Full wwPDB EM Validation Report ⓘ

Sep 23, 2024 – 01:04 PM EDT

PDB ID	:	8UXM
EMDB ID	:	EMD-42769
Title	:	Structure of PKA phosphorylated human RyR2-R420W in the open state in the presence of calcium and calmodulin
Authors	:	Miotto, M.C.; Marks, A.R.
Deposited on	:	2023-11-09
Resolution	:	3.56 Å(reported)
Based on initial model	:	7UA5

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:

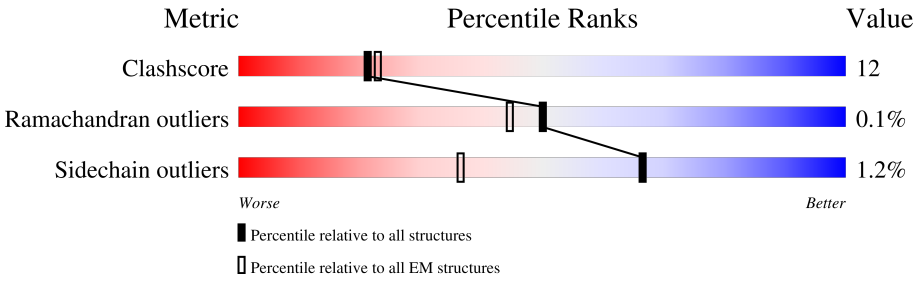
EMDB validation analysis	:	0.0.1.dev112
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.56 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	I	149	5% 52% 40%
1	J	149	5% 58% 34%
1	K	149	6% 56% 36%
1	L	149	6% 56% 36%
2	A	4967	10% 63% 21% 15%
2	B	4967	10% 63% 21% 15%
2	C	4967	10% 64% 21% 15%
2	D	4967	10% 63% 21% 15%

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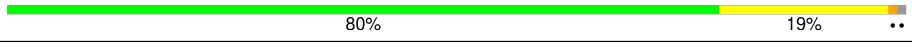
Mol	Chain	Length	Quality of chain
3	E	108	
3	F	108	
3	G	108	
3	H	108	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 143464 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 Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	I	143	Total	C	N	O	S	0	0
			1131	694	182	246	9		
1	J	143	Total	C	N	O	S	0	0
			1131	694	182	246	9		
1	L	143	Total	C	N	O	S	0	0
			1131	694	182	246	9		
1	K	143	Total	C	N	O	S	0	0
			1131	694	182	246	9		

- Molecule 2 is a protein called Ryanodine receptor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	4231	Total	C	N	O	S	2	0
			33849	21572	5764	6283	230		
2	B	4231	Total	C	N	O	S	2	0
			33849	21572	5764	6283	230		
2	C	4231	Total	C	N	O	S	2	0
			33849	21572	5764	6283	230		
2	D	4231	Total	C	N	O	S	2	0
			33849	21572	5764	6283	230		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	420	TRP	ARG	variant	UNP Q92736
B	420	TRP	ARG	variant	UNP Q92736
C	420	TRP	ARG	variant	UNP Q92736
D	420	TRP	ARG	variant	UNP Q92736

- Molecule 3 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

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

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

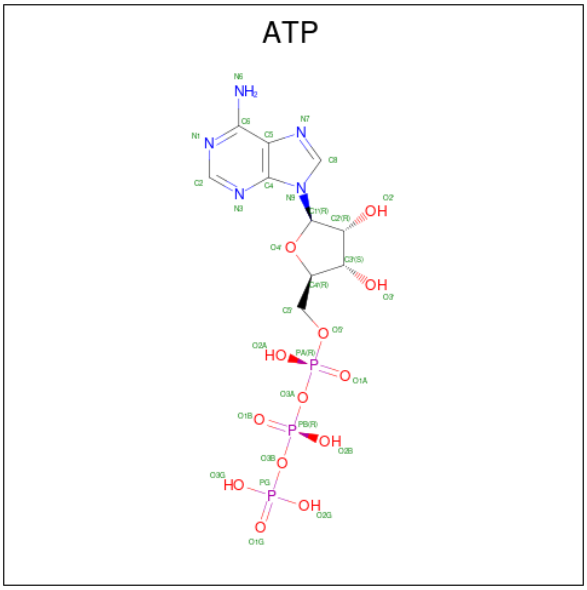
Mol	Chain	Residues	Atoms		AltConf
4	I	4	Total 4	Ca 4	0
4	A	1	Total 1	Ca 1	0
4	J	4	Total 4	Ca 4	0
4	L	4	Total 4	Ca 4	0
4	K	4	Total 4	Ca 4	0
4	B	1	Total 1	Ca 1	0
4	C	1	Total 1	Ca 1	0
4	D	1	Total 1	Ca 1	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:

$C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



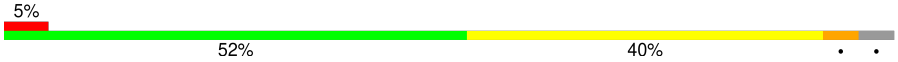
Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	D	1	Total	C	N	O	P	0
			31	10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

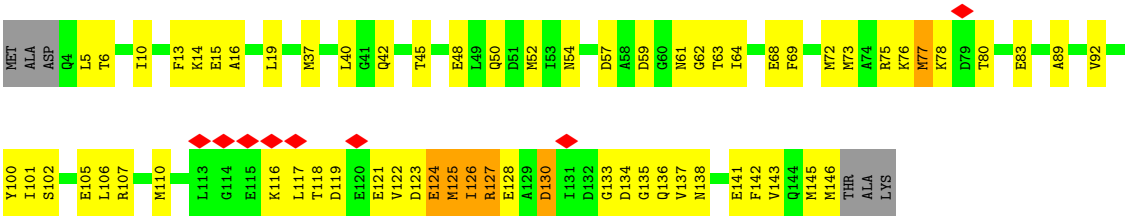
3 Residue-property plots (i)

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: Calmodulin-1

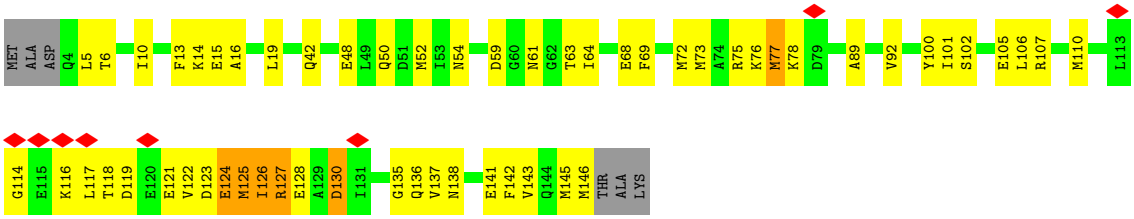
Chain I:





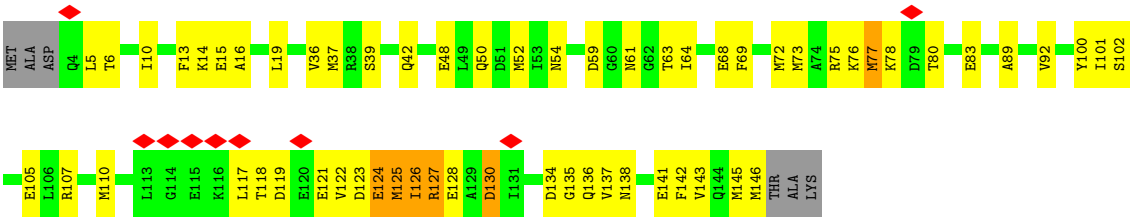
• Molecule 1: Calmodulin-1

Chain J:



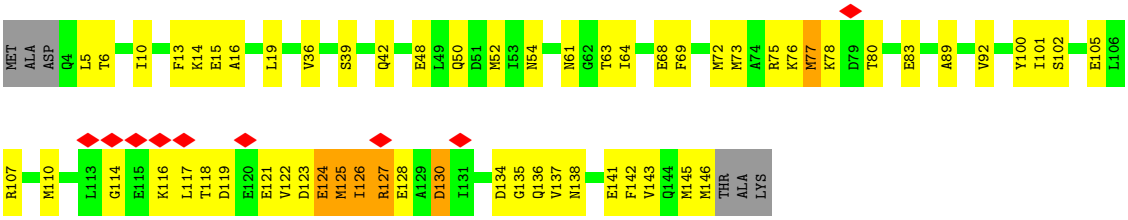
• Molecule 1: Calmodulin-1

Chain L:



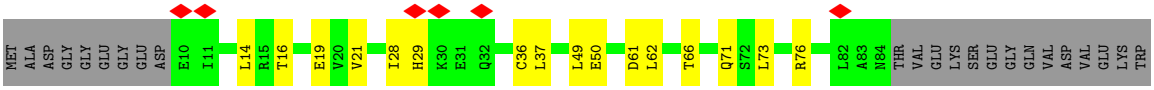
• Molecule 1: Calmodulin-1

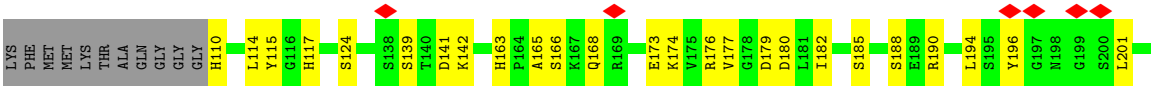
Chain K:

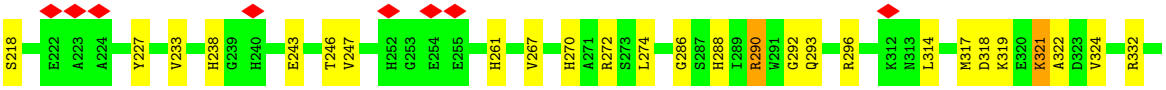


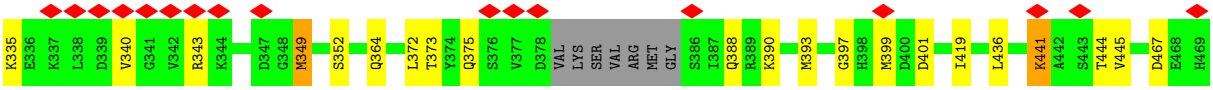
• Molecule 2: Ryanodine receptor 2

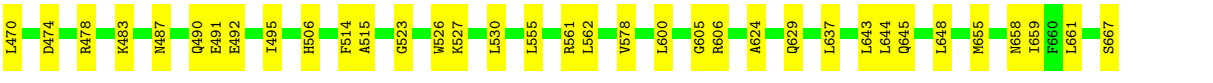
Chain A:

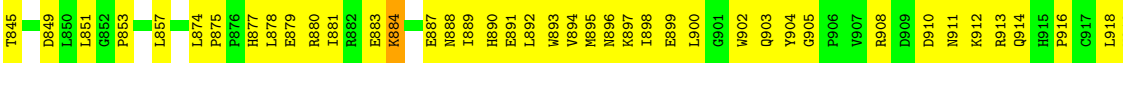


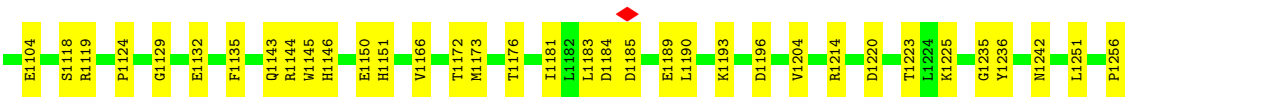


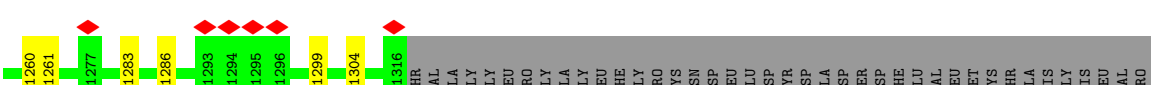


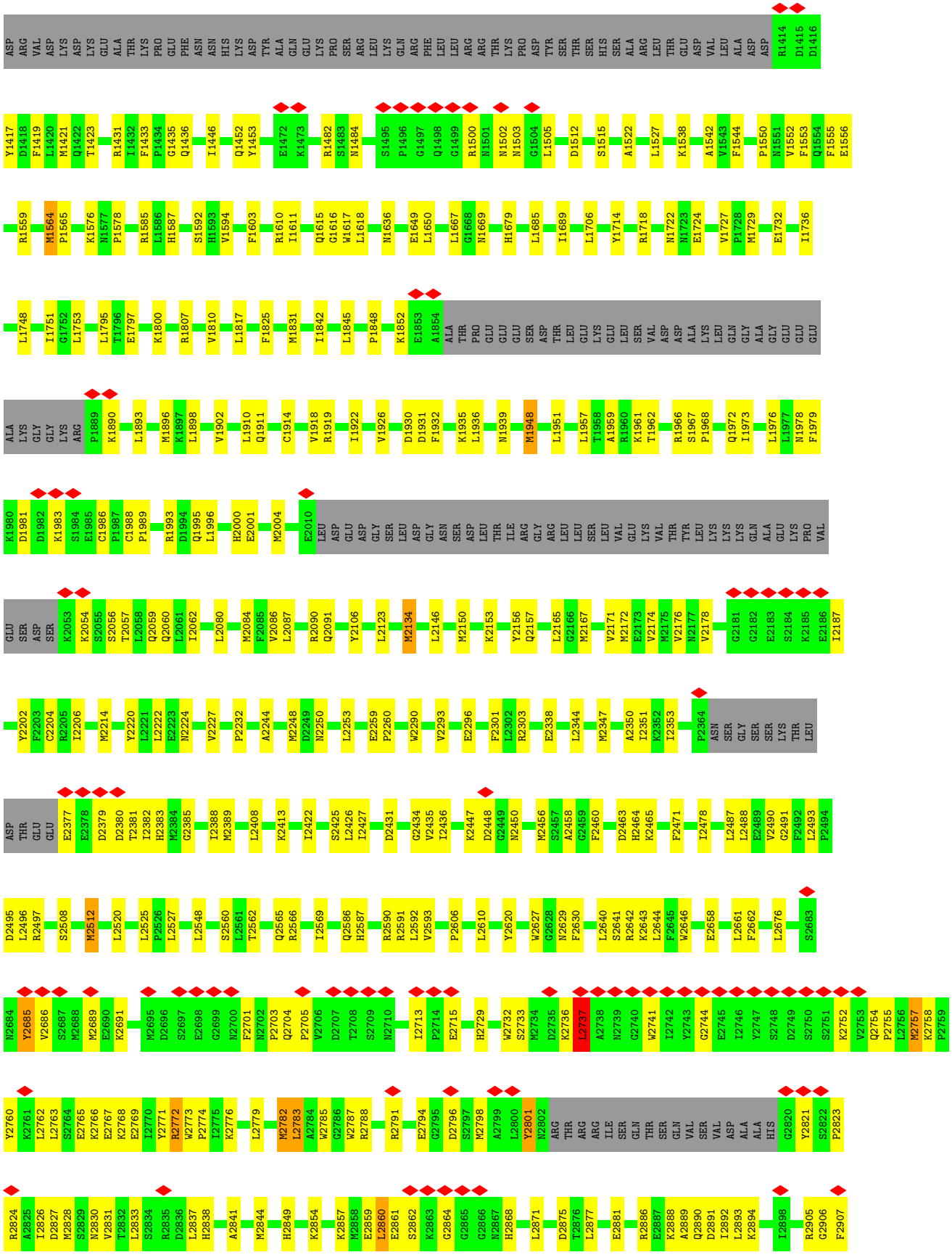


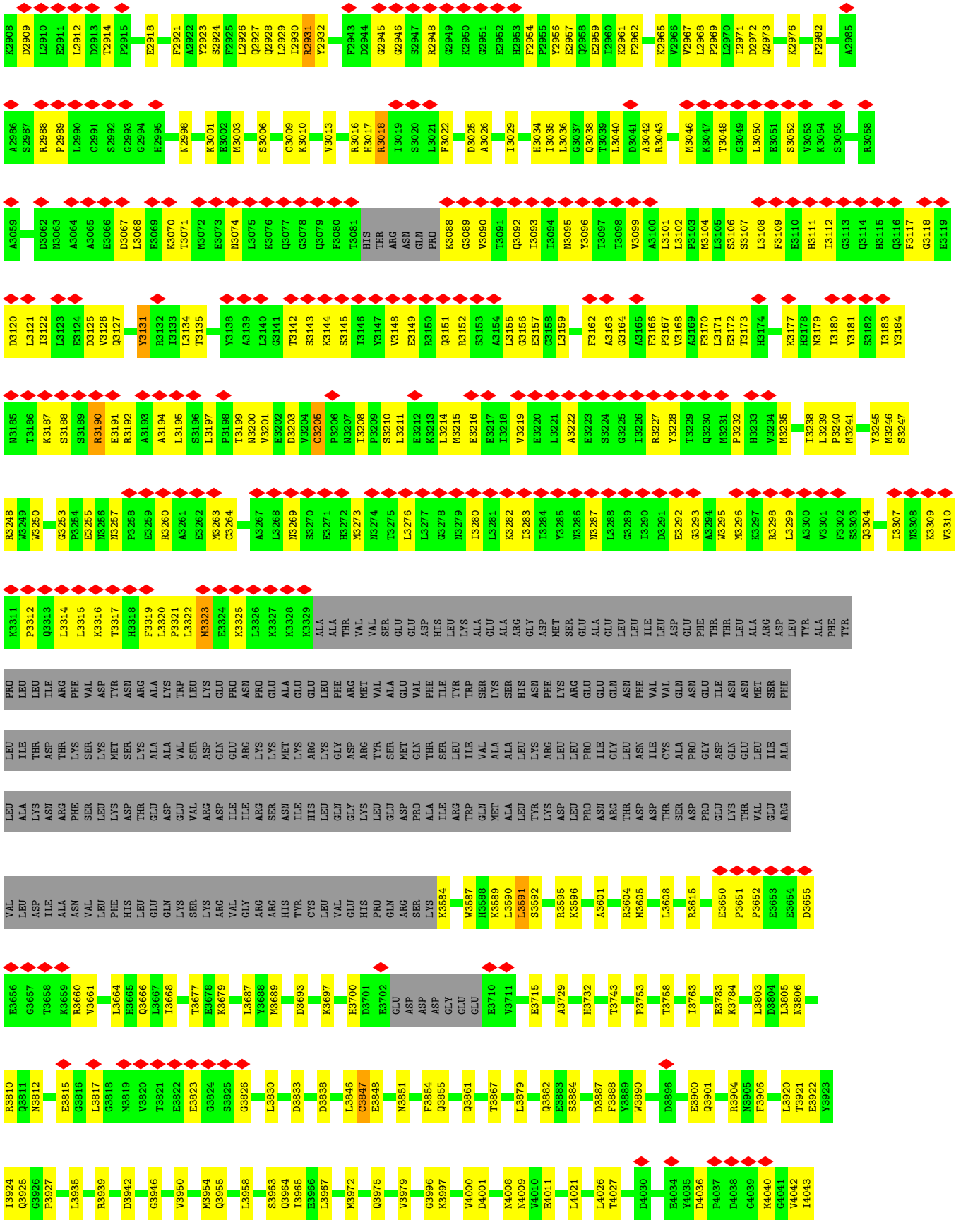









ASP ARG VAL ASP LYS ASP LYS GLU ALA THR LYS PRO GLU PHE ASN ASN HIS LYS ASP TYR ALA GLN GLU LYS PRO SER ARG LEU LYS GLN ARG PHE LEU LEU ARG ARG THR LYS PRO ASP TYR SER THR SER HIS SER ALA ARG LEU THR GLU ASP VAL LEU ALA ASP ASP
R1414 D1415 D1416
Y1417 D1418 F1419 L1420 M1421 Q1422 T1423 R1431 I1432 F1433 P1434 G1435 Q1436 I1446 Q1452 Y1453 E1472 K1473 R1482 S1483 N1484 S1495 P1496 G1497 Q1498 G1499 R1500 N1501 N1502 N1503 G1504 L1505 D1512 S1515 A1522 L1527 K1538 A1542 V1543 F1544 P1550 N1551 V1552 F1553 Q1554 F1555 E1556
R1559 M1564 P1565 K1576 N1577 P1578 R1585 L1586 H1587 S1592 H1593 V1594 F1603 R1610 I1611 Q1615 G1616 W1617 L1618 N1636 E1649 L1650 L1667 G1668 N1669 H1679 L1685 I1689 L1706 Y1714 R1718 N1722 N1723 E1724 V1727 P1728 M1729 E1732 I1736
L1748 I1751 G1752 L1753 L1795 T1796 E1797 K1800 R1807 V1810 L1817 F1825 M1831 I1842 L1845 P1848 K1852 E1853 A1854 ALA THR PRO GLU GLU GLU SER ASP THR LEU GLU LYS GLU LEU SER VAL ASP ASP ALA LYS LEU GLN GLY ALA GLY GLU GLU GLU
ALA LYS GLY GLY LYS ARG P1889 K1890 L1893 M1896 K1897 L1898 V1902 L1910 Q1911 C1914 V1918 R1919 I1922 V1926 D1930 D1931 F1932 K1935 L1936 N1939 M1948 L1961 L1957 T1958 A1959 R1960 K1961 T1962 R1966 S1967 P1968 Q1972 I1973 L1976 L1977 N1978 F1979
K1980 D1981 D1982 K1983 S1984 E1985 C1986 P1987 C1988 P1989 R1993 D1994 Q1995 L1996 H2000 E2001 M2004 E2010 LEU ASP GLU ASP GLY SER LEU ASP GLY ASN SER ASP LEU THR ILE ARG GLY ARG LEU LEU SER LEU VAL GLU LYS VAL THR TYR LEU LYS LYS LYS GLN ALA GLU LYS PRO VAL
GLU SER ASP SER K2053 K2054 S2055 S2056 T2057 L2058 Q2059 Q2060 L2061 I2062 L2080 M2084 F2085 V2086 L2087 R2090 Q2091 Y2106 L2123 M2134 L2146 M2150 K2153 Y2156 Q2157 L2165 G2166 M2167 V2171 M2172 E2173 V2174 M2175 V2176 N2177 V2178 G2181 G2182 E2183 S2184 K2185 E2186 I2187
Y2202 F2203 C2204 R2205 I2206 M2214 Y2220 L2221 L2222 E2223 N2224 V2227 P2232 A2244 M2248 D2249 N2250 L2253 E2259 P2260 W2290 V2293 E2296 F2301 L2302 R2303 E2338 L2344 M2347 A2350 I2351 K2352 I2353 P2364 ASN SER GLY SER SER LYS THR LEU
ASP THR GLU GLU E2377 E2378 D2379 D2380 T2381 I2382 H2383 M2384 G2385 I2388 M2389 L2408 K2413 I2422 S2425 L2426 I2427 D2431 G2434 V2435 I2436 K2447 D2448 G2449 N2450 M2456 S2457 A2458 G2459 F2460 D2463 H2464 K2465 F2471 I2478 L2487 L2488 E2489 V2490 G2491 F2492 L2493 P2494
D2495 L2496 R2497 S2508 M2512 L2520 L2525 P2526 L2527 L2548 S2560 L2561 T2562 Q2565 R2566 I2569 Q2586 H2587 R2590 R2591 L2592 V2593 P2606 L2610 Y2620 W2627 G2628 N2629 F2630 L2640 S2641 R2642 K2643 L2644 F2645 W2646 E2658 L2661 F2662 L2676 S2683
N2684 Y2685 V2686 S2687 M2688 M2689 E2690 K2691 M2695 D2696 S2697 E2698 G2699 N2700 F2701 N2702 P2703 Q2704 P2705 V2706 D2707 T2708 S2709 N2710 I2713 P2714 E2715 H2729 W2732 S2733 M2734 D2735 K2736 L2737 A2738 N2739 G2740 W2741 I2742 Y2743 G2744 E2745 I2746 Y2747 S2748 D2749 S2750 S2751 K2752 V2753 Q2754 P2755 L2756 M2757 K2758 P2759
Y2760 K2761 L2762 L2763 S2764 E2765 K2766 E2767 K2768 E2769 I2770 Y2771 R2772 W2773 P2774 I2775 K2776 L2779 M2782 L2783 A2784 W2785 G2786 W2787 R2788 R2791 E2794 G2795 D2796 S2797 M2798 A2799 L2800 Y2801 N2802 ARG THR ARG ARG ILE SER GLN THR SER GLN VAL SER VAL ASP ALA ALA HIS G2820 Y2821 S2822 P2823
R2824 A2825 I2826 D2827 M2828 S2829 N2830 V2831 T2832 L2833 S2834 R2835 D2836 L2837 H2838 A2841 M2844 H2849 K2854 K2857 M2858 E2859 L2860 E2861 S2862 K2863 G2864 G2865 G2866 N2867 H2868 L2871 D2875 T2876 L2877 E2881 R2886 E2887 K2888 A2889 Q2890 D2891 I2892 L2893 K2894 I2898 R2905 G2906 F2907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A2986 S2987 R2988 P2989 L2990 C2991 S2992 G2993 G2994 H2995 N2998 K3001 E3002 M3003 S3006 C3009 K3010 V3013 R3016 H3017 R3018 I3019 S3020 L3021 F3022 D3025 A3026 I3029 H3034 I3035 L3036 G3037 Q3038 T3039 L3040 D3041 A3042 R3043 M3046 K3047 T3048 G3049 L3050 E3051 S3052 V3053 K3054 S3055 R3058
A3059 D3062 N3063 A3064 A3065 E3066 D3067 L3068 E3069 K3070 T3071 M3072 E3073 N3074 L3075 K3076 Q3077 G3078 Q3079 F3080 T3081 HIS THR ARG ASN GLN PRO K3088 G3089 V3090 T3091 Q3092 I3093 T3094 N3095 Y3096 T3097 T3098 V3099 A3100 L3101 L3102 P3103 M3104 K3105 S3106 S3107 L3108 F3109 E3110 H3111 I3112 G3113 Q3114 H3115 Q3116 F3117 G3118 E3119
D3120 L3121 I3122 L3123 E3124 D3125 V3126 Q3127 Y3131 R3132 I3133 L3134 T3135 Y3138 A3139 L3140 G3141 T3142 S3143 K3144 S3145 I3146 Y3147 V3148 E3149 R3150 Q3151 R3152 S3153 A3154 L3155 G3156 E3157 C3158 L3159 F3162 A3163 G3164 A3165 F3166 P3167 V3168 A3169 F3170 L3171 E3172 T3173 H3174 K3177 H3178 N3179 I3180 Y3181 S3182 I3183 Y3184
N3185 T3186 K3187 S3188 S3189 R3190 E3191 R3192 A3193 A3194 L3195 S3196 L3197 P3198 T3199 N3200 V3201 E3202 D3203 V3204 C3205 P3206 N3207 I3208 P3209 S3210 L3211 E3212 K3213 L3214 M3215 E3216 E3217 I3218 V3219 E3220 L3221 A3222 E3223 S3224 G3225 I3226 R3227 Y3228 T3229 Q3230 M3231 P3232 H3233 V3234 M3235 I3238 L3239 P3240 M3241 Y3245 M3246 S3247
R3248 W3249 W3250 G3253 P3254 E3255 N3256 N3257 P3258 E3259 R3260 A3261 E3262 M3263 C3264 A3267 L3268 N3269 S3270 E3271 H3272 M3273 N3274 T3275 L3276 L3277 G3278 N3279 I3280 L3281 K3282 I3283 I3284 Y3285 N3286 N3287 L3288 G3289 I3290 D3291 E3292 G3293 A3294 W3295 M3296 K3297 R3298 L3299 A3300 V3301 F3302 S3303 Q3304 I3307 N3308 K3309 V3310
K3311 P3312 Q3313 L3314 L3315 K3316 T3317 H3318 F3319 L3320 P3321 L3322 M3323 E3324 K3325 L3326 K3327 K3328 K3329 ALA ALA THR VAL VAL SER GLU GLU GLY ASP HIS LEU LYS ALA GLU ALA ARG GLY ASP MET SER GLU ALA GLU LEU LEU ILE LEU ASP GLU PHE THR THR LEU ALA ARG ASP LEU TYR ALA PHE TYR
PRO LEU LEU ILE ARG PHE VAL ASP TYR ASN ARG ALA LYS TRP LEU LYS GLU PRO ASN PRO GLU ALA GLU GLU LEU PHE ARG MET VAL ALA GLU VAL PHE ILE TYR TRP SER LYS SER HIS ASN PHE LYS ARG GLU GLU GLN ASN PHE VAL VAL GLN ASN GLU ILE ASN ASN MET SER PHE
LEU ILE THR ASP THR LYS SER LYS MET SER LYS ALA ALA VAL SER ASP GLN GLU ARG LYS LYS MET LYS ARG LYS GLY ASP ARG TYR SER MET GLN THR SER LEU ILE VAL ALA ALA LEU LYS ARG LEU LEU PRO ILE GLY LEU ASN ILE CYS ALA PRO GLY ASP GLN GLU LYS THR VAL GLU LEU
LEU ALA LYS ASN ARG PHE SER LEU LYS ASP THR GLU ASP GLU VAL ARG ASP ILE ILE ARG SER ASN ILE HIS LEU GLN GLY LYS LEU GLU ASP PRO ALA ILE ARG TRP GLN MET ALA LEU TYR LYS ASP LEU PRO ASN ARG THR ASP ASP THR SER ASP PRO GLU LYS THR VAL GLU ARG
VAL LEU ASP ILE ALA ASN VAL LEU PHE HIS LEU LEU GLU GLN LYS SER LYS ARG VAL GLY ARG ARG HIS TYR CYS LEU VAL GLU HIS PRO GLN ARG SER LYS K3584 W3587 H3588 K3589 L3590 L3591 S3592 R3595 K3596 A3601 R3604 M3605 L3608 R3615 E3650 P3651 P3652 E3653 E3654 D3655
E3656 G3657 T3658 K3659 R3660 V3661 L3664 H3665 Q3666 L3667 I3668 T3677 E3678 K3679 L3687 Y3688 M3689 D3693 K3697 H3700 D3701 E3702 GLU ASP ASP ASP GLY GLU GLU E3710 V3711 E3715 A3729 H3732 T3743 P3753 T3758 I3763 E3783 K3784 L3803 D3804 L3805 N3806
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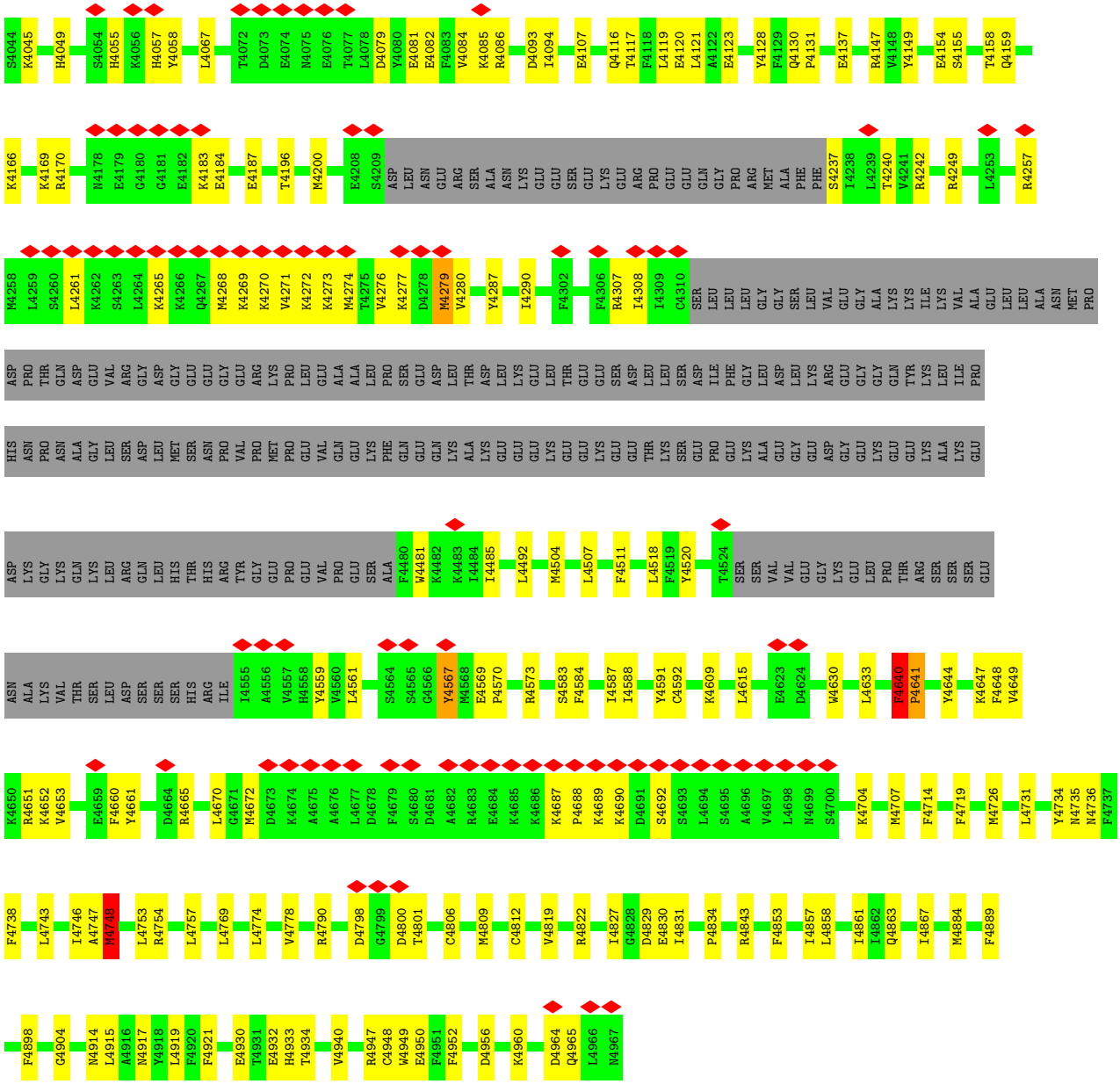
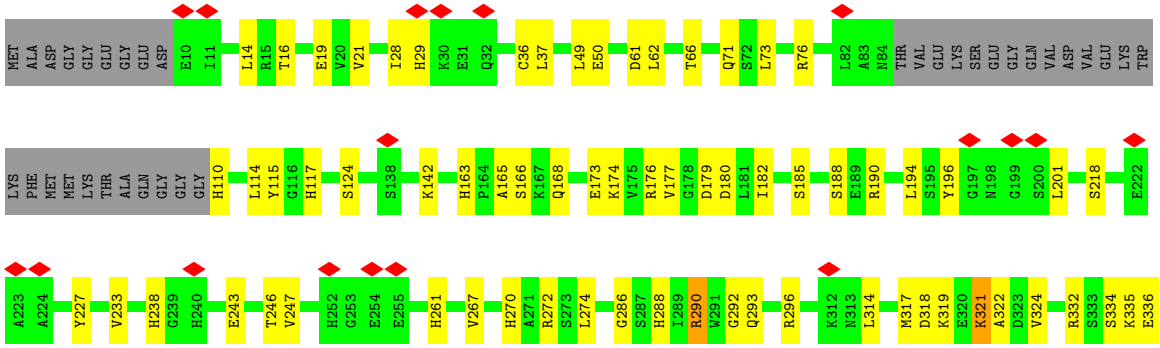
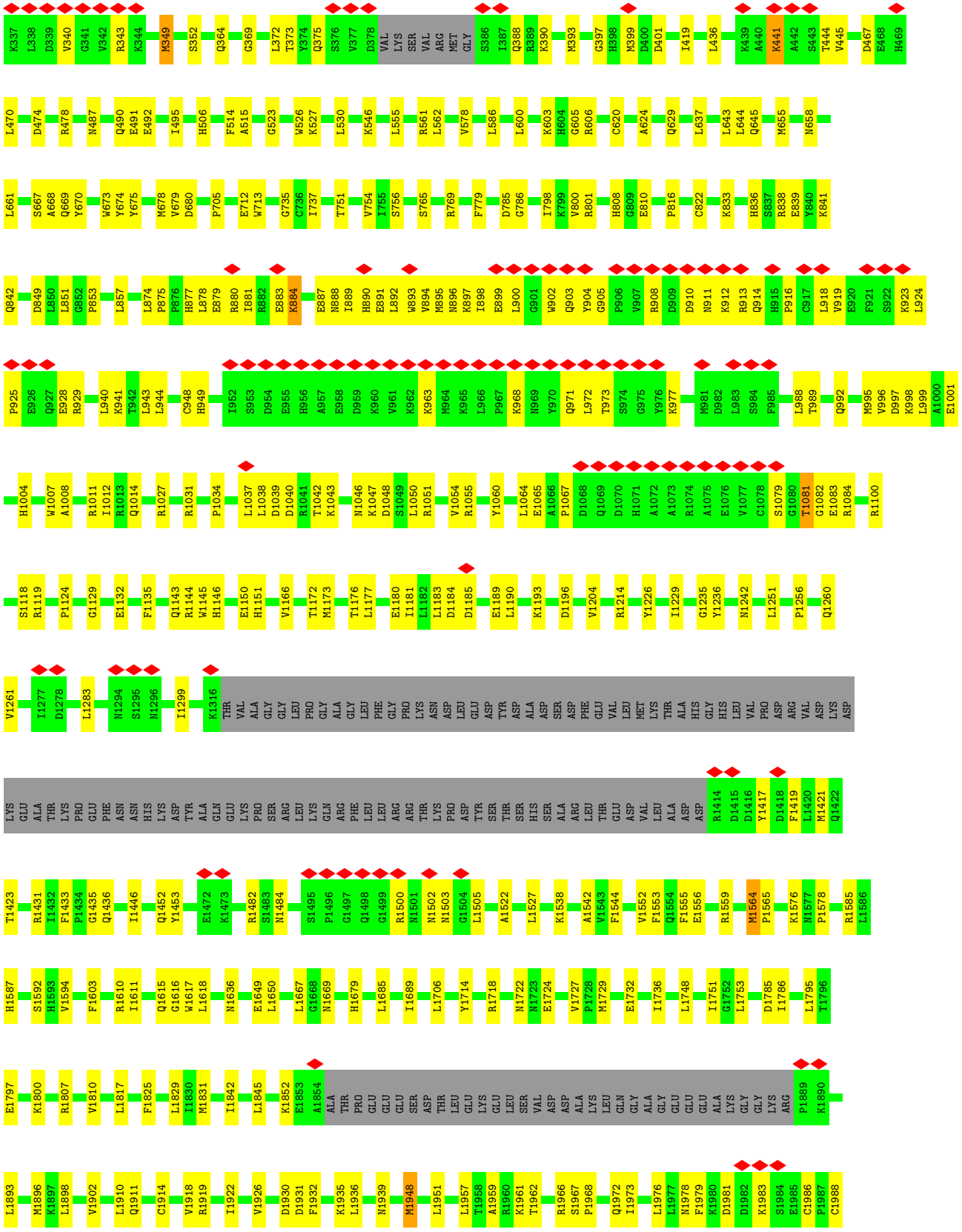
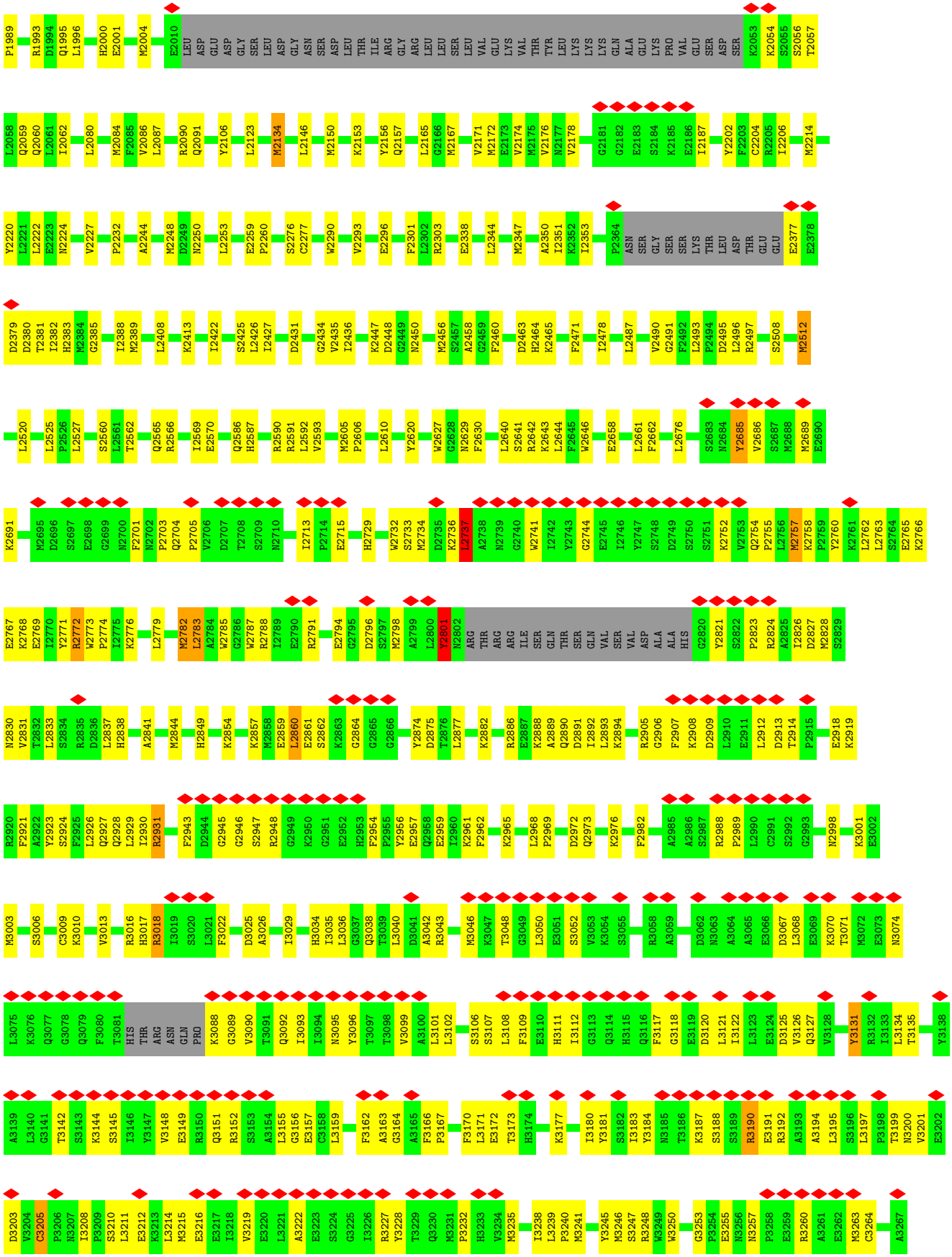


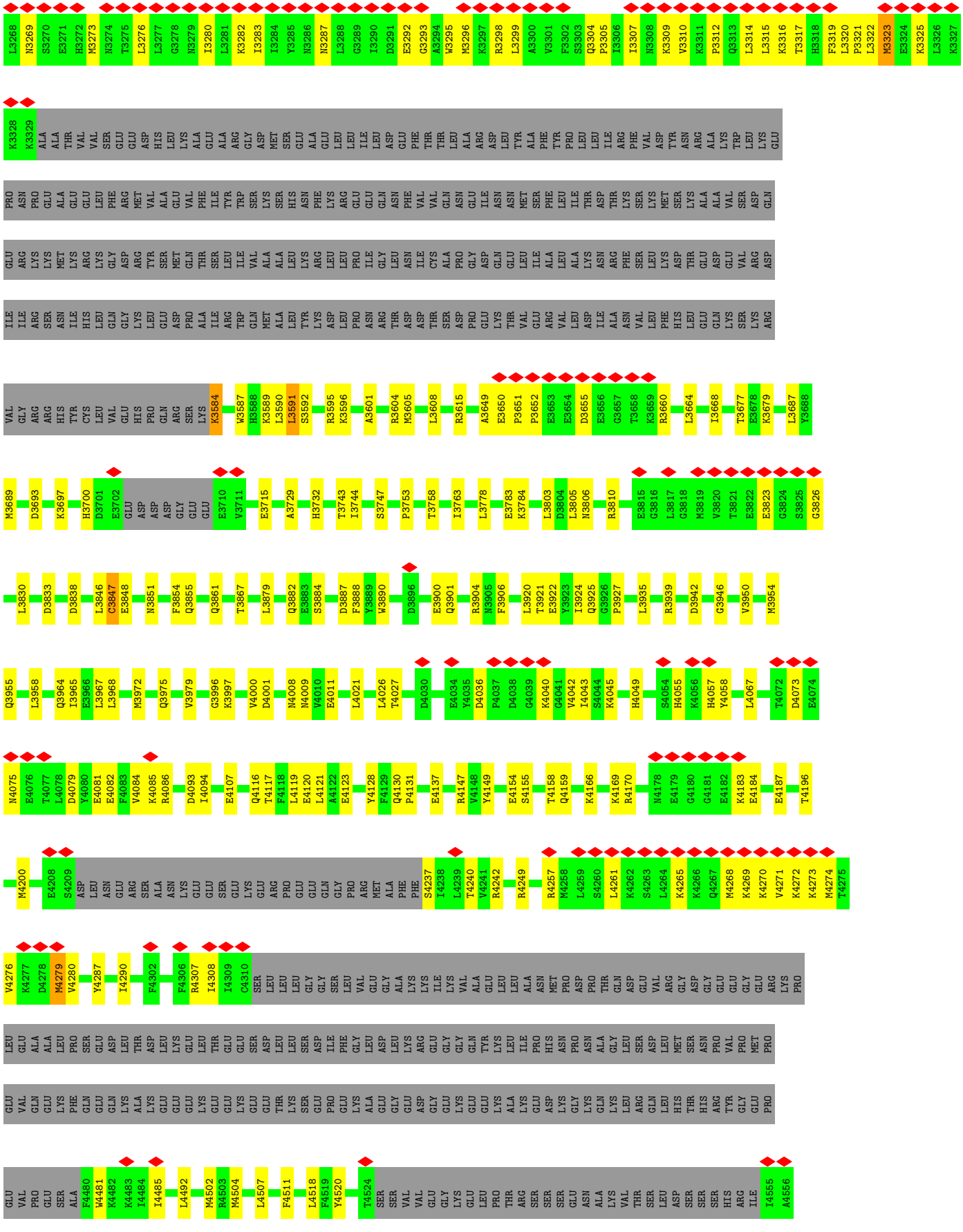
• Molecule 2: Ryanodine receptor 2

Chain B:





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K3328 K3329 ALA ALA THR VAL VAL SER GLU GLU ASP HIS LEU LYS ALA GLU ALA ARG GLY ASP MET SER GLU ALA GLU LEU LEU ILE LEU ASP GLU PHE THR THR LEU ALA ARG ASP LEU TYR ALA PHE TYR PRO LEU LEU ILE ARG PHE VAL ASP TYR ASN ARG ALA LYS TRP LEU LYS GLU
PRO ASN PRO GLU ALA GLU GLU LEU PHE ARG MET VAL ALA GLU VAL PHE ILE TYR TRP SER LYS SER HIS ASN PHE LYS ARG GLU GLU GLN ASN PHE VAL GLN GLN ASN GLU ILE ASN ASN MET SER PHE LEU ILE THR ASP THR LYS SER LYS MET SER LYS ALA ALA VAL SER ASP GLN
GLU ARG LYS LYS MET LYS ARG LYS GLY ASP ARG TYR SER MET GLN THR SER LEU ILE VAL ALA ALA LEU LYS ARG LEU LEU PRO ILE GLY LEU ASN SER PRO GLY ASP GLN GLU LEU ILE ALA LEU ALA LYS ASN ARG PHE SER LEU LEU LYS ASP THR GLU ASP GLU VAL ARG ASP
ILE ILE ARG SER ASN ILE HIS LEU GLN GLY LYS LEU GLU ASP PRO ALA ILE ARG TRP GLN MET ALA LEU TYR LYS ASP LEU PRO ASN ARG THR ASP THR SER ASP PRO GLU LYS THR VAL GLU ARG VAL LEU ASP ILE ALA ASN VAL LEU PHE HIS LEU GLU GLN LYS SER LYS ARG
VAL GLY ARG ARG HIS TYR CYS LEU VAL GLU HIS PRO GLN ARG SER LYS K3584 W3587 H3588 K3589 L3590 L3591 S3592 R3595 K3596 A3601 R3604 M3605 L3608 R3615 A3649 E3650 P3651 P3652 E3653 E3654 D3655 E3656 G3657 T3658 K3659 R3660 L3664 I3668 T3677 E3678 K3679 L3687 Y3688
M3689 D3693 K3697 H3700 D3701 E3702 GLU ASP ASP GLY GLU GLU E3710 V3711 E3715 A3729 H3732 T3743 I3744 S3747 P3753 T3758 I3763 L3778 E3783 K3784 L3803 D3804 L3805 N3806 R3810 E3815 G3816 L3817 G3818 M3819 V3820 T3821 E3822 E3823 G3824 S3825 G3826
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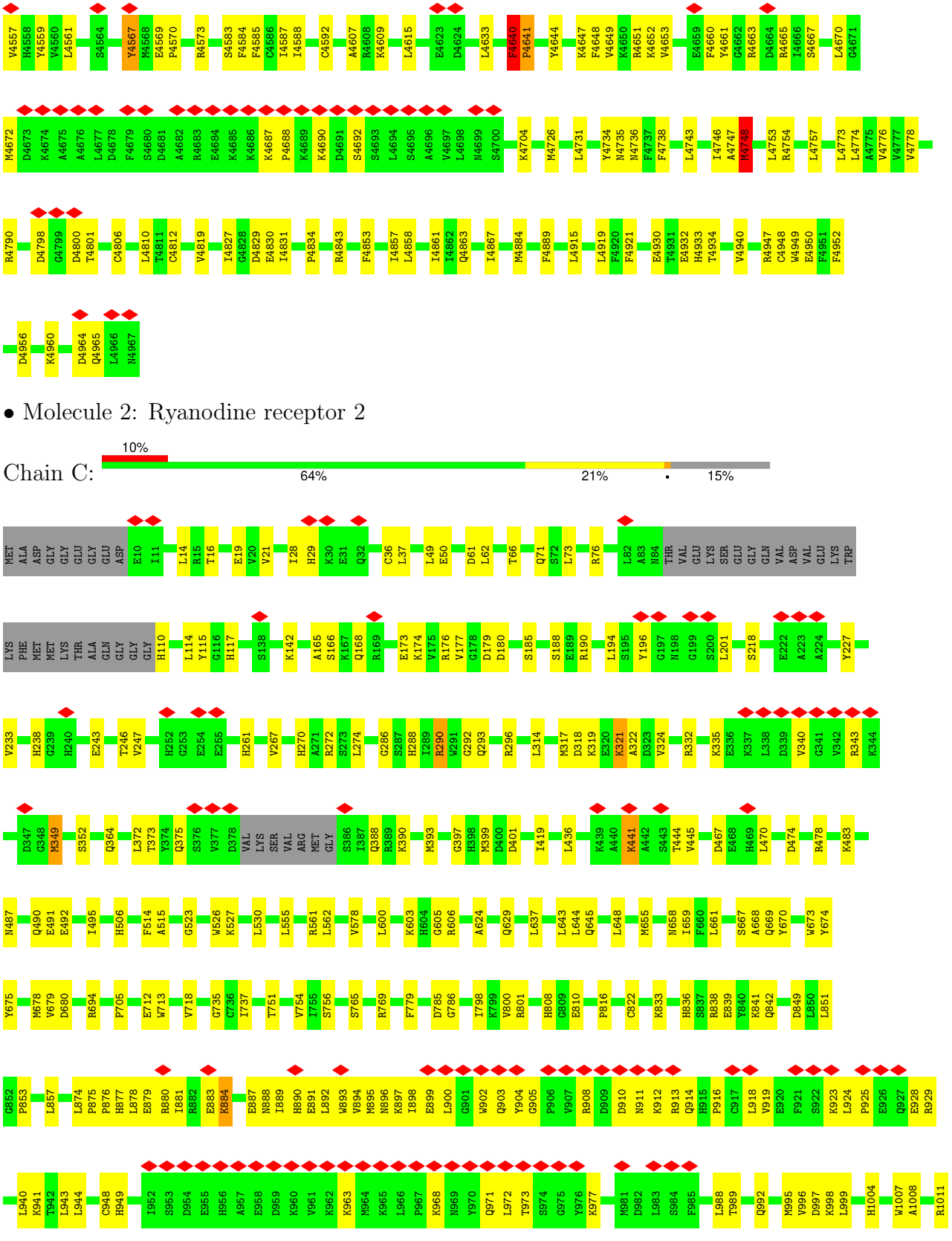
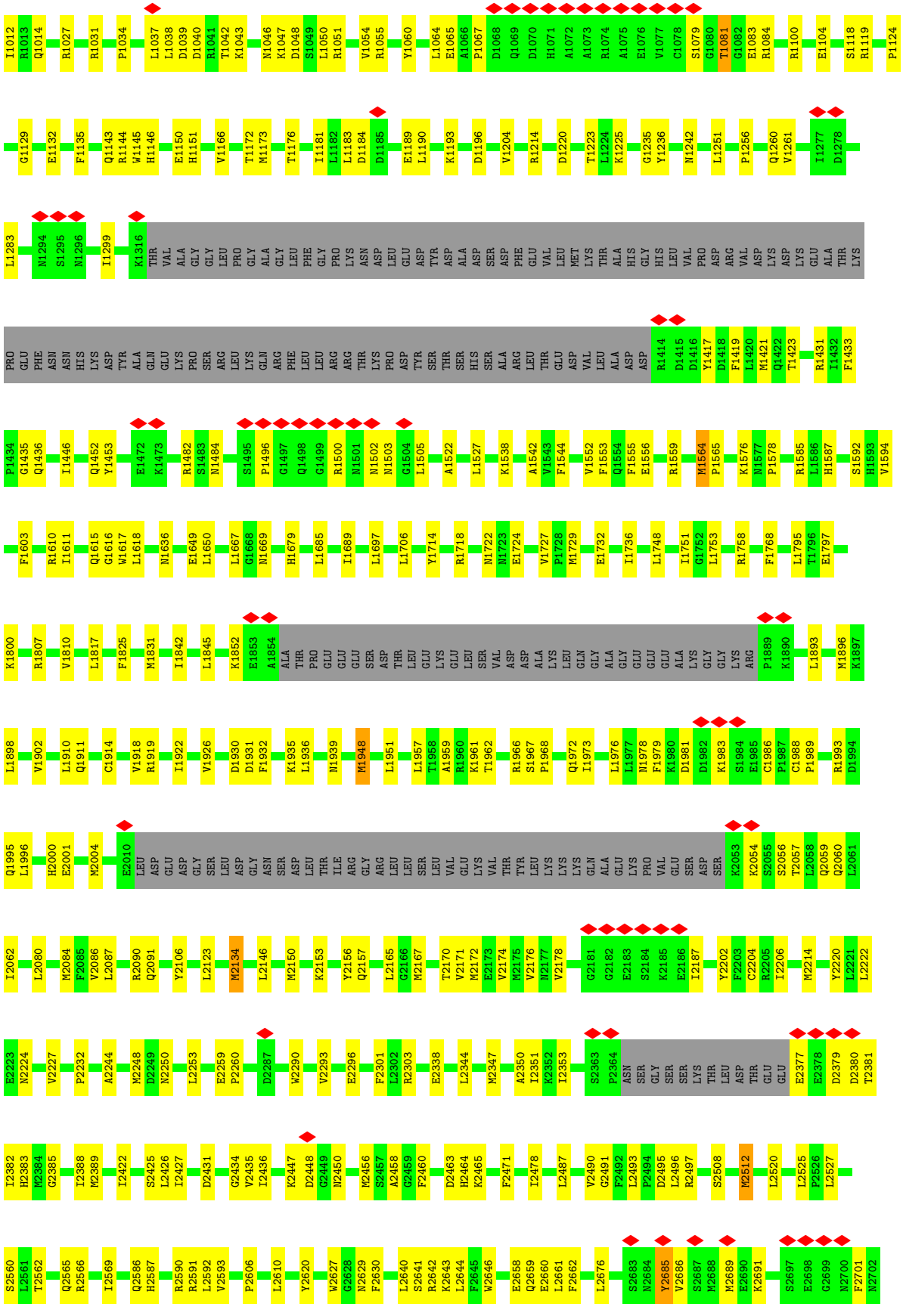
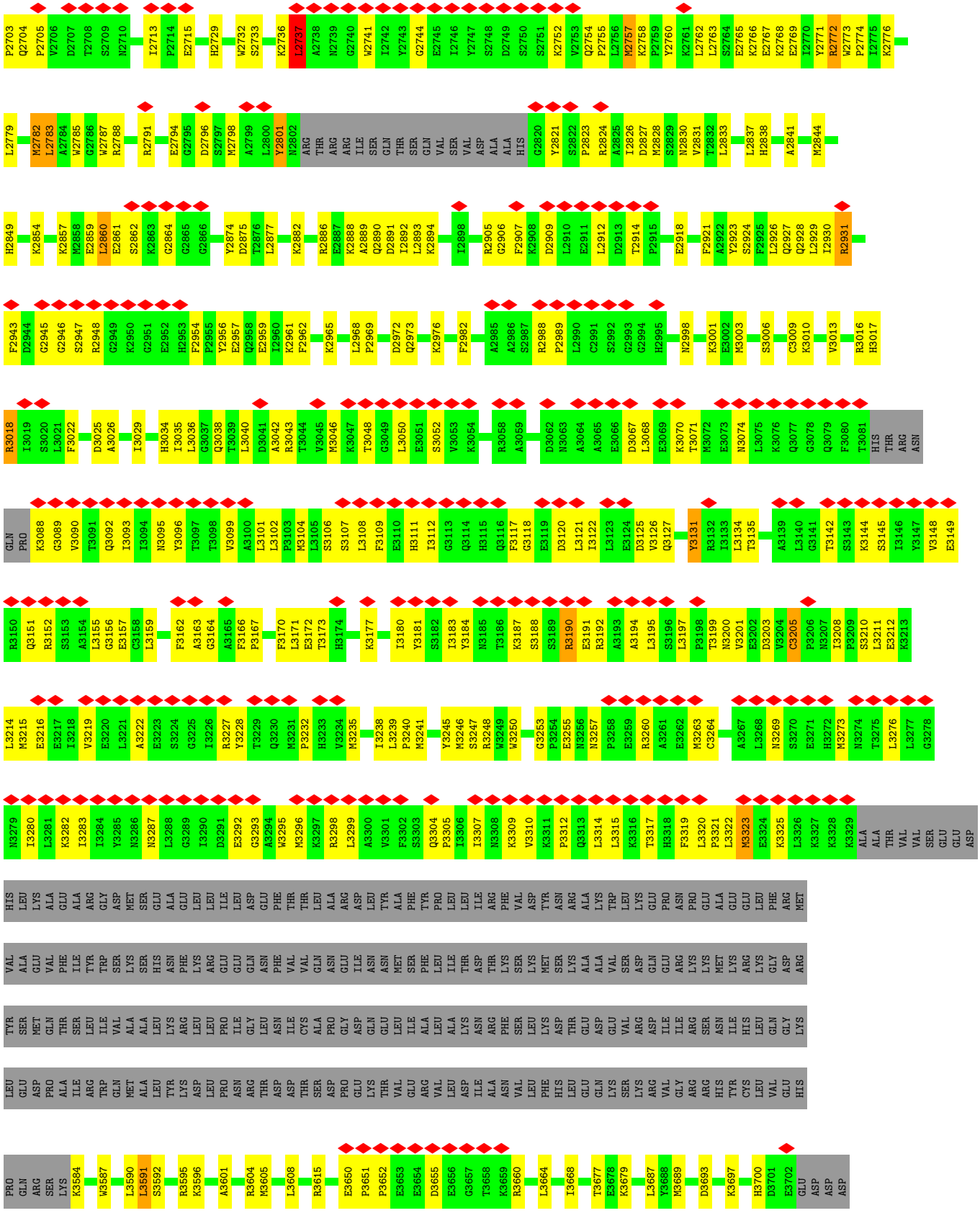
N4075 E4076 T4077 L4078 D4079 Y4080 E4081 E4082 F4083 V4084 K4085 R4086 D4093 I4094 E4107 Q4116 T4117 F4118 L4119 E4120 L4121 A4122 E4123 Y4128 F4129 Q4130 P4131 E4137 R4147 V4148 Y4149 E4154 S4155 T4158 Q4159 K4166 K4169 R4170 N4178 E4179 G4180 G4181 E4182 K4183 E4184 E4187 T4196
M4200 E4208 S4209 ASP LEU ASN GLU ARG SER ALA ASN LYS GLU GLU SER GLU GLU LYS GLU ARG PRO GLU GLU GLU GLN GLY PRO PRO ARG MET ALA PHE PHE S4237 I4238 L4239 T4240 V4241 R4242 R4249 R4257 M4258 L4259 S4260 L4261 K4262 S4263 L4264 K4265 K4266 Q4267 M4268 K4269 K4270 V4271 K4272 K4273 M4274 T4275
V4276 K4277 D4278 M4279 V4280 Y4287 I4290 F4302 F4306 R4307 I4308 I4309 C4310 SER LEU LEU LEU LEU GLY GLY SER LEU VAL GLU GLY ALA LYS LYS ILE LYS VAL ALA GLU LEU LEU ALA ASN MET PRO ASP PRO THR GLN ASP GLU VAL ARG GLY ASP GLY GLU GLU GLY GLU ARG LYS PRO
LEU GLU ALA LEU PRO SER GLU ASP LEU THR ASP LEU LYS GLU LEU THR GLU GLU SER ASP LEU LEU SER ASP ILE PHE GLY LEU ASP LEU LYS ARG GLU GLY GLY GLN TYR LYS LEU LEU PRO HIS ASN PRO ASN ALA GLY LEU SER ASP LEU LEU MET SER ASN PRO VAL PRO MET PRO
GLU VAL GLN GLU LYS PHE GLN GLU GLN LYS ALA LYS GLU LYS GLU GLU LYS GLU LYS GLU GLU THR LYS SER GLU PRO GLU LYS ALA GLU GLY GLU LYS GLU GLU LYS ALA LYS GLU ASP LYS GLY LYS GLN LYS LEU ARG GLN LEU HIS THR HIS ARG TYR GLY GLU PRO
GLU VAL PRO GLU SER ALA F4480 W4481 K4482 K4483 I4484 I4485 L4492 M4502 R4503 M4504 L4507 F4511 L4518 F4519 Y4520 T4524 SER SER VAL VAL GLU GLY LYS GLU LEU PRO THR ARG SER SER SER GLU ASN ALA LYS VAL THR SER LEU ASP SER SER HIS ARG ILE I4555 A4556



• Molecule 2: Ryanodine receptor 2

Chain C:

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L2779 M2782 L2783 A2784 W2785 G2786 W2787 R2788 R2791 E2794 G2795 D2796 S2797 M2798 A2799 L2800 Y2801 N2802 ARG THR ARG ARG ILE SER GLN THR SER GLN VAL SER VAL ASP ALA ALA HIS G2820 Y2821 S2822 P2823 R2824 A2825 I2826 D2827 M2828 S2829 N2830 V2831 T2832 L2833 L2837 H2838 A2841 M2844
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R3150 Q3151 R3152 S3153 A3154 L3155 G3156 E3157 G3158 L3159 F3162 A3163 G3164 A3165 F3166 P3167 F3170 L3171 E3172 T3173 H3174 K3177 I3180 Y3181 S3182 I3183 Y3184 N3185 T3186 K3187 S3188 S3189 R3190 E3191 R3192 A3193 A3194 L3195 S3196 L3197 P3198 T3199 N3200 V3201 E3202 D3203 V3204 C3205 P3206 N3207 I3208 P3209 S3210 L3211 E3212 K3213
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HIS LEU LYS ALA GLU ALA ARG GLY ASP MET SER GLU ALA GLU LEU LEU ILE LEU ASP GLU PHE THR THR LEU ALA ARG ASP LEU TYR ALA PHE TYR PRO LEU LEU ILE ARG PHE VAL ASP TYR ASN ARG ALA ALA LYS TRP LEU LYS GLU PRO ASN ARG PRO GLU ALA LYS LEU GLU LEU PHE ARG MET
VAL ALA GLU VAL PHE ILE TYR TRP SER LYS SER HIS ASN PHE LYS ARG GLU LEU GLN ASN PHE VAL VAL GLN ASN ARG ILE ASN ASN MET SER PHE LEU ILE THR ASP THR LYS SER LYS MET SER LYS ALA ALA VAL SER ASP GLN GLU ARG LYS LYS MET LYS ARG LYS GLY ASP ARG
TYR SER MET GLN THR SER LEU ILE VAL ALA ALA LEU LYS ARG LEU LEU PRO ILE GLY LEU ASN ILE CYS ALA PRO GLY ASP GLN GLU LEU ILE ALA LEU ALA LYS ASN ARG PHE SER LEU LYS ASP THR GLU ASP GLU VAL ARG ASP ILE ILE ARG SER ASN ILE HIS LEU GLU GLN LYS SER LYS ARG VAL GLY ARG ARG HIS TYR CYS LEU VAL GLU GLY LYS
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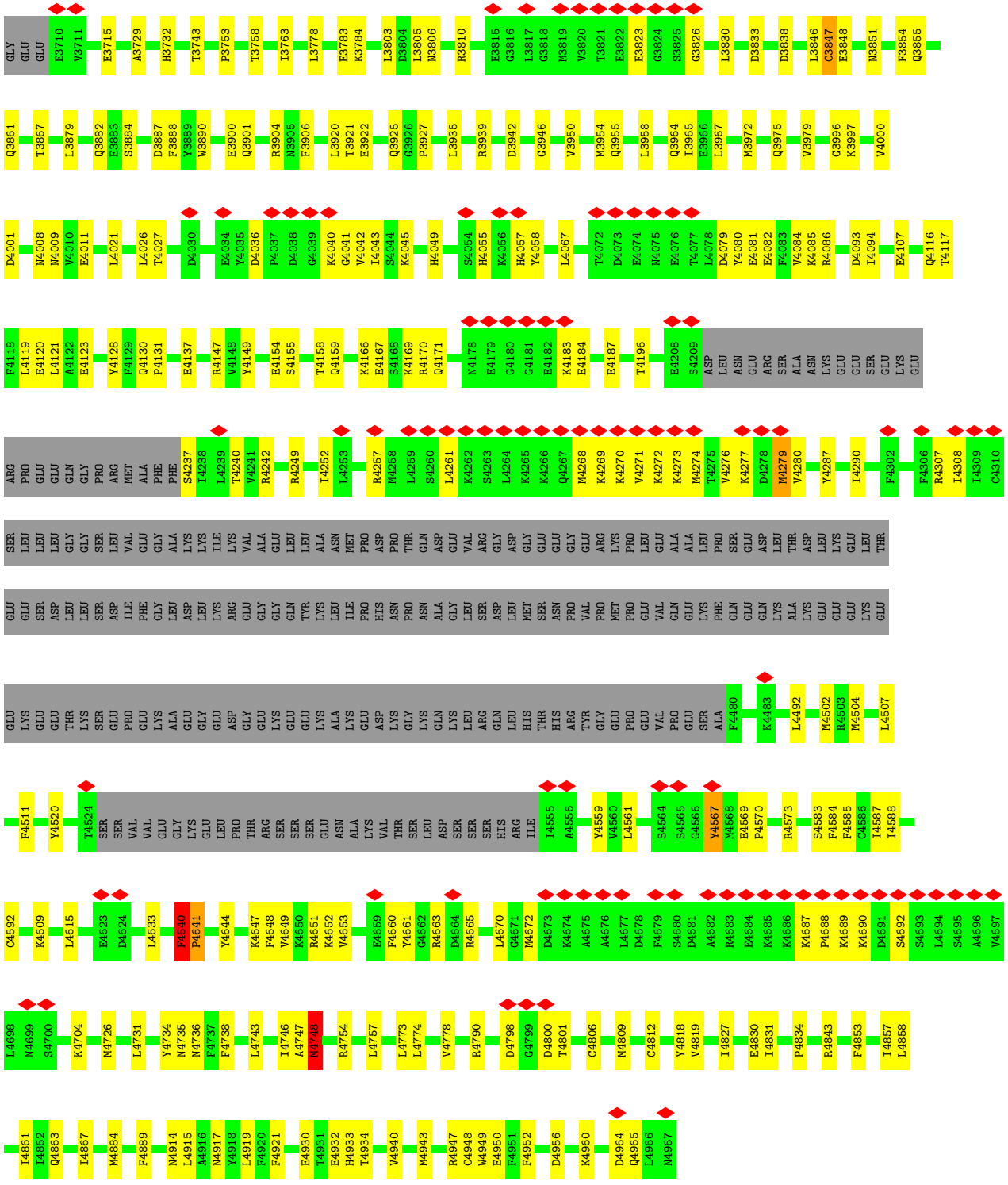
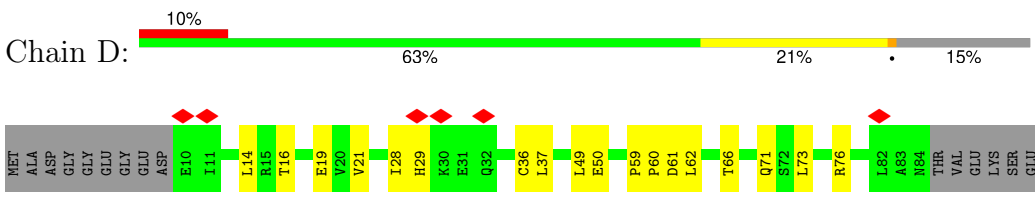
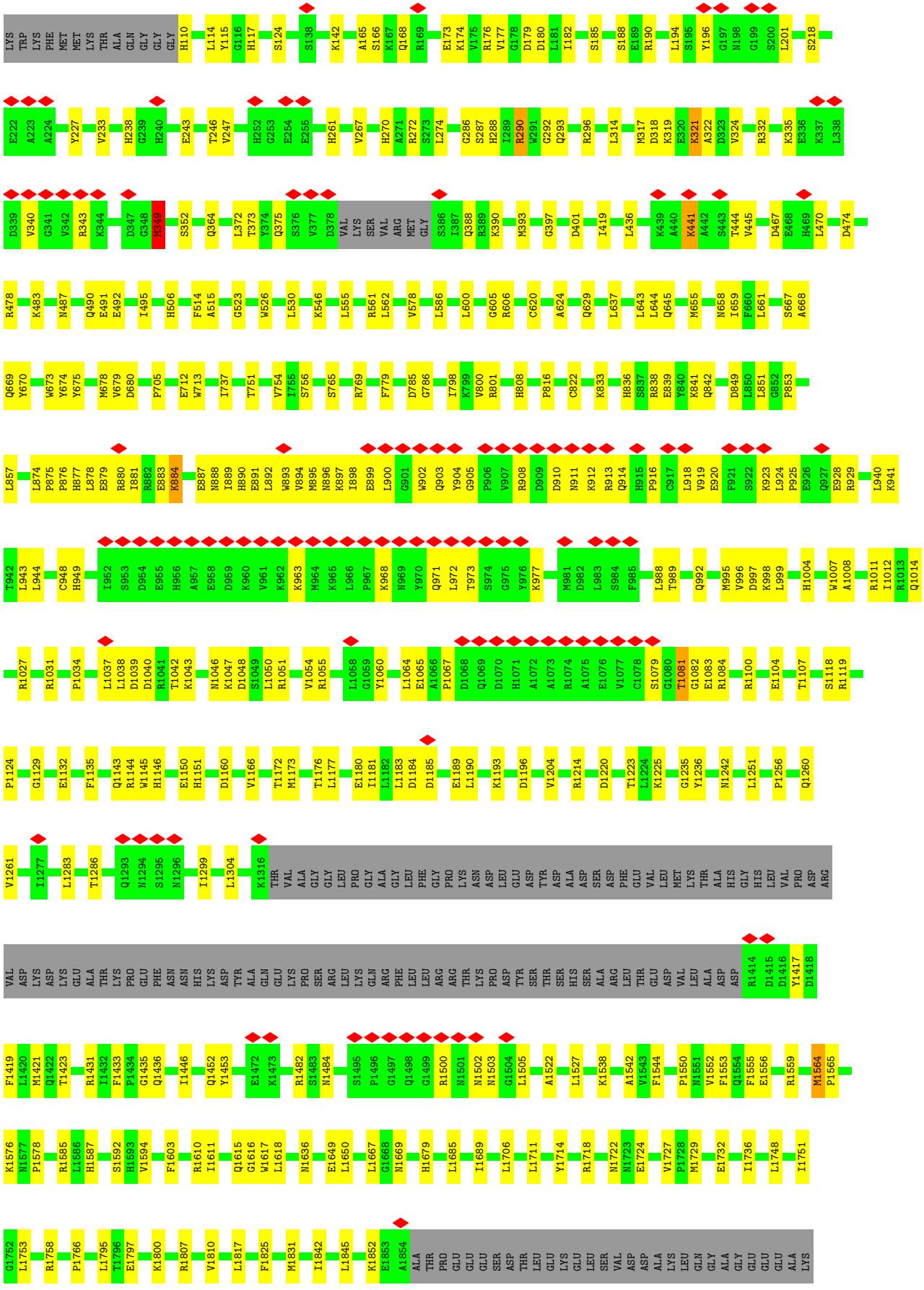


• Molecule 2: Ryanodine receptor 2

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D339 V340 G341 V342 R343 K344 D347 G348 K349 S352 Q364 L372 T373 Y374 Q375 S376 V377 D378 VAL LYS SER VAL ARG MET GLY S386 I387 Q388 R389 K390 M393 G397 D401 I419 L436 K439 A440 K441 A442 S443 T444 V445 D467 E468 H469 L470 D474
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V1261 I1277 L1283 T1286 Q1293 N1294 S1295 N1296 I1299 L1304 K1316 THR VAL ALA GLY GLY LEU PRO GLY ALA GLY LEU PHE GLY PRO LYS ASN ASP LEU GLU ASP TYR ASP ALA ASP SER ASP PHE GLU VAL LEU MET LYS THR ALA HIS GLY HIS LEU VAL PRO ASP ARG
VAL ASP LYS ASP LYS GLU ALA THR LYS PRO GLU PHE ASN ASN HIS LYS ASP TYR ALA GLN GLU LYS PRO SER ARG LEU LYS GLN ARG PHE LEU LEU ARG ARG THR LYS PRO ASP TYR SER THR SER HIS SER ALA ARG LEU THR GLU ASP VAL LEU ALA ASP ASP R1414 D1415 D1416 Y1417 D1418
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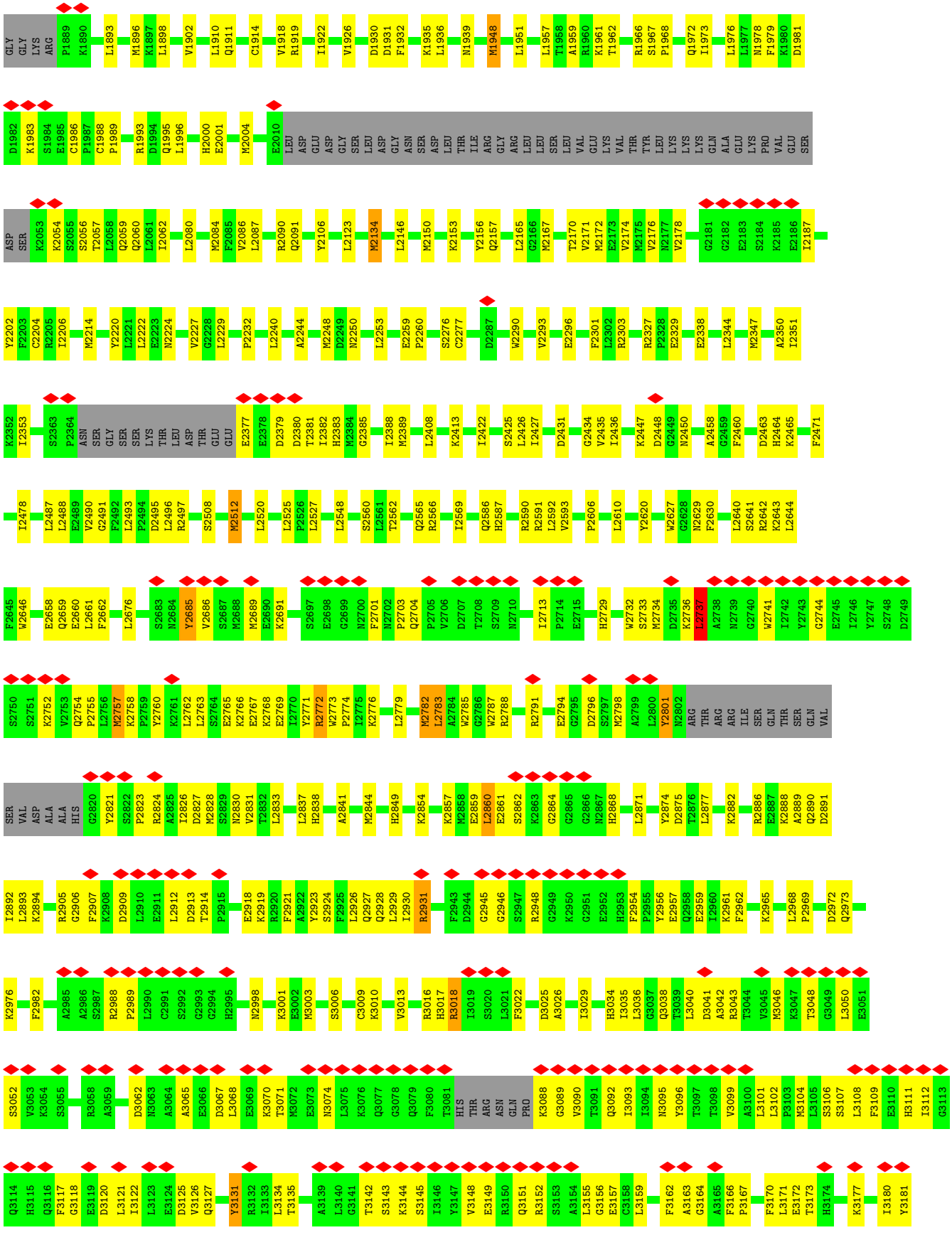
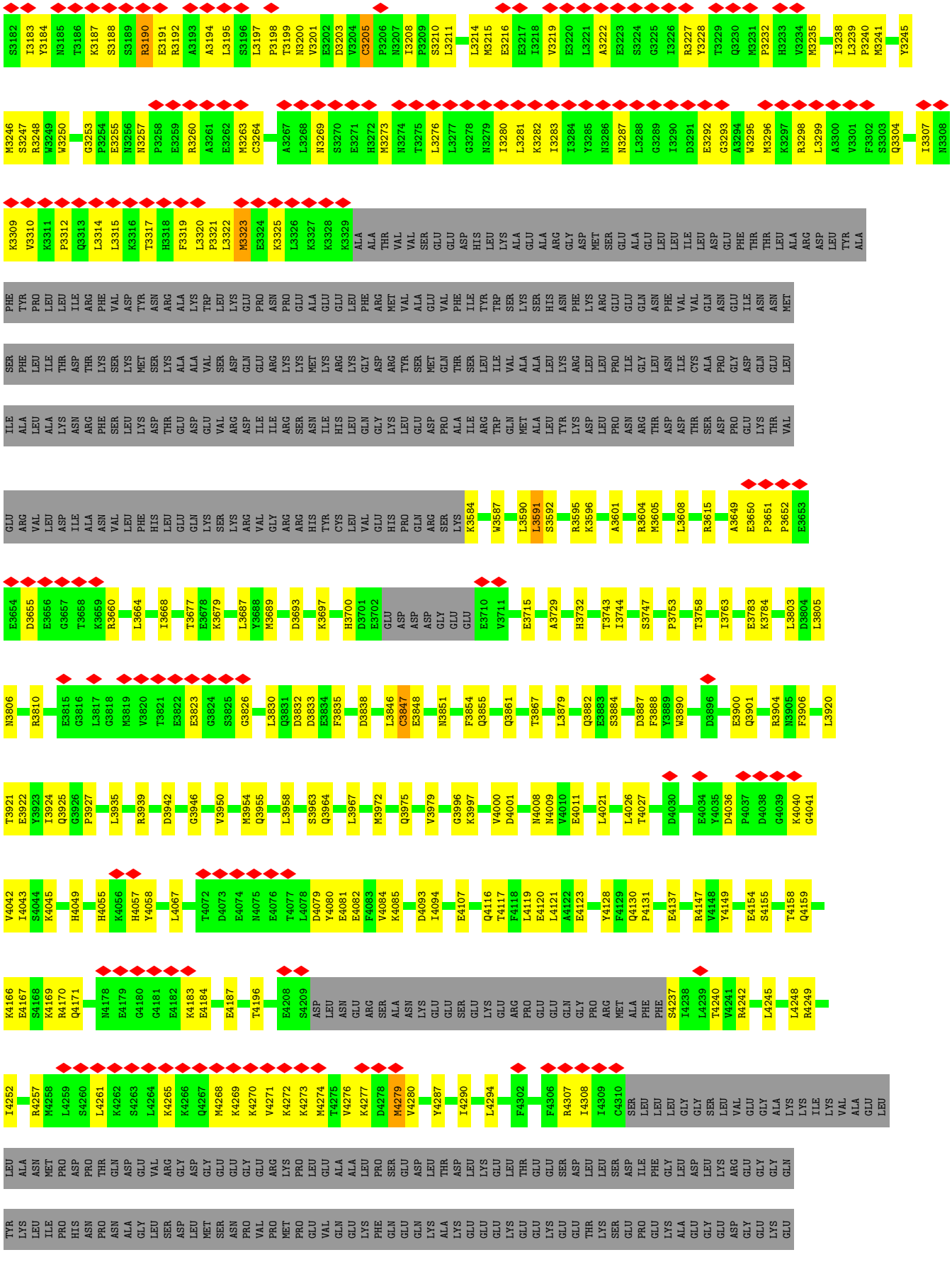
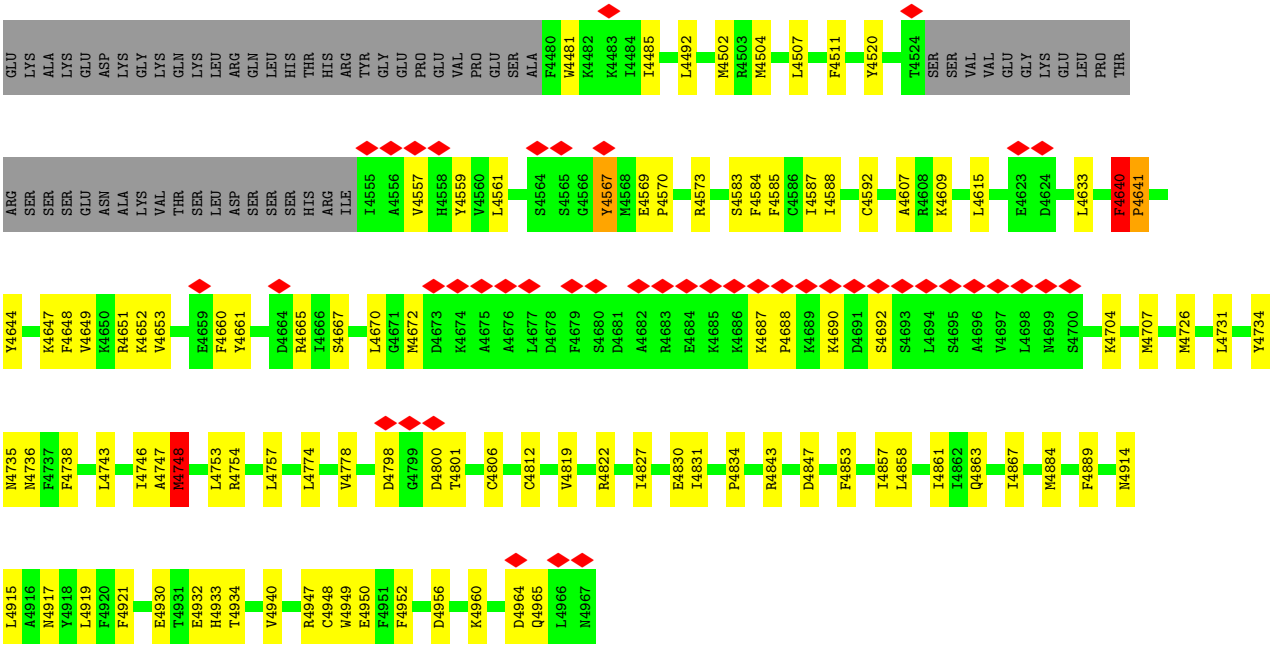
G1752 L1753 R1758 P1766 L1795 T1796 E1797 K1800 R1807 V1810 L1817 F1825 M1831 I1842 L1845 K1852 E1853 A1854 ALA THR PRO GLU GLU GLU SER ASP THR LEU GLU LYS GLU LEU SER VAL ASP ASP ALA LYS LEU GLN GLY ALA GLY GLU GLU GLU ALA LYS







• Molecule 3: Peptidyl-prolyl cis-trans isomerase FKBP1B

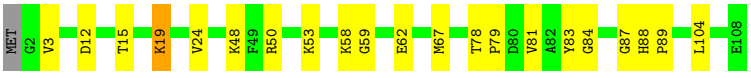
Chain E:

• Molecule 3: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F:

• Molecule 3: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain G:



• Molecule 3: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	49606	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	58	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.594	Depositor
Minimum map value	-0.010	Depositor
Average map value	0.013	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.14	Depositor
Map size (Å)	431.36, 431.36, 431.36	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8425, 0.8425, 0.8425	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	I	0.30	0/1143	0.58	1/1534 (0.1%)
1	J	0.30	0/1143	0.58	1/1534 (0.1%)
1	K	0.30	0/1143	0.58	1/1534 (0.1%)
1	L	0.30	0/1143	0.58	1/1534 (0.1%)
2	A	0.69	7/34594 (0.0%)	0.51	8/46723 (0.0%)
2	B	0.69	7/34594 (0.0%)	0.51	8/46723 (0.0%)
2	C	0.69	7/34594 (0.0%)	0.51	8/46723 (0.0%)
2	D	0.69	7/34594 (0.0%)	0.51	8/46723 (0.0%)
3	E	0.29	0/834	0.54	0/1123
3	F	0.28	0/834	0.53	0/1123
3	G	0.28	0/834	0.54	0/1123
3	H	0.28	0/834	0.54	0/1123
All	All	0.68	28/146284 (0.0%)	0.51	36/197520 (0.0%)

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
2	A	0	2
2	B	0	2
2	C	0	2
2	D	0	2
All	All	0	8

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3205	CYS	CB-SG	105.30	3.61	1.82
2	B	3205	CYS	CB-SG	105.27	3.61	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3205	CYS	CB-SG	105.27	3.61	1.82
2	C	3205	CYS	CB-SG	105.21	3.61	1.82
2	B	3131	TYR	CD2-CE2	29.66	1.83	1.39
2	A	3131	TYR	CD2-CE2	29.65	1.83	1.39
2	D	3131	TYR	CD2-CE2	29.64	1.83	1.39
2	C	3131	TYR	CD2-CE2	29.62	1.83	1.39
2	B	3131	TYR	CD1-CE1	28.64	1.82	1.39
2	C	3131	TYR	CD1-CE1	28.64	1.82	1.39
2	A	3131	TYR	CD1-CE1	28.61	1.82	1.39
2	D	3131	TYR	CD1-CE1	28.58	1.82	1.39
2	B	3131	TYR	CE2-CZ	21.85	1.67	1.38
2	C	3131	TYR	CE2-CZ	21.85	1.67	1.38
2	A	3131	TYR	CE2-CZ	21.80	1.66	1.38
2	D	3131	TYR	CE2-CZ	21.78	1.66	1.38
2	D	3131	TYR	CE1-CZ	21.53	1.66	1.38
2	A	3131	TYR	CE1-CZ	21.49	1.66	1.38
2	B	3131	TYR	CE1-CZ	21.46	1.66	1.38
2	C	3131	TYR	CE1-CZ	21.44	1.66	1.38
2	B	3131	TYR	CG-CD2	16.68	1.60	1.39
2	D	3131	TYR	CG-CD2	16.68	1.60	1.39
2	C	3131	TYR	CG-CD2	16.67	1.60	1.39
2	A	3131	TYR	CG-CD2	16.64	1.60	1.39
2	A	3131	TYR	CG-CD1	16.39	1.60	1.39
2	D	3131	TYR	CG-CD1	16.38	1.60	1.39
2	B	3131	TYR	CG-CD1	16.38	1.60	1.39
2	C	3131	TYR	CG-CD1	16.34	1.60	1.39

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	3205	CYS	CA-CB-SG	12.07	135.73	114.00
2	A	3205	CYS	CA-CB-SG	12.06	135.71	114.00
2	D	3205	CYS	CA-CB-SG	12.05	135.68	114.00
2	B	3205	CYS	CA-CB-SG	12.04	135.68	114.00
2	D	2737	LEU	CA-CB-CG	7.16	131.77	115.30
2	A	2737	LEU	CA-CB-CG	7.16	131.76	115.30
2	C	2737	LEU	CA-CB-CG	7.15	131.75	115.30
2	B	2737	LEU	CA-CB-CG	7.15	131.74	115.30
2	D	2860	LEU	CA-CB-CG	6.15	129.44	115.30
2	B	2860	LEU	CA-CB-CG	6.15	129.44	115.30
2	A	2860	LEU	CA-CB-CG	6.14	129.42	115.30
2	C	2860	LEU	CA-CB-CG	6.12	129.37	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	4567	TYR	CB-CG-CD1	6.09	124.65	121.00
2	A	4567	TYR	CB-CG-CD1	6.05	124.63	121.00
2	C	4567	TYR	CB-CG-CD1	6.04	124.62	121.00
2	B	4567	TYR	CB-CG-CD1	5.97	124.58	121.00
1	J	77	MET	CB-CG-SD	5.78	129.75	112.40
1	I	77	MET	CB-CG-SD	5.78	129.74	112.40
1	L	77	MET	CB-CG-SD	5.78	129.73	112.40
1	K	77	MET	CB-CG-SD	5.78	129.74	112.40
2	D	4640	PHE	C-N-CD	-5.38	108.77	120.60
2	A	4640	PHE	C-N-CD	-5.36	108.80	120.60
2	C	4640	PHE	C-N-CD	-5.36	108.81	120.60
2	B	4640	PHE	C-N-CD	-5.35	108.83	120.60
2	B	4748	MET	CB-CG-SD	5.34	128.43	112.40
2	C	4748	MET	CB-CG-SD	5.33	128.39	112.40
2	A	4748	MET	CB-CG-SD	5.33	128.38	112.40
2	D	4748	MET	CB-CG-SD	5.32	128.35	112.40
2	B	4567	TYR	CA-CB-CG	5.13	123.15	113.40
2	C	4567	TYR	CA-CB-CG	5.13	123.14	113.40
2	A	4567	TYR	CA-CB-CG	5.12	123.13	113.40
2	D	4567	TYR	CA-CB-CG	5.12	123.13	113.40
2	C	349	MET	CB-CG-SD	5.09	127.67	112.40
2	D	349	MET	CB-CG-SD	5.09	127.68	112.40
2	A	349	MET	CB-CG-SD	5.08	127.65	112.40
2	B	349	MET	CB-CG-SD	5.08	127.63	112.40

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	2801	TYR	Peptide
2	A	4640	PHE	Peptide
2	B	2801	TYR	Peptide
2	B	4640	PHE	Peptide
2	C	2801	TYR	Peptide
2	C	4640	PHE	Peptide
2	D	2801	TYR	Peptide
2	D	4640	PHE	Peptide

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	I	1131	0	1058	50	0
1	J	1131	0	1058	45	0
1	K	1131	0	1058	47	0
1	L	1131	0	1058	46	0
2	A	33849	0	33549	793	0
2	B	33849	0	33549	790	0
2	C	33849	0	33549	767	0
2	D	33849	0	33549	795	0
3	E	818	0	821	11	0
3	F	818	0	821	11	0
3	G	818	0	821	13	0
3	H	818	0	821	11	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
4	I	4	0	0	0	0
4	J	4	0	0	0	0
4	K	4	0	0	0	0
4	L	4	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	62	0	24	1	0
6	B	62	0	24	1	0
6	C	62	0	24	1	0
6	D	62	0	24	1	0
All	All	143464	0	141808	3297	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 12.

All (3297) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3131:TYR:CD1	2:D:3131:TYR:CE1	1.82	1.68
2:A:3131:TYR:CD1	2:A:3131:TYR:CE1	1.82	1.63
2:C:3131:TYR:CD2	2:C:3131:TYR:CE2	1.83	1.61
2:C:3131:TYR:CE1	2:C:3131:TYR:CD1	1.82	1.61
2:D:3131:TYR:CE2	2:D:3131:TYR:CD2	1.83	1.61
2:B:3131:TYR:CD2	2:B:3131:TYR:CE2	1.83	1.58
2:B:3131:TYR:CD1	2:B:3131:TYR:CE1	1.82	1.58
2:A:3131:TYR:CE2	2:A:3131:TYR:CD2	1.83	1.58
1:J:127:ARG:NH1	1:J:135:GLY:CA	1.70	1.53
1:K:127:ARG:NH1	1:K:135:GLY:CA	1.70	1.53
1:L:127:ARG:NH1	1:L:135:GLY:CA	1.70	1.50
1:I:127:ARG:NH1	1:I:135:GLY:CA	1.70	1.48
2:A:3131:TYR:CZ	2:A:3205:CYS:SG	2.37	1.17
2:B:3131:TYR:CZ	2:B:3205:CYS:SG	2.37	1.17
2:C:3131:TYR:CZ	2:C:3205:CYS:SG	2.37	1.17
2:A:3131:TYR:CE2	2:A:3205:CYS:SG	2.38	1.17
2:B:3131:TYR:CE2	2:B:3205:CYS:SG	2.38	1.17
2:C:3131:TYR:CE2	2:C:3205:CYS:SG	2.38	1.17
2:D:3131:TYR:CE2	2:D:3205:CYS:SG	2.38	1.17
2:D:3131:TYR:CZ	2:D:3205:CYS:SG	2.37	1.17
2:A:3848:GLU:OE1	2:A:3922:GLU:CD	1.87	1.13
2:B:3131:TYR:CE1	2:B:3205:CYS:SG	2.42	1.13
2:C:3848:GLU:OE1	2:C:3922:GLU:CD	1.87	1.12
2:A:3131:TYR:CE1	2:A:3205:CYS:SG	2.42	1.12
2:C:3131:TYR:CE1	2:C:3205:CYS:SG	2.42	1.11
2:D:3131:TYR:CE1	2:D:3205:CYS:SG	2.42	1.11
2:A:3131:TYR:CD2	2:A:3205:CYS:SG	2.44	1.11
2:B:3131:TYR:CD2	2:B:3205:CYS:SG	2.43	1.11
2:B:3848:GLU:OE1	2:B:3922:GLU:CD	1.87	1.11
2:D:3848:GLU:OE1	2:D:3922:GLU:CD	1.87	1.11
2:C:3131:TYR:CD2	2:C:3205:CYS:SG	2.43	1.11
2:D:3131:TYR:CD2	2:D:3205:CYS:SG	2.44	1.10
2:C:3131:TYR:CD1	2:C:3205:CYS:SG	2.46	1.09
2:D:3131:TYR:CD1	2:D:3205:CYS:SG	2.46	1.09
2:A:3131:TYR:CD1	2:A:3205:CYS:SG	2.46	1.08
2:B:3131:TYR:CD1	2:B:3205:CYS:SG	2.46	1.08
1:L:127:ARG:NH1	1:L:135:GLY:HA2	0.74	1.07
1:I:127:ARG:NH1	1:I:135:GLY:HA2	0.74	1.07
1:J:127:ARG:NH1	1:J:135:GLY:HA2	0.74	1.06
1:K:127:ARG:NH1	1:K:135:GLY:HA2	0.74	1.06
1:K:127:ARG:CZ	1:K:135:GLY:HA2	1.88	1.03
1:J:127:ARG:CZ	1:J:135:GLY:HA2	1.88	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:127:ARG:CZ	1:I:135:GLY:HA2	1.88	1.02
1:L:127:ARG:CZ	1:L:135:GLY:HA2	1.88	1.01
2:C:3131:TYR:CG	2:C:3205:CYS:SG	2.53	1.01
2:B:3131:TYR:CG	2:B:3205:CYS:SG	2.53	1.01
2:D:3131:TYR:CG	2:D:3205:CYS:SG	2.53	1.01
2:A:3131:TYR:CG	2:A:3205:CYS:SG	2.53	1.01
2:C:3131:TYR:CZ	2:C:3205:CYS:CB	2.51	0.94
2:A:3131:TYR:CZ	2:A:3205:CYS:CB	2.51	0.94
2:A:3131:TYR:CE1	2:A:3205:CYS:CB	2.51	0.94
2:B:3131:TYR:CE1	2:B:3205:CYS:CB	2.51	0.94
2:C:3131:TYR:CE2	2:C:3205:CYS:CB	2.51	0.93
2:D:3131:TYR:CE1	2:D:3205:CYS:CB	2.51	0.93
2:A:3131:TYR:CE2	2:A:3205:CYS:CB	2.51	0.93
2:B:3131:TYR:CZ	2:B:3205:CYS:CB	2.51	0.93
2:D:3131:TYR:CE2	2:D:3205:CYS:CB	2.51	0.93
1:I:127:ARG:HH11	1:I:135:GLY:HA2	1.27	0.93
2:D:3131:TYR:CZ	2:D:3205:CYS:CB	2.51	0.93
1:K:127:ARG:HH11	1:K:135:GLY:HA2	1.27	0.93
2:C:3131:TYR:CD2	2:C:3205:CYS:CB	2.52	0.93
2:C:3131:TYR:CE1	2:C:3205:CYS:CB	2.51	0.93
2:A:3131:TYR:CD2	2:A:3205:CYS:CB	2.52	0.92
2:B:3131:TYR:CE2	2:B:3205:CYS:CB	2.51	0.92
1:J:127:ARG:HH11	1:J:135:GLY:HA2	1.27	0.92
2:B:3131:TYR:CD2	2:B:3205:CYS:CB	2.52	0.92
2:D:3131:TYR:CD2	2:D:3205:CYS:CB	2.52	0.91
2:B:3131:TYR:CD1	2:B:3205:CYS:CB	2.54	0.91
2:C:3131:TYR:CD1	2:C:3205:CYS:CB	2.54	0.91
2:A:3131:TYR:CD1	2:A:3205:CYS:CB	2.54	0.90
2:D:3131:TYR:CD1	2:D:3205:CYS:CB	2.54	0.90
1:L:127:ARG:HH11	1:L:135:GLY:HA2	1.27	0.90
2:C:3131:TYR:CG	2:C:3205:CYS:CB	2.56	0.89
2:D:3131:TYR:CG	2:D:3205:CYS:CB	2.56	0.89
2:B:3131:TYR:CG	2:B:3205:CYS:CB	2.56	0.89
2:C:4834:PRO:HB3	2:C:4843:ARG:HD3	1.55	0.88
2:A:3131:TYR:CG	2:A:3205:CYS:CB	2.56	0.88
2:A:4834:PRO:HB3	2:A:4843:ARG:HD3	1.55	0.88
2:D:4834:PRO:HB3	2:D:4843:ARG:HD3	1.55	0.86
2:B:4834:PRO:HB3	2:B:4843:ARG:HD3	1.55	0.85
2:C:2425:SER:O	2:D:142:LYS:NZ	2.08	0.85
2:A:142:LYS:NZ	2:D:2425:SER:O	2.11	0.84
2:D:2512:MET:HA	2:D:2512:MET:HE2	1.60	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2788:ARG:NH1	2:B:2905:ARG:O	2.12	0.83
2:A:2788:ARG:NH1	2:A:2905:ARG:O	2.12	0.82
2:A:888:ASN:ND2	2:A:1060:TYR:OH	2.13	0.82
2:C:2788:ARG:NH1	2:C:2905:ARG:O	2.12	0.82
2:D:888:ASN:ND2	2:D:1060:TYR:OH	2.13	0.82
2:D:2788:ARG:NH1	2:D:2905:ARG:O	2.12	0.81
2:C:888:ASN:ND2	2:C:1060:TYR:OH	2.13	0.81
2:C:3890:TRP:HB3	2:D:76:ARG:HG2	1.61	0.81
2:D:2773:TRP:HE3	2:D:2776:LYS:HZ3	1.27	0.81
2:B:888:ASN:ND2	2:B:1060:TYR:OH	2.13	0.80
2:C:1559:ARG:HD2	2:C:1565:PRO:HD3	1.64	0.80
2:B:1559:ARG:HD2	2:B:1565:PRO:HD3	1.64	0.80
2:B:2773:TRP:HE3	2:B:2776:LYS:HZ3	1.28	0.79
2:C:2773:TRP:HE3	2:C:2776:LYS:HZ3	1.27	0.79
2:A:76:ARG:HG2	2:D:3890:TRP:HB3	1.64	0.79
2:A:2773:TRP:HE3	2:A:2776:LYS:HZ3	1.28	0.79
2:D:1559:ARG:HD2	2:D:1565:PRO:HD3	1.64	0.78
2:A:1559:ARG:HD2	2:A:1565:PRO:HD3	1.64	0.78
2:B:3183:ILE:HG23	2:B:3184:TYR:HD1	1.49	0.78
3:G:12:ASP:OD2	3:G:15:THR:OG1	2.03	0.77
2:A:3183:ILE:HG23	2:A:3184:TYR:HD1	1.49	0.77
2:C:3183:ILE:HG23	2:C:3184:TYR:HD1	1.49	0.77
2:C:3122:ILE:HD11	2:C:3167:PRO:HD3	1.67	0.77
2:D:3122:ILE:HD11	2:D:3167:PRO:HD3	1.67	0.77
2:D:3183:ILE:HG23	2:D:3184:TYR:HD1	1.49	0.76
3:E:12:ASP:OD2	3:E:15:THR:OG1	2.03	0.76
3:H:12:ASP:OD2	3:H:15:THR:OG1	2.03	0.76
2:A:2512:MET:HE2	2:A:2512:MET:HA	1.68	0.76
2:C:3783:GLU:OE1	2:C:3784:LYS:NZ	2.18	0.76
2:B:2957:GLU:OE1	2:B:2961:LYS:NZ	2.18	0.76
2:B:3122:ILE:HD11	2:B:3167:PRO:HD3	1.67	0.76
3:F:12:ASP:OD2	3:F:15:THR:OG1	2.02	0.76
2:B:2923:TYR:O	2:B:2927:GLN:NE2	2.19	0.76
2:C:2512:MET:HE2	2:C:2512:MET:HA	1.67	0.76
2:C:2923:TYR:O	2:C:2927:GLN:NE2	2.19	0.76
2:D:2923:TYR:O	2:D:2927:GLN:NE2	2.19	0.75
2:A:2923:TYR:O	2:A:2927:GLN:NE2	2.19	0.75
2:A:3122:ILE:HD11	2:A:3167:PRO:HD3	1.67	0.75
2:B:3050:LEU:HD23	2:B:3052:SER:H	1.51	0.75
2:D:3050:LEU:HD23	2:D:3052:SER:H	1.51	0.75
2:C:3050:LEU:HD23	2:C:3052:SER:H	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2957:GLU:OE1	2:A:2961:LYS:NZ	2.18	0.74
2:A:3222:ALA:O	2:A:3282:LYS:NZ	2.20	0.74
2:B:3783:GLU:OE1	2:B:3784:LYS:NZ	2.18	0.74
2:C:4237:SER:N	2:C:4240:THR:HG1	1.85	0.74
2:A:3050:LEU:HD23	2:A:3052:SER:H	1.51	0.74
2:B:4641:PRO:HB3	2:B:4644:TYR:HB3	1.69	0.74
2:C:4641:PRO:HB3	2:C:4644:TYR:HB3	1.69	0.74
2:D:2957:GLU:OE1	2:D:2961:LYS:NZ	2.18	0.74
2:D:3222:ALA:O	2:D:3282:LYS:NZ	2.20	0.74
2:D:4641:PRO:HB3	2:D:4644:TYR:HB3	1.69	0.74
2:C:2957:GLU:OE1	2:C:2961:LYS:NZ	2.18	0.73
2:B:2512:MET:HE2	2:B:2512:MET:HA	1.68	0.73
2:A:4641:PRO:HB3	2:A:4644:TYR:HB3	1.69	0.73
1:K:117:LEU:HD22	1:K:122:VAL:HG23	1.71	0.73
2:C:3131:TYR:CG	2:C:3205:CYS:HB3	2.23	0.73
1:K:72:MET:HA	1:K:75:ARG:HG2	1.71	0.72
2:D:3131:TYR:CG	2:D:3205:CYS:HB3	2.24	0.72
2:D:1079:SER:OG	2:D:1084:ARG:NH2	2.22	0.72
2:A:3131:TYR:CG	2:A:3205:CYS:HB3	2.23	0.72
2:C:2830:ASN:HB3	2:D:1435:GLY:HA3	1.71	0.72
2:C:3067:ASP:HA	2:C:3070:LYS:HZ3	1.55	0.72
2:C:1079:SER:OG	2:C:1084:ARG:NH2	2.22	0.72
1:L:117:LEU:HD22	1:L:122:VAL:HG23	1.71	0.72
2:B:1079:SER:OG	2:B:1084:ARG:NH2	2.22	0.72
2:C:3222:ALA:O	2:C:3282:LYS:NZ	2.20	0.72
1:J:117:LEU:HD22	1:J:122:VAL:HG23	1.71	0.72
1:L:72:MET:HA	1:L:75:ARG:HG2	1.71	0.72
1:K:137:VAL:HG13	1:K:141:GLU:HB2	1.72	0.71
2:D:3184:TYR:HB3	2:D:3192:ARG:HH21	1.55	0.71
2:A:3783:GLU:OE1	2:A:3784:LYS:NZ	2.18	0.71
2:B:3131:TYR:CG	2:B:3205:CYS:HB3	2.23	0.71
2:D:3131:TYR:CE1	2:D:3205:CYS:HB2	2.25	0.71
2:D:3247:SER:HA	2:D:3250:TRP:HD1	1.56	0.71
2:A:1079:SER:OG	2:A:1084:ARG:NH2	2.22	0.71
2:A:2703:PRO:O	2:A:2854:LYS:NZ	2.23	0.71
1:J:137:VAL:HG13	1:J:141:GLU:HB2	1.72	0.71
2:B:3067:ASP:HA	2:B:3070:LYS:HZ3	1.56	0.71
2:B:3131:TYR:CE1	2:B:3205:CYS:HB2	2.25	0.71
2:D:2703:PRO:O	2:D:2854:LYS:NZ	2.23	0.71
1:J:72:MET:HA	1:J:75:ARG:HG2	1.71	0.71
2:A:3184:TYR:HB3	2:A:3192:ARG:HH21	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:137:VAL:HG13	1:I:141:GLU:HB2	1.72	0.70
2:A:3247:SER:HA	2:A:3250:TRP:HD1	1.56	0.70
2:C:3184:TYR:HB3	2:C:3192:ARG:HH21	1.55	0.70
2:B:188:SER:HB2	2:B:190:ARG:HH11	1.56	0.70
1:I:117:LEU:HD22	1:I:122:VAL:HG23	1.71	0.70
2:C:3247:SER:HA	2:C:3250:TRP:HD1	1.56	0.70
2:A:3131:TYR:CE1	2:A:3205:CYS:HB2	2.25	0.70
2:B:2703:PRO:O	2:B:2854:LYS:NZ	2.23	0.70
1:I:72:MET:HA	1:I:75:ARG:HG2	1.71	0.70
2:B:3222:ALA:O	2:B:3282:LYS:NZ	2.20	0.70
2:B:3247:SER:HA	2:B:3250:TRP:HD1	1.56	0.70
2:A:2998:ASN:ND2	2:A:3048:THR:OG1	2.25	0.70
2:C:3131:TYR:CE1	2:C:3205:CYS:HB2	2.25	0.70
2:A:188:SER:HB2	2:A:190:ARG:HH11	1.57	0.70
1:L:137:VAL:HG13	1:L:141:GLU:HB2	1.72	0.69
2:B:875:PRO:HD2	2:B:878:LEU:HD12	1.74	0.69
2:C:188:SER:HB2	2:C:190:ARG:HH11	1.57	0.69
2:D:2389:MET:HE1	2:D:2460:PHE:HA	1.74	0.69
2:D:2998:ASN:ND2	2:D:3048:THR:OG1	2.25	0.69
2:B:2998:ASN:ND2	2:B:3048:THR:OG1	2.25	0.69
2:B:3184:TYR:HB3	2:B:3192:ARG:HH21	1.55	0.69
2:C:2703:PRO:O	2:C:2854:LYS:NZ	2.23	0.69
2:D:4237:SER:N	2:D:4240:THR:HG1	1.90	0.69
2:C:2998:ASN:ND2	2:C:3048:THR:OG1	2.25	0.69
2:D:188:SER:HB2	2:D:190:ARG:HH11	1.57	0.69
2:D:3067:ASP:HA	2:D:3070:LYS:HZ3	1.57	0.69
2:D:4687:LYS:HD2	2:D:4688:PRO:HD2	1.75	0.69
2:C:288:HIS:O	2:C:290:ARG:NH1	2.26	0.69
2:D:3783:GLU:OE1	2:D:3784:LYS:NZ	2.18	0.69
2:D:875:PRO:HD2	2:D:878:LEU:HD12	1.74	0.68
2:D:4747:ALA:HB1	2:D:4757:LEU:HD11	1.75	0.68
2:B:4687:LYS:HD2	2:B:4688:PRO:HD2	1.75	0.68
2:C:875:PRO:HD2	2:C:878:LEU:HD12	1.74	0.68
2:C:4687:LYS:HD2	2:C:4688:PRO:HD2	1.75	0.68
2:A:3067:ASP:HA	2:A:3070:LYS:HZ2	1.58	0.68
2:C:988:LEU:HD13	2:C:1055:ARG:HE	1.59	0.68
2:C:2389:MET:HE1	2:C:2460:PHE:HA	1.76	0.68
2:A:4687:LYS:HD2	2:A:4688:PRO:HD2	1.75	0.68
2:B:988:LEU:HD13	2:B:1055:ARG:HE	1.59	0.68
2:A:288:HIS:O	2:A:290:ARG:NH1	2.26	0.68
2:B:2389:MET:HE1	2:B:2460:PHE:HA	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:4747:ALA:HB1	2:C:4757:LEU:HD11	1.75	0.68
2:A:875:PRO:HD2	2:A:878:LEU:HD12	1.74	0.67
2:B:679:VAL:HG22	2:B:800:VAL:HG12	1.76	0.67
2:B:3890:TRP:HB3	2:C:76:ARG:HG2	1.76	0.67
2:A:3118:GLY:HA2	2:A:3121:LEU:HB3	1.76	0.67
2:A:1435:GLY:H	2:A:1500:ARG:HH22	1.43	0.67
2:C:4640:PHE:CD2	2:C:4641:PRO:HD3	2.30	0.67
2:D:4640:PHE:CD2	2:D:4641:PRO:HD3	2.30	0.67
2:A:988:LEU:HD13	2:A:1055:ARG:HE	1.59	0.67
2:B:4237:SER:N	2:B:4240:THR:HG1	1.92	0.67
2:C:679:VAL:HG22	2:C:800:VAL:HG12	1.77	0.67
2:C:4831:ILE:HG13	2:C:4843:ARG:HH21	1.59	0.67
1:J:137:VAL:HG21	2:B:3587:TRP:CH2	2.30	0.67
2:B:288:HIS:O	2:B:290:ARG:NH1	2.26	0.67
2:B:897:LYS:HD2	2:B:902:TRP:NE1	2.10	0.67
2:A:4237:SER:N	2:A:4240:THR:HG1	1.92	0.67
2:A:4270:LYS:HA	2:A:4273:LYS:HE2	1.77	0.67
2:A:4640:PHE:CD2	2:A:4641:PRO:HD3	2.30	0.67
2:B:4831:ILE:HG13	2:B:4843:ARG:HH21	1.59	0.67
2:D:988:LEU:HD13	2:D:1055:ARG:HE	1.59	0.67
2:D:3253:GLY:HA2	2:D:3264:CYS:HB3	1.77	0.67
2:A:2389:MET:HE1	2:A:2460:PHE:HA	1.77	0.67
2:A:4747:ALA:HB1	2:A:4757:LEU:HD11	1.75	0.67
2:C:897:LYS:HD2	2:C:902:TRP:NE1	2.10	0.67
2:C:3118:GLY:HA2	2:C:3121:LEU:HB3	1.76	0.67
2:D:4651:ARG:NH2	2:D:4672:MET:SD	2.68	0.67
2:A:3253:GLY:HA2	2:A:3264:CYS:HB3	1.77	0.67
2:B:1435:GLY:H	2:B:1500:ARG:HH22	1.43	0.67
2:B:4747:ALA:HB1	2:B:4757:LEU:HD11	1.75	0.67
2:C:3253:GLY:HA2	2:C:3264:CYS:HB3	1.77	0.67
2:D:288:HIS:O	2:D:290:ARG:NH1	2.26	0.67
2:D:3118:GLY:HA2	2:D:3121:LEU:HB3	1.76	0.67
1:I:101:ILE:N	1:I:137:VAL:O	2.25	0.67
2:A:679:VAL:HG22	2:A:800:VAL:HG12	1.77	0.67
2:A:2760:TYR:HA	2:A:2763:LEU:HD13	1.78	0.67
2:D:897:LYS:HD2	2:D:902:TRP:NE1	2.10	0.67
2:D:1435:GLY:H	2:D:1500:ARG:HH22	1.43	0.67
2:D:3142:THR:O	2:D:3144:LYS:NZ	2.28	0.67
2:A:897:LYS:HD2	2:A:902:TRP:NE1	2.10	0.66
2:C:2760:TYR:HA	2:C:2763:LEU:HD13	1.77	0.66
2:D:3848:GLU:OE1	2:D:3922:GLU:OE2	2.13	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:3142:THR:O	2:C:3144:LYS:NZ	2.28	0.66
2:C:4818:TYR:OH	2:D:4847:ASP:OD2	2.08	0.66
2:D:679:VAL:HG22	2:D:800:VAL:HG12	1.77	0.66
2:A:4120:GLU:HA	2:A:4123:GLU:HG2	1.78	0.66
2:B:4270:LYS:HA	2:B:4273:LYS:HE2	1.77	0.66
2:D:4831:ILE:HG13	2:D:4843:ARG:HH21	1.60	0.66
2:B:4640:PHE:CD2	2:B:4641:PRO:HD3	2.30	0.66
2:C:3250:TRP:HZ2	2:C:3309:LYS:HE3	1.60	0.66
2:A:3848:GLU:OE1	2:A:3922:GLU:OE2	2.13	0.66
2:B:3253:GLY:HA2	2:B:3264:CYS:HB3	1.77	0.66
2:C:2824:ARG:NH2	2:D:1502:ASN:HB3	2.10	0.66
2:C:4270:LYS:HA	2:C:4273:LYS:HE2	1.77	0.66
2:C:4651:ARG:NH2	2:C:4672:MET:SD	2.68	0.66
2:A:185:SER:HG	2:A:188:SER:HG	1.42	0.66
2:A:1172:THR:HB	2:A:1190:LEU:HD11	1.78	0.66
2:A:4831:ILE:HG13	2:A:4843:ARG:HH21	1.59	0.66
2:B:606:ARG:HH11	2:B:644:LEU:HD21	1.61	0.66
2:B:897:LYS:HD2	2:B:902:TRP:CE2	2.31	0.66
2:B:1172:THR:HB	2:B:1190:LEU:HD11	1.78	0.66
2:B:2760:TYR:HA	2:B:2763:LEU:HD13	1.77	0.66
2:B:4651:ARG:NH2	2:B:4672:MET:SD	2.68	0.66
2:C:2928:GLN:OE1	2:C:2931:ARG:NH2	2.29	0.66
2:A:897:LYS:HD2	2:A:902:TRP:CE2	2.31	0.66
2:B:3118:GLY:HA2	2:B:3121:LEU:HB3	1.76	0.66
2:B:3848:GLU:OE1	2:B:3922:GLU:OE2	2.13	0.66
2:C:1172:THR:HB	2:C:1190:LEU:HD11	1.78	0.66
2:C:1242:ASN:HB3	2:C:1807:ARG:HG3	1.77	0.66
2:D:1172:THR:HB	2:D:1190:LEU:HD11	1.78	0.66
2:A:4651:ARG:NH2	2:A:4672:MET:SD	2.68	0.66
2:D:3250:TRP:HZ2	2:D:3309:LYS:HE3	1.60	0.66
2:B:2830:ASN:HB3	2:C:1435:GLY:HA3	1.76	0.66
2:C:3848:GLU:OE1	2:C:3922:GLU:OE2	2.13	0.66
1:J:101:ILE:N	1:J:137:VAL:O	2.25	0.66
2:B:3997:LYS:NZ	2:B:4001:ASP:OD2	2.29	0.66
2:C:606:ARG:HH11	2:C:644:LEU:HD21	1.61	0.66
2:D:606:ARG:HH11	2:D:644:LEU:HD21	1.61	0.66
2:D:2760:TYR:HA	2:D:2763:LEU:HD13	1.78	0.66
2:D:4270:LYS:HA	2:D:4273:LYS:HE2	1.77	0.66
2:A:2928:GLN:OE1	2:A:2931:ARG:NH2	2.29	0.65
2:C:185:SER:HG	2:C:188:SER:HG	1.41	0.65
2:C:1435:GLY:H	2:C:1500:ARG:HH22	1.43	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1242:ASN:HB3	2:B:1807:ARG:HG3	1.77	0.65
2:B:2928:GLN:OE1	2:B:2931:ARG:NH2	2.29	0.65
2:C:874:LEU:HD13	2:C:940:LEU:HD13	1.79	0.65
2:D:897:LYS:HD2	2:D:902:TRP:CE2	2.31	0.65
2:A:606:ARG:HH11	2:A:644:LEU:HD21	1.61	0.65
2:A:1910:LEU:HD13	2:A:2062:ILE:HG12	1.79	0.65
1:K:101:ILE:N	1:K:137:VAL:O	2.25	0.65
2:B:3847:CYS:HB3	2:B:3855:GLN:HG3	1.78	0.65
2:C:897:LYS:HD2	2:C:902:TRP:CE2	2.31	0.65
2:D:16:THR:HG1	2:D:110:HIS:N	1.94	0.65
2:D:4120:GLU:HA	2:D:4123:GLU:HG2	1.78	0.65
2:B:1910:LEU:HD13	2:B:2062:ILE:HG12	1.79	0.65
2:B:3250:TRP:HZ2	2:B:3309:LYS:HE3	1.60	0.65
2:B:4120:GLU:HA	2:B:4123:GLU:HG2	1.78	0.65
2:B:16:THR:HG1	2:B:110:HIS:N	1.95	0.65
2:D:2928:GLN:OE1	2:D:2931:ARG:NH2	2.29	0.65
1:L:101:ILE:N	1:L:137:VAL:O	2.25	0.65
2:C:3847:CYS:HB3	2:C:3855:GLN:HG3	1.78	0.65
2:C:3848:GLU:OE2	2:C:3922:GLU:OE1	2.03	0.65
2:B:1936:LEU:HD11	2:B:1976:LEU:HD22	1.79	0.65
2:B:2831:VAL:HB	2:B:2894:LYS:HE3	1.79	0.65
2:C:1910:LEU:HD13	2:C:2062:ILE:HG12	1.79	0.65
2:A:1242:ASN:HB3	2:A:1807:ARG:HG3	1.78	0.65
2:B:185:SER:HG	2:B:188:SER:HG	1.44	0.65
2:C:4120:GLU:HA	2:C:4123:GLU:HG2	1.78	0.65
2:D:185:SER:HG	2:D:188:SER:HG	1.42	0.65
2:A:4822:ARG:NH1	2:B:4829:ASP:OD1	2.29	0.65
2:B:2187:ILE:HG13	2:B:2227:VAL:HG13	1.79	0.65
2:B:2801:TYR:OH	2:C:1496:PRO:O	2.14	0.65
2:D:1910:LEU:HD13	2:D:2062:ILE:HG12	1.79	0.65
2:D:3246:MET:HG2	2:D:3309:LYS:NZ	2.12	0.65
2:A:1936:LEU:HD11	2:A:1976:LEU:HD22	1.79	0.64
2:A:3250:TRP:HZ2	2:A:3309:LYS:HE3	1.60	0.64
2:D:1242:ASN:HB3	2:D:1807:ARG:HG3	1.77	0.64
2:A:874:LEU:HD13	2:A:940:LEU:HD13	1.79	0.64
2:A:3142:THR:O	2:A:3144:LYS:NZ	2.28	0.64
2:C:16:THR:HG1	2:C:110:HIS:N	1.94	0.64
2:C:2831:VAL:HB	2:C:2894:LYS:HE3	1.79	0.64
2:D:2831:VAL:HB	2:D:2894:LYS:HE3	1.79	0.64
2:B:874:LEU:HD13	2:B:940:LEU:HD13	1.79	0.64
2:D:1936:LEU:HD11	2:D:1976:LEU:HD22	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:16:THR:HG1	2:A:110:HIS:N	1.95	0.64
2:C:2187:ILE:HG13	2:C:2227:VAL:HG13	1.79	0.64
2:C:3997:LYS:NZ	2:C:4001:ASP:OD2	2.29	0.64
2:A:2187:ILE:HG13	2:A:2227:VAL:HG13	1.79	0.64
2:A:3848:GLU:OE1	2:A:3848:GLU:HA	1.97	0.64
2:B:902:TRP:CD1	2:B:918:LEU:HD12	2.33	0.64
2:B:3246:MET:HG2	2:B:3309:LYS:NZ	2.12	0.64
2:C:4690:LYS:HE3	2:C:4692:SER:HB2	1.80	0.64
2:A:2831:VAL:HB	2:A:2894:LYS:HE3	1.79	0.64
2:A:3246:MET:HG2	2:A:3309:LYS:NZ	2.12	0.64
2:D:2187:ILE:HG13	2:D:2227:VAL:HG13	1.79	0.64
2:A:3260:ARG:HG2	2:A:3263:MET:HB3	1.80	0.64
2:C:3246:MET:HG2	2:C:3309:LYS:NZ	2.12	0.64
2:A:3847:CYS:HB3	2:A:3855:GLN:HG3	1.78	0.64
2:D:3260:ARG:HG2	2:D:3263:MET:HB3	1.80	0.64
2:D:3848:GLU:OE1	2:D:3848:GLU:HA	1.97	0.64
2:D:3997:LYS:NZ	2:D:4001:ASP:OD2	2.29	0.64
2:A:902:TRP:CD1	2:A:918:LEU:HD12	2.33	0.64
2:B:4889:PHE:HD2	2:B:4915:LEU:HD21	1.63	0.64
2:D:3847:CYS:HB3	2:D:3855:GLN:HG3	1.78	0.64
2:A:3997:LYS:NZ	2:A:4001:ASP:OD2	2.29	0.64
2:C:801:ARG:NH1	2:C:1615:GLN:O	2.30	0.64
2:C:3848:GLU:OE1	2:C:3848:GLU:HA	1.97	0.64
2:A:801:ARG:NH1	2:A:1615:GLN:O	2.30	0.63
2:A:4753:LEU:HD23	2:B:4773:LEU:HD13	1.80	0.63
2:B:3142:THR:O	2:B:3144:LYS:NZ	2.28	0.63
2:C:3172:GLU:HG2	2:C:3211:LEU:HD12	1.81	0.63
2:A:3172:GLU:HG2	2:A:3211:LEU:HD12	1.80	0.63
2:B:3260:ARG:HG2	2:B:3263:MET:HB3	1.80	0.63
2:C:1936:LEU:HD11	2:C:1976:LEU:HD22	1.79	0.63
2:D:4690:LYS:HE3	2:D:4692:SER:HB2	1.80	0.63
2:C:3260:ARG:HG2	2:C:3263:MET:HB3	1.80	0.63
2:D:902:TRP:CD1	2:D:918:LEU:HD12	2.33	0.63
2:C:902:TRP:CD1	2:C:918:LEU:HD12	2.33	0.63
2:C:4276:VAL:O	2:C:4279:MET:HG3	1.99	0.63
2:D:4889:PHE:HD2	2:D:4915:LEU:HD21	1.63	0.63
2:B:3172:GLU:HG2	2:B:3211:LEU:HD12	1.81	0.63
2:D:3172:GLU:HG2	2:D:3211:LEU:HD12	1.80	0.63
2:A:4276:VAL:O	2:A:4279:MET:HG3	1.99	0.63
2:B:3848:GLU:OE1	2:B:3848:GLU:HA	1.97	0.63
2:C:655:MET:HE1	2:C:836:HIS:HA	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:893:TRP:O	2:C:897:LYS:HG2	1.99	0.63
2:A:4889:PHE:HD2	2:A:4915:LEU:HD21	1.63	0.62
2:C:2758:LYS:HB2	2:C:2762:LEU:HD23	1.81	0.62
2:C:4045:LYS:HD2	2:C:4067:LEU:HD22	1.81	0.62
2:A:655:MET:HE1	2:A:836:HIS:HA	1.81	0.62
2:A:4690:LYS:HE3	2:A:4692:SER:HB2	1.80	0.62
2:B:4276:VAL:O	2:B:4279:MET:HG3	1.99	0.62
2:B:4690:LYS:HE3	2:B:4692:SER:HB2	1.80	0.62
2:B:4045:LYS:HD2	2:B:4067:LEU:HD22	1.81	0.62
2:D:874:LEU:HD13	2:D:940:LEU:HD13	1.79	0.62
2:D:3188:SER:OG	2:D:3190:ARG:NH1	2.32	0.62
2:B:999:LEU:HB3	2:B:1050:LEU:HD11	1.82	0.62
2:C:2969:PRO:O	2:C:2973:GLN:NE2	2.33	0.62
2:D:999:LEU:HB3	2:D:1050:LEU:HD11	1.82	0.62
2:A:2969:PRO:O	2:A:2973:GLN:NE2	2.33	0.62
2:A:3211:LEU:O	2:A:3215:MET:HG2	1.99	0.62
1:L:110:MET:HA	2:D:3590:LEU:HD21	1.82	0.62
2:B:655:MET:HE1	2:B:836:HIS:HA	1.81	0.62
2:B:2833:LEU:HB3	2:B:2837:LEU:HD11	1.82	0.62
2:C:999:LEU:HB3	2:C:1050:LEU:HD11	1.82	0.62
2:C:4889:PHE:HD2	2:C:4915:LEU:HD21	1.63	0.62
2:D:893:TRP:O	2:D:897:LYS:HG2	1.99	0.62
2:D:4276:VAL:O	2:D:4279:MET:HG3	1.99	0.62
2:A:999:LEU:HB3	2:A:1050:LEU:HD11	1.82	0.62
2:A:3188:SER:OG	2:A:3190:ARG:NH1	2.32	0.62
2:B:3188:SER:OG	2:B:3190:ARG:NH1	2.32	0.62
2:C:2833:LEU:HB3	2:C:2837:LEU:HD11	1.82	0.62
2:D:1048:ASP:HA	2:D:1051:ARG:HG2	1.81	0.62
2:A:2827:ASP:OD2	2:A:2830:ASN:ND2	2.32	0.62
2:B:2758:LYS:HB2	2:B:2762:LEU:HD23	1.81	0.62
2:B:2827:ASP:OD2	2:B:2830:ASN:ND2	2.32	0.62
2:B:3211:LEU:O	2:B:3215:MET:HG2	1.99	0.62
2:C:3188:SER:OG	2:C:3190:ARG:NH1	2.32	0.62
2:D:801:ARG:NH1	2:D:1615:GLN:O	2.30	0.62
2:D:1031:ARG:NH1	6:D:5004:ATP:O3G	2.33	0.62
2:D:2827:ASP:OD2	2:D:2830:ASN:ND2	2.32	0.62
2:D:2969:PRO:O	2:D:2973:GLN:NE2	2.33	0.62
2:A:174:LYS:O	2:A:176:ARG:NH1	2.33	0.62
2:A:1031:ARG:NH1	6:A:5004:ATP:O3G	2.33	0.62
2:B:896:ASN:OD1	2:B:897:LYS:N	2.33	0.62
2:B:3848:GLU:OE2	2:B:3922:GLU:OE1	2.03	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3211:LEU:O	2:D:3215:MET:HG2	1.99	0.62
2:B:893:TRP:O	2:B:897:LYS:HG2	1.99	0.62
2:D:655:MET:HE1	2:D:836:HIS:HA	1.80	0.62
2:D:896:ASN:OD1	2:D:897:LYS:N	2.33	0.62
2:A:1119:ARG:NH2	2:A:1196:ASP:OD1	2.33	0.61
2:A:1502:ASN:OD1	2:A:1503:ASN:N	2.33	0.61
2:A:2244:ALA:O	2:A:2248:MET:HB2	2.00	0.61
2:A:2758:LYS:HB2	2:A:2762:LEU:HD23	1.81	0.61
2:C:2827:ASP:OD2	2:C:2830:ASN:ND2	2.32	0.61
2:C:2857:LYS:HA	2:C:2860:LEU:HG	1.82	0.61
2:D:1119:ARG:NH2	2:D:1196:ASP:OD1	2.33	0.61
2:A:893:TRP:O	2:A:897:LYS:HG2	1.99	0.61
2:C:896:ASN:OD1	2:C:897:LYS:N	2.33	0.61
2:C:1048:ASP:HA	2:C:1051:ARG:HG2	1.81	0.61
2:C:1502:ASN:OD1	2:C:1503:ASN:N	2.33	0.61
2:D:4045:LYS:HD2	2:D:4067:LEU:HD22	1.81	0.61
2:A:896:ASN:OD1	2:A:897:LYS:N	2.33	0.61
2:B:1119:ARG:NH2	2:B:1196:ASP:OD1	2.33	0.61
2:A:1048:ASP:HA	2:A:1051:ARG:HG2	1.81	0.61
2:A:3803:LEU:HB2	2:A:3884:SER:HB2	1.83	0.61
2:A:4045:LYS:HD2	2:A:4067:LEU:HD22	1.81	0.61
1:J:137:VAL:HG21	2:B:3587:TRP:HH2	1.66	0.61
2:B:1048:ASP:HA	2:B:1051:ARG:HG2	1.81	0.61
2:B:3192:ARG:HA	2:B:3197:LEU:HD12	1.83	0.61
2:D:174:LYS:O	2:D:176:ARG:NH1	2.33	0.61
2:A:3034:HIS:CE1	2:A:3038:GLN:HE22	2.18	0.61
2:A:3192:ARG:HA	2:A:3197:LEU:HD12	1.83	0.61
2:C:878:LEU:HA	2:C:881:ILE:HG22	1.83	0.61
2:D:878:LEU:HA	2:D:881:ILE:HG22	1.83	0.61
2:B:878:LEU:HA	2:B:881:ILE:HG22	1.83	0.61
2:B:1502:ASN:OD1	2:B:1503:ASN:N	2.33	0.61
2:B:2232:PRO:HB3	2:B:2382:ILE:HD11	1.83	0.61
2:C:3192:ARG:HA	2:C:3197:LEU:HD12	1.83	0.61
2:C:3211:LEU:O	2:C:3215:MET:HG2	2.00	0.61
2:D:2857:LYS:HA	2:D:2860:LEU:HG	1.82	0.61
2:D:3803:LEU:HB2	2:D:3884:SER:HB2	1.83	0.61
2:A:2841:ALA:HB1	2:A:2889:ALA:HB1	1.83	0.61
2:B:2733:SER:O	2:B:2737:LEU:HG	2.01	0.61
2:B:2969:PRO:O	2:B:2973:GLN:NE2	2.33	0.61
2:C:2244:ALA:O	2:C:2248:MET:HB2	2.00	0.61
2:C:3034:HIS:CE1	2:C:3038:GLN:HE22	2.18	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2244:ALA:O	2:D:2248:MET:HB2	2.00	0.61
2:D:3034:HIS:CE1	2:D:3038:GLN:HE22	2.18	0.61
2:A:2773:TRP:HB3	2:A:2774:PRO:HD3	1.83	0.61
2:A:2833:LEU:HB3	2:A:2837:LEU:HD11	1.82	0.61
2:B:2841:ALA:HB1	2:B:2889:ALA:HB1	1.83	0.61
2:D:2232:PRO:HB3	2:D:2382:ILE:HD11	1.83	0.61
2:D:2465:LYS:NZ	2:D:2495:ASP:OD2	2.30	0.61
2:D:2758:LYS:HB2	2:D:2762:LEU:HD23	1.81	0.61
2:D:4748:MET:O	2:D:4754:ARG:NH2	2.34	0.61
2:B:3148:VAL:HG13	2:B:3151:GLN:HE21	1.66	0.61
2:C:373:THR:HG21	2:C:397:GLY:HA2	1.83	0.61
2:A:1129:GLY:HA3	2:A:1145:TRP:HB3	1.83	0.61
2:A:2478:ILE:HD13	2:A:2527:LEU:HD11	1.83	0.61
2:A:2857:LYS:HA	2:A:2860:LEU:HG	1.82	0.61
2:A:4187:GLU:OE2	2:A:4947:ARG:NH2	2.34	0.61
2:A:4930:GLU:HA	2:A:4933:HIS:HD2	1.66	0.61
2:B:2244:ALA:O	2:B:2248:MET:HB2	2.00	0.61
2:C:561:ARG:HH11	2:C:561:ARG:HG3	1.66	0.61
2:C:4930:GLU:HA	2:C:4933:HIS:CD2	2.36	0.61
2:C:4930:GLU:HA	2:C:4933:HIS:HD2	1.65	0.61
2:D:2833:LEU:HB3	2:D:2837:LEU:HD11	1.82	0.61
2:A:878:LEU:HA	2:A:881:ILE:HG22	1.83	0.60
2:A:3070:LYS:O	2:A:3074:ASN:ND2	2.34	0.60
2:A:3848:GLU:OE2	2:A:3922:GLU:OE1	2.03	0.60
2:A:4748:MET:O	2:A:4754:ARG:NH2	2.34	0.60
2:C:2733:SER:O	2:C:2737:LEU:HG	2.01	0.60
2:C:3848:GLU:OE1	2:C:3922:GLU:CG	2.49	0.60
2:D:1502:ASN:OD1	2:D:1503:ASN:N	2.33	0.60
2:B:1129:GLY:HA3	2:B:1145:TRP:HB3	1.83	0.60
2:B:3070:LYS:O	2:B:3074:ASN:ND2	2.34	0.60
2:C:174:LYS:O	2:C:176:ARG:NH1	2.33	0.60
2:C:3148:VAL:HG13	2:C:3151:GLN:HE21	1.66	0.60
2:D:2773:TRP:HB3	2:D:2774:PRO:HD3	1.83	0.60
2:D:3070:LYS:O	2:D:3074:ASN:ND2	2.34	0.60
2:D:3148:VAL:HG13	2:D:3151:GLN:HE21	1.66	0.60
2:A:2232:PRO:HB3	2:A:2382:ILE:HD11	1.83	0.60
1:J:110:MET:HA	2:B:3590:LEU:HD21	1.82	0.60
2:B:1031:ARG:NH1	6:B:5004:ATP:O3G	2.33	0.60
2:B:2773:TRP:HB3	2:B:2774:PRO:HD3	1.83	0.60
2:B:2857:LYS:HA	2:B:2860:LEU:HG	1.82	0.60
2:B:3183:ILE:HG23	2:B:3184:TYR:CD1	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3939:ARG:NH2	2:B:3942:ASP:OD2	2.34	0.60
2:B:4137:GLU:HG2	2:B:4147:ARG:HG2	1.83	0.60
2:C:2232:PRO:HB3	2:C:2382:ILE:HD11	1.83	0.60
2:D:561:ARG:HH11	2:D:561:ARG:HG3	1.66	0.60
2:D:2478:ILE:HD13	2:D:2527:LEU:HD11	1.83	0.60
2:B:561:ARG:HG3	2:B:561:ARG:HH11	1.66	0.60
2:B:2425:SER:O	2:C:142:LYS:NZ	2.33	0.60
2:C:3070:LYS:O	2:C:3074:ASN:ND2	2.34	0.60
2:C:4187:GLU:OE2	2:C:4947:ARG:NH2	2.34	0.60
2:C:1031:ARG:NH1	6:C:5004:ATP:O3G	2.33	0.60
2:C:3803:LEU:HB2	2:C:3884:SER:HB2	1.83	0.60
2:C:4049:HIS:HD2	2:C:4067:LEU:HD11	1.67	0.60
2:C:4137:GLU:HG2	2:C:4147:ARG:HG2	1.83	0.60
2:D:2733:SER:O	2:D:2737:LEU:HG	2.01	0.60
2:A:373:THR:HG21	2:A:397:GLY:HA2	1.83	0.60
2:A:3148:VAL:HG13	2:A:3151:GLN:HE21	1.66	0.60
2:A:4049:HIS:HD2	2:A:4067:LEU:HD11	1.67	0.60
2:A:4829:ASP:OD1	2:D:4822:ARG:NH1	2.35	0.60
2:B:174:LYS:O	2:B:176:ARG:NH1	2.33	0.60
2:B:3803:LEU:HB2	2:B:3884:SER:HB2	1.83	0.60
2:D:3192:ARG:HA	2:D:3197:LEU:HD12	1.83	0.60
2:D:4930:GLU:HA	2:D:4933:HIS:HD2	1.66	0.60
2:B:3034:HIS:CE1	2:B:3038:GLN:HE22	2.18	0.60
2:B:4187:GLU:OE2	2:B:4947:ARG:NH2	2.34	0.60
2:C:3183:ILE:HG23	2:C:3184:TYR:CD1	2.35	0.60
2:C:4748:MET:O	2:C:4754:ARG:NH2	2.34	0.60
2:D:373:THR:HG21	2:D:397:GLY:HA2	1.83	0.60
2:A:2465:LYS:NZ	2:A:2495:ASP:OD2	2.30	0.60
2:A:4930:GLU:HA	2:A:4933:HIS:CD2	2.36	0.60
2:B:2478:ILE:HD13	2:B:2527:LEU:HD11	1.83	0.60
2:B:4049:HIS:HD2	2:B:4067:LEU:HD11	1.67	0.60
2:C:1119:ARG:NH2	2:C:1196:ASP:OD1	2.33	0.60
2:C:2773:TRP:HB3	2:C:2774:PRO:HD3	1.83	0.60
2:D:3304:GLN:HA	2:D:3307:ILE:HG12	1.84	0.60
2:D:4187:GLU:OE2	2:D:4947:ARG:NH2	2.34	0.60
2:A:4137:GLU:HG2	2:A:4147:ARG:HG2	1.83	0.60
2:B:3304:GLN:HA	2:B:3307:ILE:HG12	1.84	0.60
2:C:1129:GLY:HA3	2:C:1145:TRP:HB3	1.83	0.60
2:A:4831:ILE:HG13	2:A:4843:ARG:NH2	2.17	0.60
2:B:4107:GLU:OE2	2:B:4149:TYR:OH	2.15	0.60
2:C:4818:TYR:OH	2:D:4843:ARG:NH1	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3848:GLU:OE1	2:D:3922:GLU:CG	2.49	0.60
2:A:2733:SER:O	2:A:2737:LEU:HG	2.01	0.59
2:A:3848:GLU:OE1	2:A:3922:GLU:CG	2.49	0.59
2:B:4831:ILE:HG13	2:B:4843:ARG:NH2	2.17	0.59
2:D:2841:ALA:HB1	2:D:2889:ALA:HB1	1.83	0.59
2:D:4831:ILE:HG13	2:D:4843:ARG:NH2	2.17	0.59
2:A:561:ARG:HH11	2:A:561:ARG:HG3	1.66	0.59
2:B:902:TRP:HD1	2:B:918:LEU:HD12	1.67	0.59
2:B:904:TYR:HB2	2:B:918:LEU:HD22	1.85	0.59
2:B:4748:MET:O	2:B:4754:ARG:NH2	2.34	0.59
2:C:2841:ALA:HB1	2:C:2889:ALA:HB1	1.83	0.59
2:C:4492:LEU:HD12	2:C:4592:CYS:SG	2.43	0.59
2:D:997:ASP:HA	2:D:1047:LYS:HE2	1.84	0.59
2:A:2641:SER:HB3	2:A:2676:LEU:HD21	1.84	0.59
2:A:3183:ILE:HG23	2:A:3184:TYR:CD1	2.35	0.59
2:A:4670:LEU:HB2	2:A:4672:MET:HE1	1.84	0.59
2:D:490:GLN:HG2	2:D:495:ILE:HD12	1.84	0.59
2:D:4930:GLU:HA	2:D:4933:HIS:CD2	2.36	0.59
2:A:902:TRP:HD1	2:A:918:LEU:HD12	1.67	0.59
2:A:2338:GLU:OE1	2:A:2338:GLU:N	2.36	0.59
2:B:801:ARG:NH1	2:B:1615:GLN:O	2.30	0.59
2:B:3848:GLU:OE1	2:B:3922:GLU:CG	2.49	0.59
1:L:5:LEU:HD23	1:L:10:ILE:HG13	1.84	0.59
1:K:5:LEU:HD23	1:K:10:ILE:HG13	1.85	0.59
2:C:490:GLN:HG2	2:C:495:ILE:HD12	1.84	0.59
2:D:2641:SER:HB3	2:D:2676:LEU:HD21	1.84	0.59
2:B:2641:SER:HB3	2:B:2676:LEU:HD21	1.85	0.59
2:C:3304:GLN:HA	2:C:3307:ILE:HG12	1.84	0.59
2:C:3317:THR:H	2:C:3320:LEU:HD23	1.67	0.59
2:D:2338:GLU:OE1	2:D:2338:GLU:N	2.36	0.59
2:D:3317:THR:H	2:D:3320:LEU:HD23	1.67	0.59
2:D:4049:HIS:HD2	2:D:4067:LEU:HD11	1.67	0.59
2:A:997:ASP:HA	2:A:1047:LYS:HE2	1.84	0.59
2:B:2338:GLU:OE1	2:B:2338:GLU:N	2.36	0.59
2:B:3317:THR:H	2:B:3320:LEU:HD23	1.67	0.59
2:B:4492:LEU:HD12	2:B:4592:CYS:SG	2.43	0.59
2:B:4930:GLU:HA	2:B:4933:HIS:HD2	1.66	0.59
2:C:997:ASP:HA	2:C:1047:LYS:HE2	1.84	0.59
2:D:902:TRP:HD1	2:D:918:LEU:HD12	1.67	0.59
2:D:1129:GLY:HA3	2:D:1145:TRP:HB3	1.83	0.59
1:I:5:LEU:HD23	1:I:10:ILE:HG13	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:3304:GLN:HA	2:A:3307:ILE:HG12	1.84	0.59
2:B:373:THR:HG21	2:B:397:GLY:HA2	1.83	0.59
2:B:4930:GLU:HA	2:B:4933:HIS:CD2	2.36	0.59
2:C:2478:ILE:HD13	2:C:2527:LEU:HD11	1.83	0.59
2:C:3939:ARG:NH2	2:C:3942:ASP:OD2	2.34	0.59
2:B:894:VAL:O	2:B:898:ILE:HG12	2.03	0.59
2:B:997:ASP:HA	2:B:1047:LYS:HE2	1.84	0.59
2:B:3131:TYR:CD2	2:B:3205:CYS:HB3	2.38	0.59
2:C:902:TRP:HD1	2:C:918:LEU:HD12	1.67	0.59
2:C:904:TYR:HB2	2:C:918:LEU:HD22	1.85	0.59
2:A:904:TYR:HB2	2:A:918:LEU:HD22	1.85	0.59
2:A:4057:HIS:CE1	2:B:4660:PHE:HZ	2.21	0.59
2:A:4492:LEU:HD12	2:A:4592:CYS:SG	2.42	0.59
2:D:4137:GLU:HG2	2:D:4147:ARG:HG2	1.83	0.59
2:C:894:VAL:O	2:C:898:ILE:HG12	2.03	0.58
2:C:2338:GLU:N	2:C:2338:GLU:OE1	2.36	0.58
2:D:4492:LEU:HD12	2:D:4592:CYS:SG	2.43	0.58
2:A:884:LYS:HA	2:A:887:GLU:HG3	1.86	0.58
2:B:2926:LEU:O	2:B:2930:ILE:HD12	2.04	0.58
2:C:2465:LYS:NZ	2:C:2495:ASP:OD2	2.30	0.58
2:C:4818:TYR:HE1	2:D:4847:ASP:HB2	1.68	0.58
2:D:3939:ARG:NH2	2:D:3942:ASP:OD2	2.34	0.58
2:A:1722:ASN:O	2:A:1919:ARG:NH2	2.36	0.58
2:D:884:LYS:HA	2:D:887:GLU:HG3	1.86	0.58
2:D:1722:ASN:O	2:D:1919:ARG:NH2	2.36	0.58
2:D:3173:THR:O	2:D:3177:LYS:NZ	2.36	0.58
2:A:3317:THR:H	2:A:3320:LEU:HD23	1.67	0.58
1:J:5:LEU:HD23	1:J:10:ILE:HG13	1.85	0.58
2:B:1722:ASN:O	2:B:1919:ARG:NH2	2.36	0.58
2:D:894:VAL:O	2:D:898:ILE:HG12	2.03	0.58
2:D:1100:ARG:HH22	2:D:1235:GLY:HA3	1.69	0.58
2:A:3131:TYR:CD2	2:A:3205:CYS:HB3	2.38	0.58
2:B:2057:THR:OG1	2:B:2060:GLN:OE1	2.20	0.58
2:C:667:SER:HB2	2:C:669:GLN:HE22	1.69	0.58
2:C:884:LYS:HA	2:C:887:GLU:HG3	1.86	0.58
2:C:2982:PHE:O	2:C:3001:LYS:NZ	2.37	0.58
2:C:4831:ILE:HG13	2:C:4843:ARG:NH2	2.17	0.58
2:D:667:SER:HB2	2:D:669:GLN:HE22	1.69	0.58
2:D:904:TYR:HB2	2:D:918:LEU:HD22	1.85	0.58
2:A:490:GLN:HG2	2:A:495:ILE:HD12	1.84	0.58
2:A:2982:PHE:O	2:A:3001:LYS:NZ	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:490:GLN:HG2	2:B:495:ILE:HD12	1.84	0.58
2:B:903:GLN:H	2:B:913:ARG:HE	1.52	0.58
2:C:2202:TYR:O	2:C:2206:ILE:HG12	2.04	0.58
2:C:2641:SER:HB3	2:C:2676:LEU:HD21	1.84	0.58
2:D:2202:TYR:O	2:D:2206:ILE:HG12	2.04	0.58
2:D:2736:LYS:HB3	2:D:2741:TRP:HB2	1.86	0.58
2:D:2982:PHE:O	2:D:3001:LYS:NZ	2.37	0.58
2:A:963:LYS:HB3	2:A:977:LYS:HE2	1.86	0.58
2:A:2973:GLN:HA	2:A:2976:LYS:HZ2	1.67	0.58
1:L:42:GLN:HE21	2:D:1957:LEU:HD21	1.68	0.58
2:B:2982:PHE:O	2:B:3001:LYS:NZ	2.37	0.58
2:C:903:GLN:H	2:C:913:ARG:HE	1.52	0.58
2:C:2926:LEU:O	2:C:2930:ILE:HD12	2.04	0.58
2:A:335:LYS:NZ	2:A:401:ASP:OD2	2.37	0.58
2:A:4271:VAL:HG12	2:A:4274:MET:HE3	1.85	0.58
2:A:4518:LEU:HG	2:B:4810:LEU:HD13	1.85	0.58
2:D:903:GLN:H	2:D:913:ARG:HE	1.52	0.58
2:D:905:GLY:HA3	2:D:914:GLN:HB3	1.86	0.58
2:A:1898:LEU:HD22	2:A:1902:VAL:HG11	1.86	0.58
2:A:2736:LYS:HB3	2:A:2741:TRP:HB2	1.86	0.58
2:B:884:LYS:HA	2:B:887:GLU:HG3	1.86	0.58
2:C:1722:ASN:O	2:C:1919:ARG:NH2	2.36	0.58
2:D:247:VAL:O	2:D:272:ARG:NH1	2.37	0.58
2:D:963:LYS:HB3	2:D:977:LYS:HE2	1.86	0.58
2:D:3112:ILE:HG23	2:D:3118:GLY:HA3	1.86	0.58
2:A:247:VAL:O	2:A:272:ARG:NH1	2.37	0.57
2:B:667:SER:HB2	2:B:669:GLN:HE22	1.69	0.57
2:B:963:LYS:HB3	2:B:977:LYS:HE2	1.86	0.57
2:B:1100:ARG:HH22	2:B:1235:GLY:HA3	1.69	0.57
2:C:1100:ARG:HH22	2:C:1235:GLY:HA3	1.69	0.57
2:D:335:LYS:NZ	2:D:401:ASP:OD2	2.37	0.57
2:A:270:HIS:CD2	2:A:491:GLU:HG3	2.39	0.57
2:A:891:GLU:O	2:A:894:VAL:HG22	2.04	0.57
2:A:894:VAL:O	2:A:898:ILE:HG12	2.03	0.57
2:A:3677:THR:O	2:A:3679:LYS:NZ	2.37	0.57
2:B:270:HIS:CD2	2:B:491:GLU:HG3	2.39	0.57
2:B:2465:LYS:NZ	2:B:2495:ASP:OD2	2.30	0.57
2:C:247:VAL:O	2:C:272:ARG:NH1	2.37	0.57
2:C:2123:LEU:HD13	2:C:2167:MET:HG2	1.87	0.57
2:C:3321:PRO:O	2:C:3325:LYS:HG2	2.04	0.57
2:A:903:GLN:H	2:A:913:ARG:HE	1.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:4719:PHE:CE2	2:D:4294:LEU:HD22	2.39	0.57
1:J:106:LEU:HD22	2:B:3587:TRP:HE1	1.70	0.57
2:B:670:TYR:O	2:B:673:TRP:NE1	2.38	0.57
2:B:891:GLU:O	2:B:894:VAL:HG22	2.04	0.57
2:C:891:GLU:O	2:C:894:VAL:HG22	2.04	0.57
2:C:905:GLY:HA3	2:C:914:GLN:HB3	1.86	0.57
2:C:2972:ASP:HA	2:C:3035:ILE:HD11	1.87	0.57
2:C:3112:ILE:HG23	2:C:3118:GLY:HA3	1.86	0.57
2:D:1898:LEU:HD22	2:D:1902:VAL:HG11	1.86	0.57
2:B:335:LYS:NZ	2:B:401:ASP:OD2	2.37	0.57
2:B:2202:TYR:O	2:B:2206:ILE:HG12	2.04	0.57
2:D:2972:ASP:HA	2:D:3035:ILE:HD11	1.87	0.57
2:A:667:SER:HB2	2:A:669:GLN:HE22	1.69	0.57
2:A:1100:ARG:HH22	2:A:1235:GLY:HA3	1.69	0.57
2:A:2972:ASP:HA	2:A:3035:ILE:HD11	1.87	0.57
2:A:3321:PRO:O	2:A:3325:LYS:HG2	2.04	0.57
2:B:247:VAL:O	2:B:272:ARG:NH1	2.37	0.57
2:B:3321:PRO:O	2:B:3325:LYS:HG2	2.04	0.57
2:C:968:LYS:NZ	2:C:971:GLN:O	2.38	0.57
2:C:2057:THR:OG1	2:C:2060:GLN:OE1	2.20	0.57
2:D:2123:LEU:HD13	2:D:2167:MET:HG2	1.86	0.57
2:A:924:LEU:HD12	2:A:925:PRO:HD2	1.86	0.57
2:A:2926:LEU:O	2:A:2930:ILE:HD12	2.04	0.57
2:B:1898:LEU:HD22	2:B:1902:VAL:HG11	1.86	0.57
2:C:670:TYR:O	2:C:673:TRP:NE1	2.38	0.57
2:C:3677:THR:O	2:C:3679:LYS:NZ	2.37	0.57
2:D:670:TYR:O	2:D:673:TRP:NE1	2.38	0.57
2:D:2627:TRP:HB2	2:D:2630:PHE:HB2	1.87	0.57
2:D:3321:PRO:O	2:D:3325:LYS:HG2	2.04	0.57
1:I:102:SER:HA	1:I:136:GLN:HG3	1.87	0.57
2:A:2202:TYR:O	2:A:2206:ILE:HG12	2.04	0.57
2:B:1989:PRO:O	2:B:1993:ARG:HG3	2.05	0.57
2:C:1989:PRO:O	2:C:1993:ARG:HG3	2.05	0.57
2:D:2926:LEU:O	2:D:2930:ILE:HD12	2.04	0.57
2:D:3677:THR:O	2:D:3679:LYS:NZ	2.37	0.57
2:A:4583:SER:O	2:A:4587:ILE:HD12	2.05	0.57
2:B:3677:THR:O	2:B:3679:LYS:NZ	2.37	0.57
2:C:1898:LEU:HD22	2:C:1902:VAL:HG11	1.86	0.57
2:C:3958:LEU:HD22	2:C:3964:GLN:HG3	1.87	0.57
2:D:2973:GLN:HA	2:D:2976:LYS:HZ2	1.69	0.57
2:D:3183:ILE:HG23	2:D:3184:TYR:CD1	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:3112:ILE:HG23	2:A:3118:GLY:HA3	1.86	0.57
2:A:3173:THR:O	2:A:3177:LYS:NZ	2.36	0.57
2:B:2972:ASP:HA	2:B:3035:ILE:HD11	1.87	0.57
2:C:924:LEU:HD12	2:C:925:PRO:HD2	1.86	0.57
2:C:963:LYS:HB3	2:C:977:LYS:HE2	1.86	0.57
2:C:3163:ALA:HB1	2:C:3245:TYR:HD1	1.70	0.57
2:D:4583:SER:O	2:D:4587:ILE:HD12	2.05	0.57
2:A:3131:TYR:CZ	2:A:3205:CYS:O	2.58	0.57
2:B:1951:LEU:HD11	2:B:1961:LYS:HE3	1.87	0.57
2:C:335:LYS:NZ	2:C:401:ASP:OD2	2.37	0.57
2:D:3163:ALA:HB1	2:D:3245:TYR:HD1	1.70	0.57
2:A:4827:ILE:O	2:A:4831:ILE:HG12	2.05	0.56
2:B:924:LEU:HD12	2:B:925:PRO:HD2	1.86	0.56
2:B:968:LYS:NZ	2:B:971:GLN:O	2.38	0.56
2:B:3958:LEU:HD22	2:B:3964:GLN:HG3	1.87	0.56
2:C:3173:THR:O	2:C:3177:LYS:NZ	2.36	0.56
2:C:4040:LYS:NZ	2:C:4042:VAL:O	2.38	0.56
2:D:924:LEU:HD12	2:D:925:PRO:HD2	1.86	0.56
2:D:968:LYS:NZ	2:D:971:GLN:O	2.38	0.56
2:D:2146:LEU:O	2:D:2150:MET:HG2	2.05	0.56
2:D:3823:GLU:HG3	2:D:3826:GLY:H	1.70	0.56
2:A:670:TYR:O	2:A:673:TRP:NE1	2.38	0.56
2:A:3920:LEU:HD22	2:A:3935:LEU:HD11	1.87	0.56
2:B:1795:LEU:HD23	2:B:1842:ILE:HD11	1.87	0.56
2:B:2610:LEU:HD13	2:B:2644:LEU:HD21	1.87	0.56
2:B:3026:ALA:HA	2:B:3029:ILE:HD12	1.87	0.56
2:C:1732:GLU:HB3	2:C:1753:LEU:HD21	1.87	0.56
2:C:1795:LEU:HD23	2:C:1842:ILE:HD11	1.87	0.56
2:D:3920:LEU:HD22	2:D:3935:LEU:HD11	1.87	0.56
2:D:4040:LYS:NZ	2:D:4042:VAL:O	2.38	0.56
2:A:705:PRO:HD3	2:A:857:LEU:HD13	1.87	0.56
2:A:905:GLY:HA3	2:A:914:GLN:HB3	1.86	0.56
2:A:1435:GLY:HA3	2:D:2830:ASN:HB3	1.87	0.56
2:A:1732:GLU:HB3	2:A:1753:LEU:HD21	1.87	0.56
2:A:2123:LEU:HD13	2:A:2167:MET:HG2	1.87	0.56
2:A:2627:TRP:HB2	2:A:2630:PHE:HB2	1.87	0.56
2:A:3823:GLU:HG3	2:A:3826:GLY:H	1.70	0.56
1:L:102:SER:HA	1:L:136:GLN:HG3	1.87	0.56
1:L:102:SER:OG	1:L:105:GLU:OE1	2.22	0.56
2:B:905:GLY:HA3	2:B:914:GLN:HB3	1.86	0.56
2:B:4827:ILE:O	2:B:4831:ILE:HG12	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:270:HIS:CD2	2:C:491:GLU:HG3	2.39	0.56
2:C:3823:GLU:HG3	2:C:3826:GLY:H	1.70	0.56
2:C:4827:ILE:O	2:C:4831:ILE:HG12	2.05	0.56
2:D:270:HIS:CD2	2:D:491:GLU:HG3	2.39	0.56
2:D:3026:ALA:HA	2:D:3029:ILE:HD12	1.87	0.56
2:A:3163:ALA:HB1	2:A:3245:TYR:HD1	1.70	0.56
2:B:2123:LEU:HD13	2:B:2167:MET:HG2	1.87	0.56
2:B:3253:GLY:C	2:B:3255:GLU:H	2.09	0.56
2:B:3823:GLU:HG3	2:B:3826:GLY:H	1.70	0.56
2:C:1951:LEU:HD11	2:C:1961:LYS:HE3	1.87	0.56
2:C:4819:VAL:HG12	2:C:4830:GLU:HG3	1.88	0.56
2:D:3131:TYR:CZ	2:D:3205:CYS:O	2.58	0.56
2:A:3939:ARG:NH2	2:A:3942:ASP:OD2	2.34	0.56
2:B:1732:GLU:HB3	2:B:1753:LEU:HD21	1.87	0.56
2:B:3246:MET:HG2	2:B:3309:LYS:HZ2	1.68	0.56
2:B:4040:LYS:NZ	2:B:4042:VAL:O	2.38	0.56
2:C:4583:SER:O	2:C:4587:ILE:HD12	2.05	0.56
2:D:891:GLU:O	2:D:894:VAL:HG22	2.04	0.56
2:A:968:LYS:NZ	2:A:971:GLN:O	2.38	0.56
2:B:4583:SER:O	2:B:4587:ILE:HD12	2.05	0.56
2:C:705:PRO:HD3	2:C:857:LEU:HD13	1.87	0.56
2:C:3846:LEU:HB3	2:C:3854:PHE:CE2	2.41	0.56
2:D:3152:ARG:HD2	2:D:3232:PRO:HB2	1.87	0.56
2:A:2610:LEU:HD13	2:A:2644:LEU:HD21	1.87	0.56
2:A:3152:ARG:HD2	2:A:3232:PRO:HB2	1.87	0.56
2:A:4040:LYS:NZ	2:A:4042:VAL:O	2.38	0.56
1:K:102:SER:OG	1:K:105:GLU:OE1	2.22	0.56
2:B:1500:ARG:HG3	2:B:1505:LEU:HB2	1.88	0.56
2:B:2172:MET:HA	2:B:2172:MET:HE3	1.88	0.56
2:B:2736:LYS:HB3	2:B:2741:TRP:HB2	1.86	0.56
2:B:3112:ILE:HG23	2:B:3118:GLY:HA3	1.86	0.56
2:B:3163:ALA:HB1	2:B:3245:TYR:HD1	1.70	0.56
2:B:3846:LEU:HB3	2:B:3854:PHE:CE2	2.41	0.56
2:C:2627:TRP:HB2	2:C:2630:PHE:HB2	1.87	0.56
2:C:2736:LYS:HB3	2:C:2741:TRP:HB2	1.86	0.56
2:D:2610:LEU:HD13	2:D:2644:LEU:HD21	1.87	0.56
2:D:3958:LEU:HD22	2:D:3964:GLN:HG3	1.87	0.56
1:J:102:SER:HA	1:J:136:GLN:HG3	1.87	0.56
1:K:102:SER:HA	1:K:136:GLN:HG3	1.87	0.56
2:B:705:PRO:HD3	2:B:857:LEU:HD13	1.87	0.56
2:B:4819:VAL:HG12	2:B:4830:GLU:HG3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2610:LEU:HD13	2:C:2644:LEU:HD21	1.87	0.56
2:C:3152:ARG:HD2	2:C:3232:PRO:HB2	1.87	0.56
2:C:3235:MET:HB2	2:C:3239:LEU:HD12	1.88	0.56
2:A:2146:LEU:O	2:A:2150:MET:HG2	2.05	0.56
2:A:3026:ALA:HA	2:A:3029:ILE:HD12	1.87	0.56
1:J:122:VAL:O	1:J:126:ILE:HG23	2.06	0.56
1:K:122:VAL:O	1:K:126:ILE:HG23	2.06	0.56
2:B:3173:THR:O	2:B:3177:LYS:NZ	2.36	0.56
2:C:1500:ARG:HG3	2:C:1505:LEU:HB2	1.88	0.56
2:C:3729:ALA:HA	2:C:3732:HIS:CD2	2.41	0.56
2:A:3253:GLY:C	2:A:3255:GLU:H	2.09	0.56
2:A:3729:ALA:HA	2:A:3732:HIS:CD2	2.41	0.56
2:B:3013:VAL:O	2:B:3018:ARG:NH2	2.40	0.56
2:C:3920:LEU:HD22	2:C:3935:LEU:HD11	1.87	0.56
2:D:3192:ARG:HD3	2:D:3199:THR:HG22	1.87	0.56
2:D:3235:MET:HB2	2:D:3239:LEU:HD12	1.88	0.56
2:D:3846:LEU:HB3	2:D:3854:PHE:CE2	2.41	0.56
1:I:5:LEU:HB3	1:I:10:ILE:HD11	1.88	0.55
2:A:1989:PRO:O	2:A:1993:ARG:HG3	2.05	0.55
2:A:3013:VAL:O	2:A:3018:ARG:NH2	2.39	0.55
2:A:3846:LEU:HB3	2:A:3854:PHE:CE2	2.41	0.55
3:F:83:TYR:HB3	3:F:87:GLY:HA2	1.88	0.55
1:J:5:LEU:HB3	1:J:10:ILE:HD11	1.88	0.55
2:B:16:THR:OG1	2:B:110:HIS:N	2.39	0.55
2:B:2146:LEU:O	2:B:2150:MET:HG2	2.05	0.55
1:I:122:VAL:O	1:I:126:ILE:HG23	2.06	0.55
2:A:1951:LEU:HD11	2:A:1961:LYS:HE3	1.87	0.55
2:A:2057:THR:OG1	2:A:2060:GLN:OE1	2.20	0.55
2:A:2512:MET:HA	2:A:2512:MET:CE	2.35	0.55
2:B:514:PHE:CD2	2:B:526:TRP:HB2	2.41	0.55
2:B:2627:TRP:HB2	2:B:2630:PHE:HB2	1.87	0.55
2:B:3131:TYR:CZ	2:B:3205:CYS:O	2.58	0.55
2:C:2961:LYS:HB2	2:C:2965:LYS:NZ	2.21	0.55
2:C:3192:ARG:HD3	2:C:3199:THR:HG22	1.87	0.55
2:C:3253:GLY:C	2:C:3255:GLU:H	2.09	0.55
2:D:705:PRO:HD3	2:D:857:LEU:HD13	1.87	0.55
2:D:1795:LEU:HD23	2:D:1842:ILE:HD11	1.87	0.55
2:D:1989:PRO:O	2:D:1993:ARG:HG3	2.05	0.55
2:D:2961:LYS:HB2	2:D:2965:LYS:NZ	2.21	0.55
2:D:3729:ALA:HA	2:D:3732:HIS:CD2	2.41	0.55
2:D:3848:GLU:OE2	2:D:3922:GLU:OE1	2.03	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:3958:LEU:HD22	2:A:3964:GLN:HG3	1.87	0.55
2:B:2961:LYS:HB2	2:B:2965:LYS:NZ	2.21	0.55
2:C:798:ILE:HD12	2:C:800:VAL:HG22	1.88	0.55
2:A:1795:LEU:HD23	2:A:1842:ILE:HD11	1.87	0.55
2:A:2961:LYS:HB2	2:A:2965:LYS:NZ	2.21	0.55
3:G:83:TYR:HB3	3:G:87:GLY:HA2	1.89	0.55
3:H:83:TYR:HB3	3:H:87:GLY:HA2	1.88	0.55
1:L:122:VAL:O	1:L:126:ILE:HG23	2.06	0.55
1:K:107:ARG:NH2	1:K:119:ASP:OD2	2.40	0.55
2:C:3131:TYR:CZ	2:C:3205:CYS:O	2.58	0.55
2:D:514:PHE:CD2	2:D:526:TRP:HB2	2.41	0.55
2:D:3591:LEU:HB3	2:D:3595:ARG:NH1	2.22	0.55
2:D:4271:VAL:HG12	2:D:4274:MET:HE3	1.86	0.55
2:A:3131:TYR:CD1	2:A:3205:CYS:HB2	2.41	0.55
2:B:2512:MET:HA	2:B:2512:MET:CE	2.35	0.55
2:C:514:PHE:CD2	2:C:526:TRP:HB2	2.41	0.55
2:C:4271:VAL:HG12	2:C:4274:MET:HE3	1.89	0.55
2:D:1732:GLU:HB3	2:D:1753:LEU:HD21	1.87	0.55
2:B:3152:ARG:HD2	2:B:3232:PRO:HB2	1.87	0.55
2:B:3591:LEU:HB3	2:B:3595:ARG:NH1	2.22	0.55
2:B:3920:LEU:HD22	2:B:3935:LEU:HD11	1.87	0.55
2:C:2146:LEU:O	2:C:2150:MET:HG2	2.05	0.55
2:D:798:ILE:HD12	2:D:800:VAL:HG22	1.88	0.55
2:D:3013:VAL:O	2:D:3018:ARG:NH2	2.40	0.55
1:L:107:ARG:NH2	1:L:119:ASP:OD2	2.40	0.55
1:K:5:LEU:HB3	1:K:10:ILE:HD11	1.88	0.55
2:B:3192:ARG:HD3	2:B:3199:THR:HG22	1.87	0.55
2:C:2448:ASP:OD2	2:C:2450:ASN:ND2	2.40	0.55
2:C:4670:LEU:HB2	2:C:4672:MET:HE1	1.87	0.55
2:D:4819:VAL:HG12	2:D:4830:GLU:HG3	1.88	0.55
2:D:4827:ILE:O	2:D:4831:ILE:HG12	2.05	0.55
2:A:1500:ARG:HG3	2:A:1505:LEU:HB2	1.88	0.55
2:A:2923:TYR:HA	2:A:3003:MET:HE1	1.89	0.55
2:C:3026:ALA:HA	2:C:3029:ILE:HD12	1.87	0.55
2:C:3227:ARG:HD2	2:C:3228:TYR:H	1.72	0.55
2:D:2448:ASP:OD2	2:D:2450:ASN:ND2	2.40	0.55
2:D:2732:TRP:O	2:D:2736:LYS:HG3	2.07	0.55
2:A:514:PHE:CD2	2:A:526:TRP:HB2	2.41	0.55
2:A:1007:TRP:O	2:A:1011:ARG:HG2	2.07	0.55
2:A:2448:ASP:OD2	2:A:2450:ASN:ND2	2.40	0.55
2:B:3729:ALA:HA	2:B:3732:HIS:CD2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2512:MET:HA	2:C:2512:MET:CE	2.35	0.55
2:C:2923:TYR:HA	2:C:3003:MET:HE1	1.87	0.55
2:C:3322:LEU:HD12	2:C:3323:MET:HG3	1.89	0.55
2:D:1951:LEU:HD11	2:D:1961:LYS:HE3	1.87	0.55
2:A:246:THR:HG21	2:A:267:VAL:HG11	1.89	0.55
2:A:3131:TYR:OH	2:A:3205:CYS:O	2.23	0.55
2:A:4819:VAL:HG12	2:A:4830:GLU:HG3	1.88	0.55
1:J:102:SER:OG	1:J:105:GLU:OE1	2.22	0.55
1:J:107:ARG:NH2	1:J:119:ASP:OD2	2.40	0.55
2:B:2732:TRP:O	2:B:2736:LYS:HG3	2.07	0.55
2:B:3227:ARG:HD2	2:B:3228:TYR:H	1.72	0.55
2:B:3235:MET:HB2	2:B:3239:LEU:HD12	1.88	0.55
2:C:2436:ILE:HG22	2:C:2491:GLY:HA3	1.89	0.55
2:D:1007:TRP:O	2:D:1011:ARG:HG2	2.07	0.55
2:D:2918:GLU:HA	2:D:2923:TYR:CD1	2.42	0.55
2:D:3227:ARG:HD2	2:D:3228:TYR:H	1.72	0.55
1:I:102:SER:OG	1:I:105:GLU:OE1	2.22	0.54
2:A:629:GLN:OE1	2:A:1669:ASN:ND2	2.37	0.54
2:A:2732:TRP:O	2:A:2736:LYS:HG3	2.07	0.54
2:A:2918:GLU:HA	2:A:2923:TYR:CD1	2.42	0.54
2:A:4169:LYS:HE3	2:A:4170:ARG:HH22	1.72	0.54
3:E:83:TYR:HB3	3:E:87:GLY:HA2	1.89	0.54
2:B:4271:VAL:HG12	2:B:4274:MET:HE3	1.87	0.54
2:A:16:THR:OG1	2:A:110:HIS:N	2.39	0.54
2:A:849:ASP:OD1	2:A:1214:ARG:NE	2.37	0.54
2:A:3192:ARG:HD3	2:A:3199:THR:HG22	1.87	0.54
2:B:2918:GLU:HA	2:B:2923:TYR:CD1	2.42	0.54
2:C:2171:VAL:HA	2:C:2174:VAL:HG22	1.89	0.54
2:C:3591:LEU:HB3	2:C:3595:ARG:NH1	2.22	0.54
2:D:4169:LYS:HE3	2:D:4170:ARG:HH22	1.72	0.54
2:A:562:LEU:HG	2:A:600:LEU:HD13	1.89	0.54
2:A:2436:ILE:HG22	2:A:2491:GLY:HA3	1.89	0.54
2:A:3591:LEU:HB3	2:A:3595:ARG:NH1	2.22	0.54
1:L:5:LEU:HB3	1:L:10:ILE:HD11	1.88	0.54
2:B:296:ARG:HH21	2:B:324:VAL:HA	1.73	0.54
2:B:839:GLU:HB3	2:B:851:LEU:HD12	1.88	0.54
2:C:3901:GLN:OE1	2:C:3904:ARG:NH1	2.40	0.54
2:D:1500:ARG:HG3	2:D:1505:LEU:HB2	1.88	0.54
2:D:2057:THR:OG1	2:D:2060:GLN:OE1	2.20	0.54
2:D:3253:GLY:C	2:D:3255:GLU:H	2.09	0.54
2:D:3322:LEU:HD12	2:D:3323:MET:HG3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:134:ASP:OD1	2:A:3298:ARG:NH1	2.39	0.54
2:A:555:LEU:HD21	2:A:578:VAL:HG11	1.90	0.54
2:A:798:ILE:HD12	2:A:800:VAL:HG22	1.88	0.54
2:A:3322:LEU:HD12	2:A:3323:MET:HG3	1.89	0.54
2:A:4107:GLU:OE2	2:A:4149:TYR:OH	2.15	0.54
2:B:246:THR:HG21	2:B:267:VAL:HG11	1.89	0.54
2:B:555:LEU:HD21	2:B:578:VAL:HG11	1.90	0.54
2:B:798:ILE:HD12	2:B:800:VAL:HG22	1.88	0.54
2:B:2436:ILE:HG22	2:B:2491:GLY:HA3	1.90	0.54
2:B:3322:LEU:HD12	2:B:3323:MET:HG3	1.89	0.54
2:B:4169:LYS:HE3	2:B:4170:ARG:HH22	1.72	0.54
2:D:2171:VAL:HA	2:D:2174:VAL:HG22	1.89	0.54
2:D:2436:ILE:HG22	2:D:2491:GLY:HA3	1.89	0.54
2:A:839:GLU:HB3	2:A:851:LEU:HD12	1.88	0.54
2:A:3235:MET:HB2	2:A:3239:LEU:HD12	1.88	0.54
2:A:3312:PRO:HA	2:A:3315:LEU:HB2	1.89	0.54
2:B:2171:VAL:HA	2:B:2174:VAL:HG22	1.89	0.54
2:B:2923:TYR:HA	2:B:3003:MET:HE1	1.89	0.54
2:C:16:THR:OG1	2:C:110:HIS:N	2.39	0.54
2:C:562:LEU:HG	2:C:600:LEU:HD13	1.89	0.54
2:C:3283:ILE:O	2:C:3287:ASN:HB2	2.08	0.54
2:C:4169:LYS:HE3	2:C:4170:ARG:HH22	1.72	0.54
2:D:1842:ILE:HD12	2:D:1845:LEU:HD12	1.90	0.54
2:A:1124:PRO:HD2	2:A:1594:VAL:HG23	1.90	0.54
2:A:2171:VAL:HA	2:A:2174:VAL:HG22	1.89	0.54
1:J:100:TYR:CD1	1:J:138:ASN:HB3	2.43	0.54
2:B:238:HIS:HB3	2:B:243:GLU:HG3	1.90	0.54
2:B:562:LEU:HG	2:B:600:LEU:HD13	1.89	0.54
2:D:16:THR:OG1	2:D:110:HIS:N	2.39	0.54
2:D:839:GLU:HB3	2:D:851:LEU:HD12	1.88	0.54
2:D:4633:LEU:O	2:D:4704:LYS:NZ	2.41	0.54
2:B:1007:TRP:O	2:B:1011:ARG:HG2	2.07	0.54
2:B:2448:ASP:OD2	2:B:2450:ASN:ND2	2.40	0.54
2:B:3901:GLN:OE1	2:B:3904:ARG:NH1	2.41	0.54
2:C:2918:GLU:HA	2:C:2923:TYR:CD1	2.42	0.54
2:D:842:GLN:HB2	2:D:1603:PHE:HB2	1.90	0.54
2:D:3283:ILE:O	2:D:3287:ASN:HB2	2.08	0.54
2:D:3950:VAL:O	2:D:3954:MET:HB2	2.08	0.54
2:A:296:ARG:HH21	2:A:324:VAL:HA	1.72	0.54
2:C:238:HIS:HB3	2:C:243:GLU:HG3	1.90	0.54
2:C:849:ASP:OD1	2:C:1214:ARG:NE	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2732:TRP:O	2:C:2736:LYS:HG3	2.07	0.54
2:C:3131:TYR:CD2	2:C:3205:CYS:HB3	2.38	0.54
2:C:3950:VAL:O	2:C:3954:MET:HB2	2.08	0.54
1:I:107:ARG:NH2	1:I:119:ASP:OD2	2.40	0.54
2:A:3227:ARG:HD2	2:A:3228:TYR:H	1.72	0.54
2:B:842:GLN:HB2	2:B:1603:PHE:HB2	1.90	0.54
2:A:1435:GLY:H	2:A:1500:ARG:NH2	2.06	0.54
2:A:3950:VAL:O	2:A:3954:MET:HB2	2.08	0.54
1:K:100:TYR:CD1	1:K:138:ASN:HB3	2.43	0.54
2:C:296:ARG:HH21	2:C:324:VAL:HA	1.72	0.54
2:C:839:GLU:HB3	2:C:851:LEU:HD12	1.89	0.54
2:C:1124:PRO:HD2	2:C:1594:VAL:HG23	1.90	0.54
2:C:1842:ILE:HD12	2:C:1845:LEU:HD12	1.90	0.54
2:D:296:ARG:HH21	2:D:324:VAL:HA	1.72	0.54
2:D:562:LEU:HG	2:D:600:LEU:HD13	1.89	0.54
2:D:996:VAL:HG22	2:D:1054:VAL:HG21	1.89	0.54
2:D:2172:MET:HA	2:D:2172:MET:HE3	1.90	0.54
2:D:2593:VAL:HG12	2:D:2644:LEU:HB2	1.90	0.54
2:D:3901:GLN:OE1	2:D:3904:ARG:NH1	2.41	0.54
1:I:19:LEU:HD11	2:A:3595:ARG:HH21	1.73	0.53
2:A:605:GLY:HA2	2:A:1585:ARG:HD2	1.91	0.53
2:A:2172:MET:HA	2:A:2172:MET:HE3	1.90	0.53
2:A:3901:GLN:OE1	2:A:3904:ARG:NH1	2.41	0.53
2:B:713:TRP:HH2	2:B:1251:LEU:HD21	1.73	0.53
2:C:246:THR:HG21	2:C:267:VAL:HG11	1.89	0.53
2:C:555:LEU:HD21	2:C:578:VAL:HG11	1.90	0.53
2:C:842:GLN:HB2	2:C:1603:PHE:HB2	1.90	0.53
2:C:3312:PRO:HA	2:C:3315:LEU:HB2	1.89	0.53
2:D:2562:THR:O	2:D:2566:ARG:HG3	2.08	0.53
2:A:238:HIS:HB3	2:A:243:GLU:HG3	1.90	0.53
2:B:1979:PHE:CD1	2:B:1993:ARG:HG2	2.44	0.53
2:B:3283:ILE:O	2:B:3287:ASN:HB2	2.08	0.53
2:C:436:LEU:HG	2:C:445:VAL:HG11	1.91	0.53
2:C:713:TRP:HH2	2:C:1251:LEU:HD21	1.73	0.53
2:D:238:HIS:HB3	2:D:243:GLU:HG3	1.90	0.53
2:D:555:LEU:HD21	2:D:578:VAL:HG11	1.90	0.53
2:D:605:GLY:HA2	2:D:1585:ARG:HD2	1.90	0.53
2:D:1256:PRO:HG3	2:D:1453:TYR:HB2	1.90	0.53
2:D:3900:GLU:OE2	2:D:3904:ARG:NH2	2.41	0.53
1:L:42:GLN:HE21	2:D:1957:LEU:CD2	2.21	0.53
1:L:100:TYR:CD1	1:L:138:ASN:HB3	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:28:ILE:HG22	2:B:29:HIS:HD2	1.73	0.53
2:B:629:GLN:OE1	2:B:1669:ASN:ND2	2.37	0.53
2:B:1842:ILE:HD12	2:B:1845:LEU:HD12	1.90	0.53
2:B:4633:LEU:O	2:B:4704:LYS:NZ	2.41	0.53
2:C:801:ARG:HG2	2:C:1618:LEU:HA	1.91	0.53
2:C:1979:PHE:CD1	2:C:1993:ARG:HG2	2.44	0.53
2:C:3216:GLU:HA	2:C:3219:VAL:HG22	1.90	0.53
2:A:28:ILE:HG22	2:A:29:HIS:HD2	1.73	0.53
2:A:996:VAL:HG22	2:A:1054:VAL:HG21	1.90	0.53
2:A:1256:PRO:HG3	2:A:1453:TYR:HB2	1.90	0.53
2:A:1936:LEU:HD21	2:A:1976:LEU:HD13	1.91	0.53
2:B:1124:PRO:HD2	2:B:1594:VAL:HG23	1.90	0.53
2:C:2562:THR:O	2:C:2566:ARG:HG3	2.08	0.53
2:C:3900:GLU:OE2	2:C:3904:ARG:NH2	2.41	0.53
2:D:71:GLN:HB3	2:D:73:LEU:HD23	1.90	0.53
2:D:246:THR:HG21	2:D:267:VAL:HG11	1.89	0.53
1:I:100:TYR:CD1	1:I:138:ASN:HB3	2.43	0.53
2:A:3246:MET:HG2	2:A:3309:LYS:HZ1	1.72	0.53
2:A:3900:GLU:OE2	2:A:3904:ARG:NH2	2.41	0.53
2:B:996:VAL:HG22	2:B:1054:VAL:HG21	1.89	0.53
2:B:3312:PRO:HA	2:B:3315:LEU:HB2	1.89	0.53
2:C:4049:HIS:CD2	2:C:4067:LEU:HD11	2.43	0.53
2:C:4633:LEU:O	2:C:4704:LYS:NZ	2.41	0.53
2:D:1144:ARG:NE	2:D:1150:GLU:OE2	2.42	0.53
2:D:2512:MET:HA	2:D:2512:MET:CE	2.35	0.53
2:D:3131:TYR:CD2	2:D:3205:CYS:HB3	2.38	0.53
2:A:1144:ARG:NE	2:A:1150:GLU:OE2	2.42	0.53
2:A:2593:VAL:HG12	2:A:2644:LEU:HB2	1.90	0.53
1:K:134:ASP:OD1	2:C:3298:ARG:NH1	2.42	0.53
2:B:801:ARG:HG2	2:B:1618:LEU:HA	1.91	0.53
2:B:1936:LEU:HD21	2:B:1976:LEU:HD13	1.91	0.53
2:B:3861:GLN:H	2:B:3867:THR:HG23	1.74	0.53
2:B:3900:GLU:OE2	2:B:3904:ARG:NH2	2.41	0.53
2:B:3950:VAL:O	2:B:3954:MET:HB2	2.08	0.53
2:C:1007:TRP:O	2:C:1011:ARG:HG2	2.07	0.53
2:C:1256:PRO:HG3	2:C:1453:TYR:HB2	1.90	0.53
2:C:1957:LEU:HB2	2:C:3601:ALA:HB2	1.91	0.53
2:C:3013:VAL:O	2:C:3018:ARG:NH2	2.39	0.53
2:D:2779:LEU:O	2:D:2783:LEU:HD12	2.08	0.53
2:A:173:GLU:OE2	2:A:176:ARG:NH2	2.36	0.53
2:A:2290:TRP:CZ2	2:A:2388:ILE:HG12	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:4633:LEU:O	2:A:4704:LYS:NZ	2.41	0.53
2:B:71:GLN:HB3	2:B:73:LEU:HD23	1.90	0.53
2:B:436:LEU:HG	2:B:445:VAL:HG11	1.91	0.53
2:B:2493:LEU:HG	2:B:2497:ARG:HH21	1.74	0.53
2:B:2779:LEU:O	2:B:2783:LEU:HD12	2.08	0.53
2:D:801:ARG:HG2	2:D:1618:LEU:HA	1.91	0.53
2:D:849:ASP:OD1	2:D:1214:ARG:NE	2.37	0.53
2:D:1124:PRO:HD2	2:D:1594:VAL:HG23	1.90	0.53
2:D:2290:TRP:CZ2	2:D:2388:ILE:HG12	2.44	0.53
2:D:2779:LEU:HA	2:D:2782:MET:HG2	1.91	0.53
2:A:842:GLN:HB2	2:A:1603:PHE:HB2	1.90	0.53
2:A:3216:GLU:HA	2:A:3219:VAL:HG22	1.90	0.53
2:A:3283:ILE:O	2:A:3287:ASN:HB2	2.08	0.53
2:A:4049:HIS:CD2	2:A:4067:LEU:HD11	2.43	0.53
2:A:4559:TYR:OH	2:B:4790:ARG:NH2	2.42	0.53
2:B:185:SER:OG	2:B:188:SER:OG	2.20	0.53
2:B:1144:ARG:NE	2:B:1150:GLU:OE2	2.42	0.53
2:C:1144:ARG:NE	2:C:1150:GLU:OE2	2.42	0.53
2:D:1431:ARG:NH1	2:D:1556:GLU:OE2	2.42	0.53
2:D:2905:ARG:HE	2:D:2906:GLY:H	1.57	0.53
2:D:3125:ASP:HB2	2:D:3195:LEU:HD22	1.91	0.53
2:D:4049:HIS:CD2	2:D:4067:LEU:HD11	2.43	0.53
2:A:1979:PHE:CD1	2:A:1993:ARG:HG2	2.44	0.53
2:A:2493:LEU:HG	2:A:2497:ARG:HH21	1.74	0.53
2:A:2905:ARG:HE	2:A:2906:GLY:H	1.57	0.53
2:A:3125:ASP:HB2	2:A:3195:LEU:HD22	1.91	0.53
2:B:3102:LEU:HD21	2:B:3155:LEU:HD23	1.91	0.53
2:C:28:ILE:HG22	2:C:29:HIS:HD2	1.73	0.53
2:C:2779:LEU:O	2:C:2783:LEU:HD12	2.09	0.53
2:C:2905:ARG:HE	2:C:2906:GLY:H	1.57	0.53
2:D:658:ASN:ND2	2:D:833:LYS:HG2	2.24	0.53
2:D:3312:PRO:HA	2:D:3315:LEU:HB2	1.89	0.53
2:A:919:VAL:HB	2:A:923:LYS:HE3	1.91	0.53
2:A:2562:THR:O	2:A:2566:ARG:HG3	2.08	0.53
1:J:10:ILE:O	1:J:14:LYS:N	2.38	0.53
1:J:114:GLY:O	1:J:116:LYS:NZ	2.31	0.53
2:B:1256:PRO:HG3	2:B:1453:TYR:HB2	1.90	0.53
2:B:3125:ASP:HB2	2:B:3195:LEU:HD22	1.91	0.53
2:B:3131:TYR:CD1	2:B:3205:CYS:HB2	2.41	0.53
2:C:71:GLN:HB3	2:C:73:LEU:HD23	1.90	0.53
2:C:173:GLU:OE2	2:C:176:ARG:NH2	2.36	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2859:GLU:O	2:C:2862:SER:OG	2.23	0.53
2:C:3125:ASP:HB2	2:C:3195:LEU:HD22	1.91	0.53
2:C:3861:GLN:H	2:C:3867:THR:HG23	1.74	0.53
2:D:233:VAL:HG12	2:D:274:LEU:HD22	1.91	0.53
2:D:1419:PHE:O	2:D:1423:THR:HB	2.09	0.53
2:D:1978:ASN:HB2	2:D:1986:CYS:HB3	1.91	0.53
1:I:69:PHE:O	1:I:73:MET:HG2	2.10	0.52
2:A:713:TRP:HH2	2:A:1251:LEU:HD21	1.73	0.52
2:A:801:ARG:HG2	2:A:1618:LEU:HA	1.91	0.52
2:A:3102:LEU:HD21	2:A:3155:LEU:HD23	1.91	0.52
2:A:3890:TRP:HB3	2:B:76:ARG:HG2	1.90	0.52
3:G:50:ARG:HH21	3:G:53:LYS:HZ2	1.57	0.52
2:B:605:GLY:HA2	2:B:1585:ARG:HD2	1.91	0.52
2:B:1611:ILE:HB	2:B:1615:GLN:HB2	1.91	0.52
2:B:2059:GLN:NE2	2:B:2091:GLN:O	2.42	0.52
2:B:2593:VAL:HG12	2:B:2644:LEU:HB2	1.90	0.52
2:B:3016:ARG:O	2:B:3018:ARG:NE	2.32	0.52
2:C:668:ALA:HB2	2:C:1012:ILE:HD11	1.92	0.52
2:C:996:VAL:HG22	2:C:1054:VAL:HG21	1.90	0.52
2:D:713:TRP:HH2	2:D:1251:LEU:HD21	1.73	0.52
2:A:28:ILE:HG22	2:A:29:HIS:CD2	2.44	0.52
2:A:1184:ASP:OD2	2:A:1193:LYS:NZ	2.38	0.52
2:A:1419:PHE:O	2:A:1423:THR:HB	2.09	0.52
2:B:28:ILE:HG22	2:B:29:HIS:CD2	2.45	0.52
2:B:919:VAL:HB	2:B:923:LYS:HE3	1.91	0.52
2:B:1957:LEU:HB2	2:B:3601:ALA:HB2	1.91	0.52
2:B:2905:ARG:HE	2:B:2906:GLY:H	1.57	0.52
2:C:629:GLN:OE1	2:C:1669:ASN:ND2	2.37	0.52
2:C:658:ASN:ND2	2:C:833:LYS:HG2	2.24	0.52
2:C:1419:PHE:O	2:C:1423:THR:HB	2.09	0.52
2:D:1435:GLY:H	2:D:1500:ARG:NH2	2.06	0.52
2:D:2859:GLU:O	2:D:2862:SER:OG	2.23	0.52
2:D:2923:TYR:HA	2:D:3003:MET:HE1	1.91	0.52
2:D:3861:GLN:H	2:D:3867:THR:HG23	1.74	0.52
2:A:233:VAL:HG12	2:A:274:LEU:HD22	1.91	0.52
1:K:69:PHE:O	1:K:73:MET:HG2	2.10	0.52
2:C:3246:MET:HG2	2:C:3309:LYS:HZ1	1.75	0.52
2:D:668:ALA:HB2	2:D:1012:ILE:HD11	1.92	0.52
2:D:1979:PHE:CD1	2:D:1993:ARG:HG2	2.44	0.52
2:A:71:GLN:HB3	2:A:73:LEU:HD23	1.90	0.52
2:A:1978:ASN:HB2	2:A:1986:CYS:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:4790:ARG:HH22	2:D:4557:VAL:HG21	1.74	0.52
2:C:2831:VAL:CG2	2:D:1435:GLY:HA2	2.39	0.52
2:D:28:ILE:HG22	2:D:29:HIS:HD2	1.73	0.52
2:D:1936:LEU:HD21	2:D:1976:LEU:HD13	1.91	0.52
2:A:1957:LEU:HB2	2:A:3601:ALA:HB2	1.91	0.52
1:K:110:MET:HA	2:C:3590:LEU:HD21	1.92	0.52
2:B:3216:GLU:HA	2:B:3219:VAL:HG22	1.90	0.52
2:C:1431:ARG:NH1	2:C:1556:GLU:OE2	2.42	0.52
2:C:2290:TRP:CZ2	2:C:2388:ILE:HG12	2.44	0.52
2:C:3109:PHE:HB3	2:C:3162:PHE:HA	1.91	0.52
2:D:4081:GLU:O	2:D:4085:LYS:HG3	2.10	0.52
2:D:4520:TYR:CE2	2:D:4559:TYR:HB3	2.45	0.52
2:A:658:ASN:ND2	2:A:833:LYS:HG2	2.24	0.52
2:A:1842:ILE:HD12	2:A:1845:LEU:HD12	1.90	0.52
2:B:658:ASN:ND2	2:B:833:LYS:HG2	2.24	0.52
2:B:903:GLN:N	2:B:913:ARG:HE	2.07	0.52
2:B:2562:THR:O	2:B:2566:ARG:HG3	2.08	0.52
2:B:4049:HIS:CD2	2:B:4067:LEU:HD11	2.43	0.52
2:C:897:LYS:HD2	2:C:902:TRP:CD1	2.45	0.52
2:C:2593:VAL:HG12	2:C:2644:LEU:HB2	1.90	0.52
2:D:1611:ILE:HB	2:D:1615:GLN:HB2	1.91	0.52
2:A:2779:LEU:O	2:A:2783:LEU:HD12	2.08	0.52
2:A:3319:PHE:O	2:A:3322:LEU:HG	2.10	0.52
2:A:3861:GLN:H	2:A:3867:THR:HG23	1.74	0.52
2:B:467:ASP:HB3	2:B:470:LEU:HG	1.92	0.52
2:B:1038:LEU:O	2:B:1043:LYS:NZ	2.36	0.52
2:B:2973:GLN:HA	2:B:2976:LYS:HZ2	1.75	0.52
2:B:4518:LEU:HD12	2:C:4809:MET:HG3	1.92	0.52
2:C:1936:LEU:HD21	2:C:1976:LEU:HD13	1.91	0.52
2:C:3108:LEU:HA	2:C:3111:HIS:CD2	2.45	0.52
2:C:3134:LEU:HD22	2:C:3162:PHE:HE2	1.74	0.52
2:C:4081:GLU:O	2:C:4085:LYS:HG3	2.10	0.52
2:D:436:LEU:HG	2:D:445:VAL:HG11	1.91	0.52
2:D:919:VAL:HB	2:D:923:LYS:HE3	1.91	0.52
2:D:2059:GLN:NE2	2:D:2091:GLN:O	2.42	0.52
2:D:3319:PHE:O	2:D:3322:LEU:HG	2.10	0.52
2:A:37:LEU:HA	2:A:49:LEU:HD23	1.92	0.52
2:A:114:LEU:HB2	2:A:117:HIS:CE1	2.45	0.52
2:A:1431:ARG:NH1	2:A:1556:GLU:OE2	2.42	0.52
2:A:1611:ILE:HB	2:A:1615:GLN:HB2	1.91	0.52
2:A:4520:TYR:CE2	2:A:4559:TYR:HB3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:24:VAL:HG22	3:E:48:LYS:HG2	1.92	0.52
2:B:114:LEU:HB2	2:B:117:HIS:CE1	2.45	0.52
2:B:173:GLU:OE2	2:B:176:ARG:NH2	2.36	0.52
2:B:1431:ARG:NH1	2:B:1556:GLU:OE2	2.42	0.52
2:B:2729:HIS:HB2	2:B:2771:TYR:HE2	1.75	0.52
2:B:2779:LEU:HA	2:B:2782:MET:HG2	1.91	0.52
2:B:3134:LEU:HD22	2:B:3162:PHE:HE2	1.74	0.52
2:B:3319:PHE:O	2:B:3322:LEU:HG	2.10	0.52
2:C:233:VAL:HG12	2:C:274:LEU:HD22	1.91	0.52
2:C:2059:GLN:NE2	2:C:2091:GLN:O	2.42	0.52
2:C:4584:PHE:O	2:C:4588:ILE:HG13	2.10	0.52
2:A:903:GLN:N	2:A:913:ARG:HE	2.07	0.52
2:A:2059:GLN:NE2	2:A:2091:GLN:O	2.42	0.52
2:A:2763:LEU:HD23	2:A:2767:GLU:HG2	1.92	0.52
2:B:4584:PHE:O	2:B:4588:ILE:HG13	2.10	0.52
2:C:605:GLY:HA2	2:C:1585:ARG:HD2	1.91	0.52
2:C:1435:GLY:H	2:C:1500:ARG:NH2	2.06	0.52
2:D:114:LEU:HB2	2:D:117:HIS:CE1	2.45	0.52
2:D:3216:GLU:HA	2:D:3219:VAL:HG22	1.90	0.52
2:A:1135:PHE:CE2	2:A:1146:HIS:CD2	2.98	0.52
2:A:3125:ASP:H	2:A:3183:ILE:HD11	1.75	0.52
2:B:3109:PHE:HB3	2:B:3162:PHE:HA	1.91	0.52
2:C:114:LEU:HB2	2:C:117:HIS:CE1	2.45	0.52
2:C:1135:PHE:CE2	2:C:1146:HIS:CD2	2.98	0.52
2:C:4520:TYR:CE2	2:C:4559:TYR:HB3	2.45	0.52
2:D:1957:LEU:HB2	2:D:3601:ALA:HB2	1.91	0.52
2:D:3109:PHE:HB3	2:D:3162:PHE:HA	1.91	0.52
2:A:436:LEU:HG	2:A:445:VAL:HG11	1.91	0.51
2:A:2729:HIS:HB2	2:A:2771:TYR:HE2	1.75	0.51
2:A:3925:GLN:NE2	2:A:4934:THR:HA	2.26	0.51
2:B:2290:TRP:CZ2	2:B:2388:ILE:HG12	2.44	0.51
2:B:2763:LEU:HD23	2:B:2767:GLU:HG2	1.92	0.51
2:C:925:PRO:HB2	2:C:928:GLU:OE1	2.10	0.51
2:C:3131:TYR:CD1	2:C:3205:CYS:HB2	2.41	0.51
2:D:467:ASP:HB3	2:D:470:LEU:HG	1.92	0.51
2:D:925:PRO:HB2	2:D:928:GLU:OE1	2.10	0.51
2:D:1685:LEU:O	2:D:1689:ILE:HG12	2.10	0.51
2:D:2729:HIS:HB2	2:D:2771:TYR:HE2	1.75	0.51
2:A:1685:LEU:O	2:A:1689:ILE:HG12	2.10	0.51
1:K:42:GLN:HE21	2:C:1957:LEU:HD21	1.75	0.51
2:B:1135:PHE:CE2	2:B:1146:HIS:CD2	2.98	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1419:PHE:O	2:B:1423:THR:HB	2.09	0.51
2:C:3183:ILE:HD12	2:C:3187:LYS:HE3	1.93	0.51
2:D:185:SER:OG	2:D:188:SER:OG	2.20	0.51
2:D:897:LYS:HD2	2:D:902:TRP:CD1	2.45	0.51
2:A:897:LYS:HD2	2:A:902:TRP:CD1	2.45	0.51
2:A:3108:LEU:HA	2:A:3111:HIS:CD2	2.45	0.51
1:J:69:PHE:O	1:J:73:MET:HG2	2.10	0.51
2:B:1978:ASN:HB2	2:B:1986:CYS:HB3	1.91	0.51
2:C:919:VAL:HB	2:C:923:LYS:HE3	1.92	0.51
2:C:1611:ILE:HB	2:C:1615:GLN:HB2	1.91	0.51
2:C:2493:LEU:HG	2:C:2497:ARG:HH21	1.74	0.51
2:C:2779:LEU:HA	2:C:2782:MET:HG2	1.91	0.51
2:C:4252:ILE:HG21	2:D:4707:MET:HG2	1.92	0.51
2:D:3921:THR:O	2:D:3925:GLN:HG2	2.10	0.51
2:D:4026:LEU:HD13	2:D:4058:TYR:CE2	2.46	0.51
2:A:3183:ILE:HD12	2:A:3187:LYS:HE3	1.93	0.51
1:L:69:PHE:O	1:L:73:MET:HG2	2.10	0.51
2:B:233:VAL:HG12	2:B:274:LEU:HD22	1.91	0.51
2:B:3125:ASP:H	2:B:3183:ILE:HD11	1.75	0.51
2:C:2973:GLN:HA	2:C:2976:LYS:HZ2	1.76	0.51
2:C:3925:GLN:NE2	2:C:4934:THR:HA	2.26	0.51
2:D:37:LEU:HA	2:D:49:LEU:HD23	1.92	0.51
2:D:3102:LEU:HD21	2:D:3155:LEU:HD23	1.91	0.51
2:D:3108:LEU:HA	2:D:3111:HIS:CD2	2.45	0.51
2:A:2785:TRP:HD1	2:A:2905:ARG:HH22	1.59	0.51
2:A:3151:GLN:HE22	2:A:3155:LEU:HD11	1.76	0.51
2:A:4196:THR:HB	2:A:4919:LEU:HD11	1.93	0.51
2:A:4584:PHE:O	2:A:4588:ILE:HG13	2.10	0.51
2:A:4661:TYR:HB3	2:A:4665:ARG:NH2	2.26	0.51
2:B:1922:ILE:O	2:B:1926:VAL:HG23	2.11	0.51
2:B:3151:GLN:HE22	2:B:3155:LEU:HD11	1.76	0.51
2:B:3183:ILE:HD12	2:B:3187:LYS:HE3	1.93	0.51
2:C:28:ILE:HG22	2:C:29:HIS:CD2	2.44	0.51
2:C:1978:ASN:HB2	2:C:1986:CYS:HB3	1.91	0.51
2:D:2785:TRP:HD1	2:D:2905:ARG:HH22	1.59	0.51
2:D:3131:TYR:CD1	2:D:3205:CYS:HB2	2.41	0.51
2:D:3925:GLN:NE2	2:D:4934:THR:HA	2.26	0.51
2:D:4661:TYR:HB3	2:D:4665:ARG:NH2	2.26	0.51
2:A:2779:LEU:HA	2:A:2782:MET:HG2	1.91	0.51
2:A:3879:LEU:O	2:A:3882:GLN:HG3	2.11	0.51
2:B:4196:THR:HB	2:B:4919:LEU:HD11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:903:GLN:N	2:C:913:ARG:HE	2.07	0.51
2:C:1685:LEU:O	2:C:1689:ILE:HG12	2.10	0.51
2:C:2729:HIS:HB2	2:C:2771:TYR:HE2	1.75	0.51
2:C:4011:GLU:HG2	2:C:4121:LEU:HD13	1.93	0.51
2:D:1135:PHE:CE2	2:D:1146:HIS:CD2	2.98	0.51
2:D:2134:MET:HG2	2:D:2178:VAL:HG22	1.93	0.51
2:D:3183:ILE:HD12	2:D:3187:LYS:HE3	1.93	0.51
2:D:4670:LEU:HB2	2:D:4672:MET:HE1	1.91	0.51
2:A:3134:LEU:HD22	2:A:3162:PHE:HE2	1.74	0.51
2:B:668:ALA:HB2	2:B:1012:ILE:HD11	1.92	0.51
2:B:925:PRO:HB2	2:B:928:GLU:OE1	2.10	0.51
2:B:4011:GLU:HG2	2:B:4121:LEU:HD13	1.93	0.51
2:D:62:LEU:O	2:D:66:THR:HG23	2.11	0.51
2:D:2493:LEU:HG	2:D:2497:ARG:HH21	1.74	0.51
2:D:2587:HIS:HA	2:D:2590:ARG:HG2	1.93	0.51
2:D:3134:LEU:HD22	2:D:3162:PHE:HE2	1.74	0.51
2:D:4196:THR:HB	2:D:4919:LEU:HD11	1.93	0.51
2:D:4584:PHE:O	2:D:4588:ILE:HG13	2.10	0.51
2:A:467:ASP:HB3	2:A:470:LEU:HG	1.92	0.51
2:A:891:GLU:C	2:A:895:MET:HE1	2.31	0.51
2:A:3921:THR:O	2:A:3925:GLN:HG2	2.10	0.51
2:B:897:LYS:HD2	2:B:902:TRP:CD1	2.45	0.51
2:B:2080:LEU:O	2:B:2084:MET:HG3	2.11	0.51
2:B:3108:LEU:HA	2:B:3111:HIS:CD2	2.45	0.51
2:B:4026:LEU:HD13	2:B:4058:TYR:CE2	2.46	0.51
2:B:4661:TYR:HB3	2:B:4665:ARG:NH2	2.26	0.51
2:C:62:LEU:O	2:C:66:THR:HG23	2.11	0.51
2:C:1922:ILE:O	2:C:1926:VAL:HG23	2.11	0.51
2:C:2134:MET:HG2	2:C:2178:VAL:HG22	1.93	0.51
2:C:2905:ARG:HG3	2:C:2907:PHE:H	1.76	0.51
2:D:903:GLN:N	2:D:913:ARG:HE	2.07	0.51
2:D:2250:ASN:HB3	2:D:2253:LEU:HB2	1.93	0.51
2:D:2758:LYS:NZ	2:D:2763:LEU:HA	2.26	0.51
2:D:3151:GLN:HE22	2:D:3155:LEU:HD11	1.76	0.51
2:A:668:ALA:HB2	2:A:1012:ILE:HD11	1.92	0.51
2:A:2587:HIS:HA	2:A:2590:ARG:HG2	1.93	0.51
2:A:2765:GLU:HG3	2:A:2769:GLU:OE2	2.11	0.51
2:A:3109:PHE:HB3	2:A:3162:PHE:HA	1.91	0.51
2:A:4081:GLU:O	2:A:4085:LYS:HG3	2.10	0.51
3:F:24:VAL:HG22	3:F:48:LYS:HG2	1.92	0.51
3:H:24:VAL:HG22	3:H:48:LYS:HG2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2988:ARG:HB2	2:B:2989:PRO:HD3	1.93	0.51
2:C:2785:TRP:HD1	2:C:2905:ARG:HH22	1.59	0.51
2:C:3921:THR:O	2:C:3925:GLN:HG2	2.10	0.51
2:D:28:ILE:HG22	2:D:29:HIS:CD2	2.44	0.51
2:D:2763:LEU:HD23	2:D:2767:GLU:HG2	1.92	0.51
2:D:4011:GLU:HG2	2:D:4121:LEU:HD13	1.93	0.51
1:I:10:ILE:O	1:I:14:LYS:N	2.38	0.51
1:I:134:ASP:HA	2:A:3298:ARG:HG3	1.93	0.51
2:A:3805:LEU:HD11	2:A:3887:ASP:HB3	1.93	0.51
2:A:4026:LEU:HD13	2:A:4058:TYR:CE2	2.46	0.51
2:A:4569:GLU:HB3	2:A:4570:PRO:HD3	1.93	0.51
2:B:891:GLU:C	2:B:895:MET:HE1	2.32	0.51
2:B:3131:TYR:OH	2:B:3205:CYS:O	2.23	0.51
2:C:2080:LEU:O	2:C:2084:MET:HG3	2.11	0.51
2:C:2765:GLU:HG3	2:C:2769:GLU:OE2	2.11	0.51
2:C:3151:GLN:HE22	2:C:3155:LEU:HD11	1.76	0.51
2:C:4026:LEU:HD13	2:C:4058:TYR:CE2	2.46	0.51
2:D:629:GLN:OE1	2:D:1669:ASN:ND2	2.37	0.51
2:D:891:GLU:C	2:D:895:MET:HE1	2.31	0.51
2:D:3805:LEU:HD11	2:D:3887:ASP:HB3	1.93	0.51
2:A:3215:MET:O	2:A:3219:VAL:HG13	2.11	0.50
2:A:4011:GLU:HG2	2:A:4121:LEU:HD13	1.93	0.50
2:B:37:LEU:HA	2:B:49:LEU:HD23	1.92	0.50
2:B:1435:GLY:H	2:B:1500:ARG:NH2	2.06	0.50
2:B:3925:GLN:NE2	2:B:4934:THR:HA	2.26	0.50
2:B:4520:TYR:CE2	2:B:4559:TYR:HB3	2.45	0.50
2:C:3016:ARG:O	2:C:3018:ARG:NE	2.32	0.50
2:C:3102:LEU:HD21	2:C:3155:LEU:HD23	1.91	0.50
2:C:3125:ASP:H	2:C:3183:ILE:HD11	1.75	0.50
2:C:3319:PHE:O	2:C:3322:LEU:HG	2.10	0.50
2:D:674:TYR:HE1	2:D:756:SER:HB3	1.76	0.50
2:A:925:PRO:HB2	2:A:928:GLU:OE1	2.10	0.50
2:A:2988:ARG:HB2	2:A:2989:PRO:HD3	1.93	0.50
3:G:24:VAL:HG22	3:G:48:LYS:HG2	1.92	0.50
2:B:1685:LEU:O	2:B:1689:ILE:HG12	2.10	0.50
2:B:1935:LYS:HE3	2:B:1995:GLN:HE22	1.76	0.50
2:B:3879:LEU:O	2:B:3882:GLN:HG3	2.11	0.50
2:C:4661:TYR:HB3	2:C:4665:ARG:NH2	2.26	0.50
2:D:2988:ARG:HB2	2:D:2989:PRO:HD3	1.93	0.50
2:D:3125:ASP:H	2:D:3183:ILE:HD11	1.76	0.50
2:D:4166:LYS:O	2:D:4170:ARG:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:674:TYR:HE1	2:A:756:SER:HB3	1.76	0.50
2:A:1922:ILE:O	2:A:1926:VAL:HG23	2.11	0.50
2:A:2758:LYS:NZ	2:A:2763:LEU:HA	2.26	0.50
2:B:2905:ARG:HG3	2:B:2907:PHE:H	1.76	0.50
2:B:3215:MET:O	2:B:3219:VAL:HG13	2.11	0.50
2:B:3921:THR:O	2:B:3925:GLN:HG2	2.10	0.50
2:B:4726:MET:O	2:B:4726:MET:HE3	2.11	0.50
2:C:1935:LYS:HE3	2:C:1995:GLN:HE22	1.76	0.50
2:C:3215:MET:O	2:C:3219:VAL:HG13	2.11	0.50
2:C:4154:GLU:O	2:C:4158:THR:HG23	2.12	0.50
2:D:3016:ARG:O	2:D:3018:ARG:NE	2.32	0.50
2:D:4055:HIS:CE1	2:D:4057:HIS:CD2	3.00	0.50
2:A:4057:HIS:HE1	2:B:4660:PHE:HZ	1.57	0.50
2:A:4154:GLU:O	2:A:4158:THR:HG23	2.12	0.50
2:B:1184:ASP:OD2	2:B:1193:LYS:NZ	2.38	0.50
2:B:4081:GLU:O	2:B:4085:LYS:HG3	2.10	0.50
2:B:4166:LYS:O	2:B:4170:ARG:HG2	2.11	0.50
2:C:2763:LEU:HD23	2:C:2767:GLU:HG2	1.92	0.50
2:D:1922:ILE:O	2:D:1926:VAL:HG23	2.11	0.50
2:D:4569:GLU:HB3	2:D:4570:PRO:HD3	1.94	0.50
2:A:62:LEU:O	2:A:66:THR:HG23	2.11	0.50
2:A:2134:MET:HG2	2:A:2178:VAL:HG22	1.93	0.50
2:A:2250:ASN:HB3	2:A:2253:LEU:HB2	1.93	0.50
2:A:4166:LYS:O	2:A:4170:ARG:HG2	2.11	0.50
2:B:2782:MET:HB2	2:B:2787:TRP:HE3	1.76	0.50
2:C:3292:GLU:O	2:C:3296:MET:HE2	2.12	0.50
2:C:4569:GLU:HB3	2:C:4570:PRO:HD3	1.94	0.50
2:D:1564:MET:SD	2:D:1565:PRO:HD2	2.52	0.50
2:A:4055:HIS:CE1	2:A:4057:HIS:CD2	3.00	0.50
1:J:106:LEU:HD22	2:B:3587:TRP:NE1	2.25	0.50
1:L:127:ARG:NH1	1:L:135:GLY:C	2.58	0.50
2:B:2758:LYS:NZ	2:B:2763:LEU:HA	2.26	0.50
2:B:2765:GLU:HG3	2:B:2769:GLU:OE2	2.11	0.50
2:B:2833:LEU:HB2	2:B:2838[A]:HIS:NE2	2.27	0.50
2:B:3677:THR:HB	2:B:3679:LYS:HZ2	1.77	0.50
2:B:4154:GLU:O	2:B:4158:THR:HG23	2.12	0.50
2:B:4569:GLU:HB3	2:B:4570:PRO:HD3	1.94	0.50
2:C:37:LEU:HA	2:C:49:LEU:HD23	1.92	0.50
2:C:891:GLU:C	2:C:895:MET:HE1	2.31	0.50
2:C:1014:GLN:O	2:C:1027:ARG:NH2	2.45	0.50
2:C:2054:LYS:HE2	2:C:2056:SER:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2250:ASN:HB3	2:C:2253:LEU:HB2	1.93	0.50
2:C:2782:MET:HB2	2:C:2787:TRP:HE3	1.76	0.50
2:D:506:HIS:CE1	2:D:530:LEU:HD21	2.47	0.50
2:D:1935:LYS:HE3	2:D:1995:GLN:HE22	1.76	0.50
2:A:1748:LEU:HB3	2:A:1751:ILE:HD13	1.94	0.50
2:A:2080:LEU:O	2:A:2084:MET:HG3	2.11	0.50
2:A:2782:MET:HB2	2:A:2787:TRP:HE3	1.76	0.50
2:A:2830:ASN:HB3	2:B:1435:GLY:HA3	1.94	0.50
2:B:2134:MET:HG2	2:B:2178:VAL:HG22	1.93	0.50
2:B:2250:ASN:HB3	2:B:2253:LEU:HB2	1.93	0.50
2:B:2859:GLU:O	2:B:2862:SER:OG	2.23	0.50
2:B:4055:HIS:CE1	2:B:4057:HIS:CD2	3.00	0.50
2:C:467:ASP:HB3	2:C:470:LEU:HG	1.92	0.50
2:C:3996:GLY:O	2:C:4000:VAL:HG23	2.12	0.50
2:C:4196:THR:HB	2:C:4919:LEU:HD11	1.93	0.50
2:C:4726:MET:HE3	2:C:4726:MET:O	2.11	0.50
2:D:1299:ILE:HD11	2:D:1544:PHE:HB3	1.94	0.50
2:D:3215:MET:O	2:D:3219:VAL:HG13	2.11	0.50
2:D:3246:MET:HG2	2:D:3309:LYS:HZ1	1.75	0.50
2:D:3879:LEU:O	2:D:3882:GLN:HG3	2.11	0.50
2:A:874:LEU:CD1	2:A:940:LEU:HD13	2.42	0.50
1:K:127:ARG:NH1	1:K:135:GLY:C	2.58	0.50
2:B:506:HIS:CE1	2:B:530:LEU:HD21	2.47	0.50
2:B:1014:GLN:O	2:B:1027:ARG:NH2	2.45	0.50
2:B:2587:HIS:HA	2:B:2590:ARG:HG2	1.93	0.50
2:B:2785:TRP:HD1	2:B:2905:ARG:HH22	1.59	0.50
2:C:2831:VAL:HG22	2:D:1435:GLY:HA2	1.94	0.50
2:C:2988:ARG:HB2	2:C:2989:PRO:HD3	1.93	0.50
2:C:3295:TRP:CD1	2:C:3296:MET:SD	3.05	0.50
2:D:874:LEU:CD1	2:D:940:LEU:HD13	2.42	0.50
2:D:2080:LEU:O	2:D:2084:MET:HG3	2.11	0.50
2:D:2765:GLU:HG3	2:D:2769:GLU:OE2	2.11	0.50
2:D:4154:GLU:O	2:D:4158:THR:HG23	2.12	0.50
2:A:318:ASP:O	2:A:322:ALA:HB2	2.12	0.50
2:A:1564:MET:SD	2:A:1565:PRO:HD2	2.52	0.50
2:A:3089:GLY:O	2:A:3093:ILE:HG12	2.12	0.50
2:A:3122:ILE:HA	2:A:3126:VAL:HB	1.94	0.50
2:A:4726:MET:O	2:A:4726:MET:HE3	2.11	0.50
2:B:66:THR:OG1	2:B:124:SER:OG	2.24	0.50
2:B:674:TYR:HE1	2:B:756:SER:HB3	1.77	0.50
2:B:3089:GLY:O	2:B:3093:ILE:HG12	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3118:GLY:O	2:B:3122:ILE:HG12	2.12	0.50
2:B:4670:LEU:HB2	2:B:4672:MET:HE1	1.94	0.50
2:B:4863:GLN:O	2:B:4867:ILE:HG12	2.12	0.50
2:C:2758:LYS:NZ	2:C:2763:LEU:HA	2.26	0.50
2:C:4055:HIS:CE1	2:C:4057:HIS:CD2	3.00	0.50
2:C:4166:LYS:O	2:C:4170:ARG:HG2	2.11	0.50
2:D:238:HIS:ND1	2:D:243:GLU:OE2	2.45	0.50
2:D:2054:LYS:HE2	2:D:2056:SER:HA	1.94	0.50
2:D:3089:GLY:O	2:D:3093:ILE:HG12	2.12	0.50
2:A:474:ASP:O	2:A:478:ARG:HG2	2.12	0.49
2:A:3295:TRP:CD1	2:A:3296:MET:SD	3.05	0.49
2:B:3046:MET:HG3	2:B:3121:LEU:HA	1.94	0.49
2:B:3295:TRP:CD1	2:B:3296:MET:SD	3.05	0.49
2:C:1564:MET:SD	2:C:1565:PRO:HD2	2.52	0.49
2:C:3118:GLY:O	2:C:3122:ILE:HG12	2.12	0.49
2:C:3805:LEU:HD21	2:C:3888:PHE:HA	1.94	0.49
2:D:1014:GLN:O	2:D:1027:ARG:NH2	2.45	0.49
2:D:1184:ASP:OD2	2:D:1193:LYS:NZ	2.38	0.49
2:D:4726:MET:O	2:D:4726:MET:HE3	2.11	0.49
2:A:506:HIS:CE1	2:A:530:LEU:HD21	2.47	0.49
2:B:62:LEU:O	2:B:66:THR:HG23	2.11	0.49
2:C:317:MET:HE2	2:C:321:LYS:HD2	1.94	0.49
2:C:674:TYR:HE1	2:C:756:SER:HB3	1.76	0.49
2:C:1299:ILE:HD11	2:C:1544:PHE:HB3	1.94	0.49
2:C:3805:LEU:HD11	2:C:3887:ASP:HB3	1.93	0.49
2:D:474:ASP:O	2:D:478:ARG:HG2	2.12	0.49
2:D:2833:LEU:HB2	2:D:2838[A]:HIS:NE2	2.27	0.49
2:D:3122:ILE:HA	2:D:3126:VAL:HB	1.94	0.49
2:A:2905:ARG:HG3	2:A:2907:PHE:H	1.76	0.49
2:A:3996:GLY:O	2:A:4000:VAL:HG23	2.12	0.49
2:A:4507:LEU:HD21	2:A:4746:ILE:HG22	1.94	0.49
2:B:995:MET:HA	2:B:998:LYS:HD3	1.94	0.49
2:B:2833:LEU:HB2	2:B:2838[B]:HIS:NE2	2.28	0.49
2:C:238:HIS:ND1	2:C:243:GLU:OE2	2.45	0.49
2:C:506:HIS:CE1	2:C:530:LEU:HD21	2.47	0.49
2:C:874:LEU:CD1	2:C:940:LEU:HD13	2.42	0.49
2:C:3879:LEU:O	2:C:3882:GLN:HG3	2.11	0.49
2:D:2924:SER:O	2:D:2928:GLN:HG2	2.12	0.49
2:D:3295:TRP:CD1	2:D:3296:MET:SD	3.05	0.49
2:D:3805:LEU:HD21	2:D:3888:PHE:HA	1.94	0.49
1:I:127:ARG:NH1	1:I:135:GLY:C	2.58	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:995:MET:HA	2:A:998:LYS:HD3	1.94	0.49
2:A:1014:GLN:O	2:A:1027:ARG:NH2	2.45	0.49
2:A:2768:LYS:HB3	2:A:2772:ARG:HH21	1.77	0.49
2:B:115:TYR:OH	2:B:179:ASP:OD2	2.31	0.49
2:B:3848:GLU:OE1	2:B:3922:GLU:OE1	2.29	0.49
2:B:4021:LEU:HD22	2:B:4128:TYR:CE2	2.48	0.49
2:C:2587:HIS:HA	2:C:2590:ARG:HG2	1.93	0.49
2:C:3089:GLY:O	2:C:3093:ILE:HG12	2.12	0.49
2:D:318:ASP:O	2:D:322:ALA:HB2	2.12	0.49
2:D:2905:ARG:HG3	2:D:2907:PHE:H	1.76	0.49
2:D:3677:THR:HB	2:D:3679:LYS:HZ2	1.76	0.49
2:D:4863:GLN:O	2:D:4867:ILE:HG12	2.12	0.49
2:A:1040:ASP:HA	2:A:1043:LYS:HG2	1.95	0.49
2:A:2833:LEU:HB2	2:A:2838[A]:HIS:NE2	2.27	0.49
2:A:3046:MET:HG3	2:A:3121:LEU:HA	1.94	0.49
2:A:3118:GLY:O	2:A:3122:ILE:HG12	2.12	0.49
2:A:4769:LEU:HB3	2:D:4753:LEU:HD11	1.94	0.49
2:B:318:ASP:O	2:B:322:ALA:HB2	2.12	0.49
2:B:2691:LYS:HA	2:B:2704:GLN:HE22	1.78	0.49
2:B:3805:LEU:HD11	2:B:3887:ASP:HB3	1.93	0.49
2:B:4753:LEU:HG	2:C:4773:LEU:HD22	1.94	0.49
2:C:318:ASP:O	2:C:322:ALA:HB2	2.12	0.49
2:C:1685:LEU:HD22	2:C:1706:LEU:HB2	1.95	0.49
2:C:4055:HIS:CE1	2:C:4057:HIS:HD2	2.31	0.49
2:C:4268:MET:HA	2:C:4271:VAL:HG22	1.94	0.49
2:D:317:MET:HE2	2:D:321:LYS:HD2	1.95	0.49
2:D:3996:GLY:O	2:D:4000:VAL:HG23	2.12	0.49
2:D:4271:VAL:HA	2:D:4274:MET:HG2	1.95	0.49
2:A:1299:ILE:HD11	2:A:1544:PHE:HB3	1.94	0.49
2:A:1935:LYS:HE3	2:A:1995:GLN:HE22	1.76	0.49
2:B:238:HIS:ND1	2:B:243:GLU:OE2	2.45	0.49
2:B:317:MET:HE2	2:B:321:LYS:HD2	1.94	0.49
2:B:4667:SER:HA	2:B:4672:MET:HE3	1.94	0.49
2:C:474:ASP:O	2:C:478:ARG:HG2	2.12	0.49
2:D:1040:ASP:HA	2:D:1043:LYS:HG2	1.95	0.49
2:D:2691:LYS:HA	2:D:2704:GLN:HE22	1.78	0.49
2:A:115:TYR:OH	2:A:179:ASP:OD2	2.31	0.49
2:A:2087:LEU:O	2:A:2091:GLN:HG2	2.13	0.49
2:A:4271:VAL:HA	2:A:4274:MET:HG2	1.95	0.49
2:B:1299:ILE:HD11	2:B:1544:PHE:HB3	1.94	0.49
2:B:3996:GLY:O	2:B:4000:VAL:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4507:LEU:HD21	2:B:4746:ILE:HG22	1.94	0.49
2:C:2924:SER:O	2:C:2928:GLN:HG2	2.12	0.49
2:D:1104:GLU:OE1	2:D:1225:LYS:NZ	2.44	0.49
2:D:2961:LYS:HB2	2:D:2965:LYS:HZ3	1.78	0.49
2:D:4507:LEU:HD21	2:D:4746:ILE:HG22	1.94	0.49
2:A:889:ILE:HA	2:A:892:LEU:HD12	1.95	0.49
2:A:2859:GLU:O	2:A:2862:SER:OG	2.23	0.49
2:B:2054:LYS:HE2	2:B:2056:SER:HA	1.94	0.49
2:C:2833:LEU:HB2	2:C:2838[A]:HIS:NE2	2.27	0.49
2:D:2496:LEU:HD23	2:D:2520:LEU:HD13	1.95	0.49
2:D:2768:LYS:HB3	2:D:2772:ARG:HH21	1.77	0.49
2:D:3046:MET:HG3	2:D:3121:LEU:HA	1.94	0.49
2:A:2691:LYS:HA	2:A:2704:GLN:HE22	1.78	0.49
2:A:2833:LEU:HB2	2:A:2838[B]:HIS:NE2	2.28	0.49
1:J:59:ASP:N	1:J:68:GLU:OE2	2.33	0.49
2:B:1564:MET:SD	2:B:1565:PRO:HD2	2.52	0.49
2:B:2768:LYS:HB3	2:B:2772:ARG:HH21	1.77	0.49
2:B:3096:TYR:CE2	2:B:3101:LEU:HD13	2.48	0.49
2:B:4155:SER:O	2:B:4159:GLN:HG2	2.13	0.49
2:B:4573:ARG:NH2	2:B:4736:ASN:OD1	2.46	0.49
2:C:115:TYR:OH	2:C:179:ASP:OD2	2.31	0.49
2:C:1004:HIS:NE2	2:C:1038:LEU:HD21	2.28	0.49
2:C:1040:ASP:HA	2:C:1043:LYS:HG2	1.95	0.49
2:C:1522:ALA:HB3	2:C:1527:LEU:HD21	1.95	0.49
2:C:2156:TYR:HE1	2:C:2202:TYR:HE2	1.60	0.49
2:C:3046:MET:HG3	2:C:3121:LEU:HA	1.94	0.49
2:C:3096:TYR:CE2	2:C:3101:LEU:HD13	2.48	0.49
2:D:1685:LEU:HD22	2:D:1706:LEU:HB2	1.95	0.49
2:D:3096:TYR:CE2	2:D:3101:LEU:HD13	2.48	0.49
2:D:3118:GLY:O	2:D:3122:ILE:HG12	2.12	0.49
2:D:4055:HIS:CE1	2:D:4057:HIS:HD2	2.31	0.49
2:A:606:ARG:NH1	2:A:644:LEU:HD21	2.25	0.49
2:A:1081:THR:HG23	2:A:1083:GLU:H	1.78	0.49
2:A:3036:LEU:O	2:A:3040:LEU:HG	2.12	0.49
2:A:4863:GLN:O	2:A:4867:ILE:HG12	2.12	0.49
2:B:474:ASP:O	2:B:478:ARG:HG2	2.12	0.49
2:B:1004:HIS:NE2	2:B:1038:LEU:HD21	2.28	0.49
2:B:1081:THR:HG23	2:B:1083:GLU:H	1.78	0.49
2:B:1522:ALA:HB3	2:B:1527:LEU:HD21	1.95	0.49
2:B:3042:ALA:HB1	2:B:3121:LEU:HB2	1.95	0.49
2:B:3211:LEU:HD21	2:B:3245:TYR:CE2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3238:ILE:O	2:B:3241:MET:HB3	2.13	0.49
2:B:4268:MET:HA	2:B:4271:VAL:HG22	1.94	0.49
2:C:913:ARG:HG3	2:C:913:ARG:O	2.12	0.49
2:C:2496:LEU:HD23	2:C:2520:LEU:HD13	1.95	0.49
2:C:2691:LYS:HA	2:C:2704:GLN:HE22	1.78	0.49
2:C:3238:ILE:O	2:C:3241:MET:HB3	2.13	0.49
2:C:4021:LEU:HD22	2:C:4128:TYR:CE2	2.48	0.49
2:D:1038:LEU:O	2:D:1043:LYS:NZ	2.36	0.49
2:D:1081:THR:HG23	2:D:1083:GLU:H	1.78	0.49
2:D:2782:MET:HB2	2:D:2787:TRP:HE3	1.76	0.49
2:D:4573:ARG:NH2	2:D:4736:ASN:OD1	2.46	0.49
2:A:317:MET:HE2	2:A:321:LYS:HD2	1.94	0.48
2:A:2156:TYR:HE1	2:A:2202:TYR:HE2	1.60	0.48
2:A:2924:SER:O	2:A:2928:GLN:HG2	2.12	0.48
2:A:3096:TYR:CE2	2:A:3101:LEU:HD13	2.48	0.48
2:A:4021:LEU:HD22	2:A:4128:TYR:CE2	2.48	0.48
1:J:127:ARG:NH1	1:J:135:GLY:C	2.58	0.48
2:B:889:ILE:HA	2:B:892:LEU:HD12	1.95	0.48
2:B:3171:LEU:HD13	2:B:3214:LEU:HD12	1.95	0.48
2:C:889:ILE:HA	2:C:892:LEU:HD12	1.95	0.48
2:C:995:MET:HA	2:C:998:LYS:HD3	1.94	0.48
2:C:2831:VAL:HG22	2:D:1435:GLY:O	2.13	0.48
2:C:2857:LYS:O	2:C:2860:LEU:HG	2.13	0.48
2:C:3036:LEU:O	2:C:3040:LEU:HG	2.12	0.48
2:C:4507:LEU:HD21	2:C:4746:ILE:HG22	1.94	0.48
2:D:889:ILE:HA	2:D:892:LEU:HD12	1.95	0.48
2:D:4155:SER:O	2:D:4159:GLN:HG2	2.13	0.48
2:A:2054:LYS:HE2	2:A:2056:SER:HA	1.94	0.48
2:A:3171:LEU:HD13	2:A:3214:LEU:HD12	1.95	0.48
2:A:3211:LEU:HD21	2:A:3245:TYR:CE2	2.48	0.48
1:L:134:ASP:OD1	2:D:3298:ARG:NH1	2.46	0.48
1:L:137:VAL:HG21	2:D:3587:TRP:CH2	2.47	0.48
2:B:874:LEU:CD1	2:B:940:LEU:HD13	2.42	0.48
2:B:913:ARG:HG3	2:B:913:ARG:O	2.13	0.48
2:B:2729:HIS:CE1	2:B:2763:LEU:HD11	2.49	0.48
2:B:3036:LEU:O	2:B:3040:LEU:HG	2.12	0.48
2:B:3122:ILE:HA	2:B:3126:VAL:HB	1.94	0.48
2:B:3805:LEU:HD21	2:B:3888:PHE:HA	1.94	0.48
2:B:4055:HIS:CE1	2:B:4057:HIS:HD2	2.31	0.48
2:B:4271:VAL:HA	2:B:4274:MET:HG2	1.95	0.48
2:C:1748:LEU:HB3	2:C:1751:ILE:HD13	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:3677:THR:HB	2:C:3679:LYS:HZ2	1.77	0.48
2:D:995:MET:HA	2:D:998:LYS:HD3	1.94	0.48
2:D:1004:HIS:NE2	2:D:1038:LEU:HD21	2.28	0.48
2:D:1748:LEU:HB3	2:D:1751:ILE:HD13	1.94	0.48
2:D:2565:GLN:O	2:D:2569:ILE:HG12	2.14	0.48
2:D:2733:SER:HA	2:D:2736:LYS:NZ	2.28	0.48
2:D:4021:LEU:HD22	2:D:4128:TYR:CE2	2.48	0.48
2:A:238:HIS:ND1	2:A:243:GLU:OE2	2.45	0.48
2:B:2456:MET:SD	2:B:2512:MET:HE1	2.53	0.48
2:D:883:GLU:HG2	2:D:884:LYS:N	2.28	0.48
2:D:1522:ALA:HB3	2:D:1527:LEU:HD21	1.95	0.48
2:D:2087:LEU:O	2:D:2091:GLN:HG2	2.13	0.48
2:D:2729:HIS:CE1	2:D:2763:LEU:HD11	2.49	0.48
2:D:3036:LEU:O	2:D:3040:LEU:HG	2.12	0.48
2:D:3238:ILE:O	2:D:3241:MET:HB3	2.13	0.48
2:D:3269:ASN:O	2:D:3273:MET:HG3	2.14	0.48
2:D:4268:MET:HA	2:D:4271:VAL:HG22	1.94	0.48
2:A:2456:MET:SD	2:A:2512:MET:HE1	2.53	0.48
2:A:3238:ILE:O	2:A:3241:MET:HB3	2.13	0.48
2:A:4573:ARG:NH2	2:A:4736:ASN:OD1	2.46	0.48
2:B:606:ARG:NH1	2:B:644:LEU:HD21	2.26	0.48
2:B:1040:ASP:HA	2:B:1043:LYS:HG2	1.95	0.48
2:B:1748:LEU:HB3	2:B:1751:ILE:HD13	1.94	0.48
2:B:1797:GLU:HA	2:B:1800:LYS:HE3	1.96	0.48
2:C:2224:ASN:O	2:C:2227:VAL:HG23	2.14	0.48
2:C:2733:SER:HA	2:C:2736:LYS:NZ	2.28	0.48
2:C:3122:ILE:HA	2:C:3126:VAL:HB	1.94	0.48
2:C:3269:ASN:O	2:C:3273:MET:HG3	2.14	0.48
2:C:4271:VAL:HA	2:C:4274:MET:HG2	1.95	0.48
2:C:4573:ARG:NH2	2:C:4736:ASN:OD1	2.46	0.48
2:D:2857:LYS:O	2:D:2860:LEU:HG	2.13	0.48
2:D:3043:ARG:HA	2:D:3120:ASP:OD2	2.13	0.48
2:A:913:ARG:HG3	2:A:913:ARG:O	2.13	0.48
2:A:1004:HIS:NE2	2:A:1038:LEU:HD21	2.28	0.48
2:A:2701:PHE:CE2	2:A:2703:PRO:HG3	2.49	0.48
2:A:3295:TRP:HB3	2:A:3298:ARG:HH21	1.79	0.48
2:A:3805:LEU:HD21	2:A:3888:PHE:HA	1.94	0.48
2:A:4055:HIS:CE1	2:A:4057:HIS:HD2	2.31	0.48
3:G:88:HIS:HD2	3:G:89:PRO:HD2	1.79	0.48
2:B:2496:LEU:HD23	2:B:2520:LEU:HD13	1.95	0.48
2:B:2733:SER:HA	2:B:2736:LYS:NZ	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2924:SER:O	2:B:2928:GLN:HG2	2.12	0.48
2:C:2385:GLY:O	2:C:2389:MET:HG3	2.13	0.48
2:C:2833:LEU:HB2	2:C:2838[B]:HIS:NE2	2.28	0.48
2:C:4155:SER:O	2:C:4159:GLN:HG2	2.13	0.48
2:C:4863:GLN:O	2:C:4867:ILE:HG12	2.12	0.48
2:D:115:TYR:OH	2:D:179:ASP:OD2	2.31	0.48
2:D:3246:MET:HG2	2:D:3309:LYS:HZ2	1.78	0.48
2:A:2224:ASN:O	2:A:2227:VAL:HG23	2.14	0.48
2:A:2729:HIS:CE1	2:A:2763:LEU:HD11	2.49	0.48
2:A:3043:ARG:HA	2:A:3120:ASP:OD2	2.13	0.48
1:L:76:LYS:HB2	1:L:78:LYS:HZ2	1.78	0.48
1:L:127:ARG:HD3	1:L:127:ARG:HA	1.41	0.48
2:B:292:GLY:HA3	2:B:340:VAL:HG21	1.96	0.48
2:B:874:LEU:HD12	2:B:875:PRO:HD2	1.95	0.48
2:B:2565:GLN:O	2:B:2569:ILE:HG12	2.14	0.48
2:B:3159:LEU:HB3	2:B:3241:MET:HE2	1.95	0.48
2:C:883:GLU:HG2	2:C:884:LYS:N	2.28	0.48
2:C:1081:THR:HG23	2:C:1083:GLU:H	1.78	0.48
2:D:661:LEU:HD23	2:D:673:TRP:CD1	2.49	0.48
2:D:1034:PRO:HD2	2:D:1037:LEU:HD12	1.96	0.48
2:D:3211:LEU:HD21	2:D:3245:TYR:CE2	2.48	0.48
2:D:3295:TRP:HB3	2:D:3298:ARG:HH21	1.78	0.48
2:A:292:GLY:HA3	2:A:340:VAL:HG21	1.96	0.48
2:A:375:GLN:HB2	2:A:390:LYS:HB3	1.95	0.48
2:A:883:GLU:HG2	2:A:884:LYS:N	2.28	0.48
2:A:1797:GLU:HA	2:A:1800:LYS:HE3	1.96	0.48
2:B:165:ALA:HB3	2:B:180:ASP:HB3	1.96	0.48
2:B:849:ASP:OD1	2:B:1214:ARG:NE	2.37	0.48
2:B:3269:ASN:O	2:B:3273:MET:HG3	2.14	0.48
2:C:375:GLN:HB2	2:C:390:LYS:HB3	1.95	0.48
2:C:441:LYS:HG3	2:C:444:THR:HG23	1.96	0.48
2:C:2087:LEU:O	2:C:2091:GLN:HG2	2.13	0.48
2:C:2701:PHE:CE2	2:C:2703:PRO:HG3	2.49	0.48
2:C:3200:ASN:CB	2:C:3203:ASP:HB2	2.44	0.48
2:C:3211:LEU:HD21	2:C:3245:TYR:CE2	2.49	0.48
2:D:3068:LEU:O	2:D:3071:THR:OG1	2.27	0.48
2:A:2733:SER:HA	2:A:2736:LYS:NZ	2.28	0.48
2:A:2968:LEU:HD13	2:A:3029:ILE:HG12	1.96	0.48
3:H:88:HIS:HD2	3:H:89:PRO:HD2	1.79	0.48
2:B:1685:LEU:HD22	2:B:1706:LEU:HB2	1.95	0.48
2:B:2156:TYR:HE1	2:B:2202:TYR:HE2	1.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3295:TRP:HB3	2:B:3298:ARG:HH21	1.78	0.48
2:C:2729:HIS:CE1	2:C:2763:LEU:HD11	2.49	0.48
2:C:3131:TYR:O	2:C:3135:THR:HG23	2.14	0.48
2:D:2946:GLY:HA3	2:D:2954:PHE:HZ	1.79	0.48
2:D:2968:LEU:HD13	2:D:3029:ILE:HG12	1.96	0.48
3:E:88:HIS:HD2	3:E:89:PRO:HD2	1.79	0.48
2:B:2385:GLY:O	2:B:2389:MET:HG3	2.13	0.48
2:B:2857:LYS:O	2:B:2860:LEU:HG	2.13	0.48
2:B:3043:ARG:HA	2:B:3120:ASP:OD2	2.13	0.48
2:C:318:ASP:OD1	2:C:319:LYS:N	2.45	0.48
2:C:1435:GLY:N	2:C:1500:ARG:HH22	2.11	0.48
2:C:1967:SER:O	2:C:1972:GLN:NE2	2.41	0.48
2:C:2768:LYS:HB3	2:C:2772:ARG:HH21	1.77	0.48
2:C:3042:ALA:HB1	2:C:3121:LEU:HB2	1.95	0.48
2:D:606:ARG:NH1	2:D:644:LEU:HD21	2.25	0.48
2:D:2385:GLY:O	2:D:2389:MET:HG3	2.13	0.48
2:A:1685:LEU:HD22	2:A:1706:LEU:HB2	1.95	0.48
2:A:2857:LYS:O	2:A:2860:LEU:HG	2.13	0.48
2:A:3106:SER:OG	2:A:3157:GLU:OE1	2.21	0.48
2:A:4155:SER:O	2:A:4159:GLN:HG2	2.13	0.48
2:A:4800:ASP:OD1	2:A:4801:THR:N	2.47	0.48
2:B:2968:LEU:HD13	2:B:3029:ILE:HG12	1.96	0.48
2:B:3131:TYR:O	2:B:3135:THR:HG23	2.14	0.48
2:C:606:ARG:NH1	2:C:644:LEU:HD21	2.26	0.48
2:C:661:LEU:HD23	2:C:673:TRP:CD1	2.49	0.48
2:C:1034:PRO:HD2	2:C:1037:LEU:HD12	1.96	0.48
2:C:2565:GLN:O	2:C:2569:ILE:HG12	2.14	0.48
2:C:3184:TYR:CG	2:C:3201:VAL:HG22	2.49	0.48
2:D:318:ASP:OD1	2:D:319:LYS:N	2.45	0.48
2:D:375:GLN:HB2	2:D:390:LYS:HB3	1.95	0.48
2:D:3200:ASN:CB	2:D:3203:ASP:HB2	2.44	0.48
2:A:165:ALA:HB3	2:A:180:ASP:HB3	1.96	0.47
2:A:874:LEU:HD12	2:A:875:PRO:HD2	1.95	0.47
2:A:3269:ASN:O	2:A:3273:MET:HG3	2.14	0.47
2:B:2087:LEU:O	2:B:2091:GLN:HG2	2.13	0.47
2:B:2701:PHE:CE2	2:B:2703:PRO:HG3	2.49	0.47
2:C:19:GLU:HG2	2:C:66:THR:HB	1.95	0.47
2:C:2968:LEU:HD13	2:C:3029:ILE:HG12	1.96	0.47
2:C:3295:TRP:HB3	2:C:3298:ARG:HH21	1.79	0.47
2:D:19:GLU:HG2	2:D:66:THR:HB	1.96	0.47
2:D:913:ARG:HG3	2:D:913:ARG:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1797:GLU:HA	2:D:1800:LYS:HE3	1.96	0.47
2:D:2156:TYR:HE1	2:D:2202:TYR:HE2	1.60	0.47
2:D:3184:TYR:CG	2:D:3201:VAL:HG22	2.49	0.47
2:A:1143:GLN:HG3	2:A:1151:HIS:HA	1.96	0.47
2:A:1522:ALA:HB3	2:A:1527:LEU:HD21	1.95	0.47
2:A:3042:ALA:HB1	2:A:3121:LEU:HB2	1.95	0.47
2:A:3166:PHE:CD2	2:A:3170:PHE:HB3	2.50	0.47
2:A:4268:MET:HA	2:A:4271:VAL:HG22	1.94	0.47
2:B:441:LYS:HG3	2:B:444:THR:HG23	1.96	0.47
2:B:661:LEU:HD23	2:B:673:TRP:CD1	2.49	0.47
2:B:2431:ASP:O	2:B:2435:VAL:HG23	2.14	0.47
2:C:912:LYS:HE3	2:C:914:GLN:HG3	1.96	0.47
2:C:2431:ASP:O	2:C:2435:VAL:HG23	2.14	0.47
2:C:2912:LEU:HB3	2:C:2914:THR:HG23	1.96	0.47
2:C:3848:GLU:OE1	2:C:3922:GLU:OE1	2.29	0.47
2:D:441:LYS:HG3	2:D:444:THR:HG23	1.96	0.47
2:D:2224:ASN:O	2:D:2227:VAL:HG23	2.14	0.47
2:D:2701:PHE:CE2	2:D:2703:PRO:HG3	2.49	0.47
2:D:2833:LEU:HB2	2:D:2838[B]:HIS:NE2	2.28	0.47
2:A:19:GLU:HG2	2:A:66:THR:HB	1.96	0.47
2:A:661:LEU:HD23	2:A:673:TRP:CD1	2.49	0.47
2:A:769:ARG:NH2	2:A:816:PRO:HG3	2.30	0.47
2:A:912:LYS:HE3	2:A:914:GLN:HG3	1.96	0.47
2:A:2565:GLN:O	2:A:2569:ILE:HG12	2.14	0.47
2:B:2828:MET:O	2:B:2894:LYS:NZ	2.42	0.47
2:B:3200:ASN:CB	2:B:3203:ASP:HB2	2.44	0.47
2:C:874:LEU:HD12	2:C:875:PRO:HD2	1.95	0.47
2:C:1797:GLU:HA	2:C:1800:LYS:HE3	1.96	0.47
2:C:3159:LEU:HB3	2:C:3241:MET:HE2	1.96	0.47
2:C:3166:PHE:CD2	2:C:3170:PHE:HB3	2.50	0.47
2:D:4027:THR:HG21	2:D:4084:VAL:HG11	1.97	0.47
1:I:50:GLN:NE2	1:I:54:ASN:HD21	2.13	0.47
2:A:1104:GLU:OE1	2:A:1225:LYS:NZ	2.44	0.47
2:A:2385:GLY:O	2:A:2389:MET:HG3	2.13	0.47
2:A:2496:LEU:HD23	2:A:2520:LEU:HD13	1.95	0.47
2:A:2713:ILE:HG12	2:A:2776:LYS:HB2	1.97	0.47
1:L:50:GLN:NE2	1:L:54:ASN:HD21	2.13	0.47
2:B:2224:ASN:O	2:B:2227:VAL:HG23	2.14	0.47
2:C:2456:MET:SD	2:C:2512:MET:HE1	2.55	0.47
2:C:2744:GLY:H	2:C:2755:PRO:HA	1.79	0.47
2:C:3131:TYR:OH	2:C:3205:CYS:O	2.23	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:4735:ASN:HB3	2:C:4738:PHE:HD2	1.79	0.47
2:D:165:ALA:HB3	2:D:180:ASP:HB3	1.96	0.47
2:D:1552:VAL:HG12	2:D:1553:PHE:HD1	1.80	0.47
2:A:1034:PRO:HD2	2:A:1037:LEU:HD12	1.96	0.47
2:A:2350:ALA:HA	2:A:2353:ILE:HG22	1.96	0.47
2:A:2658:GLU:OE1	2:A:2661:LEU:N	2.37	0.47
2:A:3159:LEU:HB3	2:A:3241:MET:HE2	1.97	0.47
2:A:3200:ASN:CB	2:A:3203:ASP:HB2	2.44	0.47
2:A:4567:TYR:O	2:A:4567:TYR:CD1	2.68	0.47
3:F:88:HIS:HD2	3:F:89:PRO:HD2	1.79	0.47
2:B:3068:LEU:O	2:B:3071:THR:OG1	2.27	0.47
2:C:904:TYR:HE1	2:C:916:PRO:HA	1.80	0.47
2:C:2713:ILE:HG12	2:C:2776:LYS:HB2	1.97	0.47
2:C:3043:ARG:HA	2:C:3120:ASP:OD2	2.13	0.47
2:D:769:ARG:NH2	2:D:816:PRO:HG3	2.30	0.47
2:D:912:LYS:HE3	2:D:914:GLN:HG3	1.96	0.47
2:D:2431:ASP:O	2:D:2435:VAL:HG23	2.14	0.47
2:D:2886:ARG:HG2	2:D:2890:GLN:OE1	2.15	0.47
2:D:3042:ALA:HB1	2:D:3121:LEU:HB2	1.95	0.47
2:D:3131:TYR:O	2:D:3135:THR:HG23	2.14	0.47
2:D:4520:TYR:HD1	2:D:4561:LEU:HD13	1.79	0.47
2:D:4735:ASN:HB3	2:D:4738:PHE:HD2	1.79	0.47
2:A:4276:VAL:O	2:A:4280:VAL:HG23	2.15	0.47
2:A:4707:MET:HG2	2:D:4252:ILE:HG21	1.97	0.47
2:B:375:GLN:HB2	2:B:390:LYS:HB3	1.95	0.47
2:B:769:ARG:NH2	2:B:816:PRO:HG3	2.29	0.47
2:B:2794:GLU:HB2	2:B:2798:MET:HE1	1.97	0.47
2:B:2892:ILE:HG13	2:B:2893:LEU:N	2.30	0.47
2:B:4027:THR:HG21	2:B:4084:VAL:HG11	1.97	0.47
2:C:769:ARG:NH2	2:C:816:PRO:HG3	2.30	0.47
2:D:293:GLN:HG3	2:D:343:ARG:NH1	2.29	0.47
2:D:874:LEU:HD12	2:D:875:PRO:HD2	1.95	0.47
2:D:3171:LEU:HD13	2:D:3214:LEU:HD12	1.95	0.47
2:D:4800:ASP:OD1	2:D:4801:THR:N	2.47	0.47
1:I:126:ILE:O	1:I:130:ASP:N	2.48	0.47
2:A:624:ALA:HB2	2:A:1667:LEU:HD12	1.97	0.47
2:A:1286:THR:OG1	2:A:1550:PRO:O	2.22	0.47
2:A:1564:MET:HE1	2:A:1578:PRO:HA	1.97	0.47
2:A:2293:VAL:O	2:A:2296:GLU:HG2	2.15	0.47
2:A:2886:ARG:HG2	2:A:2890:GLN:OE1	2.15	0.47
2:A:2892:ILE:HG13	2:A:2893:LEU:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2946:GLY:HA3	2:A:2954:PHE:HZ	1.79	0.47
2:A:3184:TYR:CG	2:A:3201:VAL:HG22	2.49	0.47
2:A:4520:TYR:HD1	2:A:4561:LEU:HD13	1.79	0.47
2:B:883:GLU:HG2	2:B:884:LYS:N	2.28	0.47
2:B:996:VAL:HG13	2:B:1050:LEU:HD22	1.97	0.47
2:B:2001:GLU:OE1	2:B:2001:GLU:N	2.48	0.47
2:B:2886:ARG:HG2	2:B:2890:GLN:OE1	2.15	0.47
2:B:3042:ALA:HB1	2:B:3121:LEU:HD13	1.97	0.47
2:B:3184:TYR:HB3	2:B:3192:ARG:NH2	2.27	0.47
2:B:3184:TYR:CG	2:B:3201:VAL:HG22	2.49	0.47
2:B:4557:VAL:HG21	2:C:4790:ARG:HH22	1.80	0.47
2:B:4567:TYR:O	2:B:4567:TYR:CD1	2.68	0.47
2:C:514:PHE:HD2	2:C:526:TRP:HB2	1.80	0.47
2:C:891:GLU:O	2:C:895:MET:HE1	2.15	0.47
2:C:1552:VAL:HG12	2:C:1553:PHE:HD1	1.80	0.47
2:C:3246:MET:HG2	2:C:3309:LYS:HZ2	1.78	0.47
2:C:3715:GLU:OE2	2:C:4647:LYS:HE2	2.15	0.47
2:C:4800:ASP:OD1	2:C:4801:THR:N	2.47	0.47
2:D:292:GLY:HA3	2:D:340:VAL:HG21	1.96	0.47
2:D:1143:GLN:HG3	2:D:1151:HIS:HA	1.96	0.47
2:D:1564:MET:HE1	2:D:1578:PRO:HA	1.97	0.47
2:D:1729:MET:CE	2:D:1930:ASP:HB2	2.45	0.47
2:D:3131:TYR:OH	2:D:3205:CYS:O	2.23	0.47
2:D:3166:PHE:CD2	2:D:3170:PHE:HB3	2.50	0.47
2:A:441:LYS:HG3	2:A:444:THR:HG23	1.96	0.47
1:K:50:GLN:NE2	1:K:54:ASN:HD21	2.13	0.47
2:B:514:PHE:HD2	2:B:526:TRP:HB2	1.80	0.47
2:B:912:LYS:HE3	2:B:914:GLN:HG3	1.96	0.47
2:B:1718:ARG:HD3	2:B:1831:MET:HA	1.97	0.47
2:B:2153:LYS:HD3	2:B:2156:TYR:HD2	1.80	0.47
2:B:2744:GLY:H	2:B:2755:PRO:HA	1.79	0.47
2:B:2824:ARG:NH2	2:C:1502:ASN:HB3	2.30	0.47
2:B:4026:LEU:HD13	2:B:4058:TYR:HE2	1.80	0.47
2:C:293:GLN:HG3	2:C:343:ARG:NH1	2.30	0.47
2:C:1732:GLU:O	2:C:1736:ILE:HG13	2.15	0.47
2:C:2422:ILE:O	2:C:2426:LEU:HG	2.15	0.47
2:C:2946:GLY:HA3	2:C:2954:PHE:HZ	1.79	0.47
2:C:3171:LEU:HD13	2:C:3214:LEU:HD12	1.95	0.47
2:C:4567:TYR:CD1	2:C:4567:TYR:O	2.68	0.47
2:D:904:TYR:HE1	2:D:916:PRO:HA	1.79	0.47
2:A:293:GLN:HG3	2:A:343:ARG:NH1	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1552:VAL:HG12	2:A:1553:PHE:HD1	1.80	0.47
2:A:4806:CYS:HA	2:A:4812:CYS:HB2	1.97	0.47
2:B:1034:PRO:HD2	2:B:1037:LEU:HD12	1.96	0.47
2:B:1435:GLY:N	2:B:1500:ARG:HH22	2.11	0.47
2:B:2685:TYR:HD2	2:B:2686:VAL:O	1.98	0.47
2:B:3166:PHE:CD2	2:B:3170:PHE:HB3	2.50	0.47
2:B:3292:GLU:O	2:B:3296:MET:HE2	2.14	0.47
2:B:4800:ASP:OD1	2:B:4801:THR:N	2.47	0.47
2:C:165:ALA:HB3	2:C:180:ASP:HB3	1.96	0.47
2:C:292:GLY:HA3	2:C:340:VAL:HG21	1.96	0.47
2:C:2293:VAL:O	2:C:2296:GLU:HG2	2.15	0.47
2:C:2662:PHE:HE2	2:C:2962:PHE:HD1	1.62	0.47
2:C:3042:ALA:HB1	2:C:3121:LEU:HD13	1.97	0.47
2:D:913:ARG:HA	2:D:913:ARG:HD2	1.74	0.47
2:D:1176:THR:HG22	2:D:1181:ILE:HA	1.97	0.47
2:D:1435:GLY:N	2:D:1500:ARG:HH22	2.11	0.47
2:D:2642:ARG:HH12	2:D:2921:PHE:HA	1.80	0.47
2:D:2658:GLU:OE1	2:D:2661:LEU:N	2.37	0.47
2:D:2662:PHE:HE2	2:D:2962:PHE:HD1	1.62	0.47
2:D:2713:ILE:HG12	2:D:2776:LYS:HB2	1.97	0.47
2:D:3159:LEU:HB3	2:D:3241:MET:HE2	1.97	0.47
2:D:3166:PHE:O	2:D:3248:ARG:NH1	2.48	0.47
2:D:3715:GLU:OE2	2:D:4647:LYS:HE2	2.15	0.47
2:A:3042:ALA:HB1	2:A:3121:LEU:HD13	1.97	0.47
2:A:3131:TYR:O	2:A:3135:THR:HG23	2.14	0.47
2:A:3166:PHE:O	2:A:3248:ARG:NH1	2.48	0.47
2:A:3316:LYS:O	2:A:3317:THR:OG1	2.33	0.47
2:A:4853:PHE:HA	2:A:4857:ILE:HD12	1.97	0.47
2:B:218:SER:HB3	2:B:286:GLY:HA3	1.97	0.47
2:B:293:GLN:HG3	2:B:343:ARG:NH1	2.29	0.47
2:B:1729:MET:CE	2:B:1930:ASP:HB2	2.45	0.47
2:B:2293:VAL:O	2:B:2296:GLU:HG2	2.15	0.47
2:B:4648:PHE:CD1	2:B:4651:ARG:HG3	2.50	0.47
2:C:911:ASN:OD1	2:C:912:LYS:N	2.48	0.47
2:C:996:VAL:HG13	2:C:1050:LEU:HD22	1.97	0.47
2:C:1417:TYR:O	2:C:1421:MET:HG2	2.15	0.47
2:C:2350:ALA:HA	2:C:2353:ILE:HG22	1.96	0.47
2:C:4026:LEU:HD13	2:C:4058:TYR:HE2	1.80	0.47
2:C:4276:VAL:O	2:C:4280:VAL:HG23	2.15	0.47
2:D:972:LEU:HD23	2:D:973:THR:N	2.30	0.47
2:D:2422:ILE:O	2:D:2426:LEU:HG	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4567:TYR:O	2:D:4567:TYR:CD1	2.68	0.47
2:D:4648:PHE:CD1	2:D:4651:ARG:HG3	2.50	0.47
2:A:1718:ARG:HD3	2:A:1831:MET:HA	1.97	0.46
2:A:4648:PHE:CD1	2:A:4651:ARG:HG3	2.50	0.46
2:A:4956:ASP:HA	2:A:4960:LYS:HD3	1.97	0.46
1:J:50:GLN:NE2	1:J:54:ASN:HD21	2.13	0.46
2:B:972:LEU:HD23	2:B:973:THR:N	2.30	0.46
2:B:1732:GLU:O	2:B:1736:ILE:HG13	2.15	0.46
2:B:1981:ASP:OD2	2:B:1983:LYS:NZ	2.48	0.46
2:B:2713:ILE:HG12	2:B:2776:LYS:HB2	1.97	0.46
2:B:3310:VAL:HG13	2:B:3314:LEU:HD12	1.97	0.46
2:B:4276:VAL:O	2:B:4280:VAL:HG23	2.15	0.46
2:C:1184:ASP:OD2	2:C:1193:LYS:NZ	2.38	0.46
2:C:2642:ARG:HH12	2:C:2921:PHE:HA	1.80	0.46
2:D:1417:TYR:O	2:D:1421:MET:HG2	2.15	0.46
2:D:1718:ARG:HD3	2:D:1831:MET:HA	1.97	0.46
2:D:2001:GLU:OE1	2:D:2001:GLU:N	2.48	0.46
2:D:2153:LYS:HD3	2:D:2156:TYR:HD2	1.80	0.46
2:D:2744:GLY:H	2:D:2755:PRO:HA	1.79	0.46
2:D:2892:ILE:HG13	2:D:2893:LEU:N	2.30	0.46
2:D:3042:ALA:HB1	2:D:3121:LEU:HD13	1.97	0.46
2:D:3106:SER:OG	2:D:3157:GLU:OE1	2.21	0.46
2:D:4079:ASP:O	2:D:4082:GLU:HG3	2.15	0.46
2:D:4276:VAL:O	2:D:4280:VAL:HG23	2.15	0.46
2:A:1732:GLU:O	2:A:1736:ILE:HG13	2.15	0.46
2:A:1981:ASP:OD2	2:A:1983:LYS:NZ	2.48	0.46
2:A:2001:GLU:OE1	2:A:2001:GLU:N	2.48	0.46
2:A:2422:ILE:O	2:A:2426:LEU:HG	2.15	0.46
2:A:2431:ASP:O	2:A:2435:VAL:HG23	2.14	0.46
2:A:3043:ARG:HB3	2:A:3117:PHE:CD1	2.51	0.46
2:A:3310:VAL:HG13	2:A:3314:LEU:HD12	1.97	0.46
2:B:1143:GLN:HG3	2:B:1151:HIS:HA	1.96	0.46
2:B:2891:ASP:OD1	2:B:2892:ILE:N	2.48	0.46
2:B:4079:ASP:O	2:B:4082:GLU:HG3	2.16	0.46
2:B:4853:PHE:HA	2:B:4857:ILE:HD12	1.97	0.46
2:C:1610:ARG:HA	2:C:1617:TRP:HA	1.98	0.46
2:C:2001:GLU:N	2:C:2001:GLU:OE1	2.48	0.46
2:C:2153:LYS:HD3	2:C:2156:TYR:HD2	1.80	0.46
2:C:2891:ASP:OD1	2:C:2892:ILE:N	2.48	0.46
2:C:3043:ARG:HB3	2:C:3117:PHE:CD1	2.50	0.46
2:C:3166:PHE:O	2:C:3248:ARG:NH1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:4079:ASP:O	2:C:4082:GLU:HG3	2.16	0.46
2:C:4853:PHE:HA	2:C:4857:ILE:HD12	1.97	0.46
2:D:4806:CYS:HA	2:D:4812:CYS:HB2	1.97	0.46
1:I:10:ILE:HA	1:I:13:PHE:HB2	1.97	0.46
2:A:2733:SER:HA	2:A:2736:LYS:HZ3	1.80	0.46
2:A:4079:ASP:O	2:A:4082:GLU:HG3	2.15	0.46
2:B:904:TYR:HE1	2:B:916:PRO:HA	1.80	0.46
2:B:2912:LEU:HB3	2:B:2914:THR:HG23	1.96	0.46
2:B:3166:PHE:O	2:B:3248:ARG:NH1	2.48	0.46
2:B:3715:GLU:OE2	2:B:4647:LYS:HE2	2.15	0.46
2:C:419:ILE:HD13	2:C:492:GLU:HG3	1.97	0.46
2:C:436:LEU:HD23	2:C:436:LEU:HA	1.81	0.46
2:C:2892:ILE:HG13	2:C:2893:LEU:N	2.30	0.46
2:C:4520:TYR:HD1	2:C:4561:LEU:HD13	1.80	0.46
2:C:4774:LEU:O	2:C:4778:VAL:HG23	2.16	0.46
2:D:173:GLU:OE2	2:D:176:ARG:NH2	2.36	0.46
2:A:2891:ASP:OD1	2:A:2892:ILE:N	2.48	0.46
2:A:4026:LEU:HD13	2:A:4058:TYR:HE2	1.80	0.46
3:E:19:LYS:HB2	3:E:19:LYS:HE3	1.84	0.46
1:L:10:ILE:HA	1:L:13:PHE:HB2	1.98	0.46
1:K:137:VAL:HG21	2:C:3587:TRP:CH2	2.49	0.46
2:B:19:GLU:HG2	2:B:66:THR:HB	1.96	0.46
2:B:3925:GLN:HE22	2:B:4934:THR:HA	1.80	0.46
2:B:4806:CYS:HA	2:B:4812:CYS:HB2	1.97	0.46
2:C:2172:MET:HE3	2:C:2172:MET:HA	1.98	0.46
2:C:2685:TYR:HD2	2:C:2686:VAL:O	1.98	0.46
2:C:4648:PHE:CD1	2:C:4651:ARG:HG3	2.50	0.46
2:D:1610:ARG:HA	2:D:1617:TRP:HA	1.97	0.46
2:D:2912:LEU:HB3	2:D:2914:THR:HG23	1.96	0.46
2:D:4008:ASN:OD1	2:D:4009:ASN:N	2.49	0.46
2:D:4026:LEU:HD13	2:D:4058:TYR:HE2	1.80	0.46
2:D:4853:PHE:HA	2:D:4857:ILE:HD12	1.97	0.46
2:A:2646:TRP:CH2	2:A:2928:GLN:HG3	2.51	0.46
2:A:2685:TYR:HD2	2:A:2686:VAL:O	1.98	0.46
2:A:2912:LEU:HB3	2:A:2914:THR:HG23	1.96	0.46
2:A:3604:ARG:O	2:A:3604:ARG:HD3	2.16	0.46
2:A:4008:ASN:OD1	2:A:4009:ASN:N	2.49	0.46
2:B:1176:THR:HG22	2:B:1181:ILE:HA	1.97	0.46
2:B:2946:GLY:HA3	2:B:2954:PHE:HZ	1.79	0.46
2:B:4774:LEU:O	2:B:4778:VAL:HG23	2.16	0.46
2:C:1038:LEU:O	2:C:1043:LYS:NZ	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1143:GLN:HG3	2:C:1151:HIS:HA	1.96	0.46
2:C:1718:ARG:HD3	2:C:1831:MET:HA	1.97	0.46
2:C:4027:THR:HG21	2:C:4084:VAL:HG11	1.97	0.46
2:D:624:ALA:HB2	2:D:1667:LEU:HD12	1.97	0.46
2:D:2293:VAL:O	2:D:2296:GLU:HG2	2.15	0.46
2:D:2350:ALA:HA	2:D:2353:ILE:HG22	1.96	0.46
2:D:3925:GLN:HE22	2:D:4934:THR:HA	1.80	0.46
2:A:2744:GLY:H	2:A:2755:PRO:HA	1.79	0.46
2:B:334:SER:OG	2:B:336:GLU:OE1	2.22	0.46
2:B:1552:VAL:HG12	2:B:1553:PHE:HD1	1.80	0.46
2:B:2422:ILE:O	2:B:2426:LEU:HG	2.15	0.46
2:B:3604:ARG:O	2:B:3604:ARG:HD3	2.16	0.46
2:B:4956:ASP:HA	2:B:4960:LYS:HD3	1.97	0.46
2:C:972:LEU:HD23	2:C:973:THR:N	2.30	0.46
2:C:1014:GLN:HB3	2:C:1027:ARG:HH21	1.81	0.46
2:C:1729:MET:CE	2:C:1930:ASP:HB2	2.45	0.46
2:C:2886:ARG:HG2	2:C:2890:GLN:OE1	2.15	0.46
2:C:3184:TYR:HB3	2:C:3192:ARG:NH2	2.27	0.46
2:C:3925:GLN:HE22	2:C:4934:THR:HA	1.80	0.46
2:C:4008:ASN:OD1	2:C:4009:ASN:N	2.49	0.46
2:C:4116:GLN:HA	2:C:4119:LEU:HD12	1.98	0.46
2:D:419:ILE:HD13	2:D:492:GLU:HG3	1.97	0.46
2:D:514:PHE:HD2	2:D:526:TRP:HB2	1.80	0.46
2:D:2891:ASP:OD1	2:D:2892:ILE:N	2.48	0.46
2:D:3156:GLY:O	2:D:3240:PRO:HB2	2.16	0.46
2:D:3292:GLU:O	2:D:3296:MET:HE2	2.16	0.46
2:A:902:TRP:CD1	2:A:913:ARG:NH2	2.84	0.46
2:A:972:LEU:HD23	2:A:973:THR:N	2.30	0.46
2:A:2525:LEU:HG	2:A:2569:ILE:HD13	1.98	0.46
2:A:2779:LEU:O	2:A:2782:MET:HG3	2.16	0.46
2:A:2828:MET:O	2:A:2894:LYS:NZ	2.42	0.46
2:A:2946:GLY:HA3	2:A:2954:PHE:CZ	2.51	0.46
2:A:3022:PHE:HB3	2:A:3025:ASP:OD1	2.16	0.46
2:A:3715:GLU:OE2	2:A:4647:LYS:HE2	2.15	0.46
2:A:4027:THR:HG21	2:A:4084:VAL:HG11	1.97	0.46
2:A:4735:ASN:HB3	2:A:4738:PHE:HD2	1.79	0.46
2:A:4921:PHE:HE2	2:A:4940:VAL:HG11	1.81	0.46
2:B:1417:TYR:O	2:B:1421:MET:HG2	2.15	0.46
2:B:3022:PHE:HB3	2:B:3025:ASP:OD1	2.16	0.46
2:C:1564:MET:HE1	2:C:1578:PRO:HA	1.98	0.46
2:C:3156:GLY:O	2:C:3240:PRO:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:3293:GLY:HA3	2:C:3295:TRP:CZ3	2.51	0.46
2:C:4806:CYS:HA	2:C:4812:CYS:HB2	1.97	0.46
2:C:4956:ASP:HA	2:C:4960:LYS:HD3	1.97	0.46
2:D:902:TRP:CD1	2:D:913:ARG:NH2	2.84	0.46
2:D:2685:TYR:HD2	2:D:2686:VAL:O	1.98	0.46
1:I:110:MET:HA	2:A:3590:LEU:HD21	1.97	0.46
2:A:218:SER:HB3	2:A:286:GLY:HA3	1.98	0.46
2:A:1008:ALA:O	2:A:1012:ILE:HG12	2.16	0.46
2:A:2642:ARG:HH12	2:A:2921:PHE:HA	1.80	0.46
1:J:127:ARG:HD3	1:J:127:ARG:HA	1.41	0.46
2:B:1014:GLN:HB3	2:B:1027:ARG:HH21	1.81	0.46
2:B:2350:ALA:HA	2:B:2353:ILE:HG22	1.96	0.46
2:B:2629:ASN:OD1	2:B:2630:PHE:N	2.49	0.46
2:B:2779:LEU:O	2:B:2782:MET:HG3	2.16	0.46
2:B:3127:GLN:HG3	2:B:3183:ILE:HB	1.98	0.46
2:B:4008:ASN:OD1	2:B:4009:ASN:N	2.49	0.46
2:D:2525:LEU:HG	2:D:2569:ILE:HD13	1.98	0.46
2:D:2629:ASN:OD1	2:D:2630:PHE:N	2.49	0.46
2:D:3604:ARG:O	2:D:3604:ARG:HD3	2.16	0.46
2:D:4116:GLN:HA	2:D:4119:LEU:HD12	1.98	0.46
2:A:514:PHE:HD2	2:A:526:TRP:HB2	1.80	0.46
2:A:1014:GLN:HB3	2:A:1027:ARG:HH21	1.81	0.46
2:B:658:ASN:HD21	2:B:833:LYS:HG2	1.81	0.46
2:B:2946:GLY:HA3	2:B:2954:PHE:CZ	2.51	0.46
2:B:2956:TYR:HA	2:B:2959:GLU:OE1	2.16	0.46
2:B:3293:GLY:HA3	2:B:3295:TRP:CZ3	2.51	0.46
2:B:4520:TYR:HD1	2:B:4561:LEU:HD13	1.79	0.46
2:B:4921:PHE:HE2	2:B:4940:VAL:HG11	1.81	0.46
2:C:678:MET:HB2	2:C:754:VAL:HG22	1.98	0.46
2:C:2946:GLY:HA3	2:C:2954:PHE:CZ	2.51	0.46
2:D:1008:ALA:O	2:D:1012:ILE:HG12	2.16	0.46
2:D:1967:SER:O	2:D:1972:GLN:NE2	2.41	0.46
2:D:2779:LEU:O	2:D:2782:MET:HG3	2.16	0.46
2:D:3293:GLY:HA3	2:D:3295:TRP:CZ3	2.51	0.46
2:A:166:SER:OG	2:A:168:GLN:OE1	2.34	0.46
2:A:1176:THR:HG22	2:A:1181:ILE:HA	1.97	0.46
2:A:2629:ASN:OD1	2:A:2630:PHE:N	2.49	0.46
2:A:2662:PHE:HE2	2:A:2962:PHE:HD1	1.62	0.46
2:A:3848:GLU:OE1	2:A:3922:GLU:OE1	2.29	0.46
2:B:908:ARG:NH2	2:B:928:GLU:OE2	2.49	0.46
2:B:3316:LYS:O	2:B:3317:THR:OG1	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:785:ASP:OD1	2:C:786:GLY:N	2.49	0.46
2:C:2447:LYS:HE2	2:C:2864:GLY:HA3	1.98	0.46
2:C:2629:ASN:OD1	2:C:2630:PHE:N	2.49	0.46
2:D:194:LEU:HD11	2:D:201:LEU:HB3	1.98	0.46
2:D:658:ASN:HD21	2:D:833:LYS:HG2	1.81	0.46
2:D:785:ASP:OD1	2:D:786:GLY:N	2.49	0.46
2:D:3043:ARG:HB3	2:D:3117:PHE:CD1	2.51	0.46
2:A:1729:MET:CE	2:A:1930:ASP:HB2	2.45	0.45
1:L:48:GLU:O	1:L:52:MET:HG2	2.17	0.45
1:K:126:ILE:O	1:K:130:ASP:N	2.48	0.45
2:B:2642:ARG:HH12	2:B:2921:PHE:HA	1.80	0.45
2:B:4735:ASN:HB3	2:B:4738:PHE:HD2	1.79	0.45
2:C:1981:ASP:OD2	2:C:1983:LYS:NZ	2.48	0.45
2:C:3127:GLN:HG3	2:C:3183:ILE:HB	1.98	0.45
2:D:911:ASN:OD1	2:D:912:LYS:N	2.48	0.45
2:D:996:VAL:HG13	2:D:1050:LEU:HD22	1.97	0.45
2:D:1732:GLU:O	2:D:1736:ILE:HG13	2.15	0.45
2:D:2646:TRP:CH2	2:D:2928:GLN:HG3	2.51	0.45
2:D:4269:LYS:HA	2:D:4272:LYS:HE2	1.98	0.45
2:D:4774:LEU:O	2:D:4778:VAL:HG23	2.16	0.45
1:I:48:GLU:O	1:I:52:MET:HG2	2.17	0.45
1:I:61:ASN:ND2	1:I:63:THR:O	2.50	0.45
1:I:106:LEU:HD22	2:A:3587:TRP:HE1	1.82	0.45
2:A:66:THR:OG1	2:A:124:SER:OG	2.24	0.45
2:A:1151:HIS:ND1	2:A:1185:ASP:OD1	2.32	0.45
2:A:1417:TYR:O	2:A:1421:MET:HG2	2.15	0.45
2:A:1435:GLY:N	2:A:1500:ARG:HH22	2.12	0.45
1:J:61:ASN:ND2	1:J:63:THR:O	2.50	0.45
1:K:80:THR:OG1	1:K:83:GLU:OE2	2.32	0.45
2:B:624:ALA:HB2	2:B:1667:LEU:HD12	1.97	0.45
2:B:1610:ARG:HA	2:B:1617:TRP:HA	1.98	0.45
2:B:2703:PRO:HB2	2:B:2854:LYS:HE2	1.99	0.45
2:B:2821:TYR:CE2	2:B:2823:PRO:HG3	2.51	0.45
2:B:3043:ARG:HB3	2:B:3117:PHE:CD1	2.50	0.45
2:B:3253:GLY:O	2:B:3257:ASN:HB3	2.16	0.45
2:C:658:ASN:HD21	2:C:833:LYS:HG2	1.82	0.45
2:C:1176:THR:HG22	2:C:1181:ILE:HA	1.97	0.45
2:C:2791:ARG:NH1	2:C:2796:ASP:OD2	2.50	0.45
2:C:4921:PHE:HE2	2:C:4940:VAL:HG11	1.81	0.45
2:D:218:SER:HB3	2:D:286:GLY:HA3	1.97	0.45
2:D:891:GLU:O	2:D:895:MET:HE1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:989:THR:HG22	2:D:992:GLN:HG2	1.98	0.45
2:D:3022:PHE:HB3	2:D:3025:ASP:OD1	2.16	0.45
2:D:3310:VAL:HG13	2:D:3314:LEU:HD12	1.97	0.45
2:D:4956:ASP:HA	2:D:4960:LYS:HD3	1.97	0.45
2:A:887:GLU:O	2:A:891:GLU:HG2	2.17	0.45
2:A:911:ASN:OD1	2:A:912:LYS:N	2.48	0.45
2:A:3292:GLU:O	2:A:3296:MET:HE2	2.16	0.45
2:A:3963:SER:OG	2:A:3964:GLN:OE1	2.30	0.45
2:A:4774:LEU:O	2:A:4778:VAL:HG23	2.16	0.45
3:E:78:THR:O	3:E:81:VAL:HG12	2.17	0.45
1:J:10:ILE:HA	1:J:13:PHE:HB2	1.98	0.45
2:B:1008:ALA:O	2:B:1012:ILE:HG12	2.16	0.45
2:B:2972:ASP:OD1	2:B:2976:LYS:NZ	2.49	0.45
2:B:3156:GLY:O	2:B:3240:PRO:HB2	2.16	0.45
2:C:908:ARG:NH2	2:C:928:GLU:OE2	2.49	0.45
2:C:2592:LEU:HD22	2:C:2606:PRO:HB3	1.98	0.45
2:C:2956:TYR:HA	2:C:2959:GLU:OE1	2.16	0.45
2:C:2961:LYS:HB2	2:C:2965:LYS:HZ3	1.81	0.45
2:D:66:THR:OG1	2:D:124:SER:OG	2.24	0.45
2:D:166:SER:OG	2:D:168:GLN:OE1	2.34	0.45
2:D:2591:ARG:HH22	2:D:2875:ASP:CG	2.20	0.45
2:D:2956:TYR:HA	2:D:2959:GLU:OE1	2.16	0.45
2:D:4921:PHE:HE2	2:D:4940:VAL:HG11	1.81	0.45
2:A:785:ASP:OD1	2:A:786:GLY:N	2.49	0.45
2:A:1118:SER:HB2	2:A:1204:VAL:HG11	1.98	0.45
2:A:1979:PHE:HE1	2:A:1988:CYS:HB3	1.82	0.45
2:A:2791:ARG:NH1	2:A:2796:ASP:OD2	2.50	0.45
2:A:3156:GLY:O	2:A:3240:PRO:HB2	2.16	0.45
2:A:3293:GLY:HA3	2:A:3295:TRP:CZ3	2.51	0.45
3:H:78:THR:O	3:H:81:VAL:HG12	2.17	0.45
1:L:59:ASP:N	1:L:68:GLU:OE2	2.33	0.45
2:B:2106:TYR:HH	2:B:3615:ARG:HH12	1.64	0.45
2:B:2857:LYS:O	2:B:2861:GLU:OE1	2.34	0.45
2:B:4269:LYS:HA	2:B:4272:LYS:HE2	1.99	0.45
2:B:4609:LYS:HE3	2:B:4615:LEU:HD13	1.99	0.45
2:C:902:TRP:CD1	2:C:913:ARG:NH2	2.84	0.45
2:C:2646:TRP:CH2	2:C:2928:GLN:HG3	2.51	0.45
2:C:2779:LEU:O	2:C:2782:MET:HG3	2.16	0.45
2:C:2821:TYR:CE2	2:C:2823:PRO:HG3	2.51	0.45
2:C:2857:LYS:O	2:C:2861:GLU:OE1	2.34	0.45
2:C:3022:PHE:HB3	2:C:3025:ASP:OD1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:4242:ARG:HH22	2:C:4249:ARG:NH1	2.15	0.45
2:D:50:GLU:OE2	2:D:61:ASP:N	2.48	0.45
2:D:1981:ASP:OD2	2:D:1983:LYS:NZ	2.48	0.45
2:D:4242:ARG:HH22	2:D:4249:ARG:NH1	2.15	0.45
2:D:4858:LEU:HD23	2:D:4861:ILE:HD12	1.98	0.45
2:A:989:THR:HG22	2:A:992:GLN:HG2	1.98	0.45
2:A:1610:ARG:HA	2:A:1617:TRP:HA	1.98	0.45
2:A:2153:LYS:HD3	2:A:2156:TYR:HD2	1.80	0.45
2:A:2425:SER:O	2:B:142:LYS:NZ	2.49	0.45
2:A:2426:LEU:HB2	2:A:2427:ILE:HD12	1.99	0.45
2:A:2591:ARG:HH22	2:A:2875:ASP:CG	2.20	0.45
2:A:3276:LEU:O	2:A:3280:ILE:HG12	2.17	0.45
2:A:3664:LEU:O	2:A:3668:ILE:HG13	2.17	0.45
1:L:10:ILE:O	1:L:14:LYS:N	2.38	0.45
2:B:887:GLU:O	2:B:891:GLU:HG2	2.17	0.45
2:B:902:TRP:CD1	2:B:913:ARG:NH2	2.84	0.45
2:B:1979:PHE:HE1	2:B:1988:CYS:HB3	1.82	0.45
2:C:227:TYR:CG	2:C:352:SER:HB2	2.52	0.45
2:C:1008:ALA:O	2:C:1012:ILE:HG12	2.16	0.45
2:C:2640:LEU:HD23	2:C:2643:LYS:HZ1	1.82	0.45
2:C:3310:VAL:HG13	2:C:3314:LEU:HD12	1.97	0.45
2:D:908:ARG:NH2	2:D:928:GLU:OE2	2.49	0.45
2:D:2592:LEU:HD22	2:D:2606:PRO:HB3	1.98	0.45
2:D:3253:GLY:O	2:D:3257:ASN:HB3	2.16	0.45
2:A:658:ASN:HD21	2:A:833:LYS:HG2	1.82	0.45
2:A:678:MET:HB2	2:A:754:VAL:HG22	1.98	0.45
2:A:891:GLU:O	2:A:895:MET:HE1	2.17	0.45
2:A:904:TYR:HE1	2:A:916:PRO:HA	1.80	0.45
2:A:2821:TYR:CE2	2:A:2823:PRO:HG3	2.51	0.45
2:A:3107:SER:O	2:A:3111:HIS:HD2	2.00	0.45
2:A:4117:THR:O	2:A:4120:GLU:HG3	2.16	0.45
2:A:4269:LYS:HA	2:A:4272:LYS:HE2	1.99	0.45
2:A:4719:PHE:HE2	2:D:4294:LEU:HD22	1.79	0.45
1:K:10:ILE:HA	1:K:13:PHE:HB2	1.97	0.45
1:K:48:GLU:O	1:K:52:MET:HG2	2.17	0.45
1:K:127:ARG:HD3	1:K:127:ARG:HA	1.41	0.45
2:B:194:LEU:HD11	2:B:201:LEU:HB3	1.98	0.45
2:B:785:ASP:OD1	2:B:786:GLY:N	2.49	0.45
2:B:911:ASN:OD1	2:B:912:LYS:N	2.48	0.45
2:B:2646:TRP:CH2	2:B:2928:GLN:HG3	2.51	0.45
2:B:3107:SER:O	2:B:3111:HIS:HD2	2.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3276:LEU:O	2:B:3280:ILE:HG12	2.17	0.45
2:B:4117:THR:O	2:B:4120:GLU:HG3	2.17	0.45
2:C:2849:HIS:NE2	2:C:2877:LEU:HD11	2.32	0.45
2:C:3604:ARG:O	2:C:3604:ARG:HD3	2.16	0.45
2:C:4257:ARG:O	2:C:4261:LEU:HG	2.17	0.45
2:A:314:LEU:HD11	2:A:372:LEU:HD13	1.99	0.45
2:A:908:ARG:NH2	2:A:928:GLU:OE2	2.49	0.45
2:A:2849:HIS:NE2	2:A:2877:LEU:HD11	2.32	0.45
2:A:3187:LYS:O	2:A:3191:GLU:HB2	2.17	0.45
2:A:3925:GLN:HE22	2:A:4934:THR:HA	1.80	0.45
2:A:4714:PHE:CG	2:D:4294:LEU:HD13	2.51	0.45
3:F:78:THR:O	3:F:81:VAL:HG12	2.17	0.45
2:B:419:ILE:HD13	2:B:492:GLU:HG3	1.97	0.45
2:B:2591:ARG:HH22	2:B:2875:ASP:CG	2.20	0.45
2:B:2791:ARG:NH1	2:B:2796:ASP:OD2	2.50	0.45
2:C:624:ALA:HB2	2:C:1667:LEU:HD12	1.97	0.45
2:C:2591:ARG:HH22	2:C:2875:ASP:CG	2.20	0.45
2:C:2658:GLU:OE1	2:C:2661:LEU:N	2.37	0.45
2:C:4287:TYR:HA	2:C:4290:ILE:HD12	1.99	0.45
2:C:4609:LYS:HE3	2:C:4615:LEU:HD13	1.99	0.45
2:D:887:GLU:O	2:D:891:GLU:HG2	2.17	0.45
2:D:1151:HIS:ND1	2:D:1185:ASP:OD1	2.32	0.45
2:D:2426:LEU:HB2	2:D:2427:ILE:HD12	1.99	0.45
2:D:2640:LEU:HD23	2:D:2643:LYS:HZ1	1.81	0.45
2:D:2791:ARG:NH1	2:D:2796:ASP:OD2	2.50	0.45
2:D:2849:HIS:NE2	2:D:2877:LEU:HD11	2.32	0.45
2:D:3276:LEU:O	2:D:3280:ILE:HG12	2.17	0.45
2:D:3963:SER:OG	2:D:3964:GLN:OE1	2.30	0.45
2:D:4257:ARG:O	2:D:4261:LEU:HG	2.17	0.45
2:D:4667:SER:HA	2:D:4672:MET:HE3	1.97	0.45
2:A:436:LEU:HD23	2:A:436:LEU:HA	1.81	0.45
2:A:2347:MET:O	2:A:2351:ILE:HG12	2.17	0.45
2:A:2956:TYR:HA	2:A:2959:GLU:OE1	2.16	0.45
2:A:4257:ARG:O	2:A:4261:LEU:HG	2.17	0.45
2:B:2662:PHE:HE2	2:B:2962:PHE:HD1	1.62	0.45
2:B:2849:HIS:NE2	2:B:2877:LEU:HD11	2.32	0.45
2:B:3184:TYR:CE2	2:B:3197:LEU:HB3	2.52	0.45
2:B:4287:TYR:HA	2:B:4290:ILE:HD12	1.99	0.45
2:C:2447:LYS:HD3	2:C:2447:LYS:HA	1.80	0.45
2:D:1014:GLN:HB3	2:D:1027:ARG:HH21	1.81	0.45
2:D:3067:ASP:O	2:D:3071:THR:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3184:TYR:HB3	2:D:3192:ARG:NH2	2.27	0.45
1:I:133:GLY:O	2:A:3298:ARG:HG2	2.17	0.45
2:A:419:ILE:HD13	2:A:492:GLU:HG3	1.97	0.45
2:A:4277:LYS:HD3	2:A:4277:LYS:HA	1.75	0.45
2:A:4609:LYS:HE3	2:A:4615:LEU:HD13	1.99	0.45
3:F:3:VAL:HG21	3:F:59:GLY:HA2	1.98	0.45
1:J:76:LYS:HB2	1:J:78:LYS:HZ2	1.81	0.45
2:B:314:LEU:HD11	2:B:372:LEU:HD13	1.99	0.45
2:B:318:ASP:OD1	2:B:319:LYS:N	2.45	0.45
2:B:527:LYS:HE2	2:B:527:LYS:HB2	1.82	0.45
2:B:989:THR:HG22	2:B:992:GLN:HG2	1.98	0.45
2:B:2447:LYS:HE2	2:B:2864:GLY:HA3	1.99	0.45
2:B:2525:LEU:HG	2:B:2569:ILE:HD13	1.98	0.45
2:B:2620:TYR:HB2	2:B:2627:TRP:HD1	1.82	0.45
2:B:4242:ARG:HH22	2:B:4249:ARG:NH1	2.15	0.45
2:C:910:ASP:OD1	2:C:911:ASN:N	2.50	0.45
2:C:3171:LEU:O	2:C:3210:SER:HA	2.17	0.45
2:C:3276:LEU:O	2:C:3280:ILE:HG12	2.17	0.45
2:D:227:TYR:CG	2:D:352:SER:HB2	2.52	0.45
2:D:2794:GLU:HB2	2:D:2798:MET:CE	2.47	0.45
2:D:2857:LYS:O	2:D:2861:GLU:OE1	2.35	0.45
2:D:2946:GLY:HA3	2:D:2954:PHE:CZ	2.51	0.45
2:D:3107:SER:O	2:D:3111:HIS:HD2	2.00	0.45
2:D:3184:TYR:CE2	2:D:3197:LEU:HB3	2.52	0.45
2:A:2703:PRO:HB2	2:A:2854:LYS:HE2	1.99	0.45
3:G:3:VAL:HG21	3:G:59:GLY:HA2	1.98	0.45
2:B:2640:LEU:HD23	2:B:2643:LYS:HZ1	1.82	0.45
2:B:3067:ASP:O	2:B:3071:THR:HG23	2.17	0.45
2:B:3664:LEU:O	2:B:3668:ILE:HG13	2.17	0.45
2:B:4116:GLN:HA	2:B:4119:LEU:HD12	1.98	0.45
2:C:218:SER:HB3	2:C:286:GLY:HA3	1.97	0.45
2:C:314:LEU:HD11	2:C:372:LEU:HD13	1.99	0.45
2:C:989:THR:HG22	2:C:992:GLN:HG2	1.98	0.45
2:C:3107:SER:O	2:C:3111:HIS:HD2	2.00	0.45
2:C:3148:VAL:HA	2:C:3151:GLN:HG3	1.99	0.45
2:C:3253:GLY:O	2:C:3257:ASN:HB3	2.16	0.45
2:C:4117:THR:O	2:C:4120:GLU:HG3	2.16	0.45
2:D:2447:LYS:HE2	2:D:2864:GLY:HA3	1.99	0.45
2:D:2821:TYR:CE2	2:D:2823:PRO:HG3	2.51	0.45
2:D:3830:LEU:HB3	2:D:3833:ASP:OD1	2.17	0.45
1:I:40:LEU:HD11	2:A:3596:LYS:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1967:SER:O	2:A:1972:GLN:NE2	2.41	0.44
2:A:2715:GLU:OE1	2:A:2715:GLU:N	2.44	0.44
2:A:3171:LEU:O	2:A:3210:SER:HA	2.17	0.44
2:A:3184:TYR:CE2	2:A:3197:LEU:HB3	2.52	0.44
2:A:4116:GLN:HA	2:A:4119:LEU:HD12	1.98	0.44
2:A:4649:VAL:O	2:A:4653:VAL:HG23	2.17	0.44
3:E:3:VAL:HG21	3:E:59:GLY:HA2	1.98	0.44
1:K:19:LEU:HD11	2:C:3595:ARG:HH21	1.82	0.44
2:B:227:TYR:CG	2:B:352:SER:HB2	2.52	0.44
2:B:3187:LYS:O	2:B:3191:GLU:HB2	2.17	0.44
2:C:3200:ASN:HB3	2:C:3203:ASP:HB2	2.00	0.44
2:D:2176:VAL:HG22	2:D:2220:TYR:CZ	2.53	0.44
2:D:4287:TYR:HA	2:D:4290:ILE:HD12	1.99	0.44
2:D:4609:LYS:HE3	2:D:4615:LEU:HD13	1.99	0.44
1:I:45:THR:HG22	2:A:3817:LEU:HD23	1.99	0.44
2:A:836:HIS:ND1	2:A:841:LYS:HE3	2.32	0.44
2:A:910:ASP:OD1	2:A:911:ASN:N	2.50	0.44
2:A:2757:MET:N	2:A:2757:MET:SD	2.91	0.44
2:A:3067:ASP:O	2:A:3071:THR:HG23	2.17	0.44
2:A:3184:TYR:HB3	2:A:3192:ARG:NH2	2.27	0.44
2:A:4949:TRP:HB3	2:A:4952:PHE:HD2	1.82	0.44
2:B:678:MET:HB2	2:B:754:VAL:HG22	1.98	0.44
2:B:2961:LYS:HB2	2:B:2965:LYS:HZ3	1.82	0.44
2:B:4858:LEU:HD23	2:B:4861:ILE:HD12	1.98	0.44
2:C:1979:PHE:HE1	2:C:1988:CYS:HB3	1.82	0.44
2:C:2715:GLU:OE1	2:C:2715:GLU:N	2.44	0.44
2:C:3184:TYR:CE2	2:C:3197:LEU:HB3	2.52	0.44
2:C:4858:LEU:HD23	2:C:4861:ILE:HD12	1.98	0.44
2:D:314:LEU:HD11	2:D:372:LEU:HD13	1.99	0.44
2:D:890:HIS:O	2:D:894:VAL:HG13	2.18	0.44
2:D:3067:ASP:HA	2:D:3070:LYS:NZ	2.29	0.44
2:D:3187:LYS:O	2:D:3191:GLU:HB2	2.17	0.44
2:D:3664:LEU:O	2:D:3668:ILE:HG13	2.17	0.44
2:D:4949:TRP:HB3	2:D:4952:PHE:HD2	1.82	0.44
2:A:194:LEU:HD11	2:A:201:LEU:HB3	1.98	0.44
2:A:2377:GLU:O	2:A:2381:THR:N	2.50	0.44
2:A:2620:TYR:HB2	2:A:2627:TRP:HD1	1.82	0.44
2:A:2794:GLU:HB2	2:A:2798:MET:CE	2.47	0.44
2:A:3127:GLN:HG3	2:A:3183:ILE:HB	1.98	0.44
2:A:3253:GLY:O	2:A:3257:ASN:HB3	2.16	0.44
2:B:1948:MET:HE2	2:B:1948:MET:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2222:LEU:HD11	2:B:2301:PHE:CZ	2.52	0.44
2:B:3122:ILE:O	2:B:3127:GLN:HG2	2.18	0.44
2:B:3240:PRO:HG3	2:B:3299:LEU:HG	2.00	0.44
2:B:3830:LEU:HB3	2:B:3833:ASP:OD1	2.18	0.44
2:B:4753:LEU:HD23	2:C:4773:LEU:HD13	1.99	0.44
2:C:877:HIS:O	2:C:880:ARG:HG3	2.18	0.44
2:C:1118:SER:HB2	2:C:1204:VAL:HG11	1.98	0.44
2:C:2176:VAL:HG22	2:C:2220:TYR:CZ	2.53	0.44
2:C:2525:LEU:HG	2:C:2569:ILE:HD13	1.98	0.44
2:D:483:LYS:HE2	2:D:483:LYS:HB2	1.68	0.44
2:A:996:VAL:HG13	2:A:1050:LEU:HD22	1.97	0.44
2:A:1852:LYS:NZ	2:A:2054:LYS:HD2	2.32	0.44
2:A:2204:CYS:SG	2:A:2214:MET:HG3	2.58	0.44
2:A:3068:LEU:O	2:A:3071:THR:OG1	2.27	0.44
2:A:4287:TYR:HA	2:A:4290:ILE:HD12	1.99	0.44
2:A:4798:ASP:N	2:A:4798:ASP:OD1	2.51	0.44
3:H:3:VAL:HG21	3:H:59:GLY:HA2	1.98	0.44
2:B:1118:SER:HB2	2:B:1204:VAL:HG11	1.98	0.44
2:B:2772:ARG:HG3	2:B:2776:LYS:HZ2	1.83	0.44
2:B:3106:SER:OG	2:B:3157:GLU:OE1	2.21	0.44
2:B:3200:ASN:HB3	2:B:3203:ASP:HB2	2.00	0.44
2:C:2794:GLU:HB2	2:C:2798:MET:CE	2.47	0.44
2:C:4269:LYS:HA	2:C:4272:LYS:HE2	1.99	0.44
2:C:4649:VAL:O	2:C:4653:VAL:HG23	2.17	0.44
2:D:2831:VAL:HB	2:D:2894:LYS:CE	2.47	0.44
2:D:3001:LYS:NZ	2:D:3041:ASP:OD2	2.33	0.44
2:D:3171:LEU:O	2:D:3210:SER:HA	2.17	0.44
2:D:3200:ASN:HB3	2:D:3203:ASP:HB2	2.00	0.44
2:D:4117:THR:O	2:D:4120:GLU:HG3	2.17	0.44
2:D:4649:VAL:O	2:D:4653:VAL:HG23	2.17	0.44
2:A:227:TYR:CG	2:A:352:SER:HB2	2.52	0.44
2:A:874:LEU:HB3	2:A:879:GLU:OE2	2.18	0.44
2:A:877:HIS:O	2:A:880:ARG:HG3	2.18	0.44
2:A:1100:ARG:HB3	2:A:1236:TYR:CD2	2.53	0.44
2:A:2640:LEU:HA	2:A:2643:LYS:HZ1	1.82	0.44
2:A:3830:LEU:HB3	2:A:3833:ASP:OD1	2.17	0.44
2:C:836:HIS:ND1	2:C:841:LYS:HE3	2.32	0.44
2:C:2757:MET:N	2:C:2757:MET:SD	2.91	0.44
2:C:4511:PHE:HZ	2:C:4746:ILE:HG21	1.83	0.44
2:D:1564:MET:CE	2:D:1565:PRO:HD2	2.48	0.44
2:D:3122:ILE:O	2:D:3127:GLN:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3744:ILE:O	2:D:3747:SER:OG	2.31	0.44
2:D:4093:ASP:OD1	2:D:4094:ILE:HD12	2.18	0.44
2:A:2176:VAL:HG22	2:A:2220:TYR:CZ	2.53	0.44
3:G:78:THR:O	3:G:81:VAL:HG12	2.17	0.44
1:J:42:GLN:HE21	2:B:1957:LEU:HD21	1.82	0.44
1:L:126:ILE:O	1:L:130:ASP:N	2.48	0.44
1:K:121:GLU:O	1:K:124:GLU:HB2	2.18	0.44
2:B:335:LYS:HZ1	2:B:397:GLY:HA3	1.81	0.44
2:B:1852:LYS:NZ	2:B:2054:LYS:HD2	2.32	0.44
2:B:2176:VAL:HG22	2:B:2220:TYR:CZ	2.53	0.44
2:B:2377:GLU:O	2:B:2381:THR:N	2.50	0.44
2:B:2592:LEU:HD22	2:B:2606:PRO:HB3	1.98	0.44
2:B:4649:VAL:O	2:B:4653:VAL:HG23	2.17	0.44
2:B:4798:ASP:OD1	2:B:4798:ASP:N	2.51	0.44
2:C:194:LEU:HD11	2:C:201:LEU:HB3	1.98	0.44
2:C:1852:LYS:NZ	2:C:2054:LYS:HD2	2.32	0.44
2:C:2377:GLU:O	2:C:2381:THR:N	2.50	0.44
2:C:3067:ASP:O	2:C:3071:THR:HG23	2.17	0.44
2:D:910:ASP:OD1	2:D:911:ASN:N	2.50	0.44
2:D:949:HIS:O	2:D:1065:GLU:N	2.51	0.44
2:D:2347:MET:O	2:D:2351:ILE:HG12	2.17	0.44
2:D:3127:GLN:HG3	2:D:3183:ILE:HB	1.98	0.44
2:D:4511:PHE:HZ	2:D:4746:ILE:HG21	1.83	0.44
2:D:4798:ASP:OD1	2:D:4798:ASP:N	2.51	0.44
2:A:3200:ASN:HB3	2:A:3203:ASP:HB2	2.00	0.44
2:A:3955:GLN:HE21	2:A:3972:MET:HG2	1.83	0.44
1:L:61:ASN:ND2	1:L:63:THR:O	2.50	0.44
2:B:891:GLU:O	2:B:895:MET:HE1	2.18	0.44
2:B:1564:MET:CE	2:B:1565:PRO:HD2	2.48	0.44
2:B:2383:HIS:CG	2:B:2458:ALA:HB2	2.53	0.44
2:B:2426:LEU:HB2	2:B:2427:ILE:HD12	1.99	0.44
2:B:4093:ASP:OD1	2:B:4094:ILE:HD12	2.18	0.44
2:B:4511:PHE:HZ	2:B:4746:ILE:HG21	1.83	0.44
2:C:21:VAL:HB	2:C:36:CYS:SG	2.58	0.44
2:C:2426:LEU:HB2	2:C:2427:ILE:HD12	1.99	0.44
2:D:1100:ARG:HB3	2:D:1236:TYR:CD2	2.53	0.44
2:D:1979:PHE:HE1	2:D:1988:CYS:HB3	1.82	0.44
2:D:2222:LEU:HD11	2:D:2301:PHE:CZ	2.52	0.44
2:D:2733:SER:HA	2:D:2736:LYS:HZ3	1.82	0.44
1:I:122:VAL:HA	1:I:125:MET:HE3	2.00	0.44
2:A:515:ALA:HB2	2:A:523:GLY:HA3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2222:LEU:HD23	2:A:2222:LEU:HA	1.88	0.44
2:A:2447:LYS:HE2	2:A:2864:GLY:HA3	1.99	0.44
2:A:2857:LYS:O	2:A:2861:GLU:OE1	2.34	0.44
2:A:3122:ILE:O	2:A:3127:GLN:HG2	2.18	0.44
2:A:3246:MET:HG2	2:A:3309:LYS:HZ2	1.81	0.44
2:A:4242:ARG:HH22	2:A:4249:ARG:NH1	2.15	0.44
2:A:4707:MET:HA	2:D:4252:ILE:HG21	2.00	0.44
1:L:121:GLU:O	1:L:124:GLU:HB2	2.18	0.44
2:B:903:GLN:H	2:B:913:ARG:NE	2.16	0.44
2:B:3955:GLN:HE21	2:B:3972:MET:HG2	1.83	0.44
2:B:4257:ARG:O	2:B:4261:LEU:HG	2.17	0.44
2:C:887:GLU:O	2:C:891:GLU:HG2	2.17	0.44
2:C:2844:MET:SD	2:C:2888:LYS:NZ	2.91	0.44
2:C:3163:ALA:HB1	2:C:3245:TYR:CD1	2.52	0.44
2:C:3955:GLN:HE21	2:C:3972:MET:HG2	1.83	0.44
2:D:836:HIS:ND1	2:D:841:LYS:HE3	2.32	0.44
2:D:1286:THR:OG1	2:D:1550:PRO:O	2.22	0.44
2:D:2620:TYR:HB2	2:D:2627:TRP:HD1	1.82	0.44
1:I:121:GLU:O	1:I:124:GLU:HB2	2.18	0.44
2:A:2772:ARG:HG3	2:A:2776:LYS:HZ2	1.83	0.44
2:A:2926:LEU:HD23	2:A:2929:LEU:HD12	2.00	0.44
2:A:3240:PRO:HG3	2:A:3299:LEU:HG	2.00	0.44
2:A:4591:TYR:CD2	2:D:4287:TYR:HE1	2.36	0.44
3:G:50:ARG:HH21	3:G:53:LYS:NZ	2.16	0.44
2:B:836:HIS:ND1	2:B:841:LYS:HE3	2.33	0.44
2:B:874:LEU:HB3	2:B:879:GLU:OE2	2.18	0.44
2:B:1100:ARG:HB3	2:B:1236:TYR:CD2	2.53	0.44
2:B:2347:MET:O	2:B:2351:ILE:HG12	2.17	0.44
2:B:2794:GLU:HB2	2:B:2798:MET:CE	2.47	0.44
2:B:3171:LEU:O	2:B:3210:SER:HA	2.18	0.44
2:C:335:LYS:HZ1	2:C:397:GLY:HA3	1.83	0.44
2:C:637:LEU:HD22	2:C:1679:HIS:CD2	2.53	0.44
2:C:948:CYS:HA	2:C:1067:PRO:HD3	2.00	0.44
2:C:1100:ARG:HB3	2:C:1236:TYR:CD2	2.53	0.44
2:C:1283:LEU:HB2	2:C:1555:PHE:HB2	2.00	0.44
2:C:2620:TYR:HB2	2:C:2627:TRP:HD1	1.82	0.44
2:C:4731:LEU:HD23	2:C:4734:TYR:HD2	1.83	0.44
2:D:675:TYR:HB3	2:D:822:CYS:SG	2.58	0.44
2:D:874:LEU:HB3	2:D:879:GLU:OE2	2.18	0.44
2:D:948:CYS:HA	2:D:1067:PRO:HD3	2.00	0.44
2:D:1433:PHE:O	2:D:1500:ARG:NH1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1852:LYS:NZ	2:D:2054:LYS:HD2	2.32	0.44
2:D:2926:LEU:HD23	2:D:2929:LEU:HD12	2.00	0.44
2:D:3955:GLN:HE21	2:D:3972:MET:HG2	1.83	0.44
2:D:4731:LEU:HD23	2:D:4734:TYR:HD2	1.83	0.44
2:A:890:HIS:O	2:A:894:VAL:HG13	2.18	0.43
2:A:949:HIS:O	2:A:1065:GLU:N	2.51	0.43
2:A:2222:LEU:HD11	2:A:2301:PHE:CZ	2.52	0.43
2:A:2383:HIS:CG	2:A:2458:ALA:HB2	2.53	0.43
2:A:3292:GLU:O	2:A:3292:GLU:HG2	2.18	0.43
2:A:3589:LYS:HE2	2:A:3589:LYS:HB2	1.74	0.43
2:A:4858:LEU:HD23	2:A:4861:ILE:HD12	1.98	0.43
1:J:121:GLU:O	1:J:124:GLU:HB2	2.18	0.43
2:B:890:HIS:O	2:B:894:VAL:HG13	2.18	0.43
2:B:910:ASP:OD1	2:B:911:ASN:N	2.50	0.43
2:B:1132:GLU:HA	2:B:1146:HIS:CE1	2.53	0.43
2:B:2943:PHE:O	2:B:2947:SER:OG	2.25	0.43
2:B:3697:LYS:HA	2:B:3700:HIS:CD2	2.53	0.43
2:C:874:LEU:HB3	2:C:879:GLU:OE2	2.18	0.43
2:C:1433:PHE:O	2:C:1500:ARG:NH1	2.51	0.43
2:C:2204:CYS:SG	2:C:2214:MET:HG3	2.58	0.43
2:C:2824:ARG:O	2:C:2824:ARG:HD2	2.18	0.43
2:C:3664:LEU:O	2:C:3668:ILE:HG13	2.17	0.43
2:C:3830:LEU:HB3	2:C:3833:ASP:OD1	2.17	0.43
2:C:4949:TRP:HB3	2:C:4952:PHE:HD2	1.83	0.43
2:D:637:LEU:HD22	2:D:1679:HIS:CD2	2.53	0.43
2:D:678:MET:HB2	2:D:754:VAL:HG22	1.98	0.43
2:D:2377:GLU:O	2:D:2381:THR:N	2.50	0.43
2:D:2757:MET:SD	2:D:2757:MET:N	2.91	0.43
2:D:3188:SER:O	2:D:3192:ARG:HB2	2.18	0.43
2:A:21:VAL:HB	2:A:36:CYS:SG	2.58	0.43
2:A:675:TYR:HB3	2:A:822:CYS:SG	2.58	0.43
2:A:3148:VAL:HA	2:A:3151:GLN:HG3	2.00	0.43
2:A:4093:ASP:OD1	2:A:4094:ILE:HD12	2.18	0.43
2:A:4630:TRP:HE3	2:D:4245:LEU:HD23	1.81	0.43
3:G:83:TYR:OH	2:C:1768:PHE:O	2.24	0.43
2:B:877:HIS:O	2:B:880:ARG:HG3	2.18	0.43
2:B:2204:CYS:SG	2:B:2214:MET:HG3	2.58	0.43
2:B:3148:VAL:HA	2:B:3151:GLN:HG3	1.99	0.43
2:C:1564:MET:CE	2:C:1565:PRO:HD2	2.48	0.43
2:C:2062:ILE:HG21	2:C:2087:LEU:HG	1.99	0.43
2:C:3122:ILE:O	2:C:3127:GLN:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:3187:LYS:O	2:C:3191:GLU:HB2	2.17	0.43
2:C:4093:ASP:OD1	2:C:4094:ILE:HD12	2.18	0.43
2:D:853:PRO:HG2	2:D:1084:ARG:O	2.18	0.43
2:D:874:LEU:HD23	2:D:879:GLU:HG3	2.00	0.43
2:D:1118:SER:HB2	2:D:1204:VAL:HG11	1.98	0.43
2:D:2204:CYS:SG	2:D:2214:MET:HG3	2.58	0.43
2:D:2646:TRP:CZ3	2:D:2928:GLN:HG3	2.54	0.43
2:D:2703:PRO:HB2	2:D:2854:LYS:HE2	1.99	0.43
2:D:2828:MET:O	2:D:2894:LYS:NZ	2.42	0.43
1:I:59:ASP:N	1:I:68:GLU:OE2	2.33	0.43
1:I:137:VAL:HG21	2:A:3587:TRP:CH2	2.53	0.43
2:A:2592:LEU:HD22	2:A:2606:PRO:HB3	1.98	0.43
2:A:2646:TRP:CZ3	2:A:2928:GLN:HG3	2.53	0.43
2:A:3946:GLY:O	2:A:3950:VAL:HG23	2.18	0.43
1:J:126:ILE:O	1:J:130:ASP:N	2.48	0.43
1:L:80:THR:OG1	1:L:83:GLU:OE2	2.32	0.43
2:B:21:VAL:HB	2:B:36:CYS:SG	2.58	0.43
2:B:913:ARG:HA	2:B:913:ARG:HD2	1.74	0.43
2:B:1564:MET:HE1	2:B:1578:PRO:HA	2.00	0.43
2:B:2705:PRO:HG3	2:B:2854:LYS:HZ2	1.83	0.43
2:B:2757:MET:N	2:B:2757:MET:SD	2.91	0.43
2:B:4731:LEU:HD23	2:B:4734:TYR:HD2	1.83	0.43
2:B:4949:TRP:HB3	2:B:4952:PHE:HD2	1.83	0.43
2:C:902:TRP:CD2	2:C:913:ARG:CZ	3.01	0.43
2:C:1132:GLU:HA	2:C:1146:HIS:CE1	2.54	0.43
2:C:2222:LEU:HD11	2:C:2301:PHE:CZ	2.52	0.43
2:C:2943:PHE:O	2:C:2947:SER:OG	2.25	0.43
2:C:4277:LYS:HD3	2:C:4277:LYS:HA	1.75	0.43
2:D:877:HIS:O	2:D:880:ARG:HG3	2.18	0.43
2:D:1446:ILE:HG12	2:D:1542:ALA:HB2	2.00	0.43
2:A:1446:ILE:HG12	2:A:1542:ALA:HB2	2.00	0.43
2:A:2000:HIS:O	2:A:2004:MET:HG2	2.18	0.43
2:A:3067:ASP:HA	2:A:3070:LYS:NZ	2.29	0.43
2:A:3131:TYR:HE1	2:A:3208:ILE:HB	1.84	0.43
1:L:122:VAL:HA	1:L:125:MET:HE3	2.01	0.43
1:K:15:GLU:O	1:K:19:LEU:HG	2.19	0.43
2:B:675:TYR:HB3	2:B:822:CYS:SG	2.58	0.43
2:B:1452:GLN:HE22	2:B:1484:ASN:ND2	2.16	0.43
2:B:2150:MET:O	2:B:2156:TYR:OH	2.26	0.43
2:B:2824:ARG:HD2	2:B:2824:ARG:O	2.18	0.43
2:B:3589:LYS:HB2	2:B:3589:LYS:HE2	1.74	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2347:MET:O	2:C:2351:ILE:HG12	2.17	0.43
2:C:2383:HIS:CG	2:C:2458:ALA:HB2	2.53	0.43
2:C:2926:LEU:HD23	2:C:2929:LEU:HD12	2.00	0.43
2:D:2157:GLN:O	2:D:3615:ARG:NH2	2.52	0.43
2:D:3148:VAL:HA	2:D:3151:GLN:HG3	1.99	0.43
2:A:14:LEU:HG	2:A:177:VAL:HA	2.00	0.43
2:A:1132:GLU:HA	2:A:1146:HIS:CE1	2.54	0.43
2:A:4057:HIS:CE1	2:B:4660:PHE:CZ	3.04	0.43
2:A:4630:TRP:CH2	2:D:4248:LEU:HB3	2.54	0.43
3:H:50:ARG:HH21	3:H:53:LYS:NZ	2.16	0.43
3:H:79:PRO:O	3:H:84:GLY:HA2	2.19	0.43
2:B:897:LYS:HA	2:B:900:LEU:HB2	2.01	0.43
2:B:948:CYS:HA	2:B:1067:PRO:HD3	2.00	0.43
2:B:1039:ASP:OD1	2:B:1042:THR:HB	2.18	0.43
2:B:2844:MET:SD	2:B:2888:LYS:NZ	2.91	0.43
2:C:648:LEU:HD23	2:C:648:LEU:HA	1.89	0.43
2:C:890:HIS:O	2:C:894:VAL:HG13	2.18	0.43
2:C:1988:CYS:HA	2:C:1989:PRO:HD3	1.87	0.43
2:D:2000:HIS:O	2:D:2004:MET:HG2	2.18	0.43
2:D:3253:GLY:C	2:D:3255:GLU:N	2.72	0.43
1:I:76:LYS:HB2	1:I:78:LYS:HZ2	1.84	0.43
2:A:2926:LEU:HD23	2:A:2926:LEU:HA	1.87	0.43
2:A:3253:GLY:C	2:A:3255:GLU:N	2.72	0.43
2:A:3650:GLU:HB2	2:A:3651:PRO:HD3	2.01	0.43
1:J:48:GLU:O	1:J:52:MET:HG2	2.17	0.43
1:J:122:VAL:HA	1:J:125:MET:HE3	2.01	0.43
2:B:637:LEU:HD22	2:B:1679:HIS:CD2	2.53	0.43
2:B:2427:ILE:HD13	2:B:2471:PHE:CZ	2.54	0.43
2:B:2926:LEU:HD23	2:B:2929:LEU:HD12	2.00	0.43
2:C:483:LYS:HB2	2:C:483:LYS:HE2	1.68	0.43
2:C:897:LYS:HA	2:C:900:LEU:HB2	2.01	0.43
2:C:949:HIS:O	2:C:1065:GLU:N	2.51	0.43
2:C:2646:TRP:CZ3	2:C:2928:GLN:HG3	2.54	0.43
2:D:515:ALA:HB2	2:D:523:GLY:HA3	2.00	0.43
2:D:2785:TRP:HE1	2:D:2905:ARG:HH12	1.67	0.43
2:D:2824:ARG:HD2	2:D:2824:ARG:O	2.18	0.43
2:D:3102:LEU:HD12	2:D:3102:LEU:HA	1.86	0.43
2:D:3240:PRO:HG3	2:D:3299:LEU:HG	2.00	0.43
2:A:897:LYS:HA	2:A:900:LEU:HB2	2.01	0.43
2:A:3016:ARG:O	2:A:3018:ARG:NE	2.32	0.43
3:F:50:ARG:HH21	3:F:53:LYS:NZ	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:67:MET:HE2	3:F:104:LEU:HB2	2.01	0.43
1:K:10:ILE:O	1:K:14:LYS:N	2.38	0.43
2:B:949:HIS:O	2:B:1065:GLU:N	2.51	0.43
2:B:1433:PHE:O	2:B:1500:ARG:NH1	2.51	0.43
2:B:2658:GLU:OE1	2:B:2661:LEU:N	2.37	0.43
2:B:2945:GLY:HA2	2:B:2948:ARG:CZ	2.49	0.43
2:C:675:TYR:HB3	2:C:822:CYS:SG	2.58	0.43
2:C:694:ARG:NH1	2:C:718:VAL:O	2.49	0.43
2:C:968:LYS:HA	2:C:968:LYS:HD2	1.91	0.43
2:C:1183:LEU:HB3	2:C:1189:GLU:OE1	2.19	0.43
2:C:1260:GLN:OE1	2:C:1261:VAL:N	2.52	0.43
2:C:1538:LYS:HD2	2:C:1636:ASN:ND2	2.34	0.43
2:C:1724:GLU:HG2	2:C:2165:LEU:HD23	2.00	0.43
2:C:2000:HIS:O	2:C:2004:MET:HG2	2.18	0.43
2:C:2907:PHE:CE2	2:C:2909:ASP:HA	2.54	0.43
2:C:4107:GLU:OE2	2:C:4149:TYR:OH	2.15	0.43
2:D:902:TRP:CD2	2:D:913:ARG:CZ	3.01	0.43
2:D:1436:GLN:H	2:D:1500:ARG:HH12	1.67	0.43
2:D:2222:LEU:HD23	2:D:2222:LEU:HA	1.89	0.43
2:D:3198:PRO:O	2:D:3199:THR:OG1	2.33	0.43
2:D:3697:LYS:HA	2:D:3700:HIS:CD2	2.54	0.43
2:A:483:LYS:HE2	2:A:483:LYS:HB2	1.68	0.43
2:A:637:LEU:HD22	2:A:1679:HIS:CD2	2.53	0.43
2:A:913:ARG:HA	2:A:913:ARG:HD2	1.74	0.43
2:A:1433:PHE:O	2:A:1500:ARG:NH1	2.51	0.43
2:A:1724:GLU:HG2	2:A:2165:LEU:HD23	2.00	0.43
2:A:2436:ILE:HA	2:A:2465:LYS:HE3	2.01	0.43
2:A:3188:SER:O	2:A:3192:ARG:HB2	2.18	0.43
2:A:3697:LYS:HA	2:A:3700:HIS:CD2	2.54	0.43
2:A:4689:LYS:HD2	2:A:4689:LYS:HA	1.82	0.43
3:E:79:PRO:O	3:E:84:GLY:HA2	2.19	0.43
3:F:79:PRO:O	3:F:84:GLY:HA2	2.19	0.43
3:G:67:MET:HE2	3:G:104:LEU:HB2	2.01	0.43
3:G:79:PRO:O	3:G:84:GLY:HA2	2.19	0.43
1:J:117:LEU:HD23	1:J:118:THR:N	2.34	0.43
1:K:117:LEU:HD23	1:K:118:THR:N	2.34	0.43
2:B:902:TRP:CD2	2:B:913:ARG:CZ	3.01	0.43
2:B:1081:THR:OG1	2:B:1082:GLY:N	2.51	0.43
2:B:1283:LEU:HB2	2:B:1555:PHE:HB2	2.00	0.43
2:B:1538:LYS:HD2	2:B:1636:ASN:ND2	2.34	0.43
2:B:1714:TYR:CE2	2:B:1718:ARG:HD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:515:ALA:HB2	2:C:523:GLY:HA3	2.00	0.43
2:C:874:LEU:HD23	2:C:879:GLU:HG3	2.01	0.43
2:C:2972:ASP:OD1	2:C:2976:LYS:NZ	2.49	0.43
2:C:3188:SER:O	2:C:3192:ARG:HB2	2.18	0.43
2:D:1107:THR:OG1	2:D:1160:ASP:O	2.26	0.43
2:D:1183:LEU:HB3	2:D:1189:GLU:OE1	2.19	0.43
2:D:1260:GLN:OE1	2:D:1261:VAL:N	2.52	0.43
2:D:2106:TYR:HH	2:D:3615:ARG:HH12	1.67	0.43
2:A:902:TRP:CD2	2:A:913:ARG:CZ	3.01	0.43
2:A:1649:GLU:HG2	2:A:1650:LEU:N	2.34	0.43
2:A:2824:ARG:HD2	2:A:2824:ARG:O	2.18	0.43
2:A:2831:VAL:HB	2:A:2894:LYS:CE	2.47	0.43
2:A:2945:GLY:HA2	2:A:2948:ARG:CZ	2.49	0.43
2:A:3743:THR:HB	2:A:3758:THR:HG21	2.01	0.43
2:A:4237:SER:O	2:A:4240:THR:OG1	2.37	0.43
2:A:4511:PHE:HZ	2:A:4746:ILE:HG21	1.83	0.43
1:K:114:GLY:O	1:K:116:LYS:NZ	2.31	0.43
2:B:166:SER:OG	2:B:168:GLN:OE1	2.34	0.43
2:B:1151:HIS:ND1	2:B:1185:ASP:OD1	2.32	0.43
2:B:1183:LEU:HB3	2:B:1189:GLU:OE1	2.19	0.43
2:B:2157:GLN:O	2:B:3615:ARG:NH2	2.52	0.43
2:B:2733:SER:HA	2:B:2736:LYS:HZ3	1.83	0.43
2:B:3188:SER:O	2:B:3192:ARG:HB2	2.18	0.43
2:B:4735:ASN:HB3	2:B:4738:PHE:CD2	2.54	0.43
2:C:940:LEU:HD12	2:C:941:LYS:N	2.34	0.43
2:C:1452:GLN:HE22	2:C:1484:ASN:ND2	2.16	0.43
2:C:2427:ILE:HD13	2:C:2471:PHE:CZ	2.54	0.43
2:C:2945:GLY:HA2	2:C:2948:ARG:CZ	2.49	0.43
2:C:4663:ARG:HA	2:C:4663:ARG:HD2	1.88	0.43
2:D:21:VAL:HB	2:D:36:CYS:SG	2.58	0.43
2:D:940:LEU:HD12	2:D:941:LYS:N	2.34	0.43
2:D:1948:MET:HA	2:D:1948:MET:HE2	2.00	0.43
2:D:3655:ASP:HB2	2:D:3660:ARG:HE	1.84	0.43
1:I:80:THR:OG1	1:I:83:GLU:OE2	2.32	0.43
1:I:127:ARG:HD3	1:I:127:ARG:HA	1.41	0.43
2:A:1304:LEU:HD23	2:A:1304:LEU:HA	1.90	0.43
2:A:1512:ASP:OD2	2:A:1515:SER:OG	2.26	0.43
2:A:1931:ASP:OD1	2:A:1932:PHE:N	2.52	0.43
2:B:2062:ILE:HG21	2:B:2087:LEU:HG	2.00	0.43
2:B:3149:GLU:OE2	2:B:3232:PRO:HG2	2.19	0.43
2:B:3292:GLU:O	2:B:3292:GLU:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3946:GLY:O	2:B:3950:VAL:HG23	2.18	0.43
2:C:853:PRO:HG2	2:C:1084:ARG:O	2.18	0.43
2:C:2259:GLU:HB2	2:C:2260:PRO:HD3	2.01	0.43
2:C:2703:PRO:HB2	2:C:2854:LYS:HE2	1.99	0.43
2:C:2733:SER:HA	2:C:2736:LYS:HZ3	1.82	0.43
2:D:1714:TYR:CE2	2:D:1718:ARG:HD2	2.54	0.43
2:D:2907:PHE:CE2	2:D:2909:ASP:HA	2.54	0.43
1:I:6:THR:O	1:I:10:ILE:HD12	2.19	0.42
2:A:4731:LEU:HD23	2:A:4734:TYR:HD2	1.83	0.42
1:K:61:ASN:ND2	1:K:63:THR:O	2.50	0.42
1:K:76:LYS:HB2	1:K:78:LYS:HZ2	1.84	0.42
1:K:122:VAL:HA	1:K:125:MET:HE3	2.01	0.42
2:B:940:LEU:HD12	2:B:941:LYS:N	2.34	0.42
2:B:1166:VAL:HG23	2:B:1173:MET:HG2	2.01	0.42
2:B:2259:GLU:HB2	2:B:2260:PRO:HD3	2.01	0.42
2:B:2646:TRP:CZ3	2:B:2928:GLN:HG3	2.53	0.42
2:C:14:LEU:HG	2:C:177:VAL:HA	2.00	0.42
2:C:765:SER:HA	2:C:779:PHE:O	2.19	0.42
2:C:1039:ASP:OD1	2:C:1042:THR:HB	2.18	0.42
2:C:1649:GLU:HG2	2:C:1650:LEU:N	2.34	0.42
2:C:2157:GLN:O	2:C:3615:ARG:NH2	2.51	0.42
2:C:3149:GLU:OE2	2:C:3232:PRO:HG2	2.19	0.42
2:C:3689:MET:CE	2:C:3753:PRO:HB2	2.49	0.42
2:C:3697:LYS:HA	2:C:3700:HIS:CD2	2.54	0.42
2:D:737:ILE:HD13	2:D:1482:ARG:HD3	2.00	0.42
2:D:1132:GLU:HA	2:D:1146:HIS:CE1	2.54	0.42
2:D:2259:GLU:HB2	2:D:2260:PRO:HD3	2.01	0.42
2:D:2436:ILE:HA	2:D:2465:LYS:HE3	2.01	0.42
2:D:2844:MET:SD	2:D:2888:LYS:NZ	2.91	0.42
2:D:2945:GLY:HA2	2:D:2948:ARG:CZ	2.49	0.42
2:D:3292:GLU:O	2:D:3292:GLU:HG2	2.18	0.42
2:D:3946:GLY:O	2:D:3950:VAL:HG23	2.18	0.42
2:D:4735:ASN:HB3	2:D:4738:PHE:CD2	2.54	0.42
2:D:4964:ASP:OD1	2:D:4965:GLN:N	2.52	0.42
2:A:318:ASP:OD1	2:A:319:LYS:N	2.45	0.42
2:A:1039:ASP:OD1	2:A:1042:THR:HB	2.18	0.42
2:A:1166:VAL:HG23	2:A:1173:MET:HG2	2.01	0.42
2:A:1538:LYS:HD2	2:A:1636:ASN:ND2	2.34	0.42
2:A:2259:GLU:HB2	2:A:2260:PRO:HD3	2.01	0.42
2:A:3088:LYS:HG3	2:A:3090:VAL:HG22	2.01	0.42
2:A:3180:ILE:HG23	2:A:3181:TYR:CD1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:15:GLU:O	1:J:19:LEU:HG	2.19	0.42
1:L:19:LEU:HD11	2:D:3595:ARG:HH21	1.84	0.42
1:K:6:THR:O	1:K:10:ILE:HD12	2.19	0.42
1:K:36:VAL:O	1:K:39:SER:OG	2.27	0.42
2:B:3180:ILE:HG23	2:B:3181:TYR:CD1	2.54	0.42
2:B:3192:ARG:O	2:B:3197:LEU:HB2	2.20	0.42
2:C:274:LEU:HD23	2:C:274:LEU:HA	1.81	0.42
2:C:1962:THR:HG22	2:C:1966:ARG:HG3	2.02	0.42
2:C:3131:TYR:HE1	2:C:3208:ILE:HB	1.84	0.42
2:C:3134:LEU:HD22	2:C:3162:PHE:CE2	2.54	0.42
2:C:3188:SER:O	2:C:3192:ARG:CB	2.67	0.42
2:C:3946:GLY:O	2:C:3950:VAL:HG23	2.18	0.42
2:D:765:SER:HA	2:D:779:PHE:O	2.19	0.42
2:D:1724:GLU:HG2	2:D:2165:LEU:HD23	2.00	0.42
2:D:2383:HIS:CG	2:D:2458:ALA:HB2	2.53	0.42
2:D:3693:ASP:O	2:D:3697:LYS:HG2	2.19	0.42
1:I:15:GLU:O	1:I:19:LEU:HG	2.19	0.42
2:A:261:HIS:CE1	2:A:388:GLN:HE22	2.37	0.42
2:A:1183:LEU:HB3	2:A:1189:GLU:OE1	2.19	0.42
2:A:1220:ASP:O	2:A:1223:THR:OG1	2.37	0.42
2:A:1452:GLN:HE22	2:A:1484:ASN:ND2	2.16	0.42
2:A:1564:MET:CE	2:A:1565:PRO:HD2	2.48	0.42
2:A:1825:PHE:CE1	2:A:1842:ILE:HG12	2.54	0.42
2:A:2062:ILE:HG21	2:A:2087:LEU:HG	2.00	0.42
2:A:2427:ILE:HD13	2:A:2471:PHE:CZ	2.54	0.42
2:A:3655:ASP:HB2	2:A:3660:ARG:HE	1.84	0.42
2:A:4735:ASN:HB3	2:A:4738:PHE:CD2	2.54	0.42
2:A:4809:MET:HB2	2:D:4520:TYR:O	2.19	0.42
1:L:89:ALA:HA	1:L:92:VAL:HG22	2.01	0.42
2:B:561:ARG:HG3	2:B:561:ARG:NH1	2.34	0.42
2:B:1446:ILE:HG12	2:B:1542:ALA:HB2	2.00	0.42
2:B:1931:ASP:OD1	2:B:1932:PHE:N	2.52	0.42
2:B:3125:ASP:H	2:B:3183:ILE:CD1	2.32	0.42
2:B:3131:TYR:HE1	2:B:3208:ILE:HB	1.84	0.42
2:B:3655:ASP:HB2	2:B:3660:ARG:HE	1.84	0.42
2:B:4237:SER:O	2:B:4240:THR:OG1	2.37	0.42
2:C:166:SER:OG	2:C:168:GLN:OE1	2.34	0.42
2:C:603:LYS:HB3	2:C:603:LYS:HE2	1.88	0.42
2:C:712:GLU:HG3	2:C:838:ARG:HB3	2.02	0.42
2:C:1825:PHE:CE1	2:C:1842:ILE:HG12	2.54	0.42
2:C:2086:VAL:HG22	2:C:3687:LEU:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:3240:PRO:HG3	2:C:3299:LEU:HG	2.00	0.42
2:C:3655:ASP:HB2	2:C:3660:ARG:HE	1.84	0.42
2:C:4798:ASP:OD1	2:C:4798:ASP:N	2.51	0.42
2:D:332:ARG:NH1	2:D:364:GLN:OE1	2.52	0.42
2:D:2062:ILE:HG21	2:D:2087:LEU:HG	2.00	0.42
2:D:2741:TRP:HH2	2:D:2752:LYS:HD3	1.84	0.42
2:D:3180:ILE:HG23	2:D:3181:TYR:CD1	2.55	0.42
2:D:3650:GLU:HB2	2:D:3651:PRO:HD3	2.00	0.42
2:D:3689:MET:CE	2:D:3753:PRO:HB2	2.49	0.42
2:D:3743:THR:HB	2:D:3758:THR:HG21	2.01	0.42
2:D:4268:MET:O	2:D:4271:VAL:HG22	2.20	0.42
2:A:1948:MET:HA	2:A:1948:MET:CE	2.50	0.42
2:A:2157:GLN:O	2:A:3615:ARG:NH2	2.52	0.42
2:A:2907:PHE:CE2	2:A:2909:ASP:HA	2.54	0.42
2:A:3125:ASP:H	2:A:3183:ILE:CD1	2.32	0.42
1:L:6:THR:O	1:L:10:ILE:HD12	2.19	0.42
1:L:15:GLU:O	1:L:19:LEU:HG	2.19	0.42
1:L:76:LYS:HB2	1:L:78:LYS:NZ	2.34	0.42
1:K:76:LYS:HB2	1:K:78:LYS:NZ	2.35	0.42
2:B:332:ARG:NH1	2:B:364:GLN:OE1	2.53	0.42
2:B:902:TRP:CE2	2:B:913:ARG:CZ	3.02	0.42
2:B:2907:PHE:CE2	2:B:2909:ASP:HA	2.54	0.42
2:B:3067:ASP:HA	2:B:3070:LYS:NZ	2.29	0.42
2:B:3693:ASP:O	2:B:3697:LYS:HG2	2.19	0.42
2:B:3743:THR:HB	2:B:3758:THR:HG21	2.01	0.42
2:B:3955:GLN:NE2	2:B:3972:MET:HG2	2.35	0.42
2:C:902:TRP:CE2	2:C:913:ARG:CZ	3.03	0.42
2:C:2785:TRP:HE1	2:C:2905:ARG:HH12	1.67	0.42
2:C:3292:GLU:O	2:C:3292:GLU:HG2	2.18	0.42
2:D:1039:ASP:OD1	2:D:1042:THR:HB	2.18	0.42
2:D:1825:PHE:CE1	2:D:1842:ILE:HG12	2.54	0.42
2:D:2086:VAL:HG22	2:D:3687:LEU:HD13	2.01	0.42
2:D:4277:LYS:HA	2:D:4277:LYS:HD3	1.75	0.42
2:A:940:LEU:HD12	2:A:941:LYS:N	2.34	0.42
2:A:948:CYS:HA	2:A:1067:PRO:HD3	2.00	0.42
2:A:1714:TYR:CE2	2:A:1718:ARG:HD2	2.54	0.42
2:A:2704:GLN:HA	2:A:2705:PRO:HD3	1.91	0.42
2:A:3192:ARG:O	2:A:3197:LEU:HB2	2.20	0.42
2:B:261:HIS:CE1	2:B:388:GLN:HE22	2.37	0.42
2:B:712:GLU:HG3	2:B:838:ARG:HB3	2.02	0.42
2:B:874:LEU:HD23	2:B:879:GLU:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:332:ARG:NH1	2:C:364:GLN:OE1	2.52	0.42
2:C:737:ILE:HD13	2:C:1482:ARG:HD3	2.00	0.42
2:C:903:GLN:H	2:C:913:ARG:NE	2.16	0.42
2:C:913:ARG:HA	2:C:913:ARG:HD2	1.74	0.42
2:C:2828:MET:O	2:C:2894:LYS:NZ	2.42	0.42
2:C:3693:ASP:O	2:C:3697:LYS:HG2	2.19	0.42
2:C:4689:LYS:HA	2:C:4689:LYS:HD2	1.82	0.42
2:C:4735:ASN:HB3	2:C:4738:PHE:CD2	2.54	0.42
2:C:4964:ASP:OD1	2:C:4965:GLN:N	2.52	0.42
2:D:261:HIS:CE1	2:D:388:GLN:HE22	2.37	0.42
2:D:712:GLU:HG3	2:D:838:ARG:HB3	2.02	0.42
2:D:897:LYS:HA	2:D:900:LEU:HB2	2.00	0.42
2:D:1538:LYS:HD2	2:D:1636:ASN:ND2	2.34	0.42
2:D:1810:VAL:HB	2:D:1817:LEU:HD13	2.01	0.42
2:D:3955:GLN:NE2	2:D:3972:MET:HG2	2.35	0.42
2:A:853:PRO:HG2	2:A:1084:ARG:O	2.18	0.42
2:A:2086:VAL:HG22	2:A:3687:LEU:HD13	2.01	0.42
2:A:3188:SER:O	2:A:3192:ARG:CB	2.67	0.42
2:A:3693:ASP:O	2:A:3697:LYS:HG2	2.19	0.42
2:A:3955:GLN:NE2	2:A:3972:MET:HG2	2.35	0.42
2:A:4183:LYS:HG3	2:A:4184:GLU:HG3	2.01	0.42
2:B:1260:GLN:OE1	2:B:1261:VAL:N	2.52	0.42
2:B:1649:GLU:HG2	2:B:1650:LEU:N	2.34	0.42
2:B:2000:HIS:O	2:B:2004:MET:HG2	2.18	0.42
2:B:3006:SER:C	2:B:3010:LYS:HZ2	2.22	0.42
2:B:3650:GLU:HB2	2:B:3651:PRO:HD3	2.00	0.42
2:B:4036:ASP:HB2	2:B:4043:ILE:HD13	2.02	0.42
2:B:4964:ASP:OD1	2:B:4965:GLN:N	2.52	0.42
2:C:1220:ASP:O	2:C:1223:THR:OG1	2.37	0.42
2:C:1714:TYR:CE2	2:C:1718:ARG:HD2	2.54	0.42
2:C:1973:ILE:HG13	2:C:3608:LEU:HD11	2.02	0.42
2:C:2831:VAL:HB	2:C:2894:LYS:CE	2.47	0.42
2:C:3009:CYS:O	2:C:3013:VAL:HG23	2.19	0.42
2:C:3253:GLY:C	2:C:3255:GLU:N	2.72	0.42
2:C:3743:THR:HB	2:C:3758:THR:HG21	2.01	0.42
2:C:4237:SER:O	2:C:4240:THR:OG1	2.37	0.42
2:D:1452:GLN:HE22	2:D:1484:ASN:ND2	2.16	0.42
2:D:1914:CYS:HB3	2:D:2090:ARG:NH2	2.35	0.42
2:A:902:TRP:CE2	2:A:913:ARG:CZ	3.03	0.42
2:A:1283:LEU:HB2	2:A:1555:PHE:HB2	2.00	0.42
2:A:1436:GLN:H	2:A:1500:ARG:HH12	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1810:VAL:HB	2:A:1817:LEU:HD13	2.01	0.42
2:A:1914:CYS:HB3	2:A:2090:ARG:NH2	2.35	0.42
2:A:1979:PHE:CD2	2:A:1996:LEU:HD23	2.55	0.42
2:A:3763:ILE:HD11	2:A:3838:ASP:O	2.20	0.42
2:A:4660:PHE:HZ	2:D:4057:HIS:CE1	2.37	0.42
2:B:1979:PHE:CD2	2:B:1996:LEU:HD23	2.55	0.42
2:B:2086:VAL:HG22	2:B:3687:LEU:HD13	2.01	0.42
2:B:2831:VAL:HB	2:B:2894:LYS:CE	2.47	0.42
2:B:3095:ASN:O	2:B:3099:VAL:HG22	2.20	0.42
2:B:3188:SER:O	2:B:3192:ARG:CB	2.67	0.42
2:B:3253:GLY:C	2:B:3255:GLU:N	2.72	0.42
2:B:3806:ASN:O	2:B:3810:ARG:HG3	2.20	0.42
2:C:261:HIS:CE1	2:C:388:GLN:HE22	2.37	0.42
2:C:1104:GLU:OE1	2:C:1225:LYS:NZ	2.44	0.42
2:C:3125:ASP:H	2:C:3183:ILE:CD1	2.32	0.42
2:C:3192:ARG:O	2:C:3197:LEU:HB2	2.20	0.42
2:C:3806:ASN:O	2:C:3810:ARG:HG3	2.20	0.42
2:D:4183:LYS:HG3	2:D:4184:GLU:HG3	2.01	0.42
2:A:50:GLU:OE2	2:A:61:ASP:N	2.48	0.42
2:A:737:ILE:HD13	2:A:1482:ARG:HD3	2.00	0.42
2:A:877:HIS:CE1	2:A:878:LEU:HG	2.55	0.42
2:A:3806:ASN:O	2:A:3810:ARG:HG3	2.20	0.42
1:J:89:ALA:HA	1:J:92:VAL:HG22	2.01	0.42
1:K:127:ARG:NH1	1:K:135:GLY:N	2.55	0.42
2:B:50:GLU:OE2	2:B:61:ASP:N	2.48	0.42
2:B:515:ALA:HB2	2:B:523:GLY:HA3	2.00	0.42
2:B:853:PRO:HG2	2:B:1084:ARG:O	2.18	0.42
2:B:877:HIS:CE1	2:B:878:LEU:HG	2.55	0.42
2:B:1810:VAL:HB	2:B:1817:LEU:HD13	2.01	0.42
2:B:3689:MET:CE	2:B:3753:PRO:HB2	2.49	0.42
2:C:756:SER:HB2	2:C:769:ARG:HB3	2.02	0.42
2:C:1166:VAL:HG23	2:C:1173:MET:HG2	2.01	0.42
2:C:1446:ILE:HG12	2:C:1542:ALA:HB2	2.00	0.42
2:C:1914:CYS:HB3	2:C:2090:ARG:NH2	2.35	0.42
2:C:2436:ILE:HA	2:C:2465:LYS:HE3	2.01	0.42
2:C:3088:LYS:HG3	2:C:3090:VAL:HG22	2.01	0.42
2:C:3095:ASN:O	2:C:3099:VAL:HG22	2.20	0.42
2:C:3164:GLY:C	2:C:3248:ARG:HH12	2.23	0.42
2:D:436:LEU:HD23	2:D:436:LEU:HA	1.81	0.42
2:D:1729:MET:HE1	2:D:1930:ASP:HB2	2.01	0.42
2:D:1979:PHE:CD2	2:D:1996:LEU:HD23	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3134:LEU:HD22	2:D:3162:PHE:CE2	2.54	0.42
2:D:4743:LEU:O	2:D:4746:ILE:HG12	2.20	0.42
2:A:163:HIS:HB2	2:A:182:ILE:HG13	2.02	0.42
2:A:527:LYS:HE2	2:A:527:LYS:HB2	1.82	0.42
2:A:756:SER:HB2	2:A:769:ARG:HB3	2.02	0.42
2:A:1040:ASP:HA	2:A:1043:LYS:HZ2	1.85	0.42
2:A:1260:GLN:OE1	2:A:1261:VAL:N	2.52	0.42
2:A:1962:THR:HG22	2:A:1966:ARG:HG3	2.02	0.42
2:A:1973:ILE:HG13	2:A:3608:LEU:HD11	2.02	0.42
2:A:2447:LYS:HA	2:A:2447:LYS:HD3	1.80	0.42
2:A:2508:SER:HB3	2:A:2560:SER:HB3	2.02	0.42
2:A:3149:GLU:OE2	2:A:3232:PRO:HG2	2.19	0.42
1:L:117:LEU:HD23	1:L:118:THR:N	2.34	0.42
2:B:491:GLU:OE2	2:B:546:LYS:NZ	2.47	0.42
2:B:1724:GLU:HG2	2:B:2165:LEU:HD23	2.00	0.42
2:B:3017:HIS:O	2:B:3092:GLN:NE2	2.53	0.42
2:B:3164:GLY:C	2:B:3248:ARG:HH12	2.23	0.42
2:B:3763:ILE:HD11	2:B:3838:ASP:O	2.20	0.42
2:B:3975:GLN:O	2:B:3979:VAL:HG23	2.20	0.42
2:C:680:ASP:O	2:C:751:THR:HG23	2.20	0.42
2:C:1931:ASP:OD1	2:C:1932:PHE:N	2.52	0.42
2:C:1948:MET:HA	2:C:1948:MET:CE	2.50	0.42
2:C:2379:ASP:OD2	2:C:2380:ASP:N	2.53	0.42
2:C:2741:TRP:HH2	2:C:2752:LYS:HD3	1.84	0.42
2:C:3145:SER:H	2:C:3148:VAL:HB	1.85	0.42
2:C:3955:GLN:NE2	2:C:3972:MET:HG2	2.35	0.42
2:C:3975:GLN:O	2:C:3979:VAL:HG23	2.20	0.42
2:C:4240:THR:HG22	2:C:4308:ILE:HD13	2.02	0.42
2:D:680:ASP:O	2:D:751:THR:HG23	2.20	0.42
2:D:877:HIS:CE1	2:D:878:LEU:HG	2.55	0.42
2:D:1081:THR:OG1	2:D:1082:GLY:N	2.51	0.42
2:D:1649:GLU:HG2	2:D:1650:LEU:N	2.34	0.42
2:D:3125:ASP:H	2:D:3183:ILE:CD1	2.32	0.42
2:D:3149:GLU:OE2	2:D:3232:PRO:HG2	2.19	0.42
1:I:89:ALA:HA	1:I:92:VAL:HG22	2.01	0.42
2:A:1914:CYS:O	2:A:1918:VAL:HG23	2.20	0.42
2:A:3017:HIS:O	2:A:3092:GLN:NE2	2.53	0.42
2:A:4240:THR:HG22	2:A:4308:ILE:HD13	2.02	0.42
3:E:50:ARG:HH21	3:E:53:LYS:NZ	2.16	0.42
1:J:6:THR:O	1:J:10:ILE:HD12	2.19	0.42
2:B:14:LEU:HG	2:B:177:VAL:HA	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:896:ASN:O	2:B:899:GLU:HG3	2.20	0.42
2:B:1973:ILE:HG13	2:B:3608:LEU:HD11	2.02	0.42
2:C:1046:ASN:OD1	2:C:1047:LYS:N	2.53	0.42
2:C:1948:MET:HA	2:C:1948:MET:HE2	2.01	0.42
2:C:3006:SER:C	2:C:3010:LYS:HZ2	2.23	0.42
2:C:3017:HIS:O	2:C:3092:GLN:NE2	2.53	0.42
2:C:3106:SER:OG	2:C:3157:GLU:OE1	2.21	0.42
2:C:3763:ILE:HD11	2:C:3838:ASP:O	2.20	0.42
2:C:4268:MET:O	2:C:4271:VAL:HG22	2.20	0.42
2:D:14:LEU:HG	2:D:177:VAL:HA	2.00	0.42
2:D:896:ASN:O	2:D:899:GLU:HG3	2.20	0.42
2:D:903:GLN:H	2:D:913:ARG:NE	2.16	0.42
2:D:2736:LYS:HD2	2:D:2754:GLN:OE1	2.20	0.42
2:D:2826:ILE:H	2:D:2826:ILE:HD12	1.85	0.42
2:D:2930:ILE:HG23	2:D:3010:LYS:HE2	2.02	0.42
2:D:3009:CYS:O	2:D:3013:VAL:HG23	2.19	0.42
2:D:3095:ASN:O	2:D:3099:VAL:HG22	2.20	0.42
1:I:116:LYS:HB2	1:I:116:LYS:HE2	1.85	0.41
2:A:399:MET:SD	2:A:399:MET:N	2.92	0.41
2:A:2844:MET:SD	2:A:2888:LYS:NZ	2.91	0.41
2:A:3145:SER:H	2:A:3148:VAL:HB	1.85	0.41
2:A:3592:SER:O	2:A:3596:LYS:HD3	2.20	0.41
2:A:4237:SER:N	2:A:4240:THR:OG1	2.51	0.41
3:E:67:MET:HE2	3:E:104:LEU:HB2	2.02	0.41
1:K:42:GLN:HE21	2:C:1957:LEU:CD2	2.33	0.41
1:K:64:ILE:HG23	1:K:68:GLU:HB3	2.02	0.41
2:B:50:GLU:CD	2:B:61:ASP:H	2.22	0.41
2:B:680:ASP:O	2:B:751:THR:HG23	2.20	0.41
2:B:737:ILE:HD13	2:B:1482:ARG:HD3	2.00	0.41
2:B:808:HIS:O	2:B:1616:GLY:HA2	2.20	0.41
2:B:1914:CYS:HB3	2:B:2090:ARG:NH2	2.35	0.41
2:B:1962:THR:HG22	2:B:1966:ARG:HG3	2.02	0.41
2:B:2508:SER:HB3	2:B:2560:SER:HB3	2.02	0.41
2:B:2586:GLN:HE22	2:B:2590:ARG:NH2	2.19	0.41
2:B:3009:CYS:O	2:B:3013:VAL:HG23	2.19	0.41
2:B:3088:LYS:HG3	2:B:3090:VAL:HG22	2.02	0.41
2:B:3163:ALA:HB1	2:B:3245:TYR:CD1	2.52	0.41
2:B:4670:LEU:HB2	2:B:4672:MET:CE	2.49	0.41
2:C:808:HIS:O	2:C:1616:GLY:HA2	2.20	0.41
2:C:943:LEU:HD11	2:C:1064:LEU:HD12	2.02	0.41
2:C:1436:GLN:H	2:C:1500:ARG:HH12	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1810:VAL:HB	2:C:1817:LEU:HD13	2.01	0.41
2:C:2153:LYS:HD3	2:C:2153:LYS:HA	1.82	0.41
2:C:2736:LYS:HD2	2:C:2754:GLN:OE1	2.20	0.41
2:C:4183:LYS:HG3	2:C:4184:GLU:HG3	2.01	0.41
2:D:561:ARG:HG3	2:D:561:ARG:NH1	2.34	0.41
2:D:643:LEU:O	2:D:645:GLN:NE2	2.53	0.41
2:D:902:TRP:CE2	2:D:913:ARG:CZ	3.03	0.41
2:D:1046:ASN:OD1	2:D:1047:LYS:N	2.53	0.41
2:D:1283:LEU:HB2	2:D:1555:PHE:HB2	2.00	0.41
2:D:1948:MET:HA	2:D:1948:MET:CE	2.50	0.41
2:D:2427:ILE:HD13	2:D:2471:PHE:CZ	2.54	0.41
2:D:2508:SER:HB3	2:D:2560:SER:HB3	2.02	0.41
2:D:3188:SER:O	2:D:3192:ARG:CB	2.67	0.41
2:D:3806:ASN:O	2:D:3810:ARG:HG3	2.20	0.41
2:D:4670:LEU:HB2	2:D:4672:MET:CE	2.49	0.41
1:I:76:LYS:HB2	1:I:78:LYS:NZ	2.35	0.41
1:I:123:ASP:HA	1:I:126:ILE:HG23	2.02	0.41
2:A:2785:TRP:HE1	2:A:2905:ARG:HH12	1.67	0.41
2:A:3006:SER:C	2:A:3010:LYS:HZ2	2.23	0.41
2:A:3689:MET:CE	2:A:3753:PRO:HB2	2.49	0.41
2:A:4036:ASP:HB2	2:A:4043:ILE:HD13	2.02	0.41
2:A:4268:MET:O	2:A:4271:VAL:HG22	2.20	0.41
2:A:4743:LEU:O	2:A:4746:ILE:HG12	2.20	0.41
2:A:4964:ASP:OD1	2:A:4965:GLN:N	2.52	0.41
2:B:765:SER:HA	2:B:779:PHE:O	2.19	0.41
2:B:1962:THR:O	2:B:1966:ARG:HG3	2.20	0.41
2:B:2379:ASP:OD2	2:B:2380:ASP:N	2.53	0.41
2:B:2436:ILE:HA	2:B:2465:LYS:HE3	2.01	0.41
2:B:2908:LYS:HE2	2:B:2908:LYS:HB2	1.95	0.41
2:B:3211:LEU:HD21	2:B:3245:TYR:HE2	1.85	0.41
2:B:3906:PHE:HB3	2:B:3967:LEU:HD11	2.02	0.41
2:B:4183:LYS:HG3	2:B:4184:GLU:HG3	2.01	0.41
2:C:399:MET:SD	2:C:399:MET:N	2.92	0.41
2:C:1979:PHE:CD2	2:C:1996:LEU:HD23	2.55	0.41
2:C:2508:SER:HB3	2:C:2560:SER:HB3	2.02	0.41
2:C:3180:ILE:HG23	2:C:3181:TYR:CD1	2.54	0.41
2:C:3650:GLU:HB2	2:C:3651:PRO:HD3	2.00	0.41
2:C:4057:HIS:CE1	2:D:4660:PHE:HZ	2.38	0.41
2:D:808:HIS:O	2:D:1616:GLY:HA2	2.20	0.41
2:D:1220:ASP:O	2:D:1223:THR:OG1	2.37	0.41
2:D:1962:THR:O	2:D:1966:ARG:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2447:LYS:HD3	2:D:2447:LYS:HA	1.80	0.41
2:D:3145:SER:H	2:D:3148:VAL:HB	1.85	0.41
2:D:3164:GLY:C	2:D:3248:ARG:HH12	2.23	0.41
2:D:3192:ARG:O	2:D:3197:LEU:HB2	2.20	0.41
2:D:3592:SER:O	2:D:3596:LYS:HD3	2.20	0.41
2:D:4237:SER:O	2:D:4240:THR:OG1	2.37	0.41
2:A:712:GLU:HG3	2:A:838:ARG:HB3	2.02	0.41
2:A:2106:TYR:HH	2:A:3615:ARG:HH12	1.69	0.41
2:A:2640:LEU:HD23	2:A:2643:LYS:HZ1	1.85	0.41
2:A:2736:LYS:HD2	2:A:2754:GLN:OE1	2.20	0.41
2:A:2833:LEU:HB3	2:A:2837:LEU:CD1	2.49	0.41
2:A:3848:GLU:OE1	2:A:3922:GLU:HG3	2.20	0.41
2:B:163:HIS:HB2	2:B:182:ILE:HG13	2.02	0.41
2:B:1797:GLU:HA	2:B:1800:LYS:HG2	2.02	0.41
2:B:2741:TRP:HH2	2:B:2752:LYS:HD3	1.84	0.41
2:B:2785:TRP:HE1	2:B:2905:ARG:HH12	1.67	0.41
2:B:3134:LEU:HD22	2:B:3162:PHE:CE2	2.54	0.41
2:B:3246:MET:HG2	2:B:3309:LYS:HZ1	1.85	0.41
2:B:3679:LYS:HE2	2:B:3679:LYS:HB2	1.92	0.41
2:B:4268:MET:O	2:B:4271:VAL:HG22	2.20	0.41
2:C:487:ASN:O	2:C:491:GLU:HG2	2.21	0.41
2:C:896:ASN:O	2:C:899:GLU:HG3	2.20	0.41
2:C:1697:LEU:HD23	2:C:1697:LEU:HA	1.95	0.41
2:C:4130:GLN:HB3	2:C:4131:PRO:HD3	2.02	0.41
2:D:943:LEU:HD11	2:D:1064:LEU:HD12	2.02	0.41
2:D:3017:HIS:O	2:D:3092:GLN:NE2	2.53	0.41
2:D:3651:PRO:HB2	2:D:3652:PRO:HD3	2.03	0.41
2:D:3763:ILE:HD11	2:D:3838:ASP:O	2.20	0.41
1:I:117:LEU:HD23	1:I:118:THR:N	2.34	0.41
2:A:274:LEU:HD23	2:A:274:LEU:HA	1.81	0.41
2:A:874:LEU:HD23	2:A:879:GLU:HG3	2.01	0.41
2:A:943:LEU:HD11	2:A:1064:LEU:HD12	2.02	0.41
2:A:3163:ALA:HB1	2:A:3245:TYR:CD1	2.52	0.41
2:A:4746:ILE:HD11	2:B:4776:VAL:HG21	2.03	0.41
2:A:4753:LEU:HG	2:B:4773:LEU:HD22	2.02	0.41
1:K:89:ALA:HA	1:K:92:VAL:HG22	2.01	0.41
2:B:1046:ASN:OD1	2:B:1047:LYS:N	2.53	0.41
2:B:1967:SER:O	2:B:1972:GLN:NE2	2.41	0.41
2:B:2344:LEU:HD22	2:B:2434:GLY:HA3	2.02	0.41
2:B:2736:LYS:HD2	2:B:2754:GLN:OE1	2.20	0.41
2:B:2833:LEU:HB3	2:B:2837:LEU:CD1	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3145:SER:H	2:B:3148:VAL:HB	1.85	0.41
2:B:3592:SER:O	2:B:3596:LYS:HD3	2.20	0.41
2:B:4743:LEU:O	2:B:4746:ILE:HG12	2.20	0.41
2:C:1592:SER:OG	2:C:1594:VAL:HG12	2.21	0.41
2:C:1797:GLU:HA	2:C:1800:LYS:HG2	2.03	0.41
2:D:487:ASN:O	2:D:491:GLU:HG2	2.21	0.41
2:D:1166:VAL:HG23	2:D:1173:MET:HG2	2.01	0.41
2:D:1914:CYS:O	2:D:1918:VAL:HG23	2.20	0.41
2:D:1931:ASP:OD1	2:D:1932:PHE:N	2.52	0.41
2:D:1973:ILE:HG13	2:D:3608:LEU:HD11	2.02	0.41
2:D:4107:GLU:OE2	2:D:4149:TYR:OH	2.15	0.41
1:I:122:VAL:O	1:I:126:ILE:N	2.43	0.41
2:A:487:ASN:O	2:A:491:GLU:HG2	2.21	0.41
2:A:3211:LEU:HD21	2:A:3245:TYR:HE2	1.85	0.41
2:A:3679:LYS:HE2	2:A:3679:LYS:HB2	1.92	0.41
2:A:4858:LEU:HD23	2:A:4858:LEU:HA	1.94	0.41
3:F:58:LYS:O	3:F:62:GLU:OE1	2.39	0.41
1:J:123:ASP:HA	1:J:126:ILE:HG23	2.02	0.41
2:B:586:LEU:HD11	2:B:620:CYS:HB2	2.02	0.41
2:B:889:ILE:O	2:B:893:TRP:CE3	2.74	0.41
2:B:1436:GLN:H	2:B:1500:ARG:HH12	1.67	0.41
2:B:2715:GLU:OE1	2:B:2715:GLU:N	2.44	0.41
2:B:2930:ILE:HG23	2:B:3010:LYS:HE2	2.02	0.41
2:B:3744:ILE:O	2:B:3747:SER:OG	2.31	0.41
2:B:4130:GLN:HB3	2:B:4131:PRO:HD3	2.02	0.41
2:C:194:LEU:HD23	2:C:196:TYR:HE1	1.85	0.41
2:C:875:PRO:HA	2:C:876:PRO:HD3	1.94	0.41
2:C:2344:LEU:HD22	2:C:2434:GLY:HA3	2.02	0.41
2:C:3906:PHE:HB3	2:C:3967:LEU:HD11	2.03	0.41
2:D:335:LYS:HZ1	2:D:397:GLY:HA3	1.85	0.41
2:D:1758:ARG:HA	2:D:1758:ARG:HD2	1.83	0.41
2:D:2379:ASP:OD2	2:D:2380:ASP:N	2.53	0.41
2:D:2923:TYR:CD2	2:D:3003:MET:HE2	2.55	0.41
2:D:2945:GLY:HA2	2:D:2948:ARG:NH2	2.36	0.41
2:A:332:ARG:NH1	2:A:364:GLN:OE1	2.52	0.41
2:A:643:LEU:O	2:A:645:GLN:NE2	2.53	0.41
2:A:1727:VAL:HG11	2:A:1926:VAL:HG21	2.02	0.41
2:A:1962:THR:O	2:A:1966:ARG:HG3	2.20	0.41
2:A:2826:ILE:H	2:A:2826:ILE:HD12	1.85	0.41
2:A:2945:GLY:HA2	2:A:2948:ARG:NH2	2.36	0.41
2:A:3164:GLY:C	2:A:3248:ARG:HH12	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:4948:CYS:SG	2:A:4950:GLU:HG2	2.61	0.41
3:H:58:LYS:O	3:H:62:GLU:OE1	2.39	0.41
1:L:16:ALA:HA	1:L:19:LEU:HD12	2.03	0.41
1:K:116:LYS:HB2	1:K:116:LYS:HE2	1.85	0.41
2:B:603:LYS:HB3	2:B:603:LYS:HE2	1.88	0.41
2:B:1748:LEU:HD23	2:B:1748:LEU:HA	1.88	0.41
2:B:4649:VAL:HA	2:B:4652:LYS:HE2	2.03	0.41
2:C:877:HIS:CE1	2:C:878:LEU:HG	2.55	0.41
2:C:1585:ARG:O	2:C:1587:HIS:ND1	2.54	0.41
2:C:2824:ARG:CZ	2:D:1502:ASN:HB3	2.50	0.41
2:C:2826:ILE:H	2:C:2826:ILE:HD12	1.85	0.41
2:C:2930:ILE:HG23	2:C:3010:LYS:HE2	2.02	0.41
2:C:3068:LEU:O	2:C:3071:THR:OG1	2.27	0.41
2:C:3592:SER:O	2:C:3596:LYS:HD3	2.20	0.41
2:D:1592:SER:OG	2:D:1594:VAL:HG12	2.21	0.41
2:D:2868:HIS:HB3	2:D:2871:LEU:HD23	2.03	0.41
2:D:3131:TYR:HE1	2:D:3208:ILE:HB	1.84	0.41
2:D:3211:LEU:HD21	2:D:3245:TYR:HE2	1.85	0.41
2:D:4481:TRP:O	2:D:4485:ILE:HG12	2.21	0.41
2:D:4649:VAL:HA	2:D:4652:LYS:HE2	2.03	0.41
2:D:4948:CYS:SG	2:D:4950:GLU:HG2	2.61	0.41
2:A:390:LYS:HD2	2:A:390:LYS:HA	1.86	0.41
2:A:1729:MET:HE1	2:A:1930:ASP:HB2	2.02	0.41
2:A:2379:ASP:OD2	2:A:2380:ASP:N	2.53	0.41
2:A:2868:HIS:HB3	2:A:2871:LEU:HD23	2.03	0.41
2:A:3009:CYS:O	2:A:3013:VAL:HG23	2.19	0.41
3:E:58:LYS:O	3:E:62:GLU:OE1	2.39	0.41
3:H:43:ARG:HD3	2:D:1766:PRO:HG2	2.02	0.41
2:B:487:ASN:O	2:B:491:GLU:HG2	2.21	0.41
2:B:756:SER:HB2	2:B:769:ARG:HB3	2.02	0.41
2:B:2926:LEU:HD23	2:B:2926:LEU:HA	1.87	0.41
2:B:3212:GLU:O	2:B:3216:GLU:OE1	2.39	0.41
2:C:659:ILE:HD12	2:C:661:LEU:HD11	2.03	0.41
2:C:972:LEU:HD23	2:C:973:THR:H	1.86	0.41
2:C:1727:VAL:HG11	2:C:1926:VAL:HG21	2.02	0.41
2:C:1911:GLN:OE1	2:C:2090:ARG:NH1	2.54	0.41
2:C:3965:ILE:HG13	2:C:4086:ARG:HH11	1.86	0.41
2:D:491:GLU:OE2	2:D:546:LYS:NZ	2.47	0.41
2:D:1911:GLN:OE1	2:D:2090:ARG:NH1	2.54	0.41
2:D:2106:TYR:OH	2:D:3615:ARG:NH1	2.53	0.41
2:D:2972:ASP:OD1	2:D:2976:LYS:NZ	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3906:PHE:HB3	2:D:3967:LEU:HD11	2.02	0.41
2:D:4130:GLN:HB3	2:D:4131:PRO:HD3	2.02	0.41
1:I:64:ILE:HG23	1:I:68:GLU:HB3	2.02	0.41
2:A:50:GLU:CD	2:A:61:ASP:H	2.22	0.41
2:A:694:ARG:NH1	2:A:718:VAL:O	2.49	0.41
2:A:896:ASN:O	2:A:899:GLU:HG3	2.20	0.41
2:A:1046:ASN:OD1	2:A:1047:LYS:N	2.53	0.41
2:A:2408:LEU:HD22	2:A:2413:LYS:HD3	2.03	0.41
2:A:2741:TRP:HH2	2:A:2752:LYS:HD3	1.84	0.41
2:A:2930:ILE:HG23	2:A:3010:LYS:HE2	2.02	0.41
2:A:3651:PRO:HB2	2:A:3652:PRO:HD3	2.03	0.41
2:A:4481:TRP:O	2:A:4485:ILE:HG12	2.21	0.41
2:A:4649:VAL:HA	2:A:4652:LYS:HE2	2.03	0.41
3:G:58:LYS:O	3:G:62:GLU:OE1	2.39	0.41
3:H:67:MET:HE2	3:H:104:LEU:HB2	2.02	0.41
1:J:76:LYS:HB2	1:J:78:LYS:NZ	2.35	0.41
2:B:643:LEU:O	2:B:645:GLN:NE2	2.53	0.41
2:B:904:TYR:CE1	2:B:916:PRO:HA	2.56	0.41
2:B:972:LEU:HD23	2:B:973:THR:H	1.86	0.41
2:B:1585:ARG:O	2:B:1587:HIS:ND1	2.53	0.41
2:B:2593:VAL:HA	2:B:2644:LEU:HD13	2.03	0.41
2:B:3304:GLN:HB3	2:B:3305:PRO:HD3	2.03	0.41
2:C:1758:ARG:HA	2:C:1758:ARG:HD2	1.83	0.41
2:C:1962:THR:O	2:C:1966:ARG:HG3	2.20	0.41
2:C:2928:GLN:HA	2:C:2931:ARG:CZ	2.51	0.41
2:C:4649:VAL:HA	2:C:4652:LYS:HE2	2.03	0.41
2:C:4743:LEU:O	2:C:4746:ILE:HG12	2.20	0.41
2:C:4948:CYS:SG	2:C:4950:GLU:HG2	2.61	0.41
2:D:182:ILE:HG13	2:D:182:ILE:O	2.21	0.41
2:D:586:LEU:HD11	2:D:620:CYS:HB2	2.02	0.41
2:D:904:TYR:CE1	2:D:916:PRO:HA	2.56	0.41
2:D:1304:LEU:HD23	2:D:1304:LEU:HA	1.90	0.41
2:D:1421:MET:SD	2:D:1576:LYS:HD2	2.61	0.41
2:D:2833:LEU:HB3	2:D:2837:LEU:CD1	2.48	0.41
2:D:3924:ILE:HG21	2:D:3935:LEU:HD12	2.03	0.41
2:D:3975:GLN:O	2:D:3979:VAL:HG23	2.20	0.41
2:A:49:LEU:CD1	2:A:194:LEU:HD13	2.51	0.41
2:A:194:LEU:HD23	2:A:196:TYR:HE1	1.85	0.41
2:A:680:ASP:O	2:A:751:THR:HG23	2.20	0.41
2:A:808:HIS:O	2:A:1616:GLY:HA2	2.20	0.41
2:A:889:ILE:O	2:A:893:TRP:CE3	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:972:LEU:HD23	2:A:973:THR:H	1.86	0.41
2:A:1421:MET:SD	2:A:1576:LYS:HD2	2.61	0.41
2:A:1797:GLU:HA	2:A:1800:LYS:HG2	2.03	0.41
2:A:1893:LEU:HD23	2:A:1896:MET:SD	2.60	0.41
2:A:1948:MET:HA	2:A:1948:MET:HE2	2.03	0.41
2:A:2487:LEU:HA	2:A:2490:VAL:HG22	2.03	0.41
2:A:2586:GLN:HE22	2:A:2590:ARG:NH2	2.19	0.41
2:A:3095:ASN:O	2:A:3099:VAL:HG22	2.20	0.41
2:A:3134:LEU:HD22	2:A:3162:PHE:CE2	2.54	0.41
2:A:3143:SER:O	2:A:3148:VAL:HG11	2.21	0.41
2:A:3965:ILE:HG13	2:A:4086:ARG:HH11	1.86	0.41
2:A:3975:GLN:O	2:A:3979:VAL:HG23	2.20	0.41
2:A:4196:THR:O	2:A:4200:MET:HG3	2.21	0.41
2:A:4914:ASN:HB3	2:A:4917:ASN:ND2	2.36	0.41
3:G:19:LYS:HB2	3:G:19:LYS:HE3	1.84	0.41
1:J:16:ALA:HA	1:J:19:LEU:HD12	2.03	0.41
1:J:116:LYS:HE2	1:J:116:LYS:HB2	1.85	0.41
1:L:36:VAL:O	1:L:39:SER:OG	2.27	0.41
1:L:64:ILE:HG23	1:L:68:GLU:HB3	2.02	0.41
1:L:122:VAL:O	1:L:126:ILE:N	2.43	0.41
2:B:943:LEU:HD11	2:B:1064:LEU:HD12	2.02	0.41
2:B:1592:SER:OG	2:B:1594:VAL:HG12	2.20	0.41
2:B:1825:PHE:CE1	2:B:1842:ILE:HG12	2.54	0.41
2:B:1948:MET:HA	2:B:1948:MET:CE	2.50	0.41
2:B:2253:LEU:HD23	2:B:2253:LEU:HA	1.85	0.41
2:B:2928:GLN:HA	2:B:2931:ARG:CZ	2.51	0.41
2:B:3310:VAL:HG11	2:B:3319:PHE:CE2	2.56	0.41
2:B:3965:ILE:HG13	2:B:4086:ARG:HH11	1.86	0.41
2:B:4481:TRP:O	2:B:4485:ILE:HG12	2.21	0.41
2:B:4663:ARG:HD2	2:B:4663:ARG:HA	1.89	0.41
2:B:4948:CYS:SG	2:B:4950:GLU:HG2	2.61	0.41
2:C:643:LEU:O	2:C:645:GLN:NE2	2.53	0.41
2:C:2945:GLY:HA2	2:C:2948:ARG:NH2	2.36	0.41
2:C:3101:LEU:O	2:C:3104:MET:HB3	2.21	0.41
2:C:3212:GLU:O	2:C:3216:GLU:OE1	2.39	0.41
2:C:4036:ASP:HB2	2:C:4043:ILE:HD13	2.02	0.41
2:C:4670:LEU:HB2	2:C:4672:MET:CE	2.49	0.41
2:C:4914:ASN:HB3	2:C:4917:ASN:ND2	2.36	0.41
2:C:4943:MET:HE3	2:C:4948:CYS:O	2.21	0.41
2:D:194:LEU:HD23	2:D:196:TYR:HE1	1.85	0.41
2:D:659:ILE:HD12	2:D:661:LEU:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:889:ILE:O	2:D:893:TRP:CE3	2.74	0.41
2:D:1727:VAL:HG11	2:D:1926:VAL:HG21	2.02	0.41
2:D:1893:LEU:HD23	2:D:1896:MET:SD	2.60	0.41
2:D:1988:CYS:HA	2:D:1989:PRO:HD3	1.87	0.41
2:D:2276:SER:OG	2:D:2277:CYS:N	2.54	0.41
2:D:2408:LEU:HD22	2:D:2413:LYS:HD3	2.03	0.41
2:D:2734:MET:HE2	2:D:2737:LEU:HD11	2.03	0.41
2:D:2928:GLN:HA	2:D:2931:ARG:CZ	2.51	0.41
2:D:3163:ALA:HB1	2:D:3245:TYR:CD1	2.52	0.41
2:D:4036:ASP:HB2	2:D:4043:ILE:HD13	2.02	0.41
2:D:4041:GLY:HA2	2:D:4080:TYR:HE1	1.86	0.41
2:D:4240:THR:HG22	2:D:4308:ILE:HD13	2.02	0.41
2:A:561:ARG:HG3	2:A:561:ARG:NH1	2.34	0.41
2:A:659:ILE:HD12	2:A:661:LEU:HD11	2.03	0.41
2:A:765:SER:HA	2:A:779:PHE:O	2.20	0.41
2:A:844:ARG:HH11	2:A:845:THR:H	1.69	0.41
2:A:1585:ARG:O	2:A:1587:HIS:ND1	2.54	0.41
2:A:1592:SER:OG	2:A:1594:VAL:HG12	2.21	0.41
2:A:1911:GLN:OE1	2:A:2090:ARG:NH1	2.54	0.41
2:A:2497:ARG:NH1	2:A:2881:GLU:OE2	2.53	0.41
2:A:3088:LYS:HA	2:A:3088:LYS:HD3	1.90	0.41
2:A:3191:GLU:HA	2:A:3194:ALA:HB3	2.03	0.41
2:A:4265:LYS:O	2:A:4269:LYS:HG2	2.21	0.41
3:F:19:LYS:HB2	3:F:19:LYS:HE3	1.84	0.41
1:K:16:ALA:HA	1:K:19:LEU:HD12	2.03	0.41
2:B:2734:MET:HE2	2:B:2737:LEU:HD11	2.03	0.41
2:B:4073:ASP:OD2	2:B:4075:ASN:ND2	2.54	0.41
2:C:735:GLY:O	2:C:737:ILE:HD12	2.21	0.41
2:C:889:ILE:O	2:C:893:TRP:CE3	2.74	0.41
2:C:1893:LEU:HD23	2:C:1896:MET:SD	2.60	0.41
2:C:1914:CYS:O	2:C:1918:VAL:HG23	2.20	0.41
2:C:2487:LEU:HA	2:C:2490:VAL:HG22	2.03	0.41
2:C:2586:GLN:HE22	2:C:2590:ARG:NH2	2.19	0.41
2:C:2659:GLN:HG2	2:C:2660:GLU:N	2.36	0.41
2:C:3102:LEU:HD12	2:C:3102:LEU:HA	1.86	0.41
2:C:3651:PRO:HB2	2:C:3652:PRO:HD3	2.03	0.41
2:D:756:SER:HB2	2:D:769:ARG:HB3	2.02	0.41
2:D:2487:LEU:HA	2:D:2490:VAL:HG22	2.03	0.41
2:D:3006:SER:C	2:D:3010:LYS:HZ2	2.23	0.41
2:D:3143:SER:O	2:D:3148:VAL:HG11	2.21	0.41
1:I:16:ALA:HA	1:I:19:LEU:HD12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:37:MET:HG2	1:I:42:GLN:HB2	2.03	0.40
2:A:2928:GLN:HA	2:A:2931:ARG:CZ	2.51	0.40
2:A:3924:ILE:HG21	2:A:3935:LEU:HD12	2.03	0.40
1:J:64:ILE:HG23	1:J:68:GLU:HB3	2.02	0.40
1:L:37:MET:HG2	1:L:42:GLN:HB2	2.03	0.40
2:B:194:LEU:HD23	2:B:196:TYR:HE1	1.85	0.40
2:B:399:MET:SD	2:B:399:MET:N	2.92	0.40
2:B:810:GLU:N	2:B:810:GLU:OE2	2.54	0.40
2:B:2463:ASP:OD1	2:B:2464:HIS:N	2.55	0.40
2:B:2945:GLY:HA2	2:B:2948:ARG:NH2	2.36	0.40
2:B:3191:GLU:HA	2:B:3194:ALA:HB3	2.03	0.40
2:B:4196:THR:O	2:B:4200:MET:HG3	2.21	0.40
2:B:4265:LYS:O	2:B:4269:LYS:HG2	2.21	0.40
2:C:50:GLU:CD	2:C:61:ASP:H	2.22	0.40
2:C:527:LYS:HE2	2:C:527:LYS:HB2	1.82	0.40
2:C:2833:LEU:HB3	2:C:2837:LEU:CD1	2.49	0.40
2:C:4502:MET:SD	2:C:4585:PHE:HB3	2.61	0.40
2:D:49:LEU:CD1	2:D:194:LEU:HD13	2.51	0.40
2:D:1968:PRO:O	2:D:1972:GLN:HG3	2.21	0.40
2:D:2463:ASP:OD1	2:D:2464:HIS:N	2.54	0.40
2:D:2592:LEU:HD23	2:D:2592:LEU:HA	1.90	0.40
2:D:2593:VAL:HA	2:D:2644:LEU:HD13	2.03	0.40
2:D:3848:GLU:OE1	2:D:3922:GLU:HG3	2.21	0.40
2:D:4502:MET:SD	2:D:4585:PHE:HB3	2.61	0.40
2:A:648:LEU:HD23	2:A:648:LEU:HA	1.89	0.40
2:A:1176:THR:HG22	2:A:1181:ILE:HG13	2.03	0.40
2:A:1968:PRO:O	2:A:1972:GLN:HG3	2.21	0.40
2:A:2106:TYR:OH	2:A:3615:ARG:NH1	2.53	0.40
2:A:3906:PHE:HB3	2:A:3967:LEU:HD11	2.02	0.40
1:J:125:MET:HG3	2:B:3584:LYS:HE2	2.02	0.40
1:K:123:ASP:HA	1:K:126:ILE:HG23	2.03	0.40
2:B:274:LEU:HD23	2:B:274:LEU:HA	1.81	0.40
2:B:364:GLN:NE2	2:B:369:GLY:O	2.53	0.40
2:B:1421:MET:SD	2:B:1576:LYS:HD2	2.61	0.40
2:B:2447:LYS:HD3	2:B:2447:LYS:HA	1.80	0.40
2:B:2826:ILE:H	2:B:2826:ILE:HD12	1.85	0.40
2:C:49:LEU:CD1	2:C:194:LEU:HD13	2.51	0.40
2:C:1421:MET:SD	2:C:1576:LYS:HD2	2.61	0.40
2:C:1968:PRO:O	2:C:1972:GLN:HG3	2.21	0.40
2:C:2106:TYR:OH	2:C:3615:ARG:NH1	2.53	0.40
2:C:2170:THR:O	2:C:2174:VAL:HG13	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:3778:LEU:HD13	2:C:3854:PHE:HD1	1.87	0.40
2:C:4167:GLU:O	2:C:4171:GLN:HG2	2.22	0.40
2:D:884:LYS:HA	2:D:887:GLU:CG	2.51	0.40
2:D:920:GLU:O	2:D:924:LEU:N	2.55	0.40
2:D:1797:GLU:HA	2:D:1800:LYS:HG2	2.03	0.40
2:D:2229:LEU:HD11	2:D:2240:LEU:HD22	2.03	0.40
2:D:2344:LEU:HD22	2:D:2434:GLY:HA3	2.02	0.40
2:D:2488:LEU:HD11	2:D:2548:LEU:HD13	2.03	0.40
2:D:3088:LYS:HG3	2:D:3090:VAL:HG22	2.01	0.40
2:D:3101:LEU:O	2:D:3104:MET:HB3	2.21	0.40
2:A:182:ILE:HG13	2:A:182:ILE:O	2.21	0.40
2:A:997:ASP:O	2:A:1001:GLU:OE1	2.40	0.40
2:A:1748:LEU:HD23	2:A:1748:LEU:HA	1.88	0.40
2:A:3101:LEU:O	2:A:3104:MET:HB3	2.21	0.40
2:A:3661:VAL:HG23	2:A:3666:GLN:HG2	2.03	0.40
2:A:4130:GLN:HB3	2:A:4131:PRO:HD3	2.02	0.40
2:A:4670:LEU:HB2	2:A:4672:MET:CE	2.49	0.40
2:B:49:LEU:CD1	2:B:194:LEU:HD13	2.51	0.40
2:B:968:LYS:HA	2:B:968:LYS:HD2	1.91	0.40
2:B:1727:VAL:HG11	2:B:1926:VAL:HG21	2.02	0.40
2:B:1785:ASP:OD1	2:B:1786:ILE:N	2.55	0.40
2:B:1914:CYS:O	2:B:1918:VAL:HG23	2.20	0.40
2:B:2276:SER:OG	2:B:2277:CYS:N	2.54	0.40
2:B:2487:LEU:HA	2:B:2490:VAL:HG22	2.03	0.40
2:B:2874:TYR:O	2:B:2882:LYS:HE2	2.22	0.40
2:B:3651:PRO:HB2	2:B:3652:PRO:HD3	2.03	0.40
2:B:4240:THR:HG22	2:B:4308:ILE:HD13	2.02	0.40
2:C:884:LYS:HA	2:C:887:GLU:CG	2.51	0.40
2:C:2705:PRO:HG3	2:C:2854:LYS:HZ2	1.86	0.40
2:C:3304:GLN:HB3	2:C:3305:PRO:HD3	2.03	0.40
2:D:972:LEU:HD23	2:D:973:THR:H	1.86	0.40
2:D:1585:ARG:O	2:D:1587:HIS:ND1	2.54	0.40
2:D:2170:THR:O	2:D:2174:VAL:HG13	2.21	0.40
2:D:2586:GLN:HE22	2:D:2590:ARG:NH2	2.19	0.40
2:D:2659:GLN:HG2	2:D:2660:GLU:N	2.36	0.40
2:D:2913:ASP:HB3	2:D:2919:LYS:HE3	2.03	0.40
2:D:3281:LEU:HD22	2:D:3322:LEU:HD22	2.03	0.40
2:D:4914:ASN:HB3	2:D:4917:ASN:ND2	2.36	0.40
1:I:57:ASP:OD2	1:I:62:GLY:N	2.46	0.40
2:A:2344:LEU:HD22	2:A:2434:GLY:HA3	2.02	0.40
2:A:2488:LEU:HD11	2:A:2548:LEU:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2691:LYS:HD3	2:A:2704:GLN:NE2	2.37	0.40
2:A:2824:ARG:NH2	2:B:1502:ASN:HB3	2.37	0.40
2:A:3310:VAL:HG11	2:A:3319:PHE:CE2	2.57	0.40
2:A:3812:ASN:HA	2:A:3815:GLU:CD	2.42	0.40
1:L:123:ASP:HA	1:L:126:ILE:HG23	2.03	0.40
2:B:735:GLY:O	2:B:737:ILE:HD12	2.22	0.40
2:B:1226:TYR:HD1	2:B:1229:ILE:HD11	1.87	0.40
2:B:1829:LEU:HD12	2:B:1829:LEU:HA	1.96	0.40
2:B:1893:LEU:HD23	2:B:1896:MET:SD	2.60	0.40
2:B:1968:PRO:O	2:B:1972:GLN:HG3	2.21	0.40
2:B:2570:GLU:HG2	2:B:2605:MET:HG3	2.03	0.40
2:B:2913:ASP:HB3	2:B:2919:LYS:HE3	2.03	0.40
2:B:3183:ILE:HD12	2:B:3187:LYS:CE	2.52	0.40
2:B:3778:LEU:HD13	2:B:3854:PHE:HD1	1.87	0.40
2:B:3924:ILE:HG21	2:B:3935:LEU:HD12	2.03	0.40
2:B:3958:LEU:HB2	2:B:3968:LEU:HD13	2.03	0.40
2:B:4057:HIS:CE1	2:C:4660:PHE:HZ	2.40	0.40
2:C:810:GLU:N	2:C:810:GLU:OE2	2.55	0.40
2:C:997:ASP:OD1	2:C:1047:LYS:NZ	2.32	0.40
2:C:2874:TYR:O	2:C:2882:LYS:HE2	2.22	0.40
2:C:3184:TYR:CD1	2:C:3201:VAL:HG22	2.56	0.40
2:C:3211:LEU:HD21	2:C:3245:TYR:HE2	1.86	0.40
2:C:4041:GLY:HA2	2:C:4080:TYR:HE1	1.86	0.40
2:D:59:PRO:HA	2:D:60:PRO:HD3	1.98	0.40
2:D:287:SER:HA	2:D:349:MET:HE3	2.03	0.40
2:D:875:PRO:HA	2:D:876:PRO:HD3	1.94	0.40
2:D:1962:THR:HG22	2:D:1966:ARG:HG3	2.02	0.40
2:D:2327:ARG:HB3	2:D:2329:GLU:OE2	2.21	0.40
2:D:2874:TYR:O	2:D:2882:LYS:HE2	2.22	0.40
2:D:3649:ALA:C	2:D:3652:PRO:HD2	2.42	0.40
2:D:4167:GLU:O	2:D:4171:GLN:HG2	2.22	0.40
2:A:139:SER:O	2:A:141:ASP:N	2.54	0.40
2:A:1848:PRO:HG3	2:A:1890:LYS:NZ	2.37	0.40
2:A:2463:ASP:OD1	2:A:2464:HIS:N	2.55	0.40
2:A:2931:ARG:NH1	2:A:2932:TYR:CE1	2.90	0.40
2:A:2967:VAL:O	2:A:2971:ILE:HG13	2.22	0.40
2:A:3168:VAL:HG12	2:A:3179:ASN:ND2	2.37	0.40
2:A:4898:PHE:O	2:A:4904:GLY:HA3	2.22	0.40
1:K:10:ILE:HG22	1:K:14:LYS:NZ	2.37	0.40
2:B:884:LYS:HA	2:B:887:GLU:CG	2.51	0.40
2:B:997:ASP:O	2:B:1001:GLU:OE1	2.40	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1177:LEU:O	2:B:1180:GLU:HG3	2.22	0.40
2:B:1911:GLN:OE1	2:B:2090:ARG:NH1	2.54	0.40
2:B:2153:LYS:HD3	2:B:2153:LYS:HA	1.83	0.40
2:B:2408:LEU:HD22	2:B:2413:LYS:HD3	2.03	0.40
2:B:3649:ALA:HB1	2:B:3652:PRO:HB2	2.04	0.40
2:B:4502:MET:SD	2:B:4585:PHE:HB3	2.61	0.40
2:B:4607:ALA:HB1	2:B:4649:VAL:HG21	2.04	0.40
2:C:2463:ASP:OD1	2:C:2464:HIS:N	2.55	0.40
2:C:3191:GLU:HA	2:C:3194:ALA:HB3	2.03	0.40
2:D:1177:LEU:O	2:D:1180:GLU:HG3	2.22	0.40
2:D:1711:LEU:HB3	2:D:1831:MET:SD	2.62	0.40
2:D:3062:ASP:O	2:D:3065:ALA:HB3	2.22	0.40
2:D:3191:GLU:HA	2:D:3194:ALA:HB3	2.03	0.40
2:D:3832:ASP:HB2	2:D:3835:PHE:HB3	2.04	0.40
2:D:4265:LYS:O	2:D:4269:LYS:HG2	2.21	0.40
2:D:4607:ALA:HB1	2:D:4649:VAL:HG21	2.04	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	I	141/149 (95%)	139 (99%)	2 (1%)	0	100	100
1	J	141/149 (95%)	139 (99%)	2 (1%)	0	100	100
1	K	141/149 (95%)	139 (99%)	2 (1%)	0	100	100
1	L	141/149 (95%)	139 (99%)	2 (1%)	0	100	100
2	A	4205/4967 (85%)	4081 (97%)	119 (3%)	5 (0%)	48	79
2	B	4205/4967 (85%)	4081 (97%)	119 (3%)	5 (0%)	48	79
2	C	4205/4967 (85%)	4082 (97%)	118 (3%)	5 (0%)	48	79

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	D	4205/4967 (85%)	4080 (97%)	120 (3%)	5 (0%)	48 79
3	E	105/108 (97%)	103 (98%)	2 (2%)	0	100 100
3	F	105/108 (97%)	103 (98%)	2 (2%)	0	100 100
3	G	105/108 (97%)	103 (98%)	2 (2%)	0	100 100
3	H	105/108 (97%)	103 (98%)	2 (2%)	0	100 100
All	All	17804/20896 (85%)	17292 (97%)	492 (3%)	20 (0%)	50 79

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	3927	PRO
2	A	4641	PRO
2	B	3927	PRO
2	B	4641	PRO
2	C	3927	PRO
2	C	4641	PRO
2	D	3927	PRO
2	D	4641	PRO
2	A	1081	THR
2	A	3851	ASN
2	B	1081	THR
2	B	3851	ASN
2	C	1081	THR
2	C	3851	ASN
2	D	1081	THR
2	D	3851	ASN
2	A	1959	ALA
2	B	1959	ALA
2	C	1959	ALA
2	D	1959	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	I	123/127 (97%)	112 (91%)	11 (9%)	8 32
1	J	123/127 (97%)	112 (91%)	11 (9%)	8 32
1	K	123/127 (97%)	112 (91%)	11 (9%)	8 32
1	L	123/127 (97%)	112 (91%)	11 (9%)	8 32
2	A	3715/4358 (85%)	3678 (99%)	37 (1%)	73 85
2	B	3715/4358 (85%)	3678 (99%)	37 (1%)	73 85
2	C	3715/4358 (85%)	3678 (99%)	37 (1%)	73 85
2	D	3715/4358 (85%)	3678 (99%)	37 (1%)	73 85
3	E	88/89 (99%)	87 (99%)	1 (1%)	70 84
3	F	88/89 (99%)	87 (99%)	1 (1%)	70 84
3	G	88/89 (99%)	87 (99%)	1 (1%)	70 84
3	H	88/89 (99%)	87 (99%)	1 (1%)	70 84
All	All	15704/18296 (86%)	15508 (99%)	196 (1%)	66 83

All (196) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	77	MET
1	I	124	GLU
1	I	125	MET
1	I	126	ILE
1	I	127	ARG
1	I	128	GLU
1	I	130	ASP
1	I	142	PHE
1	I	143	VAL
1	I	145	MET
1	I	146	MET
2	A	290	ARG
2	A	321	LYS
2	A	349	MET
2	A	393	MET
2	A	441	LYS
2	A	884	LYS
2	A	929	ARG
2	A	944	LEU
2	A	1564	MET
2	A	1939	ASN
2	A	1948	MET

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Mol	Chain	Res	Type
2	A	2134	MET
2	A	2303	ARG
2	A	2512	MET
2	A	2685	TYR
2	A	2689	MET
2	A	2737	LEU
2	A	2757	MET
2	A	2766	LYS
2	A	2772	ARG
2	A	2782	MET
2	A	2783	LEU
2	A	2801	TYR
2	A	2931	ARG
2	A	3018	ARG
2	A	3190	ARG
2	A	3323	MET
2	A	3584	LYS
2	A	3591	LEU
2	A	3605	MET
2	A	3847	CYS
2	A	4279	MET
2	A	4307	ARG
2	A	4504	MET
2	A	4748	MET
2	A	4884	MET
2	A	4932	GLU
3	E	19	LYS
3	F	19	LYS
3	G	19	LYS
3	H	19	LYS
1	J	77	MET
1	J	124	GLU
1	J	125	MET
1	J	126	ILE
1	J	127	ARG
1	J	128	GLU
1	J	130	ASP
1	J	142	PHE
1	J	143	VAL
1	J	145	MET
1	J	146	MET
1	L	77	MET

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Mol	Chain	Res	Type
1	L	124	GLU
1	L	125	MET
1	L	126	ILE
1	L	127	ARG
1	L	128	GLU
1	L	130	ASP
1	L	142	PHE
1	L	143	VAL
1	L	145	MET
1	L	146	MET
1	K	77	MET
1	K	124	GLU
1	K	125	MET
1	K	126	ILE
1	K	127	ARG
1	K	128	GLU
1	K	130	ASP
1	K	142	PHE
1	K	143	VAL
1	K	145	MET
1	K	146	MET
2	B	290	ARG
2	B	321	LYS
2	B	349	MET
2	B	393	MET
2	B	441	LYS
2	B	884	LYS
2	B	929	ARG
2	B	944	LEU
2	B	1564	MET
2	B	1939	ASN
2	B	1948	MET
2	B	2134	MET
2	B	2303	ARG
2	B	2512	MET
2	B	2685	TYR
2	B	2689	MET
2	B	2737	LEU
2	B	2757	MET
2	B	2766	LYS
2	B	2772	ARG
2	B	2782	MET

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Mol	Chain	Res	Type
2	B	2783	LEU
2	B	2801	TYR
2	B	2931	ARG
2	B	3018	ARG
2	B	3190	ARG
2	B	3323	MET
2	B	3584	LYS
2	B	3591	LEU
2	B	3605	MET
2	B	3847	CYS
2	B	4279	MET
2	B	4307	ARG
2	B	4504	MET
2	B	4748	MET
2	B	4884	MET
2	B	4932	GLU
2	C	290	ARG
2	C	321	LYS
2	C	349	MET
2	C	393	MET
2	C	441	LYS
2	C	884	LYS
2	C	929	ARG
2	C	944	LEU
2	C	1564	MET
2	C	1939	ASN
2	C	1948	MET
2	C	2134	MET
2	C	2303	ARG
2	C	2512	MET
2	C	2685	TYR
2	C	2689	MET
2	C	2737	LEU
2	C	2757	MET
2	C	2766	LYS
2	C	2772	ARG
2	C	2782	MET
2	C	2783	LEU
2	C	2801	TYR
2	C	2931	ARG
2	C	3018	ARG
2	C	3190	ARG

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Mol	Chain	Res	Type
2	C	3323	MET
2	C	3584	LYS
2	C	3591	LEU
2	C	3605	MET
2	C	3847	CYS
2	C	4279	MET
2	C	4307	ARG
2	C	4504	MET
2	C	4748	MET
2	C	4884	MET
2	C	4932	GLU
2	D	290	ARG
2	D	321	LYS
2	D	349	MET
2	D	393	MET
2	D	441	LYS
2	D	884	LYS
2	D	929	ARG
2	D	944	LEU
2	D	1564	MET
2	D	1939	ASN
2	D	1948	MET
2	D	2134	MET
2	D	2303	ARG
2	D	2512	MET
2	D	2685	TYR
2	D	2689	MET
2	D	2737	LEU
2	D	2757	MET
2	D	2766	LYS
2	D	2772	ARG
2	D	2782	MET
2	D	2783	LEU
2	D	2801	TYR
2	D	2931	ARG
2	D	3018	ARG
2	D	3190	ARG
2	D	3323	MET
2	D	3584	LYS
2	D	3591	LEU
2	D	3605	MET
2	D	3847	CYS

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Mol	Chain	Res	Type
2	D	4279	MET
2	D	4307	ARG
2	D	4504	MET
2	D	4748	MET
2	D	4884	MET
2	D	4932	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	50	GLN
2	A	29	HIS
2	A	388	GLN
2	A	658	ASN
2	A	669	GLN
2	A	888	ASN
2	A	1146	HIS
2	A	1452	GLN
2	A	2217	HIS
2	A	2540	HIS
2	A	2850	ASN
2	A	2927	GLN
2	A	2998	ASN
2	A	3017	HIS
2	A	3151	GLN
2	A	3287	ASN
2	A	4049	HIS
2	A	4057	HIS
2	A	4933	HIS
1	J	54	ASN
1	L	54	ASN
1	K	50	GLN
2	B	388	GLN
2	B	658	ASN
2	B	669	GLN
2	B	888	ASN
2	B	1146	HIS
2	B	1452	GLN
2	B	2217	HIS
2	B	2540	HIS
2	B	2850	ASN
2	B	2927	GLN

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Mol	Chain	Res	Type
2	B	2998	ASN
2	B	3017	HIS
2	B	3034	HIS
2	B	3151	GLN
2	B	3287	ASN
2	B	4049	HIS
2	B	4057	HIS
2	B	4933	HIS
2	C	29	HIS
2	C	388	GLN
2	C	658	ASN
2	C	669	GLN
2	C	888	ASN
2	C	1146	HIS
2	C	1452	GLN
2	C	2217	HIS
2	C	2540	HIS
2	C	2850	ASN
2	C	2927	GLN
2	C	2998	ASN
2	C	3017	HIS
2	C	3151	GLN
2	C	3287	ASN
2	C	4049	HIS
2	C	4057	HIS
2	C	4933	HIS
2	D	388	GLN
2	D	658	ASN
2	D	669	GLN
2	D	888	ASN
2	D	1146	HIS
2	D	1452	GLN
2	D	2217	HIS
2	D	2540	HIS
2	D	2850	ASN
2	D	2927	GLN
2	D	2998	ASN
2	D	3017	HIS
2	D	3034	HIS
2	D	3151	GLN
2	D	3287	ASN
2	D	4049	HIS

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Mol	Chain	Res	Type
2	D	4057	HIS
2	D	4933	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 32 ligands modelled in this entry, 24 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	ATP	B	5002	-	28,33,33	0.75	0	34,52,52	0.75	1 (2%)
6	ATP	A	5004	-	28,33,33	0.64	0	34,52,52	0.59	1 (2%)
6	ATP	C	5004	-	28,33,33	0.65	0	34,52,52	0.59	1 (2%)
6	ATP	D	5002	-	28,33,33	0.75	0	34,52,52	0.75	1 (2%)
6	ATP	A	5002	-	28,33,33	0.75	0	34,52,52	0.75	1 (2%)
6	ATP	D	5004	-	28,33,33	0.64	0	34,52,52	0.58	1 (2%)
6	ATP	B	5004	-	28,33,33	0.64	0	34,52,52	0.59	1 (2%)
6	ATP	C	5002	-	28,33,33	0.75	0	34,52,52	0.75	1 (2%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ATP	B	5002	-	-	8/18/38/38	0/3/3/3
6	ATP	A	5004	-	-	11/18/38/38	0/3/3/3
6	ATP	C	5004	-	-	11/18/38/38	0/3/3/3
6	ATP	D	5002	-	-	8/18/38/38	0/3/3/3
6	ATP	A	5002	-	-	8/18/38/38	0/3/3/3
6	ATP	D	5004	-	-	11/18/38/38	0/3/3/3
6	ATP	B	5004	-	-	11/18/38/38	0/3/3/3
6	ATP	C	5002	-	-	8/18/38/38	0/3/3/3

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	5002	ATP	C5-C6-N6	2.35	123.88	120.31
6	B	5002	ATP	C5-C6-N6	2.33	123.86	120.31
6	C	5002	ATP	C5-C6-N6	2.33	123.86	120.31
6	A	5004	ATP	C5-C6-N6	2.32	123.84	120.31
6	C	5004	ATP	C5-C6-N6	2.32	123.84	120.31
6	D	5002	ATP	C5-C6-N6	2.32	123.84	120.31
6	B	5004	ATP	C5-C6-N6	2.31	123.83	120.31
6	D	5004	ATP	C5-C6-N6	2.30	123.81	120.31

There are no chirality outliers.

All (76) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	5002	ATP	C5'-O5'-PA-O1A
6	A	5002	ATP	C5'-O5'-PA-O2A
6	A	5002	ATP	C5'-O5'-PA-O3A
6	A	5004	ATP	PB-O3A-PA-O5'
6	A	5004	ATP	C5'-O5'-PA-O1A
6	A	5004	ATP	C5'-O5'-PA-O2A
6	A	5004	ATP	C5'-O5'-PA-O3A
6	A	5004	ATP	O4'-C4'-C5'-O5'
6	B	5002	ATP	C5'-O5'-PA-O1A
6	B	5002	ATP	C5'-O5'-PA-O2A
6	B	5002	ATP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
6	B	5004	ATP	PB-O3A-PA-O5'
6	B	5004	ATP	C5'-O5'-PA-O1A
6	B	5004	ATP	C5'-O5'-PA-O2A
6	B	5004	ATP	C5'-O5'-PA-O3A
6	B	5004	ATP	O4'-C4'-C5'-O5'
6	C	5002	ATP	C5'-O5'-PA-O1A
6	C	5002	ATP	C5'-O5'-PA-O2A
6	C	5002	ATP	C5'-O5'-PA-O3A
6	C	5004	ATP	PB-O3A-PA-O5'
6	C	5004	ATP	C5'-O5'-PA-O1A
6	C	5004	ATP	C5'-O5'-PA-O2A
6	C	5004	ATP	C5'-O5'-PA-O3A
6	C	5004	ATP	O4'-C4'-C5'-O5'
6	D	5002	ATP	C5'-O5'-PA-O1A
6	D	5002	ATP	C5'-O5'-PA-O2A
6	D	5002	ATP	C5'-O5'-PA-O3A
6	D	5004	ATP	PB-O3A-PA-O5'
6	D	5004	ATP	C5'-O5'-PA-O1A
6	D	5004	ATP	C5'-O5'-PA-O2A
6	D	5004	ATP	C5'-O5'-PA-O3A
6	D	5004	ATP	O4'-C4'-C5'-O5'
6	A	5004	ATP	C3'-C4'-C5'-O5'
6	B	5004	ATP	C3'-C4'-C5'-O5'
6	C	5004	ATP	C3'-C4'-C5'-O5'
6	D	5004	ATP	C3'-C4'-C5'-O5'
6	A	5002	ATP	C4'-C5'-O5'-PA
6	B	5002	ATP	C4'-C5'-O5'-PA
6	C	5002	ATP	C4'-C5'-O5'-PA
6	D	5002	ATP	C4'-C5'-O5'-PA
6	A	5002	ATP	O4'-C4'-C5'-O5'
6	B	5002	ATP	O4'-C4'-C5'-O5'
6	C	5002	ATP	O4'-C4'-C5'-O5'
6	D	5002	ATP	O4'-C4'-C5'-O5'
6	A	5004	ATP	PA-O3A-PB-O1B
6	B	5004	ATP	PA-O3A-PB-O1B
6	C	5004	ATP	PA-O3A-PB-O1B
6	D	5004	ATP	PA-O3A-PB-O1B
6	A	5002	ATP	PB-O3B-PG-O3G
6	A	5004	ATP	PB-O3B-PG-O3G
6	B	5002	ATP	PB-O3B-PG-O3G
6	B	5004	ATP	PB-O3B-PG-O3G
6	C	5002	ATP	PB-O3B-PG-O3G

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Mol	Chain	Res	Type	Atoms
6	C	5004	ATP	PB-O3B-PG-O3G
6	D	5002	ATP	PB-O3B-PG-O3G
6	D	5004	ATP	PB-O3B-PG-O3G
6	A	5004	ATP	PA-O3A-PB-O2B
6	B	5004	ATP	PA-O3A-PB-O2B
6	C	5004	ATP	PA-O3A-PB-O2B
6	D	5004	ATP	PA-O3A-PB-O2B
6	A	5002	ATP	PB-O3B-PG-O1G
6	B	5002	ATP	PB-O3B-PG-O1G
6	C	5002	ATP	PB-O3B-PG-O1G
6	D	5002	ATP	PB-O3B-PG-O1G
6	A	5002	ATP	PB-O3A-PA-O2A
6	A	5004	ATP	PB-O3A-PA-O1A
6	A	5004	ATP	PB-O3A-PA-O2A
6	B	5002	ATP	PB-O3A-PA-O2A
6	B	5004	ATP	PB-O3A-PA-O1A
6	B	5004	ATP	PB-O3A-PA-O2A
6	C	5002	ATP	PB-O3A-PA-O2A
6	C	5004	ATP	PB-O3A-PA-O1A
6	C	5004	ATP	PB-O3A-PA-O2A
6	D	5002	ATP	PB-O3A-PA-O2A
6	D	5004	ATP	PB-O3A-PA-O1A
6	D	5004	ATP	PB-O3A-PA-O2A

There are no ring outliers.

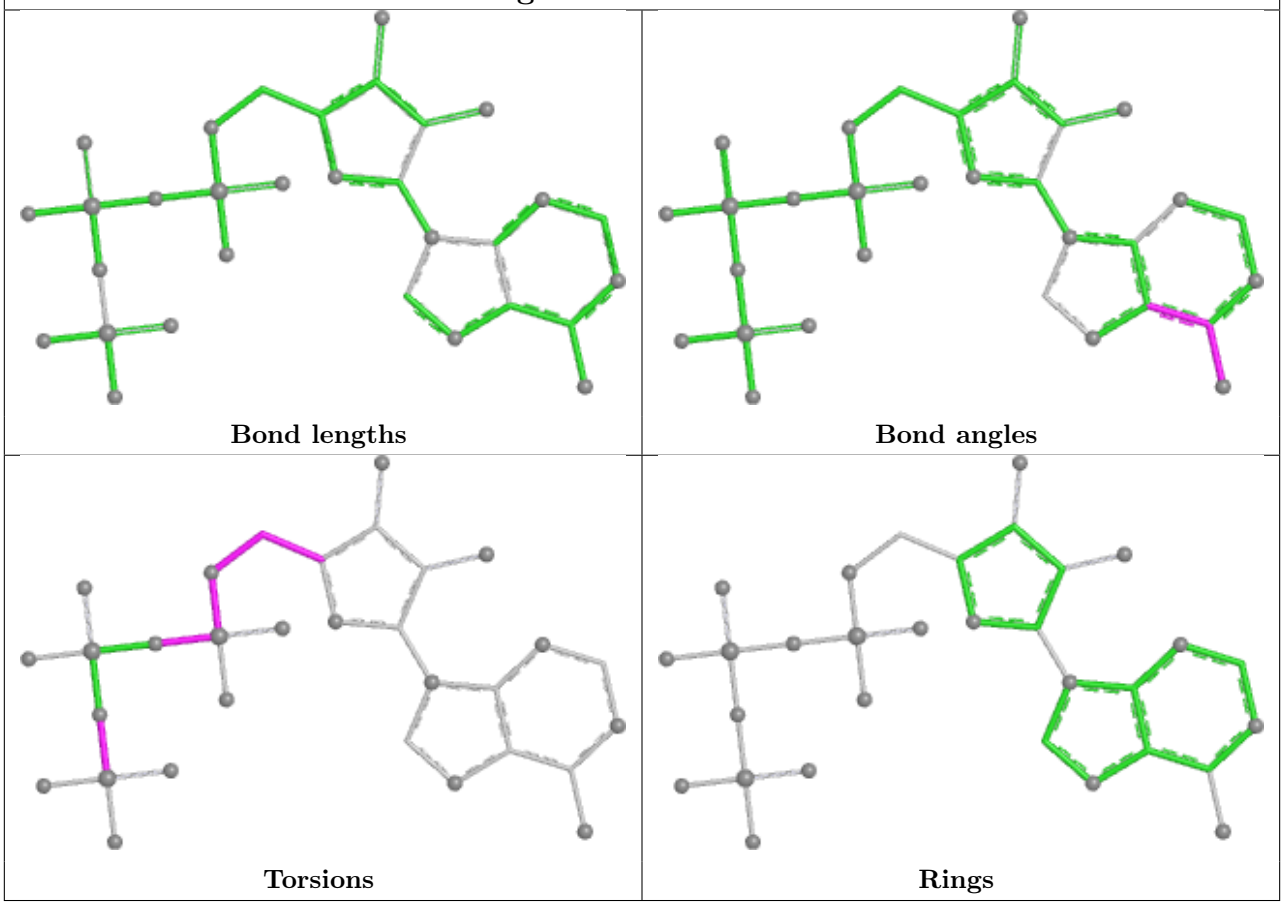
4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	5004	ATP	1	0
6	C	5004	ATP	1	0
6	D	5004	ATP	1	0
6	B	5004	ATP	1	0

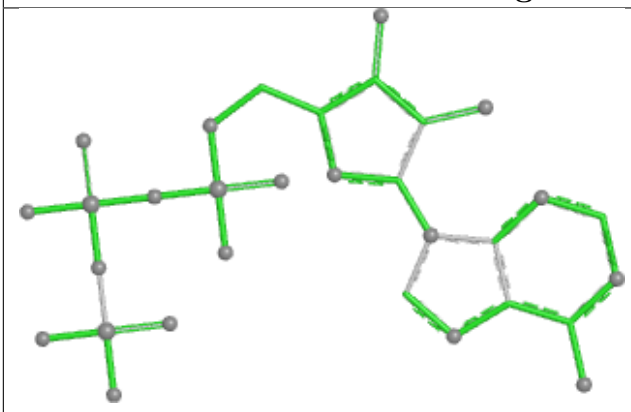
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

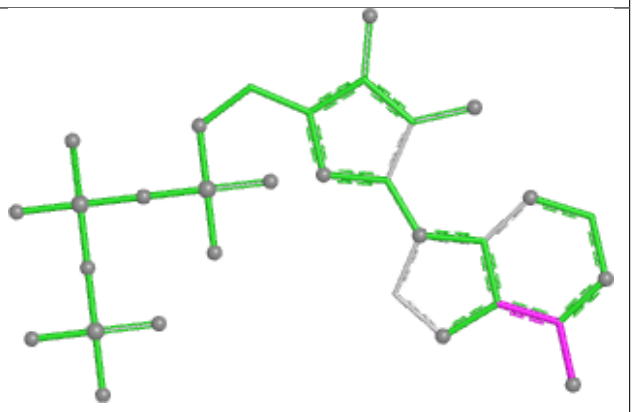
Ligand ATP B 5002



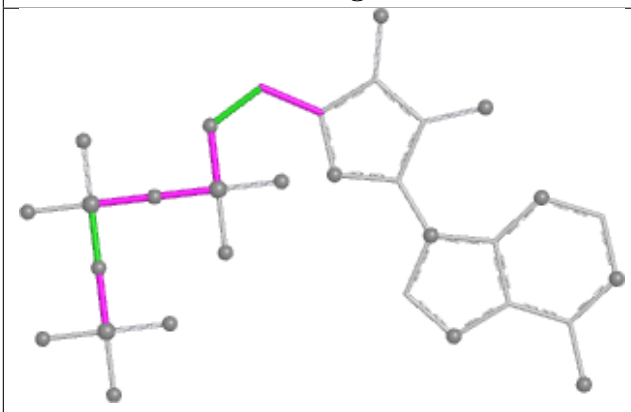
Ligand ATP A 5004



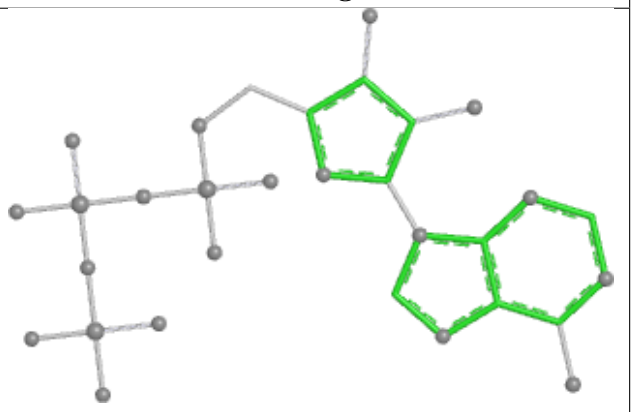
Bond lengths



Bond angles

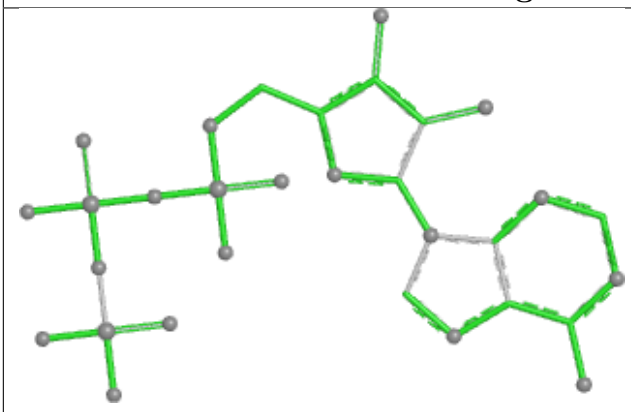


Torsions

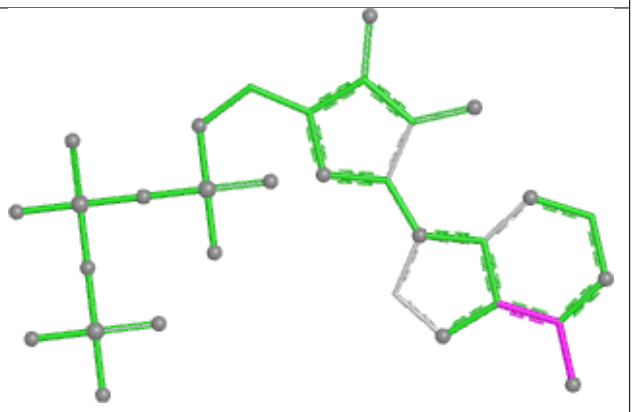


Rings

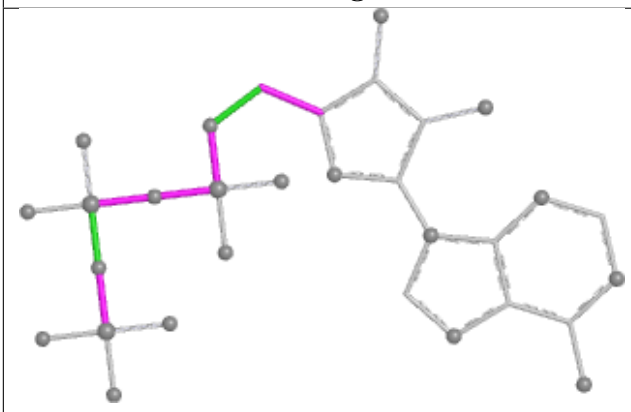
Ligand ATP C 5004



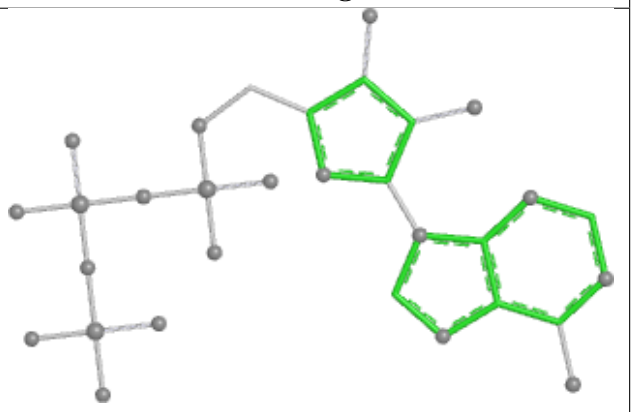
Bond lengths



Bond angles

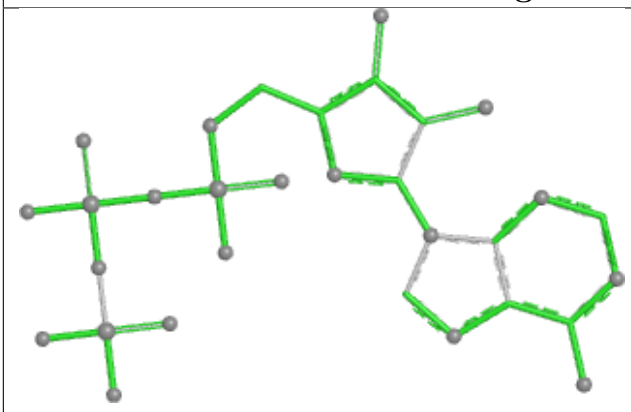


Torsions

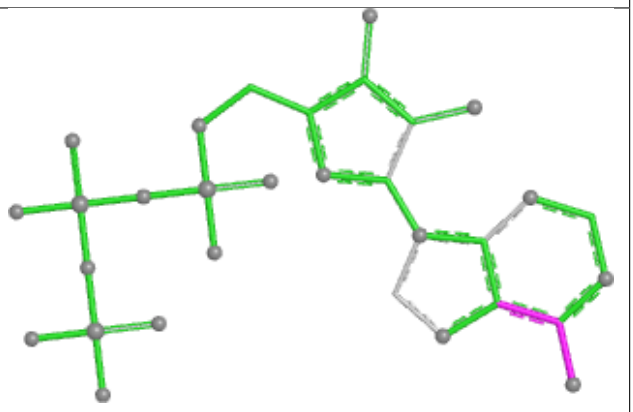


Rings

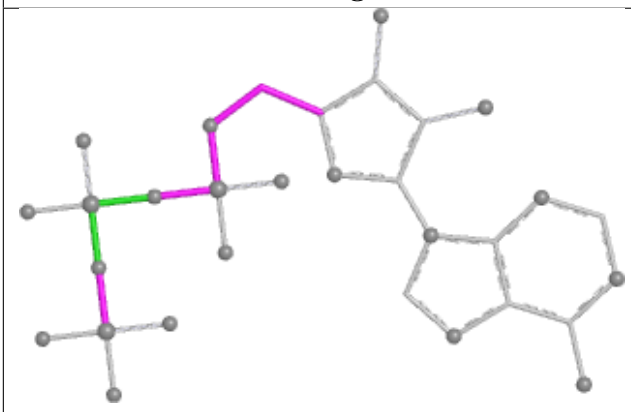
Ligand ATP D 5002



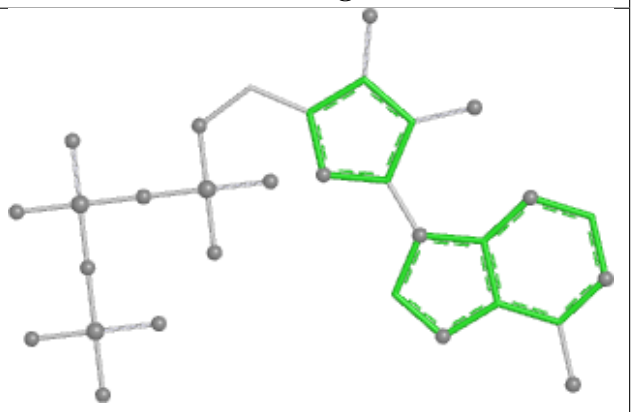
Bond lengths



Bond angles

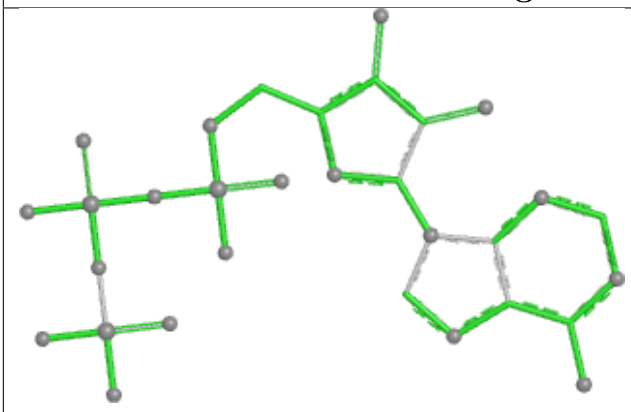


Torsions

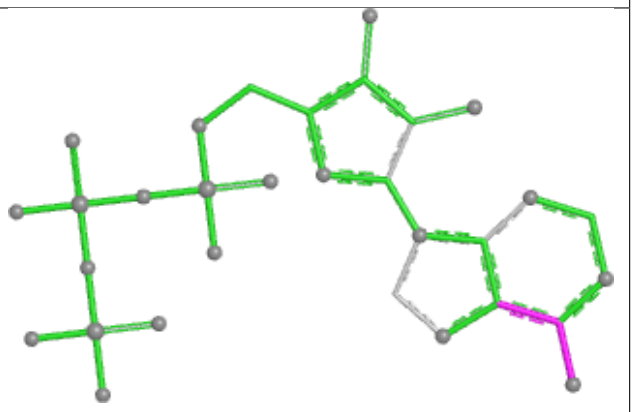


Rings

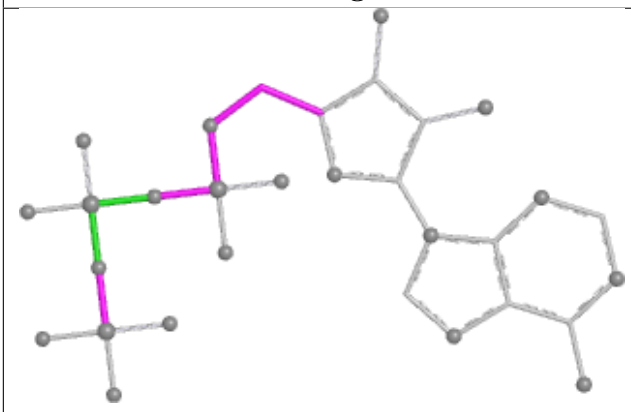
Ligand ATP A 5002



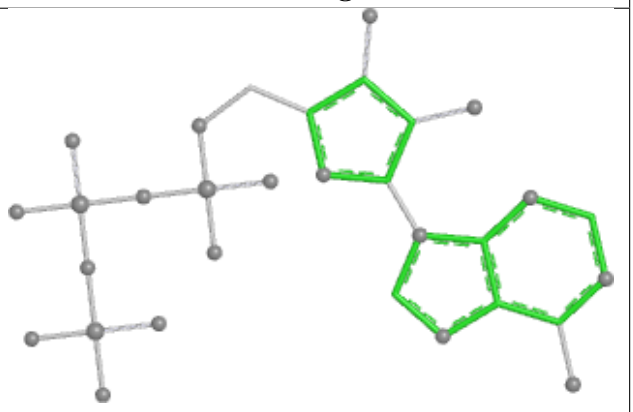
Bond lengths



Bond angles

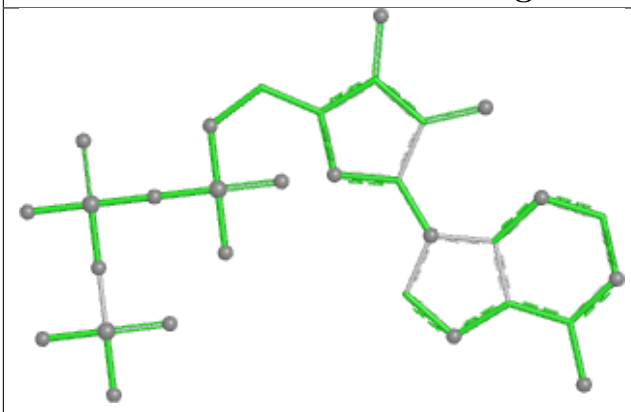


Torsions

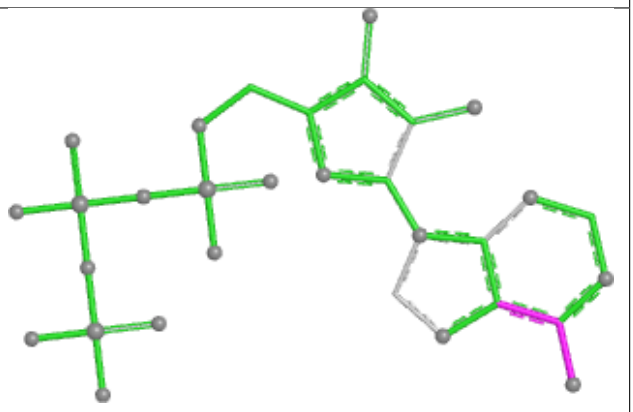


Rings

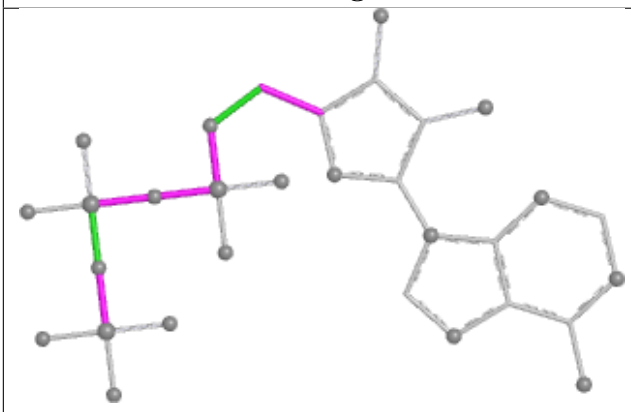
Ligand ATP D 5004



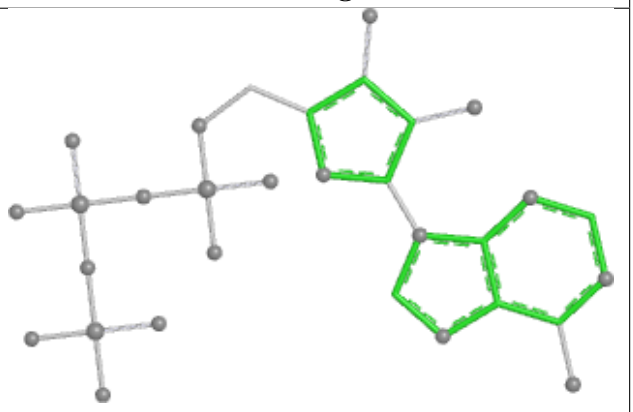
Bond lengths



Bond angles

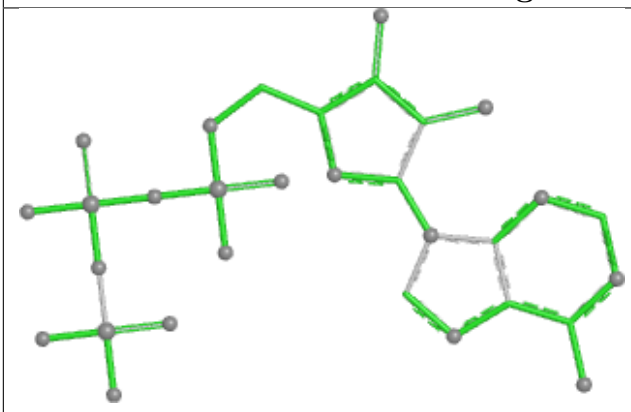


Torsions

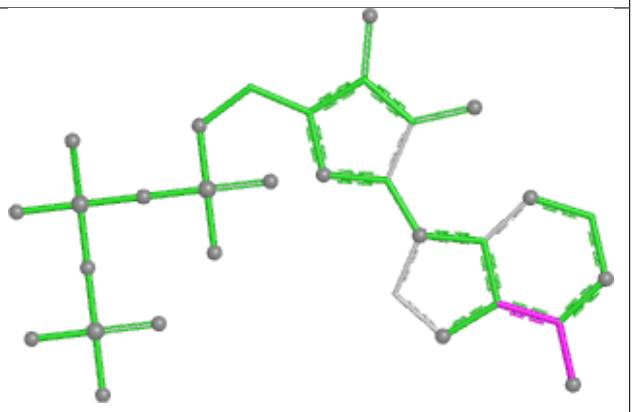


Rings

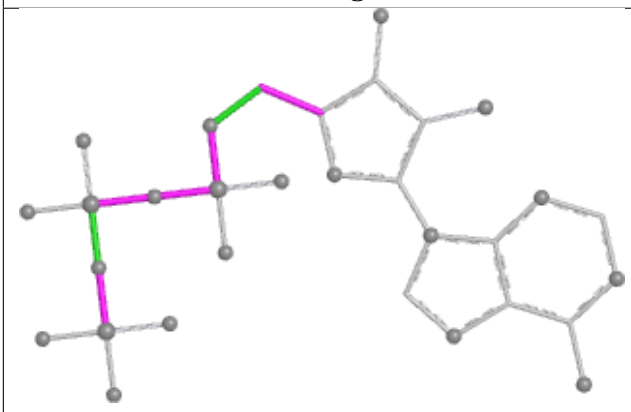
Ligand ATP B 5004



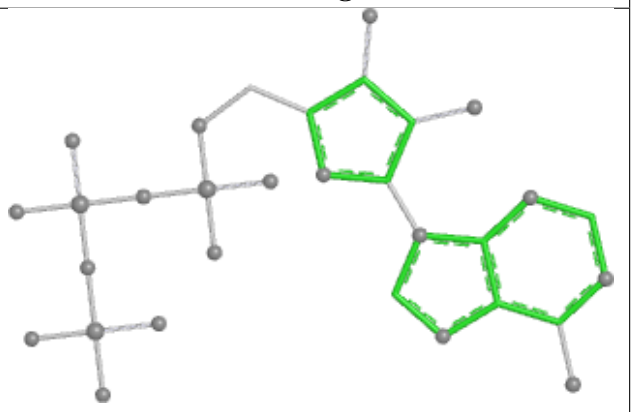
Bond lengths



Bond angles

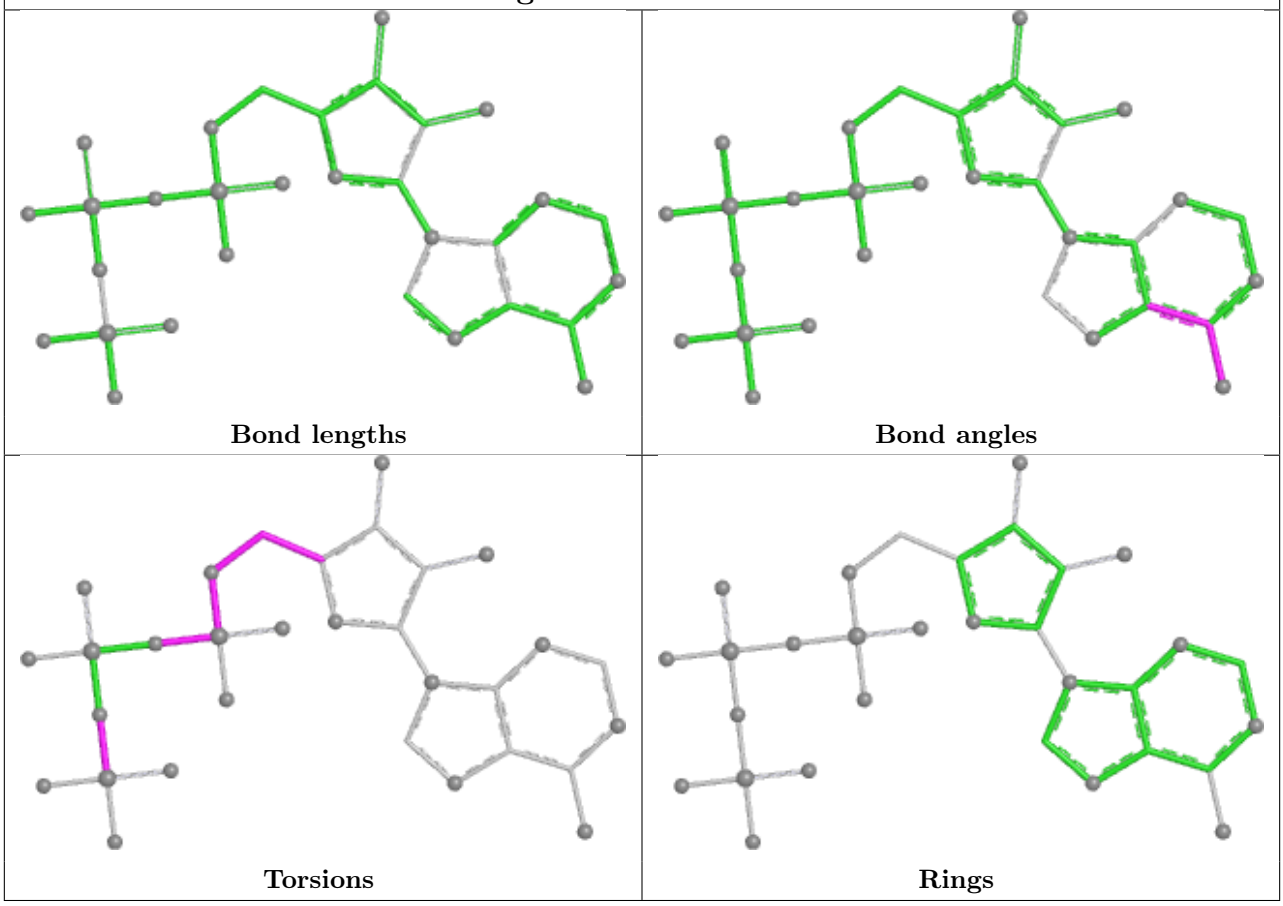


Torsions



Rings

Ligand ATP C 5002



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.

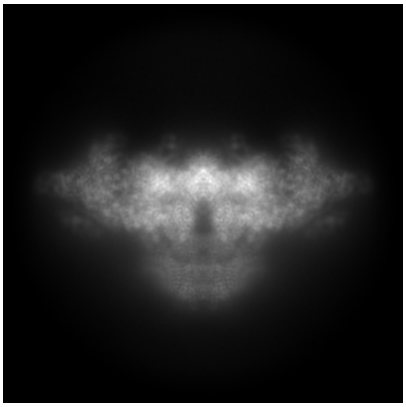
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-42769. These allow visual inspection of the internal detail of the map and identification of artifacts.

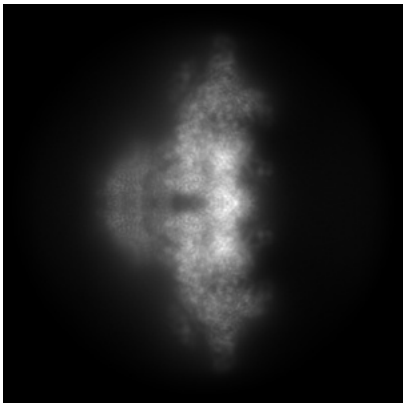
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

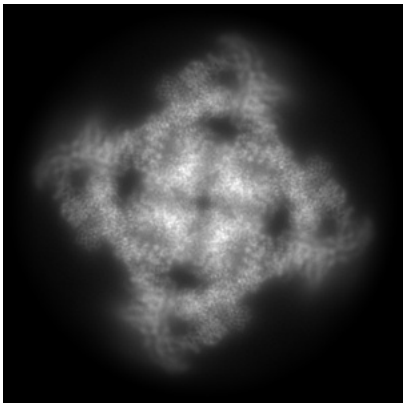
6.1.1 Primary map



X



Y

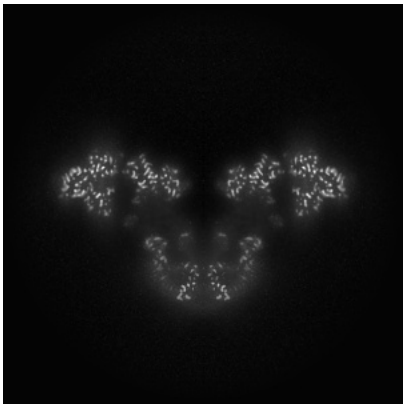


Z

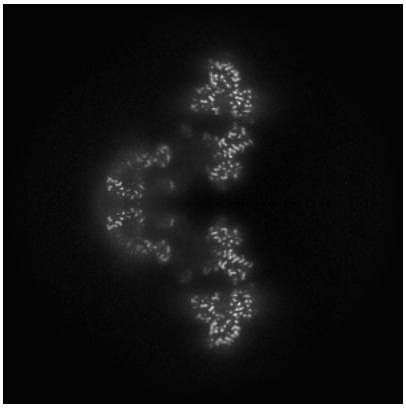
The images above show the map projected in three orthogonal directions.

6.2 Central slices

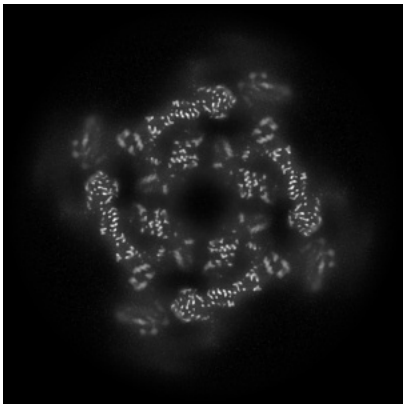
6.2.1 Primary map



X Index: 256



Y Index: 256

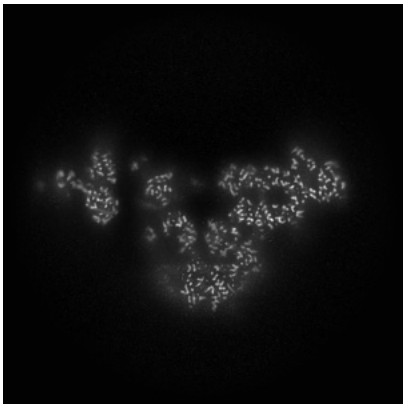


Z Index: 256

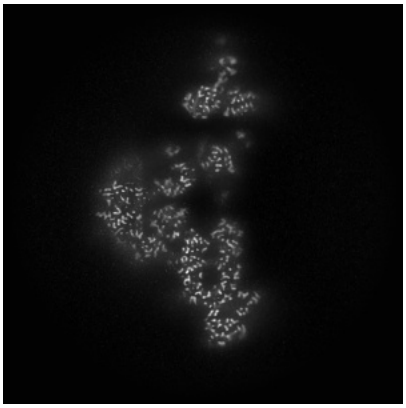
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

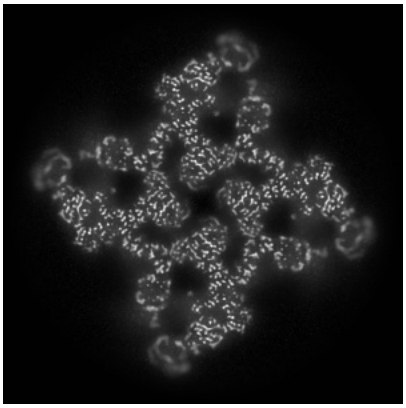
6.3.1 Primary map



X Index: 239



Y Index: 239

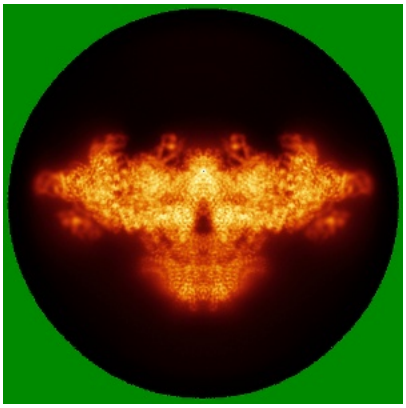


Z Index: 283

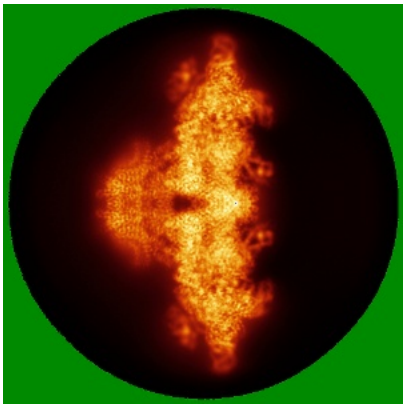
The images above show the largest variance slices of the map in three orthogonal directions.

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

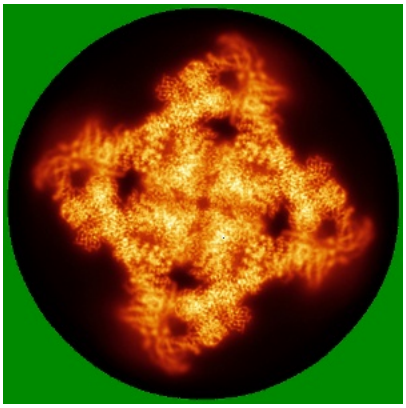
6.4.1 Primary map



X



Y

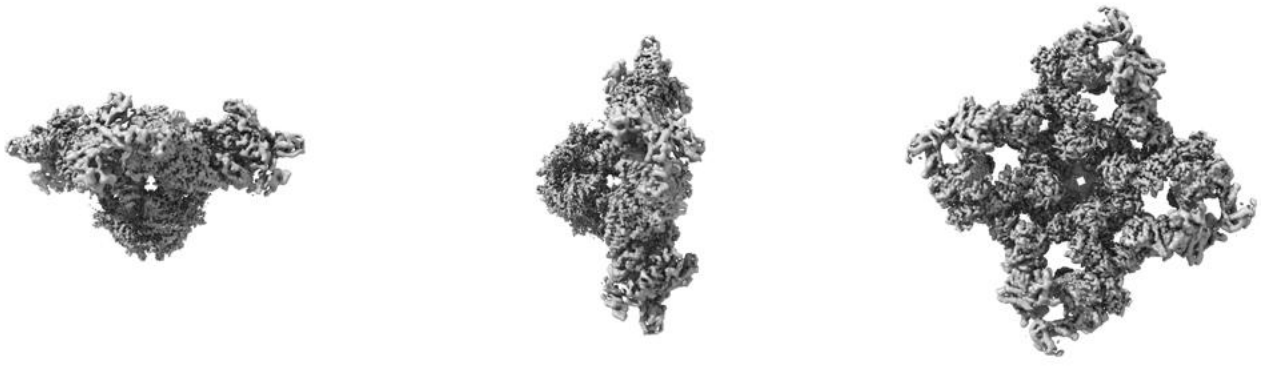


Z

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 0.14. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

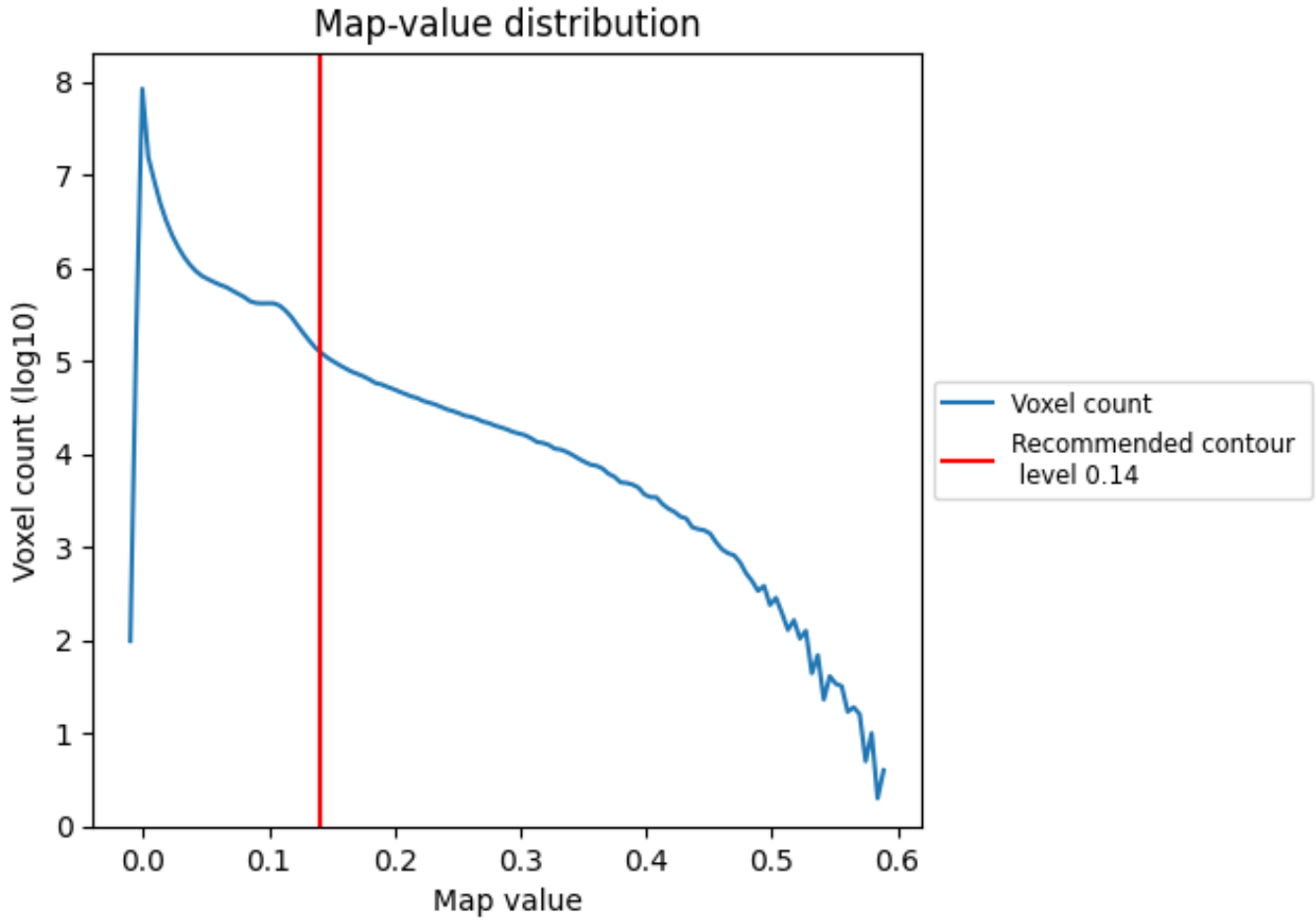
6.6 Mask visualisation (i)

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

7 Map analysis

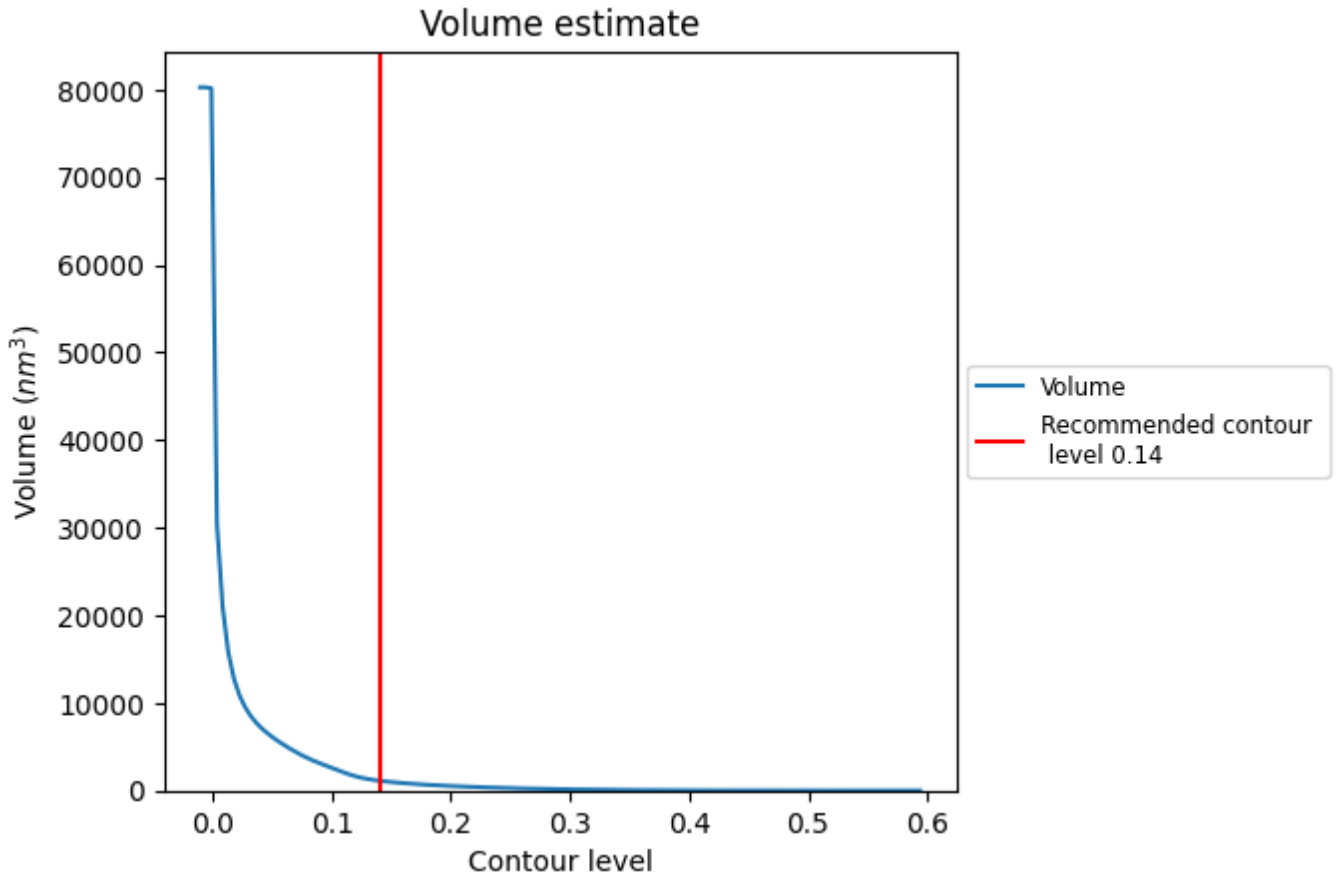
This section contains the results of statistical analysis of the map.

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.

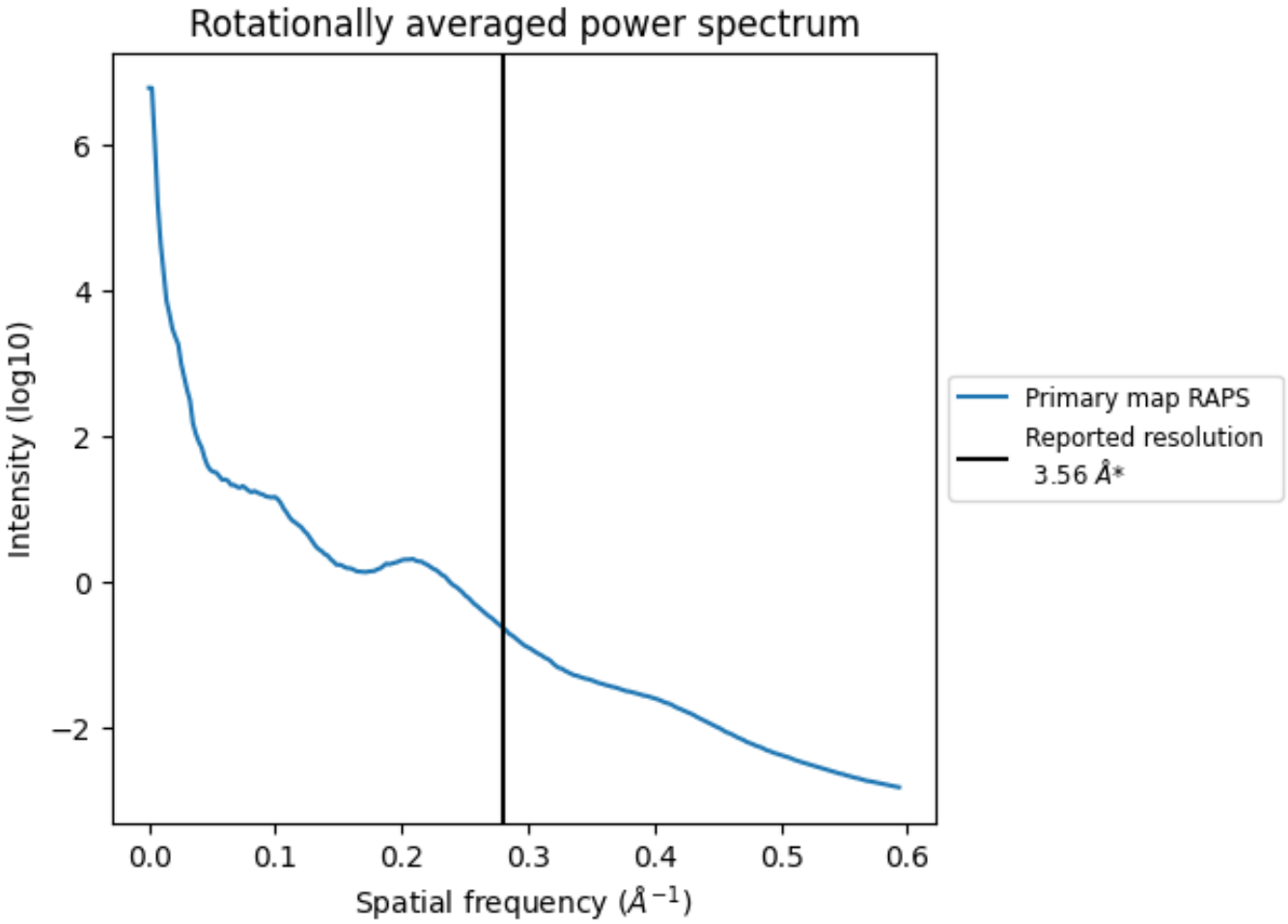
7.2 Volume estimate



The volume at the recommended contour level is 1122 nm^3; this corresponds to an approximate mass of 1014 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 0.281 $Å^{-1}$

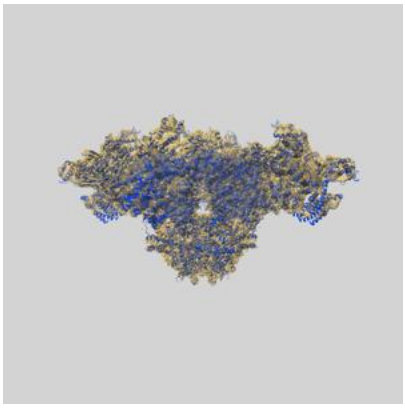
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

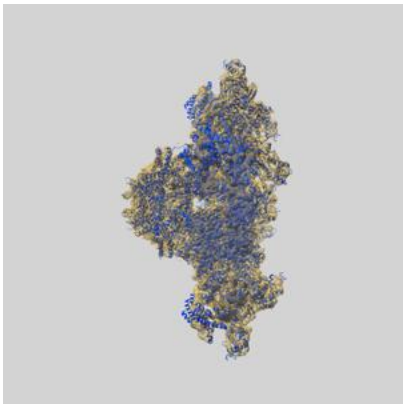
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-42769 and PDB model 8UXM. Per-residue inclusion information can be found in section 3 on page 7.

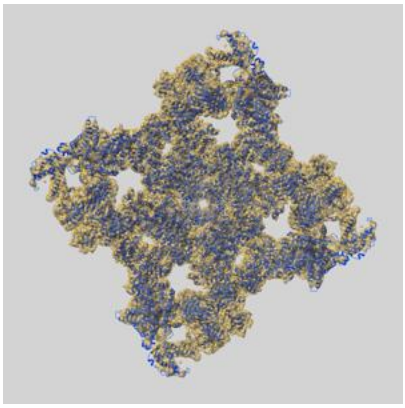
9.1 Map-model overlay



X



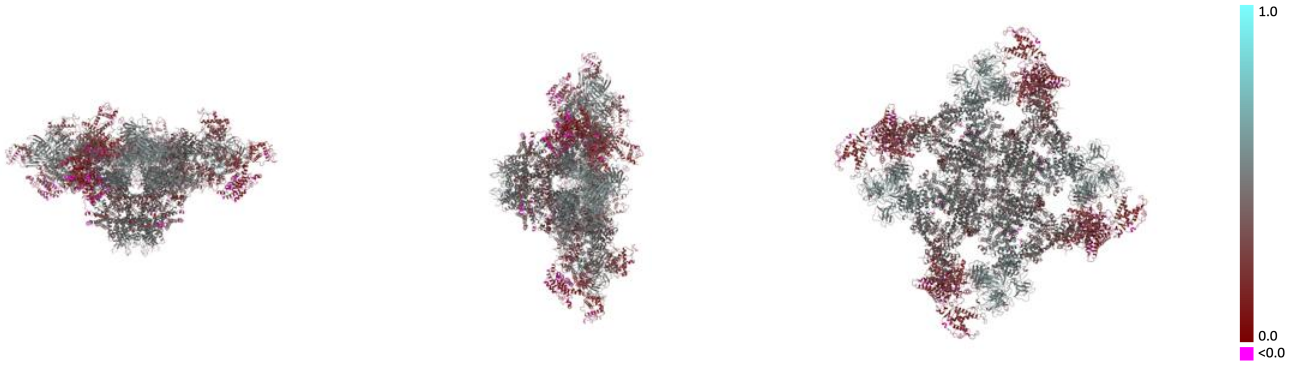
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.14 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

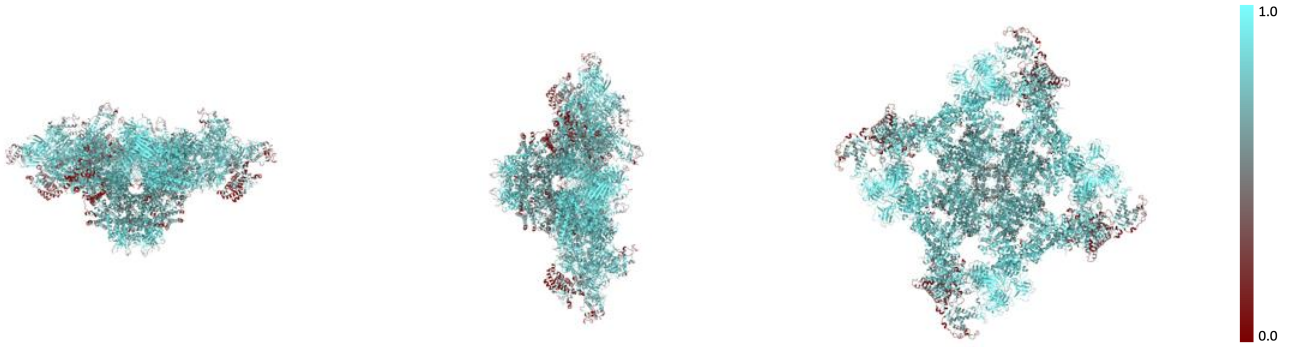
9.2 Q-score mapped to coordinate model (i)



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.

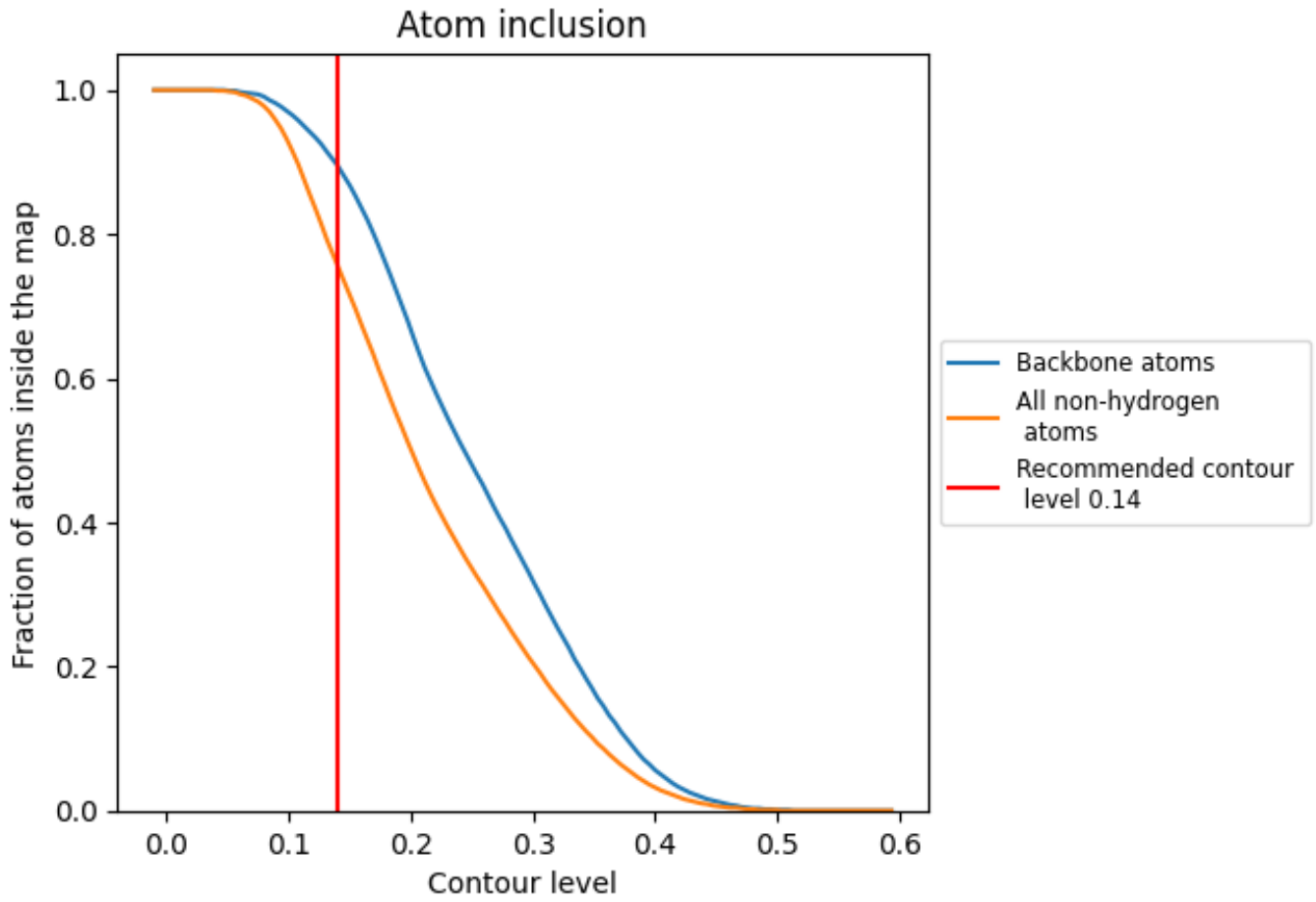
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.14).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 76% 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 (0.14) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7560	0.3810
A	0.7540	0.3840
B	0.7560	0.3860
C	0.7520	0.3800
D	0.7540	0.3820
E	0.8920	0.5130
F	0.8910	0.5110
G	0.8960	0.5120
H	0.8970	0.5110
I	0.7240	0.2220
J	0.7320	0.2220
K	0.7240	0.2220
L	0.7310	0.2190