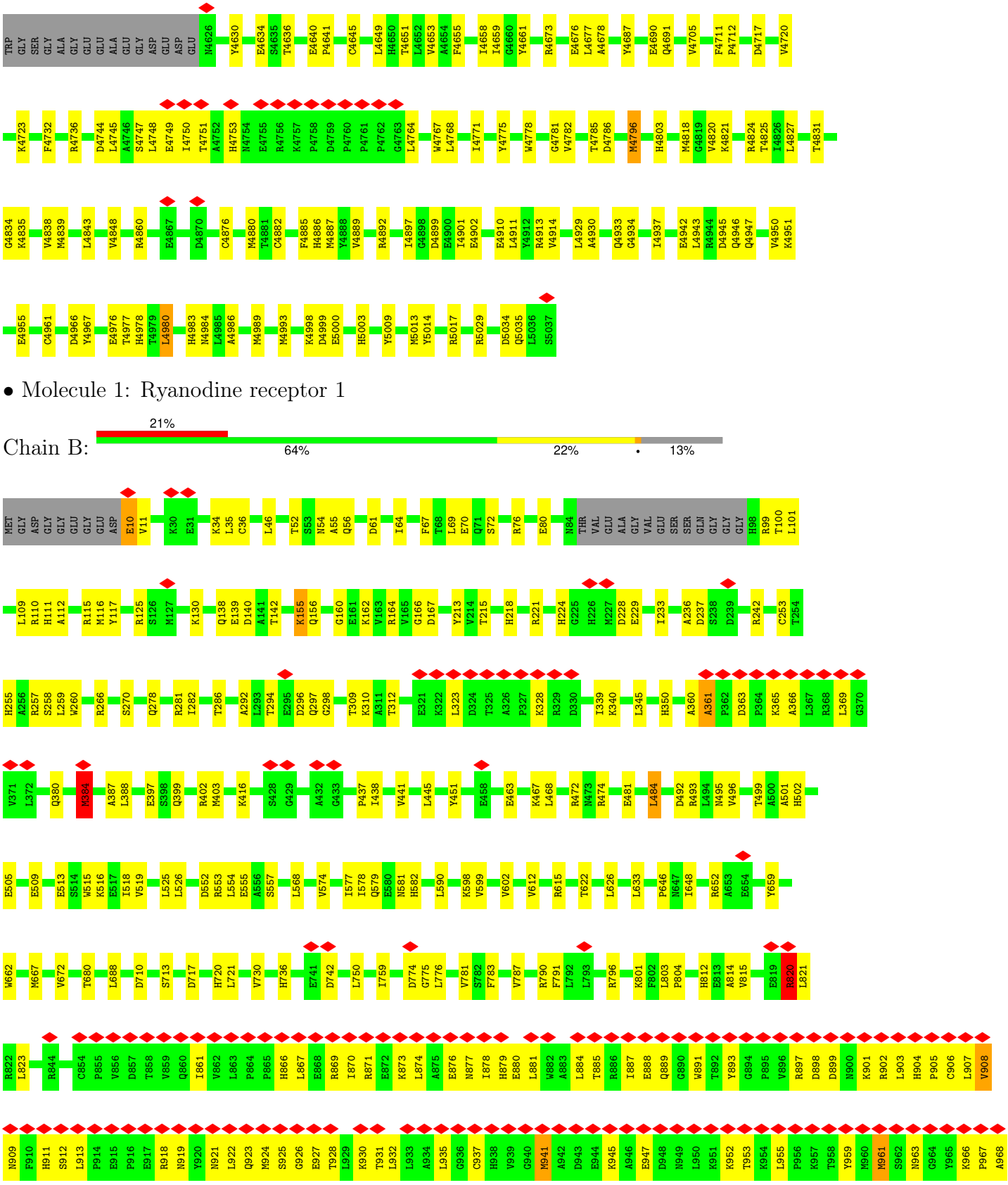
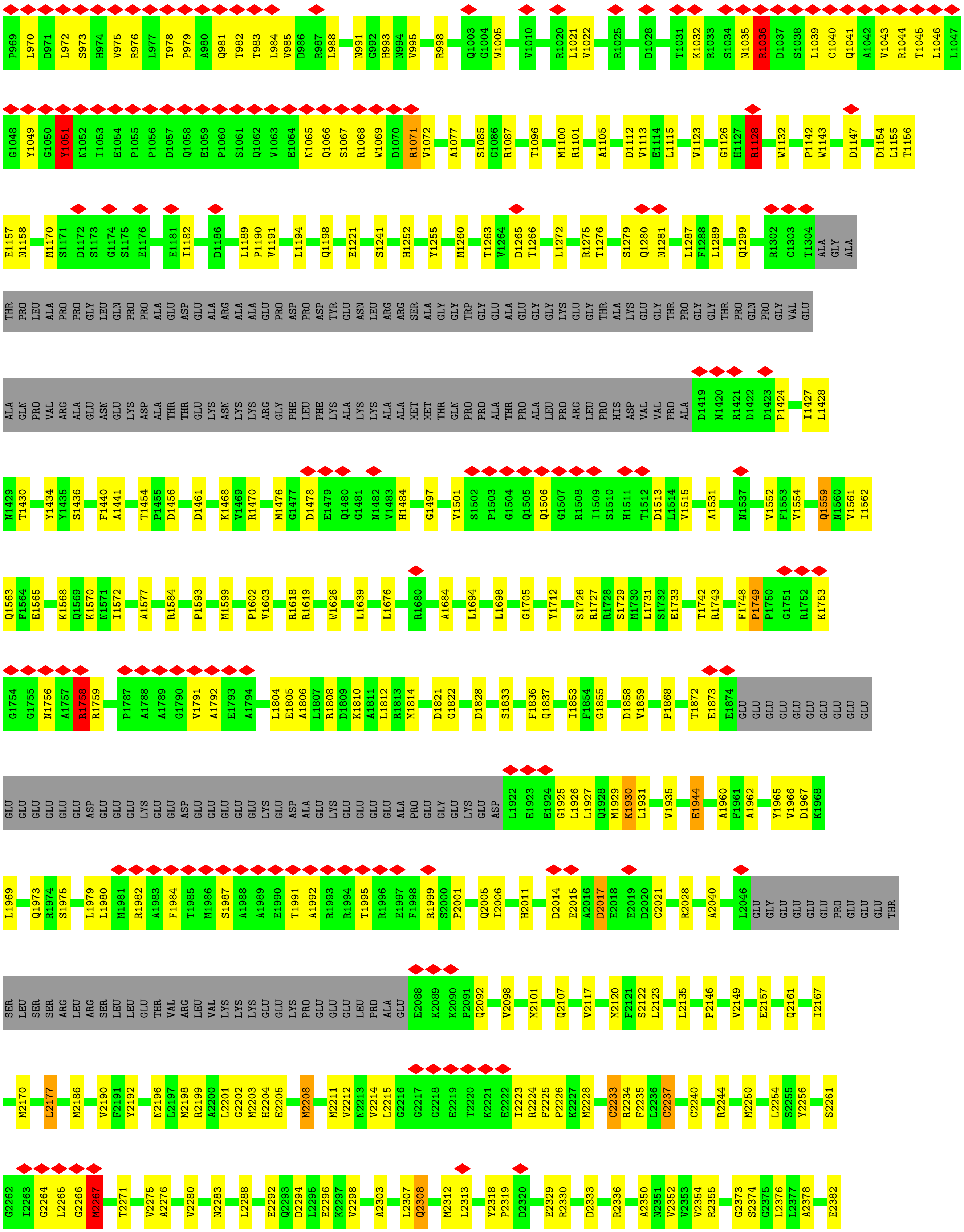
Q2599 R2600 I2603 E2604 L2607 M2608 R2612 R2615 M2618 L2623 R2624 R2625 L2626 V2627 F2628 D2629 V2630 P2631 I2632 L2633 N2634 A2637 K2638 M2639 P2640 L2641 K2642 L2643 L2644 Y2648 P2658 T2659 G2660 W2661 A2662 N2663 F2664 G2665 V2666 T2667 S2668 E2669 E2670 E2671 L2672 H2673 L2674 T2675 L2678
F2683 D2684 S2685 L2686 A2687 H2688 K2689 K2690 Y2691 D2692 Q2693 E2694 L2695 Y2696 R2697 M2698 A2699 M2700 P2701 C2702 L2703 I2706 A2707 G2708 A2709 L2710 P2711 P2712 D2713 Y2714 V2715 D2716 A2717 S2718 Y2719 S2720 S2721 K2722 A2723 E2724 K2725 LYS ALA THR VAL ASP ALA GLU GLY N2734 F2735 D2736 P2737 R2738 P2739 V2740 E2741 T2742
L2743 N2744 V2745 I2746 I2747 P2748 E2749 K2750 L2751 D2752 S2753 F2754 I2755 N2756 K2757 F2758 A2759 E2760 Y2761 T2762 H2763 E2764 K2765 W2766 A2767 F2768 D2769 K2770 I2771 Q2772 N2773 N2774 W2775 S2776 Y2777 G2778 E2779 N2780 V2781 D2782 E2783 E2784 L2785 K2786 T2787 H2788 P2789 M2790 L2791 R2792 P2793 Y2794 K2795 T2796 F2797 S2798 E2799 K2800 D2801 K2802
E2803 I2804 Y2805 R2806 W2807 P2808 I2809 K2810 E2811 S2812 L2813 K2814 A2815 M2816 I2817 A2818 W2819 E2820 W2821 T2822 I2823 E2824 K2825 A2826 R2827 E2828 G2829 E2830 GLU GLU ARG THR GLU LYS 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 M2874 A2875 E2876 Q2877 L2878 A2879 E2880 N2881 Y2882 H2883 N2884 T2885 W2886 G2887 R2888 K2889 K2890 K2891 Q2892 E2893 L2894 E2895 A2896 K2897 G2898 G2899 G2900 T2901 H2902 P2903 L2904 L2905 V2906 P2907 Y2908 D2909 T2910 L2911 T2912 A2913 K2914 E2915 K2916 A2917 R2918 D2919 R2920 E2921 K2922
A2923 Q2924 E2925 L2926 L2927 K2928 F2929 L2930 Q2931 M2932 N2933 G2934 Y2935 A2936 V2937 T2938 R2939 GLY LEU LYS ASP MET GLU L2946 D2947 T2948 S2949 S2950 I2951 E2952 K2953 R2954 F2955 F2959 L2963 W2966 M2967 D2968 I2969 S2970 Q2971 E2972 F2973 I2974 A2975 H2976 L2977 E2978 A2979 V2980 V2981 S2982 S2983 G2984 R2985 V2986 E2987
K2988 S2989 P2990 H2991 E2992 Q2993 E2994 I2995 K2996 F2997 F2998 A2999 K3000 L3003 P3004 L3005 T3006 N3007 G3008 Y3009 F3010 T3011 N3012 H3013 G3014 L3015 Y3016 F3017 T3020 P3021 A3022 K3023 V3024 L3025 G3026 S3027 G3028 G3029 H3030 A3031 S3032 N3033 K3034 E3035 K3036 I3039 L3042 F3043 L3046 A3047 A3048 L3049 V3050 R3051 H3052
R3053 V3054 S3055 L3056 F3057 G3058 T3059 D3060 A3061 P3062 V3065 N3066 C3067 L3068 H3069 I3070 L3071 A3072 R3073 S3074 L3075 D3076 A3077 R3078 T3079 V3080 M3081 K3082 S3083 G3084 P3085 E3086 I3087 V3088 L3092 R3093 S3094 F3095 F3096 A3099 S3100 E3101 D3102 I3103 E3104 K3105 W3106 Y3107 E3108 N3109 L3110 R3111 L3112 G3113 K3114 V3115 S3116
GLN ALA ARG THR GLN VAL K3123 G3124 V3125 G3126 Q3127 N3128 L3129 T3130 T3133 V3134 A3135 L3136 L3137 L3140 T3141 T3142 H3146 I3147 A3148 Q3149 H3150 Q3151 F3152 G3153 D3154 D3155 V3156 I3157 L3158 D3159 D3160 V3161 Q3162 V3163 S3164 C3165 Y3166 R3167 T3168 L3169 I3172 Y3173 S3174 L3175 G3176 T3177 T3178 K3179 N3180 T3181
Y3182 V3183 E3184 K3185 L3186 R3187 P3188 A3189 L3190 G3191 E3192 C3193 L3194 A3195 R3196 L3197 A3198 A3199 A3200 M3201 P3202 V3203 A3204 F3205 L3206 E3207 P3208 Q3209 L3210 N3211 E3212 Y3213 N3214 A3215 C3216 S3217 V3218 Y3219 T3220 T3221 K3222 S3223 P3224 R3225 E3226 R3227 A3228 I3229 L3230 G3231 L3232 P3233 N3234 S3235 V3236 E3237 E3238 M3239 C3240 P3241
D3242 I3243 P3244 V3245 L3246 D3247 R3248 L3249 M3250 T3253 G3254 G3255 L3256 A3257 E3258 S3259 Y3263 T3264 E3265 M3266 I3270 E3271 I3272 P3275 M3276 L3277 C3278 S3279 Y3280 L3281 P3282 R3283 W3284 W3285 E3286 R3287 G3288 P3289 E3290 A3291 P3292 P3293 P3294 A3295 L3296 P3297 A3298 G3299 A3300 P3301 P3302 P3303 C3304 T3305 A3306 V3307
H3311 L3312 N3313 L3316 G3317 N3318 I3319 L3320 R3321 I3322 I3323 V3324 N3325 N3326 L3327 G3328 I3329 D3330 E3331 A3332 T3333 W3334 M3335 K3336 R3337 L3338 A3339 V3340 F3341 A3342 Q3343 P3344 I3345 V3346 S3347 R3348 H3357 F3358 T3361 I3362 G3363 R3364 L3365 R3366 K3367 R3368 V3372 V3373 A3374 E3375 E3376 E3377 Q3378 L3379 R3380





• Molecule 1: Ryanodine receptor 1

Chain B: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G1048 Y1049 G1050 Y1051 N1052 I1053 E1054 P1055 P1056 D1057 Q1058 E1059 P1060 S1061 Q1062 V1063 E1064 N1065 Q1066 S1067 R1068 W1069 D1070 R1071 V1072 A1077 S1085 G1086 R1087 T1096 M1100 R1101 A1105 D1112 V1113 E1114 L1115 V1123 G1126 H1127 R1128 W1132 P1142 W1143 D1147 D1154 L1155 T1156
E1157 N1158 M1170 S1171 D1172 S1173 G1174 S1175 E1176 E1181 I1182 D1186 L1189 P1190 V1191 L1194 Q1198 E1221 S1241 H1252 Y1255 M1260 T1263 V1264 D1265 T1266 L1272 R1275 T1276 S1279 Q1280 N1281 L1287 F1288 L1289 Q1299 R1302 C1303 T1304 ALA GLY ALA
THR PRO LEU ALA PRO PRO GLY LEU GLN PRO PRO ALA GLU ASP GLU ALA ARG ALA ALA GLU PRO ASP PRO ASP TYR GLU ASN LEU ARG ARG SER ALA GLY GLY TRP GLY GLU ALA GLU GLY GLY LYS GLU GLY THR ALA LYS GLU GLY THR PRO GLY GLY THR PRO GLN PRO GLY VAL GLU
ALA GLN PRO VAL ARG ALA GLU ASN GLU LYS ASP ALA THR THR GLU LYS ASN LYS LYS ARG GLY PHE LEU PHE LYS ALA LYS LYS ALA ALA MET MET THR GLN PRO PRO ALA THR PRO ALA LEU PRO ARG LEU PRO HIS ASP VAL VAL PRO ALA D1419 N1420 R1421 D1422 D1423 P1424 I1427 L1428
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GLU GLU GLU GLU GLU GLU ASP GLU GLU GLU LYS GLU GLU ASP GLU GLU GLU GLU GLU LYS GLU ASP ALA GLU LYS GLU GLU GLU GLU ALA PRO GLU GLY GLU LYS GLU ASP L1922 E1923 E1924 G1925 L1926 L1927 Q1928 M1929 K1930 L1931 V1935 E1944 A1960 F1961 A1962 Y1965 V1966 D1967 K1968
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SER LEU SER SER ARG LEU ARG SER LEU LEU GLU THR VAL ARG LEU VAL LYS LYS LYS GLU GLU LYS PRO GLU GLU GLU LEU PRO ALA GLU E2088 K2089 K2090 P2091 Q2092 V2098 M2101 Q2107 V2117 M2120 F2121 S2122 L2123 L2135 P2146 V2149 E2157 Q2161 I2167
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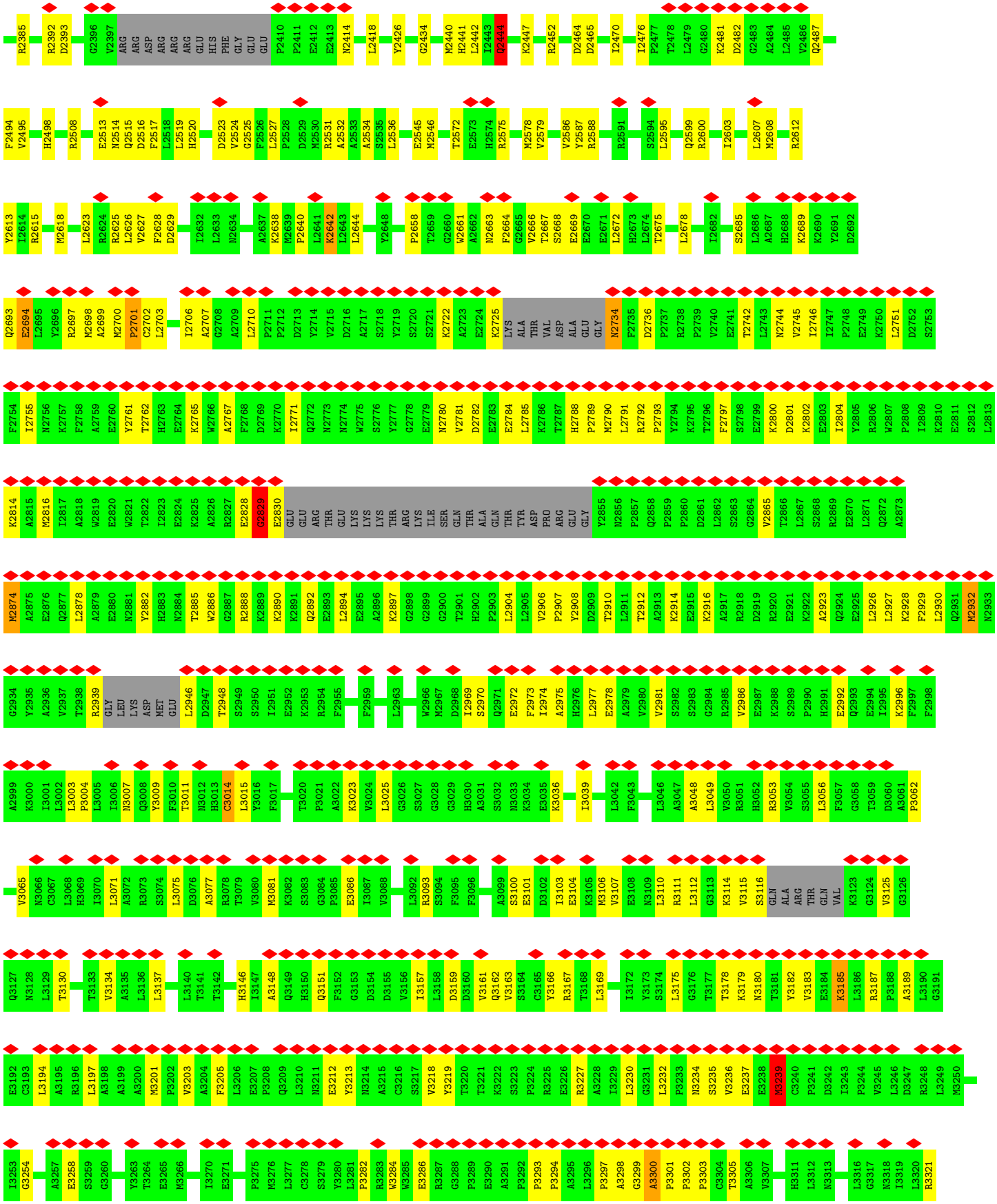
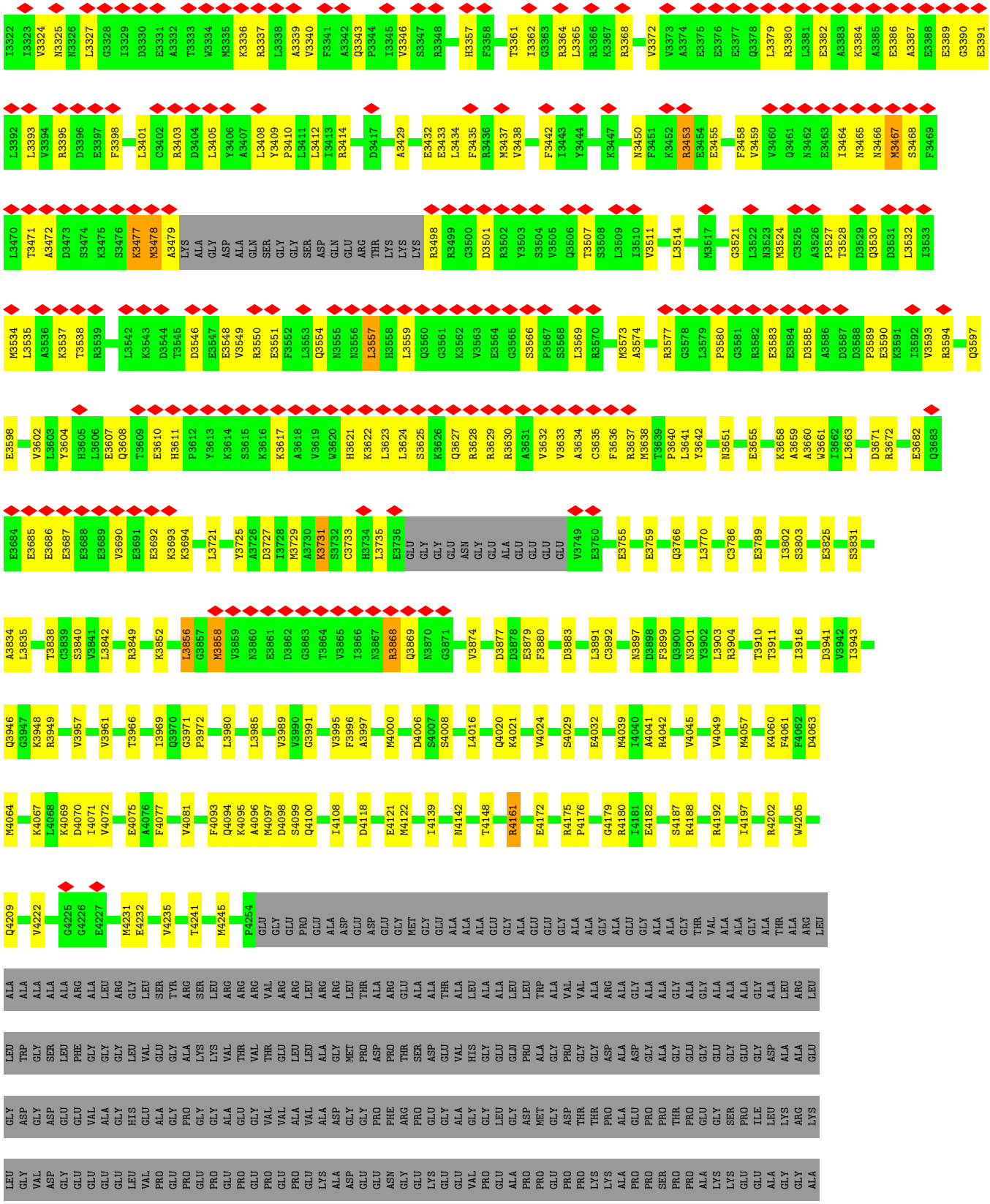
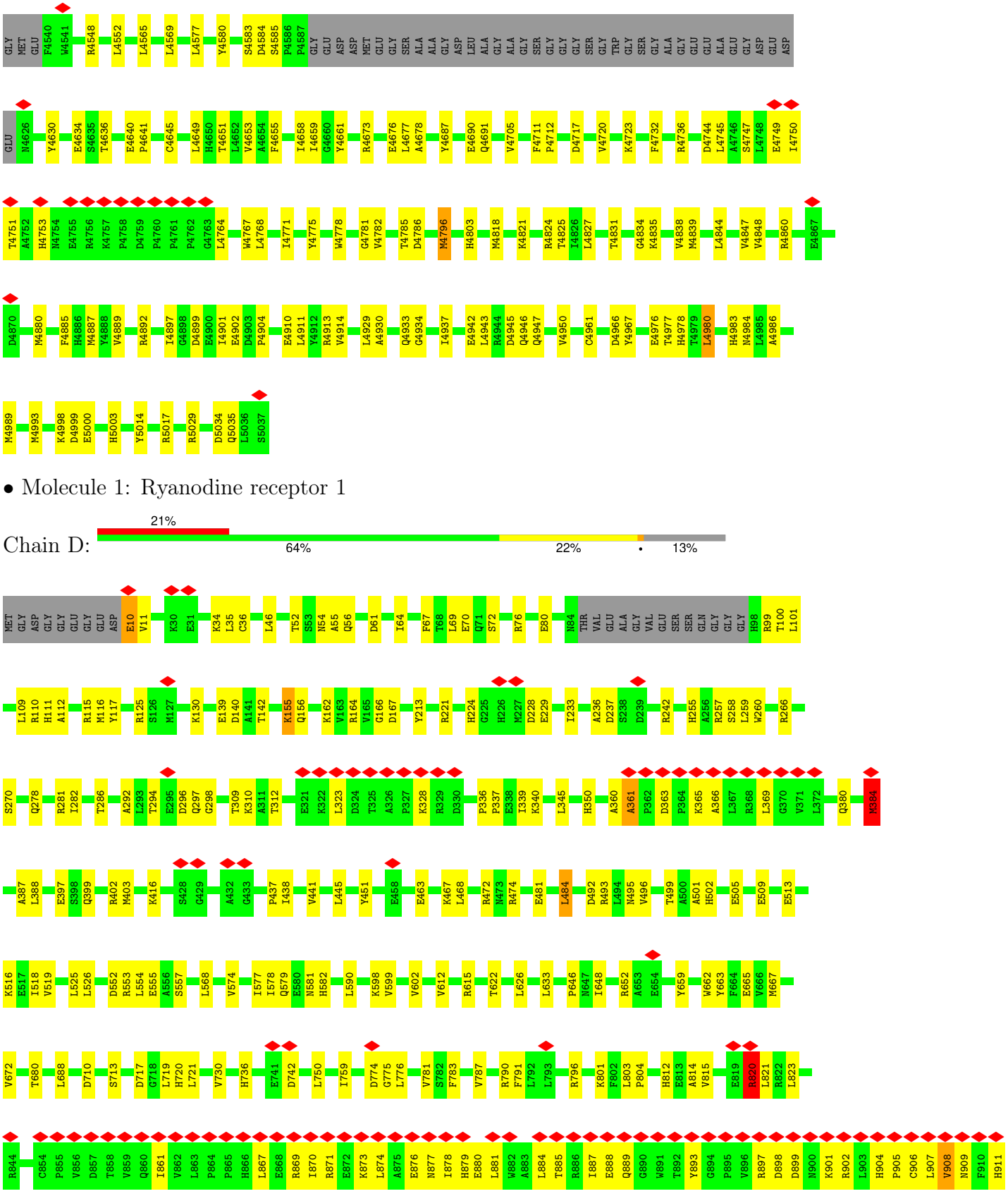
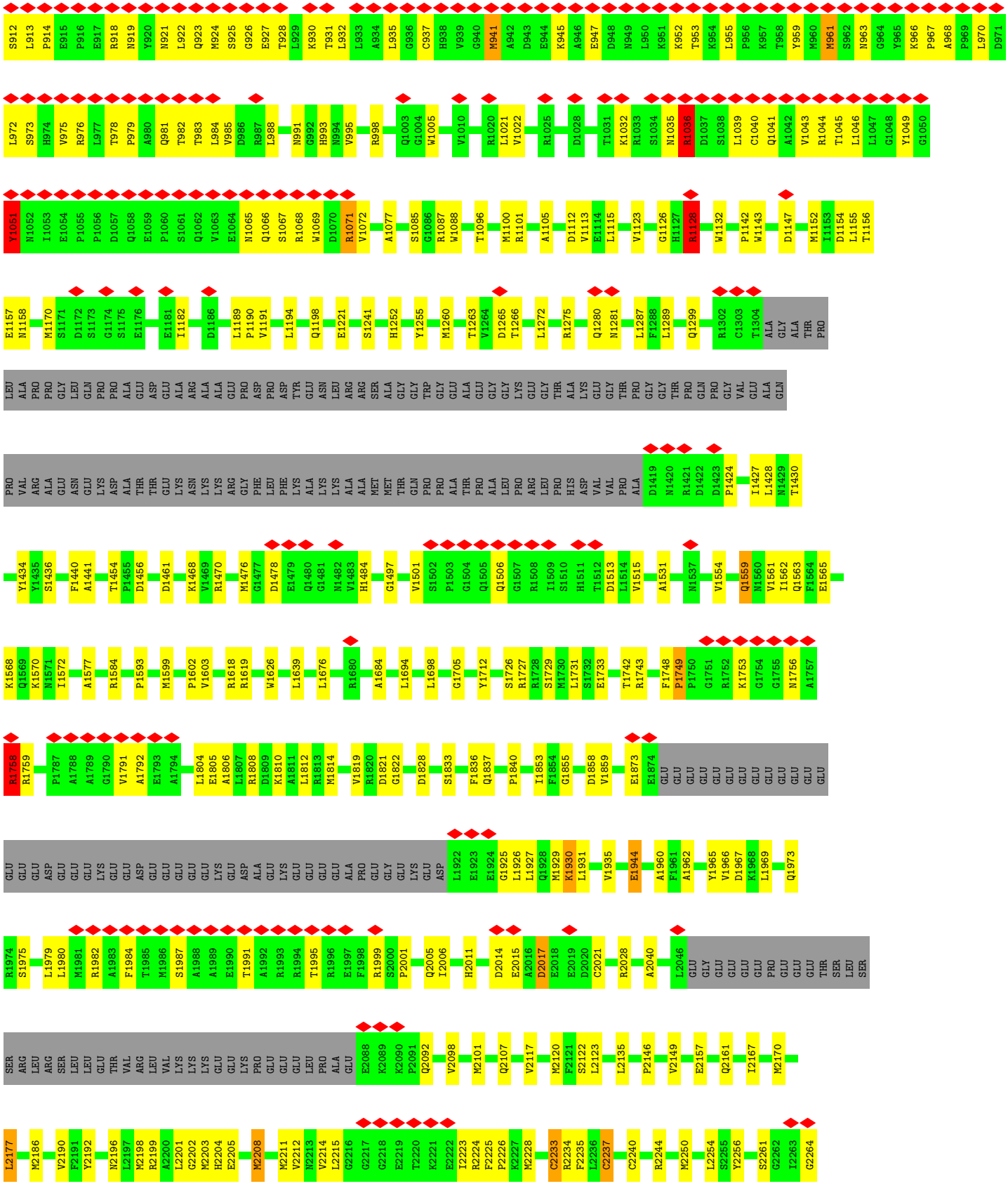






• Molecule 1: Ryanodine receptor 1

Chain D: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L972 S973 H974 V975 R976 L977 T978 P979 A980 Q981 T982 T983 L984 V985 D986 R987 L988 N991 G992 H993 N994 V995 R998 Q1003 G1004 W1005 V1010 R1020 L1021 V1022 R1025 D1028 T1031 K1032 R1033 S1034 N1035 R1036 D1037 S1038 L1039 C1040 Q1041 A1042 V1043 R1044 T1045 L1046 L1047 G1048 Y1049 G1050
V1051 N1052 I1053 E1054 P1055 P1056 D1057 Q1058 E1059 P1060 S1061 Q1062 V1063 E1064 N1065 Q1066 S1067 R1068 W1069 D1070 R1071 V1072 A1077 S1085 G1086 R1087 W1088 T1096 M1100 R1101 A1105 D1112 V1113 E1114 L1115 V1123 G1126 H1127 R1128 W1132 P1142 W1143 D1147 M1152 I1153 D1154 L1155 T1156
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LEU ALA PRO PRO GLY LEU GLN PRO PRO ASP ALA GLU ASP GLU ALA ARG ALA ALA GLU PRO ASP PRO ASP TYR GLU ASN LEU ARG ARG SER ALA GLY GLY TRP GLY GLU ALA GLU GLY GLY LYS GLU GLY THR ALA LYS GLU GLY THR PRO GLY GLY THR PRO GLN PRO GLY VAL GLU ALA GLN
PRO VAL ARG ALA GLU ASN GLU LYS ASP ALA THR THR GLU LYS ASN LYS LYS ARG GLY PHE ASP LEU PHE LYS ALA LYS LYS ALA ALA LYS LEU ARG ARG LEU PRO HIS ASP VAL VAL PRO ALA D1419 N1420 R1421 D1422 D1423 P1424 I1427 L1428 N1429 T1430
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GLU GLU GLU ASP GLU GLU GLU LYS GLU GLU ASP GLU GLU GLU GLU GLU LYS GLU ASP ALA GLU LYS GLU GLU GLU GLU ALA PRO GLU GLY GLU LYS GLU ASP L1922 E1923 E1924 G1925 L1926 L1927 Q1928 M1929 K1930 L1931 V1935 E1944 A1960 F1961 A1962 Y1965 V1966 D1967 K1968 L1969 Q1973
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SER ARG LEU ARG SER LEU LEU GLU THR VAL ARG LEU VAL LYS LYS LYS GLU GLU LYS PRO GLU GLU GLU LEU PRO ALA GLU E2088 K2089 K2090 P2091 Q2092 V2098 M2101 Q2107 V2117 M2120 F2121 S2122 L2123 L2135 P2146 V2149 E2157 Q2161 I2167 M2170
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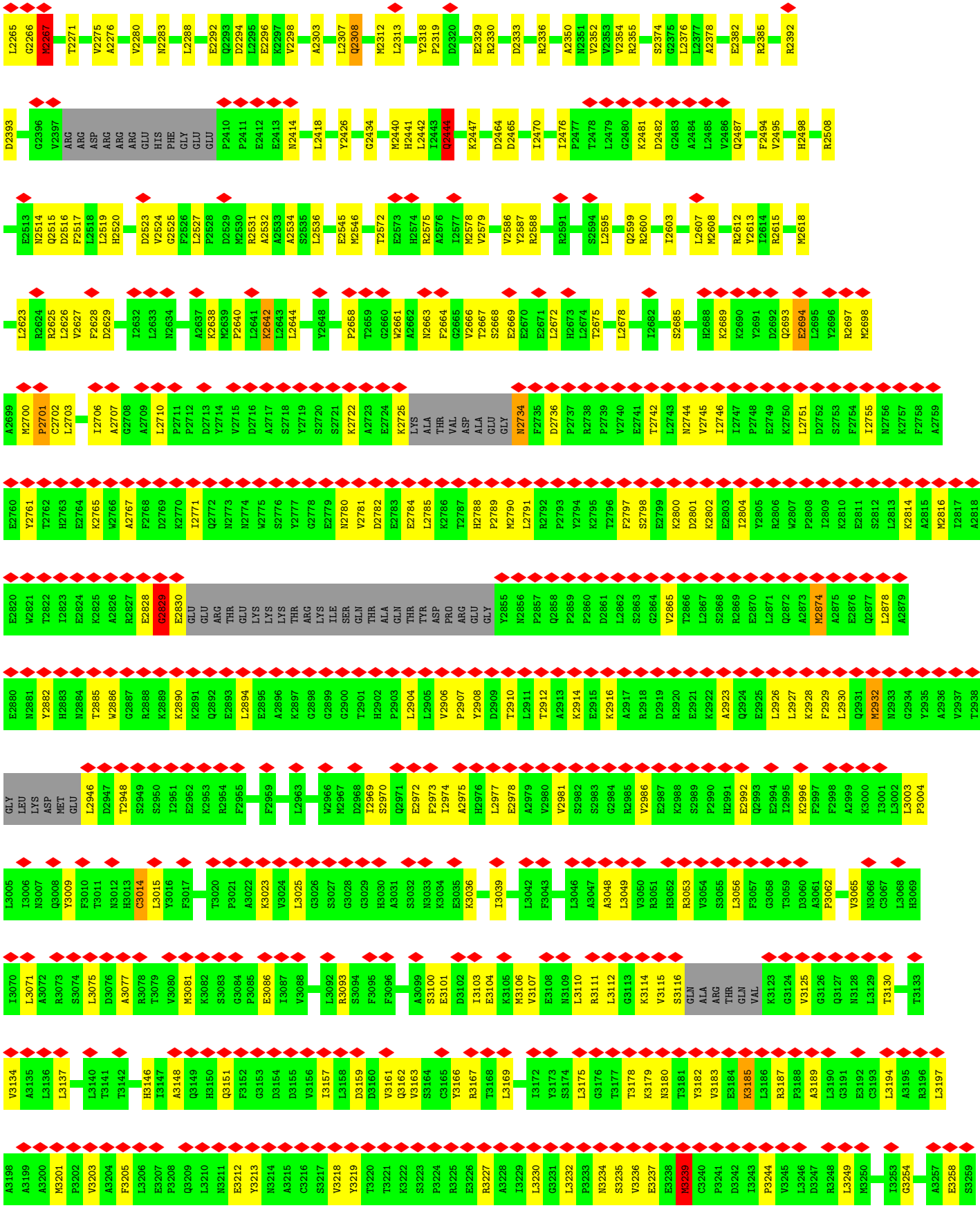
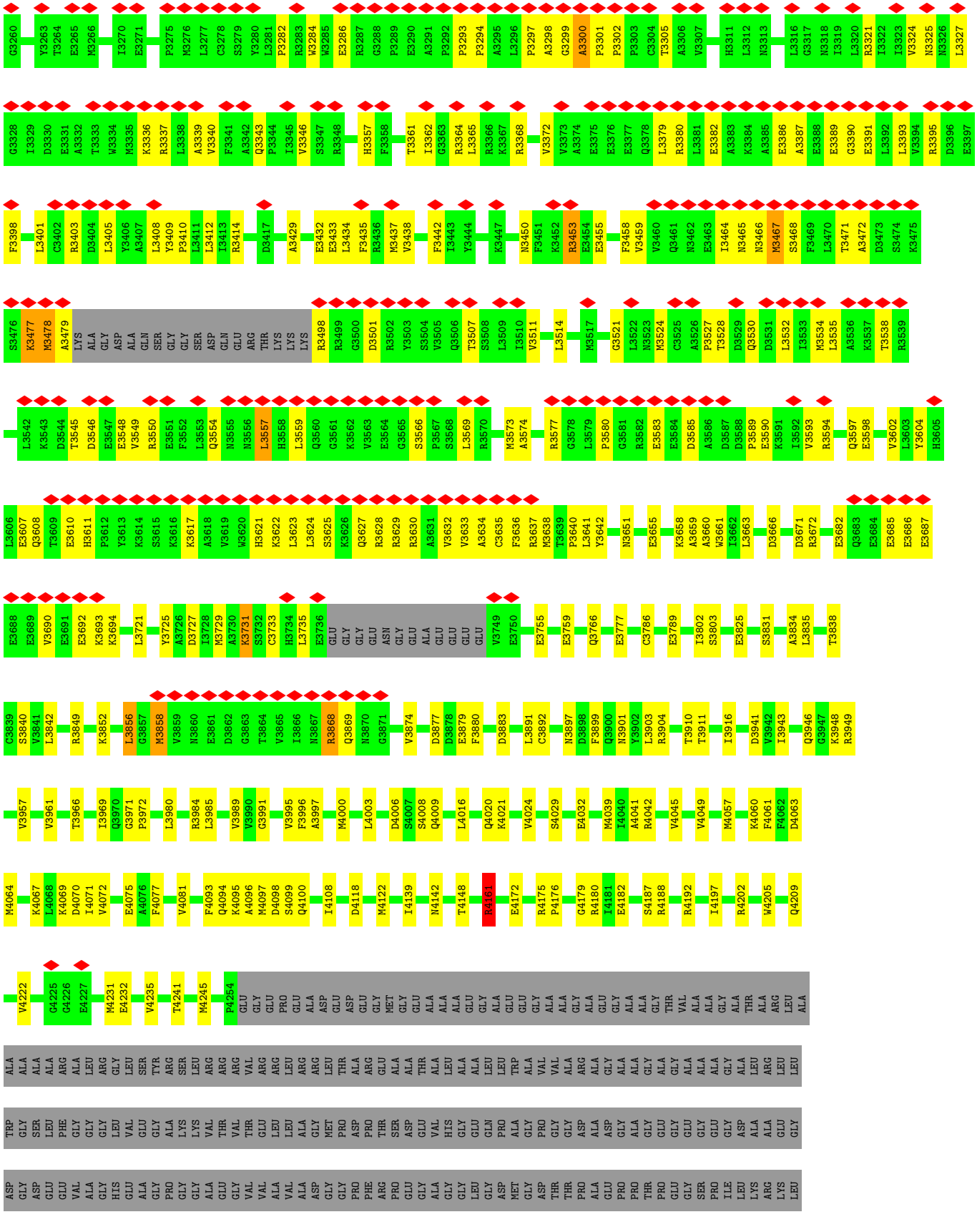
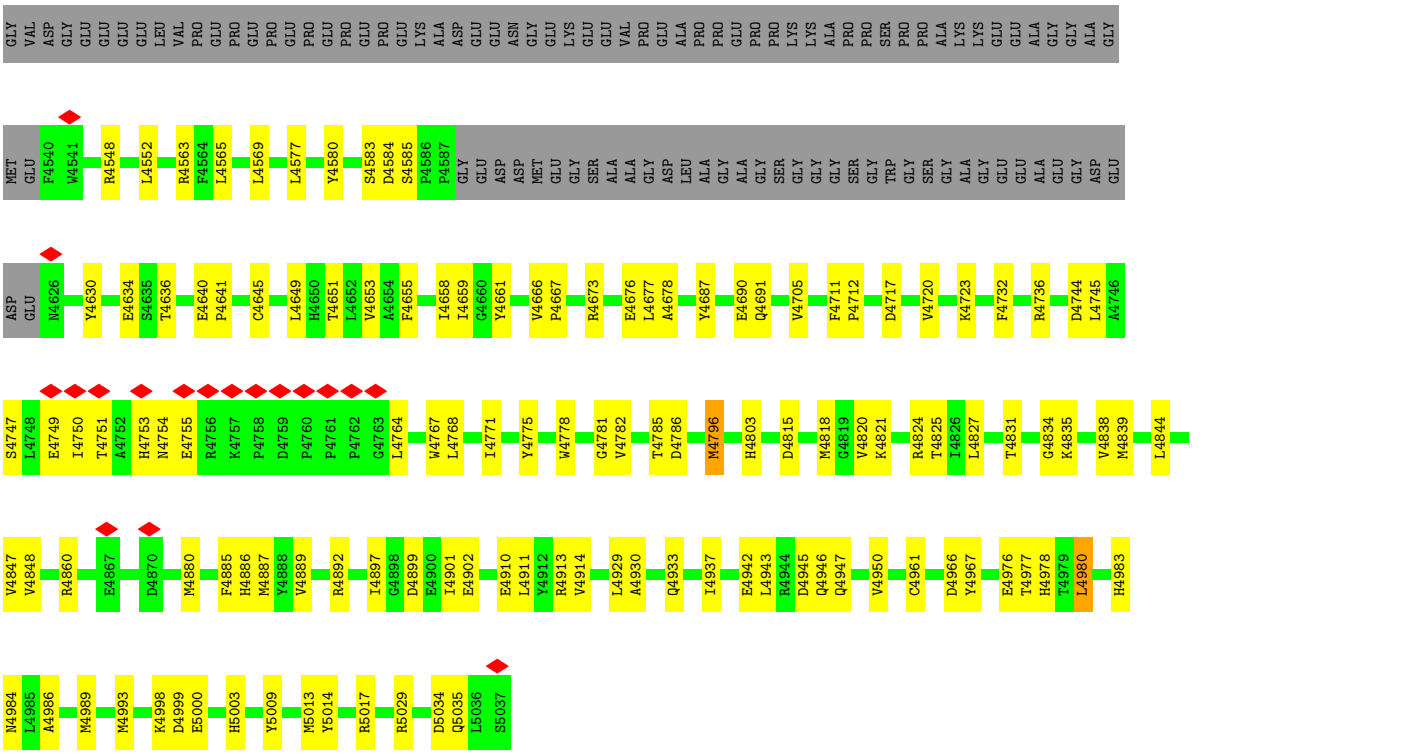
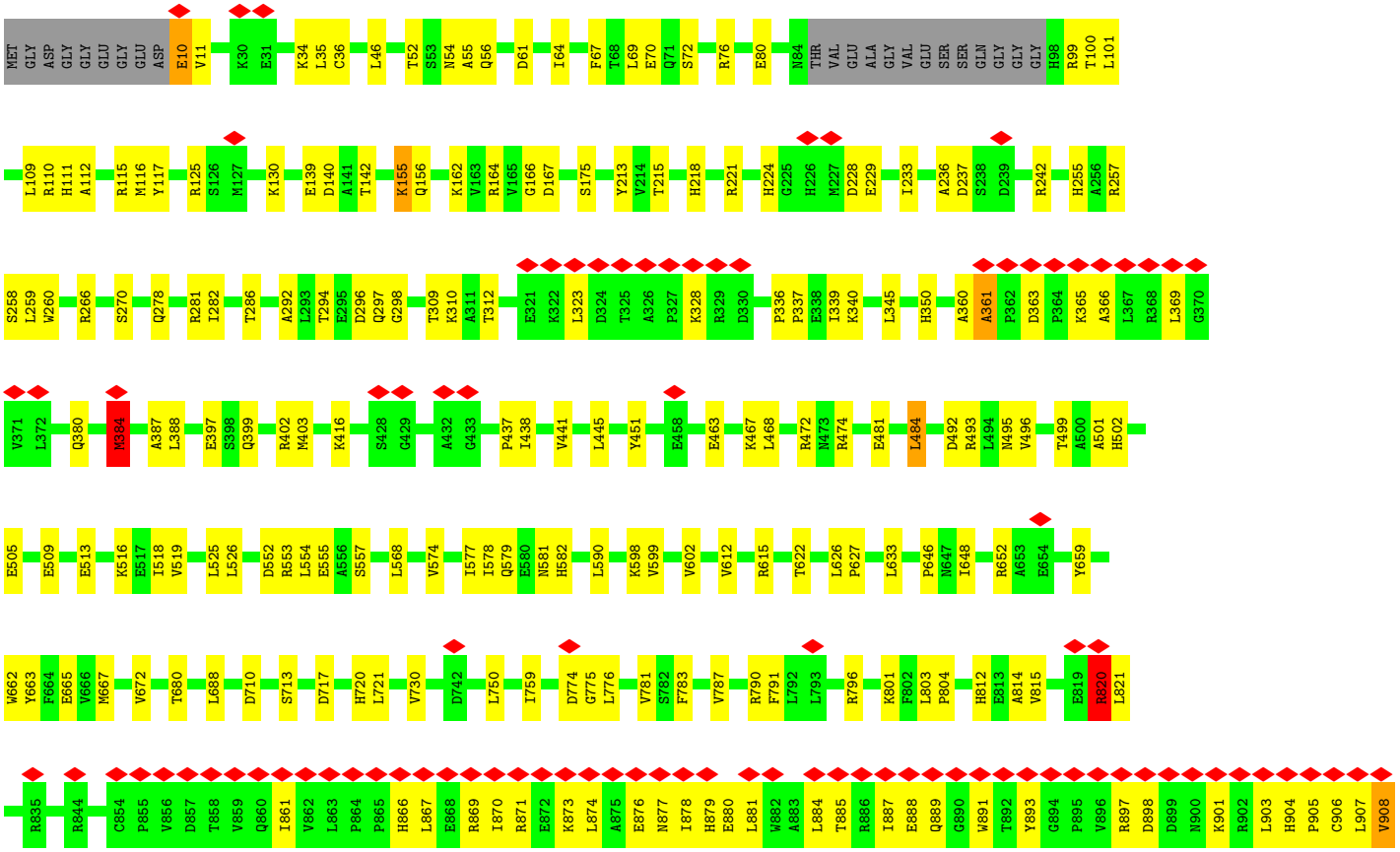


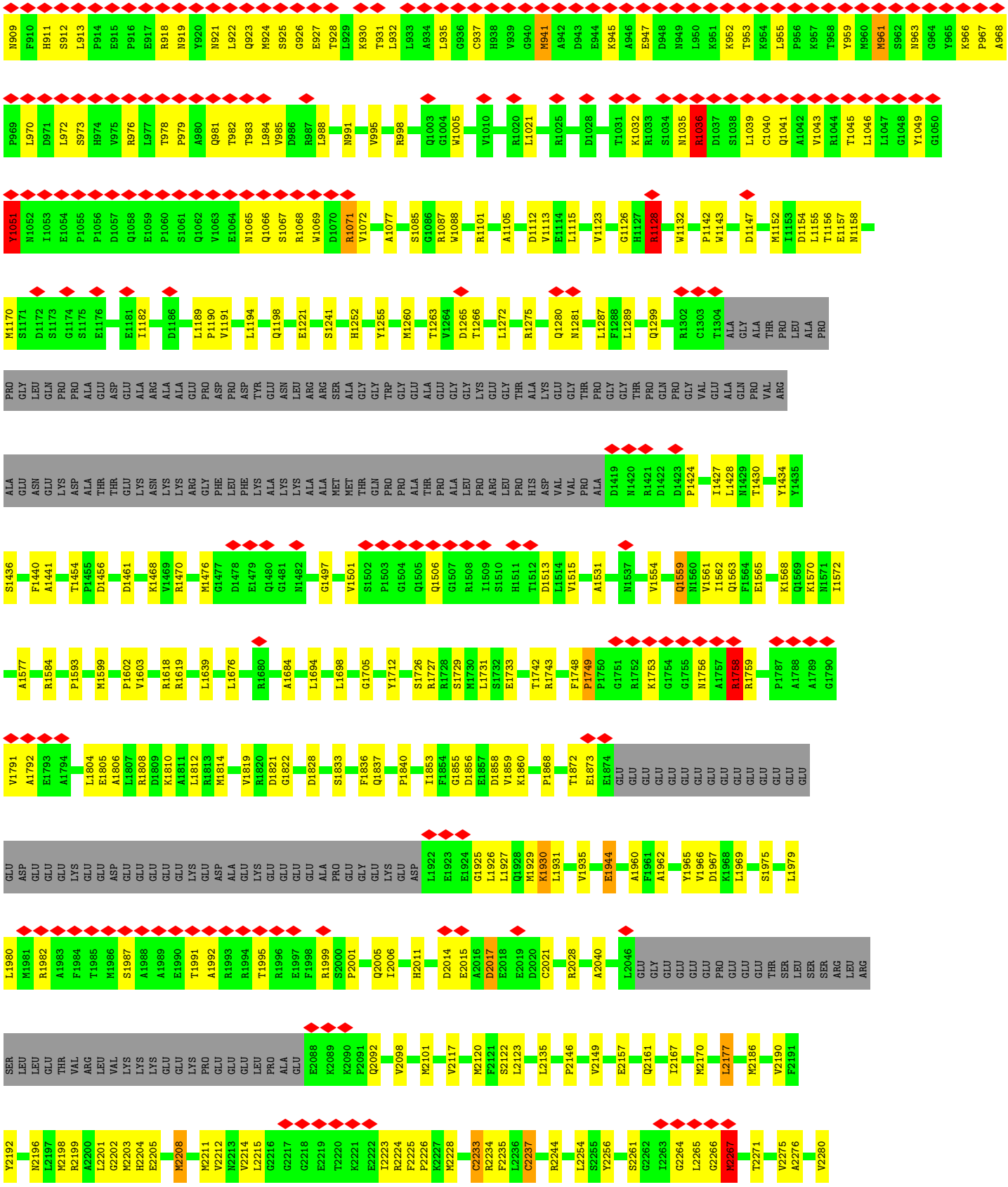




• Molecule 1: Ryanodine receptor 1

Chain C:

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Y1051 N1052 I1053 E1054 P1055 P1056 D1057 Q1058 E1059 P1060 S1061 Q1062 V1063 E1064 N1065 Q1066 S1067 R1068 W1069 D1070 R1071 V1072 A1077 S1085 G1086 R1087 W1088 R1101 A1105 D1112 V1113 E1114 L1115 V1123 G1126 H1127 R1128 W1132 P1142 W1143 D1147 M1152 I1153 D1154 L1155 T1156 E1157 N1158
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PRO GLY LEU GLN PRO PRO ALA GLU ASP GLU ALA ARG ALA ALA GLU PRO ASP PRO ASP TYR GLU ASN LEU ARG ARG SER ALA GLY GLY TRP GLY GLU GLU ALA GLU GLY GLY LYS GLU GLY THR ALA LYS GLU GLY THR PRO GLY GLY GLY THR PRO GLN PRO GLY VAL GLU ALA GLN PRO VAL ARG
ALA GLU ASN GLU LYS ASP ALA THR THR GLU LYS ASN LYS LYS ARG GLY PHE LEU PHE LYS ALA LYS LYS ALA ALA MET MET THR GLN PRO PRO ALA THR PRO ALA LEU PRO ARG LEU PRO HIS ASP VAL VAL PRO ALA D1419 N1420 R1421 D1422 D1423 P1424 I1427 L1428 N1429 T1430 Y1434 Y1435
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GLU ASP GLU GLU GLU LYS GLU GLU ASP GLU GLU GLU GLU GLU LYS GLU ASP ALA GLU LYS GLU GLU GLU GLU ALA PRO GLU GLY GLU LYS GLU ASP L1922 E1923 E1924 G1925 L1926 L1927 Q1928 M1929 K1930 L1931 V1935 E1944 A1960 F1961 A1962 Y1965 V1966 D1967 K1968 L1969 S1975 L1979
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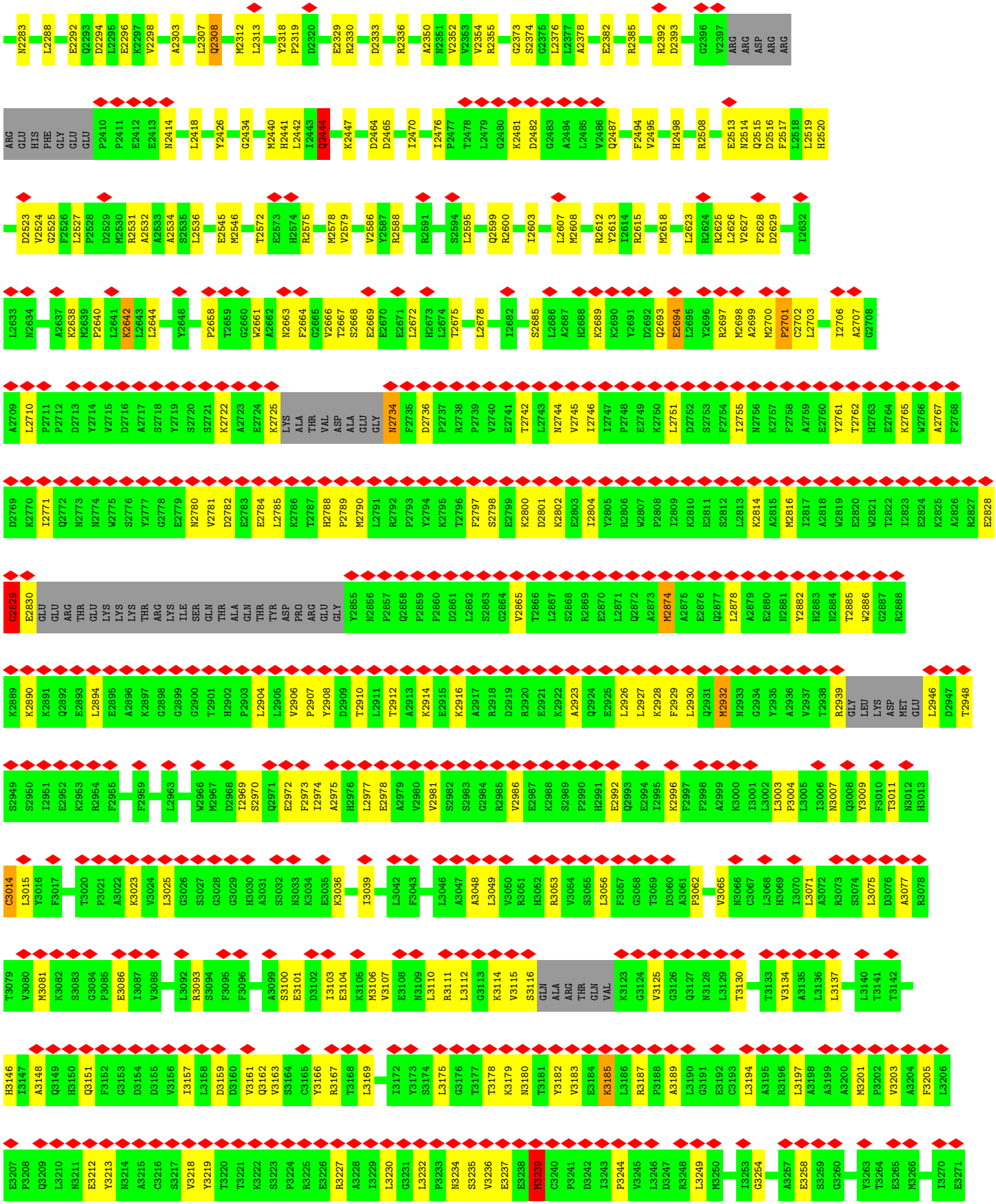
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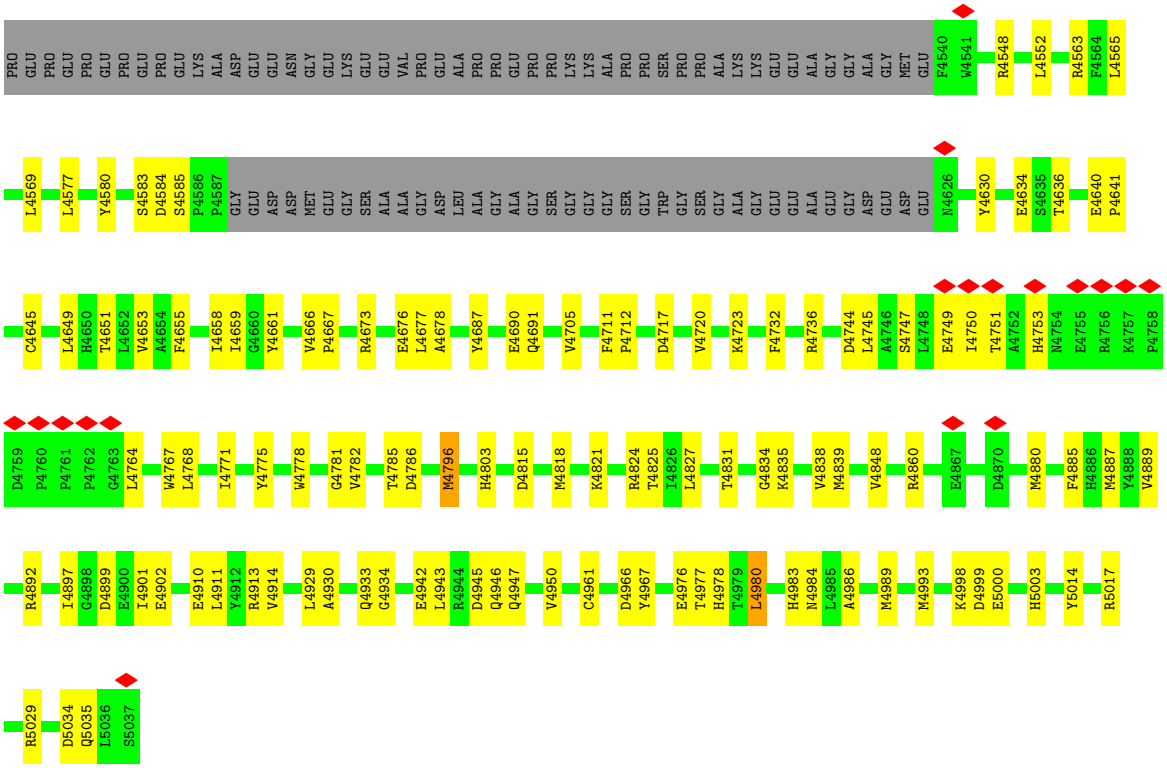
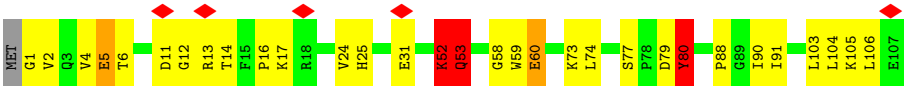
P3275 M3276 L3277 C3278 S3279 Y3280 L3281 P3282 R3283 W3284 W3285 E3286 R3287 G3288 P3289 E3290 A3291 P3292 P3293 P3294 A3295 L3296 P3297 A3298 G3299 A3300 P3301 P3302 P3303 C3304 T3305 A3306 V3307 H3311 L3312 N3313 L3316 G3317 N3318 I3319 L3320 R3321 I3322 I3323 V3324 N3325 N3326 L3327 G3328 I3329 D3330 E3331 A3332 T3333 W3334 M3335 K3336
R3337 L3338 A3339 V3340 F3341 A3342 Q3343 P3344 I3345 V3346 S3347 R3348 H3357 F3358 T3361 I3362 G3363 R3364 L3365 R3366 K3367 R3368 V3372 V3373 A3374 E3375 E3376 E3377 Q3378 L3379 R3380 L3381 E3382 A3383 K3384 A3385 E3386 A3387 E3388 E3389 G3390 E3391 L3392 L3393 V3394 R3395 D3396 E3397 F3398 L3401 C3402 R3403 D3404 L3405 Y3406 A3407
L3408 Y3409 P3410 L3411 L3412 I3413 R3414 D3417 A3429 E3432 E3433 L3434 F3435 R3436 M3437 V3438 F3442 I3443 Y3444 K3447 N3450 F3451 K3452 R3453 E3454 E3455 F3458 V3459 V3460 Q3461 N3462 E3463 I3464 N3465 N3466 M3467 S3468 F3469 L3470 T3471 A3472 D3473 S3474 K3475 S3476 K3477 M3478 A3479 LYS ALA GLY ASP ALA
GLN SER GLY GLY SER ASP GLN GLU ARG THR LYS LYS LYS R3498 R3499 G3500 D3501 R3502 Y3503 S3504 V3505 Q3506 T3507 S3508 L3509 I3510 V3511 L3514 M3517 G3521 L3522 N3523 M3524 C3525 A3526 P3527 T3528 D3529 Q3530 D3531 L3532 I3533 M3534 L3535 A3536 K3537 T3538 R3539 L3542 K3543 D3544 T3545 D3546 E3547 E3548 V3549
R3550 E3551 F3552 L3553 Q3554 N3555 N3556 L3557 H3558 L3559 Q3560 G3561 K3562 V3563 E3564 G3565 S3566 P3567 S3568 L3569 R3570 M3573 A3574 R3577 G3578 L3579 P3580 G3581 R3582 E3583 E3584 D3585 A3586 D3587 D3588 P3589 E3590 K3591 I3592 V3593 R3594 Q3597 E3598 V3602 L3603 Y3604 H3605 L3606 E3607 Q3608 T3609 E3610 H3611 P3612 Y3613 K3614
S3615 K3616 K3617 A3618 V3619 W3620 H3621 K3622 L3623 L3624 S3625 K3626 Q3627 R3628 R3629 R3630 A3631 V3632 V3633 A3634 C3635 F3636 R3637 M3638 T3639 P3640 L3641 Y3642 N3651 E3655 K3658 A3659 A3660 W3661 I3662 L3663 D3671 R3672 E3682 Q3683 E3684 E3685 E3686 E3687 E3688 E3689 V3690 E3691 E3692 K3693 K3694 L3721 Y3725
A3726 D3727 I3728 M3729 A3730 K3731 S3732 C3733 H3734 L3735 E3736 GLU GLY GLY GLU ASN GLY GLU ALA GLU GLU GLU GLU V3749 E3750 E3755 E3759 Q3766 L3770 C3786 E3789 I3802 S3803 E3825 S3831 A3834 L3835 T3838 C3839 S3840 V3841 L3842 R3849 K3852 L3856 G3857
M3858 V3859 N3860 E3861 D3862 G3863 T3864 V3865 I3866 N3867 R3868 Q3869 N3870 G3871 V3874 D3877 D3878 E3879 F3880 D3883 L3891 C3892 N3897 D3898 F3899 Q3900 N3901 Y3902 L3903 R3904 T3910 T3911 I3916 D3941 V3942 I3943 Q3946 G3947 K3948 R3949 V3957 V3961 T3966 I3969 Q3970 G3971 P3972
L3980 L3985 V3989 V3990 G3991 V3995 F3996 A3997 M4000 L4003 D4006 S4007 S4008 Q4009 L4016 Q4020 K4021 V4024 S4029 E4032 M4039 I4040 A4041 R4042 V4045 V4049 M4057 K4060 F4061 F4062 D4063 M4064 K4067 L4068 K4069 D4070 I4071 V4072 E4075 A4076 F4077
V4081 F4093 Q4094 K4095 A4096 M4097 D4098 S4099 Q4100 I4108 D4118 M4122 I4139 N4142 T4148 R4161 E4172 R4175 P4176 G4179 R4180 I4181 E4182 S4187 R4188 R4192 I4197 R4202 W4205 Q4209 V4222 G4225 G4226 E4227 M4231 E4232 V4235
T4241 M4245 P4254 GLU GLY GLU PRO GLU ALA ASP GLU ASP GLU GLY MET GLY GLU ALA ALA ALA GLU GLY ALA GLU GLU GLY ALA ALA GLY ALA GLU GLY ALA ALA GLY THR VAL ALA ALA GLY ALA THR ALA ARG LEU ALA ALA ALA ALA ALA ARG ALA LEU ARG GLY LEU SER TYR
ARG SER LEU ARG ARG ARG VAL ARG ARG LEU ARG ARG LEU THR ALA ARG GLU ALA ALA THR ALA LEU ALA ALA LEU LEU TRP ALA VAL VAL ALA ARG ALA GLY ALA ALA GLY ALA GLY ALA ALA ALA GLY ALA LEU ARG LEU LEU TRP GLY SER LEU PHE GLY GLY GLY LEU VAL GLU GLY
ALA LYS LYS VAL THR VAL THR LEU LEU LEU ALA GLY MET PRO ASP PRO THR SER ASP GLU VAL HIS GLY GLU GLN PRO ALA GLY PRO GLY GLY ASP ALA ASP GLY ALA GLY GLU GLY GLU GLY GLU GLY ASP ALA ALA GLU GLY ASP GLY ASP GLU GLU VAL ALA GLY HIS GLU ALA GLY
PRO GLY GLY ALA GLU GLY VAL VAL ALA VAL ALA ASP GLY PRO PHE ARG PRO GLU GLY ALA GLY GLY LEU GLY ASP MET GLY ASP THR THR PRO ALA GLU PRO PRO THR PRO GLU GLY SER PRO ILE LEU LYS ARG LYS LEU GLY VAL ASP GLY GLU GLU GLU GLU LEU VAL PRO GLU



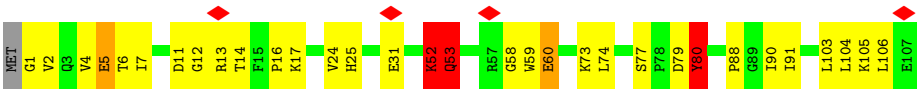
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain E:



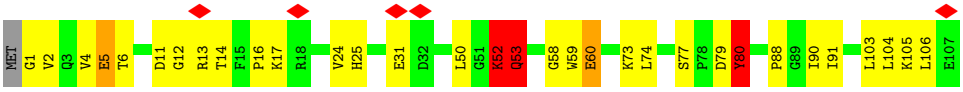
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain H:



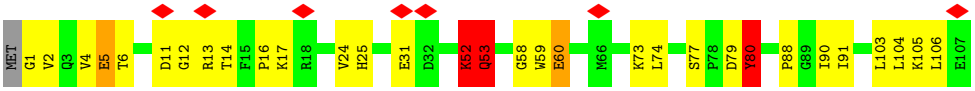
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain G:



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

Chain F:


MET
G1
V2
Q3
V4
E5
T6
D11
G12
R13
T14
F15
P16
K17
R18
V24
H25
E31
D32
K52
Q53
G58
W59
E60
M66
K73
L74
S77
P78
D79
Y80
P88
G89
I90
I91
L103
L104
K105
L106
E107

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	64353	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	58	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.555	Depositor
Minimum map value	-0.247	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	428.544, 428.544, 428.544	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.837, 0.837, 0.837	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.54	50/35977 (0.1%)	0.67	65/48726 (0.1%)
1	B	0.54	50/35977 (0.1%)	0.67	65/48726 (0.1%)
1	C	0.54	49/35977 (0.1%)	0.67	65/48726 (0.1%)
1	D	0.54	50/35977 (0.1%)	0.67	65/48726 (0.1%)
2	E	2.56	15/850 (1.8%)	3.24	24/1146 (2.1%)
2	F	2.56	15/850 (1.8%)	3.25	24/1146 (2.1%)
2	G	2.56	15/850 (1.8%)	3.24	24/1146 (2.1%)
2	H	2.56	15/850 (1.8%)	3.24	24/1146 (2.1%)
All	All	0.66	259/147308 (0.2%)	0.82	356/199488 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	14
1	B	0	14
1	C	0	14
1	D	0	14
2	E	0	5
2	F	0	5
2	G	0	5
2	H	0	5
All	All	0	76

All (259) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	80	TYR	CD1-CE1	47.33	2.10	1.39
2	F	80	TYR	CD1-CE1	47.31	2.10	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	80	TYR	CD1-CE1	47.30	2.10	1.39
2	G	80	TYR	CD1-CE1	47.26	2.10	1.39
2	G	80	TYR	CD2-CE2	36.38	1.94	1.39
2	H	80	TYR	CD2-CE2	36.34	1.93	1.39
2	F	80	TYR	CD2-CE2	36.33	1.93	1.39
2	E	80	TYR	CD2-CE2	36.32	1.93	1.39
1	A	2237	CYS	CB-SG	31.27	2.35	1.82
1	D	2237	CYS	CB-SG	31.27	2.35	1.82
1	B	2237	CYS	CB-SG	31.25	2.35	1.82
1	C	2237	CYS	CB-SG	31.25	2.35	1.82
1	A	2233	CYS	CB-SG	-30.56	1.30	1.82
1	D	2233	CYS	CB-SG	-30.56	1.30	1.82
1	C	2233	CYS	CB-SG	-30.56	1.30	1.82
1	B	2233	CYS	CB-SG	-30.53	1.30	1.82
2	F	52	LYS	CE-NZ	-23.43	0.90	1.49
2	G	52	LYS	CE-NZ	-23.40	0.90	1.49
2	H	52	LYS	CE-NZ	-23.39	0.90	1.49
2	E	52	LYS	CE-NZ	-23.38	0.90	1.49
1	D	1036	ARG	CZ-NH1	-22.60	1.03	1.33
1	A	1036	ARG	CZ-NH1	-22.58	1.03	1.33
1	B	1036	ARG	CZ-NH1	-22.58	1.03	1.33
1	C	1036	ARG	CZ-NH1	-22.58	1.03	1.33
1	B	2444	GLN	CG-CD	-19.03	1.07	1.51
1	D	2444	GLN	CG-CD	-19.03	1.07	1.51
1	A	2444	GLN	CG-CD	-19.01	1.07	1.51
1	C	2444	GLN	CG-CD	-19.01	1.07	1.51
1	A	3239	MET	CB-CG	18.46	2.10	1.51
1	D	3239	MET	CB-CG	18.46	2.10	1.51
1	B	3239	MET	CB-CG	18.45	2.10	1.51
1	C	3239	MET	CB-CG	18.45	2.10	1.51
2	H	80	TYR	CE1-CZ	-16.76	1.16	1.38
2	E	80	TYR	CE1-CZ	-16.74	1.16	1.38
2	G	80	TYR	CE1-CZ	-16.70	1.16	1.38
2	F	80	TYR	CE1-CZ	-16.69	1.16	1.38
1	B	1036	ARG	CB-CG	-16.04	1.09	1.52
1	D	1036	ARG	CB-CG	-16.02	1.09	1.52
1	A	1036	ARG	CB-CG	-16.01	1.09	1.52
1	C	1036	ARG	CB-CG	-16.01	1.09	1.52
1	B	2642	LYS	CG-CD	15.61	2.05	1.52
1	C	2642	LYS	CG-CD	15.60	2.05	1.52
1	A	2642	LYS	CG-CD	15.60	2.05	1.52
1	D	2642	LYS	CG-CD	15.58	2.05	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	80	TYR	CB-CG	-12.74	1.32	1.51
2	E	80	TYR	CB-CG	-12.71	1.32	1.51
2	F	80	TYR	CB-CG	-12.70	1.32	1.51
2	G	80	TYR	CB-CG	-12.70	1.32	1.51
1	A	1036	ARG	CG-CD	-12.48	1.20	1.51
1	B	1036	ARG	CG-CD	-12.48	1.20	1.51
1	C	1036	ARG	CG-CD	-12.48	1.20	1.51
1	D	1036	ARG	CG-CD	-12.47	1.20	1.51
1	C	416	LYS	CD-CE	-12.34	1.20	1.51
1	A	416	LYS	CD-CE	-12.32	1.20	1.51
1	B	416	LYS	CD-CE	-12.32	1.20	1.51
1	D	416	LYS	CD-CE	-12.29	1.20	1.51
1	D	820	ARG	CZ-NH1	12.21	1.49	1.33
1	A	820	ARG	CZ-NH1	12.19	1.48	1.33
1	B	820	ARG	CZ-NH1	12.19	1.48	1.33
1	C	820	ARG	CZ-NH1	12.19	1.48	1.33
1	A	3014	CYS	CB-SG	-11.73	1.62	1.82
1	D	3014	CYS	CB-SG	-11.73	1.62	1.82
1	B	3014	CYS	CB-SG	-11.70	1.62	1.82
1	C	3014	CYS	CB-SG	-11.70	1.62	1.82
1	C	3239	MET	CG-SD	11.04	2.09	1.81
1	A	3239	MET	CG-SD	11.01	2.09	1.81
1	B	3239	MET	CG-SD	10.99	2.09	1.81
1	D	3239	MET	CG-SD	10.99	2.09	1.81
1	D	2308	GLN	CB-CG	-10.38	1.24	1.52
1	C	2308	GLN	CB-CG	-10.37	1.24	1.52
1	A	2308	GLN	CB-CG	-10.37	1.24	1.52
1	B	2308	GLN	CB-CG	-10.34	1.24	1.52
2	E	5	GLU	CD-OE1	-10.05	1.14	1.25
2	H	5	GLU	CD-OE1	-10.05	1.14	1.25
2	G	5	GLU	CD-OE1	-10.02	1.14	1.25
2	F	5	GLU	CD-OE1	-10.00	1.14	1.25
2	G	53	GLN	CG-CD	10.00	1.74	1.51
2	H	53	GLN	CG-CD	9.97	1.74	1.51
2	F	53	GLN	CG-CD	9.97	1.74	1.51
2	E	53	GLN	CG-CD	9.94	1.74	1.51
1	B	3557	LEU	CG-CD1	-9.73	1.15	1.51
1	A	3557	LEU	CG-CD1	-9.71	1.16	1.51
1	C	3557	LEU	CG-CD1	-9.71	1.16	1.51
1	D	3557	LEU	CG-CD1	-9.69	1.16	1.51
1	A	1036	ARG	NE-CZ	-9.63	1.20	1.33
1	C	1036	ARG	NE-CZ	-9.63	1.20	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1036	ARG	NE-CZ	-9.59	1.20	1.33
1	D	1036	ARG	NE-CZ	-9.59	1.20	1.33
1	D	1036	ARG	CD-NE	-9.30	1.30	1.46
1	B	1036	ARG	CD-NE	-9.30	1.30	1.46
1	A	1036	ARG	CD-NE	-9.29	1.30	1.46
1	C	1036	ARG	CD-NE	-9.29	1.30	1.46
1	D	2308	GLN	CD-OE1	-9.26	1.03	1.24
1	A	2308	GLN	CD-OE1	-9.23	1.03	1.24
1	B	2308	GLN	CD-OE1	-9.23	1.03	1.24
1	C	2308	GLN	CD-OE1	-9.23	1.03	1.24
2	F	53	GLN	CB-CG	-9.15	1.27	1.52
2	H	53	GLN	CB-CG	-9.14	1.27	1.52
2	G	53	GLN	CB-CG	-9.14	1.27	1.52
2	E	53	GLN	CB-CG	-9.12	1.27	1.52
1	B	941	MET	CG-SD	-8.89	1.58	1.81
1	A	941	MET	CG-SD	-8.88	1.58	1.81
1	D	941	MET	CG-SD	-8.88	1.58	1.81
1	C	941	MET	CG-SD	-8.88	1.58	1.81
1	A	1559	GLN	CD-NE2	-8.86	1.10	1.32
1	B	1559	GLN	CD-NE2	-8.86	1.10	1.32
1	D	1559	GLN	CD-NE2	-8.86	1.10	1.32
1	C	1559	GLN	CD-NE2	-8.86	1.10	1.32
2	H	80	TYR	CE2-CZ	-8.82	1.27	1.38
2	E	80	TYR	CE2-CZ	-8.82	1.27	1.38
2	G	80	TYR	CE2-CZ	-8.81	1.27	1.38
2	F	80	TYR	CE2-CZ	-8.80	1.27	1.38
2	H	105	LYS	CE-NZ	-8.62	1.27	1.49
1	B	2308	GLN	CD-NE2	-8.60	1.11	1.32
2	G	105	LYS	CE-NZ	-8.59	1.27	1.49
2	E	105	LYS	CE-NZ	-8.59	1.27	1.49
1	A	2308	GLN	CD-NE2	-8.58	1.11	1.32
2	F	105	LYS	CE-NZ	-8.58	1.27	1.49
1	D	2308	GLN	CD-NE2	-8.57	1.11	1.32
1	C	2308	GLN	CD-NE2	-8.57	1.11	1.32
1	C	2444	GLN	CB-CG	-8.06	1.30	1.52
1	A	2444	GLN	CB-CG	-8.05	1.30	1.52
1	B	2444	GLN	CB-CG	-8.04	1.30	1.52
1	D	2444	GLN	CB-CG	-8.04	1.30	1.52
1	C	1051	TYR	CD1-CE1	8.01	1.51	1.39
1	A	1051	TYR	CD1-CE1	7.96	1.51	1.39
1	D	1051	TYR	CD1-CE1	7.96	1.51	1.39
2	H	80	TYR	CZ-OH	-7.93	1.24	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	80	TYR	CZ-OH	-7.93	1.24	1.37
2	G	80	TYR	CZ-OH	-7.91	1.24	1.37
1	B	1051	TYR	CD1-CE1	7.91	1.51	1.39
2	F	80	TYR	CZ-OH	-7.90	1.24	1.37
1	B	2177	LEU	CB-CG	-7.81	1.29	1.52
1	D	2177	LEU	CB-CG	-7.81	1.29	1.52
1	A	2177	LEU	CB-CG	-7.80	1.29	1.52
1	C	2177	LEU	CB-CG	-7.79	1.29	1.52
2	H	80	TYR	CA-CB	-7.67	1.37	1.53
2	G	80	TYR	CA-CB	-7.64	1.37	1.53
2	F	80	TYR	CA-CB	-7.63	1.37	1.53
2	E	80	TYR	CA-CB	-7.63	1.37	1.53
1	B	1559	GLN	CB-CG	-7.55	1.32	1.52
1	D	1559	GLN	CB-CG	-7.55	1.32	1.52
1	C	1559	GLN	CB-CG	-7.55	1.32	1.52
1	A	1559	GLN	CB-CG	-7.55	1.32	1.52
1	C	3478	MET	CB-CG	-7.42	1.27	1.51
1	A	3478	MET	CB-CG	-7.39	1.27	1.51
1	D	3478	MET	CB-CG	-7.39	1.27	1.51
1	B	3478	MET	CB-CG	-7.38	1.27	1.51
1	C	1944	GLU	CD-OE2	7.35	1.33	1.25
1	B	2734	ASN	CB-CG	-7.32	1.34	1.51
1	A	2734	ASN	CB-CG	-7.30	1.34	1.51
1	C	2734	ASN	CB-CG	-7.30	1.34	1.51
1	A	1944	GLU	CD-OE2	7.29	1.33	1.25
1	D	1944	GLU	CD-OE2	7.26	1.33	1.25
1	D	2734	ASN	CB-CG	-7.25	1.34	1.51
1	B	1944	GLU	CD-OE2	7.21	1.33	1.25
1	D	2722	LYS	CE-NZ	-6.99	1.31	1.49
1	A	2722	LYS	CE-NZ	-6.97	1.31	1.49
1	B	2722	LYS	CE-NZ	-6.97	1.31	1.49
1	A	1260	MET	CG-SD	-6.96	1.63	1.81
1	B	1260	MET	CG-SD	-6.96	1.63	1.81
1	D	1260	MET	CG-SD	-6.96	1.63	1.81
1	C	1260	MET	CG-SD	-6.96	1.63	1.81
1	C	2722	LYS	CE-NZ	-6.95	1.31	1.49
1	B	3467	MET	CB-CG	6.72	1.72	1.51
1	D	3467	MET	CB-CG	6.72	1.72	1.51
1	C	3467	MET	CB-CG	6.72	1.72	1.51
1	A	3467	MET	CB-CG	6.72	1.72	1.51
1	A	2874	MET	CB-CG	-6.70	1.29	1.51
1	B	2874	MET	CB-CG	-6.70	1.29	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	2874	MET	CB-CG	-6.69	1.29	1.51
1	C	2874	MET	CB-CG	-6.69	1.29	1.51
1	B	1128	ARG	CB-CG	-6.67	1.34	1.52
1	A	1128	ARG	CB-CG	-6.67	1.34	1.52
1	D	1128	ARG	CB-CG	-6.63	1.34	1.52
1	C	1128	ARG	CB-CG	-6.63	1.34	1.52
1	B	416	LYS	CE-NZ	6.49	1.65	1.49
1	D	416	LYS	CE-NZ	6.49	1.65	1.49
1	B	820	ARG	CA-CB	6.49	1.68	1.53
1	C	416	LYS	CE-NZ	6.48	1.65	1.49
1	A	416	LYS	CE-NZ	6.48	1.65	1.49
1	B	2312	MET	CB-CG	-6.48	1.30	1.51
1	D	820	ARG	CA-CB	6.48	1.68	1.53
1	C	820	ARG	CA-CB	6.48	1.68	1.53
1	A	820	ARG	CA-CB	6.47	1.68	1.53
1	A	2312	MET	CB-CG	-6.46	1.30	1.51
1	D	2312	MET	CB-CG	-6.45	1.30	1.51
1	C	2312	MET	CB-CG	-6.45	1.30	1.51
1	D	820	ARG	CG-CD	-6.35	1.36	1.51
1	A	820	ARG	CG-CD	-6.31	1.36	1.51
1	B	820	ARG	CG-CD	-6.29	1.36	1.51
1	B	820	ARG	CD-NE	6.29	1.57	1.46
1	C	820	ARG	CG-CD	-6.29	1.36	1.51
1	A	820	ARG	CD-NE	6.26	1.57	1.46
1	D	820	ARG	CD-NE	6.26	1.57	1.46
1	C	820	ARG	CD-NE	6.24	1.57	1.46
1	A	1559	GLN	CD-OE1	-6.23	1.10	1.24
1	B	1559	GLN	CD-OE1	-6.23	1.10	1.24
1	D	1559	GLN	CD-OE1	-6.23	1.10	1.24
1	C	1559	GLN	CD-OE1	-6.23	1.10	1.24
1	C	2444	GLN	CD-OE1	-5.93	1.10	1.24
1	A	2444	GLN	CD-OE1	-5.92	1.10	1.24
1	B	2444	GLN	CD-OE1	-5.92	1.10	1.24
1	D	2444	GLN	CD-OE1	-5.91	1.10	1.24
1	D	961	MET	CG-SD	-5.84	1.66	1.81
1	A	961	MET	CG-SD	-5.83	1.66	1.81
1	B	961	MET	CG-SD	-5.83	1.66	1.81
1	C	961	MET	CG-SD	-5.83	1.66	1.81
2	G	73	LYS	CE-NZ	-5.72	1.34	1.49
2	F	73	LYS	CE-NZ	-5.72	1.34	1.49
2	E	73	LYS	CE-NZ	-5.71	1.34	1.49
1	B	4161	ARG	CZ-NH1	-5.70	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	4161	ARG	CZ-NH1	-5.70	1.25	1.33
2	H	73	LYS	CE-NZ	-5.69	1.34	1.49
1	C	4161	ARG	CZ-NH1	-5.68	1.25	1.33
1	D	2267	MET	CA-CB	-5.68	1.41	1.53
1	C	2267	MET	CA-CB	-5.68	1.41	1.53
1	A	2267	MET	CA-CB	-5.67	1.41	1.53
1	B	2267	MET	CA-CB	-5.67	1.41	1.53
1	A	4161	ARG	CZ-NH1	-5.67	1.25	1.33
1	D	820	ARG	CB-CG	5.66	1.67	1.52
1	D	4161	ARG	NE-CZ	-5.66	1.25	1.33
1	A	820	ARG	CB-CG	5.65	1.67	1.52
1	A	4161	ARG	NE-CZ	-5.65	1.25	1.33
1	B	820	ARG	CB-CG	5.65	1.67	1.52
1	C	820	ARG	CB-CG	5.65	1.67	1.52
1	B	4161	ARG	NE-CZ	-5.61	1.25	1.33
1	C	4161	ARG	NE-CZ	-5.61	1.25	1.33
1	A	4796	MET	CG-SD	-5.60	1.66	1.81
1	B	4796	MET	CG-SD	-5.59	1.66	1.81
1	D	4796	MET	CG-SD	-5.59	1.66	1.81
1	C	4796	MET	CG-SD	-5.58	1.66	1.81
2	G	80	TYR	CG-CD2	-5.57	1.31	1.39
2	F	80	TYR	CG-CD2	-5.56	1.31	1.39
2	E	80	TYR	CG-CD2	-5.54	1.31	1.39
1	A	2267	MET	CG-SD	-5.52	1.66	1.81
1	D	2267	MET	CG-SD	-5.52	1.66	1.81
1	B	2267	MET	CG-SD	-5.51	1.66	1.81
1	C	2267	MET	CG-SD	-5.51	1.66	1.81
2	H	80	TYR	CG-CD2	-5.50	1.31	1.39
1	B	1036	ARG	C-N	-5.18	1.22	1.34
1	D	1036	ARG	C-N	-5.18	1.22	1.34
1	C	1036	ARG	C-N	-5.18	1.22	1.34
1	A	1036	ARG	C-N	-5.17	1.22	1.34
2	G	52	LYS	CD-CE	-5.14	1.38	1.51
1	D	1944	GLU	CB-CG	5.14	1.61	1.52
2	E	52	LYS	CD-CE	-5.14	1.38	1.51
1	B	1944	GLU	CB-CG	5.12	1.61	1.52
2	H	52	LYS	CD-CE	-5.11	1.38	1.51
2	F	52	LYS	CD-CE	-5.11	1.38	1.51
1	A	1944	GLU	CB-CG	5.10	1.61	1.52
1	B	2694	GLU	CG-CD	-5.09	1.44	1.51
1	C	1944	GLU	CB-CG	5.08	1.61	1.52
1	A	2694	GLU	CG-CD	-5.06	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	2694	GLU	CG-CD	-5.04	1.44	1.51
1	C	2694	GLU	CG-CD	-5.04	1.44	1.51
1	A	2722	LYS	CD-CE	5.01	1.63	1.51
1	B	2722	LYS	CD-CE	5.01	1.63	1.51
1	D	2722	LYS	CD-CE	5.01	1.63	1.51

All (356) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	80	TYR	CE1-CZ-CE2	-55.59	30.86	119.80
2	F	80	TYR	CE1-CZ-CE2	-55.57	30.88	119.80
2	G	80	TYR	CE1-CZ-CE2	-55.57	30.89	119.80
2	E	80	TYR	CE1-CZ-CE2	-55.56	30.90	119.80
2	F	80	TYR	CB-CG-CD2	45.56	148.33	121.00
2	G	80	TYR	CB-CG-CD2	45.46	148.28	121.00
2	H	80	TYR	CB-CG-CD2	45.45	148.27	121.00
2	E	80	TYR	CB-CG-CD2	45.40	148.24	121.00
2	H	80	TYR	CD1-CG-CD2	-44.58	68.86	117.90
2	E	80	TYR	CD1-CG-CD2	-44.55	68.89	117.90
2	G	80	TYR	CD1-CG-CD2	-44.55	68.89	117.90
2	F	80	TYR	CD1-CG-CD2	-44.54	68.91	117.90
2	F	80	TYR	CG-CD1-CE1	-39.52	89.69	121.30
2	G	80	TYR	CG-CD1-CE1	-39.50	89.70	121.30
2	E	80	TYR	CG-CD1-CE1	-39.49	89.71	121.30
2	H	80	TYR	CG-CD1-CE1	-39.46	89.73	121.30
2	E	80	TYR	CB-CG-CD1	-24.89	106.07	121.00
2	F	80	TYR	CB-CG-CD1	-24.84	106.09	121.00
2	G	80	TYR	CB-CG-CD1	-24.84	106.10	121.00
2	H	80	TYR	CB-CG-CD1	-24.83	106.10	121.00
1	B	2642	LYS	CD-CE-NZ	-23.04	58.72	111.70
1	D	2642	LYS	CD-CE-NZ	-23.03	58.73	111.70
1	A	2642	LYS	CD-CE-NZ	-23.02	58.75	111.70
1	C	2642	LYS	CD-CE-NZ	-23.02	58.76	111.70
1	A	3239	MET	CB-CG-SD	22.53	179.99	112.40
1	B	3239	MET	CB-CG-SD	22.53	179.99	112.40
1	C	3239	MET	CB-CG-SD	22.52	179.97	112.40
1	D	3239	MET	CB-CG-SD	22.52	179.97	112.40
2	G	80	TYR	CZ-CE2-CD2	-21.84	100.14	119.80
2	F	80	TYR	CZ-CE2-CD2	-21.82	100.17	119.80
2	E	80	TYR	CZ-CE2-CD2	-21.81	100.17	119.80
2	H	80	TYR	CZ-CE2-CD2	-21.79	100.19	119.80
1	B	384	MET	CG-SD-CE	-18.39	70.77	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	384	MET	CG-SD-CE	-18.38	70.79	100.20
1	C	384	MET	CG-SD-CE	-18.38	70.79	100.20
1	D	384	MET	CG-SD-CE	-18.37	70.81	100.20
1	D	384	MET	CB-CG-SD	18.25	167.14	112.40
1	A	384	MET	CB-CG-SD	18.23	167.10	112.40
1	C	384	MET	CB-CG-SD	18.22	167.07	112.40
1	B	384	MET	CB-CG-SD	18.22	167.06	112.40
1	C	2312	MET	CG-SD-CE	17.91	128.85	100.20
1	A	2312	MET	CG-SD-CE	17.89	128.83	100.20
1	B	2312	MET	CG-SD-CE	17.89	128.83	100.20
1	D	2312	MET	CG-SD-CE	17.89	128.82	100.20
1	D	3239	MET	CA-CB-CG	-17.62	83.35	113.30
1	A	3239	MET	CA-CB-CG	-17.61	83.37	113.30
1	B	3239	MET	CA-CB-CG	-17.59	83.39	113.30
1	C	3239	MET	CA-CB-CG	-17.59	83.39	113.30
1	B	384	MET	CA-CB-CG	17.09	142.36	113.30
1	D	384	MET	CA-CB-CG	17.08	142.34	113.30
1	A	384	MET	CA-CB-CG	17.07	142.33	113.30
1	C	384	MET	CA-CB-CG	17.05	142.29	113.30
1	C	1036	ARG	CG-CD-NE	16.97	147.43	111.80
1	A	1036	ARG	CG-CD-NE	16.96	147.41	111.80
1	B	1036	ARG	CG-CD-NE	16.95	147.39	111.80
1	D	1036	ARG	CG-CD-NE	16.93	147.35	111.80
2	E	80	TYR	CD1-CE1-CZ	15.81	134.03	119.80
2	G	80	TYR	CD1-CE1-CZ	15.80	134.02	119.80
2	F	80	TYR	CD1-CE1-CZ	15.79	134.01	119.80
2	H	80	TYR	CD1-CE1-CZ	15.76	133.99	119.80
2	F	5	GLU	OE1-CD-OE2	-15.06	105.23	123.30
2	G	5	GLU	OE1-CD-OE2	-15.06	105.23	123.30
2	H	5	GLU	OE1-CD-OE2	-15.05	105.24	123.30
2	E	5	GLU	OE1-CD-OE2	-15.04	105.25	123.30
1	D	1036	ARG	CD-NE-CZ	-14.54	103.24	123.60
1	A	1036	ARG	CD-NE-CZ	-14.53	103.26	123.60
1	B	1036	ARG	CD-NE-CZ	-14.51	103.28	123.60
1	C	1036	ARG	CD-NE-CZ	-14.50	103.30	123.60
2	G	53	GLN	CG-CD-OE1	14.42	150.45	121.60
2	H	53	GLN	CG-CD-OE1	14.42	150.43	121.60
2	F	53	GLN	CG-CD-OE1	14.41	150.43	121.60
2	E	53	GLN	CG-CD-OE1	14.39	150.38	121.60
1	B	1128	ARG	NE-CZ-NH1	14.37	127.48	120.30
1	C	1128	ARG	NE-CZ-NH1	14.34	127.47	120.30
1	A	1128	ARG	NE-CZ-NH1	14.33	127.47	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	1128	ARG	NE-CZ-NH1	14.33	127.47	120.30
2	E	52	LYS	CD-CE-NZ	14.26	144.51	111.70
2	H	52	LYS	CD-CE-NZ	14.25	144.48	111.70
2	G	52	LYS	CD-CE-NZ	14.24	144.46	111.70
2	F	52	LYS	CD-CE-NZ	14.24	144.45	111.70
1	B	820	ARG	CD-NE-CZ	-13.52	104.67	123.60
1	A	820	ARG	CD-NE-CZ	-13.50	104.70	123.60
1	D	820	ARG	CD-NE-CZ	-13.49	104.71	123.60
1	C	820	ARG	CD-NE-CZ	-13.49	104.71	123.60
1	C	1128	ARG	NE-CZ-NH2	-12.52	114.04	120.30
1	A	1128	ARG	NE-CZ-NH2	-12.40	114.10	120.30
2	H	53	GLN	OE1-CD-NE2	-12.40	93.38	121.90
1	B	1128	ARG	NE-CZ-NH2	-12.40	114.10	120.30
2	E	53	GLN	OE1-CD-NE2	-12.39	93.40	121.90
2	G	53	GLN	OE1-CD-NE2	-12.38	93.42	121.90
2	F	53	GLN	OE1-CD-NE2	-12.38	93.42	121.90
1	D	1128	ARG	NE-CZ-NH2	-12.35	114.12	120.30
1	C	1036	ARG	NE-CZ-NH2	-11.96	114.32	120.30
1	B	1036	ARG	NE-CZ-NH2	-11.94	114.33	120.30
1	D	1036	ARG	NE-CZ-NH2	-11.94	114.33	120.30
1	A	1036	ARG	NE-CZ-NH2	-11.91	114.34	120.30
1	B	820	ARG	CG-CD-NE	-11.80	87.02	111.80
1	A	820	ARG	CG-CD-NE	-11.79	87.03	111.80
1	D	820	ARG	CG-CD-NE	-11.79	87.04	111.80
1	C	820	ARG	CG-CD-NE	-11.78	87.06	111.80
1	A	2267	MET	CG-SD-CE	-11.47	81.85	100.20
1	B	2267	MET	CG-SD-CE	-11.47	81.85	100.20
1	D	2267	MET	CG-SD-CE	-11.47	81.85	100.20
1	C	2267	MET	CG-SD-CE	-11.47	81.86	100.20
1	B	820	ARG	NE-CZ-NH1	10.88	125.74	120.30
1	C	820	ARG	NE-CZ-NH1	10.88	125.74	120.30
1	A	820	ARG	NE-CZ-NH1	10.79	125.69	120.30
1	D	820	ARG	NE-CZ-NH1	10.75	125.67	120.30
1	C	820	ARG	CA-CB-CG	-10.74	89.78	113.40
1	B	820	ARG	CA-CB-CG	-10.73	89.79	113.40
1	D	820	ARG	CA-CB-CG	-10.73	89.78	113.40
1	A	820	ARG	CA-CB-CG	-10.73	89.80	113.40
1	C	3557	LEU	CB-CG-CD1	10.58	128.98	111.00
1	B	3557	LEU	CB-CG-CD1	10.56	128.96	111.00
1	D	3557	LEU	CB-CG-CD1	10.56	128.96	111.00
1	A	3557	LEU	CB-CG-CD1	10.56	128.96	111.00
1	B	1559	GLN	CA-CB-CG	10.31	136.08	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	1559	GLN	CA-CB-CG	10.31	136.08	113.40
1	D	1559	GLN	CA-CB-CG	10.31	136.08	113.40
1	A	1559	GLN	CA-CB-CG	10.31	136.07	113.40
1	D	3478	MET	CB-CG-SD	9.77	141.70	112.40
1	C	3478	MET	CB-CG-SD	9.76	141.67	112.40
1	A	3478	MET	CB-CG-SD	9.75	141.66	112.40
1	B	3478	MET	CB-CG-SD	9.74	141.62	112.40
2	H	105	LYS	CD-CE-NZ	9.57	133.72	111.70
2	F	105	LYS	CD-CE-NZ	9.57	133.71	111.70
2	E	105	LYS	CD-CE-NZ	9.55	133.67	111.70
2	G	105	LYS	CD-CE-NZ	9.55	133.66	111.70
2	H	53	GLN	CG-CD-NE2	-9.47	93.98	116.70
2	G	53	GLN	CG-CD-NE2	-9.46	93.99	116.70
2	F	53	GLN	CG-CD-NE2	-9.46	94.00	116.70
2	E	53	GLN	CG-CD-NE2	-9.46	94.00	116.70
1	B	2017	ASP	CB-CG-OD2	9.45	126.81	118.30
1	A	2017	ASP	CB-CG-OD2	9.42	126.78	118.30
1	D	2017	ASP	CB-CG-OD2	9.39	126.75	118.30
1	D	1036	ARG	NE-CZ-NH1	-9.37	115.62	120.30
1	C	2017	ASP	CB-CG-OD2	9.37	126.73	118.30
1	B	1036	ARG	NE-CZ-NH1	-9.31	115.64	120.30
1	A	1036	ARG	NE-CZ-NH1	-9.31	115.64	120.30
1	C	1036	ARG	NE-CZ-NH1	-9.31	115.64	120.30
1	B	4796	MET	CG-SD-CE	-9.28	85.36	100.20
1	D	4796	MET	CG-SD-CE	-9.28	85.36	100.20
1	C	4796	MET	CG-SD-CE	-9.27	85.36	100.20
1	A	4796	MET	CG-SD-CE	-9.27	85.37	100.20
1	D	3014	CYS	CA-CB-SG	9.17	130.51	114.00
1	A	3014	CYS	CA-CB-SG	9.16	130.49	114.00
1	B	3014	CYS	CA-CB-SG	9.16	130.48	114.00
1	C	3014	CYS	CA-CB-SG	9.14	130.45	114.00
1	D	3731	LYS	CD-CE-NZ	8.83	132.01	111.70
1	A	3731	LYS	CD-CE-NZ	8.82	131.99	111.70
1	D	4161	ARG	NE-CZ-NH1	-8.82	115.89	120.30
1	C	3731	LYS	CD-CE-NZ	8.82	131.98	111.70
1	B	3731	LYS	CD-CE-NZ	8.81	131.97	111.70
1	A	4161	ARG	NE-CZ-NH1	-8.77	115.92	120.30
1	B	4161	ARG	NE-CZ-NH1	-8.76	115.92	120.30
1	C	4161	ARG	NE-CZ-NH1	-8.73	115.93	120.30
1	D	3858	MET	CB-CG-SD	8.58	138.15	112.40
1	C	3858	MET	CB-CG-SD	8.58	138.13	112.40
1	A	3858	MET	CB-CG-SD	8.58	138.13	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	3858	MET	CB-CG-SD	8.57	138.12	112.40
1	D	2312	MET	CB-CG-SD	8.33	137.38	112.40
1	B	2312	MET	CB-CG-SD	8.32	137.37	112.40
1	A	2312	MET	CB-CG-SD	8.32	137.35	112.40
1	C	2312	MET	CB-CG-SD	8.31	137.32	112.40
1	C	2308	GLN	CA-CB-CG	8.26	131.56	113.40
1	D	2308	GLN	CA-CB-CG	8.26	131.56	113.40
1	A	2308	GLN	CA-CB-CG	8.25	131.55	113.40
1	B	2308	GLN	CA-CB-CG	8.23	131.51	113.40
1	A	2444	GLN	CA-CB-CG	8.01	131.02	113.40
1	C	2444	GLN	CA-CB-CG	8.01	131.01	113.40
1	B	2444	GLN	CA-CB-CG	8.00	131.01	113.40
1	D	2444	GLN	CA-CB-CG	8.00	131.01	113.40
1	D	3478	MET	CG-SD-CE	7.94	112.91	100.20
1	A	3478	MET	CG-SD-CE	7.92	112.88	100.20
1	B	3478	MET	CG-SD-CE	7.92	112.88	100.20
1	C	3478	MET	CG-SD-CE	7.92	112.88	100.20
2	G	80	TYR	N-CA-CB	-7.86	96.45	110.60
2	F	80	TYR	N-CA-CB	-7.86	96.45	110.60
2	H	80	TYR	N-CA-CB	-7.85	96.47	110.60
2	E	80	TYR	N-CA-CB	-7.85	96.47	110.60
1	D	3239	MET	CB-CA-C	-7.82	94.75	110.40
1	A	3239	MET	CB-CA-C	-7.82	94.77	110.40
1	C	2444	GLN	CG-CD-OE1	-7.82	105.97	121.60
1	B	3239	MET	CB-CA-C	-7.81	94.78	110.40
1	C	3239	MET	CB-CA-C	-7.81	94.78	110.40
2	F	53	GLN	CA-CB-CG	7.81	130.58	113.40
1	B	1260	MET	CG-SD-CE	-7.81	87.71	100.20
1	B	2444	GLN	CG-CD-OE1	-7.81	105.98	121.60
2	H	53	GLN	CA-CB-CG	7.80	130.57	113.40
1	A	1260	MET	CG-SD-CE	-7.80	87.72	100.20
1	D	1260	MET	CG-SD-CE	-7.79	87.73	100.20
1	C	1260	MET	CG-SD-CE	-7.79	87.73	100.20
1	A	2444	GLN	CG-CD-OE1	-7.79	106.01	121.60
2	E	53	GLN	CA-CB-CG	7.79	130.53	113.40
1	D	2444	GLN	CG-CD-OE1	-7.79	106.03	121.60
2	G	80	TYR	CG-CD2-CE2	-7.78	115.07	121.30
1	D	2208	MET	CG-SD-CE	-7.78	87.75	100.20
1	B	2208	MET	CG-SD-CE	-7.78	87.76	100.20
2	G	53	GLN	CA-CB-CG	7.77	130.50	113.40
1	A	2208	MET	CG-SD-CE	-7.77	87.77	100.20
1	C	2208	MET	CG-SD-CE	-7.75	87.80	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	80	TYR	CG-CD2-CE2	-7.75	115.10	121.30
2	H	80	TYR	CG-CD2-CE2	-7.75	115.10	121.30
1	A	2177	LEU	CB-CG-CD2	-7.68	97.94	111.00
1	C	2177	LEU	CB-CG-CD2	-7.68	97.95	111.00
2	F	80	TYR	CG-CD2-CE2	-7.67	115.16	121.30
1	B	2177	LEU	CB-CG-CD2	-7.67	97.96	111.00
1	D	2177	LEU	CB-CG-CD2	-7.66	97.98	111.00
1	C	3239	MET	CA-C-O	7.60	136.06	120.10
1	A	3239	MET	CA-C-O	7.60	136.05	120.10
1	B	3239	MET	CA-C-O	7.59	136.04	120.10
1	D	3239	MET	CA-C-O	7.58	136.03	120.10
1	D	3467	MET	CB-CG-SD	7.55	135.04	112.40
1	B	3467	MET	CB-CG-SD	7.54	135.04	112.40
1	A	3467	MET	CB-CG-SD	7.54	135.03	112.40
1	C	1944	GLU	OE1-CD-OE2	-7.54	114.25	123.30
1	A	1944	GLU	OE1-CD-OE2	-7.53	114.26	123.30
1	C	3467	MET	CB-CG-SD	7.53	134.99	112.40
1	B	1944	GLU	OE1-CD-OE2	-7.52	114.27	123.30
1	D	1944	GLU	OE1-CD-OE2	-7.51	114.28	123.30
1	D	3478	MET	CA-CB-CG	-7.42	100.69	113.30
1	A	3478	MET	CA-CB-CG	-7.41	100.70	113.30
1	B	3478	MET	CA-CB-CG	-7.39	100.73	113.30
1	C	3478	MET	CA-CB-CG	-7.38	100.75	113.30
1	A	4880	MET	CA-CB-CG	-7.37	100.77	113.30
1	B	4880	MET	CA-CB-CG	-7.36	100.78	113.30
1	C	4880	MET	CA-CB-CG	-7.36	100.78	113.30
1	D	4880	MET	CA-CB-CG	-7.35	100.80	113.30
1	C	2444	GLN	CB-CG-CD	7.35	130.70	111.60
1	B	2444	GLN	CB-CG-CD	7.34	130.69	111.60
1	D	2444	GLN	CB-CG-CD	7.34	130.69	111.60
1	A	2444	GLN	CB-CG-CD	7.33	130.67	111.60
1	D	1071	ARG	CG-CD-NE	7.11	126.72	111.80
1	C	1071	ARG	CG-CD-NE	7.10	126.71	111.80
1	A	1071	ARG	CG-CD-NE	7.10	126.71	111.80
1	B	1071	ARG	CG-CD-NE	7.09	126.69	111.80
1	D	4880	MET	CB-CG-SD	7.06	133.58	112.40
2	H	80	TYR	O-C-N	7.05	133.98	122.70
1	A	4880	MET	CB-CG-SD	7.05	133.54	112.40
1	B	4880	MET	CB-CG-SD	7.05	133.54	112.40
1	C	4880	MET	CB-CG-SD	7.04	133.53	112.40
2	G	80	TYR	O-C-N	7.02	133.93	122.70
2	E	80	TYR	O-C-N	7.02	133.93	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	80	TYR	O-C-N	7.02	133.93	122.70
1	C	4880	MET	CG-SD-CE	7.01	111.42	100.20
1	A	4880	MET	CG-SD-CE	7.00	111.40	100.20
1	B	4880	MET	CG-SD-CE	6.98	111.36	100.20
1	D	4880	MET	CG-SD-CE	6.97	111.36	100.20
1	D	3856	LEU	CB-CG-CD1	6.97	122.85	111.00
1	A	3856	LEU	CB-CG-CD1	6.97	122.84	111.00
1	C	3856	LEU	CB-CG-CD1	6.96	122.84	111.00
1	B	3856	LEU	CB-CG-CD1	6.94	122.80	111.00
1	B	2829	GLY	C-N-CA	6.89	138.92	121.70
1	A	2829	GLY	C-N-CA	6.88	138.91	121.70
1	D	2829	GLY	C-N-CA	6.87	138.88	121.70
1	C	2829	GLY	C-N-CA	6.87	138.88	121.70
2	H	60	GLU	OE1-CD-OE2	-6.83	115.11	123.30
2	F	60	GLU	OE1-CD-OE2	-6.81	115.12	123.30
2	E	60	GLU	OE1-CD-OE2	-6.81	115.13	123.30
2	G	60	GLU	OE1-CD-OE2	-6.79	115.15	123.30
2	G	80	TYR	CB-CA-C	6.77	123.94	110.40
2	E	80	TYR	CB-CA-C	6.77	123.93	110.40
2	H	80	TYR	CB-CA-C	6.76	123.93	110.40
2	F	80	TYR	CB-CA-C	6.75	123.91	110.40
1	D	2734	ASN	CB-CG-OD1	-6.73	108.14	121.60
1	A	2734	ASN	CB-CG-OD1	-6.71	108.17	121.60
1	B	2734	ASN	CB-CG-OD1	-6.71	108.18	121.60
1	C	2734	ASN	CB-CG-OD1	-6.71	108.19	121.60
1	D	1036	ARG	CB-CG-CD	6.59	128.74	111.60
1	A	1036	ARG	CB-CG-CD	6.58	128.72	111.60
1	B	1036	ARG	CB-CG-CD	6.57	128.69	111.60
1	C	1036	ARG	CB-CG-CD	6.57	128.67	111.60
1	B	1128	ARG	NH1-CZ-NH2	-6.23	112.55	119.40
1	A	1128	ARG	NH1-CZ-NH2	-6.22	112.56	119.40
1	D	1128	ARG	NH1-CZ-NH2	-6.21	112.56	119.40
1	C	1128	ARG	NH1-CZ-NH2	-6.19	112.60	119.40
2	F	80	TYR	OH-CZ-CE2	-6.07	103.71	120.10
2	G	80	TYR	OH-CZ-CE2	-6.05	103.77	120.10
2	E	80	TYR	OH-CZ-CE2	-6.04	103.78	120.10
2	H	80	TYR	OH-CZ-CE2	-6.03	103.81	120.10
1	C	2722	LYS	CD-CE-NZ	6.00	125.51	111.70
1	D	2722	LYS	CD-CE-NZ	6.00	125.49	111.70
1	A	2722	LYS	CD-CE-NZ	5.99	125.48	111.70
1	B	2722	LYS	CD-CE-NZ	5.98	125.45	111.70
1	D	484	LEU	CB-CG-CD2	5.91	121.05	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	484	LEU	CB-CG-CD2	5.91	121.04	111.00
1	B	484	LEU	CB-CG-CD2	5.91	121.04	111.00
1	C	484	LEU	CB-CG-CD2	5.88	121.00	111.00
1	D	4980	LEU	CB-CG-CD2	5.78	120.83	111.00
1	A	1559	GLN	CG-CD-OE1	5.77	133.14	121.60
1	B	1559	GLN	CG-CD-OE1	5.77	133.14	121.60
1	C	1559	GLN	CG-CD-OE1	5.77	133.14	121.60
1	D	1559	GLN	CG-CD-OE1	5.76	133.12	121.60
1	A	4980	LEU	CB-CG-CD2	5.76	120.79	111.00
1	C	4980	LEU	CB-CG-CD2	5.74	120.76	111.00
1	B	4980	LEU	CB-CG-CD2	5.74	120.75	111.00
1	D	3239	MET	CA-C-N	-5.62	104.83	117.20
1	A	3239	MET	CA-C-N	-5.61	104.85	117.20
1	B	3239	MET	CA-C-N	-5.60	104.88	117.20
1	C	3239	MET	CA-C-N	-5.60	104.88	117.20
1	B	2722	LYS	CG-CD-CE	-5.49	95.42	111.90
1	A	2722	LYS	CG-CD-CE	-5.48	95.46	111.90
1	C	2722	LYS	CG-CD-CE	-5.48	95.47	111.90
1	D	2722	LYS	CG-CD-CE	-5.47	95.48	111.90
1	A	10	GLU	N-CA-C	5.46	125.74	111.00
1	B	10	GLU	N-CA-C	5.46	125.74	111.00
1	A	2237	CYS	CB-CA-C	5.45	121.31	110.40
1	C	10	GLU	N-CA-C	5.45	125.72	111.00
1	B	2237	CYS	CB-CA-C	5.45	121.31	110.40
1	C	2237	CYS	CB-CA-C	5.45	121.30	110.40
1	D	10	GLU	N-CA-C	5.45	125.71	111.00
1	D	2237	CYS	CB-CA-C	5.45	121.29	110.40
2	H	52	LYS	CG-CD-CE	-5.41	95.68	111.90
2	G	52	LYS	CG-CD-CE	-5.40	95.70	111.90
2	F	52	LYS	CG-CD-CE	-5.39	95.72	111.90
2	E	52	LYS	CG-CD-CE	-5.39	95.74	111.90
1	B	2208	MET	CB-CG-SD	5.36	128.47	112.40
1	D	2208	MET	CB-CG-SD	5.35	128.46	112.40
1	A	1758	ARG	NE-CZ-NH2	-5.35	117.63	120.30
1	C	2208	MET	CB-CG-SD	5.35	128.44	112.40
1	A	2208	MET	CB-CG-SD	5.34	128.43	112.40
1	C	1758	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	D	1758	ARG	NE-CZ-NH2	-5.29	117.65	120.30
1	B	2932	MET	CG-SD-CE	5.29	108.66	100.20
1	D	2932	MET	CG-SD-CE	5.29	108.66	100.20
1	A	2932	MET	CG-SD-CE	5.29	108.66	100.20
1	B	1260	MET	CB-CG-SD	5.28	128.25	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	2932	MET	CG-SD-CE	5.28	108.64	100.20
1	D	1260	MET	CB-CG-SD	5.27	128.22	112.40
1	C	1260	MET	CB-CG-SD	5.27	128.22	112.40
1	A	1260	MET	CB-CG-SD	5.27	128.22	112.40
1	B	1758	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	B	2017	ASP	OD1-CG-OD2	-5.25	113.33	123.30
1	B	820	ARG	NH1-CZ-NH2	-5.24	113.64	119.40
2	E	5	GLU	CG-CD-OE1	5.22	128.73	118.30
1	A	2017	ASP	OD1-CG-OD2	-5.21	113.40	123.30
2	F	5	GLU	CG-CD-OE1	5.21	128.72	118.30
2	H	5	GLU	CG-CD-OE1	5.21	128.72	118.30
1	D	2017	ASP	OD1-CG-OD2	-5.20	113.42	123.30
1	A	820	ARG	NH1-CZ-NH2	-5.20	113.68	119.40
1	C	820	ARG	NH1-CZ-NH2	-5.20	113.68	119.40
1	D	820	ARG	NH1-CZ-NH2	-5.19	113.69	119.40
1	C	2017	ASP	OD1-CG-OD2	-5.18	113.45	123.30
2	G	5	GLU	CG-CD-OE1	5.18	128.66	118.30
2	H	80	TYR	CA-C-O	-5.16	109.26	120.10
2	E	80	TYR	CA-C-O	-5.16	109.27	120.10
2	G	80	TYR	CA-C-O	-5.16	109.27	120.10
2	F	80	TYR	CA-C-O	-5.15	109.28	120.10
1	B	3868	ARG	CG-CD-NE	-5.11	101.08	111.80
1	C	3868	ARG	CG-CD-NE	-5.10	101.08	111.80
1	A	3868	ARG	CG-CD-NE	-5.10	101.09	111.80
1	D	3868	ARG	CG-CD-NE	-5.09	101.11	111.80
2	E	13	ARG	NE-CZ-NH2	-5.05	117.77	120.30
2	G	13	ARG	NE-CZ-NH2	-5.04	117.78	120.30
2	H	13	ARG	NE-CZ-NH2	-5.02	117.79	120.30
2	F	13	ARG	NE-CZ-NH2	-5.01	117.80	120.30

There are no chirality outliers.

All (76) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1035	ASN	Peptide
1	A	1036	ARG	Mainchain,Sidechain
1	A	1051	TYR	Sidechain
1	A	1128	ARG	Sidechain
1	A	1749	PRO	Mainchain
1	A	1758	ARG	Sidechain
1	A	1944	GLU	Sidechain
1	A	1982	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	2444	GLN	Sidechain
1	A	2701	PRO	Peptide
1	A	3453	ARG	Sidechain
1	A	4161	ARG	Sidechain
1	A	820	ARG	Sidechain
1	B	1035	ASN	Peptide
1	B	1036	ARG	Mainchain,Sidechain
1	B	1051	TYR	Sidechain
1	B	1128	ARG	Sidechain
1	B	1749	PRO	Mainchain
1	B	1758	ARG	Sidechain
1	B	1944	GLU	Sidechain
1	B	1982	ARG	Sidechain
1	B	2444	GLN	Sidechain
1	B	2701	PRO	Peptide
1	B	3453	ARG	Sidechain
1	B	4161	ARG	Sidechain
1	B	820	ARG	Sidechain
1	C	1035	ASN	Peptide
1	C	1036	ARG	Mainchain,Sidechain
1	C	1051	TYR	Sidechain
1	C	1128	ARG	Sidechain
1	C	1749	PRO	Mainchain
1	C	1758	ARG	Sidechain
1	C	1944	GLU	Sidechain
1	C	1982	ARG	Sidechain
1	C	2444	GLN	Sidechain
1	C	2701	PRO	Peptide
1	C	3453	ARG	Sidechain
1	C	4161	ARG	Sidechain
1	C	820	ARG	Sidechain
1	D	1035	ASN	Peptide
1	D	1036	ARG	Mainchain,Sidechain
1	D	1051	TYR	Sidechain
1	D	1128	ARG	Sidechain
1	D	1749	PRO	Mainchain
1	D	1758	ARG	Sidechain
1	D	1944	GLU	Sidechain
1	D	1982	ARG	Sidechain
1	D	2444	GLN	Sidechain
1	D	2701	PRO	Peptide
1	D	3453	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	D	4161	ARG	Sidechain
1	D	820	ARG	Sidechain
2	E	5	GLU	Sidechain
2	E	52	LYS	Mainchain
2	E	53	GLN	Sidechain
2	E	60	GLU	Sidechain
2	E	80	TYR	Sidechain
2	F	5	GLU	Sidechain
2	F	52	LYS	Mainchain
2	F	53	GLN	Sidechain
2	F	60	GLU	Sidechain
2	F	80	TYR	Sidechain
2	G	5	GLU	Sidechain
2	G	52	LYS	Mainchain
2	G	53	GLN	Sidechain
2	G	60	GLU	Sidechain
2	G	80	TYR	Sidechain
2	H	5	GLU	Sidechain
2	H	52	LYS	Mainchain
2	H	53	GLN	Sidechain
2	H	60	GLU	Sidechain
2	H	80	TYR	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	35150	0	34792	993	0
1	B	35150	0	34792	985	0
1	C	35150	0	34792	973	0
1	D	35150	0	34792	984	0
2	E	831	0	831	23	0
2	F	831	0	831	23	0
2	G	831	0	831	23	0
2	H	831	0	831	23	0
3	A	31	0	12	0	0
3	B	31	0	12	0	0
3	C	31	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	31	0	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	20	0	18	3	0
6	B	20	0	18	3	0
6	C	20	0	18	3	0
6	D	20	0	18	3	0
7	A	2	0	0	0	0
7	B	2	0	0	0	0
7	C	2	0	0	0	0
7	D	2	0	0	0	0
All	All	144144	0	142612	3958	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 14.

All (3958) 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:D:3239:MET:CG	1:D:3239:MET:SD	2.09	1.41
1:A:3239:MET:CG	1:A:3239:MET:SD	2.09	1.41
1:B:3239:MET:SD	1:B:3239:MET:CG	2.09	1.39
1:C:3239:MET:SD	1:C:3239:MET:CG	2.09	1.39
1:A:2642:LYS:CD	1:A:2642:LYS:CG	2.05	1.34
1:B:2642:LYS:CG	1:B:2642:LYS:CD	2.05	1.34
1:D:2642:LYS:CG	1:D:2642:LYS:CD	2.05	1.33
1:A:1749:PRO:O	1:A:1758:ARG:NH2	1.62	1.32
1:C:2642:LYS:CG	1:C:2642:LYS:CD	2.05	1.32
1:C:1749:PRO:O	1:C:1758:ARG:NH2	1.62	1.31
1:D:3239:MET:CG	1:D:3239:MET:CB	2.10	1.30
1:A:3239:MET:CG	1:A:3239:MET:CB	2.10	1.30
1:B:1749:PRO:O	1:B:1758:ARG:NH2	1.62	1.30
1:D:1749:PRO:O	1:D:1758:ARG:NH2	1.62	1.28
1:B:3239:MET:CG	1:B:3239:MET:CB	2.10	1.28
1:C:3239:MET:CG	1:C:3239:MET:CB	2.10	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:961:MET:CE	1:C:963:ASN:HB3	1.66	1.26
1:A:961:MET:CE	1:A:963:ASN:HB3	1.66	1.25
1:D:961:MET:CE	1:D:963:ASN:HB3	1.66	1.24
1:B:961:MET:CE	1:B:963:ASN:HB3	1.66	1.23
1:B:972:LEU:HG	1:B:1041:GLN:NE2	1.59	1.18
1:C:972:LEU:HG	1:C:1041:GLN:NE2	1.59	1.18
1:A:941:MET:CE	1:A:1051:TYR:CD1	2.27	1.17
1:C:941:MET:CE	1:C:1051:TYR:CD1	2.27	1.17
1:B:941:MET:CE	1:B:1051:TYR:CD1	2.27	1.17
1:C:961:MET:HE3	1:C:963:ASN:HB3	1.24	1.17
1:D:941:MET:CE	1:D:1051:TYR:CD1	2.27	1.16
1:D:972:LEU:HG	1:D:1041:GLN:NE2	1.59	1.16
1:A:972:LEU:HG	1:A:1041:GLN:NE2	1.59	1.16
1:B:2237:CYS:SG	1:B:2237:CYS:CB	2.35	1.15
1:A:2237:CYS:CB	1:A:2237:CYS:SG	2.35	1.15
1:C:941:MET:HE1	1:C:1051:TYR:CD1	1.81	1.14
1:C:2237:CYS:SG	1:C:2237:CYS:CB	2.35	1.14
1:D:2237:CYS:SG	1:D:2275:VAL:HG22	1.88	1.13
1:D:2237:CYS:SG	1:D:2237:CYS:CB	2.35	1.13
1:C:2237:CYS:SG	1:C:2275:VAL:HG22	1.88	1.13
1:A:2237:CYS:SG	1:A:2275:VAL:HG22	1.88	1.12
1:B:2237:CYS:SG	1:B:2275:VAL:HG22	1.88	1.12
1:B:3450:ASN:OD1	1:B:3453:ARG:NH2	1.82	1.12
1:D:3450:ASN:OD1	1:D:3453:ARG:NH2	1.82	1.12
1:A:3450:ASN:OD1	1:A:3453:ARG:NH2	1.82	1.12
1:C:3450:ASN:OD1	1:C:3453:ARG:NH2	1.82	1.12
1:B:961:MET:HE3	1:B:963:ASN:HB3	1.29	1.11
1:B:941:MET:HE1	1:B:1051:TYR:CD1	1.86	1.09
1:D:961:MET:HE3	1:D:963:ASN:HB3	1.30	1.07
1:A:941:MET:HE1	1:A:1051:TYR:CD1	1.89	1.07
1:B:2233:CYS:CB	1:B:2237:CYS:SG	2.43	1.07
1:A:2233:CYS:CB	1:A:2237:CYS:SG	2.43	1.06
1:C:2233:CYS:CB	1:C:2237:CYS:SG	2.43	1.06
1:D:2233:CYS:CB	1:D:2237:CYS:SG	2.43	1.05
1:D:2642:LYS:CG	1:D:2642:LYS:NZ	2.21	1.04
1:A:961:MET:HE3	1:A:963:ASN:HB3	1.36	1.03
1:A:2642:LYS:CG	1:A:2642:LYS:NZ	2.21	1.03
1:D:941:MET:HE1	1:D:1051:TYR:CD1	1.90	1.02
1:A:2874:MET:HE2	1:A:2939:ARG:HB2	1.38	1.02
1:D:941:MET:SD	1:D:1051:TYR:CE1	2.52	1.02
1:C:972:LEU:HG	1:C:1041:GLN:HE22	0.87	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:941:MET:SD	1:A:1051:TYR:CE1	2.52	1.02
1:B:941:MET:SD	1:B:1051:TYR:CE1	2.52	1.02
1:C:941:MET:SD	1:C:1051:TYR:CE1	2.52	1.02
1:C:2642:LYS:CG	1:C:2642:LYS:NZ	2.21	1.02
1:D:2929:PHE:HA	1:D:2932:MET:HE1	1.36	1.02
1:A:2929:PHE:HA	1:A:2932:MET:HE1	1.39	1.01
1:B:2642:LYS:CG	1:B:2642:LYS:NZ	2.21	1.01
1:D:972:LEU:HG	1:D:1041:GLN:HE22	0.87	1.01
1:B:2874:MET:HE2	1:B:2939:ARG:HB2	1.42	1.00
1:A:972:LEU:HG	1:A:1041:GLN:HE22	0.87	1.00
1:B:972:LEU:HG	1:B:1041:GLN:HE22	0.87	1.00
1:C:2929:PHE:HA	1:C:2932:MET:HE1	1.44	0.99
1:B:3219:TYR:HE2	1:B:3239:MET:SD	1.86	0.99
1:C:3219:TYR:HE2	1:C:3239:MET:SD	1.86	0.99
1:D:972:LEU:CG	1:D:1041:GLN:HE22	1.77	0.98
1:A:972:LEU:CG	1:A:1041:GLN:HE22	1.77	0.98
1:A:3219:TYR:HE2	1:A:3239:MET:SD	1.86	0.98
1:B:1808:ARG:NH2	1:B:1858:ASP:OD2	1.97	0.97
1:D:3219:TYR:HE2	1:D:3239:MET:SD	1.86	0.97
1:B:2929:PHE:HA	1:B:2932:MET:HE1	1.42	0.97
1:C:972:LEU:CG	1:C:1041:GLN:HE22	1.77	0.97
1:C:2929:PHE:HA	1:C:2932:MET:CE	1.95	0.97
1:D:1808:ARG:NH2	1:D:1858:ASP:OD2	1.97	0.96
1:B:2929:PHE:HA	1:B:2932:MET:CE	1.95	0.96
1:D:2929:PHE:HA	1:D:2932:MET:CE	1.95	0.96
1:A:1808:ARG:NH2	1:A:1858:ASP:OD2	1.97	0.96
1:A:2929:PHE:HA	1:A:2932:MET:CE	1.95	0.96
1:B:2233:CYS:HB3	1:B:2237:CYS:SG	2.05	0.96
1:C:1749:PRO:C	1:C:1758:ARG:HH22	1.69	0.96
1:D:2233:CYS:HB3	1:D:2237:CYS:SG	2.04	0.96
1:C:1808:ARG:NH2	1:C:1858:ASP:OD2	1.97	0.96
1:C:2233:CYS:HB3	1:C:2237:CYS:SG	2.04	0.96
1:A:2771:ILE:HG22	1:B:1506:GLN:OE1	1.66	0.96
1:D:1749:PRO:C	1:D:1758:ARG:HH22	1.69	0.96
1:B:1749:PRO:C	1:B:1758:ARG:HH22	1.69	0.95
1:A:2233:CYS:HB3	1:A:2237:CYS:SG	2.04	0.95
1:B:972:LEU:CG	1:B:1041:GLN:HE22	1.77	0.95
1:B:3521:GLY:HA2	1:B:3524:MET:CE	1.97	0.95
1:D:3521:GLY:HA2	1:D:3524:MET:CE	1.96	0.94
1:A:3521:GLY:HA2	1:A:3524:MET:CE	1.96	0.94
1:C:3521:GLY:HA2	1:C:3524:MET:CE	1.96	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3521:GLY:HA2	1:C:3524:MET:HE3	1.49	0.94
1:D:3521:GLY:HA2	1:D:3524:MET:HE3	1.49	0.94
1:A:1749:PRO:C	1:A:1758:ARG:HH22	1.69	0.93
1:D:2874:MET:CE	1:D:2939:ARG:HB2	1.99	0.93
1:B:2874:MET:CE	1:B:2939:ARG:HB2	1.99	0.93
1:C:2874:MET:CE	1:C:2939:ARG:HB2	1.99	0.93
1:D:2874:MET:HE2	1:D:2939:ARG:HB2	1.48	0.93
1:B:2523:ASP:HB3	1:B:2578:MET:HE1	1.51	0.92
1:B:3521:GLY:HA2	1:B:3524:MET:HE3	1.49	0.92
1:C:2874:MET:HE2	1:C:2939:ARG:HB2	1.49	0.92
1:A:221:ARG:NH2	1:A:397:GLU:OE2	2.03	0.92
1:A:2874:MET:CE	1:A:2939:ARG:HB2	1.99	0.92
2:E:52:LYS:O	2:E:53:GLN:HB2	1.68	0.92
1:B:2771:ILE:HG22	1:C:1506:GLN:OE1	1.69	0.92
1:D:1506:GLN:OE1	1:C:2771:ILE:HG22	1.70	0.92
1:D:221:ARG:NH2	1:D:397:GLU:OE2	2.03	0.91
1:B:2572:THR:HG21	1:B:2579:VAL:CG2	2.00	0.91
1:C:2572:THR:HG21	1:C:2579:VAL:CG2	2.00	0.91
1:A:221:ARG:NH1	1:A:258:SER:OG	2.04	0.91
2:F:52:LYS:O	2:F:53:GLN:HB2	1.68	0.91
1:B:221:ARG:NH1	1:B:258:SER:OG	2.04	0.91
1:C:221:ARG:NH1	1:C:258:SER:OG	2.04	0.91
1:A:495:ASN:OD1	1:A:553:ARG:NH1	2.03	0.91
1:B:221:ARG:NH2	1:B:397:GLU:OE2	2.03	0.91
1:B:495:ASN:OD1	1:B:553:ARG:NH1	2.03	0.91
1:D:2011:HIS:HE1	1:D:2017:ASP:OD2	1.54	0.91
1:C:495:ASN:OD1	1:C:553:ARG:NH1	2.03	0.91
1:D:221:ARG:NH1	1:D:258:SER:OG	2.04	0.90
1:A:2011:HIS:HE1	1:A:2017:ASP:OD2	1.54	0.90
2:G:52:LYS:O	2:G:53:GLN:HB2	1.68	0.90
1:D:2628:PHE:CZ	1:D:2734:ASN:OD1	2.25	0.90
1:C:221:ARG:NH2	1:C:397:GLU:OE2	2.03	0.90
1:A:2572:THR:HG21	1:A:2579:VAL:CG2	2.00	0.90
1:D:2572:THR:HG21	1:D:2579:VAL:CG2	2.00	0.90
1:A:2628:PHE:CZ	1:A:2734:ASN:OD1	2.25	0.90
1:B:2628:PHE:CZ	1:B:2734:ASN:OD1	2.24	0.90
2:H:52:LYS:O	2:H:53:GLN:HB2	1.68	0.90
1:B:2011:HIS:HE1	1:B:2017:ASP:OD2	1.54	0.90
1:A:2226:PRO:HB3	1:A:2267:MET:HE1	1.54	0.89
1:D:495:ASN:OD1	1:D:553:ARG:NH1	2.03	0.89
1:C:2628:PHE:CZ	1:C:2734:ASN:OD1	2.25	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2011:HIS:HE1	1:C:2017:ASP:OD2	1.54	0.89
1:D:4039:MET:SD	1:D:4042:ARG:NH2	2.46	0.89
1:B:3239:MET:CG	1:B:3239:MET:CA	2.51	0.89
1:B:1454:THR:OG1	1:B:1456:ASP:OD1	1.91	0.88
1:B:2292:GLU:OE1	1:B:2352:VAL:HG11	1.74	0.88
1:C:1454:THR:OG1	1:C:1456:ASP:OD1	1.91	0.88
1:C:3239:MET:CG	1:C:3239:MET:CA	2.51	0.88
1:A:952:LYS:NZ	1:A:968:ALA:O	2.06	0.88
1:A:2292:GLU:OE1	1:A:2352:VAL:HG11	1.73	0.88
1:D:3239:MET:CG	1:D:3239:MET:CA	2.51	0.88
1:A:961:MET:SD	1:A:963:ASN:HB3	2.14	0.88
1:A:2599:GLN:O	1:A:2603:ILE:HD12	1.74	0.88
1:A:4039:MET:SD	1:A:4042:ARG:NH2	2.46	0.88
1:B:952:LYS:NZ	1:B:968:ALA:O	2.06	0.88
1:B:4039:MET:SD	1:B:4042:ARG:NH2	2.46	0.88
1:A:3239:MET:CG	1:A:3239:MET:CA	2.51	0.87
1:D:4006:ASP:OD2	1:D:4008:SER:OG	1.91	0.87
1:D:952:LYS:NZ	1:D:968:ALA:O	2.06	0.87
1:C:952:LYS:NZ	1:C:968:ALA:O	2.06	0.87
1:C:2292:GLU:OE1	1:C:2352:VAL:HG11	1.74	0.87
1:C:961:MET:SD	1:C:963:ASN:HB3	2.14	0.87
1:D:961:MET:SD	1:D:963:ASN:HB3	2.14	0.87
1:C:4006:ASP:OD2	1:C:4008:SER:OG	1.91	0.87
1:C:4039:MET:SD	1:C:4042:ARG:NH2	2.46	0.87
1:A:1506:GLN:OE1	1:D:2771:ILE:HG22	1.73	0.87
1:D:3466:ASN:ND2	1:D:3507:THR:O	2.08	0.87
1:A:1454:THR:OG1	1:A:1456:ASP:OD1	1.91	0.87
1:A:2196:ASN:OD1	1:A:2199:ARG:NH2	2.08	0.87
1:B:961:MET:SD	1:B:963:ASN:HB3	2.14	0.87
1:D:2292:GLU:OE1	1:D:2352:VAL:HG11	1.74	0.87
1:B:2196:ASN:OD1	1:B:2199:ARG:NH2	2.08	0.86
1:C:2271:THR:OG1	1:C:2330:ARG:NH2	2.08	0.86
1:C:2599:GLN:O	1:C:2603:ILE:HD12	1.74	0.86
1:B:2599:GLN:O	1:B:2603:ILE:HD12	1.74	0.86
1:D:1454:THR:OG1	1:D:1456:ASP:OD1	1.91	0.86
1:C:3466:ASN:ND2	1:C:3507:THR:O	2.08	0.86
1:D:3573:MET:HB3	1:D:3577:ARG:NH1	1.91	0.86
1:C:2196:ASN:OD1	1:C:2199:ARG:NH2	2.08	0.86
1:D:2226:PRO:HB3	1:D:2267:MET:HE1	1.57	0.86
1:A:3573:MET:HB3	1:A:3577:ARG:NH1	1.91	0.86
1:A:4006:ASP:OD2	1:A:4008:SER:OG	1.91	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2271:THR:OG1	1:B:2330:ARG:NH2	2.08	0.86
1:B:4006:ASP:OD2	1:B:4008:SER:OG	1.91	0.86
1:D:2599:GLN:O	1:D:2603:ILE:HD12	1.74	0.86
1:B:3466:ASN:ND2	1:B:3507:THR:O	2.08	0.86
1:C:3573:MET:HB3	1:C:3577:ARG:NH1	1.91	0.86
1:B:3573:MET:HB3	1:B:3577:ARG:NH1	1.91	0.86
1:B:3943:ILE:O	1:B:3948:LYS:NZ	2.09	0.86
1:A:972:LEU:CG	1:A:1041:GLN:NE2	2.38	0.85
1:A:3466:ASN:ND2	1:A:3507:THR:O	2.08	0.85
1:B:941:MET:CE	1:B:1051:TYR:CE1	2.59	0.85
1:D:3943:ILE:O	1:D:3948:LYS:NZ	2.09	0.85
1:A:3521:GLY:HA2	1:A:3524:MET:HE2	1.58	0.85
1:C:3943:ILE:O	1:C:3948:LYS:NZ	2.09	0.85
1:A:941:MET:CE	1:A:1051:TYR:CE1	2.60	0.85
1:D:2196:ASN:OD1	1:D:2199:ARG:NH2	2.08	0.85
1:D:2271:THR:OG1	1:D:2330:ARG:NH2	2.08	0.85
1:A:2271:THR:OG1	1:A:2330:ARG:NH2	2.08	0.85
1:A:3943:ILE:O	1:A:3948:LYS:NZ	2.09	0.85
1:C:3573:MET:HB3	1:C:3577:ARG:HH12	1.42	0.85
1:B:70:GLU:OE2	1:B:110:ARG:NE	2.09	0.85
1:A:70:GLU:OE2	1:A:110:ARG:NE	2.09	0.84
1:D:70:GLU:OE2	1:D:110:ARG:NE	2.09	0.84
1:C:3219:TYR:CE2	1:C:3239:MET:SD	2.70	0.84
1:C:70:GLU:OE2	1:C:110:ARG:NE	2.09	0.84
1:D:3219:TYR:CE2	1:D:3239:MET:SD	2.70	0.84
1:D:3239:MET:CA	1:D:3239:MET:HG2	2.08	0.84
1:D:3573:MET:HB3	1:D:3577:ARG:HH12	1.42	0.84
1:A:3219:TYR:CE2	1:A:3239:MET:SD	2.70	0.84
1:A:2929:PHE:HA	1:A:2932:MET:SD	2.18	0.84
1:B:2929:PHE:HA	1:B:2932:MET:SD	2.18	0.84
1:D:941:MET:CE	1:D:1051:TYR:CE1	2.60	0.84
1:B:3219:TYR:CE2	1:B:3239:MET:SD	2.70	0.83
1:C:941:MET:CE	1:C:1051:TYR:CE1	2.60	0.83
1:A:3573:MET:HB3	1:A:3577:ARG:HH12	1.42	0.83
1:C:2929:PHE:HA	1:C:2932:MET:SD	2.18	0.83
1:B:1999:ARG:HH12	1:B:3636:PHE:HA	1.44	0.83
1:B:3573:MET:HB3	1:B:3577:ARG:HH12	1.42	0.83
1:D:1999:ARG:HH12	1:D:3636:PHE:HA	1.44	0.83
1:D:2929:PHE:HA	1:D:2932:MET:SD	2.18	0.83
1:C:1156:THR:OG1	1:C:1157:GLU:OE1	1.97	0.82
1:A:1999:ARG:HH12	1:A:3636:PHE:HA	1.44	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4749:GLU:O	1:A:4753:HIS:ND1	2.13	0.82
1:C:3282:PRO:O	1:C:3286:GLU:OE1	1.97	0.82
1:B:871:ARG:HD2	1:B:926:GLY:CA	2.09	0.82
1:C:1999:ARG:HH12	1:C:3636:PHE:HA	1.44	0.82
1:A:871:ARG:HD2	1:A:926:GLY:CA	2.09	0.82
1:C:871:ARG:HD2	1:C:926:GLY:CA	2.09	0.82
1:D:871:ARG:HD2	1:D:926:GLY:CA	2.09	0.82
1:D:2237:CYS:SG	1:D:2275:VAL:CG2	2.68	0.82
1:C:4749:GLU:O	1:C:4753:HIS:ND1	2.12	0.82
1:D:1252:HIS:O	1:D:1275:ARG:NH1	2.13	0.81
1:A:3282:PRO:O	1:A:3286:GLU:OE1	1.97	0.81
1:B:3175:LEU:HD21	1:B:3183:VAL:HG13	1.63	0.81
1:D:871:ARG:HD2	1:D:926:GLY:HA2	1.62	0.81
1:D:3282:PRO:O	1:D:3286:GLU:OE1	1.97	0.81
1:D:4749:GLU:O	1:D:4753:HIS:ND1	2.13	0.81
1:C:2237:CYS:SG	1:C:2275:VAL:CG2	2.68	0.81
1:B:4961:CYS:SG	1:B:4983:HIS:ND1	2.54	0.81
1:D:2523:ASP:HB3	1:D:2578:MET:HE1	1.63	0.81
1:C:972:LEU:CG	1:C:1041:GLN:NE2	2.38	0.81
1:C:2523:ASP:HB3	1:C:2578:MET:HE1	1.61	0.81
1:B:2237:CYS:SG	1:B:2275:VAL:CG2	2.68	0.81
1:B:4749:GLU:O	1:B:4753:HIS:ND1	2.13	0.81
1:C:1252:HIS:O	1:C:1275:ARG:NH1	2.13	0.81
1:A:2237:CYS:SG	1:A:2275:VAL:CG2	2.68	0.81
1:C:4961:CYS:SG	1:C:4983:HIS:ND1	2.54	0.81
1:A:4961:CYS:SG	1:A:4983:HIS:ND1	2.54	0.81
1:B:1156:THR:OG1	1:B:1157:GLU:OE1	1.97	0.81
1:B:1252:HIS:O	1:B:1275:ARG:NH1	2.13	0.81
1:D:3175:LEU:HD21	1:D:3183:VAL:HG13	1.62	0.81
1:A:1156:THR:OG1	1:A:1157:GLU:OE1	1.97	0.81
1:D:1156:THR:OG1	1:D:1157:GLU:OE1	1.97	0.81
1:A:2523:ASP:HB3	1:A:2578:MET:CE	2.11	0.81
1:D:2523:ASP:HB3	1:D:2578:MET:CE	2.11	0.81
1:A:1252:HIS:O	1:A:1275:ARG:NH1	2.13	0.80
1:B:3465:ASN:OD1	1:B:3467:MET:HG2	1.81	0.80
1:C:885:THR:O	1:C:889:GLN:NE2	2.14	0.80
1:B:871:ARG:HD2	1:B:926:GLY:HA2	1.62	0.80
1:B:2523:ASP:HB3	1:B:2578:MET:CE	2.11	0.80
1:D:885:THR:O	1:D:889:GLN:NE2	2.14	0.80
1:B:3282:PRO:O	1:B:3286:GLU:OE1	1.97	0.80
1:C:3175:LEU:HD21	1:C:3183:VAL:HG13	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:871:ARG:HD2	1:A:926:GLY:HA2	1.62	0.80
1:A:885:THR:O	1:A:889:GLN:NE2	2.14	0.80
1:B:885:THR:O	1:B:889:GLN:NE2	2.14	0.80
1:A:3175:LEU:HD21	1:A:3183:VAL:HG13	1.62	0.80
1:D:4961:CYS:SG	1:D:4983:HIS:ND1	2.53	0.80
1:B:972:LEU:CG	1:B:1041:GLN:NE2	2.38	0.80
1:B:2226:PRO:HB3	1:B:2267:MET:HE1	1.64	0.80
1:B:3946:GLN:OE1	1:B:3949:ARG:NH1	2.15	0.80
1:A:3521:GLY:HA2	1:A:3524:MET:HE3	1.64	0.80
1:A:4075:GLU:OE1	1:B:4736:ARG:NH1	2.14	0.80
1:A:4744:ASP:OD2	1:A:4747:SER:OG	1.99	0.79
1:D:3465:ASN:OD1	1:D:3467:MET:HG2	1.82	0.79
1:C:2523:ASP:HB3	1:C:2578:MET:CE	2.11	0.79
1:C:3465:ASN:OD1	1:C:3467:MET:HG2	1.81	0.79
1:A:3465:ASN:OD1	1:A:3467:MET:HG2	1.82	0.79
1:C:4744:ASP:OD2	1:C:4747:SER:OG	1.99	0.79
1:A:3946:GLN:OE1	1:A:3949:ARG:NH1	2.15	0.79
1:B:981:GLN:O	1:B:985:VAL:HG23	1.83	0.79
1:B:1263:THR:OG1	1:B:1265:ASP:OD1	2.01	0.79
1:B:4744:ASP:OD2	1:B:4747:SER:OG	1.99	0.79
1:A:3458:PHE:HE2	1:A:3464:ILE:CD1	1.96	0.79
1:D:941:MET:HE3	1:D:1051:TYR:CD1	2.17	0.79
1:A:384:MET:SD	1:B:166:GLY:C	2.61	0.79
1:D:3946:GLN:OE1	1:D:3949:ARG:NH1	2.15	0.79
1:C:871:ARG:HD2	1:C:926:GLY:HA2	1.62	0.79
1:C:3946:GLN:OE1	1:C:3949:ARG:NH1	2.15	0.79
1:C:3458:PHE:HE2	1:C:3464:ILE:CD1	1.96	0.79
1:B:4885:PHE:O	1:B:4889:VAL:HG22	1.84	0.78
1:C:4885:PHE:O	1:C:4889:VAL:HG22	1.83	0.78
1:A:3236:VAL:HA	1:A:3239:MET:SD	2.24	0.78
1:A:4736:ARG:NH1	1:D:4075:GLU:OE1	2.16	0.78
1:B:3236:VAL:HA	1:B:3239:MET:SD	2.24	0.78
1:D:3236:VAL:HA	1:D:3239:MET:SD	2.24	0.78
1:D:1263:THR:OG1	1:D:1265:ASP:OD1	2.01	0.78
1:A:981:GLN:O	1:A:985:VAL:HG23	1.83	0.78
1:B:3458:PHE:HE2	1:B:3464:ILE:CD1	1.95	0.78
1:B:4075:GLU:OE1	1:C:4736:ARG:NH1	2.17	0.78
1:C:981:GLN:O	1:C:985:VAL:HG23	1.83	0.78
1:A:2523:ASP:HB3	1:A:2578:MET:HE1	1.66	0.78
1:A:4885:PHE:O	1:A:4889:VAL:HG22	1.84	0.78
1:D:3458:PHE:HE2	1:D:3464:ILE:CD1	1.95	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4885:PHE:O	1:D:4889:VAL:HG22	1.84	0.78
1:A:3236:VAL:HG23	1:A:3239:MET:SD	2.25	0.77
1:A:4892:ARG:NH1	1:B:4899:ASP:OD1	2.17	0.77
1:B:110:ARG:NH2	1:B:117:TYR:OH	2.17	0.77
1:D:4736:ARG:NH1	1:C:4075:GLU:OE1	2.18	0.77
1:C:3236:VAL:HA	1:C:3239:MET:SD	2.24	0.77
1:D:961:MET:SD	1:D:963:ASN:CB	2.72	0.77
1:D:4744:ASP:OD2	1:D:4747:SER:OG	1.99	0.77
1:A:110:ARG:NH2	1:A:117:TYR:OH	2.17	0.77
1:A:961:MET:SD	1:A:963:ASN:CB	2.72	0.77
1:D:2224:ARG:HG3	1:D:2225:PHE:CD2	2.20	0.77
1:C:110:ARG:NH2	1:C:117:TYR:OH	2.17	0.77
1:C:3236:VAL:HG23	1:C:3239:MET:SD	2.24	0.77
1:A:2642:LYS:HG3	1:A:2698:MET:CE	2.15	0.77
1:B:3733:CYS:O	1:B:3766:GLN:NE2	2.18	0.77
1:C:961:MET:SD	1:C:963:ASN:CB	2.72	0.77
1:C:2742:THR:HG23	1:C:2814:LYS:HE3	1.67	0.77
1:B:961:MET:SD	1:B:963:ASN:CB	2.72	0.77
1:D:2642:LYS:HG3	1:D:2698:MET:CE	2.15	0.77
1:C:4687:TYR:O	1:C:4691:GLN:NE2	2.18	0.77
1:C:3300:ALA:HB3	1:C:3301:PRO:HD3	1.67	0.77
1:A:2742:THR:HG23	1:A:2814:LYS:HE3	1.67	0.77
1:D:1753:LYS:O	1:D:1758:ARG:HD2	1.85	0.77
1:D:2742:THR:HG23	1:D:2814:LYS:HE3	1.67	0.77
1:D:3236:VAL:HG23	1:D:3239:MET:SD	2.25	0.77
1:C:2642:LYS:HG3	1:C:2698:MET:CE	2.15	0.77
1:D:972:LEU:CG	1:D:1041:GLN:NE2	2.38	0.77
1:B:4687:TYR:O	1:B:4691:GLN:NE2	2.18	0.77
1:D:2233:CYS:CB	1:D:2237:CYS:HG	1.89	0.77
1:D:4687:TYR:O	1:D:4691:GLN:NE2	2.18	0.77
1:C:3733:CYS:O	1:C:3766:GLN:NE2	2.18	0.77
1:A:4687:TYR:O	1:A:4691:GLN:NE2	2.18	0.77
1:B:2642:LYS:HG3	1:B:2698:MET:CE	2.15	0.77
1:D:110:ARG:NH2	1:D:117:TYR:OH	2.17	0.77
1:B:2628:PHE:CE2	1:B:2734:ASN:OD1	2.38	0.76
1:D:981:GLN:O	1:D:985:VAL:HG23	1.83	0.76
1:A:2224:ARG:HG3	1:A:2225:PHE:CD2	2.20	0.76
1:A:2233:CYS:CB	1:A:2237:CYS:HG	1.91	0.76
1:B:3236:VAL:HG23	1:B:3239:MET:SD	2.25	0.76
1:C:941:MET:HE1	1:C:1051:TYR:CG	2.20	0.76
1:A:3733:CYS:O	1:A:3766:GLN:NE2	2.18	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2628:PHE:CE2	1:C:2734:ASN:OD1	2.38	0.76
1:C:1753:LYS:O	1:C:1758:ARG:HD2	1.85	0.76
1:B:2742:THR:HG23	1:B:2814:LYS:HE3	1.67	0.76
1:A:2638:LYS:HE3	1:A:2694:GLU:OE1	1.86	0.76
1:B:3300:ALA:HB3	1:B:3301:PRO:HD3	1.67	0.76
1:A:710:ASP:OD1	1:A:713:SER:OG	2.03	0.76
1:B:1255:TYR:O	1:B:1275:ARG:NH1	2.19	0.76
1:D:3733:CYS:O	1:D:3766:GLN:NE2	2.18	0.76
1:B:1753:LYS:O	1:B:1758:ARG:HD2	1.85	0.76
1:C:1263:THR:OG1	1:C:1265:ASP:OD1	2.01	0.76
1:C:2224:ARG:HG3	1:C:2225:PHE:CD2	2.20	0.76
1:A:1255:TYR:O	1:A:1275:ARG:NH1	2.19	0.76
1:A:1263:THR:OG1	1:A:1265:ASP:OD1	2.01	0.76
1:C:2638:LYS:HE3	1:C:2694:GLU:OE1	1.86	0.76
1:B:1561:VAL:HG12	1:B:1562:ILE:HG23	1.67	0.75
1:D:1255:TYR:O	1:D:1275:ARG:NH1	2.19	0.75
1:D:3300:ALA:HB3	1:D:3301:PRO:HD3	1.67	0.75
1:A:1753:LYS:O	1:A:1758:ARG:HD2	1.85	0.75
1:A:2212:VAL:HG21	1:A:2256:TYR:OH	1.86	0.75
1:B:2224:ARG:HG3	1:B:2225:PHE:CD2	2.20	0.75
1:B:4902:GLU:O	1:B:4913:ARG:NH1	2.20	0.75
1:D:2628:PHE:CE2	1:D:2734:ASN:OD1	2.38	0.75
1:D:2638:LYS:HE3	1:D:2694:GLU:OE1	1.86	0.75
1:D:4902:GLU:O	1:D:4913:ARG:NH1	2.20	0.75
1:C:4902:GLU:O	1:C:4913:ARG:NH1	2.20	0.75
1:D:2212:VAL:HG21	1:D:2256:TYR:OH	1.86	0.75
1:D:1561:VAL:HG12	1:D:1562:ILE:HG23	1.67	0.75
1:A:2628:PHE:CE2	1:A:2734:ASN:OD1	2.38	0.75
1:C:1561:VAL:HG12	1:C:1562:ILE:HG23	1.67	0.75
1:A:1561:VAL:HG12	1:A:1562:ILE:HG23	1.67	0.75
1:C:1255:TYR:O	1:C:1275:ARG:NH1	2.19	0.75
1:A:870:ILE:O	1:A:874:LEU:HD12	1.87	0.74
1:A:4902:GLU:O	1:A:4913:ARG:NH1	2.20	0.74
1:B:2638:LYS:HE3	1:B:2694:GLU:OE1	1.86	0.74
1:B:2212:VAL:HG21	1:B:2256:TYR:OH	1.86	0.74
1:D:941:MET:HE3	1:D:1051:TYR:CE1	2.21	0.74
1:A:941:MET:HE3	1:A:1051:TYR:CE1	2.22	0.74
1:A:3300:ALA:HB3	1:A:3301:PRO:HD3	1.67	0.74
1:B:1999:ARG:NH1	1:B:3636:PHE:HD1	1.86	0.74
1:D:2233:CYS:HB3	1:D:2237:CYS:HG	1.47	0.74
1:C:2212:VAL:HG21	1:C:2256:TYR:OH	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3159:ASP:HA	1:A:3218:VAL:HG22	1.69	0.74
1:B:941:MET:SD	1:B:1051:TYR:CD1	2.81	0.74
1:D:941:MET:SD	1:D:1051:TYR:CD1	2.81	0.74
1:C:2226:PRO:HB3	1:C:2267:MET:HE1	1.70	0.74
1:A:2638:LYS:CE	1:A:2694:GLU:OE1	2.36	0.74
1:B:941:MET:HE3	1:B:1051:TYR:CD1	2.22	0.74
1:B:2638:LYS:CE	1:B:2694:GLU:OE1	2.36	0.74
1:D:961:MET:CE	1:D:963:ASN:CB	2.59	0.74
1:D:870:ILE:O	1:D:874:LEU:HD12	1.87	0.73
1:A:3458:PHE:HE2	1:A:3464:ILE:HD12	1.53	0.73
1:B:384:MET:SD	1:C:166:GLY:C	2.66	0.73
1:B:2974:ILE:HD13	1:B:3049:LEU:HD12	1.71	0.73
1:D:774:ASP:OD2	1:D:1470:ARG:NH2	2.21	0.73
1:A:166:GLY:C	1:D:384:MET:SD	2.67	0.73
1:A:2186:MET:O	1:A:2192:TYR:OH	2.05	0.73
1:D:3159:ASP:HA	1:D:3218:VAL:HG22	1.69	0.73
1:A:774:ASP:OD2	1:A:1470:ARG:NH2	2.21	0.73
1:A:941:MET:HE3	1:A:1051:TYR:CD1	2.19	0.73
1:B:870:ILE:O	1:B:874:LEU:HD12	1.87	0.73
1:C:2186:MET:O	1:C:2192:TYR:OH	2.05	0.73
1:A:2974:ILE:HD13	1:A:3049:LEU:HD12	1.71	0.73
1:D:911:HIS:O	1:D:918:ARG:NH2	2.22	0.73
1:D:1999:ARG:NH1	1:D:3636:PHE:HD1	1.86	0.73
1:C:870:ILE:O	1:C:874:LEU:HD12	1.87	0.73
1:C:1999:ARG:NH1	1:C:3636:PHE:HD1	1.86	0.73
1:C:2974:ILE:HD13	1:C:3049:LEU:HD12	1.71	0.73
1:C:2929:PHE:O	1:C:2932:MET:SD	2.47	0.73
1:A:911:HIS:O	1:A:918:ARG:NH2	2.22	0.72
1:B:911:HIS:O	1:B:918:ARG:NH2	2.22	0.72
1:B:961:MET:CE	1:B:963:ASN:CB	2.59	0.72
1:B:3159:ASP:HA	1:B:3218:VAL:HG22	1.69	0.72
1:C:911:HIS:O	1:C:918:ARG:NH2	2.22	0.72
1:C:2642:LYS:NZ	1:C:2642:LYS:HG3	2.04	0.72
1:A:2929:PHE:O	1:A:2932:MET:SD	2.47	0.72
1:A:2874:MET:HE2	1:A:2939:ARG:CB	2.18	0.72
2:G:77:SER:OG	2:G:79:ASP:OD1	2.08	0.72
1:B:941:MET:HE3	1:B:1051:TYR:CE1	2.24	0.72
1:B:3458:PHE:HE2	1:B:3464:ILE:HD12	1.53	0.72
1:D:2638:LYS:CE	1:D:2694:GLU:OE1	2.36	0.72
1:D:166:GLY:C	1:C:384:MET:SD	2.67	0.72
1:D:2186:MET:O	1:D:2192:TYR:OH	2.05	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3458:PHE:HE2	1:D:3464:ILE:HD12	1.53	0.72
1:C:3343:GLN:OE1	1:C:3414:ARG:NE	2.23	0.72
1:A:1999:ARG:NH1	1:A:3636:PHE:HD1	1.86	0.72
1:B:774:ASP:OD2	1:B:1470:ARG:NH2	2.21	0.72
1:A:941:MET:SD	1:A:1051:TYR:CD1	2.81	0.72
1:B:213:TYR:CD1	1:B:340:LYS:HG2	2.25	0.72
1:B:3690:VAL:O	1:B:3693:LYS:HE3	1.90	0.72
1:C:774:ASP:OD2	1:C:1470:ARG:NH2	2.21	0.72
1:C:2638:LYS:CE	1:C:2694:GLU:OE1	2.36	0.72
1:B:941:MET:HE1	1:B:1051:TYR:CG	2.24	0.72
1:B:4063:ASP:OD1	1:B:4064:MET:N	2.23	0.72
1:D:2628:PHE:HZ	1:D:2734:ASN:OD1	1.73	0.72
1:D:2929:PHE:O	1:D:2932:MET:SD	2.47	0.72
1:B:710:ASP:OD1	1:B:713:SER:OG	2.03	0.72
1:D:213:TYR:CD1	1:D:340:LYS:HG2	2.25	0.72
1:D:4899:ASP:OD1	1:C:4892:ARG:NH1	2.23	0.72
1:C:3458:PHE:HE2	1:C:3464:ILE:HD12	1.53	0.72
1:A:213:TYR:CD1	1:A:340:LYS:HG2	2.25	0.72
1:B:2642:LYS:NZ	1:B:2642:LYS:HG3	2.04	0.72
1:D:2572:THR:HG21	1:D:2579:VAL:HG21	1.71	0.72
1:D:2974:ILE:HD13	1:D:3049:LEU:HD12	1.71	0.72
1:D:3690:VAL:O	1:D:3693:LYS:HE3	1.90	0.72
1:B:2628:PHE:HZ	1:B:2734:ASN:OD1	1.73	0.71
1:B:2929:PHE:O	1:B:2932:MET:SD	2.47	0.71
1:D:4063:ASP:OD1	1:D:4064:MET:N	2.23	0.71
1:C:3891:LEU:HD13	1:C:3899:PHE:CZ	2.25	0.71
1:C:4063:ASP:OD1	1:C:4064:MET:N	2.23	0.71
1:A:961:MET:CE	1:A:963:ASN:CB	2.59	0.71
1:A:4063:ASP:OD1	1:A:4064:MET:N	2.23	0.71
1:D:2642:LYS:NZ	1:D:2642:LYS:HG3	2.04	0.71
1:A:2572:THR:HG21	1:A:2579:VAL:HG21	1.71	0.71
1:A:3690:VAL:O	1:A:3693:LYS:HE3	1.90	0.71
2:F:77:SER:OG	2:F:79:ASP:OD1	2.08	0.71
1:C:213:TYR:CD1	1:C:340:LYS:HG2	2.25	0.71
1:C:2572:THR:HG21	1:C:2579:VAL:HG21	1.71	0.71
1:C:3690:VAL:O	1:C:3693:LYS:HE3	1.90	0.71
1:B:1087:ARG:NH1	1:B:1221:GLU:O	2.23	0.71
1:C:941:MET:SD	1:C:1051:TYR:CD1	2.81	0.71
1:A:384:MET:SD	1:B:166:GLY:O	2.48	0.71
1:B:3891:LEU:HD13	1:B:3899:PHE:CZ	2.25	0.71
1:D:3891:LEU:HD13	1:D:3899:PHE:CZ	2.25	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3159:ASP:HA	1:C:3218:VAL:HG22	1.69	0.71
1:A:3321:ARG:NH1	1:A:3325:ASN:OD1	2.23	0.71
1:B:3343:GLN:OE1	1:B:3414:ARG:NE	2.23	0.71
1:D:2761:TYR:HB3	1:D:2765:LYS:NZ	2.06	0.71
2:E:77:SER:OG	2:E:79:ASP:OD1	2.08	0.71
1:C:2761:TYR:HB3	1:C:2765:LYS:NZ	2.06	0.71
1:A:3891:LEU:HD13	1:A:3899:PHE:CZ	2.25	0.71
1:D:3321:ARG:NH1	1:D:3325:ASN:OD1	2.23	0.71
1:A:4899:ASP:OD1	1:D:4892:ARG:NH1	2.23	0.71
1:B:3321:ARG:NH1	1:B:3325:ASN:OD1	2.23	0.71
1:A:3534:MET:O	1:A:3538:THR:HG23	1.91	0.70
2:E:80:TYR:CE2	2:E:80:TYR:CD1	2.38	0.70
1:B:2572:THR:HG21	1:B:2579:VAL:HG21	1.71	0.70
1:B:2761:TYR:HB3	1:B:2765:LYS:NZ	2.06	0.70
1:D:4961:CYS:SG	1:D:4978:HIS:CE1	2.84	0.70
1:A:2628:PHE:HZ	1:A:2734:ASN:OD1	1.73	0.70
1:A:2642:LYS:NZ	1:A:2642:LYS:HG3	2.04	0.70
1:A:2011:HIS:CE1	1:A:2017:ASP:OD2	2.43	0.70
1:B:4961:CYS:SG	1:B:4978:HIS:CE1	2.84	0.70
1:D:1821:ASP:OD1	1:D:1822:GLY:N	2.25	0.70
1:C:3321:ARG:NH1	1:C:3325:ASN:OD1	2.23	0.70
1:A:4961:CYS:SG	1:A:4978:HIS:CE1	2.84	0.70
2:H:77:SER:OG	2:H:79:ASP:OD1	2.08	0.70
2:G:1:GLY:HA2	2:G:80:TYR:CE2	2.27	0.70
1:D:1087:ARG:NH1	1:D:1221:GLU:O	2.24	0.70
1:C:871:ARG:NH1	1:C:922:LEU:O	2.24	0.70
1:A:2226:PRO:HB3	1:A:2267:MET:CE	2.22	0.70
1:B:871:ARG:NH1	1:B:922:LEU:O	2.24	0.70
1:B:4892:ARG:NH1	1:C:4899:ASP:OD1	2.24	0.70
1:A:871:ARG:NH1	1:A:922:LEU:O	2.24	0.70
1:D:887:ILE:HD11	1:D:907:LEU:HD22	1.73	0.70
1:C:1087:ARG:NH1	1:C:1221:GLU:O	2.23	0.70
1:A:1087:ARG:NH1	1:A:1221:GLU:O	2.24	0.70
2:H:1:GLY:HA2	2:H:80:TYR:CE2	2.27	0.70
1:B:887:ILE:HD11	1:B:907:LEU:CD2	2.22	0.70
1:B:2226:PRO:HB3	1:B:2267:MET:CE	2.22	0.70
1:A:2761:TYR:HB3	1:A:2765:LYS:NZ	2.06	0.70
1:B:3521:GLY:HA2	1:B:3524:MET:HE2	1.74	0.70
1:D:887:ILE:HD11	1:D:907:LEU:CD2	2.22	0.70
1:A:1821:ASP:OD1	1:A:1822:GLY:N	2.24	0.69
1:B:3550:ARG:NH1	1:B:3597:GLN:OE1	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2226:PRO:HB3	1:D:2267:MET:CE	2.22	0.69
1:C:710:ASP:OD1	1:C:713:SER:OG	2.03	0.69
1:C:3550:ARG:NH1	1:C:3597:GLN:OE1	2.25	0.69
1:A:1733:GLU:HG2	1:A:2201:LEU:HD23	1.74	0.69
1:A:2244:ARG:NH2	1:A:3858:MET:SD	2.65	0.69
1:B:887:ILE:HD11	1:B:907:LEU:HD22	1.73	0.69
1:D:3550:ARG:NH1	1:D:3597:GLN:OE1	2.25	0.69
1:C:69:LEU:HD13	1:C:101:LEU:HD11	1.74	0.69
1:A:3343:GLN:OE1	1:A:3414:ARG:NE	2.23	0.69
1:D:871:ARG:NH1	1:D:922:LEU:O	2.24	0.69
1:D:2244:ARG:NH2	1:D:3858:MET:SD	2.65	0.69
1:A:887:ILE:HD11	1:A:907:LEU:CD2	2.22	0.69
1:A:3550:ARG:NH1	1:A:3597:GLN:OE1	2.25	0.69
1:A:4767:TRP:CE3	1:A:4768:LEU:HD23	2.28	0.69
1:B:3534:MET:O	1:B:3538:THR:HG23	1.91	0.69
1:D:1987:SER:O	1:D:1991:THR:OG1	2.08	0.69
1:C:887:ILE:HD11	1:C:907:LEU:CD2	2.22	0.69
1:A:69:LEU:HD13	1:A:101:LEU:HD11	1.75	0.69
1:D:1808:ARG:HD2	1:D:1853:ILE:HG22	1.75	0.69
1:D:3534:MET:O	1:D:3538:THR:HG23	1.91	0.69
1:C:4961:CYS:SG	1:C:4978:HIS:CE1	2.84	0.69
1:A:941:MET:HE1	1:A:1051:TYR:CG	2.27	0.69
1:A:2011:HIS:HE1	1:A:2017:ASP:CG	1.95	0.69
1:B:4767:TRP:CE3	1:B:4768:LEU:HD23	2.28	0.69
1:D:672:VAL:O	1:D:680:THR:OG1	2.08	0.69
1:D:2970:SER:HA	1:D:2973:PHE:CE1	2.28	0.69
1:C:2244:ARG:NH2	1:C:3858:MET:SD	2.66	0.69
1:C:2628:PHE:HZ	1:C:2734:ASN:OD1	1.73	0.69
2:F:1:GLY:HA2	2:F:80:TYR:CE2	2.27	0.69
1:B:2244:ARG:NH2	1:B:3858:MET:SD	2.65	0.69
1:B:3343:GLN:O	1:B:3346:VAL:HG12	1.93	0.69
1:D:4767:TRP:CE3	1:D:4768:LEU:HD23	2.27	0.69
1:C:925:SER:O	1:C:928:THR:OG1	2.10	0.69
1:C:1821:ASP:OD1	1:C:1822:GLY:N	2.25	0.69
1:C:2226:PRO:HB3	1:C:2267:MET:CE	2.22	0.69
1:C:3343:GLN:O	1:C:3346:VAL:HG12	1.93	0.69
1:A:581:ASN:OD1	1:A:582:HIS:N	2.26	0.69
1:A:918:ARG:O	1:A:922:LEU:HD23	1.93	0.69
1:A:1808:ARG:HD2	1:A:1853:ILE:HG22	1.75	0.69
1:A:2516:ASP:OD1	1:A:2517:PHE:N	2.26	0.69
2:E:1:GLY:HA2	2:E:80:TYR:CE2	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:LEU:HD13	1:B:101:LEU:HD11	1.75	0.69
1:B:384:MET:SD	1:C:166:GLY:O	2.51	0.69
1:B:1821:ASP:OD1	1:B:1822:GLY:N	2.25	0.69
1:D:69:LEU:HD13	1:D:101:LEU:HD11	1.75	0.69
1:D:451:TYR:O	1:D:474:ARG:NH2	2.26	0.69
1:D:581:ASN:OD1	1:D:582:HIS:N	2.26	0.69
1:D:2516:ASP:OD1	1:D:2517:PHE:N	2.26	0.69
1:D:3293:PRO:HB2	1:D:3298:ALA:HB2	1.75	0.69
1:C:887:ILE:HD11	1:C:907:LEU:HD22	1.73	0.69
1:C:4767:TRP:CE3	1:C:4768:LEU:HD23	2.28	0.69
1:A:2021:CYS:O	1:A:2028:ARG:NH2	2.26	0.69
1:B:1733:GLU:HG2	1:B:2201:LEU:HD23	1.74	0.69
1:D:1733:GLU:HG2	1:D:2201:LEU:HD23	1.74	0.69
1:D:2350:ALA:O	1:D:2354:VAL:HG23	1.93	0.69
1:D:3458:PHE:CE2	1:D:3464:ILE:HD12	2.28	0.69
1:C:2011:HIS:HE1	1:C:2017:ASP:CG	1.95	0.69
1:C:3284:TRP:O	1:C:3305:THR:HG21	1.93	0.69
1:C:3293:PRO:HB2	1:C:3298:ALA:HB2	1.75	0.69
1:C:3534:MET:O	1:C:3538:THR:HG23	1.91	0.69
2:F:80:TYR:CE2	2:F:80:TYR:CD1	2.38	0.69
1:A:2970:SER:HA	1:A:2973:PHE:CE1	2.28	0.68
1:D:2021:CYS:O	1:D:2028:ARG:NH2	2.26	0.68
1:B:2288:LEU:O	1:B:3849:ARG:NH1	2.26	0.68
1:B:5014:TYR:CD1	6:B:5304:PNX:HAA3	2.29	0.68
1:D:820:ARG:NH1	1:D:821:LEU:H	1.92	0.68
1:D:3343:GLN:OE1	1:D:3414:ARG:NE	2.23	0.68
1:C:918:ARG:O	1:C:922:LEU:HD23	1.93	0.68
1:C:1808:ARG:HD2	1:C:1853:ILE:HG22	1.74	0.68
1:C:2970:SER:HA	1:C:2973:PHE:CE1	2.28	0.68
1:A:820:ARG:NH1	1:A:821:LEU:H	1.92	0.68
1:A:3343:GLN:O	1:A:3346:VAL:HG12	1.93	0.68
1:D:2211:MET:O	1:D:2214:VAL:HG12	1.93	0.68
1:C:2021:CYS:O	1:C:2028:ARG:NH2	2.26	0.68
1:A:887:ILE:HD11	1:A:907:LEU:HD22	1.73	0.68
2:H:11:ASP:OD2	2:H:12:GLY:N	2.27	0.68
1:D:918:ARG:O	1:D:922:LEU:HD23	1.93	0.68
1:D:3284:TRP:O	1:D:3305:THR:HG21	1.93	0.68
1:C:2011:HIS:CE1	1:C:2017:ASP:OD2	2.43	0.68
1:A:3458:PHE:CE2	1:A:3464:ILE:HD12	2.28	0.68
1:D:941:MET:HE1	1:D:1051:TYR:CG	2.29	0.68
1:D:2011:HIS:HE1	1:D:2017:ASP:CG	1.96	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2929:PHE:CA	1:D:2932:MET:HE1	2.19	0.68
1:D:5014:TYR:CD1	6:D:5304:PNX:HAA3	2.29	0.68
1:C:581:ASN:OD1	1:C:582:HIS:N	2.26	0.68
1:C:941:MET:HE3	1:C:1051:TYR:CE1	2.28	0.68
1:C:2211:MET:O	1:C:2214:VAL:HG12	1.93	0.68
1:C:5014:TYR:CD1	6:C:5304:PNX:HAA3	2.28	0.68
1:A:54:ASN:O	1:A:56:GLN:N	2.27	0.68
1:B:581:ASN:OD1	1:B:582:HIS:N	2.26	0.68
1:B:3458:PHE:CE2	1:B:3464:ILE:HD12	2.28	0.68
1:D:1821:ASP:OD2	1:D:1837:GLN:NE2	2.26	0.68
1:D:3521:GLY:HA2	1:D:3524:MET:HE2	1.74	0.68
1:C:820:ARG:NH1	1:C:821:LEU:H	1.92	0.68
1:C:941:MET:HE3	1:C:1051:TYR:CD1	2.27	0.68
1:A:1980:LEU:HD11	1:A:1991:THR:HG23	1.75	0.68
1:A:2350:ALA:O	1:A:2354:VAL:HG23	1.93	0.68
2:E:11:ASP:OD2	2:E:12:GLY:N	2.27	0.68
1:B:1808:ARG:HD2	1:B:1853:ILE:HG22	1.74	0.68
1:B:2970:SER:HA	1:B:2973:PHE:CE1	2.28	0.68
1:B:3293:PRO:HB2	1:B:3298:ALA:HB2	1.75	0.68
1:D:2288:LEU:O	1:D:3849:ARG:NH1	2.26	0.68
1:D:3343:GLN:O	1:D:3346:VAL:HG12	1.93	0.68
1:D:4929:LEU:O	1:D:4933:GLN:OE1	2.12	0.68
1:C:1980:LEU:HD11	1:C:1991:THR:HG23	1.75	0.68
1:A:3293:PRO:HB2	1:A:3298:ALA:HB2	1.75	0.68
2:F:11:ASP:OD2	2:F:12:GLY:N	2.27	0.68
1:B:2011:HIS:HE1	1:B:2017:ASP:CG	1.96	0.68
1:A:4929:LEU:O	1:A:4933:GLN:OE1	2.12	0.68
1:B:451:TYR:O	1:B:474:ARG:NH2	2.26	0.68
1:B:820:ARG:NH1	1:B:821:LEU:H	1.92	0.68
1:B:2021:CYS:O	1:B:2028:ARG:NH2	2.26	0.68
1:B:2211:MET:O	1:B:2214:VAL:HG12	1.93	0.68
1:B:2350:ALA:O	1:B:2354:VAL:HG23	1.93	0.68
1:D:4749:GLU:HB3	1:D:4753:HIS:HE1	1.59	0.68
1:C:54:ASN:O	1:C:56:GLN:N	2.27	0.68
1:C:1821:ASP:OD2	1:C:1837:GLN:NE2	2.26	0.68
1:C:2350:ALA:O	1:C:2354:VAL:HG23	1.93	0.68
1:C:2516:ASP:OD1	1:C:2517:PHE:N	2.26	0.68
1:A:2211:MET:O	1:A:2214:VAL:HG12	1.93	0.67
1:B:1980:LEU:HD11	1:B:1991:THR:HG23	1.75	0.67
1:C:2288:LEU:O	1:C:3849:ARG:NH1	2.26	0.67
1:A:5014:TYR:CD1	6:A:5304:PNX:HAA3	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:11:ASP:OD2	2:G:12:GLY:N	2.27	0.67
1:B:54:ASN:O	1:B:56:GLN:N	2.27	0.67
1:B:918:ARG:O	1:B:922:LEU:HD23	1.93	0.67
1:B:2186:MET:O	1:B:2192:TYR:OH	2.05	0.67
1:A:4749:GLU:HB3	1:A:4753:HIS:HE1	1.59	0.67
1:B:1821:ASP:OD2	1:B:1837:GLN:NE2	2.26	0.67
1:B:2516:ASP:OD1	1:B:2517:PHE:N	2.26	0.67
1:A:1821:ASP:OD2	1:A:1837:GLN:NE2	2.26	0.67
1:A:2288:LEU:O	1:A:3849:ARG:NH1	2.26	0.67
1:B:3284:TRP:O	1:B:3305:THR:HG21	1.93	0.67
1:D:3324:VAL:HG11	1:D:3361:THR:HG22	1.76	0.67
1:C:961:MET:CE	1:C:963:ASN:CB	2.59	0.67
1:A:166:GLY:O	1:D:384:MET:SD	2.52	0.67
1:B:3239:MET:SD	1:B:3239:MET:HG2	2.31	0.67
1:B:3324:VAL:HG11	1:B:3361:THR:HG22	1.76	0.67
1:C:908:VAL:O	1:C:963:ASN:ND2	2.28	0.67
1:C:3458:PHE:CE2	1:C:3464:ILE:HD12	2.28	0.67
1:C:493:ARG:O	1:C:496:VAL:HG22	1.94	0.67
1:C:4749:GLU:HB3	1:C:4753:HIS:HE1	1.59	0.67
1:A:3825:GLU:OE1	1:A:3825:GLU:N	2.28	0.67
1:D:166:GLY:O	1:C:384:MET:SD	2.53	0.67
1:C:3239:MET:SD	1:C:3239:MET:HG2	2.31	0.67
1:A:493:ARG:O	1:A:496:VAL:HG22	1.94	0.67
1:A:4070:ASP:OD1	1:A:4071:ILE:N	2.28	0.67
1:B:961:MET:SD	1:B:963:ASN:N	2.68	0.67
1:B:4749:GLU:HB3	1:B:4753:HIS:HE1	1.59	0.67
1:C:1733:GLU:HG2	1:C:2201:LEU:HD23	1.74	0.67
1:D:54:ASN:O	1:D:56:GLN:N	2.27	0.67
1:D:908:VAL:O	1:D:963:ASN:ND2	2.28	0.67
1:D:3239:MET:HG2	1:D:3239:MET:HA	1.76	0.67
1:C:3521:GLY:HA2	1:C:3524:MET:HE2	1.74	0.67
1:A:2233:CYS:CA	1:A:2237:CYS:SG	2.83	0.67
1:A:3324:VAL:HG11	1:A:3361:THR:HG22	1.76	0.67
1:B:4929:LEU:O	1:B:4933:GLN:OE1	2.12	0.67
1:D:1980:LEU:HD11	1:D:1991:THR:HG23	1.75	0.67
1:C:3324:VAL:HG11	1:C:3361:THR:HG22	1.76	0.67
1:B:493:ARG:O	1:B:496:VAL:HG22	1.94	0.66
1:B:2874:MET:HE2	1:B:2939:ARG:CB	2.22	0.66
1:B:3825:GLU:OE1	1:B:3825:GLU:N	2.28	0.66
1:C:4929:LEU:O	1:C:4933:GLN:OE1	2.12	0.66
1:A:2572:THR:O	1:A:2572:THR:HG22	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:493:ARG:O	1:D:496:VAL:HG22	1.94	0.66
1:C:4070:ASP:OD1	1:C:4071:ILE:N	2.28	0.66
1:A:451:TYR:O	1:A:474:ARG:NH2	2.26	0.66
1:D:1980:LEU:HD21	1:D:1995:THR:HG22	1.78	0.66
1:C:2625:ARG:NH1	1:C:2629:ASP:OD1	2.25	0.66
1:A:908:VAL:O	1:A:963:ASN:ND2	2.28	0.66
1:A:925:SER:O	1:A:928:THR:OG1	2.10	0.66
1:A:2233:CYS:O	1:A:2234:ARG:C	2.34	0.66
1:A:3284:TRP:O	1:A:3305:THR:HG21	1.93	0.66
2:H:80:TYR:CE2	2:H:80:TYR:CD1	2.38	0.66
1:B:2011:HIS:CE1	1:B:2017:ASP:OD2	2.43	0.66
1:C:961:MET:SD	1:C:963:ASN:N	2.68	0.66
1:A:1068:ARG:O	1:A:1072:VAL:HG12	1.96	0.66
1:A:4910:GLU:O	1:A:4914:VAL:HG13	1.96	0.66
2:F:1:GLY:HA2	2:F:80:TYR:HE2	1.60	0.66
1:D:2642:LYS:CG	1:D:2642:LYS:CE	2.74	0.66
1:C:1980:LEU:HD21	1:C:1995:THR:HG22	1.78	0.66
1:B:4070:ASP:OD1	1:B:4071:ILE:N	2.28	0.66
1:D:4070:ASP:OD1	1:D:4071:ILE:N	2.28	0.66
1:B:908:VAL:O	1:B:963:ASN:ND2	2.28	0.66
1:D:1424:PRO:O	1:D:1428:LEU:HD23	1.96	0.66
1:D:61:ASP:OD2	1:D:402:ARG:NH2	2.28	0.66
1:D:2233:CYS:CA	1:D:2237:CYS:SG	2.84	0.66
1:D:4910:GLU:O	1:D:4914:VAL:HG13	1.96	0.66
1:C:2233:CYS:CB	1:C:2237:CYS:HG	2.02	0.66
1:A:61:ASP:OD2	1:A:402:ARG:NH2	2.28	0.66
1:B:2572:THR:O	1:B:2572:THR:HG22	1.95	0.66
1:D:925:SER:O	1:D:928:THR:OG1	2.10	0.66
1:D:2572:THR:HG21	1:D:2579:VAL:HG23	1.78	0.66
1:C:796:ARG:HH12	1:C:1619:ARG:HH12	1.44	0.66
1:C:3825:GLU:N	1:C:3825:GLU:OE1	2.28	0.66
1:A:2572:THR:HG21	1:A:2579:VAL:HG23	1.78	0.66
1:D:1980:LEU:HD21	1:D:1995:THR:CG2	2.26	0.66
1:D:3235:SER:OG	1:D:3237:GLU:OE1	2.14	0.66
1:C:2642:LYS:CG	1:C:2642:LYS:CE	2.74	0.66
1:A:1980:LEU:HD21	1:A:1995:THR:HG22	1.78	0.65
1:D:796:ARG:HH12	1:D:1619:ARG:HH12	1.44	0.65
1:D:4148:THR:HG21	1:D:4180:ARG:HH21	1.62	0.65
1:A:796:ARG:HH12	1:A:1619:ARG:HH12	1.44	0.65
2:E:1:GLY:HA2	2:E:80:TYR:HE2	1.60	0.65
1:B:796:ARG:HH12	1:B:1619:ARG:HH12	1.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1068:ARG:O	1:D:1072:VAL:HG12	1.96	0.65
1:D:3897:ASN:OD1	1:D:3901:ASN:ND2	2.29	0.65
1:C:1975:SER:O	1:C:1979:LEU:HD23	1.96	0.65
1:C:2233:CYS:CA	1:C:2237:CYS:SG	2.84	0.65
1:C:3897:ASN:OD1	1:C:3901:ASN:ND2	2.29	0.65
1:A:1424:PRO:O	1:A:1428:LEU:HD23	1.96	0.65
1:A:1980:LEU:HD21	1:A:1995:THR:CG2	2.26	0.65
1:A:2642:LYS:CG	1:A:2642:LYS:CE	2.74	0.65
1:A:3897:ASN:OD1	1:A:3901:ASN:ND2	2.29	0.65
1:B:2233:CYS:CA	1:B:2237:CYS:SG	2.83	0.65
1:B:3235:SER:OG	1:B:3237:GLU:OE1	2.14	0.65
1:B:3897:ASN:OD1	1:B:3901:ASN:ND2	2.29	0.65
1:C:1424:PRO:O	1:C:1428:LEU:HD23	1.96	0.65
1:B:2642:LYS:CG	1:B:2642:LYS:CE	2.74	0.65
1:C:2572:THR:HG21	1:C:2579:VAL:HG23	1.78	0.65
1:B:2625:ARG:NH1	1:B:2629:ASP:OD1	2.25	0.65
1:B:3239:MET:SD	1:B:3239:MET:HG3	2.31	0.65
1:D:1032:LYS:O	1:D:1036:ARG:HG3	1.97	0.65
1:D:2625:ARG:NH1	1:D:2629:ASP:OD1	2.25	0.65
1:C:451:TYR:O	1:C:474:ARG:NH2	2.26	0.65
1:C:4148:THR:HG21	1:C:4180:ARG:HH21	1.62	0.65
1:A:941:MET:CE	1:A:1051:TYR:CG	2.79	0.65
1:B:1980:LEU:HD21	1:B:1995:THR:HG22	1.78	0.65
1:C:1980:LEU:HD21	1:C:1995:THR:CG2	2.26	0.65
1:C:2440:MET:O	1:C:2444:GLN:OE1	2.15	0.65
1:A:1032:LYS:O	1:A:1036:ARG:HG3	1.97	0.65
1:B:1980:LEU:HD21	1:B:1995:THR:CG2	2.26	0.65
1:B:2224:ARG:HE	1:B:2225:PHE:H	1.44	0.65
1:B:2523:ASP:OD1	1:B:2524:VAL:HG13	1.97	0.65
1:D:2751:LEU:O	1:D:2755:ILE:HD12	1.97	0.65
1:C:61:ASP:OD2	1:C:402:ARG:NH2	2.28	0.65
2:G:1:GLY:HA2	2:G:80:TYR:HE2	1.60	0.65
1:B:2440:MET:O	1:B:2444:GLN:OE1	2.15	0.65
1:B:4148:THR:HG21	1:B:4180:ARG:HH21	1.62	0.65
1:D:941:MET:CE	1:D:1051:TYR:CG	2.80	0.65
1:D:2523:ASP:OD1	1:D:2524:VAL:HG13	1.97	0.65
1:C:2572:THR:HG22	1:C:2572:THR:O	1.95	0.65
1:C:2751:LEU:O	1:C:2755:ILE:HD12	1.97	0.65
1:C:3235:SER:OG	1:C:3237:GLU:OE1	2.14	0.65
1:A:924:MET:O	1:A:928:THR:HG23	1.97	0.65
1:A:1975:SER:O	1:A:1979:LEU:HD23	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4148:THR:HG21	1:A:4180:ARG:HH21	1.62	0.65
1:B:61:ASP:OD2	1:B:402:ARG:NH2	2.28	0.65
1:B:1424:PRO:O	1:B:1428:LEU:HD23	1.96	0.65
1:B:4910:GLU:O	1:B:4914:VAL:HG13	1.96	0.65
1:C:568:LEU:HD12	1:C:602:VAL:HG13	1.80	0.65
1:C:1068:ARG:O	1:C:1072:VAL:HG12	1.96	0.65
1:A:2440:MET:O	1:A:2444:GLN:OE1	2.14	0.64
1:A:2751:LEU:O	1:A:2755:ILE:HD12	1.97	0.64
1:A:3235:SER:OG	1:A:3237:GLU:OE1	2.14	0.64
1:B:568:LEU:HD12	1:B:602:VAL:HG13	1.79	0.64
1:D:3239:MET:SD	1:D:3239:MET:HG3	2.31	0.64
1:B:1032:LYS:O	1:B:1036:ARG:HG3	1.97	0.64
1:B:1068:ARG:O	1:B:1072:VAL:HG12	1.96	0.64
1:D:2572:THR:O	1:D:2572:THR:HG22	1.95	0.64
1:C:2874:MET:CE	1:C:2939:ARG:CB	2.75	0.64
1:D:1975:SER:O	1:D:1979:LEU:HD23	1.96	0.64
1:D:924:MET:O	1:D:928:THR:HG23	1.97	0.64
1:D:959:TYR:HD2	1:D:966:LYS:HE2	1.63	0.64
1:C:2226:PRO:CB	1:C:2267:MET:HE3	2.28	0.64
1:A:568:LEU:HD12	1:A:602:VAL:HG13	1.79	0.64
1:A:2625:ARG:NH1	1:A:2629:ASP:OD1	2.25	0.64
1:A:4818:MET:O	1:A:4824:ARG:NH2	2.29	0.64
2:H:1:GLY:HA2	2:H:80:TYR:HE2	1.60	0.64
1:C:4910:GLU:O	1:C:4914:VAL:HG13	1.96	0.64
1:A:2224:ARG:HE	1:A:2225:PHE:H	1.44	0.64
1:A:2523:ASP:OD1	1:A:2524:VAL:HG13	1.97	0.64
1:D:721:LEU:HD12	1:D:1476:MET:HE1	1.80	0.64
1:D:2233:CYS:O	1:D:2234:ARG:C	2.34	0.64
1:C:924:MET:O	1:C:928:THR:HG23	1.97	0.64
1:C:2523:ASP:OD1	1:C:2524:VAL:HG13	1.97	0.64
1:A:2829:GLY:O	1:A:2830:GLU:OE1	2.16	0.64
1:B:941:MET:CE	1:B:1051:TYR:CG	2.79	0.64
1:B:1975:SER:O	1:B:1979:LEU:HD23	1.96	0.64
1:B:2874:MET:CE	1:B:2939:ARG:CB	2.75	0.64
1:D:2440:MET:O	1:D:2444:GLN:OE1	2.15	0.64
1:D:2615:ARG:NH1	1:D:2663:ASN:O	2.31	0.64
1:D:3825:GLU:OE1	1:D:3825:GLU:N	2.28	0.64
1:C:1032:LYS:O	1:C:1036:ARG:HG3	1.97	0.64
1:C:2224:ARG:HE	1:C:2225:PHE:H	1.45	0.64
1:B:959:TYR:HD2	1:B:966:LYS:HE2	1.63	0.64
1:B:3840:SER:OG	1:B:3877:ASP:OD1	2.15	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2011:HIS:CE1	1:D:2017:ASP:OD2	2.43	0.64
1:A:2874:MET:CE	1:A:2939:ARG:CB	2.75	0.64
1:B:2829:GLY:O	1:B:2830:GLU:OE1	2.16	0.64
1:D:2224:ARG:HE	1:D:2225:PHE:H	1.44	0.64
1:A:959:TYR:HD2	1:A:966:LYS:HE2	1.63	0.64
1:D:568:LEU:HD12	1:D:602:VAL:HG13	1.80	0.64
1:D:880:GLU:OE1	1:D:967:PRO:HB2	1.98	0.64
1:C:880:GLU:OE1	1:C:967:PRO:HB2	1.98	0.64
1:C:4658:ILE:HD12	1:C:4796:MET:SD	2.38	0.64
1:C:4747:SER:O	1:C:4751:THR:HG23	1.98	0.64
1:D:961:MET:SD	1:D:963:ASN:N	2.68	0.63
1:D:3458:PHE:CE2	1:D:3464:ILE:CD1	2.80	0.63
1:C:2829:GLY:O	1:C:2830:GLU:OE1	2.16	0.63
1:A:961:MET:SD	1:A:963:ASN:N	2.68	0.63
1:B:925:SER:O	1:B:928:THR:OG1	2.10	0.63
1:B:2751:LEU:O	1:B:2755:ILE:HD12	1.97	0.63
1:D:2829:GLY:O	1:D:2830:GLU:OE1	2.16	0.63
1:C:3840:SER:OG	1:C:3877:ASP:OD1	2.15	0.63
1:C:4711:PHE:HB3	1:C:4712:PRO:HD3	1.80	0.63
1:A:3239:MET:SD	1:A:3239:MET:HG2	2.31	0.63
1:D:2874:MET:CE	1:D:2939:ARG:CB	2.75	0.63
1:B:880:GLU:OE1	1:B:967:PRO:HB2	1.98	0.63
1:B:2615:ARG:NH1	1:B:2663:ASN:O	2.31	0.63
1:C:2644:LEU:HD13	1:C:2678:LEU:HD21	1.80	0.63
1:B:924:MET:O	1:B:928:THR:HG23	1.97	0.63
1:B:3239:MET:CG	1:B:3239:MET:CE	2.77	0.63
1:C:959:TYR:HD2	1:C:966:LYS:HE2	1.63	0.63
1:C:1987:SER:O	1:C:1991:THR:OG1	2.08	0.63
1:C:2233:CYS:O	1:C:2234:ARG:C	2.34	0.63
1:A:4711:PHE:HB3	1:A:4712:PRO:HD3	1.80	0.63
1:C:870:ILE:HD11	1:C:1049:TYR:CD2	2.34	0.63
1:C:2615:ARG:NH1	1:C:2663:ASN:O	2.31	0.63
1:C:2623:LEU:O	1:C:2627:VAL:HG23	1.99	0.63
1:A:2615:ARG:NH1	1:A:2663:ASN:O	2.31	0.63
1:A:3368:ARG:O	1:A:3372:VAL:HG23	1.99	0.63
1:B:870:ILE:HD11	1:B:1049:TYR:CD2	2.34	0.63
1:D:881:LEU:O	1:D:885:THR:HG23	1.99	0.63
1:D:2623:LEU:O	1:D:2627:VAL:HG23	1.99	0.63
1:A:2157:GLU:O	1:A:2161:GLN:NE2	2.32	0.63
1:A:2644:LEU:HD13	1:A:2678:LEU:HD21	1.80	0.63
1:B:871:ARG:CD	1:B:926:GLY:HA2	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:881:LEU:O	1:B:885:THR:HG23	1.99	0.63
1:B:2233:CYS:O	1:B:2234:ARG:C	2.34	0.63
1:D:710:ASP:OD1	1:D:713:SER:OG	2.03	0.63
1:C:881:LEU:O	1:C:885:THR:HG23	1.99	0.63
1:A:3239:MET:SD	1:A:3239:MET:HG3	2.31	0.62
1:A:4658:ILE:HD12	1:A:4796:MET:SD	2.38	0.62
1:B:2233:CYS:CB	1:B:2237:CYS:HG	2.04	0.62
1:B:2572:THR:HG21	1:B:2579:VAL:HG23	1.78	0.62
1:B:2644:LEU:HD13	1:B:2678:LEU:HD21	1.80	0.62
1:B:4711:PHE:HB3	1:B:4712:PRO:HD3	1.80	0.62
1:D:4658:ILE:HD12	1:D:4796:MET:SD	2.38	0.62
1:C:3368:ARG:O	1:C:3372:VAL:HG23	1.99	0.62
1:A:880:GLU:OE1	1:A:967:PRO:HB2	1.98	0.62
1:A:881:LEU:O	1:A:885:THR:HG23	1.99	0.62
1:B:2623:LEU:O	1:B:2627:VAL:HG23	1.99	0.62
1:C:871:ARG:CD	1:C:926:GLY:HA2	2.29	0.62
1:C:3834:ALA:O	1:C:3838:THR:HG23	1.99	0.62
1:A:1987:SER:O	1:A:1991:THR:OG1	2.08	0.62
1:A:3239:MET:CG	1:A:3239:MET:CE	2.77	0.62
1:A:4630:TYR:OH	1:B:4860:ARG:NH1	2.30	0.62
1:B:2157:GLU:O	1:B:2161:GLN:NE2	2.32	0.62
1:B:3834:ALA:O	1:B:3838:THR:HG23	1.99	0.62
1:D:3368:ARG:O	1:D:3372:VAL:HG23	1.99	0.62
1:D:4747:SER:O	1:D:4751:THR:HG23	1.98	0.62
1:A:1577:ALA:O	1:A:1584:ARG:NH1	2.32	0.62
1:A:3458:PHE:CE2	1:A:3464:ILE:CD1	2.81	0.62
1:A:4747:SER:O	1:A:4751:THR:HG23	1.98	0.62
1:D:988:LEU:HB3	1:D:1039:LEU:HD11	1.81	0.62
1:D:3840:SER:OG	1:D:3877:ASP:OD1	2.15	0.62
1:A:972:LEU:CD1	1:A:1041:GLN:NE2	2.62	0.62
1:A:3834:ALA:O	1:A:3838:THR:HG23	1.99	0.62
1:A:3840:SER:OG	1:A:3877:ASP:OD1	2.15	0.62
1:B:4658:ILE:HD12	1:B:4796:MET:SD	2.38	0.62
1:C:941:MET:CE	1:C:1051:TYR:CG	2.79	0.62
1:A:2623:LEU:O	1:A:2627:VAL:HG23	1.99	0.62
1:B:4747:SER:O	1:B:4751:THR:HG23	1.98	0.62
1:D:3834:ALA:O	1:D:3838:THR:HG23	1.99	0.62
1:C:3239:MET:CG	1:C:3239:MET:CE	2.77	0.62
1:A:3969:ILE:HG21	1:A:3980:LEU:HD12	1.82	0.62
1:B:672:VAL:O	1:B:680:THR:OG1	2.08	0.62
1:B:3368:ARG:O	1:B:3372:VAL:HG23	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4818:MET:O	1:B:4824:ARG:NH2	2.29	0.62
1:D:870:ILE:HD11	1:D:1049:TYR:CD2	2.34	0.62
1:D:2782:ASP:OD2	1:D:2785:LEU:HD22	1.99	0.62
1:D:3213:TYR:CE1	1:D:3302:PRO:HG2	2.34	0.62
1:C:2157:GLU:O	1:C:2161:GLN:NE2	2.32	0.62
1:B:988:LEU:HB3	1:B:1039:LEU:HD11	1.81	0.62
1:B:3671:ASP:OD1	1:B:3672:ARG:N	2.33	0.62
1:D:972:LEU:CD1	1:D:1041:GLN:NE2	2.62	0.62
1:D:2157:GLU:O	1:D:2161:GLN:NE2	2.32	0.62
1:D:2644:LEU:HD13	1:D:2678:LEU:HD21	1.80	0.62
1:A:870:ILE:HD11	1:A:1049:TYR:CD2	2.34	0.62
1:A:1280:GLN:O	1:A:1281:ASN:OD1	2.18	0.62
1:A:4745:LEU:O	1:A:4749:GLU:OE1	2.18	0.62
1:B:972:LEU:CD1	1:B:1041:GLN:NE2	2.62	0.62
1:D:4711:PHE:HB3	1:D:4712:PRO:HD3	1.80	0.62
1:A:3213:TYR:CE1	1:A:3302:PRO:HG2	2.34	0.62
1:D:3239:MET:CG	1:D:3239:MET:CE	2.77	0.62
1:C:721:LEU:HD12	1:C:1476:MET:HE1	1.82	0.62
1:A:2744:ASN:OD1	1:A:2745:VAL:N	2.33	0.61
1:A:3671:ASP:OD1	1:A:3672:ARG:N	2.33	0.61
2:F:16:PRO:O	2:F:17:LYS:HE2	2.00	0.61
1:B:2226:PRO:CB	1:B:2267:MET:CE	2.78	0.61
1:B:3213:TYR:CE1	1:B:3302:PRO:HG2	2.34	0.61
1:C:3213:TYR:CE1	1:C:3302:PRO:HG2	2.34	0.61
1:C:3239:MET:SD	1:C:3239:MET:HG3	2.31	0.61
1:C:3573:MET:CB	1:C:3577:ARG:HH12	2.12	0.61
1:A:2782:ASP:OD2	1:A:2785:LEU:HD22	1.99	0.61
2:E:79:ASP:OD1	2:E:80:TYR:N	2.33	0.61
1:B:281:ARG:NH2	1:B:309:THR:OG1	2.33	0.61
1:B:2744:ASN:OD1	1:B:2745:VAL:N	2.33	0.61
1:D:2265:LEU:HD12	1:D:2266:GLY:N	2.15	0.61
1:D:2642:LYS:HG3	1:D:2698:MET:HE3	1.81	0.61
1:D:3969:ILE:HG21	1:D:3980:LEU:HD12	1.82	0.61
1:A:281:ARG:NH2	1:A:309:THR:OG1	2.33	0.61
2:G:16:PRO:O	2:G:17:LYS:HE2	2.00	0.61
1:B:1577:ALA:O	1:B:1584:ARG:NH1	2.32	0.61
1:B:2782:ASP:OD2	1:B:2785:LEU:HD22	1.99	0.61
1:B:3969:ILE:HG21	1:B:3980:LEU:HD12	1.82	0.61
1:B:4584:ASP:OD1	1:B:4585:SER:N	2.33	0.61
1:C:1280:GLN:O	1:C:1281:ASN:OD1	2.18	0.61
1:C:3671:ASP:OD1	1:C:3672:ARG:N	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4634:GLU:OE1	1:C:4636:THR:OG1	2.16	0.61
1:A:2226:PRO:CB	1:A:2267:MET:CE	2.78	0.61
1:B:906:CYS:HB2	1:B:913:LEU:HB2	1.83	0.61
1:B:1929:MET:O	1:B:1930:LYS:CB	2.49	0.61
1:B:3891:LEU:HB3	1:B:3899:PHE:CE2	2.35	0.61
1:C:988:LEU:HB3	1:C:1039:LEU:HD11	1.81	0.61
1:C:2226:PRO:CB	1:C:2267:MET:CE	2.78	0.61
1:A:988:LEU:HB3	1:A:1039:LEU:HD11	1.81	0.61
1:B:1965:TYR:O	1:B:1969:LEU:HD13	2.00	0.61
1:D:871:ARG:CD	1:D:926:GLY:HA2	2.29	0.61
1:D:906:CYS:HB2	1:D:913:LEU:HB2	1.83	0.61
1:C:281:ARG:NH2	1:C:309:THR:OG1	2.33	0.61
1:C:2782:ASP:OD2	1:C:2785:LEU:HD22	1.99	0.61
1:C:3458:PHE:CE2	1:C:3464:ILE:CD1	2.81	0.61
1:C:3891:LEU:HB3	1:C:3899:PHE:CE2	2.35	0.61
1:A:906:CYS:HB2	1:A:913:LEU:HB2	1.83	0.61
1:B:1280:GLN:O	1:B:1281:ASN:OD1	2.18	0.61
1:B:2265:LEU:HD12	1:B:2266:GLY:N	2.15	0.61
1:B:4745:LEU:O	1:B:4749:GLU:OE1	2.18	0.61
1:D:1929:MET:O	1:D:1930:LYS:CB	2.49	0.61
1:D:2744:ASN:OD1	1:D:2745:VAL:N	2.33	0.61
1:D:4745:LEU:O	1:D:4749:GLU:OE1	2.18	0.61
1:C:972:LEU:CD1	1:C:1041:GLN:NE2	2.62	0.61
1:C:2744:ASN:OD1	1:C:2745:VAL:N	2.33	0.61
1:C:3969:ILE:HG21	1:C:3980:LEU:HD12	1.82	0.61
1:C:4584:ASP:OD1	1:C:4585:SER:N	2.34	0.61
1:A:721:LEU:HD12	1:A:1476:MET:CE	2.31	0.61
1:A:1965:TYR:O	1:A:1969:LEU:HD13	2.01	0.61
1:A:2929:PHE:CA	1:A:2932:MET:HE1	2.23	0.61
1:A:4584:ASP:OD1	1:A:4585:SER:N	2.34	0.61
1:A:4634:GLU:OE1	1:A:4636:THR:OG1	2.16	0.61
1:A:4705:VAL:HG13	1:A:4711:PHE:CE1	2.36	0.61
2:H:16:PRO:O	2:H:17:LYS:HE2	2.00	0.61
1:B:2658:PRO:O	1:B:2666:VAL:HG11	2.01	0.61
1:D:721:LEU:HD12	1:D:1476:MET:CE	2.31	0.61
1:D:1965:TYR:O	1:D:1969:LEU:HD13	2.01	0.61
1:C:2874:MET:HE2	1:C:2939:ARG:CB	2.28	0.61
1:C:4705:VAL:HG13	1:C:4711:PHE:CE1	2.36	0.61
1:A:672:VAL:O	1:A:680:THR:OG1	2.08	0.61
1:A:3891:LEU:HB3	1:A:3899:PHE:CE2	2.35	0.61
1:B:3007:ASN:O	1:B:3011:THR:OG1	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3573:MET:CB	1:B:3577:ARG:HH12	2.12	0.61
1:B:4705:VAL:HG13	1:B:4711:PHE:CE1	2.36	0.61
1:D:140:ASP:OD2	1:D:142:THR:OG1	2.19	0.61
1:D:1280:GLN:O	1:D:1281:ASN:OD1	2.18	0.61
1:C:1577:ALA:O	1:C:1584:ARG:NH1	2.32	0.61
1:C:2265:LEU:HD12	1:C:2266:GLY:N	2.15	0.61
1:C:2658:PRO:O	1:C:2666:VAL:HG11	2.01	0.61
1:C:2977:LEU:O	1:C:2981:VAL:HG23	2.01	0.61
2:E:16:PRO:O	2:E:17:LYS:HE2	2.00	0.61
1:D:2382:GLU:OE1	1:D:2385:ARG:NH1	2.34	0.61
1:D:3634:ALA:O	1:D:3638:MET:HG3	2.01	0.61
1:D:3671:ASP:OD1	1:D:3672:ARG:N	2.33	0.61
1:C:4745:LEU:O	1:C:4749:GLU:OE1	2.18	0.61
1:A:1929:MET:O	1:A:1930:LYS:CB	2.49	0.60
1:A:2265:LEU:HD12	1:A:2266:GLY:N	2.15	0.60
1:B:2977:LEU:O	1:B:2981:VAL:HG23	2.01	0.60
1:D:904:HIS:ND1	1:D:906:CYS:SG	2.73	0.60
1:D:4818:MET:O	1:D:4824:ARG:NH2	2.29	0.60
1:A:2977:LEU:O	1:A:2981:VAL:HG23	2.01	0.60
1:B:140:ASP:OD2	1:B:142:THR:OG1	2.19	0.60
1:D:3692:GLU:OE1	1:D:3694:LYS:N	2.35	0.60
1:D:3891:LEU:HB3	1:D:3899:PHE:CE2	2.35	0.60
1:C:1929:MET:O	1:C:1930:LYS:CB	2.49	0.60
1:A:2890:LYS:O	1:A:2894:LEU:HD13	2.02	0.60
1:B:2890:LYS:O	1:B:2894:LEU:HD13	2.02	0.60
1:D:294:THR:O	1:D:298:GLY:N	2.35	0.60
1:D:941:MET:HE3	1:D:1051:TYR:CZ	2.36	0.60
1:D:2977:LEU:O	1:D:2981:VAL:HG23	2.01	0.60
1:C:906:CYS:HB2	1:C:913:LEU:HB2	1.83	0.60
1:C:970:LEU:HD11	1:C:1049:TYR:CE1	2.37	0.60
1:C:1965:TYR:O	1:C:1969:LEU:HD13	2.00	0.60
1:C:4677:LEU:HD23	1:C:4711:PHE:CE1	2.37	0.60
1:A:871:ARG:HD2	1:A:926:GLY:N	2.17	0.60
1:A:941:MET:HE3	1:A:1051:TYR:CZ	2.37	0.60
2:H:79:ASP:OD1	2:H:80:TYR:N	2.33	0.60
1:D:281:ARG:NH2	1:D:309:THR:OG1	2.33	0.60
1:D:1577:ALA:O	1:D:1584:ARG:NH1	2.32	0.60
1:D:2226:PRO:CB	1:D:2267:MET:CE	2.78	0.60
1:A:3573:MET:CB	1:A:3577:ARG:HH12	2.12	0.60
1:A:4976:GLU:O	1:A:4980:LEU:HD13	2.02	0.60
1:B:871:ARG:HD2	1:B:926:GLY:N	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4885:PHE:CE2	1:B:4897:ILE:HD11	2.36	0.60
1:D:2464:ASP:OD1	1:D:2465:ASP:N	2.35	0.60
1:D:3573:MET:CB	1:D:3577:ARG:HH12	2.12	0.60
1:D:4677:LEU:HD23	1:D:4711:PHE:CE1	2.37	0.60
1:A:2382:GLU:OE1	1:A:2385:ARG:NH1	2.34	0.60
1:A:2642:LYS:HG3	1:A:2698:MET:HE3	1.83	0.60
1:B:1441:ALA:N	1:B:1513:ASP:OD1	2.34	0.60
1:B:2382:GLU:OE1	1:B:2385:ARG:NH1	2.34	0.60
1:D:871:ARG:HD2	1:D:926:GLY:N	2.17	0.60
1:D:4584:ASP:OD1	1:D:4585:SER:N	2.33	0.60
1:B:296:ASP:CG	1:B:297:GLN:OE1	2.40	0.60
1:B:3458:PHE:CE2	1:B:3464:ILE:CD1	2.81	0.60
1:B:3634:ALA:O	1:B:3638:MET:HG3	2.01	0.60
1:D:970:LEU:HD11	1:D:1049:TYR:CE1	2.37	0.60
1:D:4885:PHE:CE2	1:D:4897:ILE:HD11	2.36	0.60
1:C:294:THR:O	1:C:298:GLY:N	2.35	0.60
1:C:984:LEU:O	1:C:988:LEU:HD23	2.01	0.60
1:C:2464:ASP:OD1	1:C:2465:ASP:N	2.35	0.60
1:C:4976:GLU:O	1:C:4980:LEU:HD13	2.02	0.60
1:A:932:LEU:HD12	1:A:937:CYS:SG	2.42	0.60
1:A:3227:ARG:HB3	1:A:3232:LEU:HD12	1.83	0.60
1:D:985:VAL:HG13	1:D:1039:LEU:CD2	2.32	0.60
1:C:721:LEU:HD12	1:C:1476:MET:CE	2.31	0.60
1:C:1441:ALA:N	1:C:1513:ASP:OD1	2.34	0.60
1:C:4966:ASP:OD1	1:C:4967:TYR:N	2.35	0.60
1:A:871:ARG:CD	1:A:926:GLY:HA2	2.29	0.60
1:A:3634:ALA:O	1:A:3638:MET:HG3	2.02	0.60
1:D:4705:VAL:HG13	1:D:4711:PHE:CE1	2.36	0.60
1:C:140:ASP:OD2	1:C:142:THR:OG1	2.19	0.60
1:C:2382:GLU:OE1	1:C:2385:ARG:NH1	2.34	0.60
1:C:4827:LEU:O	1:C:4831:THR:HG23	2.02	0.60
1:A:296:ASP:CG	1:A:297:GLN:OE1	2.40	0.60
1:A:2233:CYS:HB3	1:A:2237:CYS:HG	1.49	0.60
1:A:2658:PRO:O	1:A:2666:VAL:HG11	2.01	0.60
1:A:4677:LEU:HD23	1:A:4711:PHE:CE1	2.37	0.60
1:B:3692:GLU:OE1	1:B:3694:LYS:N	2.35	0.60
1:B:4976:GLU:O	1:B:4980:LEU:HD13	2.02	0.60
1:D:932:LEU:HD12	1:D:937:CYS:SG	2.42	0.60
1:D:984:LEU:O	1:D:988:LEU:HD23	2.01	0.60
1:D:2658:PRO:O	1:D:2666:VAL:HG11	2.01	0.60
1:D:4976:GLU:O	1:D:4980:LEU:HD13	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:985:VAL:HG13	1:A:1039:LEU:CD2	2.32	0.59
1:B:721:LEU:HD12	1:B:1476:MET:CE	2.31	0.59
1:B:884:LEU:O	1:B:888:GLU:OE1	2.20	0.59
1:B:932:LEU:HD12	1:B:937:CYS:SG	2.42	0.59
1:C:3692:GLU:OE1	1:C:3694:LYS:N	2.35	0.59
1:A:140:ASP:OD2	1:A:142:THR:OG1	2.19	0.59
1:A:721:LEU:HD12	1:A:1476:MET:HE1	1.84	0.59
1:A:984:LEU:O	1:A:988:LEU:HD23	2.01	0.59
1:B:970:LEU:HD11	1:B:1049:TYR:CE1	2.37	0.59
1:B:4677:LEU:HD23	1:B:4711:PHE:CE1	2.37	0.59
1:B:4827:LEU:O	1:B:4831:THR:HG23	2.02	0.59
1:D:4634:GLU:OE1	1:D:4636:THR:OG1	2.16	0.59
1:C:871:ARG:HD2	1:C:926:GLY:N	2.17	0.59
1:C:932:LEU:HD12	1:C:937:CYS:SG	2.42	0.59
1:C:2890:LYS:O	1:C:2894:LEU:HD13	2.02	0.59
1:C:4885:PHE:CE2	1:C:4897:ILE:HD11	2.36	0.59
1:A:11:VAL:HG11	1:A:164:ARG:HD3	1.85	0.59
1:B:985:VAL:HG13	1:B:1039:LEU:CD2	2.32	0.59
1:D:2890:LYS:O	1:D:2894:LEU:HD13	2.02	0.59
1:A:970:LEU:HD11	1:A:1049:TYR:CE1	2.37	0.59
1:A:3327:LEU:HD12	1:A:3364:ARG:NH1	2.18	0.59
1:A:3692:GLU:OE1	1:A:3694:LYS:N	2.35	0.59
1:A:4827:LEU:O	1:A:4831:THR:HG23	2.02	0.59
1:B:233:ILE:O	1:B:257:ARG:NH1	2.35	0.59
1:B:984:LEU:O	1:B:988:LEU:HD23	2.01	0.59
1:B:3327:LEU:HD12	1:B:3364:ARG:NH1	2.18	0.59
1:D:4966:ASP:OD1	1:D:4967:TYR:N	2.35	0.59
1:C:296:ASP:CG	1:C:297:GLN:OE1	2.40	0.59
1:C:3157:ILE:HG23	1:C:3161:VAL:HG12	1.85	0.59
1:C:3634:ALA:O	1:C:3638:MET:HG3	2.02	0.59
1:A:884:LEU:O	1:A:888:GLU:OE1	2.20	0.59
1:A:4885:PHE:CE2	1:A:4897:ILE:HD11	2.36	0.59
2:G:79:ASP:OD1	2:G:80:TYR:N	2.33	0.59
2:F:79:ASP:OD1	2:F:80:TYR:N	2.33	0.59
1:D:11:VAL:HG11	1:D:164:ARG:HD3	1.85	0.59
1:D:2874:MET:HE2	1:D:2939:ARG:CB	2.27	0.59
1:C:978:THR:HG1	1:C:981:GLN:CD	2.06	0.59
1:A:64:ILE:O	1:A:111:HIS:NE2	2.36	0.59
1:A:1427:ILE:HG23	1:A:1428:LEU:HD22	1.84	0.59
1:C:985:VAL:HG13	1:C:1039:LEU:CD2	2.32	0.59
1:C:2376:LEU:HD11	1:C:2426:TYR:HB3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:THR:O	1:A:298:GLY:N	2.35	0.59
2:F:17:LYS:HE2	2:F:17:LYS:HA	1.85	0.59
1:B:978:THR:HG1	1:B:981:GLN:CD	2.06	0.59
1:B:2376:LEU:HD11	1:B:2426:TYR:HB3	1.85	0.59
1:B:2464:ASP:OD1	1:B:2465:ASP:N	2.35	0.59
1:D:1427:ILE:HG23	1:D:1428:LEU:HD22	1.84	0.59
1:D:3327:LEU:HD12	1:D:3364:ARG:NH1	2.18	0.59
1:C:2642:LYS:HG3	1:C:2698:MET:HE1	1.82	0.59
1:C:3236:VAL:O	1:C:3239:MET:HG2	2.02	0.59
1:C:3327:LEU:HD12	1:C:3364:ARG:NH1	2.18	0.59
1:C:3357:HIS:O	1:C:3361:THR:HG23	2.03	0.59
1:A:4930:ALA:HA	1:A:4933:GLN:OE1	2.03	0.59
1:B:3157:ILE:HG23	1:B:3161:VAL:HG12	1.85	0.59
1:D:3985:LEU:O	1:D:3989:VAL:HG23	2.03	0.59
1:A:2376:LEU:HD11	1:A:2426:TYR:HB3	1.85	0.59
1:A:3985:LEU:O	1:A:3989:VAL:HG23	2.03	0.59
2:E:17:LYS:HE2	2:E:17:LYS:HA	1.85	0.59
1:B:11:VAL:HG11	1:B:164:ARG:HD3	1.85	0.59
1:B:2761:TYR:HB3	1:B:2765:LYS:HZ3	1.68	0.59
1:B:3227:ARG:HB3	1:B:3232:LEU:HD12	1.83	0.59
1:D:228:ASP:OD1	1:D:229:GLU:N	2.36	0.59
1:C:3227:ARG:HB3	1:C:3232:LEU:HD12	1.83	0.59
1:A:3157:ILE:HG23	1:A:3161:VAL:HG12	1.85	0.58
2:G:17:LYS:HE2	2:G:17:LYS:HA	1.85	0.58
1:B:3985:LEU:O	1:B:3989:VAL:HG23	2.03	0.58
1:B:4930:ALA:HA	1:B:4933:GLN:OE1	2.03	0.58
1:D:2974:ILE:HD13	1:D:3049:LEU:CD1	2.33	0.58
1:C:11:VAL:HG11	1:C:164:ARG:HD3	1.85	0.58
1:C:2874:MET:HE1	1:C:2939:ARG:HB2	1.83	0.58
1:A:228:ASP:OD1	1:A:229:GLU:N	2.36	0.58
1:A:2464:ASP:OD1	1:A:2465:ASP:N	2.35	0.58
1:A:3324:VAL:CG1	1:A:3361:THR:HG22	2.33	0.58
1:A:4998:LYS:HB3	1:A:5003:HIS:HE1	1.68	0.58
1:B:64:ILE:O	1:B:111:HIS:NE2	2.36	0.58
1:B:3324:VAL:CG1	1:B:3361:THR:HG22	2.33	0.58
1:B:3357:HIS:O	1:B:3361:THR:HG23	2.03	0.58
1:B:4749:GLU:C	1:B:4753:HIS:HD1	2.07	0.58
1:A:4966:ASP:OD1	1:A:4967:TYR:N	2.35	0.58
1:D:978:THR:HG1	1:D:981:GLN:CD	2.06	0.58
1:D:3239:MET:SD	1:D:3239:MET:HG2	2.31	0.58
1:C:64:ILE:O	1:C:111:HIS:NE2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4930:ALA:HA	1:C:4933:GLN:OE1	2.03	0.58
1:A:1112:ASP:OD1	1:A:1113:VAL:HG23	2.03	0.58
1:A:3559:LEU:HD23	1:A:3559:LEU:O	2.03	0.58
2:H:17:LYS:HE2	2:H:17:LYS:HA	1.85	0.58
1:B:941:MET:HE3	1:B:1051:TYR:CZ	2.38	0.58
1:D:296:ASP:CG	1:D:297:GLN:OE1	2.40	0.58
1:D:2376:LEU:HD11	1:D:2426:TYR:HB3	1.85	0.58
1:D:3559:LEU:HD23	1:D:3559:LEU:O	2.03	0.58
1:D:4827:LEU:O	1:D:4831:THR:HG23	2.02	0.58
1:C:1427:ILE:HG23	1:C:1428:LEU:HD22	1.84	0.58
1:C:1925:GLY:O	1:C:1929:MET:HG3	2.04	0.58
1:C:2974:ILE:HD13	1:C:3049:LEU:CD1	2.33	0.58
1:C:4818:MET:O	1:C:4824:ARG:NH2	2.29	0.58
1:A:3357:HIS:O	1:A:3361:THR:HG23	2.03	0.58
1:B:228:ASP:OD1	1:B:229:GLU:N	2.36	0.58
1:B:294:THR:O	1:B:298:GLY:N	2.35	0.58
1:B:2226:PRO:CB	1:B:2267:MET:HE3	2.33	0.58
1:B:2572:THR:CG2	1:B:2579:VAL:HG21	2.33	0.58
1:B:2781:VAL:HG23	1:B:2789:PRO:HG3	1.85	0.58
1:D:69:LEU:CD1	1:D:101:LEU:HD11	2.34	0.58
1:C:1112:ASP:OD1	1:C:1113:VAL:HG23	2.03	0.58
1:A:978:THR:HG1	1:A:981:GLN:CD	2.06	0.58
1:A:2226:PRO:CB	1:A:2267:MET:HE1	2.31	0.58
1:D:64:ILE:O	1:D:111:HIS:NE2	2.36	0.58
1:D:3157:ILE:HG23	1:D:3161:VAL:HG12	1.85	0.58
1:D:3324:VAL:CG1	1:D:3361:THR:HG22	2.33	0.58
1:D:4930:ALA:HA	1:D:4933:GLN:OE1	2.03	0.58
1:A:3236:VAL:HA	1:A:3239:MET:HG2	1.85	0.58
1:A:3398:PHE:CE2	1:A:3450:ASN:HB2	2.38	0.58
1:B:1112:ASP:OD1	1:B:1113:VAL:HG23	2.03	0.58
1:B:4966:ASP:OD1	1:B:4967:TYR:N	2.35	0.58
1:D:2572:THR:CG2	1:D:2579:VAL:HG21	2.33	0.58
1:C:69:LEU:CD1	1:C:101:LEU:HD11	2.34	0.58
1:C:4749:GLU:C	1:C:4753:HIS:HD1	2.07	0.58
1:A:1925:GLY:O	1:A:1929:MET:HG3	2.04	0.58
1:C:228:ASP:OD1	1:C:229:GLU:N	2.36	0.58
1:C:884:LEU:O	1:C:888:GLU:OE1	2.20	0.58
1:C:3985:LEU:O	1:C:3989:VAL:HG23	2.03	0.58
1:A:904:HIS:ND1	1:A:906:CYS:SG	2.73	0.58
1:A:2572:THR:CG2	1:A:2579:VAL:HG21	2.33	0.58
1:B:3398:PHE:CE2	1:B:3450:ASN:HB2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3442:PHE:CG	1:B:3514:LEU:HD22	2.39	0.58
1:B:4998:LYS:HB3	1:B:5003:HIS:HE1	1.68	0.58
1:D:884:LEU:O	1:D:888:GLU:OE1	2.20	0.58
1:D:3227:ARG:HB3	1:D:3232:LEU:HD12	1.83	0.58
1:A:2974:ILE:HD13	1:A:3049:LEU:CD1	2.33	0.58
1:A:3372:VAL:CG1	1:A:3398:PHE:CE1	2.87	0.58
1:B:1925:GLY:O	1:B:1929:MET:HG3	2.04	0.58
1:B:3559:LEU:O	1:B:3559:LEU:HD23	2.03	0.58
1:C:3398:PHE:CE2	1:C:3450:ASN:HB2	2.38	0.58
1:C:3442:PHE:CG	1:C:3514:LEU:HD22	2.39	0.58
1:A:2781:VAL:HG23	1:A:2789:PRO:HG3	1.86	0.57
1:B:110:ARG:HD3	1:B:115:ARG:HE	1.70	0.57
1:D:3398:PHE:CE2	1:D:3450:ASN:HB2	2.39	0.57
1:B:1427:ILE:HG23	1:B:1428:LEU:HD22	1.84	0.57
1:D:110:ARG:HD3	1:D:115:ARG:HE	1.70	0.57
1:D:233:ILE:O	1:D:257:ARG:NH1	2.35	0.57
1:D:4749:GLU:C	1:D:4753:HIS:HD1	2.07	0.57
1:C:233:ILE:O	1:C:257:ARG:NH1	2.35	0.57
1:C:3559:LEU:O	1:C:3559:LEU:HD23	2.03	0.57
1:A:69:LEU:CD1	1:A:101:LEU:HD11	2.34	0.57
1:B:3566:SER:HB3	1:B:3569:LEU:HD12	1.86	0.57
1:D:1112:ASP:OD1	1:D:1113:VAL:HG23	2.03	0.57
1:D:3357:HIS:O	1:D:3361:THR:HG23	2.03	0.57
1:C:2586:VAL:HG13	1:C:2607:LEU:HD13	1.87	0.57
1:C:3566:SER:HB3	1:C:3569:LEU:HD12	1.86	0.57
1:A:1441:ALA:N	1:A:1513:ASP:OD1	2.34	0.57
1:B:69:LEU:CD1	1:B:101:LEU:HD11	2.34	0.57
1:B:1748:PHE:HB3	1:B:1758:ARG:NH1	2.20	0.57
1:B:4634:GLU:OE1	1:B:4636:THR:OG1	2.16	0.57
1:D:554:LEU:HD11	1:D:1593:PRO:CG	2.35	0.57
1:D:3442:PHE:CG	1:D:3514:LEU:HD22	2.39	0.57
1:C:904:HIS:ND1	1:C:906:CYS:SG	2.73	0.57
1:C:2572:THR:CG2	1:C:2579:VAL:HG21	2.33	0.57
1:A:1748:PHE:HB3	1:A:1758:ARG:NH1	2.20	0.57
1:B:3372:VAL:CG1	1:B:3398:PHE:CE1	2.87	0.57
1:B:4630:TYR:OH	1:C:4860:ARG:NH1	2.37	0.57
1:D:4998:LYS:HB3	1:D:5003:HIS:HE1	1.68	0.57
1:C:2382:GLU:OE2	1:C:2392:ARG:NH2	2.38	0.57
1:C:3372:VAL:CG1	1:C:3398:PHE:CE1	2.87	0.57
1:C:4998:LYS:HB3	1:C:5003:HIS:HE1	1.68	0.57
1:A:3254:GLY:O	1:A:3258:GLU:OE1	2.23	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1441:ALA:N	1:D:1513:ASP:OD1	2.34	0.57
1:D:3498:ARG:O	1:D:3501:ASP:N	2.38	0.57
1:C:1748:PHE:HB3	1:C:1758:ARG:NH1	2.20	0.57
1:C:3254:GLY:O	1:C:3258:GLU:OE1	2.23	0.57
1:C:3324:VAL:CG1	1:C:3361:THR:HG22	2.33	0.57
1:A:110:ARG:HD3	1:A:115:ARG:HE	1.70	0.57
1:A:554:LEU:HD11	1:A:1593:PRO:CG	2.35	0.57
1:A:2382:GLU:OE2	1:A:2392:ARG:NH2	2.38	0.57
1:A:3442:PHE:CG	1:A:3514:LEU:HD22	2.39	0.57
1:D:1748:PHE:HB3	1:D:1758:ARG:NH1	2.19	0.57
1:D:1925:GLY:O	1:D:1929:MET:HG3	2.04	0.57
1:D:3179:LYS:O	1:D:3180:ASN:ND2	2.38	0.57
1:C:1497:GLY:O	1:C:1501:VAL:HG13	2.05	0.57
1:A:3498:ARG:O	1:A:3501:ASP:N	2.38	0.57
1:B:3179:LYS:O	1:B:3180:ASN:ND2	2.38	0.57
1:B:3236:VAL:HA	1:B:3239:MET:HG2	1.86	0.57
1:D:1497:GLY:O	1:D:1501:VAL:HG13	2.05	0.57
1:B:554:LEU:HD11	1:B:1593:PRO:CG	2.35	0.57
1:B:2974:ILE:HD13	1:B:3049:LEU:CD1	2.33	0.57
1:D:3372:VAL:CG1	1:D:3398:PHE:CE1	2.87	0.57
1:C:554:LEU:HD11	1:C:1593:PRO:CG	2.35	0.57
1:C:3179:LYS:O	1:C:3180:ASN:ND2	2.38	0.57
1:A:2761:TYR:HB3	1:A:2765:LYS:HZ3	1.68	0.57
1:A:2782:ASP:N	1:A:2782:ASP:OD1	2.38	0.57
1:B:2382:GLU:OE2	1:B:2392:ARG:NH2	2.38	0.57
1:B:2586:VAL:HG13	1:B:2607:LEU:HD13	1.87	0.57
1:B:3498:ARG:O	1:B:3501:ASP:N	2.38	0.57
1:A:3179:LYS:O	1:A:3180:ASN:ND2	2.38	0.56
1:A:4749:GLU:C	1:A:4753:HIS:HD1	2.07	0.56
1:B:3137:LEU:HD23	1:B:3189:ALA:HB1	1.86	0.56
1:B:3254:GLY:O	1:B:3258:GLU:OE1	2.23	0.56
1:D:2780:ASN:OD1	1:D:2781:VAL:N	2.38	0.56
1:C:3137:LEU:HD23	1:C:3189:ALA:HB1	1.86	0.56
1:A:907:LEU:O	1:A:908:VAL:HB	2.05	0.56
1:B:812:HIS:O	1:B:815:VAL:HG12	2.05	0.56
1:D:2226:PRO:CB	1:D:2267:MET:HE1	2.34	0.56
1:D:2586:VAL:HG13	1:D:2607:LEU:HD13	1.87	0.56
1:D:3254:GLY:O	1:D:3258:GLU:OE1	2.23	0.56
1:C:110:ARG:HD3	1:C:115:ARG:HE	1.70	0.56
1:C:2780:ASN:OD1	1:C:2781:VAL:N	2.38	0.56
1:B:553:ARG:NE	1:B:555:GLU:OE2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:904:HIS:ND1	1:B:906:CYS:SG	2.73	0.56
1:B:5034:ASP:OD1	1:B:5035:GLN:N	2.38	0.56
1:D:812:HIS:O	1:D:815:VAL:HG12	2.05	0.56
1:D:1980:LEU:CD1	1:D:1991:THR:HG23	2.36	0.56
1:D:2382:GLU:OE2	1:D:2392:ARG:NH2	2.38	0.56
1:D:2782:ASP:N	1:D:2782:ASP:OD1	2.38	0.56
1:D:4860:ARG:NH1	1:C:4630:TYR:OH	2.36	0.56
1:C:812:HIS:O	1:C:815:VAL:HG12	2.05	0.56
1:C:2781:VAL:HG23	1:C:2789:PRO:HG3	1.86	0.56
1:C:3498:ARG:O	1:C:3501:ASP:N	2.38	0.56
1:B:721:LEU:HD12	1:B:1476:MET:HE1	1.87	0.56
1:B:907:LEU:O	1:B:908:VAL:HB	2.05	0.56
1:D:1461:ASP:OD2	1:D:1468:LYS:NZ	2.37	0.56
1:A:233:ILE:O	1:A:257:ARG:NH1	2.35	0.56
1:A:384:MET:CE	1:B:167:ASP:OD1	2.54	0.56
1:A:1980:LEU:CD1	1:A:1991:THR:HG23	2.35	0.56
1:A:3137:LEU:HD23	1:A:3189:ALA:HB1	1.86	0.56
1:B:991:ASN:O	1:B:995:VAL:HG23	2.05	0.56
1:B:2780:ASN:OD1	1:B:2781:VAL:N	2.38	0.56
1:D:2572:THR:O	1:D:2618:MET:HE2	2.06	0.56
1:D:2781:VAL:HG23	1:D:2789:PRO:HG3	1.85	0.56
1:D:3137:LEU:HD23	1:D:3189:ALA:HB1	1.86	0.56
1:D:5034:ASP:OD1	1:D:5035:GLN:N	2.38	0.56
1:C:1461:ASP:OD2	1:C:1468:LYS:NZ	2.37	0.56
1:C:1980:LEU:CD1	1:C:1991:THR:HG23	2.36	0.56
1:C:3629:ARG:O	1:C:3633:VAL:HG23	2.06	0.56
1:A:167:ASP:HA	1:D:384:MET:SD	2.45	0.56
1:A:1497:GLY:O	1:A:1501:VAL:HG13	2.05	0.56
1:A:5034:ASP:OD1	1:A:5035:GLN:N	2.38	0.56
1:B:861:ILE:HD13	1:B:930:LYS:HD3	1.87	0.56
1:B:1497:GLY:O	1:B:1501:VAL:HG13	2.05	0.56
1:B:3327:LEU:HD12	1:B:3364:ARG:HH12	1.70	0.56
1:B:3398:PHE:HE2	1:B:3450:ASN:HB2	1.71	0.56
1:B:4768:LEU:HA	1:B:4771:ILE:HD12	1.87	0.56
1:D:897:ARG:HB2	1:D:905:PRO:HD3	1.88	0.56
1:D:3114:LYS:HD2	1:D:3125:VAL:HG21	1.88	0.56
1:C:907:LEU:O	1:C:908:VAL:HB	2.05	0.56
1:C:5034:ASP:OD1	1:C:5035:GLN:N	2.38	0.56
1:A:812:HIS:O	1:A:815:VAL:HG12	2.05	0.56
1:A:3566:SER:HB3	1:A:3569:LEU:HD12	1.86	0.56
1:A:3629:ARG:O	1:A:3633:VAL:HG23	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2608:MET:O	1:D:2612[B]:ARG:HG3	2.06	0.56
1:C:991:ASN:O	1:C:995:VAL:HG23	2.05	0.56
1:A:554:LEU:HD11	1:A:1593:PRO:HG3	1.88	0.56
1:D:991:ASN:O	1:D:995:VAL:HG23	2.05	0.56
1:D:2212:VAL:HG21	1:D:2256:TYR:HH	1.71	0.56
1:D:4768:LEU:HA	1:D:4771:ILE:HD12	1.87	0.56
1:C:553:ARG:NE	1:C:555:GLU:OE2	2.38	0.56
1:C:3114:LYS:HD2	1:C:3125:VAL:HG21	1.88	0.56
1:C:3398:PHE:HE2	1:C:3450:ASN:HB2	1.71	0.56
1:A:2523:ASP:HB3	1:A:2578:MET:HE2	1.88	0.56
1:A:2586:VAL:HG13	1:A:2607:LEU:HD13	1.87	0.56
1:A:3852:LYS:O	1:A:3856:LEU:HG	2.06	0.56
1:B:1157:GLU:OE1	1:B:1157:GLU:N	2.39	0.56
1:B:4061:PHE:HA	1:B:4064:MET:HE3	1.88	0.56
1:D:554:LEU:HD11	1:D:1593:PRO:HG3	1.88	0.56
1:D:3566:SER:HB3	1:D:3569:LEU:HD12	1.86	0.56
1:D:3629:ARG:O	1:D:3633:VAL:HG23	2.06	0.56
1:C:897:ARG:HB2	1:C:905:PRO:HD3	1.88	0.56
1:C:941:MET:HE3	1:C:1051:TYR:CZ	2.41	0.56
1:A:167:ASP:OD1	1:D:384:MET:CE	2.54	0.56
1:A:991:ASN:O	1:A:995:VAL:HG23	2.05	0.56
1:A:3166:TYR:OH	1:A:3203:VAL:HG11	2.06	0.56
1:A:3372:VAL:HG12	1:A:3398:PHE:HE1	1.71	0.56
1:A:3398:PHE:HE2	1:A:3450:ASN:HB2	1.71	0.56
1:A:4768:LEU:HA	1:A:4771:ILE:HD12	1.87	0.56
1:C:125:ARG:HB3	1:C:125:ARG:HH11	1.71	0.56
1:C:499:THR:HG23	1:C:502:HIS:H	1.71	0.56
1:B:499:THR:HG23	1:B:502:HIS:H	1.71	0.55
1:B:897:ARG:HB2	1:B:905:PRO:HD3	1.87	0.55
1:B:2608:MET:O	1:B:2612[B]:ARG:HG3	2.06	0.55
1:D:213:TYR:CE1	1:D:340:LYS:HG2	2.42	0.55
1:D:3327:LEU:HD12	1:D:3364:ARG:HH12	1.70	0.55
1:C:2572:THR:O	1:C:2618:MET:HE2	2.06	0.55
1:C:4651:THR:CB	1:C:4803:HIS:HE2	2.19	0.55
1:A:2780:ASN:OD1	1:A:2781:VAL:N	2.38	0.55
1:A:3327:LEU:HD12	1:A:3364:ARG:HH12	1.70	0.55
1:B:1980:LEU:CD1	1:B:1991:THR:HG23	2.36	0.55
1:B:2642:LYS:HG3	1:B:2698:MET:HE3	1.86	0.55
1:B:3852:LYS:O	1:B:3856:LEU:HG	2.06	0.55
1:D:861:ILE:HD13	1:D:930:LYS:HD3	1.87	0.55
1:D:2211:MET:O	1:D:2215:LEU:HD13	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4749:GLU:HB3	1:D:4753:HIS:CE1	2.41	0.55
1:C:2608:MET:O	1:C:2612[B]:ARG:HG3	2.06	0.55
1:B:3166:TYR:OH	1:B:3203:VAL:HG11	2.06	0.55
1:B:3239:MET:CG	1:B:3239:MET:HA	2.35	0.55
1:D:125:ARG:HH11	1:D:125:ARG:HB3	1.71	0.55
1:D:907:LEU:O	1:D:908:VAL:HB	2.05	0.55
1:D:928:THR:O	1:D:932:LEU:HD23	2.07	0.55
1:C:213:TYR:CE1	1:C:340:LYS:HG2	2.42	0.55
1:C:861:ILE:HD13	1:C:930:LYS:HD3	1.87	0.55
1:C:4061:PHE:HA	1:C:4064:MET:HE3	1.88	0.55
1:A:67:PHE:HB3	1:A:109:LEU:HD22	1.89	0.55
1:A:1157:GLU:OE1	1:A:1157:GLU:N	2.39	0.55
1:A:3114:LYS:HD2	1:A:3125:VAL:HG21	1.88	0.55
1:D:3372:VAL:HG12	1:D:3398:PHE:HE1	1.71	0.55
1:C:2211:MET:O	1:C:2215:LEU:HD13	2.06	0.55
1:C:3327:LEU:HD12	1:C:3364:ARG:HH12	1.70	0.55
1:A:1931:LEU:HD22	1:A:1935:VAL:HG11	1.88	0.55
1:A:4860:ARG:NH1	1:D:4630:TYR:OH	2.39	0.55
1:B:928:THR:O	1:B:932:LEU:HD23	2.07	0.55
1:B:3629:ARG:O	1:B:3633:VAL:HG23	2.06	0.55
1:C:928:THR:O	1:C:932:LEU:HD23	2.06	0.55
1:C:1931:LEU:HD22	1:C:1935:VAL:HG11	1.88	0.55
1:C:3635:CYS:HA	1:C:3638:MET:HG3	1.88	0.55
1:C:4749:GLU:HB3	1:C:4753:HIS:CE1	2.41	0.55
1:A:861:ILE:HD13	1:A:930:LYS:HD3	1.87	0.55
1:A:897:ARG:HB2	1:A:905:PRO:HD3	1.88	0.55
1:A:2211:MET:O	1:A:2215:LEU:HD13	2.06	0.55
1:B:2211:MET:O	1:B:2215:LEU:HD13	2.06	0.55
1:D:499:THR:HG23	1:D:502:HIS:H	1.71	0.55
1:D:4061:PHE:HA	1:D:4064:MET:HE3	1.89	0.55
1:A:553:ARG:NE	1:A:555:GLU:OE2	2.38	0.55
1:A:908:VAL:O	1:A:963:ASN:CG	2.45	0.55
1:B:67:PHE:HB3	1:B:109:LEU:HD22	1.89	0.55
1:B:1726:SER:O	1:B:1729:SER:OG	2.23	0.55
1:B:4651:THR:CB	1:B:4803:HIS:HE2	2.19	0.55
1:D:2874:MET:HE1	1:D:2939:ARG:HB2	1.84	0.55
1:D:3398:PHE:HE2	1:D:3450:ASN:HB2	1.71	0.55
1:D:4205:TRP:CE3	1:D:4989:MET:HE2	2.41	0.55
1:C:2233:CYS:HB3	1:C:2237:CYS:HG	1.60	0.55
1:A:112:ALA:O	1:A:115:ARG:NH1	2.39	0.55
1:A:499:THR:HG23	1:A:502:HIS:H	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1158:ASN:ND2	1:B:1182:ILE:O	2.40	0.55
1:B:3635:CYS:HA	1:B:3638:MET:HG3	1.88	0.55
1:D:3852:LYS:O	1:D:3856:LEU:HG	2.06	0.55
1:D:4651:THR:CB	1:D:4803:HIS:HE2	2.19	0.55
1:C:1157:GLU:OE1	1:C:1157:GLU:N	2.39	0.55
1:C:1726:SER:O	1:C:1729:SER:OG	2.23	0.55
1:C:2782:ASP:OD1	1:C:2782:ASP:N	2.38	0.55
1:A:125:ARG:HB3	1:A:125:ARG:HH11	1.71	0.55
1:A:928:THR:O	1:A:932:LEU:HD23	2.06	0.55
1:A:2608:MET:O	1:A:2612[B]:ARG:HG3	2.06	0.55
1:A:4061:PHE:HA	1:A:4064:MET:HE3	1.88	0.55
1:B:112:ALA:O	1:B:115:ARG:NH1	2.38	0.55
1:B:2904:LEU:O	1:B:2904:LEU:HD23	2.07	0.55
1:C:1158:ASN:ND2	1:C:1182:ILE:O	2.40	0.55
1:C:4768:LEU:HA	1:C:4771:ILE:HD12	1.87	0.55
1:A:213:TYR:CE1	1:A:340:LYS:HG2	2.42	0.55
1:B:908:VAL:HG13	1:B:912:SER:HB2	1.89	0.55
1:C:112:ALA:O	1:C:115:ARG:NH1	2.39	0.55
1:C:931:THR:O	1:C:935:LEU:HD23	2.07	0.55
1:A:4749:GLU:HB3	1:A:4753:HIS:CE1	2.41	0.54
1:B:554:LEU:HD11	1:B:1593:PRO:HG3	1.88	0.54
1:B:3372:VAL:HG12	1:B:3398:PHE:HE1	1.71	0.54
1:D:1931:LEU:HD22	1:D:1935:VAL:HG11	1.88	0.54
1:D:2790:MET:SD	1:D:2797:PHE:HZ	2.30	0.54
1:D:2907:PRO:HB2	1:D:2910:THR:HG23	1.89	0.54
1:D:3635:CYS:HA	1:D:3638:MET:HG3	1.88	0.54
1:C:3166:TYR:OH	1:C:3203:VAL:HG11	2.06	0.54
1:A:2790:MET:SD	1:A:2797:PHE:HZ	2.30	0.54
1:A:2907:PRO:HB2	1:A:2910:THR:HG23	1.89	0.54
1:A:3635:CYS:HA	1:A:3638:MET:HG3	1.88	0.54
1:B:985:VAL:HG13	1:B:1039:LEU:HD22	1.89	0.54
1:B:2625:ARG:NH1	1:B:2629:ASP:CG	2.61	0.54
1:B:3114:LYS:HD2	1:B:3125:VAL:HG21	1.88	0.54
1:D:908:VAL:HG13	1:D:912:SER:HB2	1.89	0.54
1:D:931:THR:O	1:D:935:LEU:HD23	2.07	0.54
1:C:554:LEU:HD11	1:C:1593:PRO:HG3	1.88	0.54
1:C:908:VAL:O	1:C:963:ASN:CG	2.45	0.54
1:C:2790:MET:SD	1:C:2797:PHE:HZ	2.30	0.54
1:C:3372:VAL:HG12	1:C:3398:PHE:HE1	1.71	0.54
1:A:384:MET:SD	1:B:167:ASP:HA	2.47	0.54
1:A:1158:ASN:ND2	1:A:1182:ILE:O	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4651:THR:CB	1:A:4803:HIS:HE2	2.19	0.54
1:B:213:TYR:CE1	1:B:340:LYS:HG2	2.42	0.54
1:B:908:VAL:O	1:B:963:ASN:CG	2.45	0.54
1:B:1931:LEU:HD22	1:B:1935:VAL:HG11	1.88	0.54
1:D:67:PHE:HB3	1:D:109:LEU:HD22	1.89	0.54
1:D:2761:TYR:HB3	1:D:2765:LYS:HZ3	1.73	0.54
1:A:877:ASN:O	1:A:880:GLU:HG2	2.07	0.54
1:A:931:THR:O	1:A:935:LEU:HD23	2.07	0.54
1:B:2642:LYS:HG3	1:B:2698:MET:HE1	1.88	0.54
1:B:2907:PRO:HB2	1:B:2910:THR:HG23	1.89	0.54
1:B:4749:GLU:HB3	1:B:4753:HIS:CE1	2.41	0.54
1:D:1045:THR:HG22	1:D:1049:TYR:CE2	2.43	0.54
1:D:1157:GLU:OE1	1:D:1157:GLU:N	2.39	0.54
1:D:3442:PHE:HE1	1:D:3511:VAL:HG12	1.73	0.54
1:C:1045:THR:HG22	1:C:1049:TYR:CE2	2.43	0.54
1:C:2625:ARG:NH1	1:C:2629:ASP:CG	2.61	0.54
1:C:2907:PRO:HB2	1:C:2910:THR:HG23	1.89	0.54
1:B:125:ARG:HB3	1:B:125:ARG:HH11	1.71	0.54
1:B:931:THR:O	1:B:935:LEU:HD23	2.07	0.54
1:B:3527:PRO:HD2	1:B:3573:MET:SD	2.48	0.54
1:D:908:VAL:O	1:D:963:ASN:CG	2.45	0.54
1:C:3442:PHE:HE1	1:C:3511:VAL:HG12	1.73	0.54
1:A:3957:VAL:O	1:A:3961:VAL:HG23	2.08	0.54
1:B:1833:SER:HG	1:B:1836:PHE:HD1	1.54	0.54
1:B:4180:ARG:HD3	1:B:4192:ARG:HD3	1.89	0.54
1:D:2904:LEU:HD23	1:D:2904:LEU:O	2.07	0.54
1:C:3162:GLN:OE1	1:C:3218:VAL:HG23	2.08	0.54
1:C:3682:GLU:O	1:C:3685:GLU:N	2.41	0.54
1:B:1749:PRO:N	1:B:1758:ARG:HH12	2.06	0.54
1:B:2790:MET:SD	1:B:2797:PHE:HZ	2.30	0.54
1:D:985:VAL:HG13	1:D:1039:LEU:HD22	1.89	0.54
1:C:3527:PRO:HD2	1:C:3573:MET:SD	2.48	0.54
1:C:3727:ASP:O	1:C:3731:LYS:HG3	2.08	0.54
1:C:3852:LYS:O	1:C:3856:LEU:HG	2.06	0.54
1:A:1045:THR:HG22	1:A:1049:TYR:CE2	2.43	0.54
1:A:3197:LEU:C	1:A:3197:LEU:HD23	2.29	0.54
2:E:90:ILE:HG22	2:E:91:ILE:HG13	1.90	0.54
1:B:1045:THR:HG22	1:B:1049:TYR:CE2	2.43	0.54
1:B:1101:ARG:NH1	1:B:1115:LEU:O	2.40	0.54
1:B:3957:VAL:O	1:B:3961:VAL:HG23	2.08	0.54
1:D:3162:GLN:OE1	1:D:3218:VAL:HG23	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4945:ASP:OD1	1:D:4946:GLN:N	2.41	0.54
1:C:1101:ARG:NH1	1:C:1115:LEU:O	2.40	0.54
1:C:2904:LEU:O	1:C:2904:LEU:HD23	2.07	0.54
1:A:3379:LEU:HD12	1:A:3382:GLU:OE2	2.08	0.54
1:B:3442:PHE:HE1	1:B:3511:VAL:HG12	1.73	0.54
1:D:590:LEU:HG	1:D:599:VAL:HG11	1.90	0.54
1:A:590:LEU:HG	1:A:599:VAL:HG11	1.90	0.54
1:A:2642:LYS:NZ	1:A:2698:MET:SD	2.81	0.54
1:A:2904:LEU:HD23	1:A:2904:LEU:O	2.07	0.54
1:A:4945:ASP:OD1	1:A:4946:GLN:N	2.41	0.54
1:B:877:ASN:O	1:B:880:GLU:HG2	2.07	0.54
1:D:445:LEU:HD23	1:D:525:LEU:HD22	1.90	0.54
1:D:1101:ARG:NH1	1:D:1115:LEU:O	2.40	0.54
1:D:3786:CYS:SG	1:D:3831:SER:OG	2.65	0.54
1:C:877:ASN:O	1:C:880:GLU:HG2	2.07	0.54
1:A:2625:ARG:NH1	1:A:2629:ASP:CG	2.61	0.53
1:A:3527:PRO:HD2	1:A:3573:MET:SD	2.48	0.53
1:B:3727:ASP:O	1:B:3731:LYS:HG3	2.08	0.53
1:D:877:ASN:O	1:D:880:GLU:HG2	2.07	0.53
1:D:3166:TYR:OH	1:D:3203:VAL:HG11	2.06	0.53
1:D:3197:LEU:C	1:D:3197:LEU:HD23	2.29	0.53
1:C:590:LEU:HG	1:C:599:VAL:HG11	1.90	0.53
1:C:2294:ASP:O	1:C:2298:VAL:HG23	2.08	0.53
1:C:2638:LYS:HE2	1:C:2694:GLU:OE1	2.08	0.53
1:A:906:CYS:HB2	1:A:913:LEU:CB	2.38	0.53
1:A:1461:ASP:OD2	1:A:1468:LYS:NZ	2.37	0.53
1:B:2627:VAL:HA	1:B:2678:LEU:HD13	1.91	0.53
1:B:2638:LYS:HE2	1:B:2694:GLU:OE1	2.08	0.53
1:B:3379:LEU:HD12	1:B:3382:GLU:OE2	2.08	0.53
1:B:3682:GLU:O	1:B:3685:GLU:N	2.41	0.53
1:D:2294:ASP:O	1:D:2298:VAL:HG23	2.08	0.53
1:D:3727:ASP:O	1:D:3731:LYS:HG3	2.08	0.53
1:C:67:PHE:HB3	1:C:109:LEU:HD22	1.89	0.53
1:C:1749:PRO:N	1:C:1758:ARG:HH12	2.06	0.53
1:C:3379:LEU:HD12	1:C:3382:GLU:OE2	2.08	0.53
1:A:1749:PRO:N	1:A:1758:ARG:HH12	2.06	0.53
1:A:2882:TYR:O	1:A:2885:THR:HG22	2.09	0.53
2:G:80:TYR:CE2	2:G:80:TYR:CD1	2.38	0.53
1:B:437:PRO:O	1:B:441:VAL:HG23	2.09	0.53
1:B:3197:LEU:HD23	1:B:3197:LEU:C	2.29	0.53
1:D:1158:ASN:ND2	1:D:1182:ILE:O	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:672:VAL:O	1:C:680:THR:OG1	2.08	0.53
1:C:1833:SER:HG	1:C:1836:PHE:HD1	1.56	0.53
1:C:4945:ASP:OD1	1:C:4946:GLN:N	2.41	0.53
1:A:908:VAL:HG13	1:A:912:SER:HB2	1.89	0.53
1:A:1999:ARG:HH12	1:A:3636:PHE:CA	2.18	0.53
1:A:2294:ASP:O	1:A:2298:VAL:HG23	2.08	0.53
1:A:3727:ASP:O	1:A:3731:LYS:HG3	2.08	0.53
2:F:4:VAL:HG22	2:F:74:LEU:CD2	2.39	0.53
1:B:906:CYS:HB2	1:B:913:LEU:CB	2.38	0.53
1:B:1066:GLN:O	1:B:1071:ARG:NE	2.42	0.53
1:B:1999:ARG:HH12	1:B:3636:PHE:CA	2.18	0.53
1:B:2642:LYS:NZ	1:B:2698:MET:SD	2.81	0.53
1:B:2782:ASP:N	1:B:2782:ASP:OD1	2.38	0.53
1:D:906:CYS:HB2	1:D:913:LEU:CB	2.38	0.53
1:D:1123:VAL:HG23	1:D:1132:TRP:HB2	1.91	0.53
1:D:2882:TYR:O	1:D:2885:THR:HG22	2.09	0.53
1:C:2627:VAL:HA	1:C:2678:LEU:HD13	1.91	0.53
1:C:2761:TYR:HB3	1:C:2765:LYS:HZ3	1.73	0.53
1:C:2882:TYR:O	1:C:2885:THR:HG22	2.09	0.53
1:C:4180:ARG:HD3	1:C:4192:ARG:HD3	1.89	0.53
1:A:1066:GLN:O	1:A:1071:ARG:NE	2.42	0.53
1:A:3442:PHE:HE1	1:A:3511:VAL:HG12	1.73	0.53
2:G:4:VAL:HG22	2:G:74:LEU:CD2	2.39	0.53
1:B:1987:SER:O	1:B:1991:THR:OG1	2.08	0.53
1:D:69:LEU:HD23	1:D:109:LEU:CD2	2.39	0.53
1:D:553:ARG:NE	1:D:555:GLU:OE2	2.38	0.53
1:D:2642:LYS:NZ	1:D:2698:MET:SD	2.81	0.53
1:D:2969:ILE:O	1:D:2973:PHE:CD1	2.62	0.53
1:C:286:THR:HG21	1:C:481:GLU:OE1	2.09	0.53
1:C:437:PRO:O	1:C:441:VAL:HG23	2.09	0.53
1:C:906:CYS:HB2	1:C:913:LEU:CB	2.38	0.53
1:A:445:LEU:HD23	1:A:525:LEU:HD22	1.91	0.53
1:A:1287:LEU:HD11	1:A:1599:MET:HE3	1.90	0.53
1:A:3682:GLU:O	1:A:3685:GLU:N	2.41	0.53
1:D:2625:ARG:NH1	1:D:2629:ASP:CG	2.61	0.53
1:C:3957:VAL:O	1:C:3961:VAL:HG23	2.08	0.53
1:C:4222:VAL:HG11	1:C:4950:VAL:HA	1.90	0.53
1:A:56:GLN:O	1:A:281:ARG:NH2	2.42	0.53
1:A:652:ARG:NH1	1:A:750:LEU:O	2.42	0.53
1:A:1833:SER:HG	1:A:1836:PHE:HD1	1.56	0.53
1:A:2974:ILE:O	1:A:2978:GLU:OE1	2.27	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3372:VAL:HG12	1:B:3398:PHE:CE1	2.44	0.53
1:B:4945:ASP:OD1	1:B:4946:GLN:N	2.41	0.53
1:D:112:ALA:O	1:D:115:ARG:NH1	2.38	0.53
1:D:437:PRO:O	1:D:441:VAL:HG23	2.09	0.53
1:D:3527:PRO:HD2	1:D:3573:MET:SD	2.48	0.53
1:D:3682:GLU:O	1:D:3685:GLU:N	2.41	0.53
1:C:652:ARG:NH1	1:C:750:LEU:O	2.42	0.53
1:C:1123:VAL:HG23	1:C:1132:TRP:HB2	1.91	0.53
1:C:2874:MET:HE1	1:C:2939:ARG:CB	2.37	0.53
1:A:2969:ILE:O	1:A:2973:PHE:CD1	2.62	0.53
2:H:4:VAL:HG22	2:H:74:LEU:CD2	2.39	0.53
2:H:90:ILE:HG22	2:H:91:ILE:HG13	1.90	0.53
2:G:90:ILE:HG22	2:G:91:ILE:HG13	1.90	0.53
2:F:90:ILE:HD11	1:B:1684:ALA:HA	1.91	0.53
1:B:2294:ASP:O	1:B:2298:VAL:HG23	2.08	0.53
1:D:652:ARG:NH1	1:D:750:LEU:O	2.42	0.53
1:C:961:MET:HE3	1:C:963:ASN:CB	2.17	0.53
1:C:3239:MET:CG	1:C:3239:MET:HA	2.35	0.53
1:C:3755:GLU:O	1:C:3759:GLU:OE1	2.27	0.53
1:C:4998:LYS:HB3	1:C:5003:HIS:CE1	2.44	0.53
1:A:437:PRO:O	1:A:441:VAL:HG23	2.09	0.53
1:A:3755:GLU:O	1:A:3759:GLU:OE1	2.27	0.53
1:B:286:THR:HG21	1:B:481:GLU:OE1	2.09	0.53
1:B:590:LEU:HG	1:B:599:VAL:HG11	1.90	0.53
1:B:1123:VAL:HG23	1:B:1132:TRP:HB2	1.91	0.53
1:B:2233:CYS:HA	1:B:2237:CYS:SG	2.49	0.53
1:B:2874:MET:HE1	1:B:2939:ARG:HB2	1.90	0.53
1:B:4222:VAL:HG11	1:B:4950:VAL:HA	1.90	0.53
1:D:1287:LEU:HD11	1:D:1599:MET:HE3	1.90	0.53
1:D:1749:PRO:N	1:D:1758:ARG:HH12	2.06	0.53
1:D:3379:LEU:HD12	1:D:3382:GLU:OE2	2.08	0.53
1:C:445:LEU:HD23	1:C:525:LEU:HD22	1.91	0.53
1:C:908:VAL:HG13	1:C:912:SER:HB2	1.89	0.53
1:C:985:VAL:HG13	1:C:1039:LEU:HD22	1.89	0.53
1:C:1287:LEU:HD11	1:C:1599:MET:HE3	1.91	0.53
1:C:2642:LYS:NZ	1:C:2698:MET:SD	2.81	0.53
1:C:3197:LEU:HD23	1:C:3197:LEU:C	2.29	0.53
1:C:4205:TRP:CE3	1:C:4989:MET:HE2	2.44	0.53
1:A:3239:MET:CG	1:A:3239:MET:HA	2.34	0.53
1:A:4222:VAL:HG11	1:A:4950:VAL:HA	1.90	0.53
1:B:213:TYR:CE1	1:B:340:LYS:CG	2.92	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1855:GLY:O	1:B:1859:VAL:HG23	2.09	0.53
1:B:3162:GLN:OE1	1:B:3218:VAL:HG23	2.08	0.53
1:D:286:THR:HG21	1:D:481:GLU:OE1	2.09	0.53
1:D:2974:ILE:O	1:D:2978:GLU:OE1	2.27	0.53
1:C:633:LEU:HD13	1:C:1639:LEU:HD21	1.91	0.53
1:C:887:ILE:CG2	1:C:959:TYR:OH	2.57	0.53
1:C:1066:GLN:O	1:C:1071:ARG:NE	2.42	0.53
1:C:1749:PRO:C	1:C:1758:ARG:NH2	2.45	0.53
1:C:2969:ILE:O	1:C:2973:PHE:CD1	2.62	0.53
1:A:803:LEU:HD12	1:A:804:PRO:HD2	1.91	0.52
1:A:3162:GLN:OE1	1:A:3218:VAL:HG23	2.08	0.52
1:A:4984:ASN:OD1	1:A:4986:ALA:HB3	2.09	0.52
1:B:633:LEU:HD13	1:B:1639:LEU:HD21	1.91	0.52
1:B:2974:ILE:O	1:B:2978:GLU:OE1	2.27	0.52
1:D:803:LEU:HD12	1:D:804:PRO:HD2	1.91	0.52
1:D:4222:VAL:HG11	1:D:4950:VAL:HA	1.90	0.52
1:C:69:LEU:HD23	1:C:109:LEU:CD2	2.39	0.52
1:C:236:ALA:O	1:C:237:ASP:OD2	2.28	0.52
1:C:1855:GLY:O	1:C:1859:VAL:HG23	2.09	0.52
1:C:1926:LEU:HD23	1:C:1929:MET:SD	2.49	0.52
1:A:213:TYR:CE1	1:A:340:LYS:CG	2.92	0.52
1:A:228:ASP:OD2	1:B:155:LYS:HE2	2.08	0.52
1:A:985:VAL:HG13	1:A:1039:LEU:HD22	1.89	0.52
1:A:4180:ARG:HD3	1:A:4192:ARG:HD3	1.89	0.52
1:B:56:GLN:O	1:B:281:ARG:NH2	2.42	0.52
1:B:445:LEU:HD23	1:B:525:LEU:HD22	1.91	0.52
1:D:236:ALA:O	1:D:237:ASP:OD2	2.28	0.52
1:D:1066:GLN:O	1:D:1071:ARG:NE	2.42	0.52
1:D:1999:ARG:HH12	1:D:3636:PHE:CA	2.18	0.52
1:D:2233:CYS:HA	1:D:2237:CYS:SG	2.50	0.52
1:D:3957:VAL:O	1:D:3961:VAL:HG23	2.08	0.52
1:D:4180:ARG:HD3	1:D:4192:ARG:HD3	1.89	0.52
1:A:236:ALA:O	1:A:237:ASP:OD2	2.27	0.52
1:A:973:SER:O	1:A:976:ARG:NH1	2.43	0.52
1:A:1855:GLY:O	1:A:1859:VAL:HG23	2.09	0.52
1:A:3372:VAL:HG12	1:A:3398:PHE:CE1	2.44	0.52
2:E:4:VAL:HG22	2:E:74:LEU:CD2	2.39	0.52
1:B:69:LEU:HD23	1:B:109:LEU:CD2	2.39	0.52
1:B:1287:LEU:HD11	1:B:1599:MET:HE3	1.91	0.52
1:B:2929:PHE:CA	1:B:2932:MET:HE1	2.27	0.52
1:D:973:SER:O	1:D:976:ARG:NH1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:633:LEU:HD13	1:A:1639:LEU:HD21	1.91	0.52
1:A:1926:LEU:HD23	1:A:1929:MET:SD	2.49	0.52
1:B:3621:HIS:O	1:B:3621:HIS:ND1	2.38	0.52
1:D:1855:GLY:O	1:D:1859:VAL:HG23	2.09	0.52
1:D:4984:ASN:OD1	1:D:4986:ALA:HB3	2.09	0.52
1:C:803:LEU:HD12	1:C:804:PRO:HD2	1.91	0.52
1:A:1123:VAL:HG23	1:A:1132:TRP:HB2	1.91	0.52
1:B:688:LEU:HD12	1:B:776:LEU:O	2.10	0.52
1:D:688:LEU:HD12	1:D:776:LEU:O	2.10	0.52
1:D:1999:ARG:HH12	1:D:3636:PHE:HD1	1.58	0.52
1:D:3755:GLU:O	1:D:3759:GLU:OE1	2.27	0.52
1:A:887:ILE:CG2	1:A:959:TYR:OH	2.58	0.52
1:A:1812:LEU:HD11	1:A:1858:ASP:HB3	1.92	0.52
1:A:2233:CYS:HA	1:A:2237:CYS:SG	2.49	0.52
1:A:2626:LEU:HD22	1:A:2640:PRO:HB3	1.92	0.52
1:A:4205:TRP:CE3	1:A:4989:MET:HE2	2.44	0.52
2:F:90:ILE:HG22	2:F:91:ILE:HG13	1.90	0.52
1:B:236:ALA:O	1:B:237:ASP:OD2	2.28	0.52
1:B:3514:LEU:HD21	1:B:3602:VAL:HG13	1.92	0.52
1:D:213:TYR:CE1	1:D:340:LYS:CG	2.92	0.52
1:D:633:LEU:HD13	1:D:1639:LEU:HD21	1.91	0.52
1:D:887:ILE:CG2	1:D:959:TYR:OH	2.58	0.52
1:D:4118:ASP:OD1	1:D:4122:MET:N	2.42	0.52
1:C:973:SER:O	1:C:976:ARG:NH1	2.43	0.52
1:A:2627:VAL:HA	1:A:2678:LEU:HD13	1.90	0.52
1:A:4998:LYS:HB3	1:A:5003:HIS:CE1	2.44	0.52
1:B:652:ARG:NH1	1:B:750:LEU:O	2.42	0.52
1:B:803:LEU:HD12	1:B:804:PRO:HD2	1.91	0.52
1:B:973:SER:O	1:B:976:ARG:NH1	2.43	0.52
1:B:1926:LEU:HD23	1:B:1929:MET:SD	2.49	0.52
1:B:2969:ILE:O	1:B:2973:PHE:CD1	2.62	0.52
1:B:4677:LEU:HD23	1:B:4711:PHE:CZ	2.45	0.52
1:D:56:GLN:O	1:D:281:ARG:NH2	2.42	0.52
1:D:1812:LEU:HD11	1:D:1858:ASP:HB3	1.92	0.52
1:D:2627:VAL:HA	1:D:2678:LEU:HD13	1.90	0.52
1:D:2638:LYS:HE2	1:D:2694:GLU:OE1	2.08	0.52
1:D:3236:VAL:O	1:D:3239:MET:HG3	2.10	0.52
1:D:4241:THR:O	1:D:4245:MET:HG3	2.10	0.52
1:D:4661:TYR:OH	1:D:4786:ASP:OD2	2.26	0.52
1:C:56:GLN:O	1:C:281:ARG:NH2	2.42	0.52
1:A:69:LEU:HD23	1:A:109:LEU:CD2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3007:ASN:O	1:A:3011:THR:OG1	2.15	0.52
1:B:3755:GLU:O	1:B:3759:GLU:OE1	2.27	0.52
1:B:4984:ASN:OD1	1:B:4986:ALA:HB3	2.09	0.52
1:D:10:GLU:OE1	1:D:10:GLU:O	2.28	0.52
1:D:3532:LEU:HA	1:D:3535:LEU:HD12	1.92	0.52
1:C:688:LEU:HD12	1:C:776:LEU:O	2.10	0.52
1:C:2874:MET:HE1	1:C:2939:ARG:H	1.74	0.52
1:C:3372:VAL:HG12	1:C:3398:PHE:CE1	2.44	0.52
1:C:3607:GLU:O	1:C:3610:GLU:HG3	2.10	0.52
1:A:663:TYR:OH	1:A:665:GLU:OE2	2.27	0.52
1:B:1461:ASP:OD2	1:B:1468:LYS:NZ	2.37	0.52
1:D:1065:ASN:OD1	1:D:1066:GLN:N	2.43	0.52
1:D:1926:LEU:HD23	1:D:1929:MET:SD	2.49	0.52
1:D:2874:MET:HE1	1:D:2939:ARG:H	1.74	0.52
1:D:4677:LEU:HD23	1:D:4711:PHE:CZ	2.45	0.52
1:C:213:TYR:CE1	1:C:340:LYS:CG	2.92	0.52
1:C:3236:VAL:HA	1:C:3239:MET:HG2	1.90	0.52
1:C:4677:LEU:HD23	1:C:4711:PHE:CZ	2.45	0.52
1:C:4902:GLU:O	1:C:4913:ARG:CZ	2.58	0.52
1:A:10:GLU:OE1	1:A:10:GLU:O	2.28	0.52
1:A:286:THR:HG21	1:A:481:GLU:OE1	2.09	0.52
1:B:887:ILE:CG2	1:B:959:TYR:OH	2.58	0.52
1:B:1065:ASN:OD1	1:B:1066:GLN:N	2.43	0.52
1:B:2233:CYS:HB3	1:B:2237:CYS:HG	1.62	0.52
1:B:4705:VAL:HG13	1:B:4711:PHE:HE1	1.75	0.52
1:D:2625:ARG:HH12	1:D:2629:ASP:CG	2.12	0.52
1:D:3621:HIS:O	1:D:3622:LYS:HG2	2.10	0.52
1:C:2974:ILE:O	1:C:2978:GLU:OE1	2.27	0.52
1:C:3532:LEU:HA	1:C:3535:LEU:HD12	1.92	0.52
1:C:4984:ASN:OD1	1:C:4986:ALA:HB3	2.09	0.52
1:A:688:LEU:HD12	1:A:776:LEU:O	2.10	0.51
1:A:3589:PRO:O	1:A:3593:VAL:HG13	2.11	0.51
1:B:2882:TYR:O	1:B:2885:THR:HG22	2.09	0.51
1:B:4998:LYS:HB3	1:B:5003:HIS:CE1	2.44	0.51
1:D:4045:VAL:O	1:D:4049:VAL:HG23	2.11	0.51
1:C:2233:CYS:HA	1:C:2237:CYS:SG	2.49	0.51
1:A:1065:ASN:OD1	1:A:1066:GLN:N	2.43	0.51
1:A:4241:THR:O	1:A:4245:MET:HG3	2.10	0.51
1:B:3607:GLU:O	1:B:3610:GLU:HG3	2.10	0.51
1:D:3372:VAL:HG12	1:D:3398:PHE:CE1	2.44	0.51
1:C:3169:LEU:HD12	1:C:3194:LEU:HD11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3621:HIS:O	1:C:3622:LYS:HG2	2.10	0.51
1:A:3598:GLU:O	1:A:3602:VAL:HG23	2.11	0.51
1:A:4705:VAL:HG13	1:A:4711:PHE:HE1	1.75	0.51
1:C:4548:ARG:O	1:C:4552:LEU:HD13	2.11	0.51
1:A:3621:HIS:O	1:A:3622:LYS:HG2	2.10	0.51
1:D:2292:GLU:O	1:D:2296:GLU:OE1	2.29	0.51
1:D:3589:PRO:O	1:D:3593:VAL:HG13	2.11	0.51
1:D:4902:GLU:O	1:D:4913:ARG:CZ	2.58	0.51
1:C:1812:LEU:HD11	1:C:1858:ASP:HB3	1.92	0.51
1:C:2006:ILE:HD11	1:C:3641:LEU:HD11	1.93	0.51
1:C:3514:LEU:HD21	1:C:3602:VAL:HG13	1.92	0.51
1:A:2970:SER:O	1:A:2974:ILE:HG23	2.11	0.51
1:B:3598:GLU:O	1:B:3602:VAL:HG23	2.11	0.51
1:B:4548:ARG:O	1:B:4552:LEU:HD13	2.11	0.51
1:D:3183:VAL:O	1:D:3187:ARG:HG3	2.11	0.51
1:D:4548:ARG:O	1:D:4552:LEU:HD13	2.11	0.51
1:D:4998:LYS:HB3	1:D:5003:HIS:CE1	2.44	0.51
1:A:3372:VAL:CG1	1:A:3398:PHE:HE1	2.24	0.51
1:B:1812:LEU:HD11	1:B:1858:ASP:HB3	1.92	0.51
1:B:2572:THR:O	1:B:2618:MET:HE2	2.11	0.51
1:D:2006:ILE:HD11	1:D:3641:LEU:HD11	1.93	0.51
1:C:2626:LEU:HD22	1:C:2640:PRO:HB3	1.92	0.51
1:C:2970:SER:O	1:C:2974:ILE:HG23	2.11	0.51
1:C:4705:VAL:HG13	1:C:4711:PHE:HE1	1.75	0.51
1:A:3183:VAL:O	1:A:3187:ARG:HG3	2.11	0.51
2:G:6:THR:HG23	2:G:6:THR:O	2.11	0.51
1:B:646:PRO:HB2	1:B:648:ILE:CD1	2.41	0.51
1:B:2292:GLU:O	1:B:2296:GLU:OE1	2.29	0.51
1:B:3532:LEU:HA	1:B:3535:LEU:HD12	1.92	0.51
1:B:3621:HIS:O	1:B:3622:LYS:HG2	2.10	0.51
1:D:3169:LEU:HD12	1:D:3194:LEU:HD11	1.93	0.51
1:D:3607:GLU:O	1:D:3610:GLU:HG3	2.10	0.51
1:C:2798:SER:OG	1:C:2801:ASP:OD2	2.26	0.51
1:C:4241:THR:O	1:C:4245:MET:HG3	2.10	0.51
1:A:2520:HIS:O	1:A:2524:VAL:HG22	2.11	0.51
1:A:3554:GLN:OE1	1:A:3593:VAL:HG11	2.11	0.51
1:A:3607:GLU:O	1:A:3610:GLU:HG3	2.10	0.51
1:A:4548:ARG:O	1:A:4552:LEU:HD13	2.11	0.51
1:A:4677:LEU:HD23	1:A:4711:PHE:CZ	2.45	0.51
1:A:4902:GLU:O	1:A:4913:ARG:CZ	2.58	0.51
2:G:90:ILE:HD11	1:C:1684:ALA:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:ASP:OD2	1:C:155:LYS:HE2	2.11	0.51
1:B:3169:LEU:HD12	1:B:3194:LEU:HD11	1.93	0.51
1:B:3554:GLN:OE1	1:B:3593:VAL:HG11	2.11	0.51
1:B:3625:SER:O	1:B:3629:ARG:HG2	2.11	0.51
1:B:4902:GLU:O	1:B:4913:ARG:CZ	2.58	0.51
1:D:646:PRO:HB2	1:D:648:ILE:CD1	2.41	0.51
1:D:2626:LEU:HD22	1:D:2640:PRO:HB3	1.92	0.51
1:D:3996:PHE:HD1	1:D:4016:LEU:HD11	1.76	0.51
1:C:646:PRO:HB2	1:C:648:ILE:CD1	2.41	0.51
1:C:3372:VAL:CG1	1:C:3398:PHE:HE1	2.24	0.51
1:A:1101:ARG:NH1	1:A:1115:LEU:O	2.40	0.51
1:A:3169:LEU:HD12	1:A:3194:LEU:HD11	1.93	0.51
1:A:3621:HIS:O	1:A:3621:HIS:ND1	2.38	0.51
1:B:10:GLU:OE1	1:B:10:GLU:O	2.28	0.51
1:B:4241:THR:O	1:B:4245:MET:HG3	2.10	0.51
1:D:3299:GLY:O	1:D:3300:ALA:HB2	2.11	0.51
1:D:3514:LEU:HD21	1:D:3602:VAL:HG13	1.92	0.51
1:D:4651:THR:OG1	1:D:4803:HIS:NE2	2.05	0.51
1:C:1065:ASN:OD1	1:C:1066:GLN:N	2.43	0.51
1:C:1999:ARG:HH12	1:C:3636:PHE:CA	2.18	0.51
1:C:3589:PRO:O	1:C:3593:VAL:HG13	2.11	0.51
1:C:3996:PHE:HD1	1:C:4016:LEU:HD11	1.76	0.51
1:A:1962:ALA:O	1:A:1966:VAL:HG23	2.11	0.51
1:A:2107:GLN:O	1:A:3694:LYS:NZ	2.36	0.51
1:B:2626:LEU:HD22	1:B:2640:PRO:HB3	1.92	0.51
1:B:3589:PRO:O	1:B:3593:VAL:HG13	2.11	0.51
1:C:10:GLU:OE1	1:C:10:GLU:O	2.28	0.51
1:C:3598:GLU:O	1:C:3602:VAL:HG23	2.11	0.51
1:A:3996:PHE:HD1	1:A:4016:LEU:HD11	1.76	0.50
1:A:4098:ASP:OD1	1:A:4099:SER:N	2.44	0.50
1:A:4678:ALA:HB1	1:A:4720:VAL:HG21	1.93	0.50
1:A:4961:CYS:SG	1:A:4983:HIS:CE1	3.04	0.50
1:B:4232:GLU:OE1	1:B:5017:ARG:NH2	2.44	0.50
1:B:4583:SER:OG	1:B:4585:SER:O	2.27	0.50
1:D:2874:MET:HE1	1:D:2939:ARG:CB	2.39	0.50
1:D:4209:GLN:H	1:D:4209:GLN:CD	2.14	0.50
1:C:2292:GLU:O	1:C:2296:GLU:OE1	2.29	0.50
1:C:4045:VAL:O	1:C:4049:VAL:HG23	2.11	0.50
1:A:646:PRO:HB2	1:A:648:ILE:CD1	2.41	0.50
1:A:3532:LEU:HA	1:A:3535:LEU:HD12	1.92	0.50
1:A:4209:GLN:H	1:A:4209:GLN:CD	2.14	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:6:THR:HG23	2:F:6:THR:O	2.10	0.50
1:D:4232:GLU:OE1	1:D:5017:ARG:NH2	2.45	0.50
1:C:717:ASP:OD1	1:C:720:HIS:N	2.40	0.50
1:C:1962:ALA:O	1:C:1966:VAL:HG23	2.11	0.50
1:A:2625:ARG:HH12	1:A:2629:ASP:CG	2.12	0.50
1:A:2638:LYS:HE2	1:A:2694:GLU:OE1	2.08	0.50
1:A:3372:VAL:HG11	1:A:3398:PHE:CE1	2.47	0.50
1:A:4045:VAL:O	1:A:4049:VAL:HG23	2.11	0.50
1:B:820:ARG:CZ	1:B:820:ARG:HB3	2.24	0.50
1:B:4118:ASP:OD1	1:B:4122:MET:N	2.42	0.50
1:D:4649:LEU:O	1:D:4653:VAL:HG23	2.11	0.50
1:C:2520:HIS:O	1:C:2524:VAL:HG22	2.11	0.50
1:A:3514:LEU:HD21	1:A:3602:VAL:HG13	1.92	0.50
1:B:384:MET:SD	1:C:167:ASP:HA	2.52	0.50
1:B:2006:ILE:HD11	1:B:3641:LEU:HD11	1.93	0.50
1:B:2520:HIS:O	1:B:2524:VAL:HG22	2.11	0.50
1:B:3468:SER:O	1:B:3472:ALA:HB2	2.12	0.50
1:B:4661:TYR:OH	1:B:4786:ASP:OD2	2.27	0.50
1:B:4678:ALA:HB1	1:B:4720:VAL:HG21	1.93	0.50
1:D:2675:THR:HG23	1:D:2706:ILE:HG23	1.94	0.50
1:C:3372:VAL:HG11	1:C:3398:PHE:CE1	2.47	0.50
1:C:4678:ALA:HB1	1:C:4720:VAL:HG21	1.93	0.50
1:C:4961:CYS:SG	1:C:4983:HIS:CE1	3.04	0.50
1:A:796:ARG:NH1	1:A:1619:ARG:HH22	2.10	0.50
1:A:880:GLU:HG3	1:A:881:LEU:N	2.27	0.50
1:A:2006:ILE:HD11	1:A:3641:LEU:HD11	1.93	0.50
1:A:2572:THR:CG2	1:A:2579:VAL:CG2	2.83	0.50
1:B:2929:PHE:CA	1:B:2932:MET:SD	2.98	0.50
1:B:4045:VAL:O	1:B:4049:VAL:HG23	2.11	0.50
1:B:4098:ASP:OD1	1:B:4099:SER:N	2.44	0.50
1:B:4989:MET:SD	1:B:4993:MET:SD	3.10	0.50
1:D:323:LEU:HD23	1:D:323:LEU:H	1.77	0.50
1:D:880:GLU:HG3	1:D:881:LEU:N	2.27	0.50
1:D:3468:SER:O	1:D:3472:ALA:HB2	2.12	0.50
1:D:3598:GLU:O	1:D:3602:VAL:HG23	2.11	0.50
1:C:612:VAL:HG13	1:C:2167:ILE:O	2.12	0.50
1:C:3183:VAL:O	1:C:3187:ARG:HG3	2.11	0.50
1:C:4649:LEU:O	1:C:4653:VAL:HG23	2.11	0.50
1:A:2675:THR:HG23	1:A:2706:ILE:HG23	1.94	0.50
1:A:3468:SER:O	1:A:3472:ALA:HB2	2.12	0.50
1:A:3625:SER:O	1:A:3629:ARG:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:6:THR:HG23	2:H:6:THR:O	2.10	0.50
1:B:796:ARG:NH1	1:B:1619:ARG:HH22	2.10	0.50
1:B:2874:MET:HE1	1:B:2939:ARG:H	1.77	0.50
1:D:167:ASP:OD1	1:C:384:MET:CE	2.60	0.50
1:D:2970:SER:O	1:D:2974:ILE:HG23	2.11	0.50
1:C:323:LEU:HD23	1:C:323:LEU:H	1.77	0.50
1:C:3299:GLY:O	1:C:3300:ALA:HB2	2.11	0.50
1:C:3554:GLN:OE1	1:C:3593:VAL:HG11	2.11	0.50
1:C:4209:GLN:H	1:C:4209:GLN:CD	2.14	0.50
1:A:72:SER:O	1:A:99:ARG:NH1	2.45	0.50
1:A:2292:GLU:O	1:A:2296:GLU:OE1	2.29	0.50
1:A:2572:THR:O	1:A:2618:MET:HE2	2.12	0.50
1:A:2969:ILE:O	1:A:2972:GLU:HG3	2.11	0.50
1:A:4232:GLU:OE1	1:A:5017:ARG:NH2	2.44	0.50
1:B:781:VAL:HG13	1:B:791:PHE:CZ	2.47	0.50
1:B:1962:ALA:O	1:B:1966:VAL:HG23	2.12	0.50
1:B:2524:VAL:HG23	1:B:2525:GLY:N	2.27	0.50
1:B:3169:LEU:HD21	1:B:3205:PHE:CD2	2.47	0.50
1:B:3372:VAL:HG11	1:B:3398:PHE:CE1	2.47	0.50
1:B:4209:GLN:CD	1:B:4209:GLN:H	2.14	0.50
1:B:4649:LEU:O	1:B:4653:VAL:HG23	2.11	0.50
1:B:4961:CYS:SG	1:B:4983:HIS:CE1	3.04	0.50
1:D:1043:VAL:HA	1:D:1046:LEU:HD12	1.94	0.50
1:D:1962:ALA:O	1:D:1966:VAL:HG23	2.11	0.50
1:D:3554:GLN:OE1	1:D:3593:VAL:HG11	2.11	0.50
1:D:4678:ALA:HB1	1:D:4720:VAL:HG21	1.93	0.50
1:D:4989:MET:SD	1:D:4993:MET:SD	3.10	0.50
1:C:2470:ILE:HG22	1:C:2525:GLY:HA3	1.93	0.50
1:C:4098:ASP:OD1	1:C:4099:SER:N	2.44	0.50
1:A:612:VAL:HG13	1:A:2167:ILE:O	2.12	0.50
1:A:781:VAL:HG13	1:A:791:PHE:CZ	2.47	0.50
1:A:898:ASP:HB2	1:A:901:LYS:HG3	1.94	0.50
1:A:2524:VAL:HG23	1:A:2525:GLY:N	2.27	0.50
1:A:3299:GLY:O	1:A:3300:ALA:HB2	2.11	0.50
1:A:4649:LEU:O	1:A:4653:VAL:HG23	2.11	0.50
1:A:4989:MET:SD	1:A:4993:MET:SD	3.10	0.50
2:E:6:THR:HG23	2:E:6:THR:O	2.10	0.50
1:B:384:MET:CE	1:C:167:ASP:OD1	2.60	0.50
1:B:612:VAL:HG13	1:B:2167:ILE:O	2.12	0.50
1:B:880:GLU:HG3	1:B:881:LEU:N	2.27	0.50
1:B:2970:SER:O	1:B:2974:ILE:HG23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4060:LYS:O	1:B:4064:MET:HG3	2.12	0.50
1:D:781:VAL:HG13	1:D:791:PHE:CZ	2.47	0.50
1:D:2226:PRO:CB	1:D:2267:MET:HE3	2.41	0.50
1:D:3372:VAL:HG11	1:D:3398:PHE:CE1	2.46	0.50
1:C:3169:LEU:CD1	1:C:3194:LEU:HD11	2.41	0.50
1:C:3468:SER:O	1:C:3472:ALA:HB2	2.12	0.50
1:C:4989:MET:SD	1:C:4993:MET:SD	3.10	0.50
1:A:323:LEU:HD23	1:A:323:LEU:H	1.77	0.50
1:A:659:TYR:O	1:A:662:TRP:NE1	2.44	0.50
1:A:688:LEU:HD11	1:A:775:GLY:CA	2.42	0.50
1:B:323:LEU:H	1:B:323:LEU:HD23	1.77	0.50
1:B:3372:VAL:CG1	1:B:3398:PHE:HE1	2.24	0.50
1:B:3786:CYS:SG	1:B:3831:SER:OG	2.65	0.50
1:D:1748:PHE:C	1:D:1758:ARG:HH12	2.16	0.50
1:D:2135:LEU:HD21	1:D:3663:LEU:HD21	1.94	0.50
1:D:4098:ASP:OD1	1:D:4099:SER:N	2.44	0.50
1:C:781:VAL:HG13	1:C:791:PHE:CZ	2.47	0.50
1:C:1868:PRO:O	1:C:1872:THR:OG1	2.28	0.50
1:A:3835:LEU:HD22	1:A:3880:PHE:CZ	2.47	0.49
1:B:2107:GLN:O	1:B:3694:LYS:NZ	2.36	0.49
1:B:2923:ALA:O	1:B:2927:LEU:HD23	2.12	0.49
1:D:72:SER:O	1:D:99:ARG:NH1	2.45	0.49
1:D:612:VAL:HG13	1:D:2167:ILE:O	2.12	0.49
1:D:796:ARG:NH1	1:D:1619:ARG:HH22	2.10	0.49
1:D:898:ASP:HB2	1:D:901:LYS:HG3	1.94	0.49
1:D:2969:ILE:O	1:D:2972:GLU:HG3	2.11	0.49
1:D:3169:LEU:CD1	1:D:3194:LEU:HD11	2.42	0.49
1:D:3239:MET:CG	1:D:3239:MET:HA	2.34	0.49
1:D:3625:SER:O	1:D:3629:ARG:HG2	2.11	0.49
1:C:898:ASP:HB2	1:C:901:LYS:HG3	1.94	0.49
1:C:4565:LEU:O	1:C:4569:LEU:HD13	2.12	0.49
1:B:3183:VAL:O	1:B:3187:ARG:HG3	2.11	0.49
1:B:3996:PHE:HD1	1:B:4016:LEU:HD11	1.76	0.49
1:B:4835:LYS:O	1:B:4839:MET:HG2	2.12	0.49
1:D:155:LYS:HE2	1:C:228:ASP:OD2	2.11	0.49
1:D:2520:HIS:O	1:D:2524:VAL:HG22	2.11	0.49
1:D:4961:CYS:SG	1:D:4983:HIS:CE1	3.04	0.49
1:C:2675:THR:HG23	1:C:2706:ILE:HG23	1.94	0.49
1:C:2969:ILE:O	1:C:2972:GLU:HG3	2.11	0.49
1:C:3835:LEU:HD22	1:C:3880:PHE:CZ	2.47	0.49
1:C:4060:LYS:O	1:C:4064:MET:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4232:GLU:OE1	1:C:5017:ARG:NH2	2.44	0.49
1:A:554:LEU:CD1	1:A:1593:PRO:HG3	2.42	0.49
1:A:913:LEU:O	1:A:918:ARG:NH2	2.45	0.49
1:A:2135:LEU:HD21	1:A:3663:LEU:HD21	1.94	0.49
1:A:3169:LEU:CD1	1:A:3194:LEU:HD11	2.42	0.49
1:A:3435:PHE:CD2	1:A:3524:MET:HE1	2.47	0.49
1:A:4705:VAL:HG22	1:A:4711:PHE:HD1	1.78	0.49
1:B:667:MET:SD	1:B:790:ARG:NH2	2.85	0.49
1:B:898:ASP:HB2	1:B:901:LYS:HG3	1.94	0.49
1:B:2969:ILE:O	1:B:2972:GLU:HG3	2.11	0.49
1:B:3169:LEU:CD1	1:B:3194:LEU:HD11	2.42	0.49
1:B:3299:GLY:O	1:B:3300:ALA:HB2	2.11	0.49
1:B:4565:LEU:O	1:B:4569:LEU:HD13	2.12	0.49
1:B:4705:VAL:HG22	1:B:4711:PHE:HD1	1.78	0.49
1:D:4835:LYS:O	1:D:4839:MET:HG2	2.12	0.49
1:C:796:ARG:NH1	1:C:1619:ARG:HH22	2.10	0.49
1:C:1748:PHE:C	1:C:1758:ARG:HH12	2.16	0.49
1:C:2261:SER:O	1:C:2264:GLY:N	2.43	0.49
1:C:3169:LEU:HD21	1:C:3205:PHE:CD2	2.47	0.49
1:C:3625:SER:O	1:C:3629:ARG:HG2	2.11	0.49
1:A:2470:ILE:HG22	1:A:2525:GLY:HA3	1.93	0.49
1:A:2788:HIS:ND1	1:A:2790:MET:HB3	2.27	0.49
1:A:3230:LEU:HD12	1:A:3230:LEU:O	2.13	0.49
1:B:4976:GLU:HG2	1:B:4980:LEU:HD13	1.94	0.49
1:D:887:ILE:HD11	1:D:907:LEU:HD21	1.95	0.49
1:C:72:SER:O	1:C:99:ARG:NH1	2.45	0.49
1:C:2524:VAL:HG23	1:C:2525:GLY:N	2.27	0.49
1:C:2929:PHE:CA	1:C:2932:MET:HE1	2.30	0.49
1:A:1280:GLN:O	1:A:1281:ASN:CG	2.51	0.49
1:A:2751:LEU:HD23	1:A:2755:ILE:HD13	1.95	0.49
1:A:4060:LYS:O	1:A:4064:MET:HG3	2.12	0.49
1:B:3230:LEU:HD12	1:B:3230:LEU:O	2.13	0.49
1:D:688:LEU:HD11	1:D:775:GLY:CA	2.42	0.49
1:D:1726:SER:O	1:D:1729:SER:OG	2.24	0.49
1:D:1991:THR:O	1:D:1995:THR:HG23	2.13	0.49
1:D:3169:LEU:HD21	1:D:3205:PHE:CD2	2.47	0.49
1:C:880:GLU:HG3	1:C:881:LEU:N	2.27	0.49
1:C:2135:LEU:HD21	1:C:3663:LEU:HD21	1.94	0.49
1:C:4835:LYS:O	1:C:4839:MET:HG2	2.13	0.49
1:A:1991:THR:O	1:A:1995:THR:HG23	2.13	0.49
1:A:2693:GLN:HE22	1:A:2697:ARG:HH11	1.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2923:ALA:O	1:A:2927:LEU:HD23	2.12	0.49
1:A:2929:PHE:CA	1:A:2932:MET:SD	2.98	0.49
1:A:3786:CYS:SG	1:A:3831:SER:OG	2.65	0.49
1:B:554:LEU:CD1	1:B:1593:PRO:HG3	2.42	0.49
1:B:688:LEU:HD11	1:B:775:GLY:CA	2.42	0.49
1:B:2470:ILE:HG22	1:B:2525:GLY:HA3	1.93	0.49
1:B:2693:GLN:HE22	1:B:2697:ARG:HH11	1.60	0.49
1:B:2788:HIS:ND1	1:B:2790:MET:HB3	2.27	0.49
1:B:4732:PHE:CD2	1:B:4732:PHE:O	2.66	0.49
1:D:554:LEU:CD1	1:D:1593:PRO:HG3	2.42	0.49
1:D:667:MET:SD	1:D:790:ARG:NH2	2.86	0.49
1:D:3230:LEU:HD12	1:D:3230:LEU:O	2.12	0.49
1:D:4705:VAL:HG13	1:D:4711:PHE:HE1	1.75	0.49
1:C:554:LEU:CD1	1:C:1593:PRO:HG3	2.42	0.49
1:C:887:ILE:HD11	1:C:907:LEU:HD21	1.95	0.49
1:C:1043:VAL:HA	1:C:1046:LEU:HD12	1.94	0.49
1:C:2642:LYS:HG3	1:C:2698:MET:HE3	1.92	0.49
1:C:2751:LEU:HD23	1:C:2755:ILE:HD13	1.95	0.49
1:C:2923:ALA:O	1:C:2927:LEU:HD23	2.12	0.49
1:A:2744:ASN:OD1	1:A:2745:VAL:HG23	2.13	0.49
1:B:72:SER:O	1:B:99:ARG:NH1	2.45	0.49
1:B:296:ASP:OD1	1:B:297:GLN:OE1	2.31	0.49
1:B:1991:THR:O	1:B:1995:THR:HG23	2.13	0.49
1:B:2135:LEU:HD21	1:B:3663:LEU:HD21	1.94	0.49
1:B:4205:TRP:CE3	1:B:4989:MET:HE2	2.48	0.49
1:D:2744:ASN:OD1	1:D:2745:VAL:HG23	2.13	0.49
1:D:2923:ALA:O	1:D:2927:LEU:HD23	2.12	0.49
1:D:3835:LEU:HD22	1:D:3880:PHE:CZ	2.47	0.49
1:D:4976:GLU:HG2	1:D:4980:LEU:HD13	1.94	0.49
1:C:2929:PHE:CA	1:C:2932:MET:SD	2.98	0.49
1:C:3621:HIS:O	1:C:3621:HIS:ND1	2.38	0.49
1:A:3901:ASN:OD1	1:A:3904:ARG:NH1	2.39	0.49
1:A:4565:LEU:O	1:A:4569:LEU:HD13	2.12	0.49
1:B:979:PRO:O	1:B:983:THR:HG23	2.13	0.49
1:B:2476:ILE:HD12	1:B:2532:ALA:HB1	1.95	0.49
1:B:2751:LEU:HD23	1:B:2755:ILE:HD13	1.95	0.49
1:D:363:ASP:OD1	1:D:366:ALA:HB2	2.13	0.49
1:D:1280:GLN:O	1:D:1281:ASN:CG	2.51	0.49
1:C:913:LEU:O	1:C:918:ARG:NH2	2.45	0.49
1:C:979:PRO:O	1:C:983:THR:HG23	2.13	0.49
1:C:2476:ILE:HD12	1:C:2532:ALA:HB1	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4732:PHE:CD2	1:C:4732:PHE:O	2.66	0.49
1:A:2675:THR:HB	1:A:2710:LEU:HD21	1.95	0.49
1:B:3835:LEU:HD22	1:B:3880:PHE:CZ	2.48	0.49
1:D:4565:LEU:O	1:D:4569:LEU:HD13	2.12	0.49
1:C:1991:THR:O	1:C:1995:THR:HG23	2.12	0.49
1:C:3969:ILE:CG2	1:C:3980:LEU:HD12	2.43	0.49
1:C:4651:THR:OG1	1:C:4803:HIS:NE2	2.05	0.49
1:C:4705:VAL:HG22	1:C:4711:PHE:HD1	1.78	0.49
1:A:887:ILE:HD11	1:A:907:LEU:HD21	1.95	0.49
1:A:1743[A]:ARG:NH2	1:A:1967:ASP:OD2	2.40	0.49
1:B:360:ALA:O	1:B:361:ALA:HB3	2.13	0.49
1:B:1043:VAL:HA	1:B:1046:LEU:HD12	1.94	0.49
1:B:1810:LYS:O	1:B:1814:MET:HG3	2.13	0.49
1:B:2675:THR:HG23	1:B:2706:ILE:HG23	1.94	0.49
1:D:659:TYR:O	1:D:662:TRP:NE1	2.44	0.49
1:D:1833:SER:HG	1:D:1836:PHE:HD1	1.59	0.49
1:D:2470:ILE:HG22	1:D:2525:GLY:HA3	1.93	0.49
1:D:2524:VAL:HG23	1:D:2525:GLY:N	2.27	0.49
1:D:4705:VAL:HG22	1:D:4711:PHE:HD1	1.78	0.49
1:C:659:TYR:O	1:C:662:TRP:NE1	2.44	0.49
1:C:2974:ILE:HG13	1:C:2975:ALA:N	2.28	0.49
1:C:3590:GLU:O	1:C:3594:ARG:HG3	2.13	0.49
1:C:4976:GLU:HG2	1:C:4980:LEU:HD13	1.94	0.49
1:A:861:ILE:HD13	1:A:930:LYS:CD	2.43	0.48
1:A:1748:PHE:C	1:A:1758:ARG:HH12	2.16	0.48
1:D:2751:LEU:HD23	1:D:2755:ILE:HD13	1.95	0.48
1:D:3969:ILE:CG2	1:D:3980:LEU:HD12	2.43	0.48
1:C:667:MET:SD	1:C:790:ARG:NH2	2.85	0.48
1:C:4000:MET:SD	1:C:4020:GLN:NE2	2.79	0.48
1:A:3941:ASP:OD2	1:A:3941:ASP:N	2.46	0.48
1:A:4640:GLU:HB3	1:A:4641:PRO:HD3	1.95	0.48
1:B:861:ILE:HD13	1:B:930:LYS:CD	2.43	0.48
1:B:1999:ARG:HH12	1:B:3636:PHE:HD1	1.58	0.48
1:B:4640:GLU:HB3	1:B:4641:PRO:HD3	1.95	0.48
1:D:913:LEU:O	1:D:918:ARG:NH2	2.45	0.48
1:D:2974:ILE:HG13	1:D:2975:ALA:N	2.28	0.48
1:C:552:ASP:OD1	1:C:553:ARG:N	2.47	0.48
1:C:4834:GLY:O	1:C:4838:VAL:HG23	2.13	0.48
1:A:360:ALA:O	1:A:361:ALA:HB3	2.13	0.48
1:A:667:MET:SD	1:A:790:ARG:NH2	2.85	0.48
1:A:898:ASP:HB2	1:A:901:LYS:CG	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1043:VAL:HA	1:A:1046:LEU:HD12	1.94	0.48
1:A:1810:LYS:O	1:A:1814:MET:HG3	2.13	0.48
1:A:3442:PHE:CE1	1:A:3511:VAL:HG12	2.48	0.48
1:A:4732:PHE:O	1:A:4732:PHE:CD2	2.66	0.48
1:B:1280:GLN:O	1:B:1281:ASN:CG	2.51	0.48
1:B:3590:GLU:O	1:B:3594:ARG:HG3	2.13	0.48
1:B:4000:MET:SD	1:B:4020:GLN:NE2	2.79	0.48
1:B:5014:TYR:HD1	6:B:5304:PNX:HAA3	1.76	0.48
1:D:167:ASP:HA	1:C:384:MET:SD	2.53	0.48
1:D:663:TYR:OH	1:D:665:GLU:OE2	2.27	0.48
1:D:1810:LYS:O	1:D:1814:MET:HG3	2.13	0.48
1:D:4764:LEU:O	1:D:4768:LEU:HG	2.13	0.48
1:C:1810:LYS:O	1:C:1814:MET:HG3	2.13	0.48
1:C:4118:ASP:OD1	1:C:4122:MET:N	2.42	0.48
1:C:4717:ASP:OD2	1:C:4723:LYS:NZ	2.35	0.48
1:A:363:ASP:OD1	1:A:366:ALA:HB2	2.13	0.48
1:A:552:ASP:OD1	1:A:553:ARG:N	2.47	0.48
1:A:2642:LYS:HG3	1:A:2698:MET:HE1	1.91	0.48
1:A:2874:MET:HE1	1:A:2939:ARG:H	1.79	0.48
1:A:3169:LEU:HD21	1:A:3205:PHE:CD2	2.47	0.48
1:A:3892:CYS:HG	1:A:3899:PHE:HD2	1.61	0.48
1:A:4835:LYS:O	1:A:4839:MET:HG2	2.12	0.48
1:B:1748:PHE:C	1:B:1758:ARG:HH12	2.16	0.48
1:B:4929:LEU:C	1:B:4933:GLN:OE1	2.52	0.48
1:D:4060:LYS:O	1:D:4064:MET:HG3	2.12	0.48
1:D:4834:GLY:O	1:D:4838:VAL:HG23	2.13	0.48
1:D:5014:TYR:HD1	6:D:5304:PNX:HAA3	1.76	0.48
1:C:2742:THR:HG23	1:C:2814:LYS:CE	2.41	0.48
1:C:3442:PHE:CE1	1:C:3511:VAL:HG12	2.48	0.48
1:A:2190:VAL:HG12	1:A:2198:MET:HE3	1.96	0.48
1:A:3197:LEU:HD21	1:A:3201:MET:CE	2.44	0.48
1:A:3735:LEU:HG	1:A:3735:LEU:O	2.14	0.48
1:A:4976:GLU:HG2	1:A:4980:LEU:HD13	1.94	0.48
1:B:363:ASP:OD1	1:B:366:ALA:HB2	2.13	0.48
1:B:552:ASP:OD1	1:B:553:ARG:N	2.46	0.48
1:B:2223:ILE:HG23	1:B:2223:ILE:O	2.13	0.48
1:B:2534:ALA:HB1	1:B:2588:ARG:HD3	1.96	0.48
1:B:2974:ILE:HG13	1:B:2975:ALA:N	2.28	0.48
1:D:552:ASP:OD1	1:D:553:ARG:N	2.47	0.48
1:D:898:ASP:HB2	1:D:901:LYS:CG	2.43	0.48
1:D:2742:THR:HG23	1:D:2814:LYS:CE	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3735:LEU:HG	1:D:3735:LEU:O	2.14	0.48
1:C:360:ALA:O	1:C:361:ALA:HB3	2.13	0.48
1:C:898:ASP:HB2	1:C:901:LYS:CG	2.43	0.48
1:C:2223:ILE:O	1:C:2223:ILE:HG23	2.13	0.48
1:C:3230:LEU:O	1:C:3230:LEU:HD12	2.13	0.48
1:A:3321:ARG:O	1:A:3324:VAL:HG22	2.14	0.48
1:A:4661:TYR:OH	1:A:4786:ASP:OD2	2.27	0.48
1:B:717:ASP:OD1	1:B:720:HIS:N	2.40	0.48
1:B:2675:THR:HB	1:B:2710:LEU:HD21	1.95	0.48
1:B:3442:PHE:CE1	1:B:3511:VAL:HG12	2.48	0.48
1:D:360:ALA:O	1:D:361:ALA:HB3	2.13	0.48
1:D:2693:GLN:HE22	1:D:2697:ARG:HH11	1.60	0.48
1:C:2355:ARG:HG3	1:C:2355:ARG:HH11	1.79	0.48
1:C:2742:THR:CG2	1:C:2814:LYS:HE3	2.42	0.48
1:C:2744:ASN:OD1	1:C:2745:VAL:HG23	2.13	0.48
1:C:3197:LEU:HD21	1:C:3201:MET:CE	2.44	0.48
1:A:167:ASP:OD1	1:D:384:MET:SD	2.72	0.48
1:A:953:THR:O	1:A:968:ALA:HB1	2.14	0.48
1:A:1726:SER:O	1:A:1729:SER:OG	2.24	0.48
1:A:4929:LEU:C	1:A:4933:GLN:OE1	2.52	0.48
1:B:648:ILE:HG23	1:B:814:ALA:HB3	1.96	0.48
1:B:861:ILE:HG21	1:B:930:LYS:HD2	1.96	0.48
1:B:3471:THR:HG22	1:C:1170:MET:CE	2.44	0.48
1:B:4834:GLY:O	1:B:4838:VAL:HG23	2.13	0.48
1:D:296:ASP:OD1	1:D:297:GLN:OE1	2.31	0.48
1:D:861:ILE:HD13	1:D:930:LYS:CD	2.43	0.48
1:D:1743[A]:ARG:NH2	1:D:1967:ASP:OD2	2.39	0.48
1:D:2642:LYS:HG3	1:D:2698:MET:HE1	1.93	0.48
1:D:3941:ASP:OD2	1:D:3941:ASP:N	2.47	0.48
1:D:4911:LEU:O	1:D:4914:VAL:HG22	2.14	0.48
1:C:3007:ASN:O	1:C:3011:THR:OG1	2.15	0.48
1:C:3901:ASN:OD1	1:C:3904:ARG:NH1	2.39	0.48
1:C:5014:TYR:HD1	6:C:5304:PNX:HAA3	1.75	0.48
1:A:574:VAL:O	1:A:578:ILE:HG12	2.14	0.48
1:A:3651:ASN:O	1:A:3655:GLU:OE1	2.32	0.48
1:A:4764:LEU:O	1:A:4768:LEU:HG	2.13	0.48
1:A:4834:GLY:O	1:A:4838:VAL:HG23	2.13	0.48
1:B:913:LEU:O	1:B:918:ARG:NH2	2.45	0.48
1:B:978:THR:O	1:B:982:THR:HG23	2.14	0.48
1:B:3321:ARG:O	1:B:3324:VAL:HG22	2.14	0.48
1:B:4764:LEU:O	1:B:4768:LEU:HG	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4911:LEU:O	1:B:4914:VAL:HG22	2.14	0.48
1:D:590:LEU:HD21	1:D:599:VAL:HB	1.96	0.48
1:D:2098:VAL:HG11	1:D:2123:LEU:HG	1.96	0.48
1:D:2122:SER:HA	1:D:3721:LEU:HD11	1.96	0.48
1:D:3365:LEU:HD11	1:D:3408:LEU:HD12	1.95	0.48
1:D:3442:PHE:CE1	1:D:3511:VAL:HG12	2.48	0.48
1:D:3651:ASN:O	1:D:3655:GLU:OE1	2.32	0.48
1:C:2098:VAL:HG11	1:C:2123:LEU:HG	1.96	0.48
1:C:2204:HIS:NE2	1:C:2205:GLU:OE2	2.47	0.48
1:C:2534:ALA:HB1	1:C:2588:ARG:HD3	1.96	0.48
1:C:2788:HIS:ND1	1:C:2790:MET:HB3	2.28	0.48
1:C:3786:CYS:SG	1:C:3831:SER:OG	2.65	0.48
1:C:4929:LEU:C	1:C:4933:GLN:OE1	2.52	0.48
1:A:34:LYS:C	1:A:35:LEU:HD12	2.35	0.48
1:A:590:LEU:HD21	1:A:599:VAL:HB	1.96	0.48
1:A:861:ILE:HG21	1:A:930:LYS:HD2	1.96	0.48
1:A:2098:VAL:HG11	1:A:2123:LEU:HG	1.96	0.48
1:A:2476:ILE:HG13	1:A:2536:LEU:HD11	1.96	0.48
1:A:3627:GLN:O	1:A:3630:ARG:HG2	2.14	0.48
1:B:659:TYR:O	1:B:662:TRP:NE1	2.44	0.48
1:B:1112:ASP:OD1	1:B:1113:VAL:N	2.47	0.48
1:B:2098:VAL:HG11	1:B:2123:LEU:HG	1.96	0.48
1:B:2476:ILE:HG13	1:B:2536:LEU:HD11	1.96	0.48
1:B:3659:ALA:HA	1:B:3663:LEU:HD12	1.96	0.48
1:B:3969:ILE:CG2	1:B:3980:LEU:HD12	2.43	0.48
1:D:574:VAL:O	1:D:578:ILE:HG12	2.14	0.48
1:D:919:ASN:O	1:D:923:GLN:OE1	2.32	0.48
1:D:2534:ALA:HB1	1:D:2588:ARG:HD3	1.96	0.48
1:D:2675:THR:HB	1:D:2710:LEU:HD21	1.94	0.48
1:D:2788:HIS:ND1	1:D:2790:MET:HB3	2.27	0.48
1:D:4732:PHE:O	1:D:4732:PHE:CD2	2.66	0.48
1:C:590:LEU:HD21	1:C:599:VAL:HB	1.96	0.48
1:C:2523:ASP:HB3	1:C:2578:MET:HE2	1.93	0.48
1:C:3735:LEU:O	1:C:3735:LEU:HG	2.14	0.48
1:A:919:ASN:O	1:A:923:GLN:OE1	2.32	0.48
1:A:979:PRO:O	1:A:983:THR:HG23	2.13	0.48
1:A:2668:SER:O	1:A:2669:GLU:HB3	2.14	0.48
1:A:2974:ILE:HG13	1:A:2975:ALA:N	2.28	0.48
1:A:3659:ALA:HA	1:A:3663:LEU:HD12	1.96	0.48
1:B:2587:TYR:OH	1:B:2629:ASP:OD2	2.24	0.48
1:D:979:PRO:O	1:D:983:THR:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2107:GLN:O	1:D:3694:LYS:NZ	2.36	0.48
1:D:4640:GLU:HB3	1:D:4641:PRO:HD3	1.96	0.48
1:C:648:ILE:HG23	1:C:814:ALA:HB3	1.96	0.48
1:C:953:THR:O	1:C:968:ALA:HB1	2.14	0.48
1:C:2625:ARG:HH12	1:C:2629:ASP:CG	2.12	0.48
1:C:4911:LEU:O	1:C:4914:VAL:HG22	2.14	0.48
1:A:438:ILE:HG23	1:A:518:ILE:HD11	1.96	0.47
1:A:899:ASP:O	1:A:902:ARG:NE	2.45	0.47
1:A:4067:LYS:O	1:A:4070:ASP:OD1	2.33	0.47
1:B:3346:VAL:HG11	1:B:3414:ARG:HB2	1.96	0.47
1:D:34:LYS:C	1:D:35:LEU:HD12	2.35	0.47
1:D:1170:MET:CE	1:C:3471:THR:HG22	2.44	0.47
1:D:2329:GLU:O	1:D:2333:ASP:OD1	2.32	0.47
1:D:3627:GLN:O	1:D:3630:ARG:HG2	2.14	0.47
1:C:69:LEU:HD23	1:C:109:LEU:HD21	1.96	0.47
1:C:233:ILE:HD12	1:C:242:ARG:HB3	1.96	0.47
1:C:2392:ARG:O	1:C:2418:LEU:HD12	2.14	0.47
1:C:2693:GLN:HE22	1:C:2697:ARG:HH11	1.60	0.47
1:C:3159:ASP:O	1:C:3163:VAL:HG23	2.14	0.47
1:C:3651:ASN:O	1:C:3655:GLU:OE1	2.32	0.47
1:C:3941:ASP:OD2	1:C:3941:ASP:N	2.46	0.47
1:A:296:ASP:OD1	1:A:297:GLN:OE1	2.31	0.47
1:A:2355:ARG:HH11	1:A:2355:ARG:HG3	1.79	0.47
1:A:2373:GLY:O	1:B:130:LYS:NZ	2.44	0.47
1:A:3365:LEU:HD11	1:A:3408:LEU:HD12	1.95	0.47
1:B:221:ARG:NH2	1:B:255:HIS:O	2.48	0.47
1:B:438:ILE:HG23	1:B:518:ILE:HD11	1.96	0.47
1:B:884:LEU:HD23	1:B:955:LEU:HD11	1.97	0.47
1:B:953:THR:O	1:B:968:ALA:HB1	2.14	0.47
1:B:2204:HIS:NE2	1:B:2205:GLU:OE2	2.47	0.47
1:B:2224:ARG:HE	1:B:2225:PHE:N	2.10	0.47
1:B:2355:ARG:HH11	1:B:2355:ARG:HG3	1.79	0.47
1:B:3197:LEU:HD21	1:B:3201:MET:CE	2.44	0.47
1:B:4067:LYS:O	1:B:4070:ASP:OD1	2.33	0.47
1:D:985:VAL:HG11	1:D:1040:CYS:HB3	1.96	0.47
1:D:2929:PHE:CA	1:D:2932:MET:SD	2.98	0.47
1:D:3197:LEU:HD21	1:D:3201:MET:CE	2.44	0.47
1:D:3346:VAL:HG11	1:D:3414:ARG:HB2	1.96	0.47
1:C:363:ASP:OD1	1:C:366:ALA:HB2	2.13	0.47
1:C:688:LEU:HD11	1:C:775:GLY:CA	2.42	0.47
1:C:978:THR:O	1:C:982:THR:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1999:ARG:HH12	1:C:3636:PHE:HD1	1.58	0.47
1:C:3835:LEU:HD22	1:C:3880:PHE:HZ	1.80	0.47
1:A:46:LEU:CD2	1:A:125:ARG:HE	2.27	0.47
1:A:4118:ASP:OD1	1:A:4122:MET:N	2.42	0.47
1:B:899:ASP:O	1:B:902:ARG:NE	2.45	0.47
1:B:1749:PRO:C	1:B:1758:ARG:NH2	2.45	0.47
1:D:1112:ASP:OD1	1:D:1113:VAL:N	2.47	0.47
1:D:2204:HIS:NE2	1:D:2205:GLU:OE2	2.47	0.47
1:D:2519:LEU:HD13	1:D:2575:ARG:HG3	1.97	0.47
1:C:1280:GLN:O	1:C:1281:ASN:CG	2.51	0.47
1:C:2668:SER:O	1:C:2669:GLU:HB3	2.14	0.47
1:C:2675:THR:HB	1:C:2710:LEU:HD21	1.95	0.47
1:C:3398:PHE:CE2	1:C:3450:ASN:CB	2.97	0.47
1:A:648:ILE:HG23	1:A:814:ALA:HB3	1.96	0.47
1:A:978:THR:O	1:A:982:THR:HG23	2.14	0.47
1:A:1299:GLN:HG2	2:E:31:GLU:OE2	2.14	0.47
1:A:3159:ASP:O	1:A:3163:VAL:HG23	2.14	0.47
1:B:898:ASP:HB2	1:B:901:LYS:CG	2.43	0.47
1:B:3365:LEU:HD11	1:B:3408:LEU:HD12	1.95	0.47
1:B:3627:GLN:O	1:B:3630:ARG:HG2	2.14	0.47
1:B:4096:ALA:O	1:B:4100:GLN:HG2	2.14	0.47
1:D:380:GLN:OE1	1:D:380:GLN:N	2.45	0.47
1:D:3166:TYR:CZ	1:D:3203:VAL:HG11	2.50	0.47
1:D:3239:MET:CB	1:D:3239:MET:HG3	2.31	0.47
1:D:4929:LEU:C	1:D:4933:GLN:OE1	2.52	0.47
1:C:3627:GLN:O	1:C:3630:ARG:HG2	2.14	0.47
1:A:928:THR:O	1:A:931:THR:OG1	2.30	0.47
1:A:3346:VAL:HG11	1:A:3414:ARG:HB2	1.96	0.47
1:A:3733:CYS:HB2	1:A:3803:SER:OG	2.14	0.47
1:A:5014:TYR:HD1	6:A:5304:PNX:HAA3	1.76	0.47
2:G:2:VAL:CG2	2:G:58:GLY:HA2	2.45	0.47
1:B:3015:LEU:HD22	1:B:3025:LEU:HB3	1.96	0.47
1:B:3362:ILE:HG22	1:B:3437:MET:HB3	1.97	0.47
1:D:3362:ILE:HG22	1:D:3437:MET:HB3	1.97	0.47
1:C:1069:TRP:CE3	1:C:1602:PRO:HG2	2.50	0.47
1:C:2519:LEU:HD13	1:C:2575:ARG:HG3	1.97	0.47
1:C:4764:LEU:O	1:C:4768:LEU:HG	2.13	0.47
1:A:233:ILE:HD12	1:A:242:ARG:HB3	1.96	0.47
1:A:360:ALA:O	1:A:361:ALA:CB	2.63	0.47
1:A:384:MET:SD	1:B:167:ASP:N	2.87	0.47
1:A:2122:SER:HA	1:A:3721:LEU:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2204:HIS:NE2	1:A:2205:GLU:OE2	2.47	0.47
1:A:2476:ILE:HD12	1:A:2532:ALA:HB1	1.95	0.47
1:A:2534:ALA:HB1	1:A:2588:ARG:HD3	1.96	0.47
1:A:2742:THR:HG23	1:A:2814:LYS:CE	2.41	0.47
1:A:3362:ILE:HG22	1:A:3437:MET:HB3	1.97	0.47
1:A:3477:LYS:NZ	1:A:3479:ALA:HA	2.30	0.47
1:A:4911:LEU:O	1:A:4914:VAL:HG22	2.14	0.47
2:E:2:VAL:CG2	2:E:58:GLY:HA2	2.45	0.47
1:B:880:GLU:HB2	1:B:967:PRO:HG2	1.97	0.47
1:B:2519:LEU:HD13	1:B:2575:ARG:HG3	1.97	0.47
1:D:978:THR:O	1:D:982:THR:HG23	2.14	0.47
1:D:2223:ILE:HG23	1:D:2223:ILE:O	2.13	0.47
1:D:2392:ARG:O	1:D:2418:LEU:HD12	2.14	0.47
1:D:2742:THR:CG2	1:D:2814:LYS:HE3	2.42	0.47
1:D:3159:ASP:O	1:D:3163:VAL:HG23	2.14	0.47
1:D:3321:ARG:O	1:D:3324:VAL:HG22	2.14	0.47
1:D:3590:GLU:O	1:D:3594:ARG:HG3	2.13	0.47
1:D:3621:HIS:O	1:D:3621:HIS:ND1	2.38	0.47
1:C:574:VAL:O	1:C:578:ILE:HG12	2.14	0.47
1:C:2122:SER:HA	1:C:3721:LEU:HD11	1.96	0.47
1:C:2329:GLU:O	1:C:2333:ASP:OD1	2.32	0.47
1:C:3321:ARG:O	1:C:3324:VAL:HG22	2.14	0.47
1:C:3346:VAL:HG11	1:C:3414:ARG:HB2	1.96	0.47
1:C:3362:ILE:HG22	1:C:3437:MET:HB3	1.97	0.47
1:C:3733:CYS:HB2	1:C:3803:SER:OG	2.14	0.47
1:A:36:CYS:SG	1:A:52:THR:HG21	2.55	0.47
1:A:1112:ASP:OD1	1:A:1113:VAL:N	2.47	0.47
1:A:1427:ILE:O	1:A:1430:THR:HG22	2.15	0.47
1:A:2014:ASP:O	1:A:2015:GLU:HB3	2.15	0.47
1:A:2519:LEU:HD13	1:A:2575:ARG:HG3	1.97	0.47
1:A:2638:LYS:O	1:A:2698:MET:CE	2.63	0.47
1:A:2790:MET:SD	1:A:2797:PHE:CZ	3.08	0.47
1:A:3234:ASN:O	1:A:3234:ASN:OD1	2.33	0.47
1:A:3590:GLU:O	1:A:3594:ARG:HG3	2.13	0.47
1:A:3969:ILE:CG2	1:A:3980:LEU:HD12	2.43	0.47
1:B:233:ILE:HD12	1:B:242:ARG:HB3	1.96	0.47
1:B:360:ALA:O	1:B:361:ALA:CB	2.63	0.47
1:B:1069:TRP:CE3	1:B:1602:PRO:HG2	2.49	0.47
1:B:2011:HIS:O	1:B:2011:HIS:ND1	2.47	0.47
1:B:2261:SER:O	1:B:2264:GLY:N	2.43	0.47
1:B:2744:ASN:OD1	1:B:2745:VAL:HG23	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2790:MET:SD	1:B:2797:PHE:CZ	3.08	0.47
1:B:3166:TYR:CZ	1:B:3203:VAL:HG11	2.50	0.47
1:B:3379:LEU:HD11	1:B:3387:ALA:O	2.15	0.47
1:B:3477:LYS:NZ	1:B:3479:ALA:HA	2.30	0.47
1:D:233:ILE:HD12	1:D:242:ARG:HB3	1.96	0.47
1:D:717:ASP:OD1	1:D:720:HIS:N	2.40	0.47
1:D:953:THR:O	1:D:968:ALA:HB1	2.14	0.47
1:D:1427:ILE:O	1:D:1430:THR:HG22	2.15	0.47
1:D:2014:ASP:O	1:D:2015:GLU:HB3	2.15	0.47
1:D:2476:ILE:HD12	1:D:2532:ALA:HB1	1.95	0.47
1:D:2523:ASP:HB3	1:D:2578:MET:HE2	1.91	0.47
1:D:2668:SER:O	1:D:2669:GLU:HB3	2.14	0.47
1:D:3015:LEU:HD22	1:D:3025:LEU:HB3	1.96	0.47
1:D:3659:ALA:HA	1:D:3663:LEU:HD12	1.96	0.47
1:D:3835:LEU:HD22	1:D:3880:PHE:HZ	1.80	0.47
1:D:4583:SER:OG	1:D:4585:SER:O	2.27	0.47
1:C:221:ARG:NH2	1:C:255:HIS:O	2.48	0.47
1:C:296:ASP:OD1	1:C:297:GLN:OE1	2.31	0.47
1:C:380:GLN:OE1	1:C:380:GLN:N	2.45	0.47
1:C:861:ILE:HD13	1:C:930:LYS:CD	2.43	0.47
1:C:880:GLU:HB2	1:C:967:PRO:HG2	1.97	0.47
1:C:884:LEU:HD23	1:C:955:LEU:HD11	1.97	0.47
1:C:2014:ASP:O	1:C:2015:GLU:HB3	2.15	0.47
1:C:2224:ARG:HE	1:C:2225:PHE:N	2.10	0.47
1:C:3015:LEU:HD22	1:C:3025:LEU:HB3	1.96	0.47
1:C:3365:LEU:HD11	1:C:3408:LEU:HD12	1.95	0.47
1:C:4096:ALA:O	1:C:4100:GLN:HG2	2.14	0.47
1:C:4640:GLU:HB3	1:C:4641:PRO:HD3	1.96	0.47
1:A:2392:ARG:O	1:A:2418:LEU:HD12	2.14	0.47
1:A:3166:TYR:CZ	1:A:3203:VAL:HG11	2.50	0.47
1:A:3239:MET:CB	1:A:3239:MET:HG2	2.31	0.47
1:A:3379:LEU:HD11	1:A:3387:ALA:O	2.15	0.47
2:H:2:VAL:CG2	2:H:58:GLY:HA2	2.45	0.47
2:F:2:VAL:CG2	2:F:58:GLY:HA2	2.45	0.47
1:B:577:ILE:O	1:B:579:GLN:NE2	2.48	0.47
1:B:590:LEU:HD21	1:B:599:VAL:HB	1.96	0.47
1:B:887:ILE:HD11	1:B:907:LEU:HD21	1.95	0.47
1:B:985:VAL:HG11	1:B:1040:CYS:HB3	1.96	0.47
1:B:3234:ASN:OD1	1:B:3234:ASN:O	2.33	0.47
1:B:3835:LEU:HD22	1:B:3880:PHE:HZ	1.80	0.47
1:D:36:CYS:SG	1:D:52:THR:HG21	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:46:LEU:CD2	1:D:125:ARG:HE	2.27	0.47
1:D:648:ILE:HG23	1:D:814:ALA:HB3	1.96	0.47
1:D:3372:VAL:CG1	1:D:3398:PHE:HE1	2.24	0.47
1:C:4067:LYS:O	1:C:4070:ASP:OD1	2.33	0.47
1:A:985:VAL:HG11	1:A:1040:CYS:HB3	1.96	0.47
1:A:3398:PHE:CE2	1:A:3450:ASN:CB	2.97	0.47
1:B:69:LEU:HD23	1:B:109:LEU:HD21	1.96	0.47
1:B:919:ASN:O	1:B:923:GLN:OE1	2.32	0.47
1:B:2122:SER:HA	1:B:3721:LEU:HD11	1.96	0.47
1:B:2329:GLU:O	1:B:2333:ASP:OD1	2.32	0.47
1:B:2392:ARG:O	1:B:2418:LEU:HD12	2.14	0.47
1:B:3115:VAL:HG13	1:B:3116:SER:N	2.30	0.47
1:B:3239:MET:CB	1:B:3239:MET:HG2	2.31	0.47
1:B:3651:ASN:O	1:B:3655:GLU:OE1	2.32	0.47
1:D:69:LEU:HD23	1:D:109:LEU:HD21	1.96	0.47
1:D:438:ILE:HG23	1:D:518:ILE:HD11	1.96	0.47
1:D:2146:PRO:HA	1:D:2149:VAL:HG23	1.97	0.47
1:D:3100:SER:O	1:D:3104:GLU:OE1	2.33	0.47
1:D:3733:CYS:HB2	1:D:3803:SER:OG	2.14	0.47
1:D:4096:ALA:O	1:D:4100:GLN:HG2	2.14	0.47
1:C:34:LYS:C	1:C:35:LEU:HD12	2.35	0.47
1:C:985:VAL:HG11	1:C:1040:CYS:HB3	1.96	0.47
1:C:3166:TYR:CZ	1:C:3203:VAL:HG11	2.50	0.47
1:C:3182:TYR:O	1:C:3185:LYS:HG3	2.15	0.47
1:C:3659:ALA:HA	1:C:3663:LEU:HD12	1.96	0.47
1:A:577:ILE:O	1:A:579:GLN:NE2	2.48	0.47
1:A:2434:GLY:O	1:A:2508:ARG:NE	2.43	0.47
1:B:553:ARG:O	1:B:557:SER:OG	2.29	0.47
1:B:2190:VAL:HG12	1:B:2198:MET:HE3	1.97	0.47
1:B:2572:THR:HG23	1:B:2575:ARG:HB2	1.97	0.47
1:B:2638:LYS:O	1:B:2698:MET:CE	2.63	0.47
1:B:3159:ASP:O	1:B:3163:VAL:HG23	2.14	0.47
1:B:3733:CYS:HB2	1:B:3803:SER:OG	2.14	0.47
1:D:577:ILE:O	1:D:579:GLN:NE2	2.48	0.47
1:D:1749:PRO:C	1:D:1758:ARG:NH2	2.45	0.47
1:D:2476:ILE:HG13	1:D:2536:LEU:HD11	1.96	0.47
1:D:2572:THR:HG23	1:D:2575:ARG:HB2	1.97	0.47
1:D:2745:VAL:HG12	1:D:2746:ILE:N	2.30	0.47
1:D:2790:MET:SD	1:D:2797:PHE:CZ	3.08	0.47
1:D:4067:LYS:O	1:D:4070:ASP:OD1	2.33	0.47
1:C:919:ASN:O	1:C:923:GLN:OE1	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1570:LYS:O	1:C:1572:ILE:HD12	2.15	0.47
1:C:2146:PRO:HA	1:C:2149:VAL:HG23	1.97	0.47
1:C:2745:VAL:HG12	1:C:2746:ILE:N	2.30	0.47
1:C:3062:PRO:HA	1:C:3065:VAL:HG22	1.97	0.47
1:C:3100:SER:O	1:C:3104:GLU:OE1	2.33	0.47
1:A:1069:TRP:CE3	1:A:1602:PRO:HG2	2.50	0.46
1:A:2329:GLU:O	1:A:2333:ASP:OD1	2.32	0.46
1:A:3048:ALA:O	1:A:3053:ARG:NH2	2.49	0.46
1:A:4096:ALA:O	1:A:4100:GLN:HG2	2.14	0.46
1:B:574:VAL:O	1:B:578:ILE:HG12	2.14	0.46
1:B:2668:SER:O	1:B:2669:GLU:HB3	2.14	0.46
1:B:3157:ILE:HG22	1:B:3162:GLN:HG2	1.97	0.46
1:B:3735:LEU:HG	1:B:3735:LEU:O	2.14	0.46
1:B:4848:VAL:HG11	1:B:4887:MET:HG2	1.97	0.46
1:D:861:ILE:HG21	1:D:930:LYS:HD2	1.96	0.46
1:D:1115:LEU:HD13	1:D:1123:VAL:HG11	1.97	0.46
1:D:2190:VAL:HG12	1:D:2198:MET:HE3	1.96	0.46
1:D:2638:LYS:O	1:D:2698:MET:CE	2.63	0.46
1:D:3048:ALA:O	1:D:3053:ARG:NH2	2.49	0.46
1:D:3901:ASN:OD1	1:D:3904:ARG:NH1	2.39	0.46
1:C:1112:ASP:OD1	1:C:1113:VAL:N	2.47	0.46
1:C:2790:MET:SD	1:C:2797:PHE:CZ	3.08	0.46
1:C:3157:ILE:HG22	1:C:3162:GLN:HG2	1.97	0.46
1:A:2226:PRO:CB	1:A:2267:MET:HE3	2.44	0.46
1:A:2742:THR:CG2	1:A:2814:LYS:HE3	2.42	0.46
1:A:3015:LEU:HD22	1:A:3025:LEU:HB3	1.96	0.46
1:A:4747:SER:HA	1:A:4750:ILE:HG12	1.97	0.46
1:B:34:LYS:C	1:B:35:LEU:HD12	2.35	0.46
1:B:1115:LEU:HD13	1:B:1123:VAL:HG11	1.97	0.46
1:D:100:THR:HG21	1:D:162:LYS:HE2	1.98	0.46
1:D:884:LEU:HD23	1:D:955:LEU:HD11	1.97	0.46
1:D:1570:LYS:O	1:D:1572:ILE:HD12	2.15	0.46
1:C:46:LEU:CD2	1:C:125:ARG:HE	2.27	0.46
1:C:100:THR:HG21	1:C:162:LYS:HE2	1.98	0.46
1:C:577:ILE:O	1:C:579:GLN:NE2	2.48	0.46
1:C:3048:ALA:O	1:C:3053:ARG:NH2	2.49	0.46
1:A:961:MET:HE1	1:A:963:ASN:HB3	1.79	0.46
1:A:1115:LEU:HD13	1:A:1123:VAL:HG11	1.97	0.46
1:A:2223:ILE:HG23	1:A:2223:ILE:O	2.13	0.46
1:A:3062:PRO:HA	1:A:3065:VAL:HG22	1.97	0.46
1:A:4705:VAL:HG13	1:A:4711:PHE:CD1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1554:VAL:HG21	1:B:1561:VAL:CG1	2.45	0.46
1:B:2014:ASP:O	1:B:2015:GLU:HB3	2.15	0.46
1:B:3100:SER:O	1:B:3104:GLU:OE1	2.33	0.46
1:D:574:VAL:HA	1:D:577:ILE:HG12	1.98	0.46
1:D:1554:VAL:HG21	1:D:1561:VAL:CG1	2.45	0.46
1:D:2355:ARG:HH11	1:D:2355:ARG:HG3	1.79	0.46
1:D:2912:THR:HG22	1:D:2914:LYS:H	1.81	0.46
1:D:3062:PRO:HA	1:D:3065:VAL:HG22	1.97	0.46
1:D:3157:ILE:HG22	1:D:3162:GLN:HG2	1.97	0.46
1:C:1115:LEU:HD13	1:C:1123:VAL:HG11	1.97	0.46
1:C:1427:ILE:O	1:C:1430:THR:HG22	2.15	0.46
1:C:2534:ALA:HB1	1:C:2588:ARG:CD	2.46	0.46
1:A:2745:VAL:HG12	1:A:2746:ILE:N	2.30	0.46
1:A:4690:GLU:O	1:A:4691:GLN:HB2	2.16	0.46
1:A:4732:PHE:HE2	1:A:4736:ARG:HG2	1.81	0.46
1:B:46:LEU:CD2	1:B:125:ARG:HE	2.27	0.46
1:B:2211:MET:O	1:B:2214:VAL:CG1	2.64	0.46
1:B:2434:GLY:O	1:B:2508:ARG:NE	2.43	0.46
1:B:2874:MET:HE1	1:B:2939:ARG:CB	2.44	0.46
1:B:3398:PHE:CE2	1:B:3450:ASN:CB	2.97	0.46
1:B:4767:TRP:CE3	1:B:4768:LEU:CD2	2.99	0.46
1:D:1069:TRP:CE3	1:D:1602:PRO:HG2	2.49	0.46
1:D:2767:ALA:O	1:D:2771:ILE:HG12	2.16	0.46
1:D:3379:LEU:HD11	1:D:3387:ALA:O	2.15	0.46
1:C:438:ILE:HG23	1:C:518:ILE:HD11	1.96	0.46
1:C:1456:ASP:OD1	1:C:1456:ASP:N	2.47	0.46
1:C:2170:MET:HG3	1:C:2225:PHE:CE2	2.50	0.46
1:C:2476:ILE:HG13	1:C:2536:LEU:HD11	1.96	0.46
1:C:3379:LEU:HD11	1:C:3387:ALA:O	2.15	0.46
1:C:4661:TYR:OH	1:C:4786:ASP:OD2	2.27	0.46
1:A:884:LEU:O	1:A:887:ILE:HB	2.16	0.46
1:A:921:ASN:HA	1:A:924:MET:SD	2.56	0.46
1:A:1973:GLN:NE2	1:A:2005:GLN:OE1	2.44	0.46
1:A:1999:ARG:HH12	1:A:3636:PHE:HD1	1.58	0.46
1:A:2011:HIS:CE1	1:A:2017:ASP:CG	2.84	0.46
1:A:3100:SER:O	1:A:3104:GLU:OE1	2.33	0.46
1:A:3182:TYR:O	1:A:3185:LYS:HG3	2.15	0.46
1:B:667:MET:SD	1:B:801:LYS:NZ	2.86	0.46
1:B:2170:MET:HG3	1:B:2225:PHE:CE2	2.50	0.46
1:B:2534:ALA:HB1	1:B:2588:ARG:CD	2.46	0.46
1:B:3048:ALA:O	1:B:3053:ARG:NH2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3062:PRO:HA	1:B:3065:VAL:HG22	1.97	0.46
1:B:4651:THR:OG1	1:B:4803:HIS:NE2	2.05	0.46
1:D:2170:MET:HG3	1:D:2225:PHE:CE2	2.50	0.46
1:D:2233:CYS:SG	1:D:2275:VAL:CG2	3.04	0.46
1:D:2515:GLN:O	1:D:2519:LEU:HG	2.16	0.46
1:D:4848:VAL:HG11	1:D:4887:MET:HG2	1.96	0.46
1:C:574:VAL:HA	1:C:577:ILE:HG12	1.98	0.46
1:C:861:ILE:HG21	1:C:930:LYS:HD2	1.96	0.46
1:C:921:ASN:HA	1:C:924:MET:SD	2.56	0.46
1:C:2233:CYS:SG	1:C:2275:VAL:CG2	3.04	0.46
1:C:2515:GLN:O	1:C:2519:LEU:HG	2.16	0.46
1:C:2638:LYS:O	1:C:2698:MET:CE	2.63	0.46
1:C:4041:ALA:O	1:C:4045:VAL:HG23	2.16	0.46
1:C:4690:GLU:O	1:C:4691:GLN:HB2	2.16	0.46
1:A:100:THR:HG21	1:A:162:LYS:HE2	1.98	0.46
1:A:2233:CYS:SG	1:A:2275:VAL:CG2	3.04	0.46
1:A:2586:VAL:CG1	1:A:2607:LEU:HD13	2.46	0.46
1:A:2703:LEU:CD2	1:A:2706:ILE:HD12	2.46	0.46
1:A:3115:VAL:HG13	1:A:3116:SER:N	2.30	0.46
1:A:4583:SER:OG	1:A:4585:SER:O	2.27	0.46
1:A:4934:GLY:HA2	1:D:4937:ILE:HG12	1.97	0.46
1:B:884:LEU:O	1:B:887:ILE:HB	2.16	0.46
1:B:921:ASN:HA	1:B:924:MET:SD	2.56	0.46
1:B:2146:PRO:HA	1:B:2149:VAL:HG23	1.97	0.46
1:B:2742:THR:HG23	1:B:2814:LYS:CE	2.41	0.46
1:D:360:ALA:O	1:D:361:ALA:CB	2.63	0.46
1:D:2011:HIS:ND1	1:D:2011:HIS:O	2.47	0.46
1:D:3115:VAL:HG13	1:D:3116:SER:N	2.30	0.46
1:C:879:HIS:CE1	1:C:913:LEU:HD13	2.51	0.46
1:C:3234:ASN:OD1	1:C:3234:ASN:O	2.33	0.46
1:C:3339:ALA:O	1:C:3343:GLN:HG2	2.16	0.46
1:C:3477:LYS:NZ	1:C:3479:ALA:HA	2.30	0.46
1:A:880:GLU:HB2	1:A:967:PRO:HG2	1.97	0.46
1:A:884:LEU:HD23	1:A:955:LEU:HD11	1.97	0.46
1:A:3530:GLN:O	1:A:3534:MET:HG2	2.16	0.46
1:A:3835:LEU:HD22	1:A:3880:PHE:HZ	1.80	0.46
1:A:3991:GLY:O	1:A:3995:VAL:HG23	2.16	0.46
1:B:869:ARG:HD2	1:B:870:ILE:N	2.31	0.46
1:B:2233:CYS:SG	1:B:2275:VAL:CG2	3.04	0.46
1:B:2494:PHE:HD1	1:B:2498:HIS:HD1	1.64	0.46
1:B:2586:VAL:CG1	1:B:2607:LEU:HD13	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2703:LEU:CD2	1:B:2706:ILE:HD12	2.46	0.46
1:B:3901:ASN:OD1	1:B:3904:ARG:NH1	2.40	0.46
1:D:3234:ASN:OD1	1:D:3234:ASN:O	2.33	0.46
1:D:3530:GLN:O	1:D:3534:MET:HG2	2.16	0.46
1:C:884:LEU:O	1:C:887:ILE:HB	2.16	0.46
1:C:4176:PRO:O	1:C:4202:ARG:NH2	2.49	0.46
1:A:574:VAL:HA	1:A:577:ILE:HG12	1.98	0.46
1:A:2767:ALA:O	1:A:2771:ILE:HG12	2.16	0.46
1:A:3910:THR:HG23	1:A:3911:THR:HG23	1.98	0.46
1:A:4848:VAL:HG11	1:A:4887:MET:HG2	1.97	0.46
1:B:879:HIS:CE1	1:B:913:LEU:HD13	2.51	0.46
1:B:2745:VAL:HG12	1:B:2746:ILE:N	2.30	0.46
1:B:3339:ALA:O	1:B:3343:GLN:HG2	2.16	0.46
1:B:3910:THR:HG23	1:B:3911:THR:HG23	1.98	0.46
1:B:3991:GLY:O	1:B:3995:VAL:HG23	2.16	0.46
1:B:4717:ASP:OD2	1:B:4723:LYS:NZ	2.35	0.46
1:B:4732:PHE:HE2	1:B:4736:ARG:HG2	1.81	0.46
1:D:463:GLU:O	1:D:467:LYS:HG2	2.16	0.46
1:D:2198:MET:HB3	1:D:2203:MET:SD	2.56	0.46
1:D:2534:ALA:HB1	1:D:2588:ARG:CD	2.46	0.46
1:D:2661:TRP:HB3	1:D:2664:PHE:HD1	1.81	0.46
1:D:2908:TYR:OH	1:D:2916:LYS:HA	2.16	0.46
1:D:3910:THR:HG23	1:D:3911:THR:HG23	1.98	0.46
1:C:360:ALA:O	1:C:361:ALA:CB	2.63	0.46
1:C:2233:CYS:O	1:C:2235:PHE:N	2.49	0.46
1:C:2703:LEU:CD2	1:C:2706:ILE:HD12	2.46	0.46
1:C:2767:ALA:O	1:C:2771:ILE:HG12	2.16	0.46
1:A:384:MET:SD	1:B:167:ASP:OD1	2.74	0.46
1:A:1554:VAL:HG21	1:A:1561:VAL:CG1	2.45	0.46
1:A:2170:MET:HG3	1:A:2225:PHE:CE2	2.50	0.46
1:A:2224:ARG:HE	1:A:2225:PHE:N	2.10	0.46
1:A:2908:TYR:OH	1:A:2916:LYS:HA	2.16	0.46
1:B:36:CYS:SG	1:B:52:THR:HG21	2.55	0.46
1:B:2742:THR:CG2	1:B:2814:LYS:HE3	2.42	0.46
1:D:880:GLU:HB2	1:D:967:PRO:HG2	1.97	0.46
1:D:921:ASN:HA	1:D:924:MET:SD	2.56	0.46
1:D:3401:LEU:O	1:D:3405:LEU:HD13	2.16	0.46
1:D:4645:CYS:O	1:D:4649:LEU:HD13	2.16	0.46
1:D:4705:VAL:HG13	1:D:4711:PHE:CD1	2.51	0.46
1:C:2198:MET:HB3	1:C:2203:MET:SD	2.56	0.46
1:C:2586:VAL:CG1	1:C:2607:LEU:HD13	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1749:PRO:C	1:A:1758:ARG:NH2	2.45	0.46
1:A:4041:ALA:O	1:A:4045:VAL:HG23	2.16	0.46
1:B:4041:ALA:O	1:B:4045:VAL:HG23	2.16	0.46
1:B:4690:GLU:O	1:B:4691:GLN:HB2	2.16	0.46
1:D:2233:CYS:O	1:D:2235:PHE:N	2.49	0.46
1:D:2233:CYS:SG	1:D:2275:VAL:HG23	2.57	0.46
1:D:3182:TYR:O	1:D:3185:LYS:HG3	2.15	0.46
1:D:3339:ALA:O	1:D:3343:GLN:HG2	2.16	0.46
1:D:3398:PHE:CE2	1:D:3450:ASN:CB	2.98	0.46
1:C:2661:TRP:HB3	1:C:2664:PHE:HD1	1.81	0.46
1:C:2912:THR:HG22	1:C:2914:LYS:H	1.81	0.46
1:C:3401:LEU:O	1:C:3405:LEU:HD13	2.16	0.46
1:C:3910:THR:HG23	1:C:3911:THR:HG23	1.98	0.46
1:A:69:LEU:HD23	1:A:109:LEU:HD21	1.96	0.45
1:A:213:TYR:HA	1:A:339:ILE:O	2.16	0.45
1:A:2011:HIS:O	1:A:2011:HIS:ND1	2.47	0.45
1:A:2146:PRO:HA	1:A:2149:VAL:HG23	1.97	0.45
1:A:2198:MET:HB3	1:A:2203:MET:SD	2.56	0.45
1:A:2303:ALA:O	1:A:2307:LEU:HD13	2.17	0.45
1:A:2515:GLN:O	1:A:2519:LEU:HG	2.16	0.45
1:A:2782:ASP:OD2	1:A:2785:LEU:HD13	2.17	0.45
1:A:3336:LYS:O	1:A:3340:VAL:HG23	2.16	0.45
1:A:3339:ALA:O	1:A:3343:GLN:HG2	2.16	0.45
1:B:463:GLU:O	1:B:467:LYS:HG2	2.16	0.45
1:B:1427:ILE:O	1:B:1430:THR:HG22	2.15	0.45
1:B:2198:MET:HB3	1:B:2203:MET:SD	2.56	0.45
1:B:2515:GLN:O	1:B:2519:LEU:HG	2.16	0.45
1:B:2767:ALA:O	1:B:2771:ILE:HG12	2.16	0.45
1:B:2782:ASP:OD2	1:B:2785:LEU:HD13	2.17	0.45
1:B:2828:GLU:O	1:B:2829:GLY:O	2.34	0.45
1:B:2908:TYR:OH	1:B:2916:LYS:HA	2.16	0.45
1:B:2912:THR:HG22	1:B:2914:LYS:H	1.81	0.45
1:B:4176:PRO:O	1:B:4202:ARG:NH2	2.49	0.45
1:B:4705:VAL:HG13	1:B:4711:PHE:CD1	2.51	0.45
1:B:4942:GLU:O	1:B:4945:ASP:OD1	2.34	0.45
1:D:1929:MET:O	1:D:1930:LYS:HB3	2.16	0.45
1:D:2703:LEU:CD2	1:D:2706:ILE:HD12	2.46	0.45
1:D:3477:LYS:NZ	1:D:3479:ALA:HA	2.30	0.45
1:D:4041:ALA:O	1:D:4045:VAL:HG23	2.16	0.45
1:C:213:TYR:HA	1:C:339:ILE:O	2.16	0.45
1:C:869:ARG:HD2	1:C:870:ILE:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2494:PHE:HD1	1:C:2498:HIS:HD1	1.64	0.45
1:C:2572:THR:HG23	1:C:2575:ARG:HB2	1.97	0.45
1:C:3115:VAL:HG13	1:C:3116:SER:N	2.30	0.45
1:A:1570:LYS:O	1:A:1572:ILE:HD12	2.15	0.45
1:A:2482:ASP:C	1:A:2482:ASP:OD1	2.55	0.45
1:A:3899:PHE:CZ	1:A:3903:LEU:HD21	2.52	0.45
1:B:100:THR:HG21	1:B:162:LYS:HE2	1.98	0.45
1:B:1570:LYS:O	1:B:1572:ILE:HD12	2.15	0.45
1:B:2233:CYS:O	1:B:2235:PHE:N	2.49	0.45
1:B:2280:VAL:HG22	1:B:2280:VAL:O	2.16	0.45
1:B:4016:LEU:O	1:B:4020:GLN:HG3	2.16	0.45
1:B:4172:GLU:OE1	1:B:4175:ARG:NH1	2.50	0.45
1:D:820:ARG:HB3	1:D:820:ARG:CZ	2.24	0.45
1:D:4148:THR:HG21	1:D:4180:ARG:NH2	2.31	0.45
1:C:2011:HIS:O	1:C:2011:HIS:ND1	2.47	0.45
1:C:2928:LYS:O	1:C:2932:MET:HE3	2.17	0.45
1:C:3398:PHE:HE2	1:C:3450:ASN:CB	2.29	0.45
1:C:3530:GLN:O	1:C:3534:MET:HG2	2.16	0.45
1:C:4148:THR:HG21	1:C:4180:ARG:NH2	2.31	0.45
1:C:4172:GLU:OE1	1:C:4175:ARG:NH1	2.50	0.45
1:C:4732:PHE:HE2	1:C:4736:ARG:HG2	1.81	0.45
1:A:224:HIS:HA	1:A:388:LEU:HD23	1.98	0.45
1:A:260:TRP:CE3	1:A:282:ILE:HG22	2.51	0.45
1:A:463:GLU:O	1:A:467:LYS:HG2	2.16	0.45
1:A:1929:MET:O	1:A:1930:LYS:HB3	2.16	0.45
1:A:2280:VAL:O	1:A:2280:VAL:HG22	2.16	0.45
1:A:2534:ALA:HB1	1:A:2588:ARG:CD	2.46	0.45
1:A:3324:VAL:HA	1:A:3327:LEU:HG	1.99	0.45
1:A:4075:GLU:CD	1:B:4736:ARG:NH1	2.69	0.45
1:A:4942:GLU:O	1:A:4945:ASP:OD1	2.34	0.45
2:G:25:HIS:CD2	2:G:104:LEU:HD21	2.51	0.45
1:B:213:TYR:HA	1:B:339:ILE:O	2.16	0.45
1:B:2707:ALA:HB1	1:B:3009:TYR:CD1	2.52	0.45
1:D:867:LEU:HA	1:D:870:ILE:HG22	1.98	0.45
1:D:2707:ALA:HB1	1:D:3009:TYR:CD1	2.52	0.45
1:D:3891:LEU:HD13	1:D:3899:PHE:HZ	1.79	0.45
1:D:4577:LEU:HD23	1:D:4580:TYR:CE1	2.52	0.45
1:C:36:CYS:SG	1:C:52:THR:HG21	2.55	0.45
1:C:260:TRP:CE3	1:C:282:ILE:HG22	2.51	0.45
1:C:2233:CYS:SG	1:C:2275:VAL:HG23	2.57	0.45
1:C:4705:VAL:HG13	1:C:4711:PHE:CD1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:ARG:NH2	1:A:255:HIS:O	2.48	0.45
1:A:2912:THR:HG22	1:A:2914:LYS:H	1.81	0.45
1:A:3157:ILE:HG22	1:A:3162:GLN:HG2	1.97	0.45
1:A:4172:GLU:OE1	1:A:4175:ARG:NH1	2.50	0.45
1:A:4645:CYS:O	1:A:4649:LEU:HD13	2.16	0.45
1:B:574:VAL:HA	1:B:577:ILE:HG12	1.98	0.45
1:B:927:GLU:O	1:B:931:THR:HG23	2.16	0.45
1:B:3182:TYR:O	1:B:3185:LYS:HG3	2.15	0.45
1:B:3336:LYS:O	1:B:3340:VAL:HG23	2.16	0.45
1:B:3530:GLN:O	1:B:3534:MET:HG2	2.16	0.45
1:B:4645:CYS:O	1:B:4649:LEU:HD13	2.16	0.45
1:B:4747:SER:HA	1:B:4750:ILE:HG12	1.98	0.45
1:D:1791:VAL:O	1:D:1792:ALA:HB3	2.16	0.45
1:D:2828:GLU:O	1:D:2829:GLY:O	2.34	0.45
1:D:3409:TYR:O	1:D:3412:LEU:N	2.50	0.45
1:D:4176:PRO:O	1:D:4202:ARG:NH2	2.49	0.45
1:D:4690:GLU:O	1:D:4691:GLN:HB2	2.16	0.45
1:D:4747:SER:HA	1:D:4750:ILE:HG12	1.97	0.45
1:C:867:LEU:HA	1:C:870:ILE:HG22	1.98	0.45
1:C:927:GLU:O	1:C:931:THR:HG23	2.16	0.45
1:C:985:VAL:HA	1:C:1039:LEU:HD22	1.98	0.45
1:C:1929:MET:O	1:C:1930:LYS:HB3	2.16	0.45
1:C:2280:VAL:O	1:C:2280:VAL:HG22	2.16	0.45
1:C:2782:ASP:OD2	1:C:2785:LEU:HD13	2.17	0.45
1:C:4016:LEU:O	1:C:4020:GLN:HG3	2.16	0.45
1:A:365:LYS:O	1:A:369:LEU:HG	2.17	0.45
1:A:759:ILE:O	1:A:759:ILE:HG23	2.17	0.45
1:A:869:ARG:HD2	1:A:870:ILE:N	2.31	0.45
1:A:879:HIS:CE1	1:A:913:LEU:HD13	2.51	0.45
1:A:1272:LEU:HD22	1:A:1289:LEU:HD11	1.98	0.45
1:A:2211:MET:O	1:A:2214:VAL:CG1	2.64	0.45
1:A:2233:CYS:SG	1:A:2275:VAL:HG23	2.56	0.45
1:A:2254:LEU:CD1	1:A:2276:ALA:HB1	2.47	0.45
1:A:2261:SER:O	1:A:2264:GLY:N	2.43	0.45
1:A:2572:THR:HG23	1:A:2575:ARG:HB2	1.97	0.45
1:A:3036:LYS:O	1:A:3039:ILE:HG22	2.16	0.45
1:A:3401:LEU:O	1:A:3405:LEU:HD13	2.16	0.45
1:A:4577:LEU:HD23	1:A:4580:TYR:CE1	2.52	0.45
1:A:4902:GLU:O	1:A:4913:ARG:NH2	2.50	0.45
2:F:25:HIS:HD2	2:F:104:LEU:HD21	1.82	0.45
1:B:365:LYS:O	1:B:369:LEU:HG	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:880:GLU:O	1:B:884:LEU:HD13	2.17	0.45
1:B:941:MET:SD	1:B:1051:TYR:HE1	2.32	0.45
1:B:1272:LEU:HD22	1:B:1289:LEU:HD11	1.98	0.45
1:B:2233:CYS:SG	1:B:2275:VAL:HG23	2.56	0.45
1:D:2011:HIS:CE1	1:D:2017:ASP:CG	2.84	0.45
1:D:2280:VAL:O	1:D:2280:VAL:HG22	2.16	0.45
1:D:2782:ASP:OD2	1:D:2785:LEU:HD13	2.17	0.45
1:D:4172:GLU:OE1	1:D:4175:ARG:NH1	2.50	0.45
1:C:553:ARG:NH2	1:C:555:GLU:OE2	2.50	0.45
1:C:880:GLU:O	1:C:884:LEU:HD13	2.17	0.45
1:C:1791:VAL:O	1:C:1792:ALA:HB3	2.16	0.45
1:C:2211:MET:O	1:C:2214:VAL:CG1	2.64	0.45
1:C:4645:CYS:O	1:C:4649:LEU:HD13	2.16	0.45
1:C:4848:VAL:HG11	1:C:4887:MET:HG2	1.97	0.45
1:A:2661:TRP:HB3	1:A:2664:PHE:HD1	1.81	0.45
2:H:25:HIS:CD2	2:H:104:LEU:HD21	2.51	0.45
2:F:25:HIS:CD2	2:F:104:LEU:HD21	2.51	0.45
1:B:260:TRP:CE3	1:B:282:ILE:HG22	2.51	0.45
1:B:553:ARG:NH2	1:B:555:GLU:OE2	2.50	0.45
1:B:2572:THR:CG2	1:B:2579:VAL:CG2	2.83	0.45
1:D:1272:LEU:HD22	1:D:1289:LEU:HD11	1.98	0.45
1:D:2303:ALA:O	1:D:2307:LEU:HD13	2.17	0.45
1:D:3036:LYS:O	1:D:3039:ILE:HG22	2.16	0.45
1:C:224:HIS:HA	1:C:388:LEU:HD23	1.98	0.45
1:C:759:ILE:HG23	1:C:759:ILE:O	2.17	0.45
1:C:1272:LEU:HD22	1:C:1289:LEU:HD11	1.98	0.45
1:C:1554:VAL:HG21	1:C:1561:VAL:CG1	2.45	0.45
1:C:2214:VAL:HG11	1:C:2228:MET:HE3	1.98	0.45
1:A:2494:PHE:HD1	1:A:2498:HIS:HD1	1.64	0.45
1:A:2886:TRP:O	1:A:2890:LYS:HG2	2.17	0.45
1:A:3086:GLU:OE2	1:A:3093:ARG:NH1	2.50	0.45
1:B:759:ILE:HG23	1:B:759:ILE:O	2.17	0.45
1:B:2303:ALA:O	1:B:2307:LEU:HD13	2.17	0.45
1:B:2886:TRP:O	1:B:2890:LYS:HG2	2.17	0.45
1:D:365:LYS:O	1:D:369:LEU:HG	2.17	0.45
1:D:985:VAL:HA	1:D:1039:LEU:HD22	1.98	0.45
1:D:2244:ARG:NH2	1:D:2283:ASN:OD1	2.50	0.45
1:D:3213:TYR:CD1	1:D:3302:PRO:HG2	2.52	0.45
1:D:3324:VAL:HA	1:D:3327:LEU:HG	1.99	0.45
1:D:3390:GLY:HA2	1:D:3393:LEU:HD13	1.99	0.45
1:D:3414:ARG:HH22	1:D:3472:ALA:CB	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3899:PHE:CZ	1:D:3903:LEU:HD21	2.52	0.45
1:D:3991:GLY:O	1:D:3995:VAL:HG23	2.16	0.45
1:C:463:GLU:O	1:C:467:LYS:HG2	2.16	0.45
1:C:941:MET:SD	1:C:1051:TYR:HE1	2.32	0.45
1:C:1105:ALA:O	1:C:1189:LEU:N	2.50	0.45
1:C:2254:LEU:CD1	1:C:2276:ALA:HB1	2.47	0.45
1:C:2908:TYR:OH	1:C:2916:LYS:HA	2.16	0.45
1:C:3409:TYR:O	1:C:3412:LEU:N	2.50	0.45
1:C:3899:PHE:CZ	1:C:3903:LEU:HD21	2.52	0.45
1:C:3991:GLY:O	1:C:3995:VAL:HG23	2.16	0.45
1:C:4747:SER:HA	1:C:4750:ILE:HG12	1.98	0.45
1:A:717:ASP:OD1	1:A:720:HIS:N	2.40	0.45
1:A:985:VAL:HA	1:A:1039:LEU:HD22	1.98	0.45
1:A:3106:MET:O	1:A:3110:LEU:HD23	2.17	0.45
1:A:3566:SER:CB	1:A:3569:LEU:HD12	2.47	0.45
2:E:25:HIS:HD2	2:E:104:LEU:HD21	1.82	0.45
1:B:2254:LEU:CD1	1:B:2276:ALA:HB1	2.47	0.45
1:B:3628:ARG:HD2	1:B:3632:VAL:HG13	1.99	0.45
1:D:759:ILE:HG23	1:D:759:ILE:O	2.17	0.45
1:D:1105:ALA:O	1:D:1189:LEU:N	2.50	0.45
1:D:2586:VAL:CG1	1:D:2607:LEU:HD13	2.46	0.45
1:D:3086:GLU:OE2	1:D:3093:ARG:NH1	2.50	0.45
1:C:2244:ARG:NH2	1:C:2283:ASN:OD1	2.50	0.45
1:C:2828:GLU:O	1:C:2829:GLY:O	2.34	0.45
1:C:3390:GLY:HA2	1:C:3393:LEU:HD13	1.99	0.45
1:C:3566:SER:CB	1:C:3569:LEU:HD12	2.47	0.45
1:A:2233:CYS:O	1:A:2235:PHE:N	2.49	0.45
1:A:3802:ILE:HD11	1:A:3883:ASP:O	2.17	0.45
1:A:4016:LEU:O	1:A:4020:GLN:HG3	2.16	0.45
2:G:25:HIS:HD2	2:G:104:LEU:HD21	1.81	0.45
1:B:1873:GLU:OE1	1:B:1873:GLU:N	2.50	0.45
1:B:1929:MET:O	1:B:1930:LYS:HB3	2.16	0.45
1:B:2661:TRP:HB3	1:B:2664:PHE:HD1	1.81	0.45
1:B:3398:PHE:HE2	1:B:3450:ASN:CB	2.30	0.45
1:D:260:TRP:CE3	1:D:282:ILE:HG22	2.51	0.45
1:D:2224:ARG:HE	1:D:2225:PHE:N	2.10	0.45
1:D:4732:PHE:HE2	1:D:4736:ARG:HG2	1.81	0.45
1:D:4902:GLU:O	1:D:4913:ARG:NH2	2.50	0.45
1:C:2303:ALA:O	1:C:2307:LEU:HD13	2.17	0.45
1:C:2685:SER:O	1:C:2689:LYS:HG2	2.17	0.45
1:C:3213:TYR:CD1	1:C:3302:PRO:HG2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3324:VAL:HA	1:C:3327:LEU:HG	1.99	0.45
1:C:3414:ARG:HH22	1:C:3472:ALA:CB	2.30	0.45
1:C:3802:ILE:HD11	1:C:3883:ASP:O	2.17	0.45
1:C:4577:LEU:HD23	1:C:4580:TYR:CE1	2.52	0.45
1:C:4821:LYS:O	1:C:4825:THR:HG23	2.17	0.45
1:C:4942:GLU:O	1:C:4945:ASP:OD1	2.34	0.45
1:A:380:GLN:OE1	1:A:380:GLN:N	2.45	0.45
1:A:622:THR:HA	1:A:626:LEU:HD13	1.99	0.45
1:A:1791:VAL:O	1:A:1792:ALA:HB3	2.16	0.45
1:A:2904:LEU:O	1:A:2906:VAL:HG22	2.17	0.45
1:A:3213:TYR:CD1	1:A:3302:PRO:HG2	2.52	0.45
1:A:3414:ARG:HH22	1:A:3472:ALA:CB	2.30	0.45
1:A:4176:PRO:O	1:A:4202:ARG:NH2	2.49	0.45
1:A:4821:LYS:O	1:A:4825:THR:HG23	2.17	0.45
1:B:155:LYS:HD2	1:B:156:GLN:N	2.32	0.45
1:B:345:LEU:HD12	1:B:387:ALA:HB1	1.99	0.45
1:B:721:LEU:HD12	1:B:1476:MET:HE2	1.98	0.45
1:B:820:ARG:CZ	1:B:820:ARG:CB	2.80	0.45
1:B:1126:GLY:HA3	1:B:1143:TRP:CE3	2.52	0.45
1:B:2685:SER:O	1:B:2689:LYS:HG2	2.17	0.45
1:B:3230:LEU:HD12	1:B:3232:LEU:HG	1.99	0.45
1:B:3401:LEU:O	1:B:3405:LEU:HD13	2.16	0.45
1:B:3409:TYR:O	1:B:3412:LEU:N	2.50	0.45
1:B:3566:SER:CB	1:B:3569:LEU:HD12	2.47	0.45
1:B:3899:PHE:CZ	1:B:3903:LEU:HD21	2.52	0.45
1:D:221:ARG:NH2	1:D:255:HIS:O	2.47	0.45
1:D:879:HIS:CE1	1:D:913:LEU:HD13	2.51	0.45
1:D:2303:ALA:O	1:D:2307:LEU:CD1	2.65	0.45
1:D:3580:PRO:O	1:D:3583:GLU:OE2	2.35	0.45
1:D:3891:LEU:CB	1:D:3899:PHE:CE2	3.00	0.45
1:D:3966:THR:HG23	1:D:4029:SER:OG	2.17	0.45
1:D:4095:LYS:O	1:D:4098:ASP:OD1	2.35	0.45
1:C:365:LYS:O	1:C:369:LEU:HG	2.17	0.45
1:C:2303:ALA:O	1:C:2307:LEU:CD1	2.65	0.45
1:C:3107:VAL:O	1:C:3111:ARG:HG2	2.17	0.45
1:A:155:LYS:HD2	1:A:156:GLN:N	2.32	0.44
1:A:336:PRO:HA	1:A:337:PRO:HD3	1.91	0.44
1:A:345:LEU:HD12	1:A:387:ALA:HB1	2.00	0.44
1:A:880:GLU:O	1:A:884:LEU:HD13	2.17	0.44
1:A:927:GLU:O	1:A:931:THR:HG23	2.16	0.44
1:A:2707:ALA:HB1	1:A:3009:TYR:CD1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3327:LEU:O	1:A:3403:ARG:NH2	2.50	0.44
1:A:3409:TYR:O	1:A:3412:LEU:N	2.50	0.44
1:B:3036:LYS:O	1:B:3039:ILE:HG22	2.16	0.44
1:B:3324:VAL:HA	1:B:3327:LEU:HG	1.99	0.44
1:B:3414:ARG:HH22	1:B:3472:ALA:CB	2.30	0.44
1:B:4148:THR:HG21	1:B:4180:ARG:NH2	2.31	0.44
1:D:155:LYS:HD2	1:D:156:GLN:N	2.32	0.44
1:D:1515:VAL:O	1:D:1531:ALA:O	2.36	0.44
1:D:1805:GLU:HG2	1:D:1806:ALA:N	2.33	0.44
1:D:2261:SER:O	1:D:2264:GLY:N	2.43	0.44
1:D:3546:ASP:O	1:D:3549:VAL:HG22	2.17	0.44
1:D:4016:LEU:O	1:D:4020:GLN:HG3	2.16	0.44
1:C:820:ARG:HB3	1:C:820:ARG:CZ	2.24	0.44
1:C:2675:THR:CG2	1:C:2706:ILE:HG23	2.48	0.44
1:A:1126:GLY:HA3	1:A:1143:TRP:CE3	2.52	0.44
1:A:1515:VAL:O	1:A:1531:ALA:O	2.36	0.44
2:H:7:ILE:HA	1:D:719:LEU:HD11	1.99	0.44
1:B:224:HIS:HA	1:B:388:LEU:HD23	1.98	0.44
1:B:1742:THR:O	1:B:1960:ALA:HB2	2.18	0.44
1:B:1805:GLU:HG2	1:B:1806:ALA:N	2.33	0.44
1:B:2373:GLY:O	1:C:130:LYS:NZ	2.49	0.44
1:B:3106:MET:O	1:B:3110:LEU:HD23	2.17	0.44
1:B:3842:LEU:HD23	1:B:3874:VAL:CG1	2.47	0.44
1:B:3941:ASP:OD2	1:B:3941:ASP:N	2.46	0.44
1:B:4095:LYS:O	1:B:4098:ASP:OD1	2.35	0.44
1:D:884:LEU:O	1:D:887:ILE:HB	2.16	0.44
1:D:2494:PHE:HD1	1:D:2498:HIS:HD1	1.64	0.44
1:D:3465:ASN:OD1	1:D:3467:MET:CG	2.60	0.44
1:D:4942:GLU:O	1:D:4945:ASP:OD1	2.34	0.44
1:C:553:ARG:O	1:C:557:SER:OG	2.29	0.44
1:C:2226:PRO:HB2	1:C:2267:MET:HE3	1.99	0.44
1:C:3036:LYS:O	1:C:3039:ILE:HG22	2.16	0.44
1:C:3580:PRO:O	1:C:3583:GLU:OE2	2.35	0.44
1:C:3966:THR:HG23	1:C:4029:SER:OG	2.17	0.44
1:C:4094:GLN:HG3	1:C:4108:ILE:HG21	1.99	0.44
1:C:4583:SER:OG	1:C:4585:SER:O	2.27	0.44
1:A:941:MET:SD	1:A:1051:TYR:HE1	2.32	0.44
1:A:2244:ARG:NH2	1:A:2283:ASN:OD1	2.50	0.44
1:A:4094:GLN:HG3	1:A:4108:ILE:HG21	2.00	0.44
1:A:4937:ILE:HG12	1:B:4934:GLY:HA2	1.99	0.44
1:B:985:VAL:HA	1:B:1039:LEU:HD22	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2214:VAL:HG11	1:B:2228:MET:CE	2.48	0.44
1:B:2303:ALA:O	1:B:2307:LEU:CD1	2.65	0.44
1:B:3107:VAL:O	1:B:3111:ARG:HG2	2.17	0.44
1:B:3802:ILE:HD11	1:B:3883:ASP:O	2.17	0.44
1:B:3966:THR:HG23	1:B:4029:SER:OG	2.17	0.44
1:B:4902:GLU:O	1:B:4913:ARG:NH2	2.50	0.44
1:D:76:ARG:O	1:D:80:GLU:HG2	2.18	0.44
1:D:213:TYR:HA	1:D:339:ILE:O	2.16	0.44
1:D:622:THR:HA	1:D:626:LEU:HD13	1.99	0.44
1:D:2482:ASP:C	1:D:2482:ASP:OD1	2.55	0.44
1:D:2791:LEU:HD13	1:D:2791:LEU:HA	1.89	0.44
1:D:3802:ILE:HD11	1:D:3883:ASP:O	2.17	0.44
1:D:4821:LYS:O	1:D:4825:THR:HG23	2.17	0.44
1:C:2482:ASP:C	1:C:2482:ASP:OD1	2.55	0.44
1:C:2572:THR:CG2	1:C:2579:VAL:CG2	2.83	0.44
1:C:3842:LEU:HD23	1:C:3874:VAL:CG1	2.47	0.44
1:C:4093:PHE:O	1:C:4097:MET:HG2	2.17	0.44
1:C:4943:LEU:O	1:C:4947:GLN:HG2	2.17	0.44
1:A:553:ARG:NH2	1:A:555:GLU:OE2	2.50	0.44
1:A:3230:LEU:HD12	1:A:3232:LEU:HG	1.99	0.44
1:A:3528:THR:HG23	1:A:3573:MET:SD	2.58	0.44
1:A:3546:ASP:O	1:A:3549:VAL:HG22	2.17	0.44
1:A:3842:LEU:HD23	1:A:3874:VAL:CG1	2.47	0.44
1:A:4820:VAL:HG11	1:B:4839:MET:CE	2.47	0.44
2:E:25:HIS:CD2	2:E:104:LEU:HD21	2.51	0.44
2:H:25:HIS:HD2	2:H:104:LEU:HD21	1.82	0.44
1:B:1791:VAL:O	1:B:1792:ALA:HB3	2.16	0.44
1:B:3327:LEU:O	1:B:3403:ARG:NH2	2.50	0.44
1:D:869:ARG:HD2	1:D:870:ILE:N	2.31	0.44
1:D:927:GLU:O	1:D:931:THR:HG23	2.16	0.44
1:D:959:TYR:CD2	1:D:966:LYS:HE2	2.50	0.44
1:D:1456:ASP:OD1	1:D:1456:ASP:N	2.47	0.44
1:D:4093:PHE:O	1:D:4097:MET:HG2	2.17	0.44
1:D:4094:GLN:HG3	1:D:4108:ILE:HG21	1.99	0.44
1:D:4943:LEU:O	1:D:4947:GLN:HG2	2.18	0.44
1:C:984:LEU:HD23	1:C:988:LEU:HD23	2.00	0.44
1:C:1515:VAL:O	1:C:1531:ALA:O	2.35	0.44
1:C:1873:GLU:N	1:C:1873:GLU:OE1	2.50	0.44
1:C:2701:PRO:C	1:C:2702:CYS:SG	2.96	0.44
1:C:2707:ALA:HB1	1:C:3009:TYR:CD1	2.52	0.44
1:C:2904:LEU:O	1:C:2906:VAL:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3336:LYS:O	1:C:3340:VAL:HG23	2.16	0.44
1:C:4029:SER:HA	1:C:4032:GLU:HG3	2.00	0.44
1:A:2675:THR:CG2	1:A:2706:ILE:HG23	2.47	0.44
1:A:2828:GLU:O	1:A:2829:GLY:O	2.34	0.44
1:A:3107:VAL:O	1:A:3111:ARG:HG2	2.17	0.44
1:A:3398:PHE:HE2	1:A:3450:ASN:CB	2.30	0.44
1:A:4736:ARG:NH1	1:D:4075:GLU:CD	2.70	0.44
1:A:4778:TRP:O	1:A:4782:VAL:HG23	2.18	0.44
1:B:380:GLN:OE1	1:B:380:GLN:N	2.45	0.44
1:B:961:MET:SD	1:B:963:ASN:HB2	2.57	0.44
1:B:2482:ASP:OD1	1:B:2482:ASP:C	2.55	0.44
1:B:2675:THR:CG2	1:B:2706:ILE:HG23	2.47	0.44
1:B:2904:LEU:O	1:B:2906:VAL:HG22	2.17	0.44
1:B:3075:LEU:O	1:B:3146:HIS:NE2	2.51	0.44
1:B:3086:GLU:OE2	1:B:3093:ARG:NH1	2.50	0.44
1:B:3604:TYR:CD1	1:B:3608:GLN:OE1	2.71	0.44
1:B:4093:PHE:O	1:B:4097:MET:HG2	2.17	0.44
1:B:4094:GLN:HG3	1:B:4108:ILE:HG21	2.00	0.44
1:B:4977:THR:OG1	1:B:5029:ARG:NH2	2.51	0.44
1:D:880:GLU:O	1:D:884:LEU:HD13	2.17	0.44
1:D:3628:ARG:HD2	1:D:3632:VAL:HG13	1.99	0.44
1:D:3842:LEU:HD23	1:D:3874:VAL:CG1	2.47	0.44
1:D:4029:SER:HA	1:D:4032:GLU:HG3	2.00	0.44
1:D:4977:THR:OG1	1:D:5029:ARG:NH2	2.51	0.44
1:C:663:TYR:OH	1:C:665:GLU:OE2	2.27	0.44
1:C:1126:GLY:HA3	1:C:1143:TRP:CE3	2.52	0.44
1:C:3086:GLU:OE2	1:C:3093:ARG:NH1	2.50	0.44
1:C:3528:THR:HG23	1:C:3573:MET:SD	2.58	0.44
1:C:3546:ASP:O	1:C:3549:VAL:HG22	2.17	0.44
1:A:1170:MET:CE	1:D:3471:THR:HG22	2.47	0.44
1:A:1805:GLU:HG2	1:A:1806:ALA:N	2.33	0.44
1:A:3580:PRO:O	1:A:3583:GLU:OE2	2.35	0.44
1:B:867:LEU:HA	1:B:870:ILE:HG22	1.98	0.44
1:B:984:LEU:HD23	1:B:988:LEU:HD23	2.00	0.44
1:B:1868:PRO:O	1:B:1872:THR:OG1	2.28	0.44
1:B:2701:PRO:C	1:B:2702:CYS:SG	2.96	0.44
1:B:4077:PHE:O	1:B:4081:VAL:HG23	2.18	0.44
1:B:4732:PHE:CE2	1:B:4736:ARG:HG2	2.53	0.44
1:D:345:LEU:HD12	1:D:387:ALA:HB1	2.00	0.44
1:D:553:ARG:NH2	1:D:555:GLU:OE2	2.50	0.44
1:D:3106:MET:O	1:D:3110:LEU:HD23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3343:GLN:HE22	1:D:3410:PRO:HB2	1.83	0.44
1:D:3971:GLY:N	1:D:3972:PRO:HA	2.33	0.44
1:D:4778:TRP:O	1:D:4782:VAL:HG23	2.18	0.44
1:C:345:LEU:HD12	1:C:387:ALA:HB1	2.00	0.44
1:C:4902:GLU:O	1:C:4913:ARG:NH2	2.50	0.44
1:C:4977:THR:OG1	1:C:5029:ARG:NH2	2.51	0.44
1:A:155:LYS:HE2	1:D:228:ASP:OD2	2.17	0.44
1:A:345:LEU:HD12	1:A:387:ALA:CB	2.48	0.44
1:A:1873:GLU:OE1	1:A:1873:GLU:N	2.50	0.44
1:A:3984:ARG:NH1	1:B:160:GLY:O	2.48	0.44
1:A:4767:TRP:CE3	1:A:4768:LEU:CD2	2.99	0.44
1:B:1067:SER:O	1:B:1071:ARG:HG3	2.18	0.44
1:B:3537:LYS:NZ	1:B:3607:GLU:OE2	2.33	0.44
1:D:224:HIS:HA	1:D:388:LEU:HD23	1.98	0.44
1:D:598:LYS:O	1:D:602:VAL:HG23	2.18	0.44
1:D:1742:THR:O	1:D:1960:ALA:HB2	2.18	0.44
1:D:3327:LEU:O	1:D:3403:ARG:NH2	2.50	0.44
1:D:3336:LYS:O	1:D:3340:VAL:HG23	2.17	0.44
1:D:3566:SER:CB	1:D:3569:LEU:HD12	2.47	0.44
1:C:622:THR:HA	1:C:626:LEU:HD13	1.99	0.44
1:C:646:PRO:HB2	1:C:648:ILE:HD13	2.00	0.44
1:C:1805:GLU:HG2	1:C:1806:ALA:N	2.33	0.44
1:C:2886:TRP:O	1:C:2890:LYS:HG2	2.17	0.44
1:C:3455:GLU:O	1:C:3459:VAL:HG23	2.17	0.44
1:A:730:VAL:HG23	1:A:1476:MET:SD	2.58	0.44
1:A:867:LEU:HA	1:A:870:ILE:HG22	1.98	0.44
1:A:941:MET:HE3	1:A:1051:TYR:CG	2.49	0.44
1:A:1067:SER:O	1:A:1071:ARG:HG3	2.18	0.44
1:A:2303:ALA:O	1:A:2307:LEU:CD1	2.65	0.44
1:A:2701:PRO:C	1:A:2702:CYS:SG	2.96	0.44
1:A:2929:PHE:CD1	1:A:2932:MET:SD	3.11	0.44
1:A:3343:GLN:HE22	1:A:3410:PRO:HB2	1.83	0.44
1:A:3628:ARG:HD2	1:A:3632:VAL:HG13	1.99	0.44
1:A:4977:THR:OG1	1:A:5029:ARG:NH2	2.51	0.44
2:H:103:LEU:HD21	2:H:106:LEU:HD11	2.00	0.44
1:B:76:ARG:O	1:B:80:GLU:HG2	2.18	0.44
1:B:259:LEU:HD11	1:B:397:GLU:HG2	2.00	0.44
1:B:730:VAL:HG23	1:B:1476:MET:SD	2.58	0.44
1:B:3390:GLY:HA2	1:B:3393:LEU:HD13	1.99	0.44
1:B:3971:GLY:N	1:B:3972:PRO:HA	2.33	0.44
1:B:4943:LEU:O	1:B:4947:GLN:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:345:LEU:HD12	1:D:387:ALA:CB	2.48	0.44
1:D:2481:LYS:O	1:D:2482:ASP:CG	2.57	0.44
1:D:2904:LEU:O	1:D:2906:VAL:HG22	2.17	0.44
1:D:2929:PHE:CD1	1:D:2932:MET:SD	3.11	0.44
1:D:3455:GLU:O	1:D:3459:VAL:HG23	2.17	0.44
1:D:3789:GLU:OE1	1:D:3789:GLU:N	2.51	0.44
1:D:4767:TRP:CE3	1:D:4768:LEU:CD2	2.99	0.44
1:C:2214:VAL:HG11	1:C:2228:MET:CE	2.48	0.44
1:C:2330:ARG:O	1:C:2333:ASP:OD1	2.36	0.44
1:C:2527:LEU:O	1:C:2531:ARG:HG3	2.18	0.44
1:A:783:PHE:HB2	1:A:787:VAL:HG21	2.00	0.44
1:A:2330:ARG:O	1:A:2333:ASP:OD1	2.36	0.44
1:A:3390:GLY:HA2	1:A:3393:LEU:HD13	1.99	0.44
1:A:4095:LYS:O	1:A:4098:ASP:OD1	2.35	0.44
1:B:266:ARG:O	1:B:270:SER:OG	2.34	0.44
1:B:345:LEU:HD12	1:B:387:ALA:CB	2.48	0.44
1:B:1515:VAL:O	1:B:1531:ALA:O	2.36	0.44
1:B:2926:LEU:O	1:B:2930:LEU:HD13	2.18	0.44
1:B:3343:GLN:HE22	1:B:3410:PRO:HB2	1.83	0.44
1:B:4577:LEU:HD23	1:B:4580:TYR:CE1	2.52	0.44
1:D:941:MET:HE3	1:D:1051:TYR:CG	2.48	0.44
1:D:1694:LEU:O	1:D:1698:LEU:HG	2.18	0.44
1:D:2798:SER:OG	1:D:2801:ASP:OD2	2.26	0.44
1:D:5009:TYR:CZ	1:D:5013:MET:HE3	2.52	0.44
6:D:5304:PNX:HAK1	6:D:5304:PNX:HAA1	2.00	0.44
1:C:155:LYS:HD2	1:C:156:GLN:N	2.32	0.44
1:C:345:LEU:HD12	1:C:387:ALA:CB	2.48	0.44
1:C:1067:SER:O	1:C:1071:ARG:HG3	2.18	0.44
1:C:2929:PHE:CD1	1:C:2932:MET:SD	3.11	0.44
1:C:3327:LEU:O	1:C:3403:ARG:NH2	2.50	0.44
1:C:3429:ALA:HA	1:C:3432:GLU:OE1	2.18	0.44
1:C:4767:TRP:HE3	1:C:4768:LEU:HD23	1.80	0.44
1:A:1077:ALA:HB2	1:A:1190:PRO:HG2	2.00	0.43
1:A:2926:LEU:O	1:A:2930:LEU:HD13	2.18	0.43
1:A:3604:TYR:CD1	1:A:3608:GLN:OE1	2.71	0.43
1:A:4182:GLU:HB2	1:A:4983:HIS:CD2	2.53	0.43
2:F:31:GLU:OE2	1:B:1299:GLN:HG2	2.18	0.43
1:B:2481:LYS:O	1:B:2482:ASP:CG	2.57	0.43
1:B:3455:GLU:O	1:B:3459:VAL:HG23	2.17	0.43
1:B:4778:TRP:O	1:B:4782:VAL:HG23	2.18	0.43
1:D:646:PRO:HB2	1:D:648:ILE:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:667:MET:SD	1:D:801:LYS:NZ	2.85	0.43
1:D:2434:GLY:O	1:D:2508:ARG:NE	2.43	0.43
1:D:2701:PRO:C	1:D:2702:CYS:SG	2.96	0.43
1:D:3107:VAL:O	1:D:3111:ARG:HG2	2.17	0.43
1:D:3429:ALA:HA	1:D:3432:GLU:OE1	2.18	0.43
1:D:3528:THR:HG23	1:D:3573:MET:SD	2.58	0.43
1:C:76:ARG:O	1:C:80:GLU:HG2	2.18	0.43
1:C:309:THR:O	1:C:309:THR:HG22	2.18	0.43
1:C:3212:GLU:OE2	1:C:3213:TYR:CZ	2.71	0.43
1:C:3343:GLN:HE22	1:C:3410:PRO:HB2	1.83	0.43
1:C:3891:LEU:CB	1:C:3899:PHE:CE2	3.00	0.43
1:C:4095:LYS:O	1:C:4098:ASP:OD1	2.35	0.43
1:C:4182:GLU:HB2	1:C:4983:HIS:CD2	2.53	0.43
1:C:4732:PHE:CE2	1:C:4736:ARG:HG2	2.53	0.43
6:C:5304:PNX:HAA1	6:C:5304:PNX:HAK1	2.00	0.43
1:A:259:LEU:HD11	1:A:397:GLU:HG2	2.00	0.43
1:A:1694:LEU:O	1:A:1698:LEU:HG	2.18	0.43
1:A:2214:VAL:HG11	1:A:2228:MET:CE	2.48	0.43
1:A:3212:GLU:OE2	1:A:3213:TYR:CZ	2.72	0.43
1:A:4093:PHE:O	1:A:4097:MET:HG2	2.17	0.43
2:H:31:GLU:OE2	1:D:1299:GLN:HG2	2.18	0.43
1:B:598:LYS:O	1:B:602:VAL:HG23	2.18	0.43
1:B:615:ARG:NH2	1:B:1676:LEU:O	2.50	0.43
1:B:646:PRO:HB2	1:B:648:ILE:HD13	2.00	0.43
1:B:1694:LEU:O	1:B:1698:LEU:HG	2.18	0.43
1:B:2527:LEU:O	1:B:2531:ARG:HG3	2.18	0.43
1:B:2929:PHE:CD1	1:B:2932:MET:SD	3.11	0.43
1:B:3789:GLU:N	1:B:3789:GLU:OE1	2.51	0.43
1:B:3891:LEU:CB	1:B:3899:PHE:CE2	3.00	0.43
1:B:4029:SER:HA	1:B:4032:GLU:HG3	2.00	0.43
1:D:730:VAL:HG23	1:D:1476:MET:SD	2.58	0.43
1:D:1126:GLY:HA3	1:D:1143:TRP:CE3	2.52	0.43
1:D:1705:GLY:HA3	1:D:1836:PHE:CD2	2.53	0.43
1:D:1873:GLU:OE1	1:D:1873:GLU:N	2.50	0.43
1:D:2254:LEU:CD1	1:D:2276:ALA:HB1	2.47	0.43
1:D:2675:THR:CG2	1:D:2706:ILE:HG23	2.47	0.43
1:D:2685:SER:O	1:D:2689:LYS:HG2	2.17	0.43
1:D:2926:LEU:O	1:D:2930:LEU:HD13	2.18	0.43
1:D:3104:GLU:OE2	1:D:3167:ARG:HB3	2.19	0.43
1:D:3604:TYR:CD1	1:D:3608:GLN:OE1	2.71	0.43
1:C:1045:THR:HG22	1:C:1049:TYR:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1705:GLY:HA3	1:C:1836:PHE:CD2	2.53	0.43
1:C:2514:ASN:OD1	1:C:2517:PHE:HB3	2.19	0.43
1:C:3628:ARG:HD2	1:C:3632:VAL:HG13	1.99	0.43
1:C:4778:TRP:O	1:C:4782:VAL:HG23	2.18	0.43
1:A:598:LYS:O	1:A:602:VAL:HG23	2.18	0.43
1:A:646:PRO:HB2	1:A:648:ILE:HD13	2.00	0.43
1:A:1980:LEU:CD2	1:A:1995:THR:HG22	2.48	0.43
1:A:3604:TYR:CE1	1:A:3608:GLN:OE1	2.72	0.43
1:A:3789:GLU:OE1	1:A:3789:GLU:N	2.51	0.43
2:E:88:PRO:O	2:E:90:ILE:HD12	2.19	0.43
2:F:103:LEU:HD21	2:F:106:LEU:HD11	2.00	0.43
1:B:783:PHE:HB2	1:B:787:VAL:HG21	2.00	0.43
1:B:1743[A]:ARG:NH2	1:B:1967:ASP:OD2	2.40	0.43
1:B:2514:ASN:OD1	1:B:2517:PHE:HB3	2.18	0.43
1:B:2791:LEU:HD13	1:B:2791:LEU:HA	1.89	0.43
1:B:3213:TYR:CD1	1:B:3302:PRO:HG2	2.52	0.43
1:D:309:THR:O	1:D:309:THR:HG22	2.18	0.43
1:D:1077:ALA:HB2	1:D:1190:PRO:HG2	2.00	0.43
1:D:2886:TRP:O	1:D:2890:LYS:HG2	2.17	0.43
1:D:3075:LEU:O	1:D:3146:HIS:NE2	2.51	0.43
1:D:3574:ALA:HA	1:D:3577:ARG:NH2	2.33	0.43
1:D:4182:GLU:HB2	1:D:4983:HIS:CD2	2.53	0.43
1:D:4673:ARG:O	1:D:4676:GLU:HG3	2.18	0.43
1:D:4732:PHE:CE2	1:D:4736:ARG:HG2	2.53	0.43
1:C:116:MET:HG2	1:C:139:GLU:HA	2.00	0.43
1:C:336:PRO:HA	1:C:337:PRO:HD3	1.91	0.43
1:C:2092:GLN:O	1:C:2092:GLN:HG2	2.19	0.43
1:C:3604:TYR:CE1	1:C:3608:GLN:OE1	2.72	0.43
1:A:2527:LEU:O	1:A:2531:ARG:HG3	2.18	0.43
1:A:2801:ASP:OD1	1:A:2802:LYS:N	2.52	0.43
1:A:3130:THR:O	1:A:3134:VAL:HG23	2.19	0.43
1:A:3966:THR:HG23	1:A:4029:SER:OG	2.17	0.43
1:A:4029:SER:HA	1:A:4032:GLU:HG3	2.00	0.43
1:A:4651:THR:OG1	1:A:4803:HIS:NE2	2.05	0.43
1:A:4655:PHE:CE2	1:A:4659:ILE:HD11	2.54	0.43
1:A:4732:PHE:CE2	1:A:4736:ARG:HG2	2.53	0.43
1:B:116:MET:HG2	1:B:139:GLU:HA	2.00	0.43
1:B:928:THR:O	1:B:931:THR:OG1	2.30	0.43
1:B:2330:ARG:O	1:B:2333:ASP:OD1	2.36	0.43
1:B:2393:ASP:OD1	1:B:2418:LEU:N	2.52	0.43
1:B:2801:ASP:OD1	1:B:2802:LYS:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3162:GLN:O	1:B:3166:TYR:CD2	2.72	0.43
1:B:3580:PRO:O	1:B:3583:GLU:OE2	2.35	0.43
1:B:4060:LYS:O	1:B:4063:ASP:OD1	2.37	0.43
1:B:4821:LYS:O	1:B:4825:THR:HG23	2.17	0.43
1:D:941:MET:SD	1:D:1051:TYR:HE1	2.32	0.43
1:D:2214:VAL:HG11	1:D:2228:MET:CE	2.48	0.43
1:D:2330:ARG:O	1:D:2333:ASP:OD1	2.36	0.43
1:D:2816:MET:HG3	1:D:2878:LEU:HD13	2.01	0.43
1:D:4655:PHE:CE2	1:D:4659:ILE:HD11	2.54	0.43
1:C:959:TYR:CD2	1:C:966:LYS:HE2	2.50	0.43
1:C:3686:GLU:O	1:C:3687:GLU:HB2	2.18	0.43
1:C:3789:GLU:OE1	1:C:3789:GLU:N	2.51	0.43
1:A:76:ARG:O	1:A:80:GLU:HG2	2.18	0.43
1:A:667:MET:SD	1:A:801:LYS:NZ	2.86	0.43
1:A:3455:GLU:O	1:A:3459:VAL:HG23	2.17	0.43
1:A:3686:GLU:O	1:A:3687:GLU:HB2	2.18	0.43
1:A:3891:LEU:CB	1:A:3899:PHE:CE2	3.00	0.43
1:A:4077:PHE:O	1:A:4081:VAL:HG23	2.18	0.43
1:B:1005:TRP:HB3	1:B:1021:LEU:CD1	2.48	0.43
1:B:1077:ALA:HB2	1:B:1190:PRO:HG2	2.00	0.43
1:B:3574:ALA:HA	1:B:3577:ARG:NH2	2.33	0.43
1:B:4182:GLU:HB2	1:B:4983:HIS:CD2	2.53	0.43
6:B:5304:PNX:HAK1	6:B:5304:PNX:HAA1	2.00	0.43
1:D:615:ARG:NH2	1:D:1676:LEU:O	2.49	0.43
1:D:2393:ASP:OD1	1:D:2418:LEU:N	2.52	0.43
1:D:4717:ASP:OD2	1:D:4723:LYS:NZ	2.35	0.43
1:C:598:LYS:O	1:C:602:VAL:HG23	2.18	0.43
1:C:730:VAL:HG23	1:C:1476:MET:SD	2.58	0.43
1:C:1980:LEU:CD2	1:C:1995:THR:HG22	2.48	0.43
1:C:2393:ASP:OD1	1:C:2418:LEU:N	2.52	0.43
1:C:2481:LYS:O	1:C:2482:ASP:CG	2.56	0.43
1:C:2736:ASP:OD1	1:C:2736:ASP:O	2.36	0.43
1:C:3162:GLN:O	1:C:3166:TYR:CD2	2.72	0.43
1:A:310:LYS:O	1:A:350:HIS:NE2	2.51	0.43
1:A:985:VAL:HG13	1:A:1039:LEU:HD23	2.00	0.43
1:A:2393:ASP:OD1	1:A:2418:LEU:N	2.52	0.43
1:A:3429:ALA:HA	1:A:3432:GLU:OE1	2.18	0.43
1:A:3971:GLY:N	1:A:3972:PRO:HA	2.33	0.43
1:A:4943:LEU:O	1:A:4947:GLN:HG2	2.17	0.43
2:E:24:VAL:HG12	2:E:103:LEU:HA	2.01	0.43
2:H:11:ASP:OD1	2:H:14:THR:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:88:PRO:O	2:H:90:ILE:HD12	2.19	0.43
2:G:24:VAL:HG12	2:G:103:LEU:HA	2.01	0.43
2:G:88:PRO:O	2:G:90:ILE:HD12	2.19	0.43
2:G:103:LEU:HD21	2:G:106:LEU:HD11	2.00	0.43
2:F:11:ASP:OD1	2:F:14:THR:HG23	2.19	0.43
1:B:622:THR:HA	1:B:626:LEU:HD13	1.99	0.43
1:B:874:LEU:O	1:B:878:ILE:HG12	2.19	0.43
1:B:1804:LEU:HD13	1:B:1853:ILE:HD12	2.00	0.43
1:B:2092:GLN:O	1:B:2092:GLN:HG2	2.19	0.43
1:B:2736:ASP:OD1	1:B:2736:ASP:O	2.36	0.43
1:B:2992:GLU:O	1:B:2996:LYS:HG2	2.19	0.43
1:D:874:LEU:O	1:D:878:ILE:HG12	2.19	0.43
1:D:961:MET:SD	1:D:963:ASN:HB2	2.57	0.43
1:D:1126:GLY:O	1:D:1142:PRO:HA	2.19	0.43
1:D:1804:LEU:HD13	1:D:1853:ILE:HD12	2.00	0.43
1:D:2514:ASN:OD1	1:D:2517:PHE:HB3	2.19	0.43
1:D:3104:GLU:O	1:D:3107:VAL:HG22	2.19	0.43
1:D:3398:PHE:HE2	1:D:3450:ASN:CB	2.30	0.43
1:D:3623:LEU:HD12	1:D:3624:LEU:N	2.34	0.43
1:D:3686:GLU:O	1:D:3687:GLU:HB2	2.18	0.43
1:C:1694:LEU:O	1:C:1698:LEU:HG	2.18	0.43
1:C:1742:THR:O	1:C:1960:ALA:HB2	2.18	0.43
1:C:3106:MET:O	1:C:3110:LEU:HD23	2.17	0.43
1:C:3230:LEU:HD12	1:C:3232:LEU:HG	1.99	0.43
1:C:3574:ALA:HA	1:C:3577:ARG:NH2	2.33	0.43
1:C:3604:TYR:CD1	1:C:3608:GLN:OE1	2.71	0.43
1:A:1742:THR:O	1:A:1960:ALA:HB2	2.18	0.43
1:A:2514:ASN:OD1	1:A:2517:PHE:HB3	2.18	0.43
1:A:3104:GLU:O	1:A:3107:VAL:HG22	2.19	0.43
1:A:3465:ASN:OD1	1:A:3467:MET:CG	2.60	0.43
1:A:3640:PRO:HB2	1:A:3642:TYR:CE1	2.54	0.43
6:A:5304:PNX:HAK1	6:A:5304:PNX:HAA1	2.00	0.43
1:B:941:MET:HE3	1:B:1051:TYR:CG	2.52	0.43
1:B:1045:THR:HG22	1:B:1049:TYR:CZ	2.53	0.43
1:B:1705:GLY:HA3	1:B:1836:PHE:CD2	2.53	0.43
1:B:3429:ALA:HA	1:B:3432:GLU:OE1	2.18	0.43
1:B:3528:THR:HG23	1:B:3573:MET:SD	2.58	0.43
1:B:3546:ASP:O	1:B:3549:VAL:HG22	2.17	0.43
1:B:3604:TYR:CE1	1:B:3608:GLN:OE1	2.72	0.43
1:B:3693:LYS:HA	1:B:3693:LYS:HE2	2.01	0.43
1:D:984:LEU:HD23	1:D:988:LEU:HD23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1154:ASP:OD1	1:D:1156:THR:OG1	2.37	0.43
1:D:2092:GLN:HG2	1:D:2092:GLN:O	2.19	0.43
1:C:310:LYS:O	1:C:350:HIS:NE2	2.51	0.43
1:C:1154:ASP:OD1	1:C:1156:THR:OG1	2.37	0.43
1:C:2190:VAL:HG12	1:C:2198:MET:HE3	2.00	0.43
1:C:2816:MET:HG3	1:C:2878:LEU:HD13	2.01	0.43
1:C:2986:VAL:O	1:C:2986:VAL:HG13	2.19	0.43
1:C:3640:PRO:HB2	1:C:3642:TYR:CE1	2.54	0.43
1:C:4077:PHE:O	1:C:4081:VAL:HG23	2.18	0.43
1:A:1154:ASP:OD1	1:A:1156:THR:OG1	2.37	0.43
1:A:1804:LEU:HD13	1:A:1853:ILE:HD12	2.00	0.43
1:A:3623:LEU:HD12	1:A:3624:LEU:N	2.34	0.43
1:A:3693:LYS:HE2	1:A:3693:LYS:HA	2.01	0.43
1:A:4673:ARG:O	1:A:4676:GLU:HG3	2.18	0.43
1:A:4677:LEU:HD23	1:A:4711:PHE:HE1	1.83	0.43
2:H:24:VAL:HG12	2:H:103:LEU:HA	2.01	0.43
1:B:484:LEU:HD12	1:B:526:LEU:HD12	2.01	0.43
1:B:2244:ARG:NH2	1:B:2283:ASN:OD1	2.50	0.43
1:B:3104:GLU:OE2	1:B:3167:ARG:HB3	2.19	0.43
1:D:259:LEU:HD11	1:D:397:GLU:HG2	2.00	0.43
1:D:985:VAL:HG13	1:D:1039:LEU:HD23	2.00	0.43
1:D:1005:TRP:HB3	1:D:1021:LEU:CD1	2.48	0.43
1:D:1067:SER:O	1:D:1071:ARG:HG3	2.18	0.43
1:D:2211:MET:O	1:D:2214:VAL:CG1	2.64	0.43
1:D:2801:ASP:OD1	1:D:2802:LYS:N	2.52	0.43
1:D:3197:LEU:HD21	1:D:3201:MET:HE3	2.01	0.43
1:D:4000:MET:SD	1:D:4020:GLN:NE2	2.79	0.43
1:C:259:LEU:HD11	1:C:397:GLU:HG2	2.00	0.43
1:C:2801:ASP:OD1	1:C:2802:LYS:N	2.52	0.43
1:C:2992:GLU:O	1:C:2996:LYS:HG2	2.19	0.43
1:C:3104:GLU:O	1:C:3107:VAL:HG22	2.19	0.43
1:C:3583:GLU:HB3	1:C:3585:ASP:OD1	2.19	0.43
1:C:3971:GLY:N	1:C:3972:PRO:HA	2.33	0.43
1:A:266:ARG:O	1:A:270:SER:OG	2.34	0.43
1:A:984:LEU:HD23	1:A:988:LEU:HD23	2.00	0.43
1:A:1705:GLY:HA3	1:A:1836:PHE:CD2	2.53	0.43
1:A:2800:LYS:O	1:A:2804:ILE:HG13	2.19	0.43
1:A:2816:MET:HG3	1:A:2878:LEU:HD13	2.01	0.43
1:A:3391:GLU:O	1:A:3395:ARG:HD2	2.19	0.43
1:A:3777:GLU:OE1	1:A:3777:GLU:N	2.47	0.43
1:B:309:THR:HG22	1:B:309:THR:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:LYS:O	1:B:350:HIS:NE2	2.51	0.43
1:B:1126:GLY:O	1:B:1142:PRO:HA	2.19	0.43
1:B:3212:GLU:OE2	1:B:3213:TYR:CZ	2.72	0.43
1:B:3682:GLU:O	1:B:3686:GLU:OE2	2.37	0.43
1:B:3725:TYR:O	1:B:3729:MET:HG3	2.19	0.43
1:D:1045:THR:HG22	1:D:1049:TYR:CZ	2.53	0.43
1:D:1828:ASP:N	1:D:1828:ASP:OD1	2.52	0.43
1:D:1980:LEU:CD2	1:D:1995:THR:HG22	2.48	0.43
1:D:3693:LYS:HE2	1:D:3693:LYS:HA	2.01	0.43
1:D:3777:GLU:OE1	1:D:3777:GLU:N	2.47	0.43
1:D:4946:GLN:O	1:D:4950:VAL:HG23	2.19	0.43
1:C:1077:ALA:HB2	1:C:1190:PRO:HG2	2.01	0.43
1:C:3075:LEU:O	1:C:3146:HIS:NE2	2.51	0.43
1:C:3104:GLU:OE2	1:C:3167:ARG:HB3	2.19	0.43
1:A:116:MET:HG2	1:A:139:GLU:HA	2.00	0.43
1:A:820:ARG:HB3	1:A:820:ARG:CZ	2.24	0.43
1:A:2481:LYS:O	1:A:2482:ASP:CG	2.56	0.43
1:A:2685:SER:O	1:A:2689:LYS:HG2	2.17	0.43
1:A:2736:ASP:O	1:A:2736:ASP:OD1	2.36	0.43
1:A:3104:GLU:OE2	1:A:3167:ARG:HB3	2.19	0.43
1:A:4148:THR:HG21	1:A:4180:ARG:NH2	2.31	0.43
1:A:4182:GLU:HB2	1:A:4983:HIS:NE2	2.34	0.43
2:F:24:VAL:HG12	2:F:103:LEU:HA	2.01	0.43
1:B:1440:PHE:CZ	1:B:1563:GLN:HG3	2.54	0.43
1:B:1828:ASP:OD1	1:B:1828:ASP:N	2.52	0.43
1:B:2800:LYS:O	1:B:2804:ILE:HG13	2.19	0.43
1:B:3686:GLU:O	1:B:3687:GLU:HB2	2.18	0.43
1:B:4901:ILE:HG13	1:B:4913:ARG:NH2	2.34	0.43
1:D:167:ASP:OD1	1:C:384:MET:SD	2.77	0.43
1:D:2736:ASP:O	1:D:2736:ASP:OD1	2.36	0.43
1:D:2800:LYS:O	1:D:2804:ILE:HG13	2.19	0.43
1:D:3162:GLN:O	1:D:3166:TYR:CD2	2.72	0.43
1:D:3175:LEU:O	1:D:3175:LEU:HD23	2.19	0.43
1:D:3212:GLU:OE2	1:D:3213:TYR:CZ	2.71	0.43
1:D:3230:LEU:HD12	1:D:3232:LEU:HG	1.99	0.43
1:D:4781:GLY:O	1:D:4785:THR:HG23	2.19	0.43
1:C:874:LEU:O	1:C:878:ILE:HG12	2.19	0.43
1:C:2725:LYS:HE3	1:C:2734:ASN:O	2.19	0.43
1:C:3239:MET:CB	1:C:3239:MET:HG2	2.31	0.43
1:C:3891:LEU:HD13	1:C:3899:PHE:HZ	1.79	0.43
1:C:4655:PHE:CE2	1:C:4659:ILE:HD11	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4673:ARG:O	1:C:4676:GLU:HG3	2.18	0.43
1:C:4781:GLY:O	1:C:4785:THR:HG23	2.19	0.43
1:A:908:VAL:O	1:A:909:ASN:HB2	2.19	0.42
1:A:1105:ALA:HB2	1:A:1191:VAL:HG11	2.00	0.42
1:A:1143:TRP:HB2	1:A:1147:ASP:HB2	2.01	0.42
1:A:3162:GLN:O	1:A:3166:TYR:CD2	2.72	0.42
1:A:3583:GLU:HB3	1:A:3585:ASP:OD1	2.19	0.42
1:A:4000:MET:SD	1:A:4020:GLN:NE2	2.79	0.42
1:A:4060:LYS:O	1:A:4063:ASP:OD1	2.37	0.42
1:A:4901:ILE:HG13	1:A:4913:ARG:NH2	2.34	0.42
2:E:11:ASP:OD1	2:E:14:THR:HG23	2.19	0.42
1:B:1154:ASP:OD1	1:B:1156:THR:OG1	2.37	0.42
1:B:1756:ASN:OD1	1:B:2040:ALA:HB2	2.19	0.42
1:B:3239:MET:CB	1:B:3239:MET:HG3	2.31	0.42
1:B:3380:ARG:NH1	1:B:3391:GLU:OE2	2.50	0.42
1:D:2527:LEU:O	1:D:2531:ARG:HG3	2.18	0.42
1:D:2572:THR:CG2	1:D:2579:VAL:CG2	2.83	0.42
1:D:3868:ARG:HG2	1:D:3869:GLN:N	2.34	0.42
1:D:4077:PHE:O	1:D:4081:VAL:HG23	2.18	0.42
1:C:484:LEU:HD12	1:C:526:LEU:HD12	2.01	0.42
1:C:783:PHE:HB2	1:C:787:VAL:HG21	2.00	0.42
1:C:961:MET:SD	1:C:963:ASN:HB2	2.57	0.42
1:C:1436:SER:OG	1:C:1565:GLU:HB2	2.19	0.42
1:C:2969:ILE:O	1:C:2973:PHE:HD1	2.02	0.42
1:C:3682:GLU:O	1:C:3686:GLU:OE2	2.37	0.42
1:C:3693:LYS:HE2	1:C:3693:LYS:HA	2.01	0.42
1:A:1005:TRP:HB3	1:A:1021:LEU:CD1	2.48	0.42
1:A:1045:THR:HG22	1:A:1049:TYR:CZ	2.54	0.42
1:A:1436:SER:OG	1:A:1565:GLU:HB2	2.19	0.42
1:A:1756:ASN:OD1	1:A:2040:ALA:HB2	2.19	0.42
1:A:2992:GLU:O	1:A:2996:LYS:HG2	2.19	0.42
1:A:4946:GLN:O	1:A:4950:VAL:HG23	2.19	0.42
2:G:31:GLU:OE2	1:C:1299:GLN:HG2	2.19	0.42
1:B:1105:ALA:HB2	1:B:1191:VAL:HG11	2.00	0.42
1:B:1105:ALA:O	1:B:1189:LEU:N	2.50	0.42
1:B:2595:LEU:O	1:B:2600:ARG:NH2	2.52	0.42
1:B:3573:MET:CB	1:B:3577:ARG:NH1	2.73	0.42
1:B:3623:LEU:HD12	1:B:3624:LEU:N	2.34	0.42
1:B:4673:ARG:O	1:B:4676:GLU:HG3	2.18	0.42
1:D:928:THR:O	1:D:931:THR:OG1	2.30	0.42
1:D:3604:TYR:CE1	1:D:3608:GLN:OE1	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3725:TYR:O	1:D:3729:MET:HG3	2.19	0.42
1:D:4231:MET:O	1:D:4235:VAL:HG23	2.20	0.42
1:C:1005:TRP:HB3	1:C:1021:LEU:CD1	2.48	0.42
1:C:2208:MET:O	1:C:2212:VAL:HG22	2.19	0.42
1:C:2434:GLY:O	1:C:2508:ARG:NE	2.43	0.42
1:C:3197:LEU:HD21	1:C:3201:MET:HE3	2.01	0.42
1:C:3725:TYR:O	1:C:3729:MET:HG3	2.19	0.42
1:C:4060:LYS:O	1:C:4063:ASP:OD1	2.37	0.42
1:C:4182:GLU:HB2	1:C:4983:HIS:NE2	2.34	0.42
1:A:553:ARG:O	1:A:557:SER:OG	2.29	0.42
1:A:893:TYR:HD1	1:A:907:LEU:O	2.03	0.42
1:A:921:ASN:O	1:A:924:MET:HG2	2.19	0.42
1:A:2874:MET:HE1	1:A:2939:ARG:HB2	1.95	0.42
1:A:2986:VAL:HG13	1:A:2986:VAL:O	2.19	0.42
1:A:3071:LEU:O	1:A:3075:LEU:HG	2.19	0.42
1:A:3471:THR:HG22	1:B:1170:MET:CE	2.49	0.42
1:B:921:ASN:O	1:B:924:MET:HG2	2.19	0.42
1:B:2700:MET:O	1:B:2702:CYS:SG	2.78	0.42
1:B:3130:THR:O	1:B:3134:VAL:HG23	2.19	0.42
1:D:492:ASP:O	1:D:496:VAL:HG13	2.19	0.42
1:D:2414:ASN:OD1	1:D:2414:ASN:C	2.58	0.42
1:D:4182:GLU:HB2	1:D:4983:HIS:NE2	2.34	0.42
1:C:266:ARG:O	1:C:270:SER:OG	2.34	0.42
1:C:1743[A]:ARG:NH2	1:C:1967:ASP:OD2	2.39	0.42
1:C:2865:VAL:HG11	1:C:2928:LYS:HE2	2.02	0.42
1:C:2926:LEU:O	1:C:2930:LEU:HD13	2.18	0.42
1:C:3197:LEU:HD23	1:C:3197:LEU:O	2.20	0.42
1:C:3879:GLU:HG2	1:C:3880:PHE:N	2.35	0.42
1:C:4021:LYS:N	1:C:4139:ILE:HD13	2.35	0.42
1:C:4563:ARG:NH2	1:C:4815:ASP:OD1	2.53	0.42
1:A:2414:ASN:OD1	1:A:2414:ASN:C	2.58	0.42
2:F:24:VAL:HG21	2:F:59:TRP:HZ3	1.85	0.42
1:B:2816:MET:HG3	1:B:2878:LEU:HD13	2.01	0.42
1:B:4021:LYS:N	1:B:4139:ILE:HD13	2.35	0.42
1:B:4182:GLU:HB2	1:B:4983:HIS:NE2	2.34	0.42
1:B:4231:MET:O	1:B:4235:VAL:HG23	2.20	0.42
1:D:783:PHE:HB2	1:D:787:VAL:HG21	2.00	0.42
1:D:921:ASN:O	1:D:924:MET:HG2	2.19	0.42
1:D:1194:LEU:HD23	1:D:1198:GLN:O	2.19	0.42
1:D:1434:TYR:HB2	1:D:1572:ILE:HG21	2.01	0.42
1:D:2986:VAL:HG13	1:D:2986:VAL:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3640:PRO:HB2	1:D:3642:TYR:CE1	2.54	0.42
1:D:3892:CYS:HG	1:D:3899:PHE:HD2	1.67	0.42
1:C:908:VAL:O	1:C:909:ASN:HB2	2.19	0.42
1:C:1194:LEU:HD23	1:C:1198:GLN:O	2.19	0.42
1:C:1828:ASP:OD1	1:C:1828:ASP:N	2.52	0.42
1:C:2612[B]:ARG:NH1	1:C:2613:TYR:OH	2.53	0.42
1:A:998:ARG:HG2	1:A:998:ARG:HH11	1.84	0.42
1:A:3682:GLU:O	1:A:3686:GLU:OE2	2.37	0.42
1:A:4781:GLY:O	1:A:4785:THR:HG23	2.19	0.42
2:E:103:LEU:HD21	2:E:106:LEU:HD11	2.00	0.42
2:G:11:ASP:OD1	2:G:14:THR:HG23	2.19	0.42
1:B:893:TYR:HD1	1:B:907:LEU:O	2.03	0.42
1:B:2703:LEU:HD22	1:B:2706:ILE:HD12	2.02	0.42
1:B:3071:LEU:O	1:B:3075:LEU:HG	2.19	0.42
1:B:3175:LEU:O	1:B:3175:LEU:HD23	2.19	0.42
1:B:3197:LEU:HD23	1:B:3197:LEU:O	2.20	0.42
1:B:3868:ARG:HG2	1:B:3869:GLN:N	2.34	0.42
1:B:3879:GLU:HG2	1:B:3880:PHE:N	2.35	0.42
1:B:4781:GLY:O	1:B:4785:THR:HG23	2.19	0.42
1:D:116:MET:HG2	1:D:139:GLU:HA	2.00	0.42
1:D:266:ARG:O	1:D:270:SER:OG	2.34	0.42
1:D:998:ARG:HG2	1:D:998:ARG:HH11	1.84	0.42
1:D:1143:TRP:HB2	1:D:1147:ASP:HB2	2.01	0.42
1:D:2595:LEU:O	1:D:2600:ARG:NH2	2.52	0.42
1:D:3879:GLU:HG2	1:D:3880:PHE:N	2.34	0.42
1:C:1105:ALA:HB2	1:C:1191:VAL:HG11	2.00	0.42
1:C:1143:TRP:HB2	1:C:1147:ASP:HB2	2.01	0.42
1:C:2595:LEU:O	1:C:2600:ARG:NH2	2.52	0.42
1:C:2667:THR:HG21	1:C:2672:LEU:HG	2.01	0.42
1:C:3294:PRO:HB2	1:C:3297:PRO:HD2	2.01	0.42
1:C:3435:PHE:CD2	1:C:3524:MET:CE	3.03	0.42
1:C:3573:MET:CB	1:C:3577:ARG:NH1	2.73	0.42
1:C:4946:GLN:O	1:C:4950:VAL:HG23	2.19	0.42
1:A:309:THR:O	1:A:309:THR:HG22	2.18	0.42
1:A:484:LEU:HD12	1:A:526:LEU:HD12	2.01	0.42
1:A:492:ASP:O	1:A:496:VAL:HG13	2.19	0.42
1:A:2700:MET:O	1:A:2702:CYS:SG	2.78	0.42
1:A:2703:LEU:HD22	1:A:2706:ILE:HD12	2.02	0.42
1:A:3725:TYR:O	1:A:3729:MET:HG3	2.19	0.42
1:A:3879:GLU:HG2	1:A:3880:PHE:N	2.35	0.42
1:A:4021:LYS:N	1:A:4139:ILE:HD13	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:908:VAL:O	1:B:909:ASN:HB2	2.19	0.42
1:B:1436:SER:OG	1:B:1565:GLU:HB2	2.20	0.42
1:B:1727:ARG:O	1:B:1731:LEU:HG	2.20	0.42
1:B:2667:THR:HG21	1:B:2672:LEU:HG	2.01	0.42
1:B:2977:LEU:HD23	1:B:3056:LEU:HD11	2.02	0.42
1:B:3435:PHE:CD2	1:B:3524:MET:CE	3.03	0.42
1:B:3640:PRO:HB2	1:B:3642:TYR:CE1	2.54	0.42
1:D:908:VAL:O	1:D:909:ASN:HB2	2.19	0.42
1:D:1927:LEU:HD22	1:D:2101:MET:SD	2.60	0.42
1:D:3610:GLU:OE1	1:D:3611:HIS:CD2	2.73	0.42
1:D:4060:LYS:O	1:D:4063:ASP:OD1	2.37	0.42
1:C:921:ASN:O	1:C:924:MET:HG2	2.20	0.42
1:C:1804:LEU:HD13	1:C:1853:ILE:HD12	2.00	0.42
1:C:3391:GLU:O	1:C:3395:ARG:HD2	2.19	0.42
1:A:1440:PHE:CZ	1:A:1563:GLN:HG3	2.54	0.42
1:A:1828:ASP:N	1:A:1828:ASP:OD1	2.52	0.42
1:A:1992:ALA:O	1:A:1995:THR:OG1	2.29	0.42
1:A:2092:GLN:HG2	1:A:2092:GLN:O	2.19	0.42
1:A:2545:GLU:HG2	1:A:2546:MET:N	2.35	0.42
1:A:2595:LEU:O	1:A:2600:ARG:NH2	2.52	0.42
1:A:3386:GLU:O	1:A:3389:GLU:O	2.38	0.42
1:A:3574:ALA:HA	1:A:3577:ARG:NH2	2.33	0.42
2:F:88:PRO:O	2:F:90:ILE:HD12	2.19	0.42
1:B:278:GLN:HG3	1:B:328:LYS:NZ	2.35	0.42
1:B:873:LYS:O	1:B:876:GLU:HG2	2.20	0.42
1:B:1194:LEU:HD23	1:B:1198:GLN:O	2.19	0.42
1:B:1276:THR:O	1:B:1279:SER:OG	2.27	0.42
1:B:1927:LEU:HD22	1:B:2101:MET:SD	2.60	0.42
1:B:2208:MET:O	1:B:2212:VAL:HG22	2.19	0.42
1:D:69:LEU:CD2	1:D:109:LEU:HD21	2.50	0.42
1:D:2208:MET:O	1:D:2212:VAL:HG22	2.19	0.42
1:D:3130:THR:O	1:D:3134:VAL:HG23	2.19	0.42
1:D:3660:ALA:HB3	1:D:3661:TRP:HD1	1.85	0.42
1:D:3899:PHE:HE2	1:D:3903:LEU:HD11	1.85	0.42
1:C:69:LEU:CD2	1:C:109:LEU:HD21	2.50	0.42
1:C:1126:GLY:O	1:C:1142:PRO:HA	2.19	0.42
1:C:1927:LEU:HD22	1:C:2101:MET:SD	2.60	0.42
1:C:3175:LEU:HD23	1:C:3175:LEU:O	2.19	0.42
1:C:4179:GLY:CA	1:C:4197:ILE:HD11	2.50	0.42
1:A:167:ASP:N	1:D:384:MET:SD	2.92	0.42
1:A:468:LEU:O	1:A:472:ARG:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:874:LEU:O	1:A:878:ILE:HG12	2.19	0.42
1:A:1194:LEU:HD23	1:A:1198:GLN:O	2.19	0.42
1:A:1927:LEU:HD22	1:A:2101:MET:SD	2.60	0.42
1:A:2798:SER:OG	1:A:2801:ASP:OD2	2.26	0.42
1:A:3478:MET:O	1:A:3478:MET:HG3	2.19	0.42
1:A:4999:ASP:OD1	1:A:5000:GLU:N	2.53	0.42
1:B:1434:TYR:HB2	1:B:1572:ILE:HG21	2.01	0.42
1:B:2414:ASN:OD1	1:B:2414:ASN:C	2.58	0.42
1:D:1756:ASN:OD1	1:D:2040:ALA:HB2	2.19	0.42
1:D:2313:LEU:HB3	1:D:2318:TYR:HB2	2.02	0.42
1:D:2587:TYR:OH	1:D:2629:ASP:OD2	2.24	0.42
1:D:2992:GLU:O	1:D:2996:LYS:HG2	2.19	0.42
1:D:3682:GLU:O	1:D:3686:GLU:OE2	2.37	0.42
1:C:292:ALA:HB2	1:C:312:THR:HG22	2.02	0.42
1:C:468:LEU:O	1:C:472:ARG:HG2	2.20	0.42
1:C:873:LYS:O	1:C:876:GLU:HG2	2.20	0.42
1:C:2001:PRO:O	1:C:2005:GLN:HG3	2.20	0.42
1:C:2545:GLU:HG2	1:C:2546:MET:N	2.35	0.42
1:C:3458:PHE:CE2	1:C:3464:ILE:HD11	2.54	0.42
1:A:869:ARG:NH2	1:A:947:GLU:OE2	2.52	0.42
1:A:1126:GLY:O	1:A:1142:PRO:HA	2.19	0.42
1:A:1434:TYR:HB2	1:A:1572:ILE:HG21	2.01	0.42
1:A:3294:PRO:HB2	1:A:3297:PRO:HD2	2.01	0.42
1:A:4843:LEU:HD21	1:D:4827:LEU:HD21	2.02	0.42
1:B:292:ALA:HB2	1:B:312:THR:HG22	2.02	0.42
1:B:309:THR:O	1:B:309:THR:CG2	2.68	0.42
1:B:468:LEU:O	1:B:472:ARG:HG2	2.20	0.42
1:B:516:LYS:O	1:B:519:VAL:HG22	2.20	0.42
1:B:3103:ILE:O	1:B:3107:VAL:HG13	2.20	0.42
1:B:3148:ALA:O	1:B:3151:GLN:NE2	2.53	0.42
1:B:3478:MET:O	1:B:3478:MET:HG3	2.19	0.42
1:B:4187:SER:O	1:B:4188:ARG:HB2	2.20	0.42
1:B:4705:VAL:HG23	1:B:4775:TYR:HD2	1.85	0.42
1:D:292:ALA:HB2	1:D:312:THR:HG22	2.02	0.42
1:D:309:THR:O	1:D:309:THR:CG2	2.68	0.42
1:D:516:LYS:O	1:D:519:VAL:HG22	2.20	0.42
1:D:887:ILE:HD13	1:D:887:ILE:HA	1.87	0.42
1:D:893:TYR:HD1	1:D:907:LEU:O	2.03	0.42
1:D:1105:ALA:HB2	1:D:1191:VAL:HG11	2.00	0.42
1:D:1265:ASP:OD1	1:D:1266:THR:N	2.53	0.42
1:D:1440:PHE:CZ	1:D:1563:GLN:HG3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2545:GLU:HG2	1:D:2546:MET:N	2.35	0.42
1:D:3148:ALA:O	1:D:3151:GLN:NE2	2.53	0.42
1:D:3321:ARG:HA	1:D:3324:VAL:HG22	2.02	0.42
1:D:3583:GLU:HB3	1:D:3585:ASP:OD1	2.19	0.42
1:D:4021:LYS:N	1:D:4139:ILE:HD13	2.35	0.42
1:D:4179:GLY:CA	1:D:4197:ILE:HD11	2.50	0.42
1:C:1434:TYR:HB2	1:C:1572:ILE:HG21	2.01	0.42
1:C:2700:MET:O	1:C:2702:CYS:SG	2.78	0.42
1:C:2977:LEU:HD23	1:C:3056:LEU:HD11	2.02	0.42
1:C:3623:LEU:HD12	1:C:3624:LEU:N	2.34	0.42
1:A:484:LEU:HD11	1:A:526:LEU:HD11	2.02	0.42
1:A:4179:GLY:HA3	1:A:4197:ILE:HD11	2.02	0.42
2:E:24:VAL:HG21	2:E:59:TRP:HZ3	1.85	0.42
1:B:384:MET:SD	1:C:167:ASP:OD1	2.78	0.42
1:B:484:LEU:HD11	1:B:526:LEU:HD11	2.02	0.42
1:B:2865:VAL:HG11	1:B:2928:LYS:HE2	2.02	0.42
1:B:3391:GLU:O	1:B:3395:ARG:HD2	2.19	0.42
1:B:3997:ALA:HB1	1:B:4057:MET:SD	2.60	0.42
1:B:4655:PHE:CE2	1:B:4659:ILE:HD11	2.54	0.42
1:D:310:LYS:O	1:D:350:HIS:NE2	2.51	0.42
1:D:484:LEU:HD12	1:D:526:LEU:HD12	2.01	0.42
1:D:2441:HIS:CE1	1:D:2442:LEU:HD12	2.55	0.42
1:D:2612[B]:ARG:NH1	1:D:2613:TYR:OH	2.53	0.42
1:D:3197:LEU:HD23	1:D:3197:LEU:O	2.20	0.42
1:D:3478:MET:O	1:D:3478:MET:HG3	2.19	0.42
1:D:4069:LYS:O	1:D:4072:VAL:HG22	2.20	0.42
1:C:484:LEU:HD11	1:C:526:LEU:HD11	2.02	0.42
1:C:484:LEU:CD1	1:C:526:LEU:CD1	2.98	0.42
1:C:1440:PHE:CZ	1:C:1563:GLN:HG3	2.54	0.42
1:C:1756:ASN:OD1	1:C:2040:ALA:HB2	2.19	0.42
1:C:2800:LYS:O	1:C:2804:ILE:HG13	2.19	0.42
1:C:2946:LEU:N	1:C:2948:THR:HG23	2.35	0.42
1:C:3478:MET:HG3	1:C:3478:MET:O	2.19	0.42
1:C:4999:ASP:OD1	1:C:5000:GLU:N	2.53	0.42
1:A:1265:ASP:OD1	1:A:1266:THR:N	2.53	0.41
1:A:1684:ALA:HA	2:E:90:ILE:HD11	2.02	0.41
1:A:2495:VAL:HG22	1:A:2498:HIS:CE1	2.55	0.41
1:A:2667:THR:HG21	1:A:2672:LEU:HG	2.01	0.41
1:A:3111:ARG:O	1:A:3112:LEU:HB2	2.20	0.41
1:A:3148:ALA:O	1:A:3151:GLN:NE2	2.53	0.41
1:A:3175:LEU:O	1:A:3175:LEU:HD23	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3321:ARG:HA	1:A:3324:VAL:HG22	2.02	0.41
1:A:3997:ALA:HB1	1:A:4057:MET:SD	2.60	0.41
1:A:4231:MET:O	1:A:4235:VAL:HG23	2.20	0.41
1:B:484:LEU:CD1	1:B:526:LEU:CD1	2.98	0.41
1:B:998:ARG:HG2	1:B:998:ARG:HH11	1.84	0.41
1:B:2928:LYS:O	1:B:2932:MET:HE3	2.20	0.41
1:B:3077:ALA:O	1:B:3081:MET:HG2	2.20	0.41
1:B:3104:GLU:O	1:B:3107:VAL:HG22	2.19	0.41
1:B:3633:VAL:O	1:B:3637:ARG:HD3	2.20	0.41
1:B:4179:GLY:CA	1:B:4197:ILE:HD11	2.50	0.41
1:B:4179:GLY:HA3	1:B:4197:ILE:HD11	2.02	0.41
1:D:484:LEU:HD11	1:D:526:LEU:HD11	2.02	0.41
1:D:1819:VAL:HG22	1:D:1926:LEU:HD21	2.02	0.41
1:D:2495:VAL:HG22	1:D:2498:HIS:CE1	2.55	0.41
1:D:3294:PRO:HB2	1:D:3297:PRO:HD2	2.02	0.41
1:D:3458:PHE:CE2	1:D:3464:ILE:HD11	2.54	0.41
1:D:4999:ASP:OD1	1:D:5000:GLU:N	2.53	0.41
1:C:492:ASP:O	1:C:496:VAL:HG13	2.19	0.41
1:C:509:GLU:O	1:C:513:GLU:CD	2.59	0.41
1:C:926:GLY:O	1:C:930:LYS:HG3	2.20	0.41
1:C:998:ARG:HG2	1:C:998:ARG:HH11	1.84	0.41
1:C:1265:ASP:OD1	1:C:1266:THR:N	2.53	0.41
1:C:1727:ARG:O	1:C:1731:LEU:HG	2.20	0.41
1:C:2117:VAL:O	1:C:2120:MET:HG2	2.21	0.41
1:C:2135:LEU:HD12	1:C:3658:LYS:HG3	2.02	0.41
1:C:2313:LEU:HB3	1:C:2318:TYR:HB2	2.02	0.41
1:C:2487:GLN:NE2	1:C:2545:GLU:OE1	2.53	0.41
1:C:3660:ALA:HB3	1:C:3661:TRP:HD1	1.85	0.41
1:C:4231:MET:O	1:C:4235:VAL:HG23	2.20	0.41
1:A:509:GLU:O	1:A:513:GLU:CD	2.59	0.41
1:A:885:THR:HA	1:A:888:GLU:OE1	2.20	0.41
1:A:2001:PRO:O	1:A:2005:GLN:HG3	2.20	0.41
1:A:2374:SER:OG	1:A:2378:ALA:HB3	2.21	0.41
1:A:2444:GLN:OE1	1:A:2444:GLN:N	2.53	0.41
1:A:3610:GLU:OE1	1:A:3611:HIS:CD2	2.73	0.41
1:A:3899:PHE:HE2	1:A:3903:LEU:HD11	1.85	0.41
1:A:4705:VAL:HG23	1:A:4775:TYR:HD2	1.85	0.41
2:G:24:VAL:HG21	2:G:59:TRP:HZ3	1.85	0.41
1:B:384:MET:SD	1:C:167:ASP:N	2.93	0.41
1:B:492:ASP:O	1:B:496:VAL:HG13	2.19	0.41
1:B:1676:LEU:HD22	1:B:2167:ILE:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2202:GLY:HA2	1:B:2205:GLU:OE1	2.20	0.41
1:B:2487:GLN:NE2	1:B:2545:GLU:OE1	2.53	0.41
1:B:2495:VAL:HG22	1:B:2498:HIS:CE1	2.55	0.41
1:B:2725:LYS:HE3	1:B:2734:ASN:O	2.19	0.41
1:B:2986:VAL:O	1:B:2986:VAL:HG13	2.19	0.41
1:B:3003:LEU:HB2	1:B:3004:PRO:HD3	2.02	0.41
1:B:3111:ARG:HH21	1:B:3178:THR:CB	2.33	0.41
1:B:3916:ILE:HD12	1:B:3916:ILE:H	1.86	0.41
1:B:4069:LYS:O	1:B:4072:VAL:HG22	2.21	0.41
1:D:336:PRO:HA	1:D:337:PRO:HD3	1.91	0.41
1:D:873:LYS:O	1:D:876:GLU:HG2	2.20	0.41
1:D:1085:SER:N	1:D:1155:LEU:HD22	2.35	0.41
1:D:1727:ARG:O	1:D:1731:LEU:HG	2.20	0.41
1:D:3386:GLU:O	1:D:3389:GLU:O	2.38	0.41
1:D:3391:GLU:O	1:D:3395:ARG:HD2	2.19	0.41
1:D:3409:TYR:N	1:D:3410:PRO:HD2	2.35	0.41
1:D:3997:ALA:HB1	1:D:4057:MET:SD	2.60	0.41
1:D:4024:VAL:HG11	1:D:4142:ASN:HB3	2.02	0.41
1:D:4705:VAL:HG23	1:D:4775:TYR:HD2	1.85	0.41
1:C:1992:ALA:O	1:C:1995:THR:OG1	2.29	0.41
1:C:2441:HIS:CE1	1:C:2442:LEU:HD12	2.55	0.41
1:C:2642:LYS:NZ	1:C:2698:MET:HE1	2.36	0.41
1:C:3239:MET:CB	1:C:3239:MET:HG3	2.31	0.41
1:C:4024:VAL:HG11	1:C:4142:ASN:HB3	2.02	0.41
1:A:292:ALA:HB2	1:A:312:THR:HG22	2.02	0.41
1:A:399:GLN:O	1:A:403:MET:HG3	2.21	0.41
1:A:1085:SER:N	1:A:1155:LEU:HD22	2.35	0.41
1:A:1568:LYS:HB2	1:A:1572:ILE:O	2.20	0.41
1:A:1727:ARG:O	1:A:1731:LEU:HG	2.20	0.41
1:A:2208:MET:O	1:A:2212:VAL:HG22	2.19	0.41
1:A:2625:ARG:O	1:A:2628:PHE:HB3	2.21	0.41
1:A:3197:LEU:HD21	1:A:3201:MET:HE1	2.02	0.41
1:A:4069:LYS:O	1:A:4072:VAL:HG22	2.20	0.41
1:A:4187:SER:O	1:A:4188:ARG:HB2	2.20	0.41
1:A:5009:TYR:CZ	1:A:5013:MET:HE3	2.55	0.41
1:B:1999:ARG:NH1	1:B:3636:PHE:CD1	2.76	0.41
1:B:2313:LEU:HB3	1:B:2318:TYR:HB2	2.02	0.41
1:B:2374:SER:OG	1:B:2378:ALA:HB3	2.21	0.41
1:B:2444:GLN:OE1	1:B:2444:GLN:N	2.54	0.41
1:B:3583:GLU:HB3	1:B:3585:ASP:OD1	2.19	0.41
1:B:3610:GLU:OE1	1:B:3611:HIS:CD2	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3660:ALA:HB3	1:B:3661:TRP:HD1	1.85	0.41
1:B:4677:LEU:HD23	1:B:4711:PHE:HE1	1.83	0.41
1:B:4946:GLN:O	1:B:4950:VAL:HG23	2.19	0.41
1:D:2202:GLY:HA2	1:D:2205:GLU:OE1	2.20	0.41
1:D:2700:MET:O	1:D:2702:CYS:SG	2.78	0.41
1:D:3899:PHE:CE2	1:D:3903:LEU:HD11	2.55	0.41
1:D:4901:ILE:HG13	1:D:4913:ARG:NH2	2.34	0.41
1:C:1676:LEU:HD22	1:C:2167:ILE:HD12	2.03	0.41
1:C:2011:HIS:CE1	1:C:2017:ASP:CG	2.84	0.41
1:C:2703:LEU:HD22	1:C:2706:ILE:HD12	2.02	0.41
1:C:3071:LEU:O	1:C:3075:LEU:HG	2.19	0.41
1:C:3148:ALA:O	1:C:3151:GLN:NE2	2.53	0.41
1:C:3610:GLU:OE1	1:C:3611:HIS:CD2	2.73	0.41
1:C:3628:ARG:HH11	1:C:3632:VAL:HG11	1.85	0.41
1:C:3899:PHE:CE2	1:C:3903:LEU:HD11	2.55	0.41
1:C:4677:LEU:HD23	1:C:4711:PHE:HE1	1.83	0.41
1:C:5000:GLU:HA	1:C:5003:HIS:CD2	2.56	0.41
1:A:501:ALA:O	1:A:505:GLU:HG3	2.20	0.41
1:A:516:LYS:O	1:A:519:VAL:HG22	2.20	0.41
1:A:873:LYS:O	1:A:876:GLU:HG2	2.20	0.41
1:A:2487:GLN:NE2	1:A:2545:GLU:OE1	2.53	0.41
1:A:2977:LEU:HD23	1:A:3056:LEU:HD11	2.02	0.41
1:A:3003:LEU:HB2	1:A:3004:PRO:HD3	2.02	0.41
1:A:3137:LEU:HD23	1:A:3189:ALA:CB	2.50	0.41
2:F:4:VAL:HG22	2:F:74:LEU:HD22	2.03	0.41
1:B:501:ALA:O	1:B:505:GLU:HG3	2.20	0.41
1:B:926:GLY:O	1:B:930:LYS:HG3	2.20	0.41
1:B:1552:VAL:HG11	1:B:1562:ILE:HD13	2.02	0.41
1:B:1992:ALA:O	1:B:1995:THR:OG1	2.29	0.41
1:B:2452:ARG:HG3	1:C:175:SER:O	2.20	0.41
1:B:2545:GLU:HG2	1:B:2546:MET:N	2.35	0.41
1:B:4093:PHE:CE1	1:B:4097:MET:HE2	2.56	0.41
1:D:399:GLN:O	1:D:403:MET:HG3	2.21	0.41
1:D:509:GLU:O	1:D:513:GLU:CD	2.59	0.41
1:D:1088:TRP:O	1:D:1152:MET:HA	2.21	0.41
1:D:2725:LYS:HE3	1:D:2734:ASN:O	2.19	0.41
1:C:2414:ASN:C	1:C:2414:ASN:OD1	2.58	0.41
1:C:3130:THR:O	1:C:3134:VAL:HG23	2.19	0.41
1:C:3386:GLU:O	1:C:3389:GLU:O	2.38	0.41
1:C:3633:VAL:O	1:C:3637:ARG:HD3	2.20	0.41
1:C:4069:LYS:O	1:C:4072:VAL:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4187:SER:O	1:C:4188:ARG:HB2	2.20	0.41
1:C:4901:ILE:HG13	1:C:4913:ARG:NH2	2.34	0.41
1:A:1676:LEU:HD22	1:A:2167:ILE:HD12	2.03	0.41
1:A:2330:ARG:HA	1:A:2333:ASP:OD1	2.21	0.41
1:A:3075:LEU:O	1:A:3146:HIS:NE2	2.51	0.41
1:A:3114:LYS:HD3	1:A:3116:SER:H	1.85	0.41
1:A:3409:TYR:N	1:A:3410:PRO:HD2	2.35	0.41
1:A:3435:PHE:CD2	1:A:3524:MET:CE	3.03	0.41
1:A:3660:ALA:HB3	1:A:3661:TRP:HD1	1.85	0.41
1:A:3891:LEU:HD13	1:A:3899:PHE:HZ	1.79	0.41
1:A:4179:GLY:CA	1:A:4197:ILE:HD11	2.50	0.41
1:B:125:ARG:NH1	1:B:125:ARG:CB	2.84	0.41
1:B:221:ARG:NH1	1:B:255:HIS:O	2.54	0.41
1:B:869:ARG:NH2	1:B:947:GLU:OE2	2.52	0.41
1:B:1143:TRP:HB2	1:B:1147:ASP:HB2	2.01	0.41
1:B:1265:ASP:OD1	1:B:1266:THR:N	2.53	0.41
1:B:2612[B]:ARG:NH1	1:B:2613:TYR:OH	2.53	0.41
1:B:2625:ARG:O	1:B:2628:PHE:HB3	2.21	0.41
1:B:3294:PRO:HB2	1:B:3297:PRO:HD2	2.01	0.41
1:B:3458:PHE:CE2	1:B:3464:ILE:HD11	2.54	0.41
1:B:4705:VAL:HG23	1:B:4775:TYR:CD2	2.56	0.41
1:D:885:THR:HA	1:D:888:GLU:OE1	2.20	0.41
1:D:1568:LYS:HB2	1:D:1572:ILE:O	2.21	0.41
1:D:2117:VAL:O	1:D:2120:MET:HG2	2.21	0.41
1:D:2865:VAL:HG11	1:D:2928:LYS:HE2	2.02	0.41
1:D:3380:ARG:NH1	1:D:3391:GLU:OE2	2.50	0.41
1:C:125:ARG:NH1	1:C:125:ARG:CB	2.84	0.41
1:C:2330:ARG:HA	1:C:2333:ASP:OD1	2.21	0.41
1:C:3077:ALA:O	1:C:3081:MET:HG2	2.20	0.41
1:C:3103:ILE:O	1:C:3107:VAL:HG13	2.20	0.41
1:C:3380:ARG:NH2	1:C:3391:GLU:OE2	2.52	0.41
1:C:3997:ALA:HB1	1:C:4057:MET:SD	2.60	0.41
1:C:4767:TRP:CE3	1:C:4768:LEU:CD2	2.99	0.41
1:A:215:THR:HG1	1:A:218:HIS:CE1	2.37	0.41
1:A:631:LEU:HD23	1:A:631:LEU:HA	1.96	0.41
1:A:820:ARG:CZ	1:A:820:ARG:CB	2.80	0.41
1:A:973:SER:O	1:A:976:ARG:NH2	2.54	0.41
1:A:1819:VAL:HG22	1:A:1926:LEU:HD21	2.03	0.41
1:A:2476:ILE:HD11	1:A:2536:LEU:HG	2.03	0.41
1:A:2894:LEU:O	1:A:2897:LYS:HG2	2.21	0.41
1:A:2946:LEU:N	1:A:2948:THR:HG23	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2969:ILE:O	1:A:2973:PHE:HD1	2.03	0.41
1:A:3197:LEU:HD23	1:A:3197:LEU:O	2.20	0.41
2:H:90:ILE:HD11	1:D:1684:ALA:HA	2.02	0.41
1:B:399:GLN:O	1:B:403:MET:HG3	2.21	0.41
1:B:509:GLU:O	1:B:513:GLU:CD	2.59	0.41
1:B:975:VAL:HG11	1:B:1044:ARG:HA	2.03	0.41
1:B:2011:HIS:CE1	1:B:2017:ASP:CG	2.84	0.41
1:B:3434:LEU:O	1:B:3438:VAL:HG13	2.21	0.41
1:B:3729:MET:HB3	1:B:3770:LEU:HD11	2.03	0.41
1:B:3899:PHE:CE2	1:B:3903:LEU:HD11	2.55	0.41
1:B:3899:PHE:HE2	1:B:3903:LEU:HD11	1.85	0.41
1:D:1676:LEU:HD22	1:D:2167:ILE:HD12	2.03	0.41
1:D:2444:GLN:OE1	1:D:2444:GLN:N	2.54	0.41
1:D:2946:LEU:N	1:D:2948:THR:HG23	2.35	0.41
1:D:2977:LEU:HD23	1:D:3056:LEU:HD11	2.02	0.41
1:D:3628:ARG:HH11	1:D:3632:VAL:HG11	1.85	0.41
1:D:3633:VAL:O	1:D:3637:ARG:HD3	2.20	0.41
1:D:3916:ILE:H	1:D:3916:ILE:HD12	1.85	0.41
1:D:4989:MET:O	1:D:4993:MET:HG3	2.21	0.41
1:C:2202:GLY:HA2	1:C:2205:GLU:OE1	2.20	0.41
1:C:2495:VAL:HG22	1:C:2498:HIS:CE1	2.55	0.41
1:C:3409:TYR:N	1:C:3410:PRO:HD2	2.35	0.41
1:C:3435:PHE:CD2	1:C:3524:MET:HE1	2.56	0.41
1:A:484:LEU:CD1	1:A:526:LEU:CD1	2.98	0.41
1:A:1552:VAL:HG11	1:A:1562:ILE:HD13	2.03	0.41
1:A:2117:VAL:O	1:A:2120:MET:HG2	2.21	0.41
1:A:2513:GLU:OE1	1:A:2513:GLU:N	2.54	0.41
1:A:3077:ALA:O	1:A:3081:MET:HG2	2.20	0.41
1:A:3899:PHE:CE2	1:A:3903:LEU:HD11	2.55	0.41
1:B:69:LEU:CD2	1:B:109:LEU:HD21	2.50	0.41
1:B:1085:SER:N	1:B:1155:LEU:HD22	2.35	0.41
1:B:1568:LYS:HB2	1:B:1572:ILE:O	2.21	0.41
1:B:1973:GLN:NE2	1:B:2005:GLN:OE1	2.44	0.41
1:B:2135:LEU:HD12	1:B:3658:LYS:HG3	2.02	0.41
1:B:2330:ARG:HA	1:B:2333:ASP:OD1	2.21	0.41
1:B:3137:LEU:HD23	1:B:3189:ALA:CB	2.50	0.41
1:B:3433:GLU:HG3	1:B:3437:MET:HE1	2.02	0.41
1:B:3891:LEU:HD13	1:B:3899:PHE:HZ	1.79	0.41
1:B:4930:ALA:CA	1:B:4933:GLN:OE1	2.69	0.41
1:D:278:GLN:HG3	1:D:328:LYS:NZ	2.35	0.41
1:D:501:ALA:O	1:D:505:GLU:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:869:ARG:NH2	1:D:947:GLU:OE2	2.52	0.41
1:D:973:SER:O	1:D:976:ARG:NH2	2.54	0.41
1:D:2135:LEU:HD12	1:D:3658:LYS:HG3	2.02	0.41
1:D:2330:ARG:HA	1:D:2333:ASP:OD1	2.21	0.41
1:D:2667:THR:HG21	1:D:2672:LEU:HG	2.02	0.41
1:D:3071:LEU:O	1:D:3075:LEU:HG	2.19	0.41
1:D:3103:ILE:O	1:D:3107:VAL:HG13	2.20	0.41
1:D:4161:ARG:HH11	1:D:4161:ARG:HD2	1.54	0.41
1:D:4563:ARG:NH2	1:D:4815:ASP:OD1	2.53	0.41
1:C:887:ILE:HD13	1:C:887:ILE:HA	1.87	0.41
1:C:1021:LEU:HD23	1:C:1021:LEU:O	2.21	0.41
1:C:3465:ASN:OD1	1:C:3467:MET:CG	2.60	0.41
1:A:160:GLY:O	1:D:3984:ARG:NH1	2.49	0.41
1:A:278:GLN:HG3	1:A:328:LYS:NZ	2.35	0.41
1:A:1088:TRP:O	1:A:1152:MET:HA	2.21	0.41
1:A:1105:ALA:O	1:A:1189:LEU:N	2.50	0.41
1:A:1805:GLU:O	1:A:1808:ARG:HG2	2.21	0.41
1:A:2214:VAL:HG11	1:A:2228:MET:HE3	2.01	0.41
1:A:2442:LEU:HD23	1:A:2447:LYS:CE	2.51	0.41
1:A:2905:LEU:HD23	1:A:2905:LEU:HA	1.98	0.41
1:A:3103:ILE:O	1:A:3107:VAL:HG13	2.20	0.41
1:A:3434:LEU:O	1:A:3438:VAL:HG13	2.21	0.41
1:A:4717:ASP:OD2	1:A:4723:LYS:NZ	2.35	0.41
1:B:2001:PRO:O	1:B:2005:GLN:HG3	2.20	0.41
1:B:2699:ALA:O	1:B:2702:CYS:HB3	2.21	0.41
1:B:3321:ARG:HA	1:B:3324:VAL:HG22	2.02	0.41
1:B:3892:CYS:HG	1:B:3899:PHE:HD2	1.69	0.41
1:B:4999:ASP:OD1	1:B:5000:GLU:N	2.53	0.41
1:B:5000:GLU:HA	1:B:5003:HIS:CD2	2.56	0.41
1:D:468:LEU:O	1:D:472:ARG:HG2	2.20	0.41
1:D:484:LEU:CD1	1:D:526:LEU:CD1	2.98	0.41
1:D:553:ARG:O	1:D:557:SER:OG	2.29	0.41
1:D:926:GLY:O	1:D:930:LYS:HG3	2.20	0.41
1:D:1436:SER:OG	1:D:1565:GLU:HB2	2.20	0.41
1:D:1805:GLU:O	1:D:1808:ARG:HG2	2.21	0.41
1:D:1821:ASP:OD1	1:D:1821:ASP:C	2.59	0.41
1:D:1973:GLN:NE2	1:D:2005:GLN:OE1	2.44	0.41
1:D:2703:LEU:HD22	1:D:2706:ILE:HD12	2.02	0.41
1:D:3077:ALA:O	1:D:3081:MET:HG2	2.20	0.41
1:D:3114:LYS:HD3	1:D:3116:SER:H	1.85	0.41
1:D:3435:PHE:CD2	1:D:3524:MET:CE	3.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3604:TYR:O	1:D:3608:GLN:OE1	2.39	0.41
1:D:4179:GLY:HA3	1:D:4197:ILE:HD11	2.02	0.41
1:D:4767:TRP:HE3	1:D:4768:LEU:HD23	1.80	0.41
1:D:5000:GLU:HA	1:D:5003:HIS:CD2	2.56	0.41
1:C:874:LEU:HD21	1:C:1046:LEU:HG	2.03	0.41
1:C:885:THR:HA	1:C:888:GLU:OE1	2.20	0.41
1:C:1085:SER:N	1:C:1155:LEU:HD22	2.35	0.41
1:C:1568:LYS:HB2	1:C:1572:ILE:O	2.20	0.41
1:C:2374:SER:OG	1:C:2378:ALA:HB3	2.20	0.41
1:C:3111:ARG:HH21	1:C:3178:THR:CB	2.33	0.41
1:C:3336:LYS:HG3	1:C:3337:ARG:N	2.36	0.41
1:C:4705:VAL:HG23	1:C:4775:TYR:CD2	2.56	0.41
1:C:4989:MET:O	1:C:4993:MET:HG3	2.21	0.41
1:A:69:LEU:CD2	1:A:109:LEU:HD21	2.50	0.41
1:A:117:TYR:O	1:A:138:GLN:N	2.51	0.41
1:A:160:GLY:O	1:D:3984:ARG:NH2	2.52	0.41
1:A:721:LEU:HD12	1:A:1476:MET:HE2	2.01	0.41
1:A:823:LEU:HD13	1:A:1626:TRP:CE3	2.56	0.41
1:A:926:GLY:O	1:A:930:LYS:HG3	2.20	0.41
1:A:1021:LEU:O	1:A:1021:LEU:HD23	2.21	0.41
1:A:2202:GLY:HA2	1:A:2205:GLU:OE1	2.20	0.41
1:A:2313:LEU:HB3	1:A:2318:TYR:HB2	2.02	0.41
1:A:2725:LYS:HE3	1:A:2734:ASN:O	2.19	0.41
1:A:2865:VAL:HG11	1:A:2928:LYS:HE2	2.02	0.41
1:A:3336:LYS:HG3	1:A:3337:ARG:N	2.36	0.41
1:A:3384:LYS:H	1:A:3387:ALA:HB3	1.86	0.41
1:A:3458:PHE:HE2	1:A:3464:ILE:HD11	1.82	0.41
1:A:3573:MET:CB	1:A:3577:ARG:NH1	2.73	0.41
1:A:3604:TYR:O	1:A:3608:GLN:OE1	2.39	0.41
1:A:3628:ARG:HH11	1:A:3632:VAL:HG11	1.85	0.41
1:A:3633:VAL:O	1:A:3637:ARG:HD3	2.20	0.41
1:A:3969:ILE:HD11	1:A:4029:SER:HB2	2.02	0.41
1:A:4024:VAL:HG11	1:A:4142:ASN:HB3	2.02	0.41
1:A:4839:MET:CE	1:D:4820:VAL:HG11	2.50	0.41
1:A:5000:GLU:HA	1:A:5003:HIS:CD2	2.56	0.41
2:H:24:VAL:HG21	2:H:59:TRP:HZ3	1.85	0.41
1:B:117:TYR:O	1:B:138:GLN:N	2.51	0.41
1:B:365:LYS:HD3	1:B:369:LEU:HD21	2.03	0.41
1:B:823:LEU:HD13	1:B:1626:TRP:CE3	2.56	0.41
1:B:885:THR:HA	1:B:888:GLU:OE1	2.21	0.41
1:B:973:SER:O	1:B:976:ARG:NH2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:985:VAL:HG13	1:B:1039:LEU:HD23	2.00	0.41
1:B:1096:THR:O	1:B:1100:MET:HE1	2.21	0.41
1:B:2441:HIS:CE1	1:B:2442:LEU:HD12	2.55	0.41
1:B:2442:LEU:HD23	1:B:2447:LYS:CE	2.51	0.41
1:B:2476:ILE:HD11	1:B:2536:LEU:HG	2.02	0.41
1:B:2946:LEU:N	1:B:2948:THR:HG23	2.35	0.41
1:B:2969:ILE:O	1:B:2973:PHE:HD1	2.02	0.41
1:B:3062:PRO:O	1:B:3065:VAL:HG22	2.21	0.41
1:B:3101:GLU:HA	1:B:3104:GLU:OE1	2.21	0.41
1:B:3114:LYS:HD3	1:B:3116:SER:H	1.85	0.41
1:B:3336:LYS:HG3	1:B:3337:ARG:N	2.36	0.41
1:B:3384:LYS:H	1:B:3387:ALA:HB3	1.86	0.41
1:B:3386:GLU:O	1:B:3389:GLU:O	2.38	0.41
1:B:3435:PHE:CD2	1:B:3524:MET:HE1	2.56	0.41
1:B:3628:ARG:HH11	1:B:3632:VAL:HG11	1.85	0.41
1:B:3969:ILE:HD11	1:B:4029:SER:HB2	2.02	0.41
1:B:4075:GLU:CD	1:C:4736:ARG:NH1	2.73	0.41
1:D:130:LYS:NZ	1:C:2373:GLY:O	2.50	0.41
1:D:874:LEU:HD21	1:D:1046:LEU:HG	2.03	0.41
1:D:877:ASN:O	1:D:880:GLU:CG	2.69	0.41
1:D:1712:TYR:CG	1:D:1840:PRO:HB3	2.56	0.41
1:D:2374:SER:OG	1:D:2378:ALA:HB3	2.21	0.41
1:D:2442:LEU:HD23	1:D:2447:LYS:CE	2.51	0.41
1:D:2487:GLN:NE2	1:D:2545:GLU:OE1	2.53	0.41
1:D:3111:ARG:HH21	1:D:3178:THR:CB	2.33	0.41
1:D:3111:ARG:O	1:D:3112:LEU:HB2	2.20	0.41
1:D:3380:ARG:NH2	1:D:3391:GLU:OE2	2.52	0.41
1:D:3434:LEU:O	1:D:3438:VAL:HG13	2.21	0.41
1:D:3545:THR:HG23	1:D:3548:GLU:H	1.86	0.41
1:D:4705:VAL:HG23	1:D:4775:TYR:CD2	2.56	0.41
1:C:215:THR:HG1	1:C:218:HIS:CE1	2.39	0.41
1:C:399:GLN:O	1:C:403:MET:HG3	2.21	0.41
1:C:985:VAL:HG13	1:C:1039:LEU:HD23	2.00	0.41
1:C:1088:TRP:O	1:C:1152:MET:HA	2.21	0.41
1:C:2212:VAL:HG21	1:C:2256:TYR:HH	1.79	0.41
1:C:2442:LEU:HD23	1:C:2447:LYS:CE	2.51	0.41
1:C:2444:GLN:OE1	1:C:2444:GLN:N	2.53	0.41
1:C:2625:ARG:O	1:C:2628:PHE:HB3	2.21	0.41
1:C:2762:THR:HA	1:C:2765:LYS:HE2	2.03	0.41
1:C:3062:PRO:O	1:C:3065:VAL:HG22	2.21	0.41
1:C:3101:GLU:HA	1:C:3104:GLU:OE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3111:ARG:O	1:C:3112:LEU:HB2	2.20	0.41
1:C:3434:LEU:O	1:C:3438:VAL:HG13	2.21	0.41
1:A:221:ARG:NH1	1:A:255:HIS:O	2.54	0.41
1:A:1926:LEU:HA	1:A:1929:MET:SD	2.61	0.41
1:A:2369[B]:ARG:HD3	1:A:2369[B]:ARG:HA	1.92	0.41
1:A:2441:HIS:CE1	1:A:2442:LEU:HD12	2.55	0.41
1:A:3545:THR:HG23	1:A:3548:GLU:H	1.86	0.41
1:A:4705:VAL:HG23	1:A:4775:TYR:CD2	2.56	0.41
1:B:866:HIS:CD2	1:B:867:LEU:CD2	3.04	0.41
1:B:1980:LEU:HD21	1:B:1995:THR:HG23	2.02	0.41
1:B:2762:THR:HA	1:B:2765:LYS:HE2	2.03	0.41
1:B:2792:ARG:HB3	1:B:2793:PRO:HD2	2.03	0.41
1:B:3197:LEU:HD21	1:B:3201:MET:HE1	2.02	0.41
1:D:975:VAL:HG11	1:D:1044:ARG:HA	2.03	0.41
1:D:1096:THR:O	1:D:1100:MET:HE1	2.20	0.41
1:D:1241:SER:HA	1:D:1603:VAL:HG22	2.03	0.41
1:D:1478:ASP:HB2	1:D:1484:HIS:CE1	2.56	0.41
1:D:1748:PHE:HA	1:D:1749:PRO:HD3	1.92	0.41
1:D:2625:ARG:O	1:D:2628:PHE:HB3	2.21	0.41
1:D:3336:LYS:HG3	1:D:3337:ARG:N	2.36	0.41
1:D:3666:ASP:OD1	1:D:3666:ASP:O	2.39	0.41
1:C:501:ALA:O	1:C:505:GLU:HG3	2.20	0.41
1:C:516:LYS:O	1:C:519:VAL:HG22	2.20	0.41
1:C:615:ARG:NH2	1:C:1676:LEU:O	2.50	0.41
1:C:879:HIS:HE1	1:C:913:LEU:HD13	1.86	0.41
1:C:973:SER:O	1:C:976:ARG:NH2	2.54	0.41
1:C:1241:SER:HA	1:C:1603:VAL:HG22	2.03	0.41
1:C:1712:TYR:CG	1:C:1840:PRO:HB3	2.56	0.41
1:C:3244:PRO:HD2	1:C:3249:LEU:HD21	2.03	0.41
1:C:3892:CYS:HG	1:C:3899:PHE:HD2	1.69	0.41
1:C:3899:PHE:HE2	1:C:3903:LEU:HD11	1.85	0.41
1:C:4705:VAL:HG23	1:C:4775:TYR:HD2	1.85	0.41
1:A:125:ARG:NH1	1:A:125:ARG:CB	2.84	0.40
1:A:515:TRP:O	1:A:519:VAL:HG13	2.21	0.40
1:A:1241:SER:HA	1:A:1603:VAL:HG22	2.03	0.40
1:A:3101:GLU:HA	1:A:3104:GLU:OE1	2.21	0.40
1:A:3111:ARG:HH21	1:A:3178:THR:CB	2.33	0.40
1:A:3666:ASP:O	1:A:3666:ASP:OD1	2.40	0.40
1:A:3729:MET:HB3	1:A:3770:LEU:HD11	2.03	0.40
1:A:3868:ARG:HG2	1:A:3869:GLN:N	2.34	0.40
1:A:4748:LEU:O	1:A:4751:THR:OG1	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4876:CYS:HA	1:A:4882:CYS:HB2	2.04	0.40
2:E:4:VAL:HG22	2:E:74:LEU:HD22	2.03	0.40
2:G:50:LEU:HA	2:G:50:LEU:HD12	1.89	0.40
1:B:1478:ASP:HB2	1:B:1484:HIS:CE1	2.56	0.40
1:B:1984:PHE:HA	1:B:1991:THR:HG21	2.03	0.40
1:B:2784:GLU:OE2	1:B:2785:LEU:HD12	2.21	0.40
1:B:3302:PRO:HA	1:B:3303:PRO:HD3	2.00	0.40
1:D:736:HIS:NE2	1:D:742:ASP:OD2	2.55	0.40
1:D:2319:PRO:HG2	1:D:2392:ARG:HA	2.03	0.40
1:D:3062:PRO:O	1:D:3065:VAL:HG22	2.21	0.40
1:D:3244:PRO:HD2	1:D:3249:LEU:HD21	2.03	0.40
1:D:4093:PHE:CE1	1:D:4097:MET:HE2	2.56	0.40
1:D:4187:SER:O	1:D:4188:ARG:HB2	2.20	0.40
1:C:221:ARG:NH1	1:C:255:HIS:O	2.54	0.40
1:C:626:LEU:N	1:C:627:PRO:HD2	2.37	0.40
1:C:820:ARG:CZ	1:C:820:ARG:CB	2.80	0.40
1:C:869:ARG:NH2	1:C:947:GLU:OE2	2.52	0.40
1:C:1819:VAL:HG22	1:C:1926:LEU:HD21	2.03	0.40
1:C:1856:ASP:O	1:C:1860:LYS:HG3	2.21	0.40
1:C:3321:ARG:HA	1:C:3324:VAL:HG22	2.02	0.40
1:C:3868:ARG:HG2	1:C:3869:GLN:N	2.34	0.40
1:A:1008:SER:HB3	1:A:1017:ARG:HB3	2.03	0.40
1:A:1821:ASP:OD1	1:A:1821:ASP:C	2.59	0.40
1:A:2319:PRO:HG2	1:A:2392:ARG:HA	2.03	0.40
1:A:2699:ALA:O	1:A:2702:CYS:HB3	2.21	0.40
1:A:3622:LYS:HB2	1:A:3625:SER:HB3	2.03	0.40
1:A:3916:ILE:H	1:A:3916:ILE:HD12	1.85	0.40
1:A:4989:MET:O	1:A:4993:MET:HG3	2.21	0.40
1:B:215:THR:HG1	1:B:218:HIS:CE1	2.39	0.40
1:B:891:TRP:CE3	1:B:903:LEU:HA	2.56	0.40
1:B:1021:LEU:O	1:B:1021:LEU:HD23	2.21	0.40
1:B:2319:PRO:HG2	1:B:2392:ARG:HA	2.03	0.40
1:B:2894:LEU:O	1:B:2897:LYS:HG2	2.21	0.40
1:B:4024:VAL:HG11	1:B:4142:ASN:HB3	2.03	0.40
1:D:125:ARG:NH1	1:D:125:ARG:CB	2.84	0.40
1:D:906:CYS:HA	1:D:914:PRO:HD3	2.04	0.40
1:D:1984:PHE:HA	1:D:1991:THR:HG21	2.03	0.40
1:D:2001:PRO:O	1:D:2005:GLN:HG3	2.20	0.40
1:D:2476:ILE:HD11	1:D:2536:LEU:HG	2.03	0.40
1:D:3183:VAL:HG12	1:D:3187:ARG:HE	1.87	0.40
1:C:309:THR:O	1:C:309:THR:CG2	2.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2513:GLU:OE1	1:C:2513:GLU:N	2.54	0.40
1:C:2699:ALA:O	1:C:2702:CYS:HB3	2.21	0.40
1:C:3114:LYS:HD3	1:C:3116:SER:H	1.86	0.40
1:C:3916:ILE:H	1:C:3916:ILE:HD12	1.85	0.40
1:A:309:THR:O	1:A:309:THR:CG2	2.68	0.40
1:A:2135:LEU:HD12	1:A:3658:LYS:HG3	2.02	0.40
1:A:2240:CYS:SG	1:A:2250:MET:HG3	2.62	0.40
1:A:2784:GLU:OE2	1:A:2785:LEU:HD12	2.21	0.40
1:A:3458:PHE:CE2	1:A:3464:ILE:HD11	2.54	0.40
1:B:221:ARG:NE	1:B:253:CYS:O	2.55	0.40
1:B:515:TRP:O	1:B:519:VAL:HG13	2.21	0.40
1:B:736:HIS:NE2	1:B:742:ASP:OD2	2.55	0.40
1:B:993:HIS:NE2	1:B:1022:VAL:O	2.53	0.40
1:B:1241:SER:HA	1:B:1603:VAL:HG22	2.03	0.40
1:B:1926:LEU:HA	1:B:1929:MET:SD	2.61	0.40
1:B:2117:VAL:O	1:B:2120:MET:HG2	2.21	0.40
1:B:2240:CYS:SG	1:B:2250:MET:HG3	2.62	0.40
1:B:2513:GLU:N	1:B:2513:GLU:OE1	2.54	0.40
1:B:3111:ARG:O	1:B:3112:LEU:HB2	2.20	0.40
1:B:3409:TYR:N	1:B:3410:PRO:HD2	2.35	0.40
1:D:870:ILE:HD12	1:D:870:ILE:HA	1.98	0.40
1:D:993:HIS:NE2	1:D:1022:VAL:O	2.53	0.40
1:D:1926:LEU:HA	1:D:1929:MET:SD	2.61	0.40
1:D:2240:CYS:SG	1:D:2250:MET:HG3	2.62	0.40
1:D:2969:ILE:O	1:D:2973:PHE:HD1	2.02	0.40
1:D:3003:LEU:HB2	1:D:3004:PRO:HD3	2.02	0.40
1:D:3532:LEU:HD23	1:D:3535:LEU:HD12	2.03	0.40
1:D:4003:LEU:HA	1:D:4009:GLN:OE1	2.22	0.40
1:C:667:MET:SD	1:C:801:LYS:NZ	2.86	0.40
1:C:891:TRP:CE3	1:C:903:LEU:HA	2.57	0.40
1:C:893:TYR:CD1	1:C:907:LEU:O	2.75	0.40
1:C:893:TYR:HD1	1:C:907:LEU:O	2.03	0.40
1:C:2476:ILE:HD11	1:C:2536:LEU:HG	2.03	0.40
1:C:2638:LYS:O	1:C:2698:MET:HE2	2.22	0.40
1:C:3254:GLY:C	1:C:3258:GLU:OE1	2.60	0.40
1:C:3532:LEU:HD23	1:C:3535:LEU:HD12	2.02	0.40
1:A:350:HIS:O	1:A:354:GLY:N	2.49	0.40
1:A:874:LEU:HD21	1:A:1046:LEU:HG	2.03	0.40
1:A:975:VAL:HG11	1:A:1044:ARG:HA	2.03	0.40
1:A:1478:ASP:HB2	1:A:1484:HIS:CE1	2.56	0.40
1:A:1712:TYR:CG	1:A:1840:PRO:HB3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2630:VAL:N	1:A:2631:PRO:CD	2.85	0.40
1:A:3239:MET:CB	1:A:3239:MET:HG3	2.31	0.40
1:A:3254:GLY:C	1:A:3258:GLU:OE1	2.60	0.40
1:B:1821:ASP:OD1	1:B:1821:ASP:C	2.59	0.40
1:B:4844:LEU:O	1:B:4847:VAL:HG22	2.21	0.40
1:B:4989:MET:O	1:B:4993:MET:HG3	2.21	0.40
1:D:167:ASP:N	1:C:384:MET:SD	2.95	0.40
1:D:823:LEU:HD13	1:D:1626:TRP:CE3	2.56	0.40
1:D:899:ASP:O	1:D:902:ARG:NE	2.45	0.40
1:D:3969:ILE:HD11	1:D:4029:SER:HB2	2.02	0.40
1:D:4666:VAL:N	1:D:4667:PRO:CD	2.85	0.40
1:D:4844:LEU:O	1:D:4847:VAL:HG22	2.21	0.40
1:C:866:HIS:CD2	1:C:867:LEU:CD2	3.04	0.40
1:C:1805:GLU:O	1:C:1808:ARG:HG2	2.21	0.40
1:C:2319:PRO:HG2	1:C:2392:ARG:HA	2.03	0.40
1:C:2520:HIS:HA	1:C:2523:ASP:OD2	2.22	0.40
1:C:2784:GLU:OE2	1:C:2785:LEU:HD12	2.21	0.40
1:C:3003:LEU:HB2	1:C:3004:PRO:HD3	2.02	0.40
1:C:3545:THR:HG23	1:C:3548:GLU:H	1.86	0.40
1:C:3729:MET:HB3	1:C:3770:LEU:HD11	2.03	0.40
1:A:736:HIS:NE2	1:A:742:ASP:OD2	2.55	0.40
1:A:866:HIS:CD2	1:A:867:LEU:CD2	3.04	0.40
1:A:891:TRP:CE3	1:A:903:LEU:HA	2.56	0.40
1:A:973:SER:O	1:A:976:ARG:CZ	2.70	0.40
1:A:2165:LEU:HD21	1:A:2177:LEU:HD22	2.04	0.40
1:A:3239:MET:CA	1:A:3239:MET:HG2	2.46	0.40
1:A:3254:GLY:O	1:A:3255:GLY:C	2.60	0.40
1:A:4767:TRP:HE3	1:A:4768:LEU:HD23	1.80	0.40
1:A:4848:VAL:HG13	1:A:4886:HIS:HB3	2.03	0.40
1:A:4951:LYS:O	1:A:4955:GLU:OE1	2.40	0.40
1:B:1698:LEU:HD22	1:B:1712:TYR:CE2	2.57	0.40
1:B:2888:ARG:O	1:B:2892:GLN:HG2	2.22	0.40
1:B:3548:GLU:O	1:B:3551:GLU:HG3	2.22	0.40
1:B:3622:LYS:HB2	1:B:3625:SER:HB3	2.03	0.40
1:B:4118:ASP:OD1	1:B:4121:GLU:N	2.55	0.40
1:B:4904:PRO:HB3	1:B:4913:ARG:HD3	2.04	0.40
1:B:4937:ILE:HG12	1:C:4934:GLY:HA2	2.03	0.40
1:D:2442:LEU:HD23	1:D:2447:LYS:HE3	2.03	0.40
1:D:2784:GLU:OE2	1:D:2785:LEU:HD12	2.21	0.40
1:D:3101:GLU:HA	1:D:3104:GLU:OE1	2.21	0.40
1:D:3433:GLU:HG3	1:D:3437:MET:HE1	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4754:ASN:OD1	1:D:4755:GLU:N	2.55	0.40
1:D:4848:VAL:HG13	1:D:4886:HIS:HB3	2.03	0.40
1:C:278:GLN:HG3	1:C:328:LYS:NZ	2.35	0.40
1:C:365:LYS:HD3	1:C:369:LEU:HD21	2.03	0.40
1:C:4003:LEU:HA	1:C:4009:GLN:OE1	2.22	0.40
1:C:4666:VAL:N	1:C:4667:PRO:CD	2.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	4385/5037 (87%)	4268 (97%)	109 (2%)	8 (0%)	44	66
1	B	4385/5037 (87%)	4268 (97%)	109 (2%)	8 (0%)	44	66
1	C	4385/5037 (87%)	4268 (97%)	109 (2%)	8 (0%)	44	66
1	D	4385/5037 (87%)	4268 (97%)	109 (2%)	8 (0%)	44	66
2	E	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
2	F	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
2	G	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
2	H	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
All	All	17960/20580 (87%)	17480 (97%)	448 (2%)	32 (0%)	45	66

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	908	VAL
1	A	2829	GLY
1	A	3239	MET
1	A	3300	ALA

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Mol	Chain	Res	Type
1	B	908	VAL
1	B	2829	GLY
1	B	3239	MET
1	B	3300	ALA
1	D	908	VAL
1	D	2829	GLY
1	D	3239	MET
1	D	3300	ALA
1	C	908	VAL
1	C	2829	GLY
1	C	3239	MET
1	C	3300	ALA
1	A	55	ALA
1	A	1930	LYS
1	B	55	ALA
1	B	1930	LYS
1	D	55	ALA
1	D	1930	LYS
1	C	55	ALA
1	C	1930	LYS
1	A	1036	ARG
1	B	1036	ARG
1	D	1036	ARG
1	C	1036	ARG
1	A	361	ALA
1	B	361	ALA
1	D	361	ALA
1	C	361	ALA

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	3836/4276 (90%)	3816 (100%)	20 (0%)	86 95
1	B	3836/4276 (90%)	3816 (100%)	20 (0%)	86 95
1	C	3836/4276 (90%)	3816 (100%)	20 (0%)	86 95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	3836/4276 (90%)	3815 (100%)	21 (0%)	86 95
2	E	89/90 (99%)	89 (100%)	0	100 100
2	F	89/90 (99%)	89 (100%)	0	100 100
2	G	89/90 (99%)	89 (100%)	0	100 100
2	H	89/90 (99%)	89 (100%)	0	100 100
All	All	15700/17464 (90%)	15619 (100%)	81 (0%)	85 95

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	155	LYS
1	A	384	MET
1	A	820	ARG
1	A	945	LYS
1	A	1036	ARG
1	A	1128	ARG
1	A	1559	GLN
1	A	1618	ARG
1	A	1759	ARG
1	A	2177	LEU
1	A	2267	MET
1	A	2308	GLN
1	A	2336	ARG
1	A	2444	GLN
1	A	3014	CYS
1	A	3023	LYS
1	A	3185	LYS
1	A	3477	LYS
1	A	3557	LEU
1	A	3617	LYS
1	B	155	LYS
1	B	384	MET
1	B	820	ARG
1	B	945	LYS
1	B	1036	ARG
1	B	1128	ARG
1	B	1559	GLN
1	B	1618	ARG
1	B	1759	ARG
1	B	2177	LEU

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Mol	Chain	Res	Type
1	B	2267	MET
1	B	2308	GLN
1	B	2336	ARG
1	B	2444	GLN
1	B	3014	CYS
1	B	3023	LYS
1	B	3185	LYS
1	B	3477	LYS
1	B	3557	LEU
1	B	3617	LYS
1	D	155	LYS
1	D	384	MET
1	D	820	ARG
1	D	945	LYS
1	D	1036	ARG
1	D	1128	ARG
1	D	1559	GLN
1	D	1618	ARG
1	D	1759	ARG
1	D	2177	LEU
1	D	2267	MET
1	D	2308	GLN
1	D	2336	ARG
1	D	2444	GLN
1	D	3014	CYS
1	D	3023	LYS
1	D	3185	LYS
1	D	3239	MET
1	D	3477	LYS
1	D	3557	LEU
1	D	3617	LYS
1	C	155	LYS
1	C	384	MET
1	C	820	ARG
1	C	945	LYS
1	C	1036	ARG
1	C	1128	ARG
1	C	1559	GLN
1	C	1618	ARG
1	C	1759	ARG
1	C	2177	LEU
1	C	2267	MET

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Mol	Chain	Res	Type
1	C	2308	GLN
1	C	2336	ARG
1	C	2444	GLN
1	C	3014	CYS
1	C	3023	LYS
1	C	3185	LYS
1	C	3477	LYS
1	C	3557	LEU
1	C	3617	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	HIS
1	A	879	HIS
1	A	889	GLN
1	A	963	ASN
1	A	1041	GLN
1	A	1299	GLN
1	A	2011	HIS
1	A	2161	GLN
1	A	2734	ASN
1	A	3605	HIS
1	A	3611	HIS
1	A	5003	HIS
1	B	105	HIS
1	B	879	HIS
1	B	889	GLN
1	B	963	ASN
1	B	1041	GLN
1	B	1299	GLN
1	B	2011	HIS
1	B	2161	GLN
1	B	2734	ASN
1	B	3605	HIS
1	B	3611	HIS
1	B	5003	HIS
1	D	105	HIS
1	D	879	HIS
1	D	889	GLN
1	D	963	ASN
1	D	1041	GLN

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Mol	Chain	Res	Type
1	D	1299	GLN
1	D	2011	HIS
1	D	2161	GLN
1	D	2734	ASN
1	D	3605	HIS
1	D	3611	HIS
1	D	5003	HIS
1	C	105	HIS
1	C	879	HIS
1	C	889	GLN
1	C	963	ASN
1	C	1041	GLN
1	C	1299	GLN
1	C	2011	HIS
1	C	2161	GLN
1	C	2734	ASN
1	C	3605	HIS
1	C	3611	HIS
1	C	5003	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	ATP	B	5301	-	28,33,33	0.63	0	34,52,52	1.04	4 (11%)
3	ATP	D	5301	-	28,33,33	0.63	0	34,52,52	1.04	4 (11%)
6	PNX	C	5304	-	13,21,21	0.79	1 (7%)	13,30,30	2.92	3 (23%)
6	PNX	A	5304	-	13,21,21	0.79	1 (7%)	13,30,30	2.92	3 (23%)
3	ATP	A	5301	-	28,33,33	0.63	0	34,52,52	1.03	4 (11%)
6	PNX	B	5304	-	13,21,21	0.79	0	13,30,30	2.91	3 (23%)
6	PNX	D	5304	-	13,21,21	0.81	1 (7%)	13,30,30	2.94	3 (23%)
3	ATP	C	5301	-	28,33,33	0.63	0	34,52,52	1.03	4 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	B	5301	-	-	4/18/38/38	0/3/3/3
3	ATP	D	5301	-	-	4/18/38/38	0/3/3/3
6	PNX	C	5304	-	-	5/7/7/7	0/2/2/2
6	PNX	A	5304	-	-	5/7/7/7	0/2/2/2
3	ATP	A	5301	-	-	4/18/38/38	0/3/3/3
6	PNX	B	5304	-	-	5/7/7/7	0/2/2/2
6	PNX	D	5304	-	-	5/7/7/7	0/2/2/2
3	ATP	C	5301	-	-	4/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	5304	PNX	C6-N1	2.08	1.41	1.38
6	C	5304	PNX	C6-N1	2.04	1.41	1.38
6	A	5304	PNX	C6-N1	2.02	1.41	1.38

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	5304	PNX	C5-C6-N1	-9.08	111.31	120.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	5304	PNX	C5-C6-N1	-9.03	111.36	120.27
6	B	5304	PNX	C5-C6-N1	-9.03	111.37	120.27
6	A	5304	PNX	C5-C6-N1	-9.02	111.37	120.27
6	D	5304	PNX	C4-C5-C6	4.46	123.36	119.96
6	A	5304	PNX	C4-C5-C6	4.44	123.34	119.96
6	C	5304	PNX	C4-C5-C6	4.43	123.33	119.96
6	B	5304	PNX	C4-C5-C6	4.35	123.27	119.96
6	A	5304	PNX	CAC-N3-C4	2.88	121.94	118.20
6	D	5304	PNX	CAC-N3-C4	2.88	121.93	118.20
6	B	5304	PNX	CAC-N3-C4	2.85	121.90	118.20
6	C	5304	PNX	CAC-N3-C4	2.84	121.89	118.20
3	D	5301	ATP	C5-C6-N6	2.39	123.95	120.31
3	B	5301	ATP	O4'-C1'-N9	-2.36	105.61	108.75
3	B	5301	ATP	C5-C6-N6	2.36	123.91	120.31
3	A	5301	ATP	O4'-C1'-N9	-2.36	105.62	108.75
3	D	5301	ATP	O4'-C1'-N9	-2.35	105.62	108.75
3	C	5301	ATP	C5-C6-N6	2.35	123.90	120.31
3	A	5301	ATP	C5-C6-N6	2.35	123.89	120.31
3	C	5301	ATP	O4'-C1'-N9	-2.35	105.63	108.75
3	D	5301	ATP	O3'-C3'-C4'	-2.09	105.09	111.08
3	C	5301	ATP	O3'-C3'-C4'	-2.07	105.12	111.08
3	A	5301	ATP	O3'-C3'-C4'	-2.07	105.13	111.08
3	B	5301	ATP	O3'-C3'-C4'	-2.06	105.15	111.08
3	C	5301	ATP	O3'-C3'-C2'	-2.05	105.25	111.82
3	B	5301	ATP	O3'-C3'-C2'	-2.05	105.26	111.82
3	A	5301	ATP	O3'-C3'-C2'	-2.05	105.26	111.82
3	D	5301	ATP	O3'-C3'-C2'	-2.04	105.27	111.82

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	5301	ATP	PB-O3B-PG-O3G
3	B	5301	ATP	PB-O3B-PG-O3G
3	D	5301	ATP	PB-O3B-PG-O3G
3	C	5301	ATP	PB-O3B-PG-O3G
6	A	5304	PNX	CAH-CAI-CAK-N1
6	B	5304	PNX	CAH-CAI-CAK-N1
6	D	5304	PNX	CAH-CAI-CAK-N1
6	C	5304	PNX	CAH-CAI-CAK-N1
6	A	5304	PNX	CAI-CAH-CAJ-CAM
6	B	5304	PNX	CAI-CAH-CAJ-CAM

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Mol	Chain	Res	Type	Atoms
6	D	5304	PNX	CAI-CAH-CAJ-CAM
6	C	5304	PNX	CAI-CAH-CAJ-CAM
6	A	5304	PNX	CAH-CAJ-CAM-CAA
6	A	5304	PNX	CAH-CAJ-CAM-OAD
6	B	5304	PNX	CAH-CAJ-CAM-CAA
6	B	5304	PNX	CAH-CAJ-CAM-OAD
6	D	5304	PNX	CAH-CAJ-CAM-CAA
6	D	5304	PNX	CAH-CAJ-CAM-OAD
6	C	5304	PNX	CAH-CAJ-CAM-CAA
6	C	5304	PNX	CAH-CAJ-CAM-OAD
3	A	5301	ATP	C3'-C4'-C5'-O5'
3	B	5301	ATP	C3'-C4'-C5'-O5'
3	D	5301	ATP	C3'-C4'-C5'-O5'
3	C	5301	ATP	C3'-C4'-C5'-O5'
6	D	5304	PNX	CAJ-CAH-CAI-CAK
6	B	5304	PNX	CAJ-CAH-CAI-CAK
6	C	5304	PNX	CAJ-CAH-CAI-CAK
6	A	5304	PNX	CAJ-CAH-CAI-CAK
3	A	5301	ATP	O4'-C4'-C5'-O5'
3	B	5301	ATP	O4'-C4'-C5'-O5'
3	D	5301	ATP	O4'-C4'-C5'-O5'
3	C	5301	ATP	O4'-C4'-C5'-O5'
3	A	5301	ATP	PG-O3B-PB-O1B
3	B	5301	ATP	PG-O3B-PB-O1B
3	D	5301	ATP	PG-O3B-PB-O1B
3	C	5301	ATP	PG-O3B-PB-O1B

There are no ring outliers.

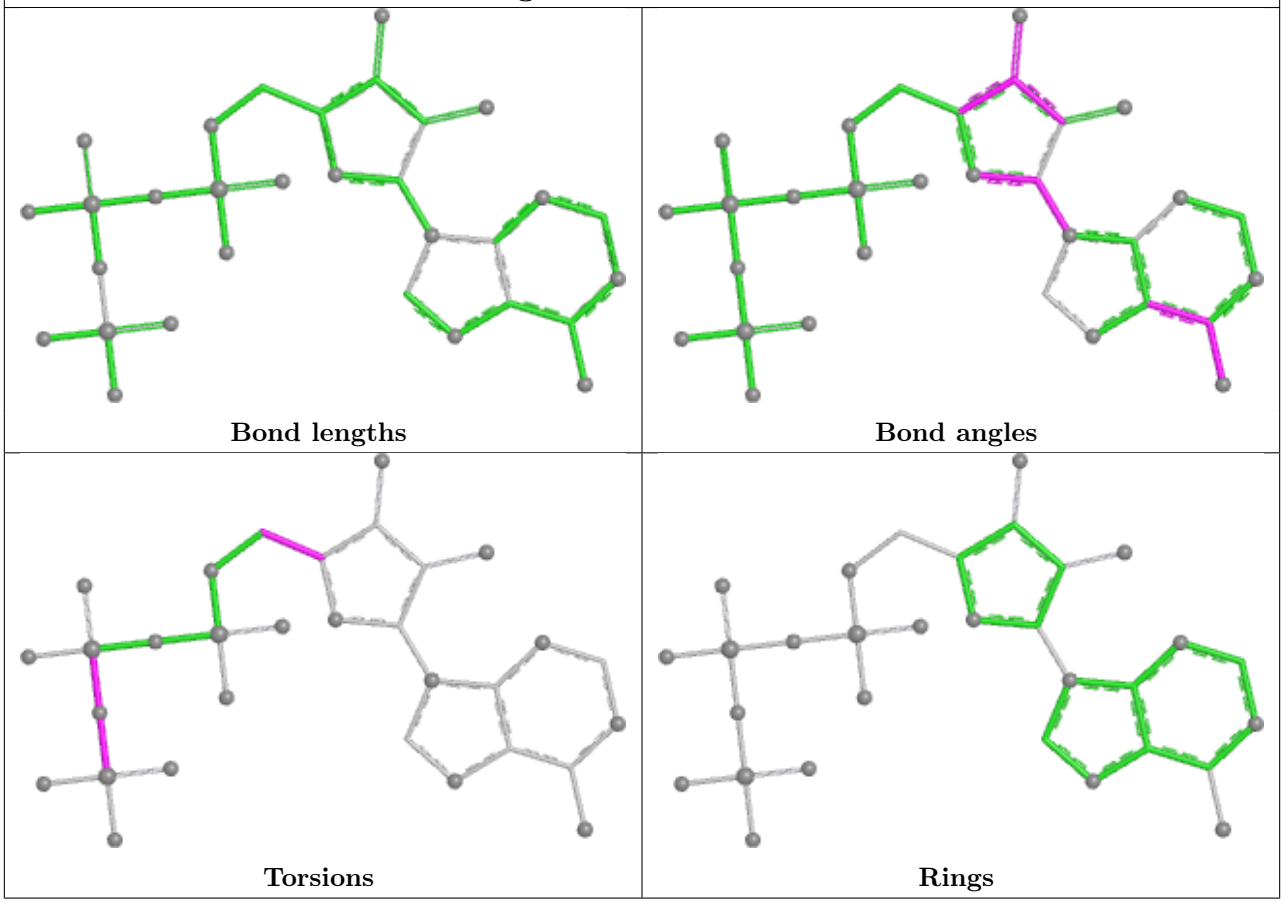
4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	5304	PNX	3	0
6	A	5304	PNX	3	0
6	B	5304	PNX	3	0
6	D	5304	PNX	3	0

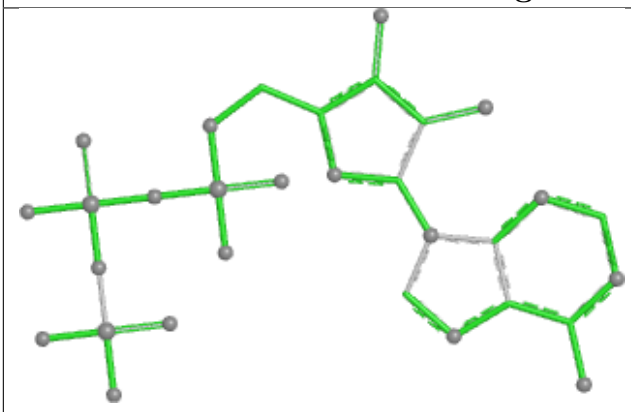
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

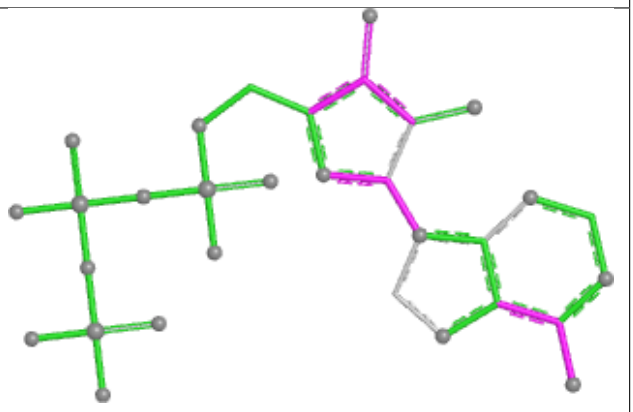
Ligand ATP B 5301



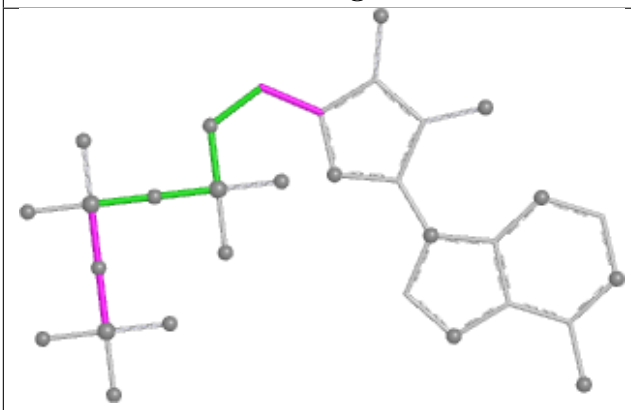
Ligand ATP D 5301



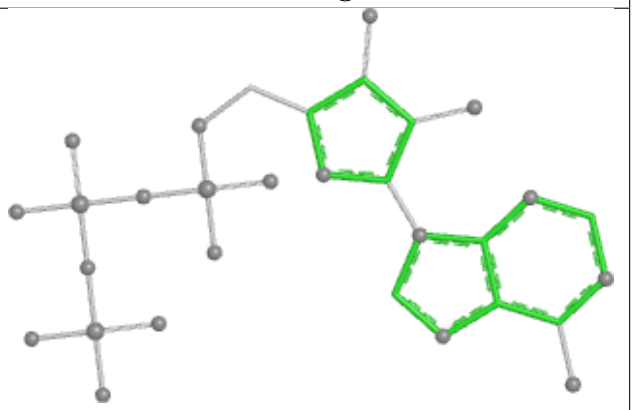
Bond lengths



Bond angles

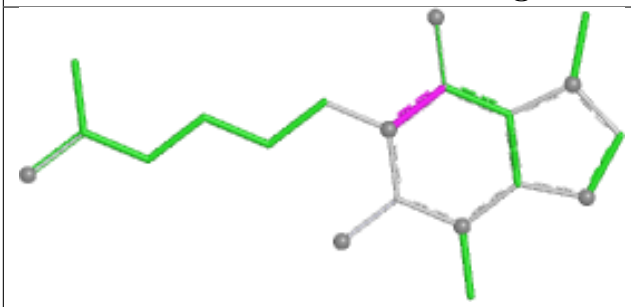


Torsions

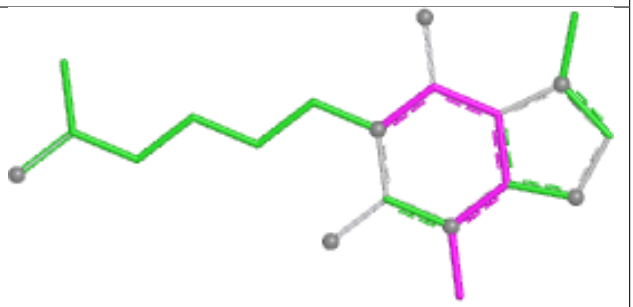


Rings

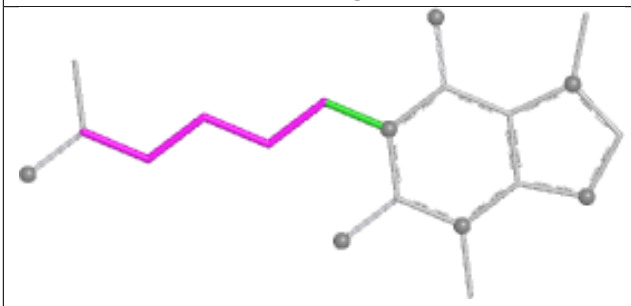
Ligand PNX C 5304



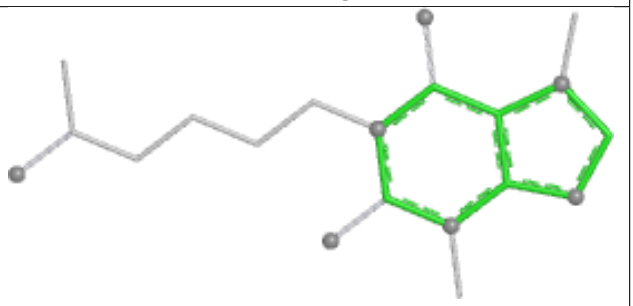
Bond lengths



Bond angles

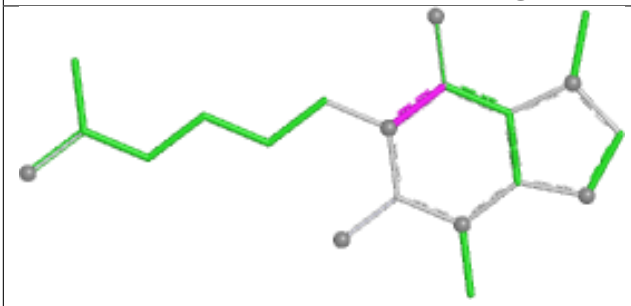


Torsions

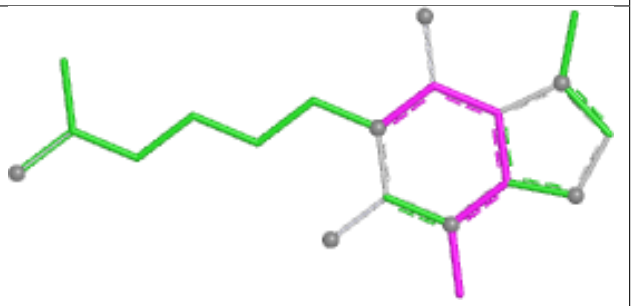


Rings

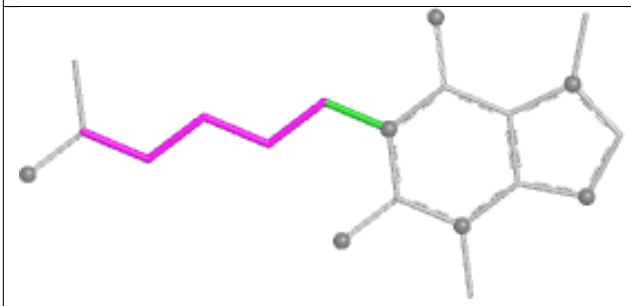
Ligand PNX A 5304



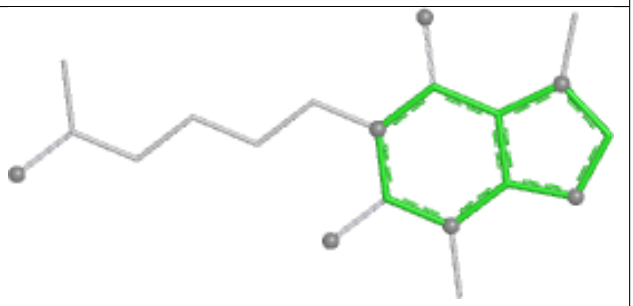
Bond lengths



Bond angles

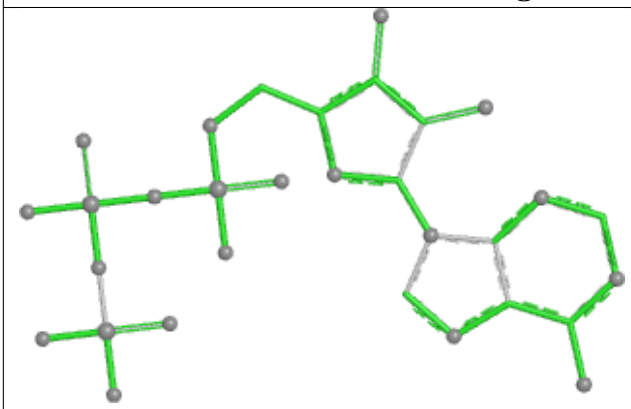


Torsions

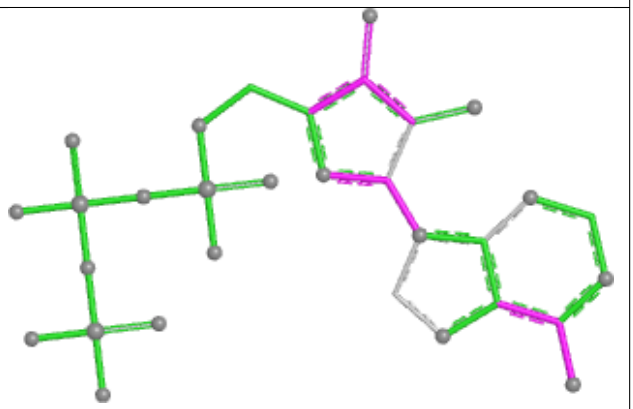


Rings

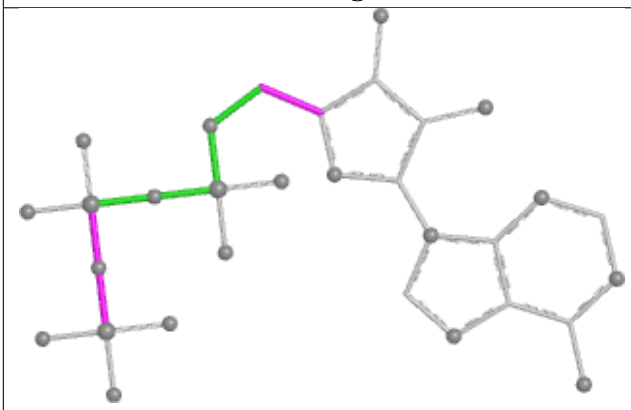
Ligand ATP A 5301



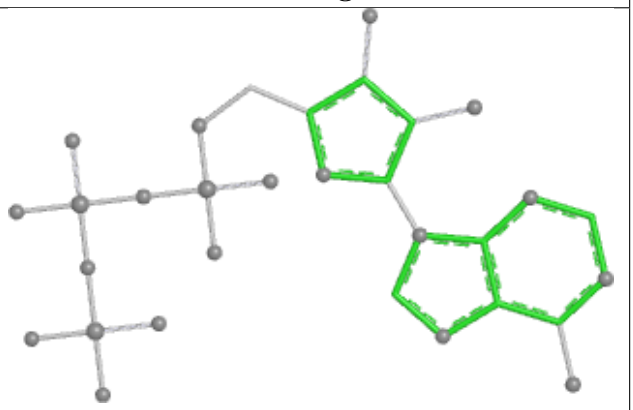
Bond lengths



Bond angles

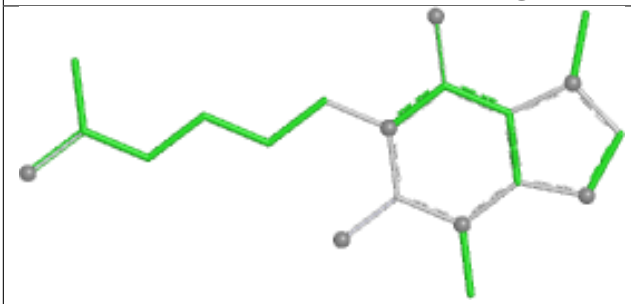


Torsions

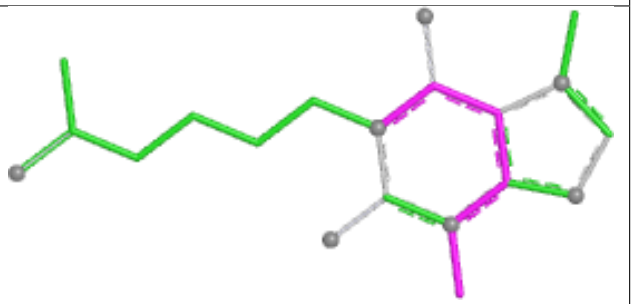


Rings

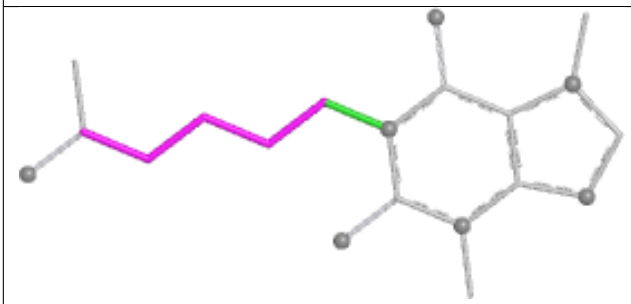
Ligand PNX B 5304



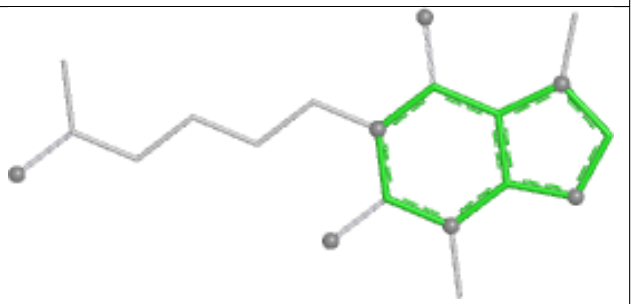
Bond lengths



Bond angles

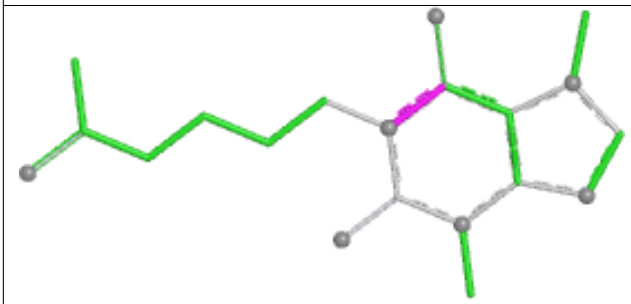


Torsions

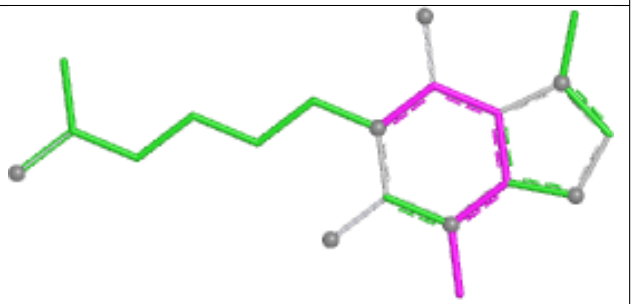


Rings

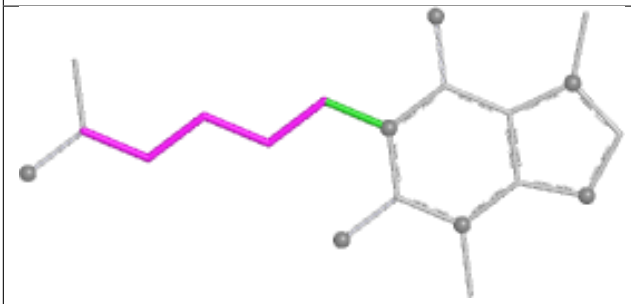
Ligand PNX D 5304



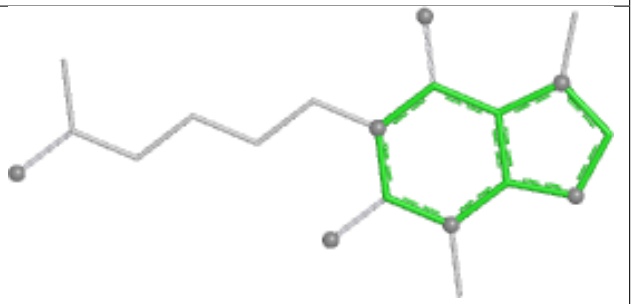
Bond lengths



Bond angles

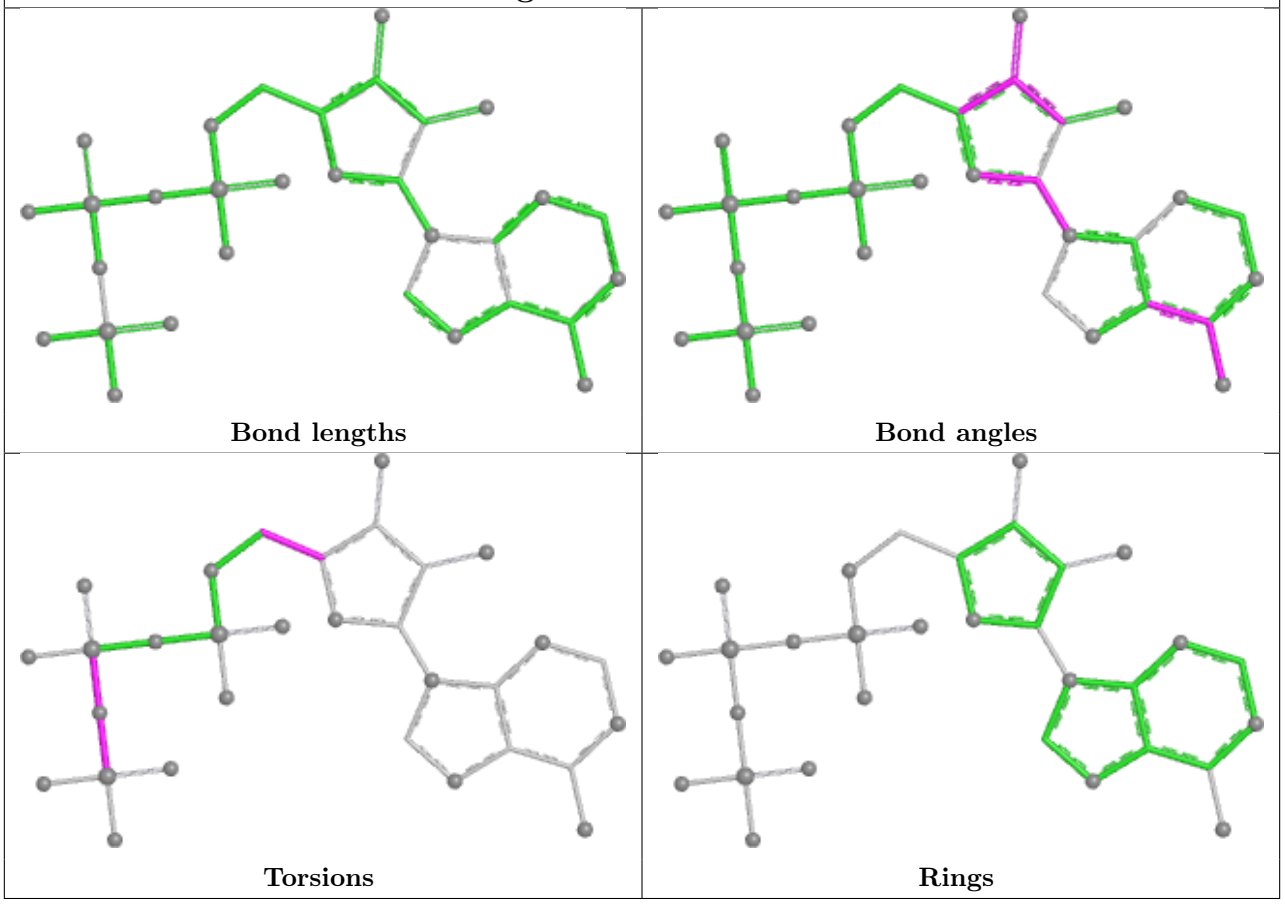


Torsions



Rings

Ligand ATP C 5301



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.

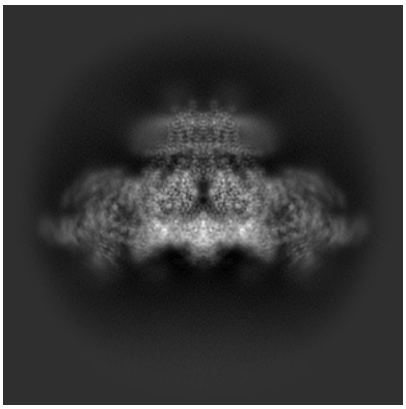
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-47385. These allow visual inspection of the internal detail of the map and identification of artifacts.

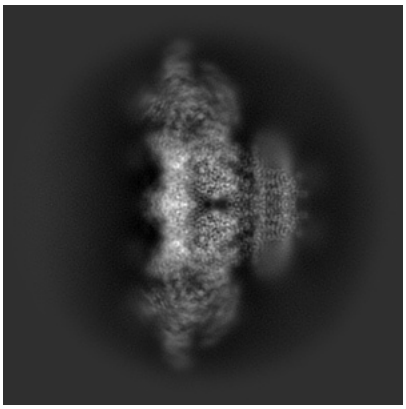
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

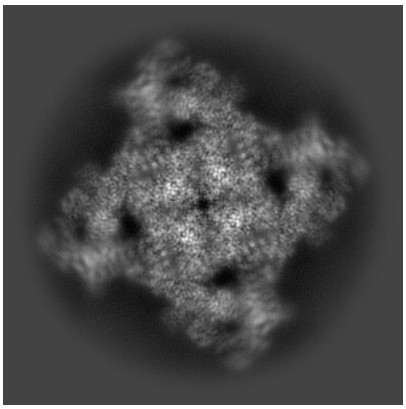
6.1.1 Primary map



X

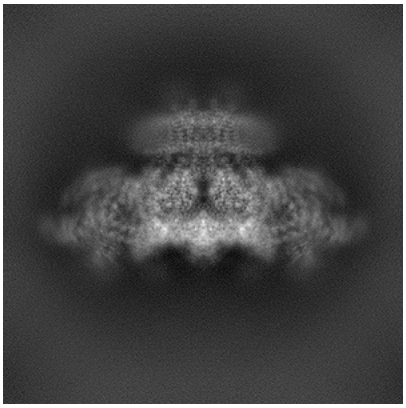


Y

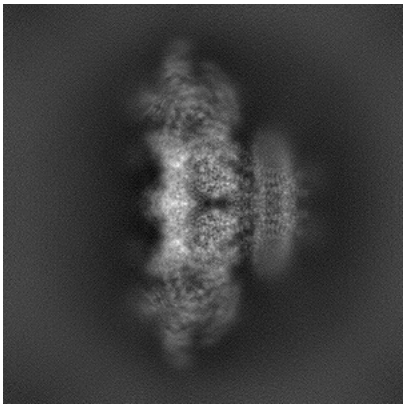


Z

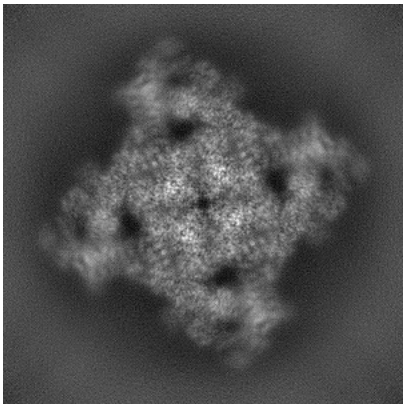
6.1.2 Raw map



X



Y

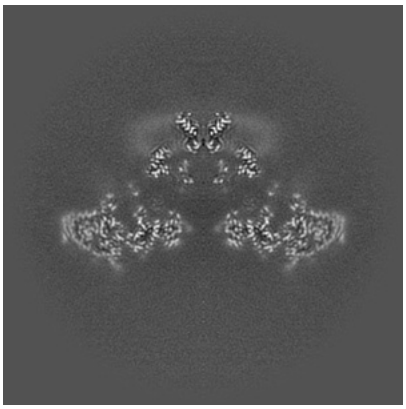


Z

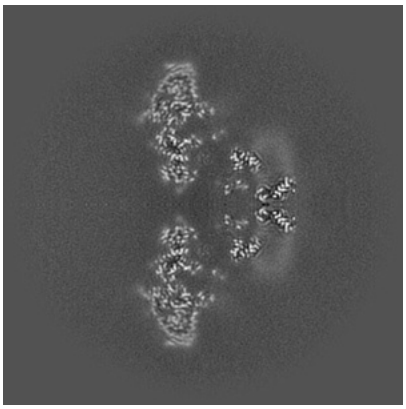
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

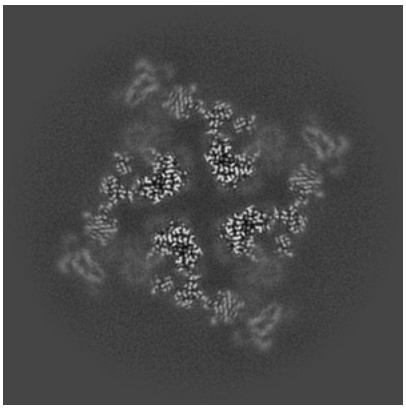
6.2.1 Primary map



X Index: 256

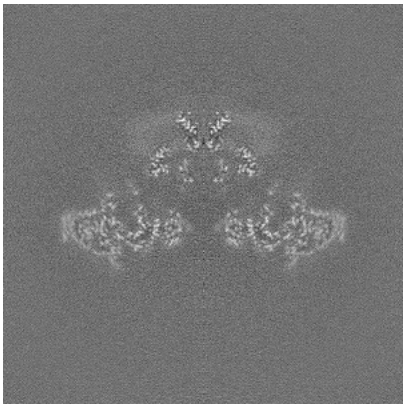


Y Index: 256

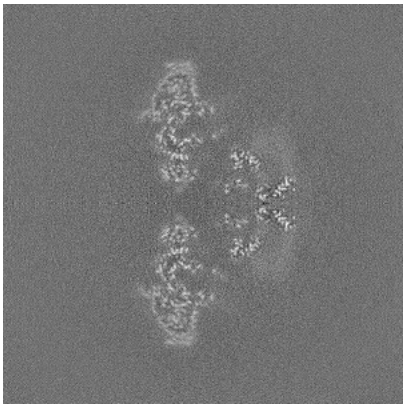


Z Index: 256

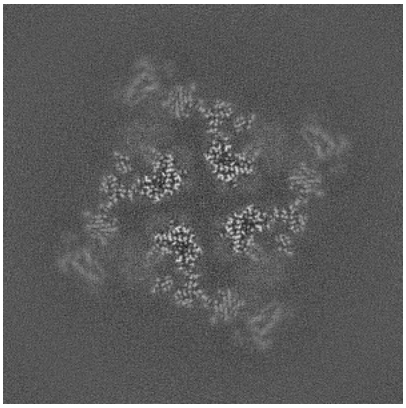
6.2.2 Raw map



X Index: 256



Y Index: 256

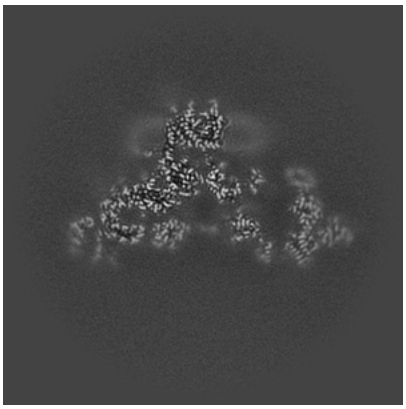


Z Index: 256

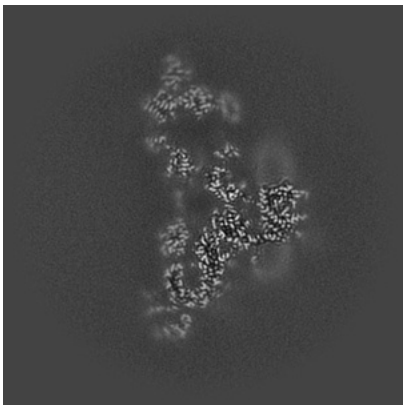
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

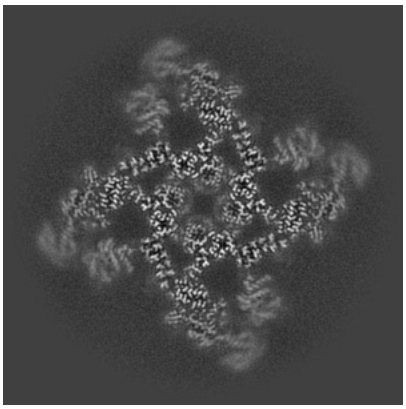
6.3.1 Primary map



X Index: 239



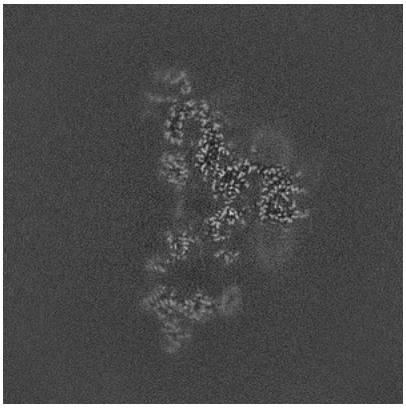
Y Index: 273



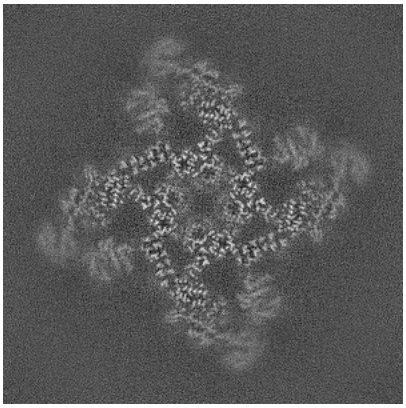
Z Index: 229

6.3.2 Raw map

X Index: 239



Y Index: 239

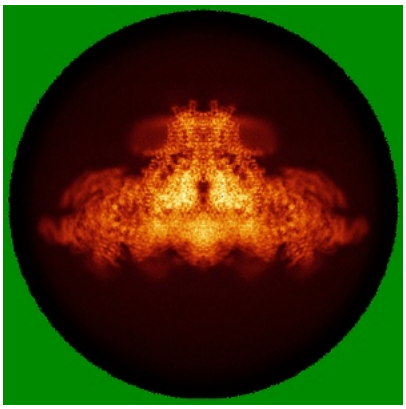


Z Index: 229

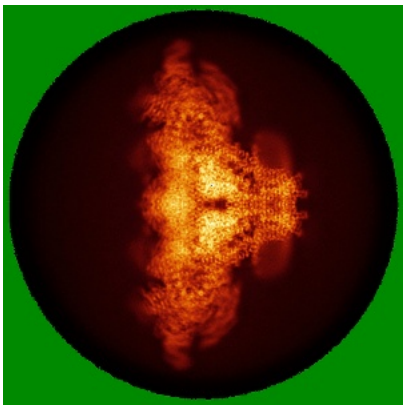
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

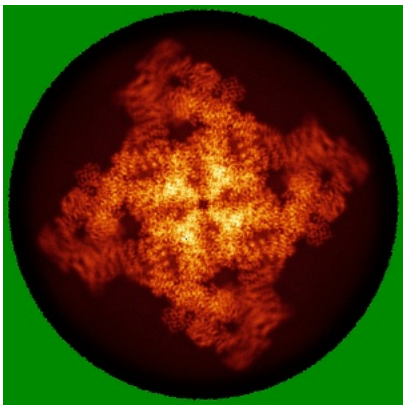
6.4.1 Primary map



X

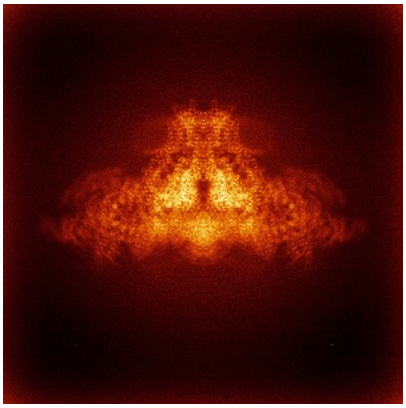


Y

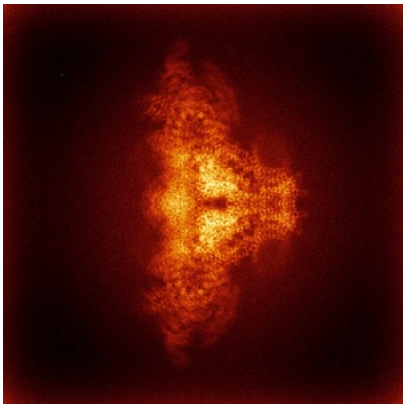


Z

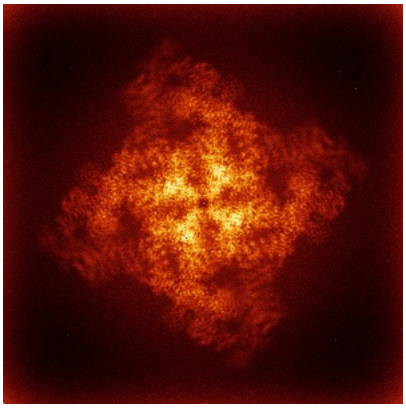
6.4.2 Raw map



X



Y

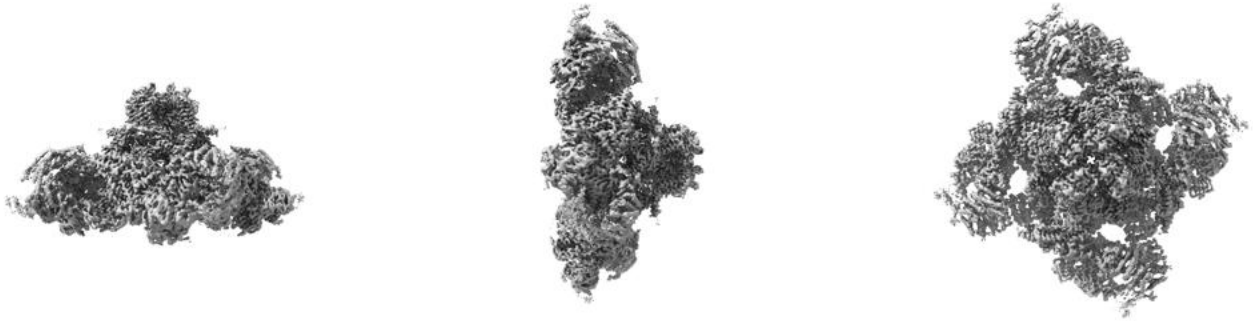


Z

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)

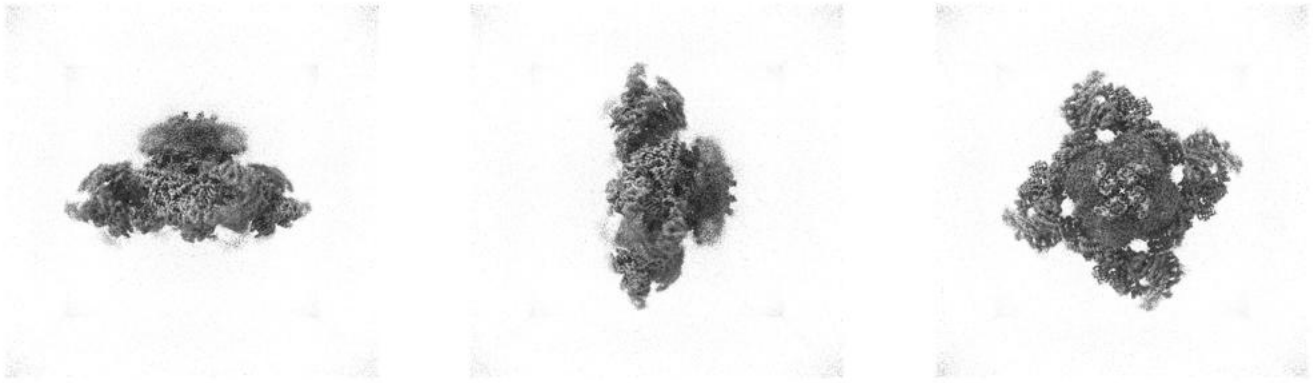
6.5.1 Primary map



X Y Z

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

6.5.2 Raw map



X Y Z

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.

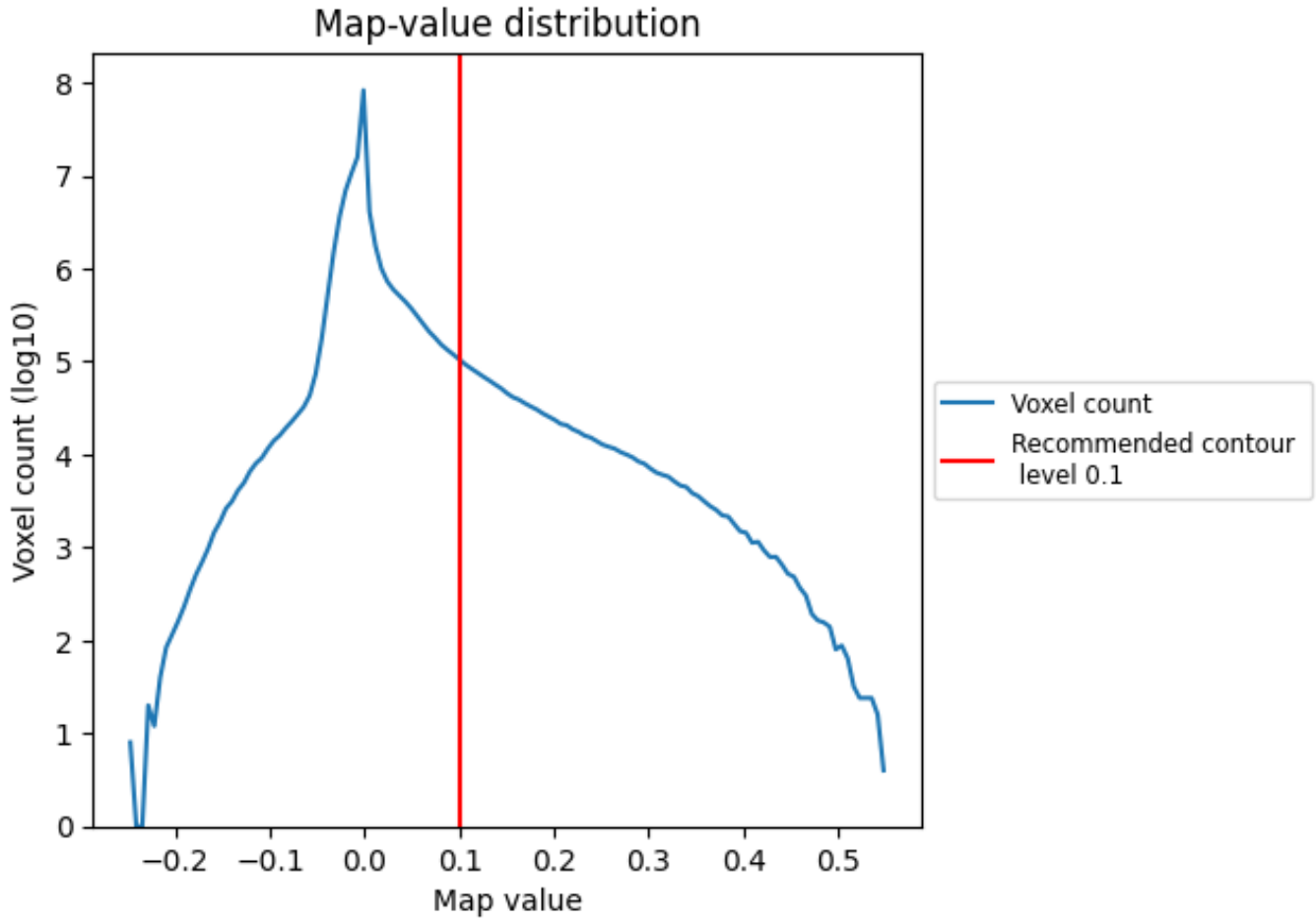
6.6 Mask visualisation (i)

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

7 Map analysis

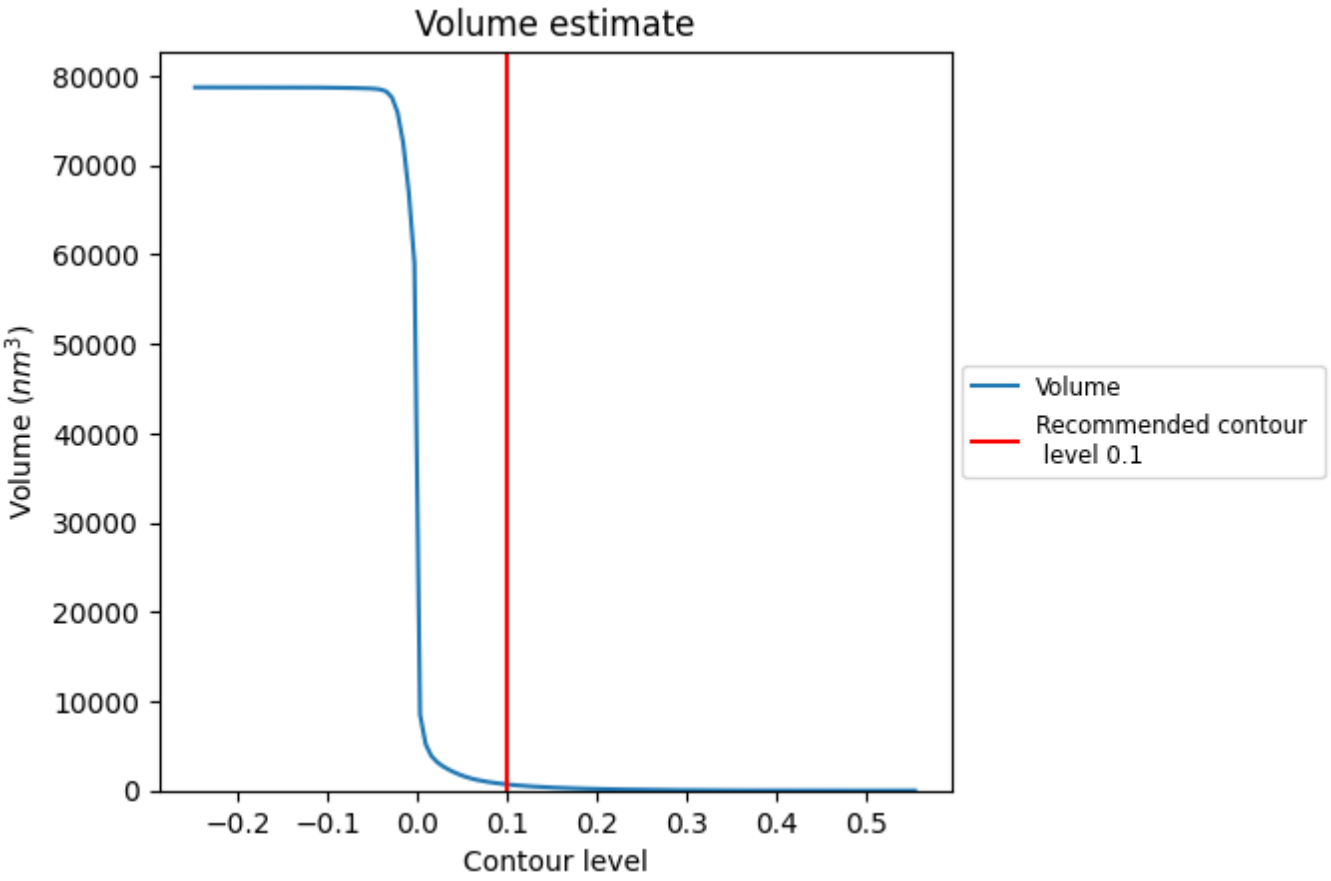
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

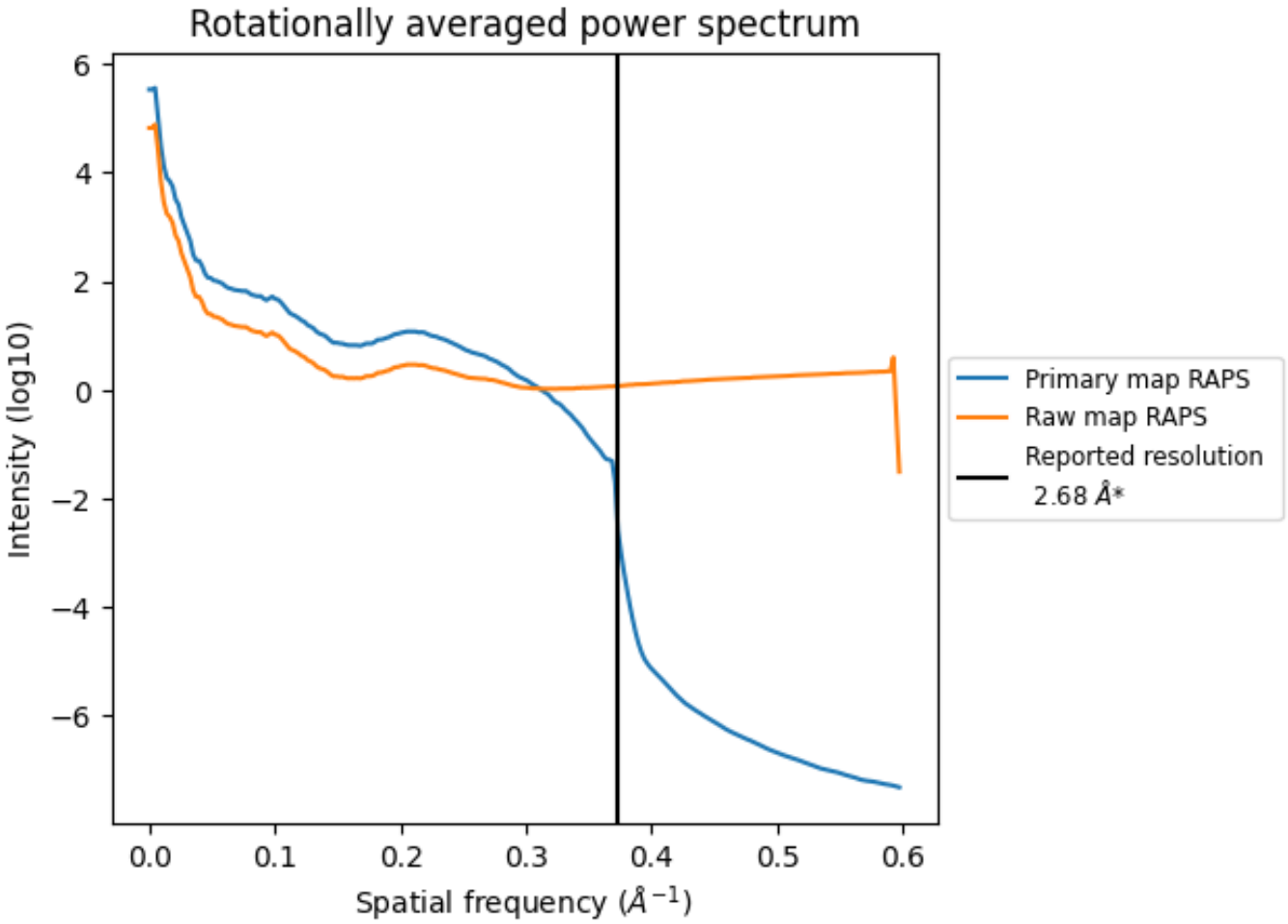
7.2 Volume estimate



The volume at the recommended contour level is 692 nm^3; this corresponds to an approximate mass of 625 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 (i)

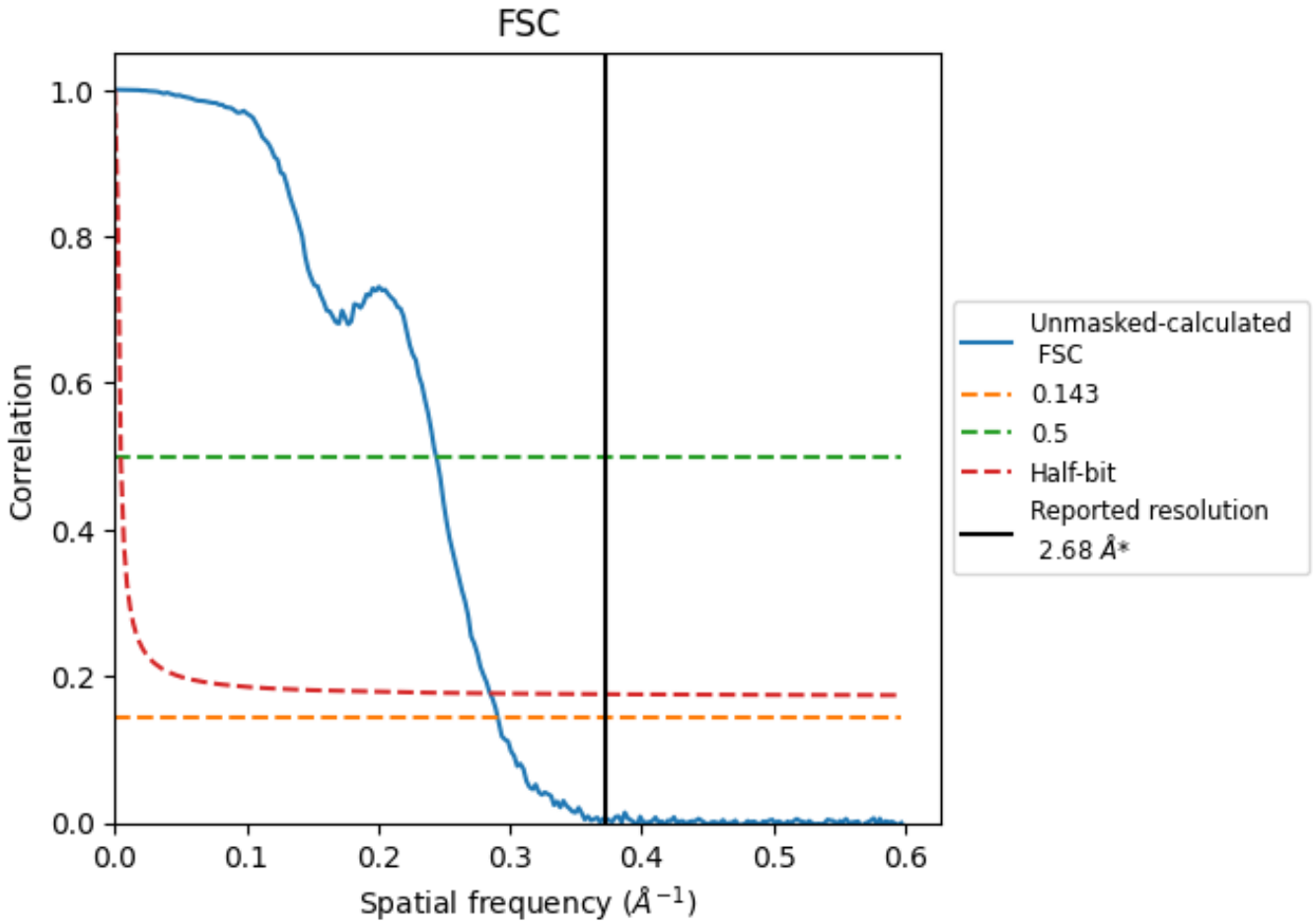


*Reported resolution corresponds to spatial frequency of 0.373 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.373 Å^{-1}

8.2 Resolution estimates (i)

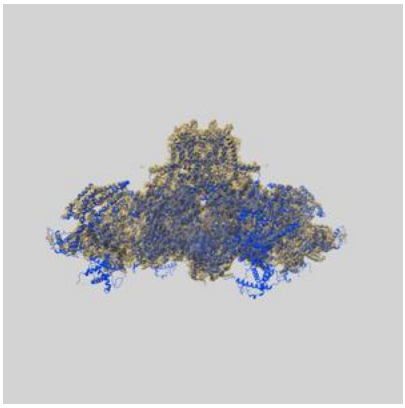
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.68	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.44	4.10	3.51

*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 3.44 differs from the reported value 2.68 by more than 10 %

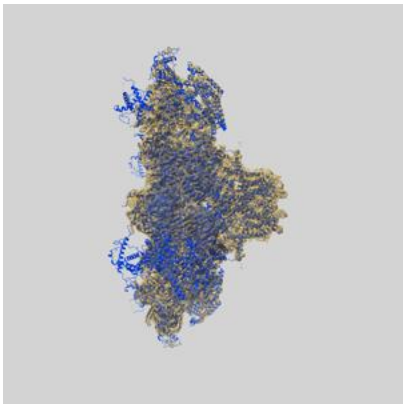
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-47385 and PDB model 9E18. Per-residue inclusion information can be found in section 3 on page 7.

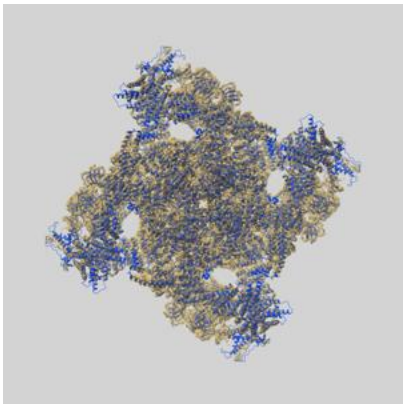
9.1 Map-model overlay



X



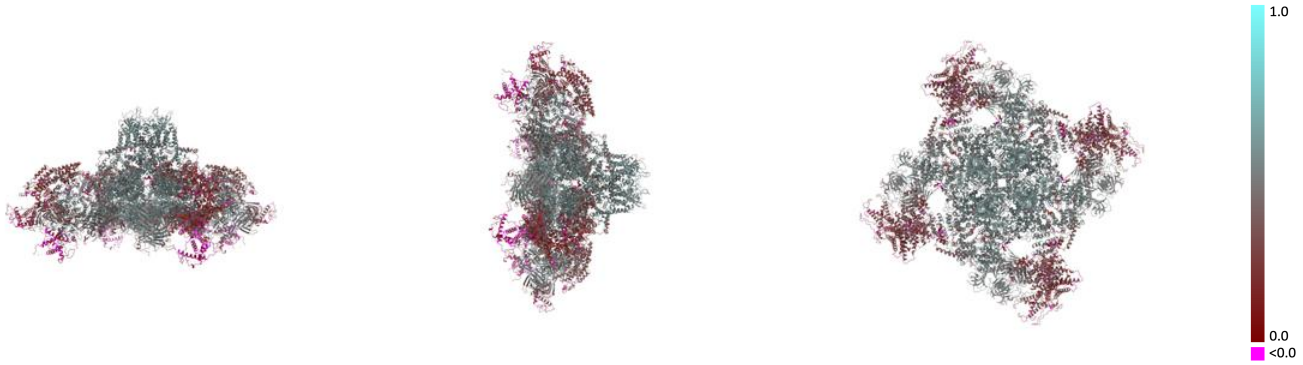
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

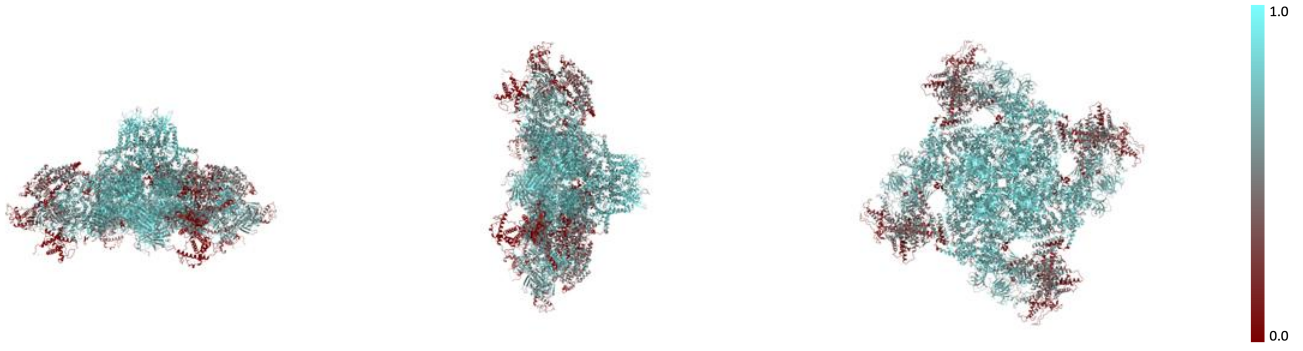
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according 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.

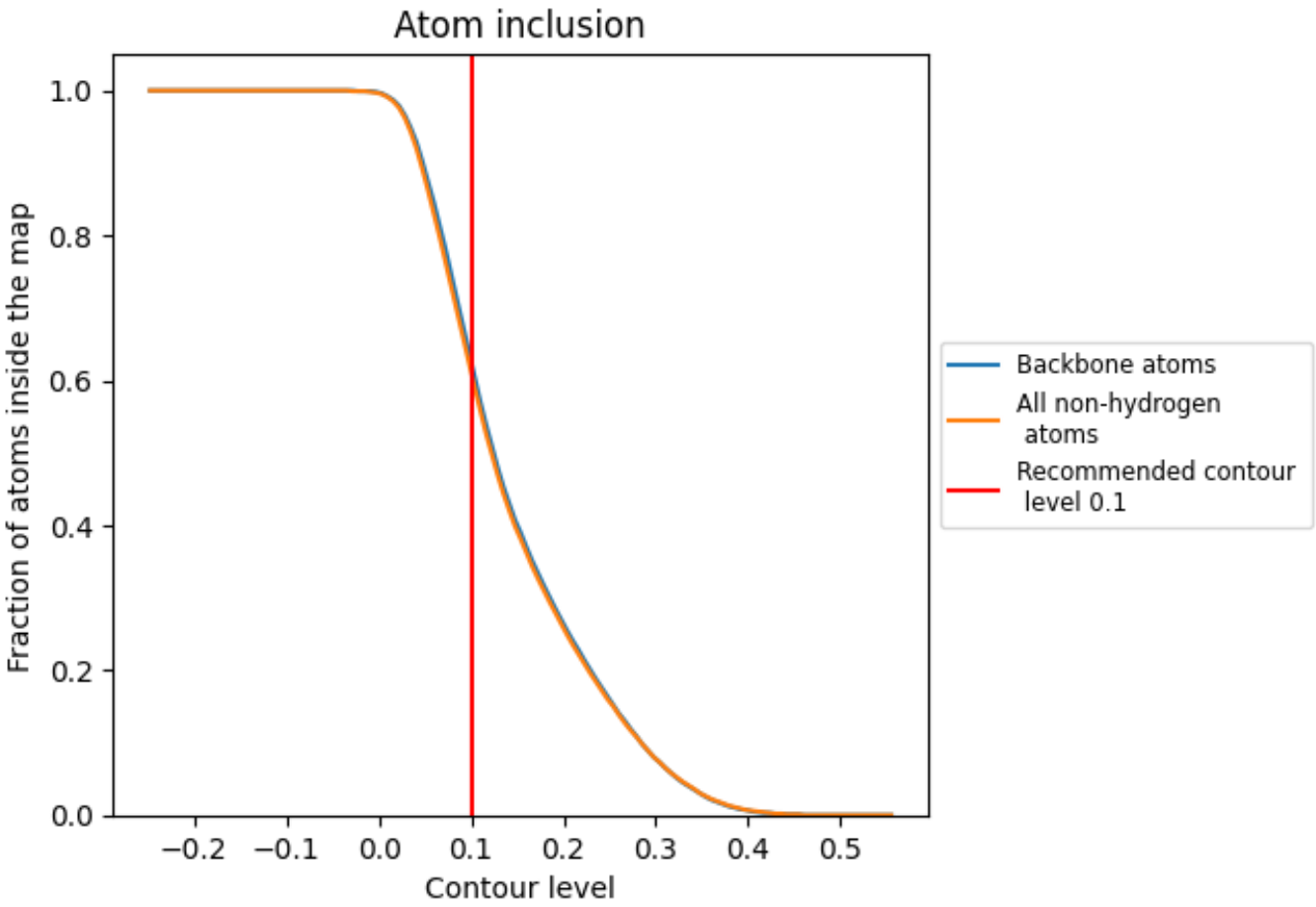
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).

9.4 Atom inclusion (i)



At the recommended contour level, 63% of all backbone atoms, 61% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6110	0.4160
A	0.6180	0.4140
B	0.6180	0.4150
C	0.6180	0.4140
D	0.6180	0.4140
E	0.6470	0.5000
F	0.6500	0.4970
G	0.6430	0.4940
H	0.6470	0.4960