Full wwPDB EM Validation Report (i)

Mar 6, 2026 – 10:12 AM UTC

PDB ID	:	8RRV / pdb_00008rrv
EMDB ID	:	EMD-19466
Title	:	Structure of RyR1 in detergent in close state in complex with FKBP and Nb9657.
Authors	:	Li, C.; Efremov, R.G.
Deposited on	:	2024-01-23
Resolution	:	3.20 Å(reported)

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 (i) 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 (i)) were used in the production of this report:

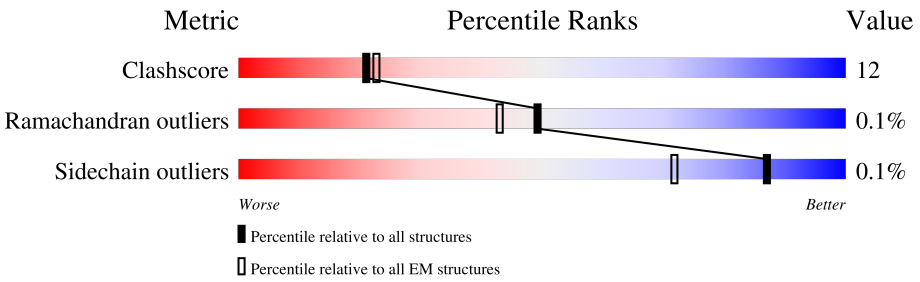
EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh &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

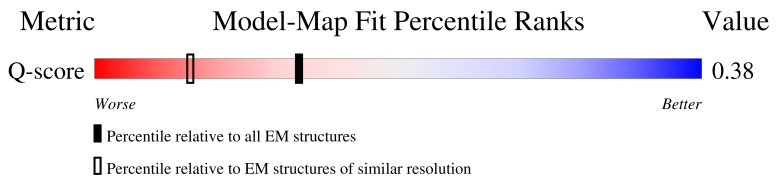
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

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	B	5037	63% 22% 15%
1	E	5037	63% 22% 15%
1	G	5037	63% 22% 15%
1	J	5037	63% 22% 15%

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Mol	Chain	Length	Quality of chain
2	A	107	77% 23%
2	D	107	77% 23%
2	H	107	75% 25%
2	I	107	75% 25%
3	C	137	18% 62% 30% 8%
3	F	137	18% 64% 28% 8%
3	K	137	18% 63% 29% 8%
3	M	137	17% 64% 28% 8%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 142968 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	4290	33956	21639	5852	6236	229	1	0
1	E	4290	33956	21639	5852	6236	229	1	0
1	G	4290	33956	21639	5852	6236	229	1	0
1	J	4290	33956	21639	5852	6236	229	1	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	3221	SER	THR	conflict	UNP P11716
E	3221	SER	THR	conflict	UNP P11716
G	3221	SER	THR	conflict	UNP P11716
J	3221	SER	THR	conflict	UNP P11716

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	107	818	516	144	154	4	0	0
2	D	107	818	516	144	154	4	0	0
2	H	107	818	516	144	154	4	0	0
2	I	107	818	516	144	154	4	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ASP	GLY	conflict	UNP Q8HYX6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	100	ASP	GLY	conflict	UNP Q8HYX6
H	100	ASP	GLY	conflict	UNP Q8HYX6
I	100	ASP	GLY	conflict	UNP Q8HYX6

- Molecule 3 is a protein called nanobody9657.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	126	967	597	170	195	5	0	0
3	F	126	967	597	170	195	5	0	0
3	K	126	967	597	170	195	5	0	0
3	M	126	967	597	170	195	5	0	0

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

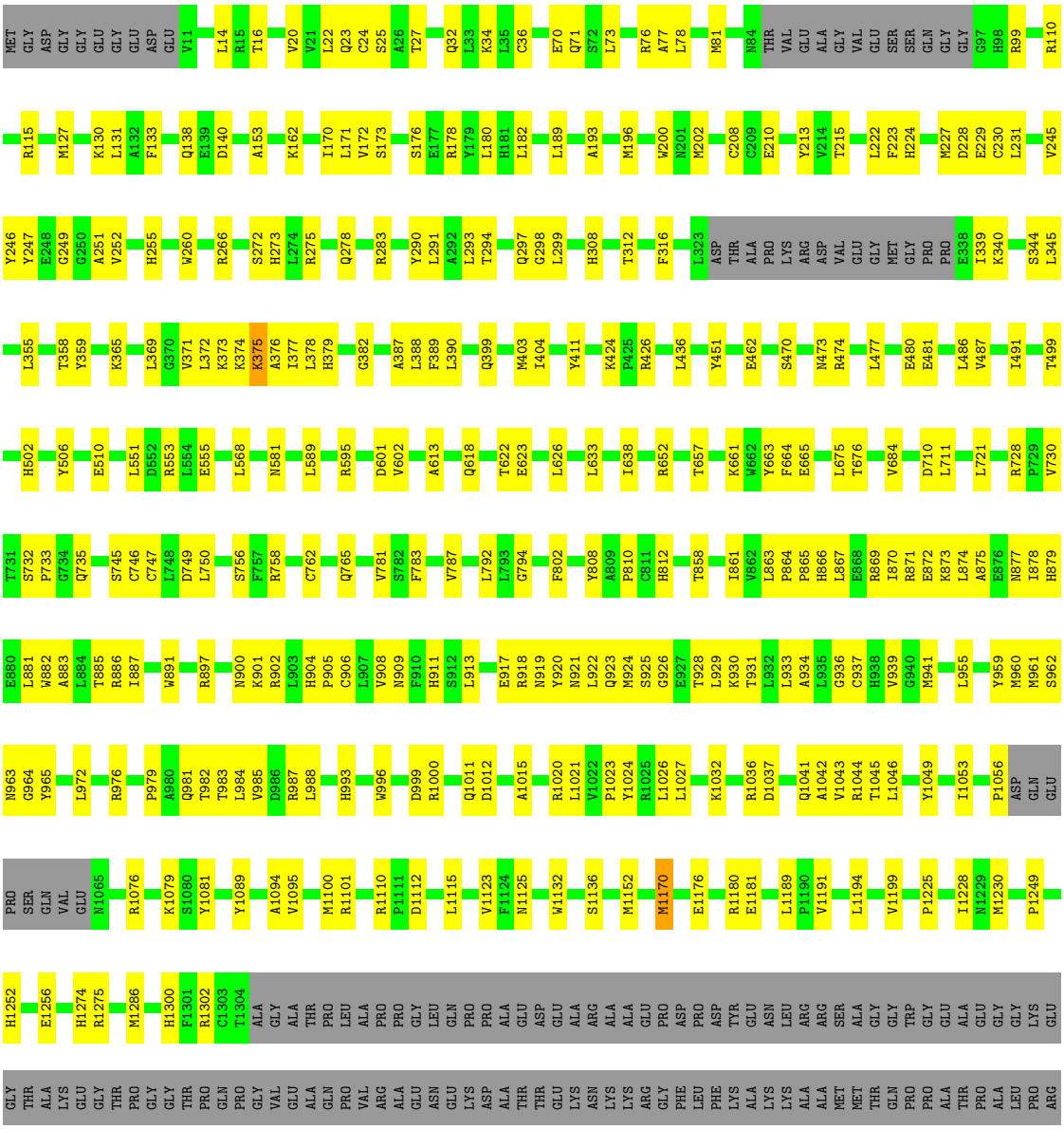
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
4	B	1	1	1	0
4	E	1	1	1	0
4	G	1	1	1	0
4	J	1	1	1	0

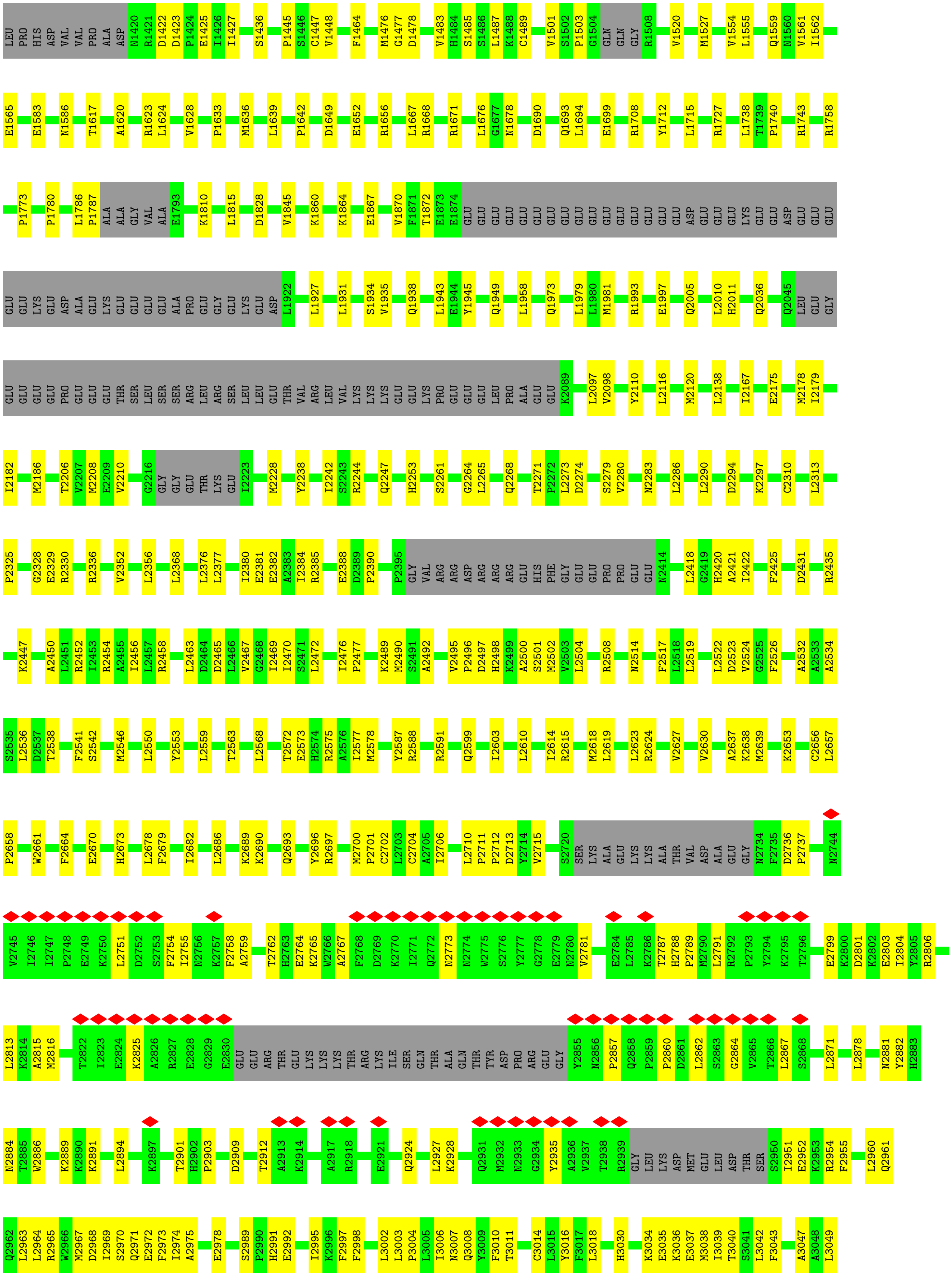
3 Residue-property plots (i)

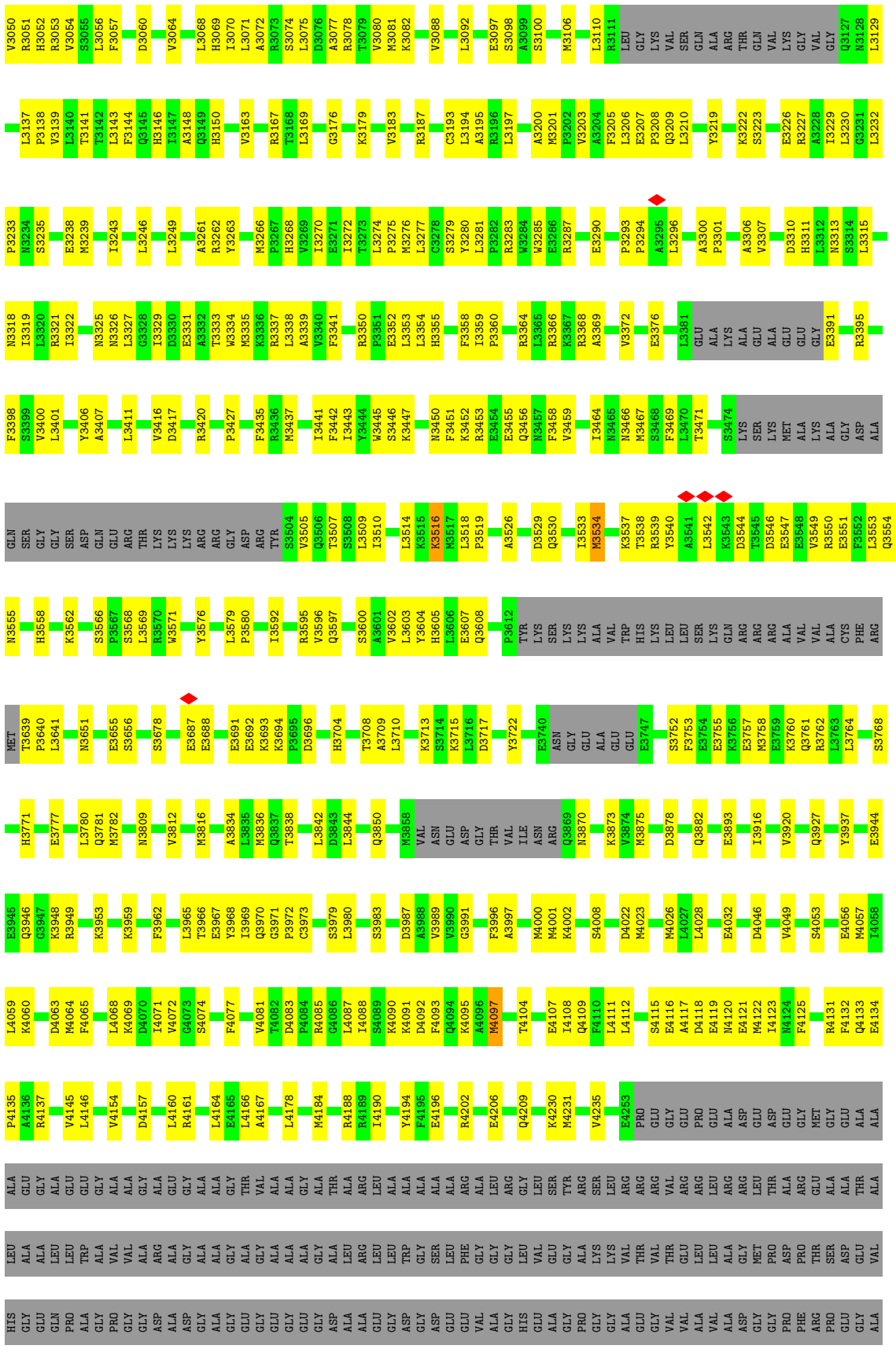
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Ryanodine receptor 1

Chain B:




LEU PRO HIS ASP VAL VAL PRO ALA ASP N1420 R1421 D1422 D1423 P1424 E1425 I1426 I1427 S1436 P1445 S1446 C1447 V1448 F1464 M1476 G1477 D1478 V1483 H1484 S1485 S1486 L1487 K1488 C1489 V1501 S1502 P1503 G1504 GLN GLN GLY R1508 V1520 M1527 V1554 L1555 Q1559 N1560 V1561 I1562
E1565 E1583 N1586 T1617 A1620 R1623 L1624 V1628 P1633 M1636 L1639 P1642 D1649 E1652 R1656 L1667 R1668 R1671 L1676 G1677 N1678 D1690 Q1693 L1694 E1699 R1708 Y1712 L1715 R1727 L1738 T1739 P1740 R1743 R1758
P1773 P1780 L1786 P1787 ALA ALA GLY VAL ALA E1793 K1810 L1815 D1828 V1845 K1860 K1864 E1867 V1870 F1871 T1872 E1873 E1874 GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU ASP GLU GLU GLU LYS GLU GLU ASP GLU GLU GLU
GLU GLU LYS GLU ASP ALA GLU LYS GLU GLU GLU GLU ALA PRO GLU GLY GLU LYS GLU ASP L1922 L1927 L1931 S1934 V1935 Q1938 L1943 E1944 Y1945 Q1949 L1958 Q1973 L1979 L1980 M1981 R1993 E1997 Q2005 L2010 H2011 Q2036 Q2045 LEU GLU GLY
GLU GLU GLU GLU PRO GLU GLU GLU THR SER LEU SER SER SER ARG LEU ARG SER LEU LEU GLU THR VAL ARG LEU VAL LYS LYS LYS GLU GLU LYS PRO GLU GLU GLU LEU PRO ALA GLU GLU K2089 L2097 V2098 Y2110 L2116 M2120 L2138 I2167 E2175 M2178 I2179
I2182 M2186 T2206 V2207 M2208 E2209 V2210 G2216 GLY GLY GLU THR LYS GLU I2223 M2228 Y2238 I2242 S2243 R2244 Q2247 H2253 S2261 G2264 L2265 Q2268 T2271 P2272 L2273 D2274 S2279 V2280 N2283 L2286 L2290 D2294 K2297 C2310 L2313
P2325 G2328 E2329 R2330 R2336 V2352 L2356 L2368 L2376 L2377 I2380 E2381 E2382 A2383 I2384 R2385 E2388 D2389 P2390 P2395 GLY VAL ARG ARG ASP ARG ARG ARG GLU HIS PHE GLY GLU GLU PRO PRO GLU GLU N2414 L2418 G2419 H2420 A2421 I2422 F2425 D2431 R2435
K2447 A2450 L2451 R2452 I2453 R2454 A2455 I2456 L2457 R2458 L2463 D2464 D2465 L2466 V2467 G2468 I2469 I2470 S2471 L2472 I2476 P2477 K2489 M2490 S2491 A2492 V2495 P2496 D2497 H2498 K2499 A2500 S2501 M2502 V2503 L2504 R2508 N2514 F2517 L2518 L2519 L2522 D2523 V2524 G2525 F2526 A2532 A2533 A2534
S2535 L2536 D2537 T2538 F2541 S2542 M2546 L2550 Y2553 L2559 T2563 L2568 T2572 E2573 H2574 R2575 A2576 I2577 M2578 Y2587 R2588 R2591 Q2599 I2603 L2610 I2614 R2615 M2618 L2619 L2623 R2624 V2627 V2630 A2637 K2638 M2639 K2653 C2656 L2657
P2658 W2661 F2664 E2670 H2673 L2678 F2679 I2682 L2686 K2689 K2690 Q2693 Y2696 R2697 M2700 P2701 C2702 L2703 C2704 A2705 I2706 L2710 P2711 P2712 D2713 Y2714 V2715 S2720 SER LYS ALA GLU LYS LYS ALA THR VAL ASP ALA GLU GLY N2734 F2735 D2736 P2737 N2744
V2745 I2746 I2747 P2748 E2749 K2750 L2751 D2752 S2753 F2754 I2755 N2756 K2757 F2758 A2759 T2762 H2763 E2764 K2765 W2766 A2767 F2768 D2769 K2770 I2771 Q2772 N2773 N2774 W2775 S2776 Y2777 G2778 E2779 N2780 V2781 E2784 L2785 K2786 T2787 H2788 P2789 M2790 L2791 R2792 P2793 Y2794 K2795 T2796 E2799 K2800 D2801 K2802 E2803 I2804 Y2805 R2806
L2813 K2814 A2815 M2816 T2822 I2823 E2824 K2825 A2826 R2827 E2828 G2829 E2830 GLU GLU ARG THR GLU LYS LYS LYS THR ARG LYS ILE SER GLN THR ALA GLN THR TYR ASP PRO ARG GLU GLY Y2855 N2856 P2857 Q2858 P2859 P2860 D2861 L2862 S2863 G2864 V2865 T2866 L2867 S2868 L2871 L2878 N2881 Y2882 H2883
N2884 T2885 W2886 K2889 K2890 K2891 L2894 K2897 T2901 H2902 P2903 D2909 T2912 A2913 K2914 A2917 R2918 E2921 Q2924 L2927 K2928 Q2931 M2932 N2933 G2934 Y2935 A2936 V2937 T2938 R2939 GLY LEU LYS ASP MET GLU LEU ASP THR SER S2950 I2951 E2952 K2953 R2954 F2955 L2960 Q2961
Q2962 L2963 L2964 R2965 W2966 M2967 D2968 I2969 S2970 Q2971 E2972 F2973 I2974 A2975 E2978 S2989 P2990 H2991 E2992 I2995 K2996 F2997 F2998 L3002 L3003 P3004 L3005 I3006 N3007 Q3008 Y3009 F3010 T3011 C3014 L3015 Y3016 F3017 L3018 H3030 K3034 E3035 K3036 E3037 M3038 I3039 T3040 S3041 L3042 F3043 A3047 A3048 L3049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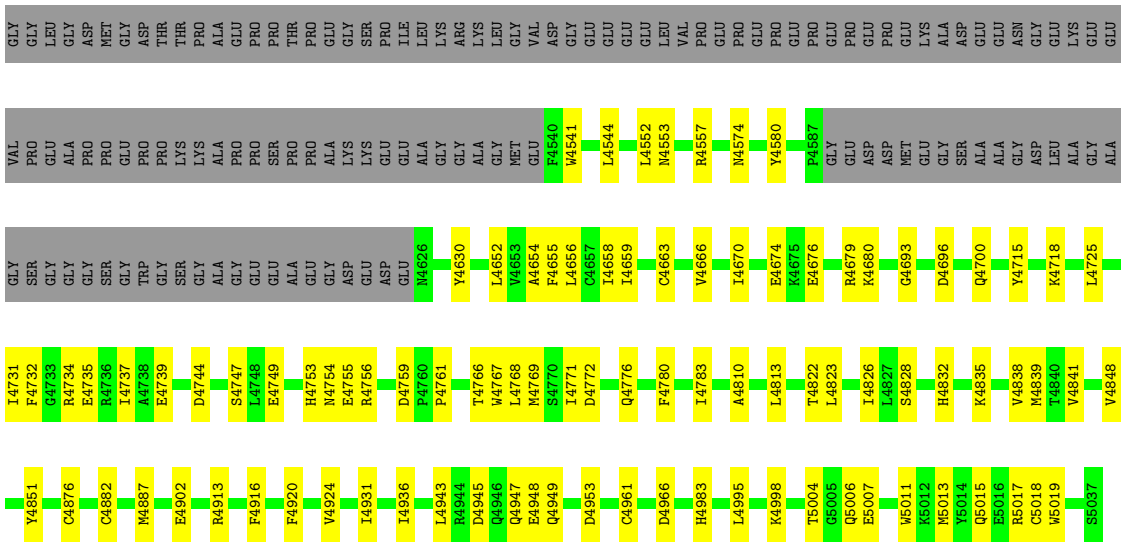
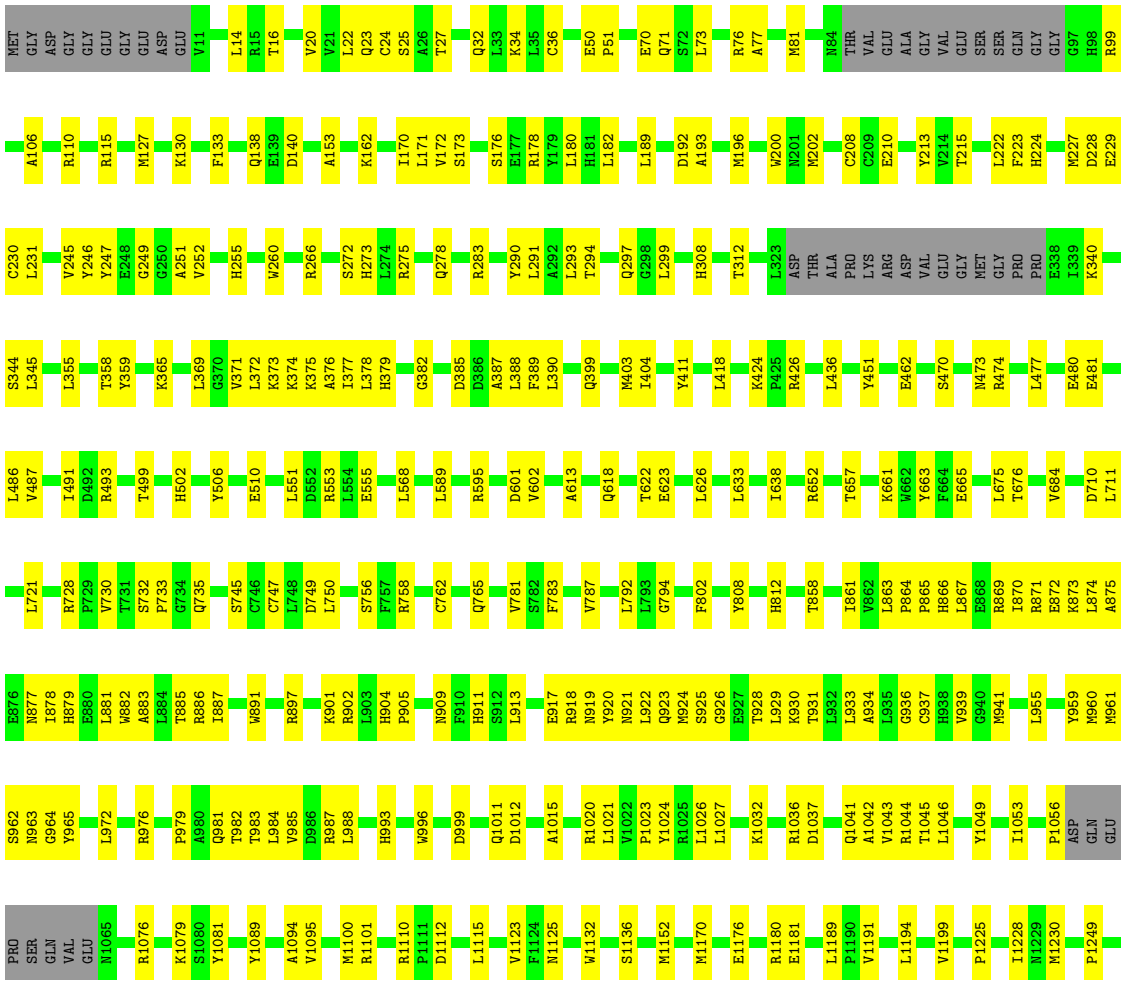
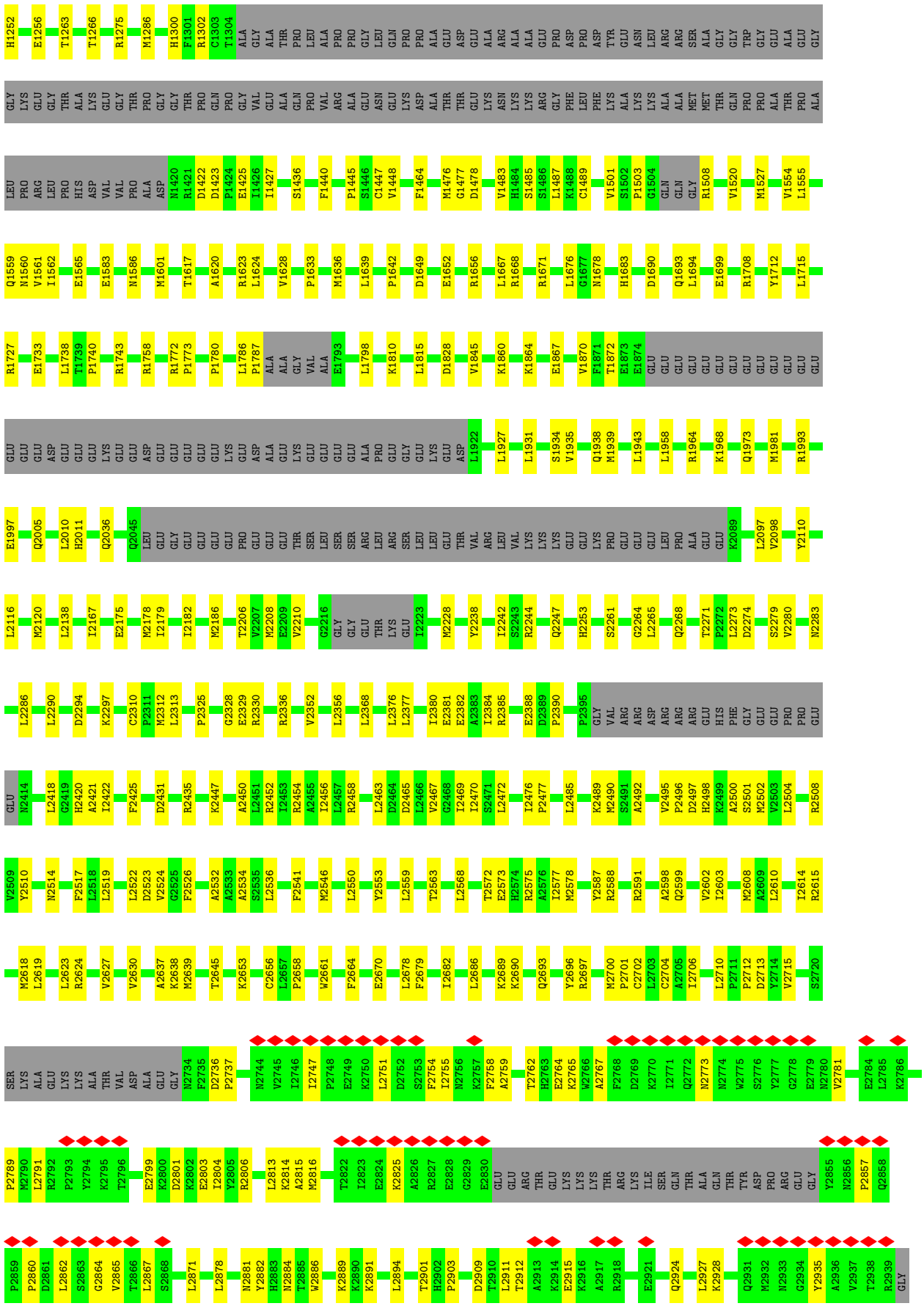
L3137 P3138 V3139 L3140 T3141 T3142 L3143 F3144 Q3145 H3146 I3147 A3148 Q3149 H3150 V3163 R3167 T3168 L3169 G3176 K3179 V3183 R3187 C3193 L3194 A3195 R3196 L3197 A3200 M3201 P3202 V3203 A3204 F3205 L3206 E3207 P3208 Q3209 L3210 Y3219 K3222 S3223 E3226 R3227 A3228 I3229 L3230 G3231 L3232
P3233 N3234 S3235 E3238 M3239 I3243 L3246 L3249 A3261 R3262 Y3263 M3266 P3267 H3268 V3269 I3270 E3271 I3272 T3273 L3274 P3275 M3276 L3277 C3278 S3279 Y3280 L3281 P3282 R3283 W3284 W3285 E3286 R3287 E3290 P3293 P3294 A3295 L3296 A3300 P3301 A3306 V3307 D3310 H3311 L3312 N3313 S3314 L3315
N3318 I3319 L3320 R3321 I3322 N3325 N3326 L3327 G3328 I3329 D3330 E3331 A3332 T3333 W3334 M3335 K3336 R3337 L3338 A3339 V3340 F3341 R3350 P3351 E3352 L3353 L3354 H3355 F3358 I3359 P3360 R3364 L3365 R3366 K3367 R3368 A3369 V3372 E3376 L3381 GLU ALA LYS ALA GLU ALA GLU GLU GLY E3391 R3395
F3398 S3399 V3400 L3401 Y3406 A3407 L3411 V3416 D3417 R3420 P3427 F3435 R3436 M3437 I3441 F3442 I3443 Y3444 W3445 S3446 K3447 N3450 F3451 K3452 R3453 E3454 E3455 Q3456 N3457 F3458 V3459 I3464 N3465 N3466 M3467 S3468 F3469 L3470 T3471 S3474 LYS SER LYS MET ALA LYS ALA GLY ASP ALA
GLN SER GLY GLY SER ASP GLN GLU ARG THR LYS LYS LYS ARG ARG GLY ASP ARG TYR S3504 V3505 Q3506 T3507 S3508 L3509 I3510 L3514 K3515 K3516 M3517 L3518 P3519 A3526 D3529 Q3530 I3533 M3534 K3537 T3538 R3539 Y3540 A3541 L3542 K3543 D3544 T3545 D3546 E3547 E3548 V3549 R3550 E3551 F3552 L3553 Q3554
N3555 H3558 K3562 S3566 P3567 S3568 L3569 R3570 W3571 Y3576 L3579 P3580 I3592 R3595 V3596 Q3597 S3600 A3601 V3602 L3603 Y3604 H3605 L3606 E3607 Q3608 P3612 TYR LYS SER LYS LYS LYS VAL TRP HIS LYS LEU LEU SER LYS GLN ARG ARG ARG ALA VAL VAL ALA CYS PHE ARG
MET T3639 P3640 L3641 N3651 E3655 S3656 S3678 E3687 E3688 E3691 E3692 K3693 K3694 P3695 D3696 H3704 T3708 A3709 L3710 K3713 S3714 K3715 L3716 D3717 Y3722 E3740 ASN GLY GLU ALA GLU GLU E3747 S3752 F3753 E3754 E3755 K3756 E3757 M3758 E3759 K3760 Q3761 R3762 L3763 L3764 S3768
H3771 E3777 L3780 Q3781 M3782 N3809 V3812 M3816 A3834 L3835 M3836 Q3837 T3838 L3842 D3843 L3844 Q3850 M3858 VAL ASN GLU ASP GLY THR VAL ILE ASN ARG Q3869 N3870 K3873 V3874 M3875 D3878 Q3882 E3893 I3916 V3920 Q3927 Y3937 E3944
E3945 Q3946 G3947 K3948 R3949 K3953 K3959 F3962 L3965 T3966 E3967 Y3968 I3969 Q3970 G3971 P3972 C3973 S3979 L3980 S3983 D3987 A3988 V3989 V3990 G3991 F3996 A3997 M4000 M4001 K4002 S4008 D4022 M4023 M4026 L4027 L4028 E4032 D4046 V4049 S4053 E4056 M4057 I4058
L4059 K4060 D4063 M4064 F4065 L4068 K4069 D4070 I4071 V4072 G4073 S4074 F4077 V4081 T4082 D4083 P4084 R4085 G4086 L4087 I4088 S4089 K4090 K4091 D4092 F4093 Q4094 K4095 A4096 M4097 T4104 E4107 I4108 Q4109 F4110 L4111 L4112 S4115 E4116 A4117 D4118 E4119 N4120 E4121 M4122 I4123 M4124 F4125 R4131 F4132 Q4133 E4134
P4135 A4136 R4137 V4145 L4146 V4154 D4157 L4160 R4161 L4164 E4165 L4166 A4167 L4178 M4184 R4188 R4189 I4190 Y4194 F4195 E4196 R4202 E4206 Q4209 K4230 M4231 V4235 E4253 PRO GLU GLY GLU PRO GLU ALA ASP GLU GLU GLY MET GLY GLU ALA ALA
ALA GLU GLY ALA GLU GLU GLY ALA GLY ALA GLU GLY ALA ALA ALA GLY ALA THR ALA ARG LEU LEU ALA ALA ALA ARG ARG ARG ARG ARG LEU ARG SER LEU ARG ARG ARG VAL ARG ARG LEU LEU ARG ARG ARG LEU ARG GLU ALA ALA THR ALA
LEU ALA ALA LEU LEU TRP ALA VAL ALA ALA ALA GLY ALA GLY GLY VAL ALA ALA GLY GLY ALA ALA ALA GLY ALA LEU ARG LEU LEU TRP GLY SER LEU PHE GLY GLY GLY LEU VAL THR VAL THR GLU LEU LEU ALA GLY MET PRO ASP PRO THR SER ASP GLU VAL
HIS GLY GLU GLN PRO ALA GLY GLY ASP ALA ALA GLU GLY GLU GLU GLU GLY GLY ASP GLY ASP GLU GLU GLU HIS GLU ALA GLY PRO GLY GLY ALA GLU GLY VAL VAL ALA VAL ALA ASP GLY GLY PRO PHE ARG PRO GLU GLY ALA



- Molecule 1: Ryanodine receptor 1

Chain E:




H1252 E1256 T1263 T1266 R1275 M1286 H1300 F1301 R1302 C1303 T1304 ALA GLY ALA THR PRO LEU ALA PRO PRO GLY LEU GLN PRO PRO ALA GLU ASP GLU ALA ARG ALA ALA GLU PRO ASP PRO ASP TYR GLU ASN LEU ARG ARG SER ALA GLY GLY GLY TRP GLY GLU ALA GLU GLY
GLY LYS GLU GLY THR ALA LYS GLU GLY THR PRO GLY GLY THR PRO GLN PRO GLY VAL GLU ALA GLN PRO VAL ARG ALA GLU ASN GLU LYS ASP ALA THR THR GLU LYS ASN LYS LYS ARG GLY PHE LEU PHE LYS ALA LYS LYS ALA ALA MET MET THR GLN PRO PRO ALA THR PRO ALA
LEU PRO ARG LEU PRO HIS ASP VAL VAL PRO ALA ASP N1420 R1421 D1422 D1423 P1424 E1425 I1426 I1427 S1436 F1440 P1445 S1446 C1447 V1448 F1464 M1476 G1477 D1478 V1483 H1484 S1485 S1486 L1487 K1488 C1489 V1501 S1502 P1503 G1504 GLN GLN GLY R1508 V1520 M1527 V1554 L1555
Q1559 N1560 V1561 I1562 E1565 E1583 N1586 M1601 T1617 A1620 R1623 L1624 V1628 P1633 M1636 L1639 P1642 D1649 E1652 R1656 L1667 R1668 R1671 L1676 G1677 N1678 H1683 D1690 Q1693 L1694 E1699 R1708 Y1712 L1715
R1727 E1733 L1738 T1739 P1740 R1743 R1758 R1772 P1773 P1780 L1786 P1787 ALA ALA GLY VAL ALA E1793 L1798 K1810 L1815 D1828 V1845 K1860 K1864 E1867 V1870 F1871 T1872 E1873 E1874 GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU
GLU GLU GLU ASP GLU GLU GLU LYS GLU GLU ASP GLU GLU GLU GLU GLU GLU LYS GLU ASP ALA GLU LYS GLU GLU ALA PRO GLU GLY GLU LYS GLU ASP L1922 L1927 L1931 S1934 V1935 Q1938 M1939 L1943 L1958 R1964 K1968 Q1973 M1981 R1993
E1997 Q2005 L2010 H2011 Q2036 Q2045 LEU GLU GLY GLU GLU GLU GLU PRO GLU GLU GLU THR SER LEU SER SER ARG LEU ARG SER LEU LEU GLU THR VAL ARG LEU VAL LYS LYS LYS GLU GLU LYS PRO GLU GLU GLU LEU PRO ALA GLU GLU K2089 L2097 V2098 Y2110
L2116 M2120 L2138 I2167 E2175 M2178 I2179 I2182 M2186 T2206 V2207 M2208 E2209 V2210 G2216 GLY GLY GLU THR LYS GLU I2223 M2228 Y2238 I2242 S2243 R2244 Q2247 H2253 S2261 G2264 L2265 Q2268 T2271 P2272 L2273 D2274 S2279 V2280 N2283
L2286 L2290 D2294 K2297 C2310 P2311 M2312 L2313 P2325 G2328 E2329 R2330 R2336 V2352 L2356 L2368 L2376 L2377 I2380 E2381 E2382 A2383 I2384 R2385 E2388 D2389 P2390 P2395 GLY VAL ARG ARG ASP ARG ARG ARG GLU HIS PHE GLY GLU GLU PRO PRO GLU
GLU N2414 L2418 G2419 H2420 A2421 I2422 F2425 D2431 R2435 K2447 A2450 L2451 R2452 I2453 R2454 A2455 I2456 L2457 R2458 L2463 D2464 D2465 L2466 V2467 G2468 I2469 I2470 S2471 L2472 I2476 P2477 L2485 K2489 M2490 S2491 A2492 V2495 P2496 D2497 H2498 K2499 A2500 S2501 M2502 V2503 L2504 R2508
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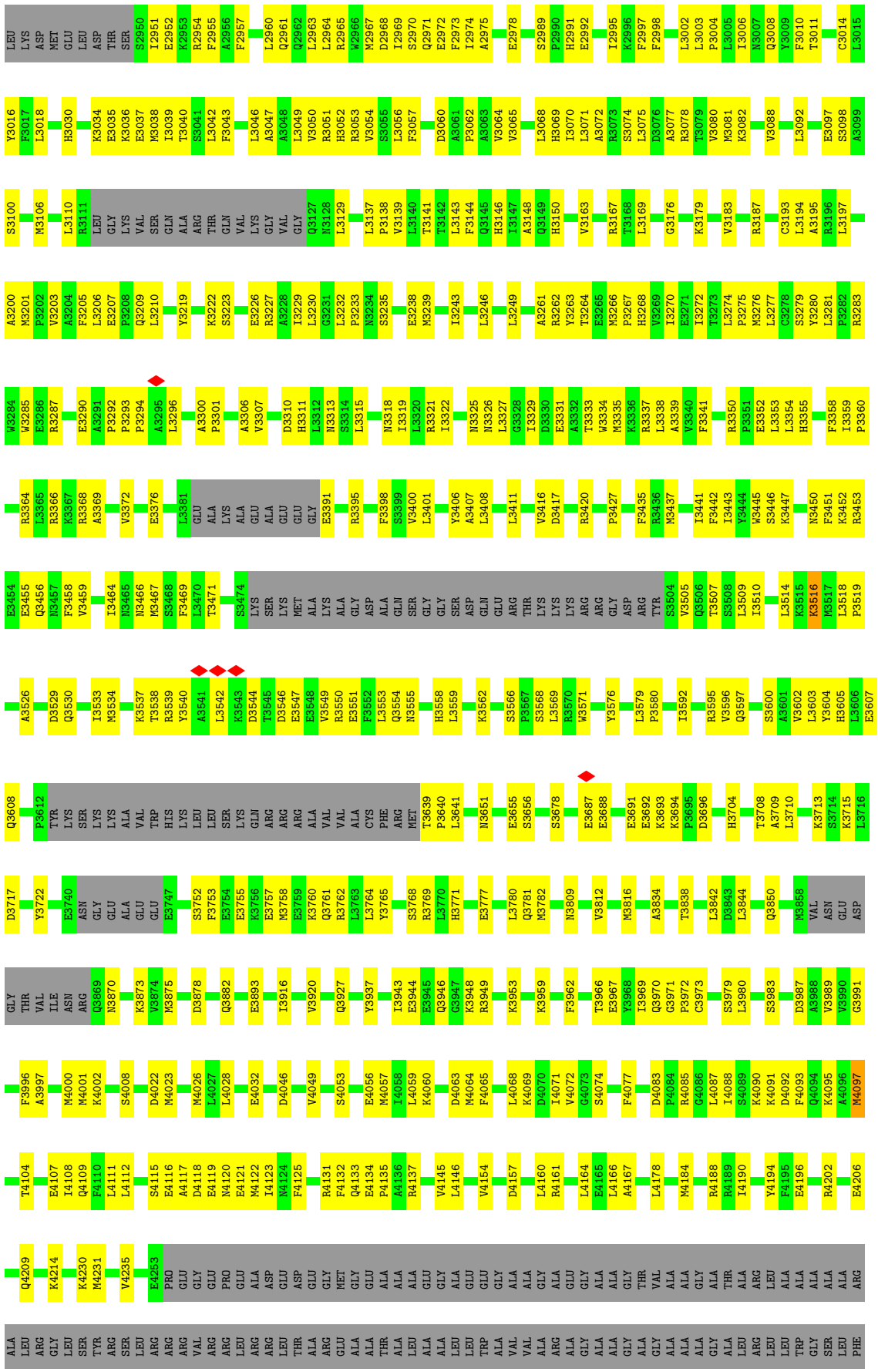

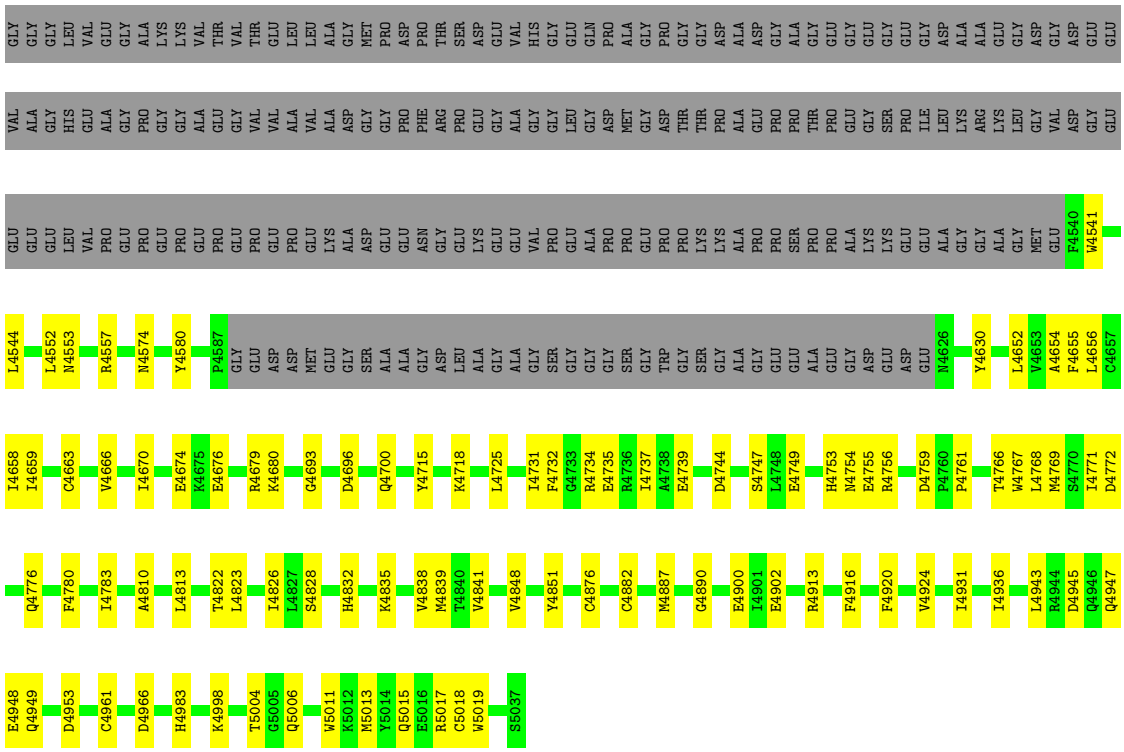

- Molecule 1: Ryanodine receptor 1

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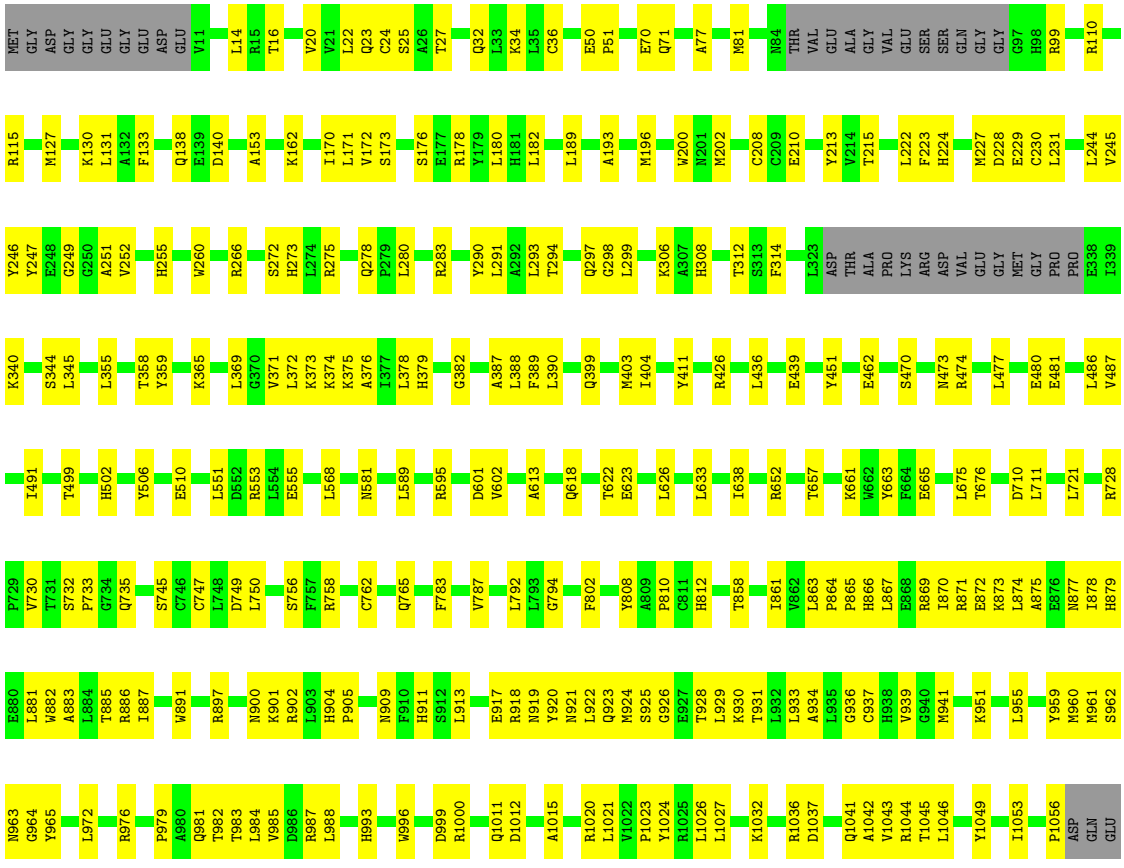

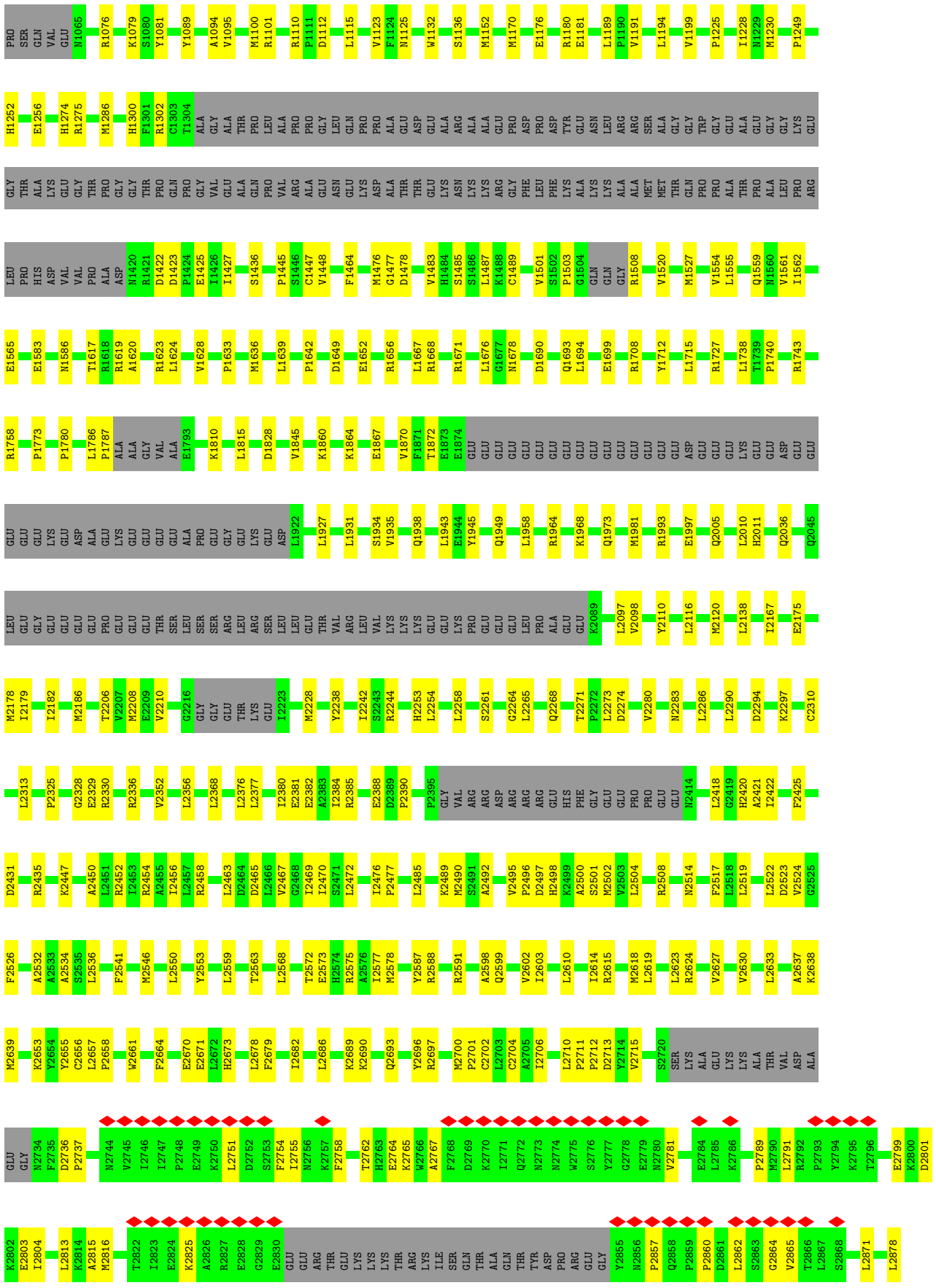
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H1252 E1256 H1274 R1275 M1286 H1300 F1301 R1302 C1303 T1304 ALA GLY ALA THR PRO LEU ALA PRO PRO GLY LEU GLN PRO PRO ALA GLU ASP GLU ALA ARG ALA ALA GLU PRO GLU LEU PHE TYR GLU ASN LEU ARG SER ALA GLY GLY TRP GLY GLU ALA GLU GLY GLY LYS GLU
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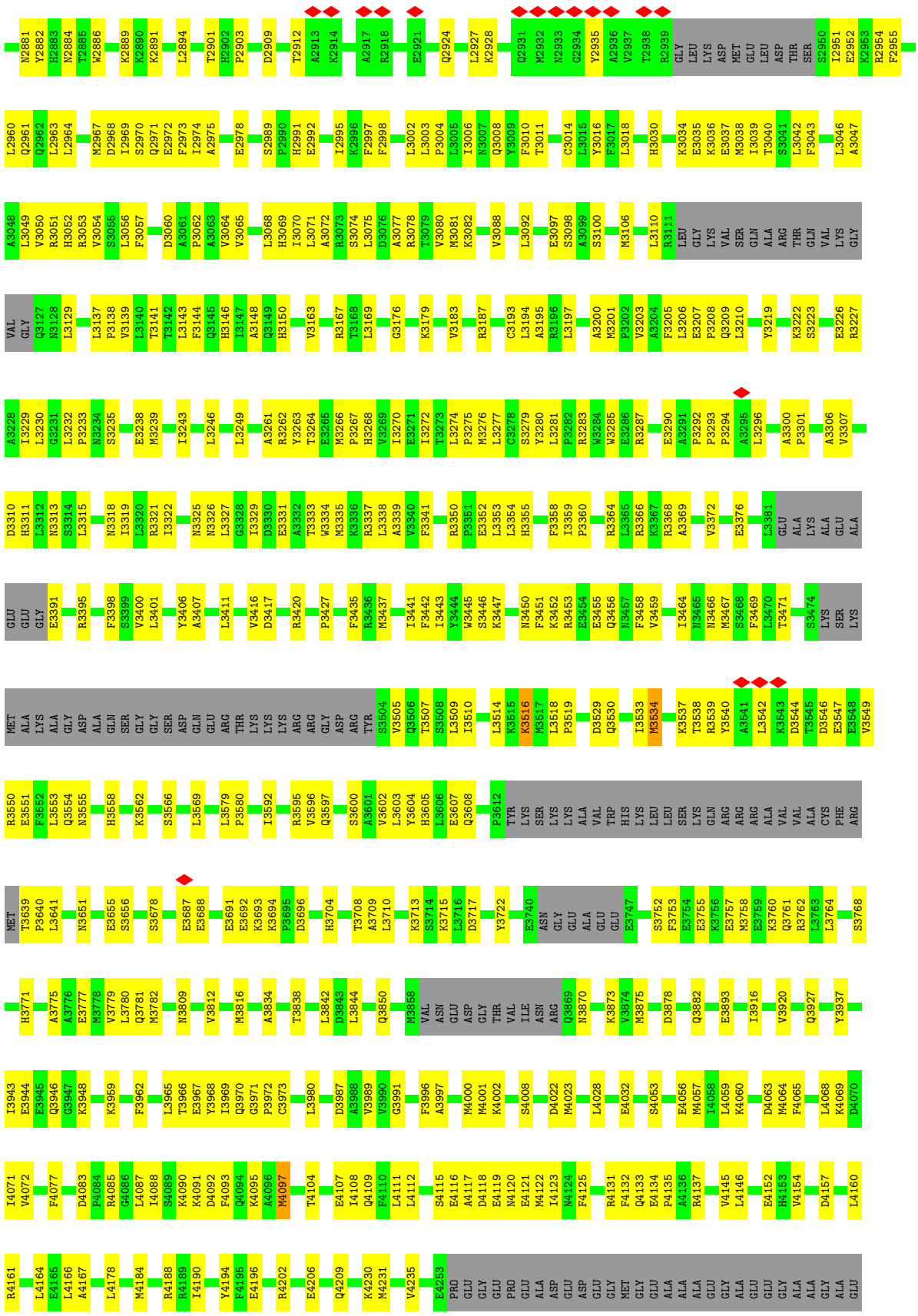
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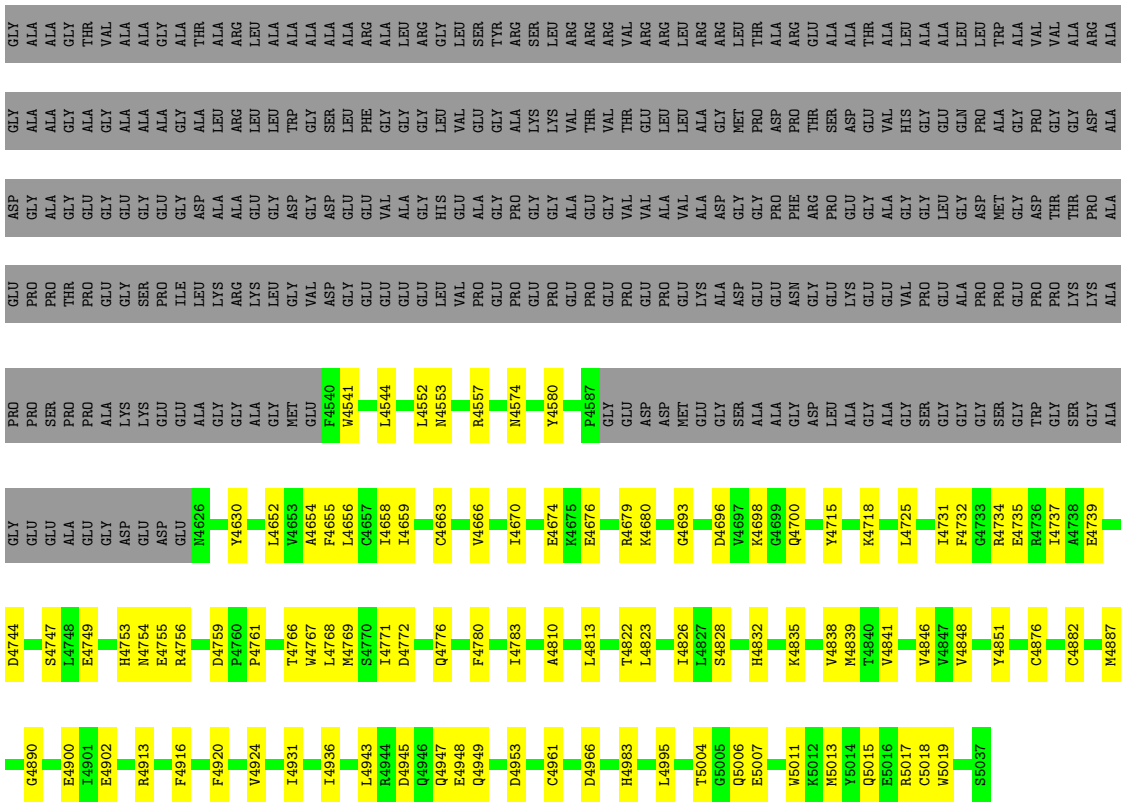

- Molecule 1: Ryanodine receptor 1

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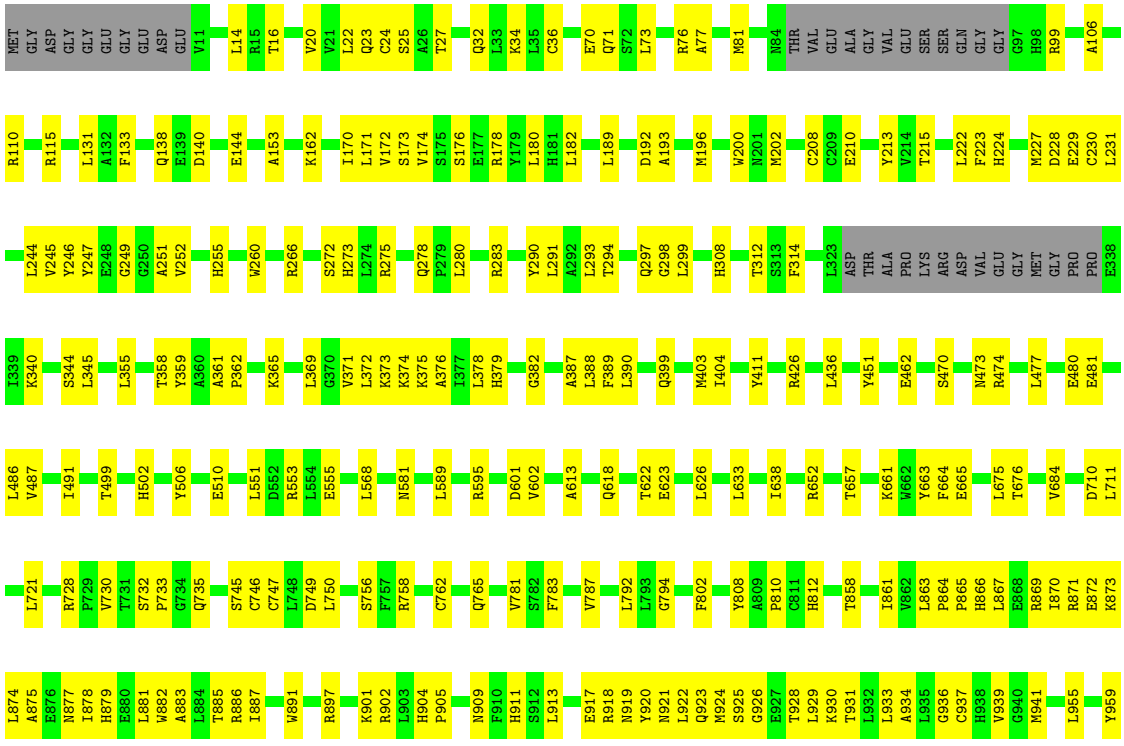

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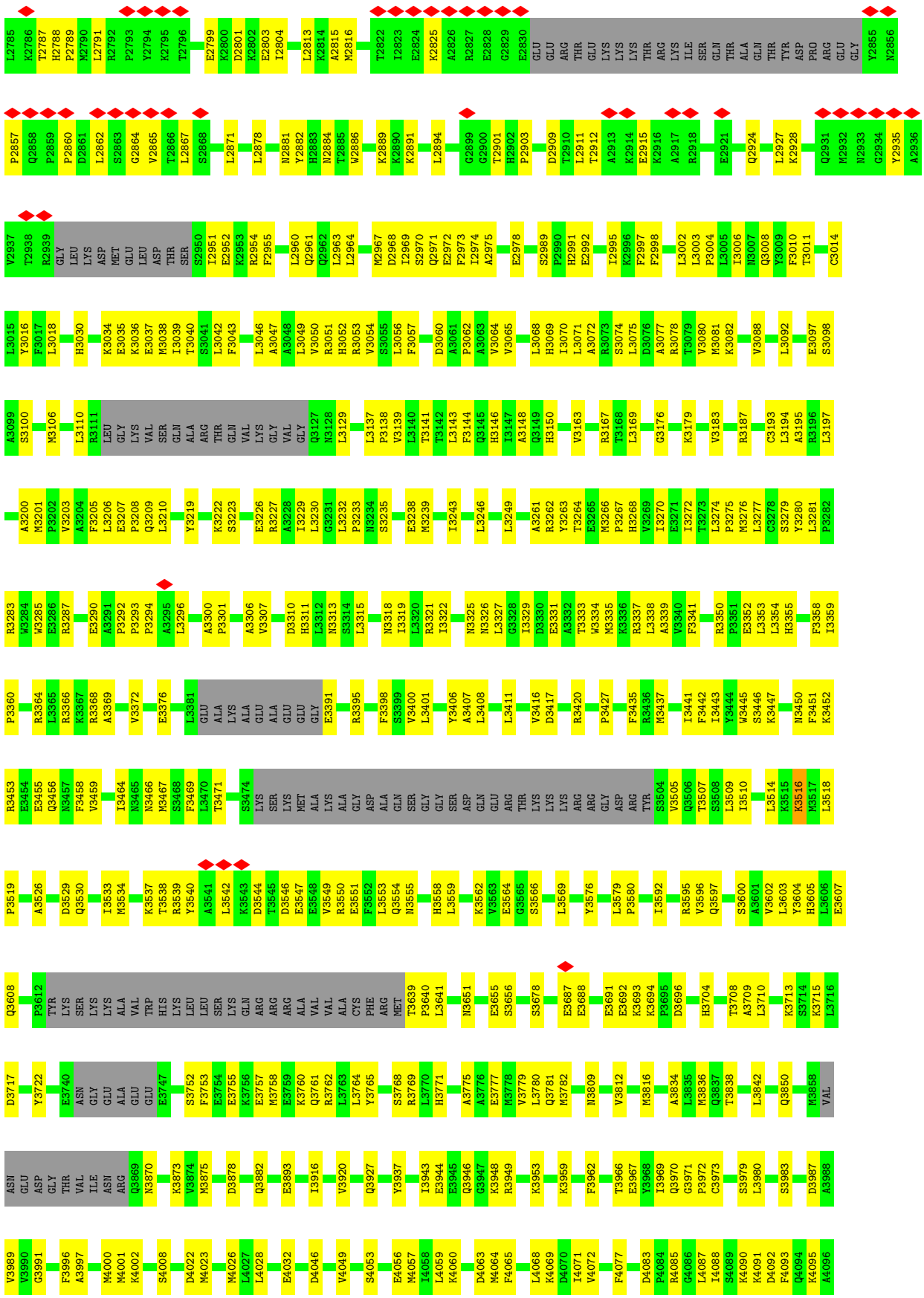
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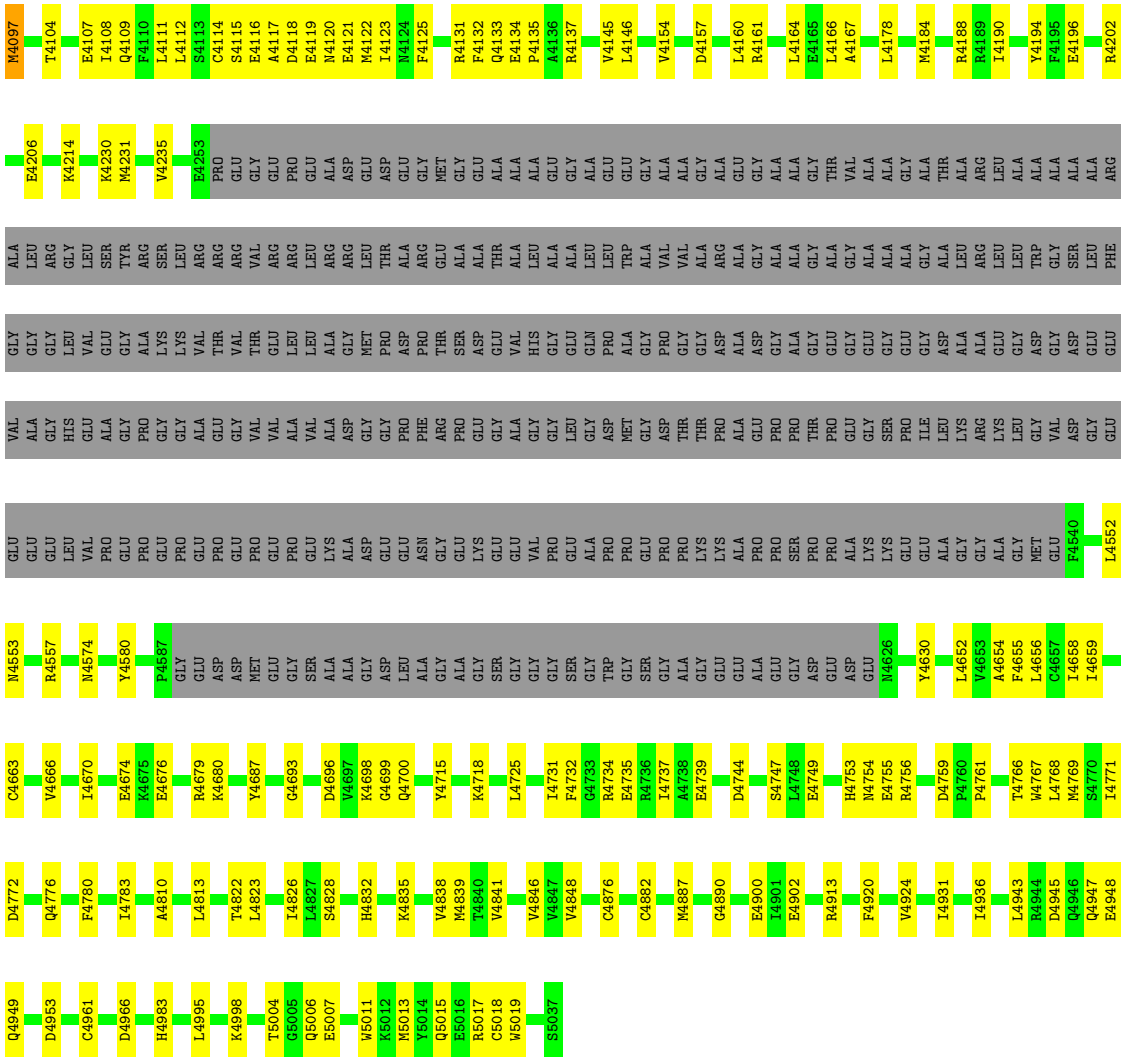
V2937 T2938 R2939 GLY LEU LYS ASP MET GLU LEU ASP THR SER S2950 I2951 E2952 K2953 R2954 F2955 L2960 Q2961 Q2962 L2963 L2964 M2967 D2968 I2969 S2970 Q2971 E2972 F2973 I2974 A2975 E2978 S2989 P2990 H2991 E2992 I2995 K2996 F2997 F2998 L3002 L3003 P3004 L3005 I3006 N3007 Q3008 Y3009 F3010 T3011 C3014
L3015 Y3016 F3017 L3018 H3030 K3034 E3035 K3036 E3037 M3038 I3039 T3040 S3041 L3042 F3043 L3046 A3047 A3048 L3049 V3050 R3051 H3052 R3053 V3054 S3055 L3056 F3057 D3060 A3061 P3062 A3063 V3064 V3065 L3068 H3069 I3070 L3071 A3072 R3073 S3074 L3075 D3076 A3077 R3078 T3079 V3080 M3081 K3082 V3088 L3092 E3097 S3098
A3099 S3100 M3106 L3110 R3111 LEU GLY LYS VAL SER GLN ALA ARG THR GLN VAL LYS GLY VAL GLY Q3127 N3128 L3129 L3137 P3138 V3139 L3140 T3141 T3142 L3143 F3144 Q3145 H3146 I3147 A3148 Q3149 H3150 V3163 R3167 T3168 L3169 G3176 K3179 V3183 R3187 C3193 L3194 A3195 R3196 L3197
A3200 M3201 P3202 V3203 A3204 F3205 L3206 E3207 P3208 Q3209 L3210 Y3219 K3222 S3223 E3226 R3227 A3228 I3229 L3230 G3231 L3232 P3233 N3234 S3235 E3238 M3239 I3243 L3246 L3249 A3261 R3262 Y3263 T3264 E3265 M3266 P3267 H3268 V3269 I3270 E3271 I3272 T3273 L3274 P3275 M3276 L3277 C3278 S3279 Y3280 L3281 P3282
R3283 W3284 W3285 E3286 R3287 E3290 A3291 P3292 P3293 P3294 A3295 L3296 A3300 P3301 A3306 V3307 D3310 H3311 L3312 N3313 S3314 L3315 N3318 I3319 L3320 R3321 I3322 N3325 N3326 L3327 G3328 I3329 D3330 E3331 A3332 T3333 W3334 M3335 K3336 R3337 L3338 A3339 V3340 F3341 R3350 P3351 E3352 L3353 L3354 H3355 F3358 I3359
P3360 R3364 L3365 R3366 K3367 R3368 A3369 V3372 E3376 L3381 GLU ALA LYS ALA GLU ALA GLU GLU GLY E3391 R3395 F3398 S3399 V3400 L3401 Y3406 A3407 L3408 L3411 V3416 D3417 R3420 P3427 F3435 R3436 M3437 I3441 F3442 I3443 Y3444 W3445 S3446 K3447 N3450 F3451 K3452
R3453 E3454 E3455 Q3456 N3457 F3458 V3459 I3464 N3465 N3466 M3467 S3468 F3469 L3470 T3471 S3474 LYS SER LYS MET ALA LYS ALA GLY ASP ALA GLN SER GLY GLY GLY SER ASP GLN GLU ARG THR LYS LYS LYS ARG ARG GLY ASP ARG TYR S3504 V3505 Q3506 T3507 S3508 L3509 I3510 L3514 K3515 K3516 M3517 L3518
P3519 A3526 D3529 Q3530 I3533 M3534 K3537 T3538 R3539 Y3540 A3541 L3542 K3543 D3544 T3545 D3546 E3547 E3548 V3549 R3550 E3551 F3552 L3553 Q3554 N3555 H3558 L3559 K3562 V3563 E3564 G3565 S3566 L3569 Y3576 L3579 P3580 I3592 R3595 V3596 Q3597 S3600 A3601 V3602 L3603 Y3604 H3605 L3606 E3607
Q3608 P3612 TYR LYS SER LYS LYS LYS ALA VAL TRP HIS LYS LEU LEU SER LYS GLN ARG ARG ARG ALA VAL VAL ALA CYS PHE ARG MET T3639 P3640 L3641 N3651 E3655 S3656 S3678 E3687 E3688 E3691 E3692 K3693 K3694 P3695 D3696 H3704 T3708 A3709 L3710 K3713 S3714 K3715 L3716
D3717 Y3722 E3740 ASN GLY GLU ALA GLU GLU E3747 S3752 F3753 E3754 E3755 K3756 E3757 M3758 E3759 K3760 Q3761 R3762 L3763 L3764 Y3765 S3768 R3769 L3770 H3771 A3775 A3776 E3777 M3778 V3779 L3780 Q3781 M3782 N3809 V3812 M3816 A3834 L3835 M3836 Q3837 T3838 L3842 Q3850 M3858 VAL
ASN GLU ASP GLY THR VAL ILE ASN ARG Q3869 N3870 K3873 V3874 M3875 D3878 Q3882 E3883 I3916 V3920 Q3927 Y3937 I3943 E3944 E3945 Q3946 G3947 K3948 R3949 K3953 K3959 F3962 T3966 E3967 Y3968 I3969 Q3970 G3971 P3972 C3973 S3979 L3980 S3983 D3987 A3988
V3989 V3990 G3991 F3996 A3997 M4000 M4001 K4002 S4008 D4022 M4023 M4026 L4027 L4028 E4032 D4046 V4049 S4053 E4056 M4057 I4058 L4059 K4060 D4063 M4064 F4065 L4068 K4069 D4070 I4071 V4072 F4077 D4083 P4084 R4085 G4086 L4087 I4088 S4089 K4090 K4091 D4092 F4093 Q4094 K4095 A4096



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

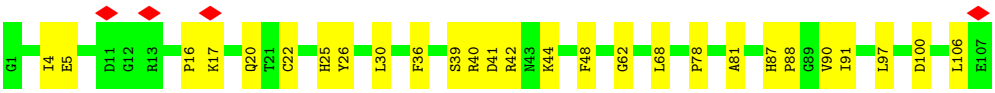
Chain A:

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

Chain D:

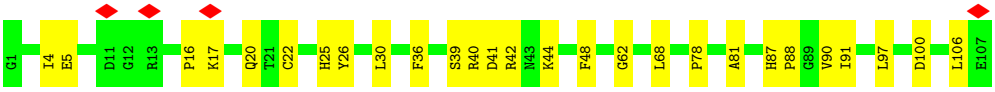
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H:



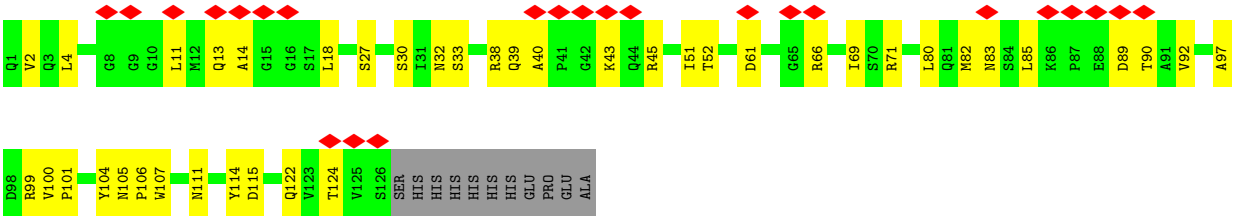
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain I:



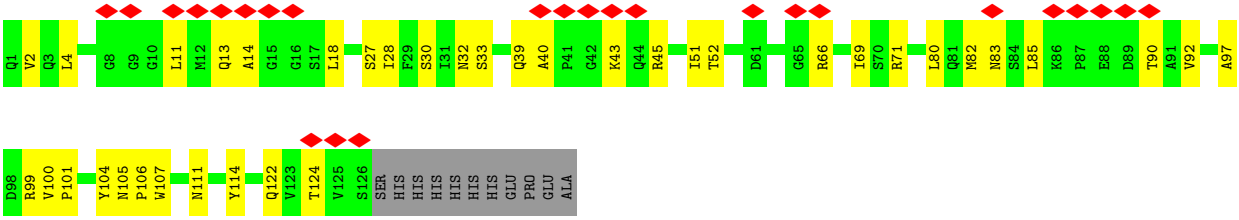
• Molecule 3: nanobody9657

Chain C:



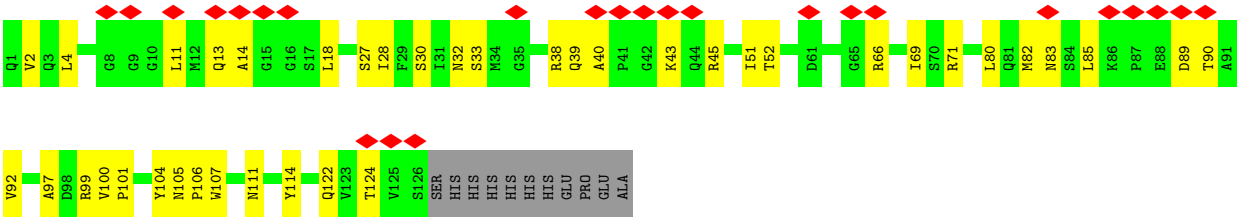
• Molecule 3: nanobody9657

Chain F:



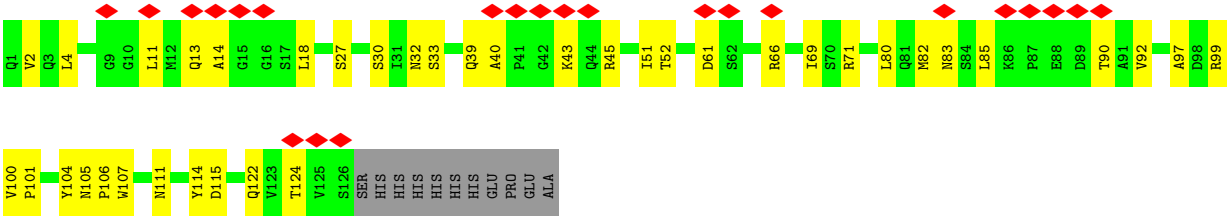
• Molecule 3: nanobody9657

Chain K:



• Molecule 3: nanobody9657

Chain M:


Q1
V2
Q3
L4
G9
G10
L11
M12
Q13
A14
G15
G16
S17
L18
S27
S30
I31
N32
S33
Q39
A40
P41
G42
K43
Q44
R45
I51
T52
D61
S62
R66
I69
S70
R71
L80
Q81
M82
N83
S84
L85
K86
P87
E88
D89
T90
A91
V92
A97
D98
R99

V100
P101
Y104
N105
P106
W107
N111
Y114
D115
Q122
V123
T124
V125
S126
SER
HIS
HIS
HIS
HIS
HIS
HIS
GLU
PRO
GLU
ALA

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	171023	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	6.350	Depositor
Minimum map value	-0.105	Depositor
Average map value	0.076	Depositor
Map value standard deviation	0.164	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	499.96802, 499.96802, 499.96802	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.488, 1.488, 1.488	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: 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	B	0.12	0/34727	0.32	2/47063 (0.0%)
1	E	0.13	0/34727	0.32	2/47063 (0.0%)
1	G	0.13	0/34727	0.32	2/47063 (0.0%)
1	J	0.13	0/34727	0.32	2/47063 (0.0%)
2	A	0.10	0/834	0.30	0/1123
2	D	0.10	0/834	0.30	0/1123
2	H	0.10	0/834	0.30	0/1123
2	I	0.10	0/834	0.30	0/1123
3	C	0.16	0/987	0.44	0/1340
3	F	0.15	0/987	0.44	0/1340
3	K	0.15	0/987	0.44	0/1340
3	M	0.15	0/987	0.44	0/1340
All	All	0.13	0/146192	0.32	8/198104 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1503	PRO	N-CA-CB	6.96	110.19	103.51
1	E	1503	PRO	N-CA-CB	6.96	110.19	103.51
1	G	1503	PRO	N-CA-CB	6.91	110.14	103.51
1	J	1503	PRO	N-CA-CB	6.91	110.14	103.51
1	E	4097	MET	CB-CG-SD	-5.25	96.94	112.70
1	B	4097	MET	CB-CG-SD	-5.25	96.96	112.70
1	G	4097	MET	CB-CG-SD	-5.24	96.99	112.70
1	J	4097	MET	CB-CG-SD	-5.24	96.99	112.70

There are no chirality outliers.

There are no planarity outliers.

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	B	33956	0	33378	793	0
1	E	33956	0	33378	807	0
1	G	33956	0	33378	788	0
1	J	33956	0	33378	814	0
2	A	818	0	824	17	0
2	D	818	0	824	17	0
2	H	818	0	824	19	0
2	I	818	0	824	19	0
3	C	967	0	916	39	0
3	F	967	0	916	37	0
3	K	967	0	916	38	0
3	M	967	0	916	40	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	J	1	0	0	0	0
All	All	142968	0	140472	3373	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 (3373) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:4961:CYS:SG	1:J:4983:HIS:CE1	2.58	0.97
1:B:4961:CYS:SG	1:B:4983:HIS:CE1	2.58	0.96
1:E:4961:CYS:SG	1:E:4983:HIS:CE1	2.58	0.96
1:G:4961:CYS:SG	1:G:4983:HIS:CE1	2.58	0.95
1:B:870:ILE:HA	1:B:873:LYS:HE2	1.57	0.86
1:B:1520:VAL:HG23	1:B:1527:MET:HG2	1.58	0.86
1:J:870:ILE:HA	1:J:873:LYS:HE2	1.57	0.85
1:E:1520:VAL:HG23	1:E:1527:MET:HG2	1.58	0.84
1:G:870:ILE:HA	1:G:873:LYS:HE2	1.57	0.84
1:E:870:ILE:HA	1:E:873:LYS:HE2	1.57	0.84
1:G:1520:VAL:HG23	1:G:1527:MET:HG2	1.58	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1520:VAL:HG23	1:J:1527:MET:HG2	1.58	0.83
1:E:210:GLU:HB3	1:E:213:TYR:HB2	1.61	0.82
1:B:210:GLU:HB3	1:B:213:TYR:HB2	1.61	0.82
1:B:897:ARG:HB2	1:B:905:PRO:HB3	1.62	0.81
1:J:210:GLU:HB3	1:J:213:TYR:HB2	1.61	0.81
1:J:897:ARG:HB2	1:J:905:PRO:HB3	1.62	0.81
1:B:3534:MET:HA	1:B:3537:LYS:HE2	1.63	0.81
1:E:897:ARG:HB2	1:E:905:PRO:HB3	1.62	0.81
1:E:917:GLU:HB2	3:F:104:TYR:HE2	1.46	0.81
1:G:3534:MET:HA	1:G:3537:LYS:HE2	1.63	0.81
1:J:917:GLU:HB2	3:K:104:TYR:HE2	1.45	0.81
1:G:210:GLU:HB3	1:G:213:TYR:HB2	1.61	0.81
1:E:3534:MET:HA	1:E:3537:LYS:HE2	1.63	0.81
1:J:3534:MET:HA	1:J:3537:LYS:HE2	1.63	0.80
1:G:897:ARG:HB2	1:G:905:PRO:HB3	1.62	0.80
1:B:3227:ARG:HB3	1:B:3232:LEU:HB2	1.64	0.79
1:B:917:GLU:HB2	3:C:104:TYR:HE2	1.48	0.79
1:E:3227:ARG:HB3	1:E:3232:LEU:HB2	1.64	0.79
1:G:3227:ARG:HB3	1:G:3232:LEU:HB2	1.64	0.78
1:J:3227:ARG:HB3	1:J:3232:LEU:HB2	1.64	0.78
1:G:981:GLN:HA	1:G:984:LEU:HD12	1.66	0.77
1:E:1422:ASP:HB2	1:E:1427:ILE:HD11	1.67	0.77
1:J:919:ASN:O	1:J:923:GLN:NE2	2.12	0.77
1:J:1422:ASP:HB2	1:J:1427:ILE:HD11	1.67	0.77
1:J:2951:ILE:HD12	1:J:2954:ARG:HD2	1.67	0.77
1:J:981:GLN:HA	1:J:984:LEU:HD12	1.66	0.77
1:B:981:GLN:HA	1:B:984:LEU:HD12	1.66	0.76
1:E:2951:ILE:HD12	1:E:2954:ARG:HD2	1.67	0.76
1:G:917:GLU:HB2	3:M:104:TYR:HE2	1.49	0.76
1:B:2951:ILE:HD12	1:B:2954:ARG:HD2	1.67	0.76
1:B:1422:ASP:HB2	1:B:1427:ILE:HD11	1.67	0.76
1:E:981:GLN:HA	1:E:984:LEU:HD12	1.66	0.75
1:B:919:ASN:O	1:B:923:GLN:NE2	2.12	0.75
1:G:919:ASN:O	1:G:923:GLN:NE2	2.12	0.75
1:G:1422:ASP:HB2	1:G:1427:ILE:HD11	1.67	0.75
1:B:3416:VAL:HB	1:B:3516:LYS:NZ	2.02	0.74
1:E:3416:VAL:HB	1:E:3516:LYS:HZ1	1.52	0.74
1:J:3416:VAL:HB	1:J:3516:LYS:NZ	2.02	0.74
1:E:3416:VAL:HB	1:E:3516:LYS:NZ	2.02	0.74
1:J:4060:LYS:O	1:J:4064:MET:HG2	1.87	0.74
1:B:4060:LYS:O	1:B:4064:MET:HG2	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3416:VAL:HB	1:G:3516:LYS:NZ	2.02	0.74
1:E:2998:PHE:HA	1:E:3002:LEU:HD23	1.70	0.74
1:G:4060:LYS:O	1:G:4064:MET:HG2	1.87	0.74
1:J:917:GLU:HB2	3:K:104:TYR:CE2	2.22	0.74
1:B:2998:PHE:HA	1:B:3002:LEU:HD23	1.70	0.74
1:E:3262:ARG:HG3	1:E:3326:ASN:HD21	1.52	0.74
1:G:924:MET:HE1	3:M:106:PRO:HB2	1.68	0.74
1:G:2998:PHE:HA	1:G:3002:LEU:HD23	1.70	0.74
1:E:4060:LYS:O	1:E:4064:MET:HG2	1.88	0.74
1:J:2998:PHE:HA	1:J:3002:LEU:HD23	1.70	0.74
1:B:917:GLU:HB2	3:C:104:TYR:CE2	2.23	0.74
1:E:917:GLU:HB2	3:F:104:TYR:CE2	2.22	0.73
1:G:2951:ILE:HD12	1:G:2954:ARG:HD2	1.67	0.73
3:F:111:ASN:HA	3:F:114:TYR:HB2	1.69	0.73
3:K:111:ASN:HA	3:K:114:TYR:HB2	1.69	0.73
1:G:3262:ARG:HG3	1:G:3326:ASN:HD21	1.52	0.73
1:J:3262:ARG:HG3	1:J:3326:ASN:HD21	1.52	0.73
1:J:3687:GLU:HB3	1:J:3693:LYS:HE2	1.71	0.73
1:E:919:ASN:O	1:E:923:GLN:NE2	2.12	0.73
1:E:3368:ARG:HH22	1:E:3400:VAL:HG22	1.54	0.73
1:G:3687:GLU:HB3	1:G:3693:LYS:HE2	1.71	0.73
1:G:2700:MET:HE3	1:G:2701:PRO:HD3	1.71	0.72
1:B:2700:MET:HE3	1:B:2701:PRO:HD3	1.71	0.72
1:J:2700:MET:HE3	1:J:2701:PRO:HD3	1.71	0.72
1:E:2700:MET:HE3	1:E:2701:PRO:HD3	1.71	0.72
1:G:4735:GLU:OE1	1:G:4735:GLU:N	2.22	0.72
3:F:105:ASN:HD21	3:F:107:TRP:HD1	1.37	0.72
1:B:3687:GLU:HB3	1:B:3693:LYS:HE2	1.71	0.72
1:J:920:TYR:HA	1:J:923:GLN:HG2	1.72	0.72
1:E:2704:CYS:HB3	1:E:3008:GLN:HG2	1.72	0.72
1:J:3368:ARG:HH22	1:J:3400:VAL:HG22	1.54	0.72
1:B:3368:ARG:HH22	1:B:3400:VAL:HG22	1.54	0.72
1:B:2704:CYS:HB3	1:B:3008:GLN:HG2	1.72	0.72
1:B:3262:ARG:HG3	1:B:3326:ASN:HD21	1.52	0.72
3:K:105:ASN:HD21	3:K:107:TRP:HD1	1.37	0.72
1:E:920:TYR:HA	1:E:923:GLN:HG2	1.72	0.71
1:G:920:TYR:HA	1:G:923:GLN:HG2	1.72	0.71
1:G:917:GLU:HB2	3:M:104:TYR:CE2	2.24	0.71
1:G:3368:ARG:HH22	1:G:3400:VAL:HG22	1.54	0.71
1:J:3235:SER:HB3	1:J:3238:GLU:HG3	1.72	0.71
1:B:4735:GLU:OE1	1:B:4735:GLU:N	2.22	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1256:GLU:HB2	1:J:1275:ARG:HE	1.56	0.71
1:E:3687:GLU:HB3	1:E:3693:LYS:HE2	1.71	0.71
3:M:111:ASN:HA	3:M:114:TYR:HB2	1.73	0.71
1:E:2974:ILE:HD11	1:E:3049:LEU:HD22	1.72	0.71
3:C:105:ASN:HD21	3:C:107:TRP:HD1	1.39	0.71
1:B:920:TYR:HA	1:B:923:GLN:HG2	1.72	0.71
1:B:2974:ILE:HD11	1:B:3049:LEU:HD22	1.72	0.71
3:C:111:ASN:HA	3:C:114:TYR:HB2	1.71	0.70
1:B:3235:SER:HB3	1:B:3238:GLU:HG3	1.72	0.70
1:G:4574:ASN:HD21	1:G:4810:ALA:HA	1.56	0.70
1:J:4735:GLU:OE1	1:J:4735:GLU:N	2.22	0.70
1:G:3319:ILE:HG12	1:G:3338:LEU:HD21	1.72	0.70
1:J:4574:ASN:HD21	1:J:4810:ALA:HA	1.56	0.70
1:B:875:ALA:O	1:B:879:HIS:ND1	2.25	0.70
1:E:3603:LEU:O	1:E:3607:GLU:HG3	1.91	0.70
1:G:2704:CYS:HB3	1:G:3008:GLN:HG2	1.72	0.70
1:E:3319:ILE:HG12	1:E:3338:LEU:HD21	1.72	0.70
1:G:875:ALA:O	1:G:879:HIS:ND1	2.25	0.70
1:J:2974:ILE:HD11	1:J:3049:LEU:HD22	1.72	0.70
1:J:2704:CYS:HB3	1:J:3008:GLN:HG2	1.72	0.70
1:E:3235:SER:HB3	1:E:3238:GLU:HG3	1.72	0.70
1:B:247:TYR:CD2	1:B:372:LEU:HB3	2.26	0.70
1:E:1256:GLU:HB2	1:E:1275:ARG:HE	1.56	0.70
1:G:3235:SER:HB3	1:G:3238:GLU:HG3	1.72	0.70
1:B:3603:LEU:O	1:B:3607:GLU:HG3	1.91	0.70
1:G:2974:ILE:HD11	1:G:3049:LEU:HD22	1.72	0.70
1:G:1256:GLU:HB2	1:G:1275:ARG:HE	1.56	0.69
1:G:3603:LEU:O	1:G:3607:GLU:HG3	1.91	0.69
1:J:3319:ILE:HG12	1:J:3338:LEU:HD21	1.72	0.69
1:E:3533:ILE:O	1:E:3537:LYS:HG3	1.92	0.69
1:E:4574:ASN:HD21	1:E:4810:ALA:HA	1.56	0.69
1:B:3319:ILE:HG12	1:B:3338:LEU:HD21	1.72	0.69
1:E:3537:LYS:HB3	1:E:3604:TYR:CD1	2.27	0.69
1:E:4735:GLU:OE1	1:E:4735:GLU:N	2.22	0.69
1:G:3533:ILE:O	1:G:3537:LYS:HG3	1.92	0.69
1:J:2638:LYS:HB2	1:J:2639:MET:HE2	1.74	0.69
1:B:3537:LYS:HB3	1:B:3604:TYR:CD1	2.27	0.69
1:J:3603:LEU:O	1:J:3607:GLU:HG3	1.91	0.69
1:B:3533:ILE:O	1:B:3537:LYS:HG3	1.92	0.69
1:E:2638:LYS:HB2	1:E:2639:MET:HE2	1.74	0.69
1:E:3233:PRO:HD2	1:E:3239:MET:HG2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1740:PRO:HA	1:J:1743:ARG:HG2	1.74	0.69
1:B:4574:ASN:HD21	1:B:4810:ALA:HA	1.56	0.69
1:E:4725:LEU:HD11	1:E:4734:ARG:HG3	1.75	0.69
1:G:4679:ARG:NH1	1:G:4715:TYR:OH	2.26	0.69
1:B:4725:LEU:HD11	1:B:4734:ARG:HG3	1.75	0.69
1:E:875:ALA:O	1:E:879:HIS:ND1	2.25	0.69
1:E:3453:ARG:NH1	1:E:3456:GLN:OE1	2.26	0.69
1:G:675:LEU:HG	1:G:676:THR:HG23	1.75	0.69
1:J:3233:PRO:HD2	1:J:3239:MET:HG2	1.74	0.69
1:J:3453:ARG:NH1	1:J:3456:GLN:OE1	2.26	0.69
1:B:675:LEU:HG	1:B:676:THR:HG23	1.75	0.69
1:G:3416:VAL:HB	1:G:3516:LYS:HZ1	1.58	0.69
1:G:3537:LYS:HB3	1:G:3604:TYR:CD1	2.27	0.69
1:J:3018:LEU:HB3	1:J:3074:SER:HA	1.74	0.69
1:J:3533:ILE:O	1:J:3537:LYS:HG3	1.92	0.69
1:B:1740:PRO:HA	1:B:1743:ARG:HG2	1.74	0.68
1:E:223:PHE:O	1:E:389:PHE:N	2.21	0.68
1:E:1740:PRO:HA	1:E:1743:ARG:HG2	1.74	0.68
1:B:1256:GLU:HB2	1:B:1275:ARG:HE	1.56	0.68
1:E:675:LEU:HG	1:E:676:THR:HG23	1.75	0.68
1:E:3018:LEU:HB3	1:E:3074:SER:HA	1.74	0.68
1:E:4679:ARG:NH1	1:E:4715:TYR:OH	2.26	0.68
1:J:875:ALA:O	1:J:879:HIS:ND1	2.25	0.68
1:J:2963:LEU:O	1:J:2967:MET:HG2	1.94	0.68
1:J:4090:LYS:HZ1	1:J:4115:SER:HB2	1.58	0.68
1:J:4679:ARG:NH1	1:J:4715:TYR:OH	2.26	0.68
1:B:4116:GLU:O	1:B:4118:ASP:N	2.27	0.68
1:B:3233:PRO:HD2	1:B:3239:MET:HG2	1.74	0.68
1:B:2638:LYS:HB2	1:B:2639:MET:HE2	1.74	0.68
1:J:4116:GLU:O	1:J:4118:ASP:N	2.27	0.68
1:B:4679:ARG:NH1	1:B:4715:TYR:OH	2.26	0.68
1:G:4116:GLU:O	1:G:4118:ASP:N	2.27	0.68
1:E:3036:LYS:HD3	1:E:3039:ILE:HD12	1.76	0.68
1:E:4580:TYR:HE2	1:E:4630:TYR:HB3	1.59	0.68
1:G:2638:LYS:HB2	1:G:2639:MET:HE2	1.74	0.68
1:B:2963:LEU:O	1:B:2967:MET:HG2	1.93	0.68
1:B:3018:LEU:HB3	1:B:3074:SER:HA	1.74	0.68
1:G:4725:LEU:HD11	1:G:4734:ARG:HG3	1.75	0.68
1:G:1740:PRO:HA	1:G:1743:ARG:HG2	1.74	0.68
1:G:3233:PRO:HD2	1:G:3239:MET:HG2	1.74	0.68
1:J:675:LEU:HG	1:J:676:THR:HG23	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:3537:LYS:HB3	1:J:3604:TYR:CD1	2.27	0.68
1:G:2963:LEU:O	1:G:2967:MET:HG2	1.94	0.67
1:J:4725:LEU:HD11	1:J:4734:ARG:HG3	1.75	0.67
1:G:3937:TYR:O	1:G:4002:LYS:NZ	2.27	0.67
1:J:3036:LYS:HD3	1:J:3039:ILE:HD12	1.76	0.67
1:J:4580:TYR:HE2	1:J:4630:TYR:HB3	1.59	0.67
1:B:223:PHE:O	1:B:389:PHE:N	2.21	0.67
1:B:3036:LYS:HD3	1:B:3039:ILE:HD12	1.76	0.67
1:E:2963:LEU:O	1:E:2967:MET:HG2	1.93	0.67
1:E:3376:GLU:OE2	1:E:3450:ASN:ND2	2.28	0.67
1:E:4116:GLU:O	1:E:4118:ASP:N	2.27	0.67
1:G:3018:LEU:HB3	1:G:3074:SER:HA	1.74	0.67
1:G:3036:LYS:HD3	1:G:3039:ILE:HD12	1.76	0.67
1:J:3376:GLU:OE2	1:J:3450:ASN:ND2	2.28	0.67
1:B:375:LYS:HG2	1:B:377:ILE:HD11	1.75	0.67
1:E:3937:TYR:O	1:E:4002:LYS:NZ	2.27	0.67
1:G:4580:TYR:HE2	1:G:4630:TYR:HB3	1.59	0.67
1:E:2712:PRO:HA	1:E:2955:PHE:HB3	1.76	0.67
1:J:2712:PRO:HA	1:J:2955:PHE:HB3	1.76	0.67
1:E:293:LEU:HD12	1:E:378:LEU:HD13	1.75	0.67
1:G:3376:GLU:OE2	1:G:3450:ASN:ND2	2.28	0.67
1:G:4090:LYS:HZ1	1:G:4115:SER:HB2	1.60	0.67
3:F:105:ASN:HD21	3:F:107:TRP:CD1	2.13	0.67
1:G:2577:ILE:HG23	1:G:2578:MET:SD	2.35	0.67
3:K:104:TYR:HE1	3:K:106:PRO:HG3	1.60	0.67
1:B:2577:ILE:HG23	1:B:2578:MET:SD	2.35	0.67
1:B:3376:GLU:OE2	1:B:3450:ASN:ND2	2.28	0.67
1:G:874:LEU:HA	1:G:877:ASN:HD21	1.60	0.67
1:G:2952:GLU:OE1	1:G:2961:GLN:NE2	2.28	0.67
1:B:3937:TYR:O	1:B:4002:LYS:NZ	2.27	0.67
1:B:4580:TYR:HE2	1:B:4630:TYR:HB3	1.59	0.67
1:J:2952:GLU:OE1	1:J:2961:GLN:NE2	2.28	0.67
3:K:105:ASN:HD21	3:K:107:TRP:CD1	2.13	0.67
1:B:2952:GLU:OE1	1:B:2961:GLN:NE2	2.28	0.66
1:G:2712:PRO:HA	1:G:2955:PHE:HB3	1.76	0.66
1:G:247:TYR:CD2	1:G:372:LEU:HB3	2.30	0.66
1:B:924:MET:HE1	3:C:106:PRO:HB2	1.76	0.66
1:J:3937:TYR:O	1:J:4002:LYS:NZ	2.27	0.66
1:E:345:LEU:HB3	1:E:387:ALA:HB1	1.78	0.66
1:G:2536:LEU:HD13	1:G:2541:PHE:HB3	1.78	0.66
1:B:2536:LEU:HD13	1:B:2541:PHE:HB3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2712:PRO:HA	1:B:2955:PHE:HB3	1.76	0.66
1:J:2116:LEU:O	1:J:2120:MET:HG2	1.96	0.66
1:E:2577:ILE:HG23	1:E:2578:MET:SD	2.35	0.66
1:E:2952:GLU:OE1	1:E:2961:GLN:NE2	2.28	0.66
1:J:874:LEU:HA	1:J:877:ASN:HD21	1.60	0.66
1:B:1300:HIS:O	1:B:1302:ARG:NH1	2.29	0.66
1:J:246:TYR:HE1	1:J:375:LYS:HZ3	1.43	0.66
1:E:1300:HIS:O	1:E:1302:ARG:NH1	2.29	0.66
1:G:665:GLU:HB3	1:G:792:LEU:HB2	1.78	0.66
1:G:2469:ILE:HA	1:G:2472:LEU:HD23	1.78	0.66
1:G:3453:ARG:NH1	1:G:3456:GLN:OE1	2.26	0.66
1:B:2469:ILE:HA	1:B:2472:LEU:HD23	1.78	0.66
1:E:874:LEU:HA	1:E:877:ASN:HD21	1.60	0.65
1:E:2116:LEU:O	1:E:2120:MET:HG2	1.96	0.65
1:B:345:LEU:HB3	1:B:387:ALA:HB1	1.78	0.65
1:G:227:MET:HE1	1:G:249:GLY:HA2	1.78	0.65
1:G:1300:HIS:O	1:G:1302:ARG:NH1	2.29	0.65
1:J:247:TYR:CD2	1:J:372:LEU:HB3	2.30	0.65
1:E:4090:LYS:HZ1	1:E:4115:SER:HB2	1.59	0.65
1:J:293:LEU:HD12	1:J:378:LEU:HD13	1.78	0.65
1:J:2577:ILE:HG23	1:J:2578:MET:SD	2.35	0.65
1:B:874:LEU:HA	1:B:877:ASN:HD21	1.60	0.65
1:B:2116:LEU:O	1:B:2120:MET:HG2	1.96	0.65
1:E:3996:PHE:O	1:E:4000:MET:HG3	1.96	0.65
1:G:3996:PHE:O	1:G:4000:MET:HG3	1.96	0.65
1:B:227:MET:HE1	1:B:249:GLY:HA2	1.77	0.65
1:B:1089:TYR:HD1	1:B:1152:MET:HG2	1.61	0.65
1:G:293:LEU:HD12	1:G:378:LEU:HD13	1.78	0.65
1:J:665:GLU:HB3	1:J:792:LEU:HB2	1.78	0.65
1:E:227:MET:HE1	1:E:249:GLY:HA2	1.77	0.65
1:E:3176:GLY:HA2	1:E:3272:ILE:HD12	1.79	0.65
1:G:293:LEU:HD11	1:G:355:LEU:HD12	1.79	0.65
1:J:2536:LEU:HD13	1:J:2541:PHE:HB3	1.78	0.65
1:E:2536:LEU:HD13	1:E:2541:PHE:HB3	1.78	0.65
1:G:3081:MET:HE2	1:G:3092:LEU:HD23	1.79	0.65
1:J:293:LEU:HD11	1:J:355:LEU:HD12	1.79	0.65
1:J:960:MET:HE3	1:J:962:SER:HB2	1.79	0.65
1:J:1300:HIS:O	1:J:1302:ARG:NH1	2.29	0.65
1:B:374:LYS:O	1:B:375:LYS:C	2.40	0.65
1:B:4902:GLU:O	1:B:4913:ARG:NH2	2.30	0.65
1:E:2469:ILE:HA	1:E:2472:LEU:HD23	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:223:PHE:O	1:G:389:PHE:N	2.21	0.65
1:G:2116:LEU:O	1:G:2120:MET:HG2	1.96	0.65
1:G:4131:ARG:O	1:G:4133:GLN:HG2	1.97	0.65
1:G:4902:GLU:O	1:G:4913:ARG:NH2	2.30	0.65
1:J:345:LEU:HB3	1:J:387:ALA:HB1	1.78	0.65
1:J:3081:MET:HE2	1:J:3092:LEU:HD23	1.79	0.65
1:J:3270:ILE:HA	1:J:3274:LEU:HD23	1.79	0.65
1:B:3081:MET:HE2	1:B:3092:LEU:HD23	1.79	0.64
1:E:1089:TYR:HD1	1:E:1152:MET:HG2	1.61	0.64
1:G:345:LEU:HB3	1:G:387:ALA:HB1	1.78	0.64
1:J:227:MET:HE1	1:J:249:GLY:HA2	1.77	0.64
3:F:104:TYR:HE1	3:F:106:PRO:HG3	1.59	0.64
1:B:3996:PHE:O	1:B:4000:MET:HG3	1.96	0.64
1:G:3270:ILE:HA	1:G:3274:LEU:HD23	1.79	0.64
1:G:3989:VAL:HG13	1:G:4023:MET:HE2	1.79	0.64
1:J:3996:PHE:O	1:J:4000:MET:HG3	1.96	0.64
1:G:3445:TRP:HA	1:G:3451:PHE:HD1	1.63	0.64
1:B:665:GLU:HB3	1:B:792:LEU:HB2	1.78	0.64
1:B:2377:LEU:HA	1:B:2469:ILE:HD11	1.79	0.64
1:B:3453:ARG:NH1	1:B:3456:GLN:OE1	2.26	0.64
1:E:652:ARG:HD3	1:E:750:LEU:HB3	1.80	0.64
1:J:2469:ILE:HA	1:J:2472:LEU:HD23	1.78	0.64
1:J:3176:GLY:HA2	1:J:3272:ILE:HD12	1.79	0.64
1:J:3553:LEU:HD11	1:J:3597:GLN:HG3	1.79	0.64
1:B:983:THR:O	1:B:987:ARG:HG3	1.98	0.64
1:B:3270:ILE:HA	1:B:3274:LEU:HD23	1.79	0.64
1:B:3445:TRP:HA	1:B:3451:PHE:HD1	1.63	0.64
1:E:3270:ILE:HA	1:E:3274:LEU:HD23	1.79	0.64
1:E:3445:TRP:HA	1:E:3451:PHE:HD1	1.63	0.64
1:J:3445:TRP:HA	1:J:3451:PHE:HD1	1.63	0.64
1:G:960:MET:HE3	1:G:962:SER:HB2	1.79	0.64
1:G:983:THR:O	1:G:987:ARG:HG3	1.98	0.64
1:G:2377:LEU:HA	1:G:2469:ILE:HD11	1.79	0.64
1:J:4131:ARG:O	1:J:4133:GLN:HG2	1.97	0.64
1:B:4131:ARG:O	1:B:4133:GLN:HG2	1.97	0.64
1:E:3989:VAL:HG13	1:E:4023:MET:HE2	1.80	0.64
3:M:105:ASN:HD21	3:M:107:TRP:HD1	1.46	0.64
1:B:3553:LEU:HD11	1:B:3597:GLN:HG3	1.79	0.64
1:E:247:TYR:H	1:E:374:LYS:H	1.46	0.64
1:J:983:THR:O	1:J:987:ARG:HG3	1.98	0.64
1:B:293:LEU:HD12	1:B:378:LEU:HD13	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3176:GLY:HA2	1:B:3272:ILE:HD12	1.79	0.64
1:B:3987:ASP:OD2	1:E:162:LYS:NZ	2.29	0.64
1:E:665:GLU:HB3	1:E:792:LEU:HB2	1.78	0.64
1:G:1089:TYR:HD1	1:G:1152:MET:HG2	1.61	0.64
1:J:1089:TYR:HD1	1:J:1152:MET:HG2	1.61	0.64
1:E:293:LEU:HD11	1:E:355:LEU:HD12	1.79	0.64
1:E:960:MET:HE3	1:E:962:SER:HB2	1.79	0.64
1:E:2377:LEU:HA	1:E:2469:ILE:HD11	1.79	0.64
1:E:4131:ARG:O	1:E:4133:GLN:HG2	1.97	0.64
1:B:652:ARG:HD3	1:B:750:LEU:HB3	1.80	0.63
1:E:3081:MET:HE2	1:E:3092:LEU:HD23	1.79	0.63
1:J:2862:LEU:HG	1:J:2864:GLY:H	1.63	0.63
1:J:3194:LEU:HG	1:J:3279:SER:HB2	1.80	0.63
1:E:983:THR:O	1:E:987:ARG:HG3	1.98	0.63
1:G:246:TYR:HE1	1:G:375:LYS:HZ3	1.45	0.63
1:G:3176:GLY:HA2	1:G:3272:ILE:HD12	1.79	0.63
1:J:4902:GLU:O	1:J:4913:ARG:NH2	2.30	0.63
1:B:293:LEU:HD11	1:B:355:LEU:HD12	1.79	0.63
1:E:4902:GLU:O	1:E:4913:ARG:NH2	2.30	0.63
3:F:33:SER:HA	3:F:52:THR:HA	1.80	0.63
3:K:33:SER:HA	3:K:52:THR:HA	1.79	0.63
1:B:960:MET:HE3	1:B:962:SER:HB2	1.79	0.63
1:E:3194:LEU:HG	1:E:3279:SER:HB2	1.80	0.63
1:E:3842:LEU:HD23	1:E:3875:MET:HG3	1.81	0.63
1:G:404:ILE:HD13	1:G:481:GLU:HG3	1.81	0.63
1:G:2862:LEU:HG	1:G:2864:GLY:H	1.63	0.63
1:B:224:HIS:HA	1:B:388:LEU:HA	1.81	0.63
1:J:404:ILE:HD13	1:J:481:GLU:HG3	1.81	0.63
1:J:652:ARG:HD3	1:J:750:LEU:HB3	1.80	0.63
1:B:404:ILE:HD13	1:B:481:GLU:HG3	1.81	0.63
1:B:2447:LYS:HG2	1:B:2450:ALA:H	1.63	0.63
1:B:2862:LEU:HG	1:B:2864:GLY:H	1.63	0.63
1:B:3842:LEU:HD23	1:B:3875:MET:HG3	1.81	0.63
1:B:3970:GLN:HE21	1:B:5004:THR:HA	1.63	0.63
1:G:3553:LEU:HD11	1:G:3597:GLN:HG3	1.79	0.63
1:J:2377:LEU:HA	1:J:2469:ILE:HD11	1.79	0.63
1:E:2447:LYS:HG2	1:E:2450:ALA:H	1.63	0.63
1:E:3141:THR:OG1	1:E:3193:CYS:SG	2.56	0.63
1:G:224:HIS:HA	1:G:388:LEU:HA	1.81	0.63
1:G:359:TYR:HA	1:G:376:ALA:HA	1.80	0.63
1:G:3141:THR:OG1	1:G:3193:CYS:SG	2.56	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:3989:VAL:HG13	1:J:4023:MET:HE2	1.80	0.63
1:E:404:ILE:HD13	1:E:481:GLU:HG3	1.81	0.63
1:E:3141:THR:HG1	1:E:3193:CYS:HG	1.43	0.63
1:G:633:LEU:HD13	1:G:1639:LEU:HD21	1.81	0.63
1:J:224:HIS:HA	1:J:388:LEU:HA	1.81	0.63
3:C:105:ASN:HD21	3:C:107:TRP:CD1	2.15	0.63
1:E:224:HIS:HA	1:E:388:LEU:HA	1.81	0.63
1:E:3987:ASP:OD2	1:J:162:LYS:NZ	2.30	0.63
1:J:3141:THR:OG1	1:J:3193:CYS:SG	2.56	0.63
1:J:3416:VAL:HB	1:J:3516:LYS:HZ3	1.62	0.63
1:B:2261:SER:HA	1:B:2265:LEU:HD23	1.81	0.62
1:B:3989:VAL:HG13	1:B:4023:MET:HE2	1.81	0.62
1:G:3194:LEU:HG	1:G:3279:SER:HB2	1.80	0.62
3:C:33:SER:HA	3:C:52:THR:HA	1.81	0.62
1:E:3553:LEU:HD11	1:E:3597:GLN:HG3	1.79	0.62
1:E:2261:SER:HA	1:E:2265:LEU:HD23	1.81	0.62
1:E:4090:LYS:H	1:E:4121:GLU:HB3	1.64	0.62
1:G:2447:LYS:HG2	1:G:2450:ALA:H	1.63	0.62
1:J:2376:LEU:HB2	1:J:2465:ASP:HB3	1.82	0.62
3:M:66:ARG:NH1	3:M:83:ASN:O	2.32	0.62
1:B:633:LEU:HD13	1:B:1639:LEU:HD21	1.81	0.62
1:G:2376:LEU:HB2	1:G:2465:ASP:HB3	1.82	0.62
1:J:2447:LYS:HG2	1:J:2450:ALA:H	1.63	0.62
1:J:4090:LYS:H	1:J:4121:GLU:HB3	1.64	0.62
1:E:633:LEU:HD13	1:E:1639:LEU:HD21	1.81	0.62
1:G:652:ARG:HD3	1:G:750:LEU:HB3	1.80	0.62
1:J:633:LEU:HD13	1:J:1639:LEU:HD21	1.81	0.62
1:B:3077:ALA:HA	1:B:3080:VAL:HG22	1.82	0.62
1:E:2862:LEU:HG	1:E:2864:GLY:H	1.63	0.62
1:E:294:THR:HG23	1:E:297:GLN:H	1.65	0.62
1:E:3077:ALA:HA	1:E:3080:VAL:HG22	1.82	0.62
1:G:3466:ASN:ND2	1:G:3507:THR:HG23	2.15	0.62
1:G:3842:LEU:HD23	1:G:3875:MET:HG3	1.81	0.62
1:G:3970:GLN:HE21	1:G:5004:THR:HA	1.64	0.62
1:J:3842:LEU:HD23	1:J:3875:MET:HG3	1.80	0.62
1:J:4059:LEU:HD13	1:J:4167:ALA:HB2	1.82	0.62
1:B:4059:LEU:HD13	1:B:4167:ALA:HB2	1.82	0.61
1:B:4154:VAL:O	1:B:4161:ARG:NH2	2.33	0.61
1:E:4059:LEU:HD13	1:E:4167:ALA:HB2	1.82	0.61
1:G:2261:SER:HA	1:G:2265:LEU:HD23	1.82	0.61
1:J:359:TYR:HA	1:J:376:ALA:HA	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3194:LEU:HG	1:B:3279:SER:HB2	1.80	0.61
1:E:4154:VAL:O	1:E:4161:ARG:NH2	2.33	0.61
1:J:2781:VAL:HA	1:J:2789:PRO:HB2	1.82	0.61
3:F:66:ARG:NH1	3:F:83:ASN:O	2.32	0.61
1:B:1981:MET:HE2	1:B:1981:MET:HA	1.82	0.61
1:B:3141:THR:OG1	1:B:3193:CYS:SG	2.56	0.61
1:B:4654:ALA:O	1:B:4658:ILE:HG12	2.00	0.61
1:G:2781:VAL:HA	1:G:2789:PRO:HB2	1.83	0.61
1:G:3077:ALA:HA	1:G:3080:VAL:HG22	1.82	0.61
1:B:2376:LEU:HB2	1:B:2465:ASP:HB3	1.82	0.61
1:B:4090:LYS:H	1:B:4121:GLU:HB3	1.64	0.61
1:E:2781:VAL:HA	1:E:2789:PRO:HB2	1.82	0.61
1:G:891:TRP:HA	1:G:902:ARG:HB3	1.83	0.61
1:G:1981:MET:HE2	1:G:1981:MET:HA	1.82	0.61
1:J:2522:LEU:HA	1:J:2526:PHE:HD2	1.66	0.61
1:B:1583:GLU:OE1	1:B:1586:ASN:ND2	2.34	0.61
1:B:2781:VAL:HA	1:B:2789:PRO:HB2	1.82	0.61
1:B:3466:ASN:ND2	1:B:3507:THR:HG23	2.15	0.61
1:E:3466:ASN:ND2	1:E:3507:THR:HG23	2.15	0.61
1:E:4654:ALA:O	1:E:4658:ILE:HG12	2.00	0.61
1:G:4059:LEU:HD13	1:G:4167:ALA:HB2	1.82	0.61
1:J:891:TRP:HE1	1:J:904:HIS:HA	1.66	0.61
1:E:3097:GLU:OE1	1:E:3167:ARG:NH1	2.34	0.61
1:J:3466:ASN:ND2	1:J:3507:THR:HG23	2.15	0.61
3:C:66:ARG:NH1	3:C:83:ASN:O	2.32	0.61
1:B:891:TRP:HA	1:B:902:ARG:HB3	1.83	0.61
1:E:2376:LEU:HB2	1:E:2465:ASP:HB3	1.82	0.61
1:G:2522:LEU:HA	1:G:2526:PHE:HD2	1.66	0.61
2:H:42:ARG:HB3	2:H:44:LYS:HE2	1.83	0.61
1:B:182:LEU:HD11	1:B:189:LEU:HB3	1.83	0.61
1:B:294:THR:HG23	1:B:297:GLN:H	1.65	0.61
1:B:1024:TYR:HA	1:B:1027:LEU:HD12	1.83	0.61
1:B:3997:ALA:HA	1:B:4000:MET:HE2	1.82	0.61
1:G:4090:LYS:H	1:G:4121:GLU:HB3	1.64	0.61
1:J:182:LEU:HD11	1:J:189:LEU:HB3	1.83	0.61
1:B:359:TYR:HA	1:B:376:ALA:HA	1.83	0.61
1:B:3038:MET:C	1:B:3038:MET:HE2	2.26	0.61
1:B:3539:ARG:HA	1:B:3542:LEU:HB2	1.83	0.61
1:E:3997:ALA:HA	1:E:4000:MET:HE2	1.82	0.61
1:G:182:LEU:HD11	1:G:189:LEU:HB3	1.83	0.61
1:G:2615:ARG:HG3	1:G:2664:PHE:HB3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3537:LYS:HB3	1:G:3604:TYR:CE1	2.36	0.61
1:J:223:PHE:O	1:J:389:PHE:N	2.21	0.61
1:J:2261:SER:HA	1:J:2265:LEU:HD23	1.82	0.61
1:J:3077:ALA:HA	1:J:3080:VAL:HG22	1.82	0.61
1:B:2599:GLN:O	1:B:2603:ILE:HG12	2.01	0.60
1:E:2522:LEU:HA	1:E:2526:PHE:HD2	1.66	0.60
1:J:3539:ARG:HA	1:J:3542:LEU:HB2	1.83	0.60
2:I:42:ARG:HB3	2:I:44:LYS:HE2	1.83	0.60
1:B:2989:SER:HB2	1:B:2992:GLU:HB3	1.83	0.60
1:B:3416:VAL:HB	1:B:3516:LYS:HZ1	1.64	0.60
1:B:3441:ILE:HG22	1:B:3510:ILE:HD11	1.84	0.60
1:E:1981:MET:HE2	1:E:1981:MET:HA	1.82	0.60
1:G:266:ARG:HH12	1:G:273:HIS:CE1	2.19	0.60
1:G:3997:ALA:HA	1:G:4000:MET:HE2	1.82	0.60
1:J:266:ARG:HH12	1:J:273:HIS:CE1	2.19	0.60
1:J:4835:LYS:O	1:J:4839:MET:HG3	2.01	0.60
1:B:399:GLN:O	1:B:403:MET:HG3	2.02	0.60
1:B:2522:LEU:HA	1:B:2526:PHE:HD2	1.66	0.60
1:E:891:TRP:HE1	1:E:904:HIS:HA	1.66	0.60
1:E:1583:GLU:OE1	1:E:1586:ASN:ND2	2.34	0.60
1:E:2989:SER:HB2	1:E:2992:GLU:HB3	1.83	0.60
1:J:3537:LYS:HB3	1:J:3604:TYR:CE1	2.36	0.60
1:E:266:ARG:HH12	1:E:273:HIS:CE1	2.20	0.60
1:E:399:GLN:O	1:E:403:MET:HG3	2.02	0.60
1:G:3539:ARG:HA	1:G:3542:LEU:HB2	1.83	0.60
1:J:294:THR:HG23	1:J:297:GLN:H	1.66	0.60
1:J:3201:MET:SD	1:J:3203:VAL:HG12	2.42	0.60
1:J:3970:GLN:HE21	1:J:5004:THR:HA	1.65	0.60
2:A:42:ARG:HB3	2:A:44:LYS:HE2	1.83	0.60
1:E:3038:MET:HE2	1:E:3038:MET:C	2.26	0.60
1:E:3441:ILE:HG22	1:E:3510:ILE:HD11	1.83	0.60
1:G:399:GLN:O	1:G:403:MET:HG3	2.02	0.60
1:G:676:THR:HG21	1:G:1633:PRO:HB3	1.84	0.60
1:G:1024:TYR:HA	1:G:1027:LEU:HD12	1.83	0.60
1:J:2599:GLN:O	1:J:2603:ILE:HG12	2.01	0.60
1:J:2989:SER:HB2	1:J:2992:GLU:HB3	1.83	0.60
1:B:891:TRP:HE1	1:B:904:HIS:HA	1.66	0.60
1:E:1024:TYR:HA	1:E:1027:LEU:HD12	1.83	0.60
1:G:4835:LYS:O	1:G:4839:MET:HG3	2.01	0.60
1:J:891:TRP:HA	1:J:902:ARG:HB3	1.83	0.60
1:J:3097:GLU:OE1	1:J:3167:ARG:NH1	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:4767:TRP:HE1	1:J:4771:ILE:HD11	1.67	0.60
1:B:4835:LYS:O	1:B:4839:MET:HG3	2.01	0.60
1:E:4835:LYS:O	1:E:4839:MET:HG3	2.01	0.60
1:G:294:THR:HG23	1:G:297:GLN:H	1.66	0.60
1:G:2989:SER:HB2	1:G:2992:GLU:HB3	1.83	0.60
1:G:3201:MET:SD	1:G:3203:VAL:HG12	2.42	0.60
1:G:4654:ALA:O	1:G:4658:ILE:HG12	2.00	0.60
1:J:365:LYS:HE2	1:J:369:LEU:HD21	1.83	0.60
1:J:1583:GLU:OE1	1:J:1586:ASN:ND2	2.34	0.60
1:J:3441:ILE:HG22	1:J:3510:ILE:HD11	1.84	0.60
1:J:3997:ALA:HA	1:J:4000:MET:HE2	1.82	0.60
1:B:266:ARG:HH12	1:B:273:HIS:CE1	2.19	0.60
1:B:3263:TYR:HA	1:B:3270:ILE:HG13	1.84	0.60
1:B:3537:LYS:HB3	1:B:3604:TYR:CE1	2.36	0.60
1:E:355:LEU:HD13	1:E:378:LEU:O	2.02	0.60
1:E:3537:LYS:HB3	1:E:3604:TYR:CE1	2.36	0.60
1:E:3539:ARG:HA	1:E:3542:LEU:HB2	1.83	0.60
1:G:900:ASN:ND2	3:M:61:ASP:OD1	2.34	0.60
1:G:2273:LEU:HD23	1:G:2330:ARG:HB3	1.84	0.60
1:G:2599:GLN:O	1:G:2603:ILE:HG12	2.01	0.60
1:G:3038:MET:C	1:G:3038:MET:HE2	2.26	0.60
1:G:3263:TYR:HA	1:G:3270:ILE:HG13	1.84	0.60
1:G:4154:VAL:O	1:G:4161:ARG:NH2	2.33	0.60
1:G:4767:TRP:HE1	1:G:4771:ILE:HD11	1.67	0.60
2:D:42:ARG:HB3	2:D:44:LYS:HE2	1.83	0.60
1:E:247:TYR:CD2	1:E:372:LEU:HB3	2.37	0.60
1:E:891:TRP:HA	1:E:902:ARG:HB3	1.83	0.60
1:E:2615:ARG:HG3	1:E:2664:PHE:HB3	1.83	0.60
1:E:4767:TRP:HE1	1:E:4771:ILE:HD11	1.67	0.60
1:G:365:LYS:HE2	1:G:369:LEU:HD21	1.84	0.60
1:G:3441:ILE:HG22	1:G:3510:ILE:HD11	1.83	0.60
1:J:2376:LEU:O	1:J:2380:ILE:HG12	2.02	0.60
1:J:3038:MET:C	1:J:3038:MET:HE2	2.26	0.60
1:J:4654:ALA:O	1:J:4658:ILE:HG12	2.00	0.60
1:B:676:THR:HG21	1:B:1633:PRO:HB3	1.84	0.60
1:E:182:LEU:HD11	1:E:189:LEU:HB3	1.83	0.60
1:E:676:THR:HG21	1:E:1633:PRO:HB3	1.84	0.60
1:E:3201:MET:SD	1:E:3203:VAL:HG12	2.42	0.60
1:G:1583:GLU:OE1	1:G:1586:ASN:ND2	2.34	0.60
1:G:3097:GLU:OE1	1:G:3167:ARG:NH1	2.34	0.60
1:G:3339:ALA:HB2	1:G:3407:ALA:HA	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3097:GLU:OE1	1:B:3167:ARG:NH1	2.34	0.59
1:E:2599:GLN:O	1:E:2603:ILE:HG12	2.01	0.59
1:E:3970:GLN:HE21	1:E:5004:THR:HA	1.66	0.59
1:J:399:GLN:O	1:J:403:MET:HG3	2.02	0.59
1:J:1981:MET:HE2	1:J:1981:MET:HA	1.82	0.59
1:J:4154:VAL:O	1:J:4161:ARG:NH2	2.33	0.59
1:J:941:MET:HE1	1:J:1049:TYR:HB3	1.84	0.59
1:J:3263:TYR:HA	1:J:3270:ILE:HG13	1.84	0.59
1:B:2615:ARG:HG3	1:B:2664:PHE:HB3	1.83	0.59
1:B:4767:TRP:HE1	1:B:4771:ILE:HD11	1.67	0.59
1:G:891:TRP:HE1	1:G:904:HIS:HA	1.66	0.59
1:E:941:MET:HE1	1:E:1049:TYR:HB3	1.84	0.59
1:E:972:LEU:HB2	1:E:1044:ARG:HE	1.67	0.59
1:E:3263:TYR:HA	1:E:3270:ILE:HG13	1.84	0.59
1:J:2273:LEU:HD23	1:J:2330:ARG:HB3	1.84	0.59
1:B:941:MET:HE1	1:B:1049:TYR:HB3	1.84	0.59
1:J:1447:CYS:HB3	1:J:1555:LEU:HB3	1.84	0.59
1:B:4091:LYS:O	1:B:4095:LYS:HG2	2.03	0.59
1:J:1024:TYR:HA	1:J:1027:LEU:HD12	1.83	0.59
1:J:2615:ARG:HG3	1:J:2664:PHE:HB3	1.83	0.59
1:J:2961:GLN:HA	1:J:2964:LEU:HD12	1.85	0.59
1:B:247:TYR:HD2	1:B:372:LEU:HB3	1.68	0.59
1:B:2961:GLN:HA	1:B:2964:LEU:HD12	1.85	0.59
1:B:3201:MET:SD	1:B:3203:VAL:HG12	2.42	0.59
1:G:2376:LEU:O	1:G:2380:ILE:HG12	2.02	0.59
1:G:2575:ARG:NH2	1:G:2578:MET:HE3	2.18	0.59
1:B:972:LEU:HB2	1:B:1044:ARG:HE	1.67	0.59
1:B:2575:ARG:NH2	1:B:2578:MET:HE3	2.18	0.59
1:E:224:HIS:NE2	1:E:230:CYS:SG	2.76	0.59
1:E:365:LYS:HE2	1:E:369:LEU:HD21	1.83	0.59
1:G:2961:GLN:HA	1:G:2964:LEU:HD12	1.85	0.59
1:J:676:THR:HG21	1:J:1633:PRO:HB3	1.84	0.59
1:J:1423:ASP:OD2	1:J:1425:GLU:HG2	2.03	0.59
2:D:90:VAL:HG12	2:D:91:ILE:HG13	1.85	0.59
3:M:105:ASN:HD21	3:M:107:TRP:CD1	2.20	0.59
1:B:3339:ALA:HB2	1:B:3407:ALA:HA	1.84	0.59
1:E:2376:LEU:O	1:E:2380:ILE:HG12	2.02	0.59
1:G:985:VAL:HG22	1:G:1043:VAL:HG21	1.85	0.59
1:G:3537:LYS:HA	1:G:3540:TYR:HD2	1.68	0.59
1:J:3331:GLU:HG3	1:J:3334:TRP:HB3	1.85	0.59
1:B:2273:LEU:HD23	1:B:2330:ARG:HB3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2961:GLN:HA	1:E:2964:LEU:HD12	1.85	0.58
1:B:1447:CYS:HB3	1:B:1555:LEU:HB3	1.84	0.58
1:E:2736:ASP:OD1	1:E:2736:ASP:N	2.37	0.58
1:E:3331:GLU:HG3	1:E:3334:TRP:HB3	1.85	0.58
1:E:3537:LYS:HA	1:E:3540:TYR:HD2	1.68	0.58
3:M:33:SER:HA	3:M:52:THR:HA	1.84	0.58
1:B:229:GLU:HG2	1:B:252:VAL:HG13	1.85	0.58
1:E:1095:VAL:HB	1:E:1199:VAL:HG23	1.85	0.58
1:E:1423:ASP:OD2	1:E:1425:GLU:HG2	2.03	0.58
1:E:2273:LEU:HD23	1:E:2330:ARG:HB3	1.84	0.58
1:G:941:MET:HE1	1:G:1049:TYR:HB3	1.84	0.58
1:G:972:LEU:HB2	1:G:1044:ARG:HE	1.67	0.58
1:J:224:HIS:NE2	1:J:230:CYS:SG	2.76	0.58
1:J:1095:VAL:HB	1:J:1199:VAL:HG23	1.86	0.58
2:A:90:VAL:HG12	2:A:91:ILE:HG13	1.85	0.58
1:B:2376:LEU:O	1:B:2380:ILE:HG12	2.02	0.58
1:G:1780:PRO:O	2:H:42:ARG:NH1	2.36	0.58
1:J:985:VAL:HG22	1:J:1043:VAL:HG21	1.85	0.58
1:E:3230:LEU:HG	1:E:3232:LEU:HG	1.86	0.58
1:E:3360:PRO:O	1:E:3364:ARG:HG2	2.04	0.58
1:G:229:GLU:HG2	1:G:252:VAL:HG13	1.85	0.58
1:G:1447:CYS:HB3	1:G:1555:LEU:HB3	1.84	0.58
1:B:208:CYS:HB3	1:B:272:SER:HB3	1.86	0.58
1:B:1095:VAL:HB	1:B:1199:VAL:HG23	1.86	0.58
1:B:3230:LEU:HG	1:B:3232:LEU:HG	1.86	0.58
1:E:1447:CYS:HB3	1:E:1555:LEU:HB3	1.84	0.58
1:E:2310:CYS:HB3	1:E:2313:LEU:HG	1.86	0.58
1:E:3339:ALA:HB2	1:E:3407:ALA:HA	1.84	0.58
1:E:4091:LYS:O	1:E:4095:LYS:HG2	2.03	0.58
1:G:1423:ASP:OD2	1:G:1425:GLU:HG2	2.03	0.58
3:K:66:ARG:NH1	3:K:83:ASN:O	2.32	0.58
1:B:3360:PRO:O	1:B:3364:ARG:HG2	2.04	0.58
1:G:1095:VAL:HB	1:G:1199:VAL:HG23	1.86	0.58
1:G:4091:LYS:O	1:G:4095:LYS:HG2	2.03	0.58
2:I:90:VAL:HG12	2:I:91:ILE:HG13	1.85	0.58
3:C:4:LEU:HD21	3:C:97:ALA:HB2	1.86	0.58
3:K:4:LEU:HD21	3:K:97:ALA:HB2	1.86	0.58
1:B:224:HIS:NE2	1:B:230:CYS:SG	2.76	0.58
1:B:231:LEU:HA	1:B:245:VAL:HB	1.86	0.58
1:B:985:VAL:HG22	1:B:1043:VAL:HG21	1.85	0.58
1:E:1448:VAL:HG12	1:E:1554:VAL:HG23	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3051:ARG:HH21	1:E:3098:SER:HB3	1.69	0.58
1:J:972:LEU:HB2	1:J:1044:ARG:HE	1.67	0.58
1:J:2175:GLU:O	1:J:2179:ILE:HG12	2.03	0.58
1:J:3246:LEU:HD23	1:J:3246:LEU:H	1.69	0.58
1:B:1423:ASP:OD2	1:B:1425:GLU:HG2	2.03	0.58
1:B:2418:LEU:O	1:B:2422:ILE:HG12	2.04	0.58
1:B:2736:ASP:OD1	1:B:2736:ASP:N	2.37	0.58
1:B:3331:GLU:HG3	1:B:3334:TRP:HB3	1.86	0.58
1:B:3537:LYS:HA	1:B:3540:TYR:HD2	1.68	0.58
1:E:2418:LEU:O	1:E:2422:ILE:HG12	2.04	0.58
1:G:162:LYS:NZ	1:J:3987:ASP:OD2	2.33	0.58
1:G:224:HIS:NE2	1:G:230:CYS:SG	2.76	0.58
1:G:2310:CYS:HB3	1:G:2313:LEU:HG	1.86	0.58
1:G:2418:LEU:O	1:G:2422:ILE:HG12	2.04	0.58
1:G:3230:LEU:HG	1:G:3232:LEU:HG	1.86	0.58
1:J:3360:PRO:O	1:J:3364:ARG:HG2	2.04	0.58
3:M:4:LEU:HD21	3:M:97:ALA:HB2	1.86	0.58
1:B:23:GLN:HG2	1:B:36:CYS:HB3	1.86	0.58
1:B:2175:GLU:O	1:B:2179:ILE:HG12	2.03	0.58
1:B:2310:CYS:HB3	1:B:2313:LEU:HG	1.86	0.58
1:B:2476:ILE:HD11	1:B:2536:LEU:HD21	1.86	0.58
1:B:3709:ALA:HB2	1:B:3782:MET:HE2	1.86	0.58
1:E:2534:ALA:HB1	1:E:2588:ARG:HD2	1.86	0.58
1:E:3709:ALA:HB2	1:E:3782:MET:HE2	1.86	0.58
1:G:2476:ILE:HD11	1:G:2536:LEU:HD21	1.86	0.58
1:J:3051:ARG:HH21	1:J:3098:SER:HB3	1.69	0.58
1:J:3230:LEU:HG	1:J:3232:LEU:HG	1.86	0.58
2:H:90:VAL:HG12	2:H:91:ILE:HG13	1.85	0.58
1:G:2534:ALA:HB1	1:G:2588:ARG:HD2	1.86	0.57
1:G:3246:LEU:H	1:G:3246:LEU:HD23	1.69	0.57
1:J:2310:CYS:HB3	1:J:2313:LEU:HG	1.86	0.57
1:B:2182:ILE:O	1:B:2186:MET:HG2	2.05	0.57
1:E:2175:GLU:O	1:E:2179:ILE:HG12	2.04	0.57
1:E:2182:ILE:O	1:E:2186:MET:HG2	2.05	0.57
1:E:3205:PHE:HE2	1:E:3243:ILE:HG21	1.69	0.57
1:E:3326:ASN:HB3	1:E:3329:ILE:HB	1.86	0.57
1:E:3540:TYR:CE2	1:E:3549:VAL:HG11	2.40	0.57
1:J:3205:PHE:HE2	1:J:3243:ILE:HG21	1.69	0.57
1:E:208:CYS:HB3	1:E:272:SER:HB3	1.86	0.57
1:E:231:LEU:HA	1:E:245:VAL:HB	1.85	0.57
1:E:985:VAL:HG22	1:E:1043:VAL:HG21	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2575:ARG:NH2	1:E:2578:MET:HE3	2.18	0.57
1:G:2736:ASP:OD1	1:G:2736:ASP:N	2.36	0.57
1:G:3331:GLU:HG3	1:G:3334:TRP:HB3	1.85	0.57
1:G:3540:TYR:CE2	1:G:3549:VAL:HG11	2.39	0.57
1:J:3339:ALA:HB2	1:J:3407:ALA:HA	1.84	0.57
1:J:3537:LYS:HA	1:J:3540:TYR:HD2	1.68	0.57
1:J:4091:LYS:O	1:J:4095:LYS:HG2	2.03	0.57
3:M:30:SER:HB3	3:M:99:ARG:HB3	1.87	0.57
1:B:2591:ARG:HH12	1:B:2637:ALA:HA	1.70	0.57
1:E:4056:GLU:HG2	1:E:4166:LEU:HD13	1.86	0.57
1:G:208:CYS:HB3	1:G:272:SER:HB3	1.86	0.57
1:J:1780:PRO:O	2:I:42:ARG:NH1	2.38	0.57
1:E:229:GLU:HG2	1:E:252:VAL:HG13	1.85	0.57
1:J:23:GLN:HG2	1:J:36:CYS:HB3	1.86	0.57
1:J:2534:ALA:HB1	1:J:2588:ARG:HD2	1.86	0.57
1:J:3709:ALA:HB2	1:J:3782:MET:HE2	1.86	0.57
1:B:2382:GLU:HA	1:B:2385:ARG:HE	1.70	0.57
1:B:3540:TYR:CE2	1:B:3549:VAL:HG11	2.40	0.57
1:B:4072:VAL:HG23	1:B:4125:PHE:HE2	1.70	0.57
1:G:3360:PRO:O	1:G:3364:ARG:HG2	2.04	0.57
1:G:4072:VAL:HG23	1:G:4125:PHE:HE2	1.70	0.57
1:J:4056:GLU:HG2	1:J:4166:LEU:HD13	1.86	0.57
3:C:30:SER:HB3	3:C:99:ARG:HB3	1.87	0.57
3:F:4:LEU:HD21	3:F:97:ALA:HB2	1.86	0.57
1:E:765:GLN:NE2	1:E:1478:ASP:O	2.38	0.57
1:G:23:GLN:HG2	1:G:36:CYS:HB3	1.86	0.57
1:G:2175:GLU:O	1:G:2179:ILE:HG12	2.04	0.57
1:G:3051:ARG:HH21	1:G:3098:SER:HB3	1.69	0.57
1:J:2476:ILE:HD11	1:J:2536:LEU:HD21	1.86	0.57
1:B:359:TYR:HB2	1:B:374:LYS:HB3	1.86	0.57
1:B:3246:LEU:HD23	1:B:3246:LEU:H	1.69	0.57
1:G:2382:GLU:HA	1:G:2385:ARG:HE	1.70	0.57
1:J:2575:ARG:NH2	1:J:2578:MET:HE3	2.18	0.57
1:J:3540:TYR:CE2	1:J:3549:VAL:HG11	2.39	0.57
1:B:4053:SER:O	1:B:4057:MET:HG3	2.05	0.57
1:E:877:ASN:ND2	1:E:1045:THR:HG21	2.20	0.57
1:E:1011:GLN:OE1	1:E:1020:ARG:NH2	2.35	0.57
1:G:877:ASN:ND2	1:G:1045:THR:HG21	2.20	0.57
1:G:3450:ASN:HA	1:G:3453:ARG:HB2	1.87	0.57
1:J:231:LEU:HA	1:J:245:VAL:HB	1.86	0.57
1:J:2382:GLU:HA	1:J:2385:ARG:HE	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:3534:MET:SD	1:J:3537:LYS:NZ	2.75	0.57
1:J:4072:VAL:HG23	1:J:4125:PHE:HE2	1.70	0.57
1:B:224:HIS:HD2	1:B:388:LEU:HB3	1.70	0.57
1:B:1448:VAL:HG12	1:B:1554:VAL:HG23	1.86	0.57
1:G:2591:ARG:HH12	1:G:2637:ALA:HA	1.69	0.57
1:G:2755:ILE:HG23	1:G:2813:LEU:HD13	1.87	0.57
1:J:229:GLU:HG2	1:J:252:VAL:HG13	1.85	0.57
1:J:1023:PRO:HD2	1:J:1026:LEU:HD12	1.87	0.57
1:B:1225:PRO:HG2	1:B:1228:ILE:HB	1.87	0.56
1:B:3326:ASN:HB3	1:B:3329:ILE:HB	1.86	0.56
1:E:4072:VAL:HG23	1:E:4125:PHE:HE2	1.70	0.56
1:G:224:HIS:HD2	1:G:388:LEU:HB3	1.70	0.56
1:G:231:LEU:HA	1:G:245:VAL:HB	1.86	0.56
1:G:1023:PRO:HD2	1:G:1026:LEU:HD12	1.87	0.56
1:G:2175:GLU:HG3	1:G:2228:MET:HB2	1.86	0.56
1:G:4053:SER:O	1:G:4057:MET:HG3	2.05	0.56
1:B:3169:LEU:HD13	1:B:3197:LEU:HD11	1.88	0.56
1:E:224:HIS:HD2	1:E:388:LEU:HB3	1.70	0.56
1:E:1225:PRO:HG2	1:E:1228:ILE:HB	1.87	0.56
1:E:4053:SER:O	1:E:4057:MET:HG3	2.05	0.56
1:G:924:MET:HE1	3:M:106:PRO:CB	2.34	0.56
1:G:1448:VAL:HG12	1:G:1554:VAL:HG23	1.86	0.56
1:G:2182:ILE:O	1:G:2186:MET:HG2	2.05	0.56
1:J:208:CYS:HB3	1:J:272:SER:HB3	1.86	0.56
1:J:1448:VAL:HG12	1:J:1554:VAL:HG23	1.86	0.56
1:J:2175:GLU:HG3	1:J:2228:MET:HB2	1.86	0.56
1:B:3205:PHE:HE2	1:B:3243:ILE:HG21	1.69	0.56
1:E:462:GLU:HG2	1:E:3710:LEU:HD13	1.88	0.56
1:E:2591:ARG:HH12	1:E:2637:ALA:HA	1.69	0.56
1:E:3246:LEU:HD23	1:E:3246:LEU:H	1.69	0.56
1:E:3455:GLU:O	1:E:3459:VAL:HG23	2.06	0.56
1:G:765:GLN:NE2	1:G:1478:ASP:O	2.38	0.56
1:G:1225:PRO:HG2	1:G:1228:ILE:HB	1.87	0.56
1:G:3326:ASN:HB3	1:G:3329:ILE:HB	1.86	0.56
1:J:224:HIS:HD2	1:J:388:LEU:HB3	1.70	0.56
1:J:765:GLN:NE2	1:J:1478:ASP:O	2.38	0.56
1:J:1225:PRO:HG2	1:J:1228:ILE:HB	1.87	0.56
1:J:2418:LEU:O	1:J:2422:ILE:HG12	2.04	0.56
1:J:3311:HIS:O	1:J:3315:LEU:HG	2.06	0.56
1:J:3326:ASN:HB3	1:J:3329:ILE:HB	1.86	0.56
1:J:3455:GLU:O	1:J:3459:VAL:HG23	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:4001:MET:HE1	1:J:4057:MET:HB3	1.88	0.56
1:J:4053:SER:O	1:J:4057:MET:HG3	2.05	0.56
3:C:11:LEU:HG	3:C:124:THR:HB	1.87	0.56
1:B:4001:MET:HE1	1:B:4057:MET:HB3	1.88	0.56
1:G:2470:ILE:HG12	1:G:2502:MET:HE3	1.88	0.56
1:G:3205:PHE:HE2	1:G:3243:ILE:HG21	1.69	0.56
1:J:3169:LEU:HD13	1:J:3197:LEU:HD11	1.88	0.56
3:C:104:TYR:HE1	3:C:106:PRO:HG3	1.71	0.56
1:B:16:THR:HG22	1:B:99:ARG:H	1.71	0.56
1:B:2500:ALA:HB2	1:B:2553:TYR:HD1	1.71	0.56
1:B:3051:ARG:HH21	1:B:3098:SER:HB3	1.69	0.56
1:B:3971:GLY:O	1:B:3973:CYS:N	2.39	0.56
1:E:2175:GLU:HG3	1:E:2228:MET:HB2	1.86	0.56
1:E:2476:ILE:HD11	1:E:2536:LEU:HD21	1.86	0.56
1:E:2500:ALA:HB2	1:E:2553:TYR:HD1	1.71	0.56
1:G:2490:MET:HA	1:G:2490:MET:HE3	1.88	0.56
1:G:2500:ALA:HB2	1:G:2553:TYR:HD1	1.71	0.56
1:G:3466:ASN:HA	1:G:3469:PHE:CD2	2.41	0.56
1:G:3555:ASN:O	1:G:3558:HIS:ND1	2.37	0.56
1:G:3709:ALA:HB2	1:G:3782:MET:HE2	1.86	0.56
1:J:2755:ILE:HG23	1:J:2813:LEU:HD13	1.87	0.56
1:J:3537:LYS:O	1:J:3540:TYR:HB2	2.06	0.56
1:B:4056:GLU:HG2	1:B:4166:LEU:HD13	1.86	0.56
1:E:20:VAL:HG11	1:E:202:MET:HG3	1.88	0.56
1:E:23:GLN:HG2	1:E:36:CYS:HB3	1.86	0.56
1:E:377:ILE:HB	1:E:379:HIS:CE1	2.40	0.56
1:E:2737:PRO:HD2	1:E:2891:LYS:HD3	1.88	0.56
1:E:3534:MET:SD	1:E:3537:LYS:NZ	2.75	0.56
1:E:3537:LYS:O	1:E:3540:TYR:HB2	2.06	0.56
1:E:4001:MET:HE1	1:E:4057:MET:HB3	1.88	0.56
1:G:3311:HIS:O	1:G:3315:LEU:HG	2.06	0.56
1:J:877:ASN:ND2	1:J:1045:THR:HG21	2.20	0.56
1:J:2470:ILE:HG12	1:J:2502:MET:HE3	1.88	0.56
1:J:2591:ARG:HH12	1:J:2637:ALA:HA	1.69	0.56
1:B:2755:ILE:HG23	1:B:2813:LEU:HD13	1.87	0.56
1:E:2382:GLU:HA	1:E:2385:ARG:HE	1.70	0.56
1:E:3466:ASN:HA	1:E:3469:PHE:CD2	2.41	0.56
1:G:16:THR:HG22	1:G:99:ARG:H	1.71	0.56
1:G:3537:LYS:O	1:G:3540:TYR:HB2	2.06	0.56
3:K:30:SER:HB3	3:K:99:ARG:HB3	1.88	0.56
1:B:3003:LEU:HB2	1:B:3004:PRO:HD3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3450:ASN:HA	1:B:3453:ARG:HB2	1.87	0.56
1:B:3466:ASN:HA	1:B:3469:PHE:CD2	2.41	0.56
1:B:3534:MET:SD	1:B:3537:LYS:NZ	2.75	0.56
1:E:2470:ILE:HG12	1:E:2502:MET:HE3	1.88	0.56
1:E:2755:ILE:HG23	1:E:2813:LEU:HD13	1.87	0.56
1:G:3757:GLU:O	1:G:3761:GLN:HG2	2.06	0.56
1:G:4001:MET:HE1	1:G:4057:MET:HB3	1.88	0.56
1:J:20:VAL:HG11	1:J:202:MET:HG3	1.88	0.56
1:J:3466:ASN:HA	1:J:3469:PHE:CD2	2.41	0.56
1:B:765:GLN:NE2	1:B:1478:ASP:O	2.38	0.56
1:B:877:ASN:ND2	1:B:1045:THR:HG21	2.20	0.56
1:B:2534:ALA:HB1	1:B:2588:ARG:HD2	1.86	0.56
1:G:1011:GLN:OE1	1:G:1020:ARG:NH2	2.35	0.56
1:G:3003:LEU:HB2	1:G:3004:PRO:HD3	1.88	0.56
1:G:4056:GLU:HG2	1:G:4166:LEU:HD13	1.86	0.56
1:J:3355:HIS:O	1:J:3359:ILE:HD12	2.06	0.56
1:J:3450:ASN:HA	1:J:3453:ARG:HB2	1.87	0.56
1:J:3757:GLU:O	1:J:3761:GLN:HG2	2.06	0.56
1:J:3971:GLY:O	1:J:3973:CYS:N	2.39	0.56
1:B:2470:ILE:HG12	1:B:2502:MET:HE3	1.88	0.56
1:E:16:THR:HG22	1:E:99:ARG:H	1.71	0.56
1:E:3311:HIS:O	1:E:3315:LEU:HG	2.06	0.56
1:E:3450:ASN:HA	1:E:3453:ARG:HB2	1.87	0.56
1:G:2271:THR:HG23	1:G:2274:ASP:H	1.71	0.56
1:G:3110:LEU:HD11	1:G:3129:LEU:HD22	1.87	0.56
1:G:3455:GLU:O	1:G:3459:VAL:HG23	2.06	0.56
1:B:1023:PRO:HD2	1:B:1026:LEU:HD12	1.87	0.55
1:E:358:THR:HG21	1:E:382:GLY:HA2	1.88	0.55
1:E:2653:LYS:HB2	1:E:2661:TRP:NE1	2.21	0.55
1:J:2653:LYS:HB2	1:J:2661:TRP:NE1	2.21	0.55
1:J:3040:THR:HA	1:J:3043:PHE:CD1	2.41	0.55
3:K:11:LEU:HG	3:K:124:THR:HB	1.87	0.55
1:B:2175:GLU:HG3	1:B:2228:MET:HB2	1.86	0.55
1:B:3040:THR:HA	1:B:3043:PHE:CD1	2.41	0.55
1:B:3455:GLU:O	1:B:3459:VAL:HG23	2.06	0.55
1:J:358:THR:HG21	1:J:382:GLY:HA2	1.88	0.55
1:J:2178:MET:HE2	1:J:2210:VAL:HG11	1.88	0.55
1:J:2500:ALA:HB2	1:J:2553:TYR:HD1	1.71	0.55
1:J:3003:LEU:HB2	1:J:3004:PRO:HD3	1.88	0.55
1:J:3219:TYR:HD1	1:J:3227:ARG:HD2	1.71	0.55
3:M:11:LEU:HG	3:M:124:THR:HB	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:TYR:HB3	1:B:373:LYS:HA	1.88	0.55
1:B:462:GLU:HG2	1:B:3710:LEU:HD13	1.88	0.55
1:B:1477:GLY:HA2	1:B:1483:VAL:HA	1.88	0.55
1:B:3311:HIS:O	1:B:3315:LEU:HG	2.06	0.55
1:E:1477:GLY:HA2	1:E:1483:VAL:HA	1.89	0.55
1:E:1652:GLU:OE1	1:E:1656:ARG:NH1	2.40	0.55
1:E:2630:VAL:HG12	1:E:2682:ILE:HD11	1.88	0.55
1:E:3355:HIS:O	1:E:3359:ILE:HD12	2.06	0.55
1:G:3040:THR:HA	1:G:3043:PHE:CD1	2.41	0.55
1:G:3355:HIS:O	1:G:3359:ILE:HD12	2.06	0.55
1:J:462:GLU:HG2	1:J:3710:LEU:HD13	1.88	0.55
1:J:733:PRO:HG2	1:J:762:CYS:HB3	1.88	0.55
1:J:2182:ILE:O	1:J:2186:MET:HG2	2.05	0.55
1:E:1023:PRO:HD2	1:E:1026:LEU:HD12	1.87	0.55
1:G:358:THR:HG21	1:G:382:GLY:HA2	1.88	0.55
1:G:733:PRO:HG2	1:G:762:CYS:HB3	1.88	0.55
1:G:3971:GLY:O	1:G:3973:CYS:N	2.39	0.55
1:J:1652:GLU:OE1	1:J:1656:ARG:NH1	2.40	0.55
1:J:3040:THR:HA	1:J:3043:PHE:HD1	1.72	0.55
3:C:101:PRO:HG2	3:C:104:TYR:CE2	2.42	0.55
1:B:308:HIS:O	1:B:312:THR:OG1	2.24	0.55
1:B:909:ASN:HB2	1:B:964:GLY:H	1.71	0.55
1:B:2737:PRO:HD2	1:B:2891:LYS:HD3	1.88	0.55
1:B:3040:THR:HA	1:B:3043:PHE:HD1	1.72	0.55
1:B:3537:LYS:O	1:B:3540:TYR:HB2	2.06	0.55
1:B:3757:GLU:O	1:B:3761:GLN:HG2	2.06	0.55
1:E:2271:THR:HG23	1:E:2274:ASP:H	1.71	0.55
1:E:2368:LEU:HD11	1:E:2376:LEU:HD22	1.88	0.55
1:E:3335:MET:HE2	1:E:3335:MET:HA	1.89	0.55
1:G:462:GLU:HG2	1:G:3710:LEU:HD13	1.88	0.55
1:J:2736:ASP:OD1	1:J:2736:ASP:N	2.36	0.55
1:B:2476:ILE:HD12	1:B:2477:PRO:HD2	1.89	0.55
1:B:2490:MET:HE3	1:B:2490:MET:HA	1.88	0.55
1:B:2653:LYS:HB2	1:B:2661:TRP:NE1	2.21	0.55
1:E:3040:THR:HA	1:E:3043:PHE:CD1	2.41	0.55
1:E:3110:LEU:HD11	1:E:3129:LEU:HD22	1.87	0.55
1:G:20:VAL:HG11	1:G:202:MET:HG3	1.88	0.55
1:G:3169:LEU:HD13	1:G:3197:LEU:HD11	1.87	0.55
1:J:909:ASN:HB2	1:J:964:GLY:H	1.71	0.55
3:F:11:LEU:HG	3:F:124:THR:HB	1.87	0.55
1:E:2490:MET:HA	1:E:2490:MET:HE3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3219:TYR:HD1	1:E:3227:ARG:HD2	1.71	0.55
1:G:874:LEU:HA	1:G:877:ASN:ND2	2.22	0.55
1:G:2881:ASN:HA	1:G:2884:ASN:HD21	1.72	0.55
1:J:2737:PRO:HD2	1:J:2891:LYS:HD3	1.88	0.55
1:J:3467:MET:O	1:J:3471:THR:HG22	2.07	0.55
1:B:20:VAL:HG11	1:B:202:MET:HG3	1.88	0.55
1:B:3110:LEU:HD11	1:B:3129:LEU:HD22	1.87	0.55
1:E:3040:THR:HA	1:E:3043:PHE:HD1	1.72	0.55
1:G:1477:GLY:HA2	1:G:1483:VAL:HA	1.88	0.55
1:G:3040:THR:HA	1:G:3043:PHE:HD1	1.72	0.55
1:J:2630:VAL:HG12	1:J:2682:ILE:HD11	1.88	0.55
1:B:3948:LYS:NZ	1:B:4008:SER:O	2.40	0.55
1:B:4823:LEU:HD13	1:B:4826:ILE:HD11	1.88	0.55
1:E:2476:ILE:HD12	1:E:2477:PRO:HD2	1.89	0.55
1:J:2490:MET:HE3	1:J:2490:MET:HA	1.88	0.55
1:J:3335:MET:HA	1:J:3335:MET:HE2	1.89	0.55
1:J:3948:LYS:NZ	1:J:4008:SER:O	2.40	0.55
1:B:618:GLN:OE1	1:B:1678:ASN:ND2	2.38	0.55
1:E:2587:TYR:CZ	1:E:2591:ARG:HD2	2.42	0.55
1:E:3003:LEU:HB2	1:E:3004:PRO:HD3	1.88	0.55
1:G:2368:LEU:HD11	1:G:2376:LEU:HD22	1.88	0.55
1:G:3534:MET:SD	1:G:3537:LYS:NZ	2.75	0.55
1:J:308:HIS:O	1:J:312:THR:OG1	2.24	0.55
1:B:622:THR:HG23	1:B:626:LEU:HD12	1.89	0.54
1:B:900:ASN:ND2	3:C:61:ASP:OD1	2.37	0.54
1:B:2960:LEU:HB3	1:B:3038:MET:HE3	1.89	0.54
1:B:3355:HIS:O	1:B:3359:ILE:HD12	2.06	0.54
1:E:3467:MET:O	1:E:3471:THR:HG22	2.07	0.54
1:J:3110:LEU:HD11	1:J:3129:LEU:HD22	1.87	0.54
1:J:4823:LEU:HD13	1:J:4826:ILE:HD11	1.88	0.54
3:F:30:SER:HB3	3:F:99:ARG:HB3	1.89	0.54
1:B:733:PRO:HG2	1:B:762:CYS:HB3	1.88	0.54
1:B:874:LEU:HA	1:B:877:ASN:ND2	2.22	0.54
1:E:909:ASN:HB2	1:E:964:GLY:H	1.71	0.54
1:E:2178:MET:HE2	1:E:2210:VAL:HG11	1.88	0.54
1:G:2630:VAL:HG12	1:G:2682:ILE:HD11	1.88	0.54
1:G:2653:LYS:HB2	1:G:2661:TRP:NE1	2.21	0.54
1:G:3219:TYR:HD1	1:G:3227:ARG:HD2	1.72	0.54
1:B:2765:LYS:HZ3	1:B:2857:PRO:HG2	1.71	0.54
1:B:3313:ASN:HB3	1:B:3353:LEU:HD13	1.90	0.54
1:E:3169:LEU:HD13	1:E:3197:LEU:HD11	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3971:GLY:O	1:E:3973:CYS:N	2.39	0.54
1:G:308:HIS:O	1:G:312:THR:OG1	2.24	0.54
1:G:909:ASN:HB2	1:G:964:GLY:H	1.71	0.54
1:B:358:THR:HG21	1:B:382:GLY:HA2	1.88	0.54
1:B:2271:THR:HG23	1:B:2274:ASP:H	1.71	0.54
1:B:3049:LEU:HB3	1:B:3057:PHE:HE1	1.73	0.54
1:B:3335:MET:HA	1:B:3335:MET:HE2	1.88	0.54
1:E:622:THR:HG23	1:E:626:LEU:HD12	1.89	0.54
1:E:2572:THR:HB	1:E:2575:ARG:HB2	1.90	0.54
1:G:3467:MET:O	1:G:3471:THR:HG22	2.07	0.54
1:J:16:THR:HG22	1:J:99:ARG:H	1.71	0.54
1:J:4780:PHE:HA	1:J:4783:ILE:HG22	1.90	0.54
3:F:100:VAL:HG13	3:F:104:TYR:O	2.07	0.54
1:B:2587:TYR:CZ	1:B:2591:ARG:HD2	2.42	0.54
1:B:2881:ASN:HA	1:B:2884:ASN:HD21	1.72	0.54
1:E:359:TYR:CE1	1:E:385:ASP:HB2	2.43	0.54
1:E:874:LEU:HA	1:E:877:ASN:ND2	2.22	0.54
1:E:1780:PRO:O	2:D:42:ARG:NH1	2.40	0.54
1:E:3757:GLU:O	1:E:3761:GLN:HG2	2.06	0.54
1:G:275:ARG:HB2	1:G:278:GLN:HB2	1.89	0.54
1:G:3948:LYS:NZ	1:G:4008:SER:O	2.40	0.54
1:J:2587:TYR:CZ	1:J:2591:ARG:HD2	2.42	0.54
1:J:2881:ASN:HA	1:J:2884:ASN:HD21	1.72	0.54
1:B:2178:MET:HE2	1:B:2210:VAL:HG11	1.88	0.54
1:B:2630:VAL:HG12	1:B:2682:ILE:HD11	1.88	0.54
1:B:3139:VAL:O	1:B:3143:LEU:HG	2.07	0.54
1:B:3809:ASN:OD1	1:B:3812:VAL:HG22	2.08	0.54
1:E:3948:LYS:NZ	1:E:4008:SER:O	2.40	0.54
1:G:2178:MET:HE2	1:G:2210:VAL:HG11	1.88	0.54
1:G:2587:TYR:CZ	1:G:2591:ARG:HD2	2.42	0.54
1:G:2737:PRO:HD2	1:G:2891:LYS:HD3	1.88	0.54
1:G:3313:ASN:HB3	1:G:3353:LEU:HD13	1.90	0.54
1:G:4780:PHE:HA	1:G:4783:ILE:HG22	1.90	0.54
1:G:4823:LEU:HD13	1:G:4826:ILE:HD11	1.88	0.54
1:J:275:ARG:HB2	1:J:278:GLN:HB2	1.89	0.54
1:J:2271:THR:HG23	1:J:2274:ASP:H	1.71	0.54
1:J:2476:ILE:HD12	1:J:2477:PRO:HD2	1.89	0.54
3:K:100:VAL:HG13	3:K:104:TYR:O	2.07	0.54
1:B:1652:GLU:OE1	1:B:1656:ARG:NH1	2.40	0.54
1:B:3467:MET:O	1:B:3471:THR:HG22	2.07	0.54
1:E:2881:ASN:HA	1:E:2884:ASN:HD21	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3809:ASN:OD1	1:E:3812:VAL:HG22	2.08	0.54
1:E:3893:GLU:HA	1:E:3967:GLU:OE2	2.08	0.54
1:G:1652:GLU:OE1	1:G:1656:ARG:NH1	2.40	0.54
1:G:3049:LEU:HB3	1:G:3057:PHE:HE1	1.73	0.54
1:G:3285:TRP:HE1	1:G:3306:ALA:HB3	1.73	0.54
1:J:924:MET:HE1	3:K:106:PRO:HB2	1.89	0.54
1:J:2368:LEU:HD11	1:J:2376:LEU:HD22	1.88	0.54
3:C:100:VAL:HG13	3:C:104:TYR:O	2.07	0.54
1:B:2710:LEU:HD21	1:B:2955:PHE:CE2	2.43	0.54
1:B:3219:TYR:HD1	1:B:3227:ARG:HD2	1.72	0.54
1:B:4780:PHE:HA	1:B:4783:ILE:HG22	1.90	0.54
1:E:3230:LEU:HD23	1:E:3230:LEU:H	1.73	0.54
1:E:3313:ASN:HB3	1:E:3353:LEU:HD13	1.90	0.54
1:E:4780:PHE:HA	1:E:4783:ILE:HG22	1.90	0.54
1:G:2960:LEU:HB3	1:G:3038:MET:HE3	1.89	0.54
1:J:3281:LEU:HD12	1:J:3341:PHE:CD1	2.43	0.54
1:J:3566:SER:HB3	1:J:3569:LEU:HD23	1.89	0.54
1:E:3566:SER:HB3	1:E:3569:LEU:HD23	1.89	0.54
1:E:4693:GLY:O	1:E:4700:GLN:NE2	2.41	0.54
1:G:4134:GLU:HB3	1:G:4135:PRO:HD3	1.90	0.54
1:G:4693:GLY:O	1:G:4700:GLN:NE2	2.41	0.54
1:J:874:LEU:HA	1:J:877:ASN:ND2	2.22	0.54
1:J:1477:GLY:HA2	1:J:1483:VAL:HA	1.89	0.54
1:J:2325:PRO:O	1:J:2329:GLU:HG2	2.08	0.54
1:J:2960:LEU:HB3	1:J:3038:MET:HE3	1.89	0.54
1:J:3049:LEU:HB3	1:J:3057:PHE:HE1	1.73	0.54
1:B:275:ARG:HB2	1:B:278:GLN:HB2	1.89	0.54
1:B:3230:LEU:HD23	1:B:3230:LEU:H	1.73	0.54
1:B:3566:SER:HB3	1:B:3569:LEU:HD23	1.89	0.54
1:E:3139:VAL:O	1:E:3143:LEU:HG	2.07	0.54
1:E:4823:LEU:HD13	1:E:4826:ILE:HD11	1.88	0.54
1:G:618:GLN:OE1	1:G:1678:ASN:ND2	2.38	0.54
1:G:2765:LYS:HZ2	1:G:2860:PRO:HA	1.71	0.54
1:G:3809:ASN:OD1	1:G:3812:VAL:HG22	2.08	0.54
1:B:3579:LEU:HD12	1:B:3580:PRO:HD2	1.90	0.53
1:B:4693:GLY:O	1:B:4700:GLN:NE2	2.41	0.53
1:E:3579:LEU:HD12	1:E:3580:PRO:HD2	1.90	0.53
1:G:3566:SER:HB3	1:G:3569:LEU:HD23	1.89	0.53
1:J:2710:LEU:HD21	1:J:2955:PHE:CE2	2.43	0.53
1:B:2368:LEU:HD11	1:B:2376:LEU:HD22	1.88	0.53
1:E:3049:LEU:HB3	1:E:3057:PHE:HE1	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3139:VAL:O	1:G:3143:LEU:HG	2.07	0.53
1:G:3230:LEU:HD23	1:G:3230:LEU:H	1.73	0.53
3:K:101:PRO:HG2	3:K:104:TYR:CE2	2.43	0.53
1:E:275:ARG:HB2	1:E:278:GLN:HB2	1.89	0.53
1:E:2011:HIS:O	1:E:2011:HIS:ND1	2.41	0.53
1:E:2325:PRO:O	1:E:2329:GLU:HG2	2.08	0.53
1:G:231:LEU:O	1:G:260:TRP:NE1	2.41	0.53
1:G:622:THR:HG23	1:G:626:LEU:HD12	1.89	0.53
1:G:2710:LEU:HD21	1:G:2955:PHE:CE2	2.43	0.53
3:K:13:GLN:OE1	3:K:13:GLN:N	2.37	0.53
1:B:2238:TYR:O	1:B:2242:ILE:HG12	2.09	0.53
1:E:733:PRO:HG2	1:E:762:CYS:HB3	1.88	0.53
1:E:2575:ARG:HH21	1:E:2578:MET:HE3	1.74	0.53
1:E:3281:LEU:HD12	1:E:3341:PHE:CD1	2.43	0.53
1:G:2476:ILE:HD12	1:G:2477:PRO:HD2	1.89	0.53
1:G:2572:THR:HB	1:G:2575:ARG:HB2	1.90	0.53
1:J:622:THR:HG23	1:J:626:LEU:HD12	1.89	0.53
1:J:4693:GLY:O	1:J:4700:GLN:NE2	2.41	0.53
1:B:3201:MET:HA	1:B:3201:MET:HE2	1.90	0.53
1:B:4090:LYS:HZ1	1:B:4115:SER:HB2	1.73	0.53
1:B:4848:VAL:HG11	1:B:4887:MET:HG2	1.91	0.53
1:G:3281:LEU:HD12	1:G:3341:PHE:CD1	2.43	0.53
1:G:3368:ARG:HH21	1:G:3401:LEU:HD23	1.74	0.53
1:G:3768:SER:HA	1:G:3771:HIS:CE1	2.44	0.53
3:F:101:PRO:HG2	3:F:104:TYR:CE2	2.43	0.53
1:B:2572:THR:HB	1:B:2575:ARG:HB2	1.90	0.53
1:E:1676:LEU:HD22	1:E:2167:ILE:HD12	1.90	0.53
1:E:2710:LEU:HD21	1:E:2955:PHE:CE2	2.43	0.53
1:G:2238:TYR:O	1:G:2242:ILE:HG12	2.09	0.53
1:J:2572:THR:HB	1:J:2575:ARG:HB2	1.89	0.53
1:B:2881:ASN:HA	1:B:2884:ASN:ND2	2.24	0.53
1:E:3285:TRP:HE1	1:E:3306:ALA:HB3	1.73	0.53
1:E:3411:LEU:H	1:E:3411:LEU:HD12	1.74	0.53
1:G:3335:MET:HA	1:G:3335:MET:HE2	1.89	0.53
1:G:4848:VAL:HG11	1:G:4887:MET:HG2	1.91	0.53
1:J:2881:ASN:HA	1:J:2884:ASN:ND2	2.24	0.53
1:J:3230:LEU:HD23	1:J:3230:LEU:H	1.73	0.53
1:J:3313:ASN:HB3	1:J:3353:LEU:HD13	1.90	0.53
2:A:87:HIS:HD2	2:A:91:ILE:HD12	1.74	0.53
3:C:13:GLN:OE1	3:C:13:GLN:N	2.37	0.53
1:B:3285:TRP:HE1	1:B:3306:ALA:HB3	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:374:LYS:O	1:G:375:LYS:C	2.51	0.53
1:G:1676:LEU:HD22	1:G:2167:ILE:HD12	1.90	0.53
1:J:2238:TYR:O	1:J:2242:ILE:HG12	2.09	0.53
1:J:3139:VAL:O	1:J:3143:LEU:HG	2.07	0.53
1:B:3368:ARG:HH21	1:B:3401:LEU:HD23	1.74	0.53
1:B:3768:SER:HA	1:B:3771:HIS:CE1	2.44	0.53
1:B:4134:GLU:HB3	1:B:4135:PRO:HD3	1.90	0.53
1:E:308:HIS:O	1:E:312:THR:OG1	2.24	0.53
1:E:2765:LYS:HZ3	1:E:2857:PRO:HG2	1.73	0.53
1:G:2325:PRO:O	1:G:2329:GLU:HG2	2.08	0.53
1:G:3201:MET:HE2	1:G:3201:MET:HA	1.90	0.53
1:J:3411:LEU:H	1:J:3411:LEU:HD12	1.74	0.53
1:J:3555:ASN:O	1:J:3558:HIS:ND1	2.37	0.53
1:J:4134:GLU:HB3	1:J:4135:PRO:HD3	1.90	0.53
3:M:100:VAL:HG13	3:M:104:TYR:O	2.09	0.53
1:B:231:LEU:O	1:B:260:TRP:NE1	2.41	0.53
1:E:1286:MET:HE2	1:E:1464:PHE:HB3	1.91	0.53
1:J:3287:ARG:HG2	1:J:3294:PRO:HD2	1.90	0.53
2:D:87:HIS:HD2	2:D:91:ILE:HD12	1.74	0.53
2:H:87:HIS:HD2	2:H:91:ILE:HD12	1.74	0.53
3:F:105:ASN:ND2	3:F:107:TRP:HD1	2.06	0.53
1:B:162:LYS:NZ	1:G:3987:ASP:OD2	2.32	0.52
1:B:369:LEU:HB2	1:B:371:VAL:HG23	1.90	0.52
1:E:2238:TYR:O	1:E:2242:ILE:HG12	2.09	0.52
1:E:2881:ASN:HA	1:E:2884:ASN:ND2	2.24	0.52
1:E:3768:SER:HA	1:E:3771:HIS:CE1	2.44	0.52
1:G:1286:MET:HE2	1:G:1464:PHE:HB3	1.91	0.52
1:G:2573:GLU:OE1	1:G:2573:GLU:N	2.42	0.52
1:J:1286:MET:HE2	1:J:1464:PHE:HB3	1.91	0.52
1:J:2206:THR:O	1:J:2210:VAL:HG23	2.09	0.52
1:J:3201:MET:HA	1:J:3201:MET:HE2	1.90	0.52
1:J:3579:LEU:HD12	1:J:3580:PRO:HD2	1.90	0.52
3:M:104:TYR:HE1	3:M:106:PRO:HG3	1.74	0.52
1:B:3281:LEU:HD12	1:B:3341:PHE:CD1	2.43	0.52
1:E:979:PRO:O	1:E:983:THR:HG23	2.10	0.52
1:E:3290:GLU:HG3	1:E:3307:VAL:HG22	1.92	0.52
1:E:3691:GLU:HG2	1:E:3692:GLU:HG3	1.92	0.52
1:E:4848:VAL:HG11	1:E:4887:MET:HG2	1.91	0.52
1:G:196:MET:HE2	1:G:196:MET:N	2.25	0.52
1:G:2206:THR:O	1:G:2210:VAL:HG23	2.09	0.52
1:G:3411:LEU:H	1:G:3411:LEU:HD12	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:3290:GLU:HG3	1:J:3307:VAL:HG22	1.92	0.52
1:J:3369:ALA:HA	1:J:3401:LEU:HD11	1.91	0.52
1:J:3809:ASN:OD1	1:J:3812:VAL:HG22	2.08	0.52
1:J:3893:GLU:HA	1:J:3967:GLU:OE2	2.08	0.52
1:J:4848:VAL:HG11	1:J:4887:MET:HG2	1.91	0.52
1:B:196:MET:H	1:B:196:MET:HE2	1.74	0.52
1:B:1286:MET:HE2	1:B:1464:PHE:HB3	1.91	0.52
1:B:3144:PHE:CD2	1:B:3197:LEU:HB3	2.44	0.52
1:B:3287:ARG:HG2	1:B:3294:PRO:HD2	1.90	0.52
1:E:196:MET:HE2	1:E:196:MET:N	2.25	0.52
1:E:411:TYR:HB2	1:E:486:LEU:HD21	1.92	0.52
1:E:2206:THR:O	1:E:2210:VAL:HG23	2.09	0.52
1:E:2960:LEU:HB3	1:E:3038:MET:HE3	1.89	0.52
1:E:2968:ASP:O	1:E:2971:GLN:HG2	2.10	0.52
1:G:2575:ARG:HH21	1:G:2578:MET:HE3	1.73	0.52
1:J:196:MET:H	1:J:196:MET:HE2	1.74	0.52
1:J:2011:HIS:ND1	1:J:2011:HIS:O	2.41	0.52
1:J:3310:ASP:HA	1:J:3313:ASN:HD21	1.75	0.52
1:J:4069:LYS:HD2	1:J:4133:GLN:HG3	1.91	0.52
2:I:87:HIS:HD2	2:I:91:ILE:HD12	1.74	0.52
1:B:2206:THR:O	1:B:2210:VAL:HG23	2.09	0.52
1:B:2325:PRO:O	1:B:2329:GLU:HG2	2.08	0.52
1:B:3442:PHE:CD2	1:B:3514:LEU:HD11	2.44	0.52
1:E:924:MET:HE1	3:F:106:PRO:HB2	1.90	0.52
1:G:3144:PHE:CD2	1:G:3197:LEU:HB3	2.45	0.52
1:J:374:LYS:O	1:J:375:LYS:C	2.51	0.52
1:J:1623:ARG:NE	1:J:1623:ARG:O	2.43	0.52
1:J:3768:SER:HA	1:J:3771:HIS:CE1	2.44	0.52
1:J:3959:LYS:HG3	1:J:4022:ASP:OD2	2.10	0.52
1:B:3411:LEU:H	1:B:3411:LEU:HD12	1.74	0.52
1:B:3416:VAL:HB	1:B:3516:LYS:HZ3	1.73	0.52
1:E:1623:ARG:NE	1:E:1623:ARG:O	2.43	0.52
1:E:3144:PHE:CD2	1:E:3197:LEU:HB3	2.44	0.52
1:J:2573:GLU:OE1	1:J:2573:GLU:N	2.42	0.52
1:J:3368:ARG:HH21	1:J:3401:LEU:HD23	1.74	0.52
1:B:196:MET:HE2	1:B:196:MET:N	2.25	0.52
1:B:1676:LEU:HD22	1:B:2167:ILE:HD12	1.90	0.52
1:B:2710:LEU:HD21	1:B:2955:PHE:HE2	1.75	0.52
1:B:3310:ASP:HA	1:B:3313:ASN:HD21	1.75	0.52
1:B:3691:GLU:HG2	1:B:3692:GLU:HG3	1.92	0.52
1:E:196:MET:HE2	1:E:196:MET:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:595:ARG:HH22	1:E:1642:PRO:HD2	1.75	0.52
1:E:2573:GLU:OE1	1:E:2573:GLU:N	2.42	0.52
1:E:3201:MET:HE2	1:E:3201:MET:HA	1.90	0.52
1:E:3310:ASP:HA	1:E:3313:ASN:HD21	1.75	0.52
1:E:3959:LYS:HG3	1:E:4022:ASP:OD2	2.10	0.52
1:E:4069:LYS:HD2	1:E:4133:GLN:HG3	1.91	0.52
1:G:2011:HIS:O	1:G:2011:HIS:ND1	2.41	0.52
1:G:2881:ASN:HA	1:G:2884:ASN:ND2	2.24	0.52
1:G:3442:PHE:CD2	1:G:3514:LEU:HD11	2.44	0.52
1:J:979:PRO:O	1:J:983:THR:HG23	2.10	0.52
1:J:2871:LEU:HG	1:J:2927:LEU:HD11	1.91	0.52
1:J:4670:ILE:O	1:J:4674:GLU:HG3	2.10	0.52
1:B:2575:ARG:HH21	1:B:2578:MET:HE3	1.73	0.52
1:G:979:PRO:O	1:G:983:THR:HG23	2.09	0.52
1:G:3310:ASP:HA	1:G:3313:ASN:HD21	1.75	0.52
1:J:1676:LEU:HD22	1:J:2167:ILE:HD12	1.90	0.52
1:J:3144:PHE:CD2	1:J:3197:LEU:HB3	2.45	0.52
1:J:3285:TRP:HE1	1:J:3306:ALA:HB3	1.73	0.52
1:J:3442:PHE:CD2	1:J:3514:LEU:HD11	2.44	0.52
1:J:3691:GLU:HG2	1:J:3692:GLU:HG3	1.92	0.52
1:E:3555:ASN:O	1:E:3558:HIS:ND1	2.37	0.52
1:E:4134:GLU:HB3	1:E:4135:PRO:HD3	1.90	0.52
1:G:1958:LEU:HD23	1:G:2138:LEU:HD21	1.92	0.52
1:G:3287:ARG:HG2	1:G:3294:PRO:HD2	1.90	0.52
1:G:3579:LEU:HD12	1:G:3580:PRO:HD2	1.90	0.52
2:I:68:LEU:HD13	2:I:106:LEU:HB2	1.92	0.52
3:C:14:ALA:HA	3:C:85:LEU:HB2	1.92	0.52
3:F:14:ALA:HA	3:F:85:LEU:HB2	1.92	0.52
3:K:14:ALA:HA	3:K:85:LEU:HB2	1.92	0.52
1:B:291:LEU:HD11	1:B:299:LEU:HD12	1.92	0.52
1:B:1958:LEU:HD23	1:B:2138:LEU:HD21	1.92	0.52
1:E:1263:THR:OG1	1:E:1266:THR:OG1	2.26	0.52
1:E:3293:PRO:HD2	1:E:3296:LEU:HD22	1.92	0.52
1:E:3442:PHE:CD2	1:E:3514:LEU:HD11	2.44	0.52
1:G:196:MET:HE2	1:G:196:MET:H	1.74	0.52
1:G:2710:LEU:HD21	1:G:2955:PHE:HE2	1.75	0.52
1:G:2968:ASP:O	1:G:2971:GLN:HG2	2.10	0.52
1:G:3893:GLU:HA	1:G:3967:GLU:OE2	2.08	0.52
1:J:3137:LEU:HB3	1:J:3138:PRO:HD3	1.92	0.52
3:M:14:ALA:HA	3:M:85:LEU:HB2	1.92	0.52
1:B:411:TYR:HB2	1:B:486:LEU:HD21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:867:LEU:HA	1:B:871:ARG:HG2	1.92	0.52
1:B:2573:GLU:OE1	1:B:2573:GLU:N	2.42	0.52
1:B:2871:LEU:HG	1:B:2927:LEU:HD11	1.91	0.52
1:B:3137:LEU:HB3	1:B:3138:PRO:HD3	1.92	0.52
1:B:3290:GLU:HG3	1:B:3307:VAL:HG22	1.92	0.52
1:E:3287:ARG:HG2	1:E:3294:PRO:HD2	1.90	0.52
1:G:2751:LEU:O	1:G:2755:ILE:HG12	2.10	0.52
1:G:4670:ILE:O	1:G:4674:GLU:HG3	2.10	0.52
1:J:595:ARG:HH22	1:J:1642:PRO:HD2	1.75	0.52
1:B:881:LEU:O	1:B:885:THR:HG23	2.10	0.51
1:B:2968:ASP:O	1:B:2971:GLN:HG2	2.10	0.51
1:E:3368:ARG:HH21	1:E:3401:LEU:HD23	1.74	0.51
1:E:4137:ARG:NH2	1:E:4196:GLU:OE2	2.43	0.51
1:E:5013:MET:HG2	1:E:5018:CYS:HB2	1.92	0.51
1:G:595:ARG:HH22	1:G:1642:PRO:HD2	1.75	0.51
1:G:3369:ALA:HA	1:G:3401:LEU:HD11	1.91	0.51
1:J:510:GLU:OE1	1:J:510:GLU:N	2.43	0.51
1:J:2575:ARG:HH21	1:J:2578:MET:HE3	1.73	0.51
1:J:2751:LEU:O	1:J:2755:ILE:HG12	2.10	0.51
2:A:68:LEU:HD13	2:A:106:LEU:HB2	1.92	0.51
1:B:595:ARG:HH22	1:B:1642:PRO:HD2	1.75	0.51
1:B:858:THR:HG21	1:B:931:THR:HG23	1.92	0.51
1:B:924:MET:HE1	3:C:106:PRO:CB	2.40	0.51
1:B:3293:PRO:HD2	1:B:3296:LEU:HD22	1.92	0.51
1:E:291:LEU:HD11	1:E:299:LEU:HD12	1.92	0.51
1:G:1623:ARG:NE	1:G:1623:ARG:O	2.43	0.51
1:G:3037:GLU:HG2	1:G:3088:VAL:HG21	1.93	0.51
1:G:3290:GLU:HG3	1:G:3307:VAL:HG22	1.92	0.51
1:J:196:MET:HE2	1:J:196:MET:N	2.25	0.51
1:J:231:LEU:O	1:J:260:TRP:NE1	2.41	0.51
1:J:618:GLN:OE1	1:J:1678:ASN:ND2	2.38	0.51
1:J:2968:ASP:O	1:J:2971:GLN:HG2	2.10	0.51
3:C:39:GLN:OE1	3:C:45:ARG:NH2	2.39	0.51
1:B:3037:GLU:HG2	1:B:3088:VAL:HG21	1.93	0.51
1:B:3369:ALA:HA	1:B:3401:LEU:HD11	1.91	0.51
1:E:2767:ALA:HB2	1:E:2791:LEU:HD11	1.92	0.51
1:G:266:ARG:HH12	1:G:273:HIS:HE1	1.58	0.51
1:G:867:LEU:HA	1:G:871:ARG:HG2	1.92	0.51
1:G:3959:LYS:HG3	1:G:4022:ASP:OD2	2.10	0.51
1:J:881:LEU:O	1:J:885:THR:HG23	2.10	0.51
1:J:3539:ARG:HB3	1:J:3544:ASP:CG	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:30:LEU:HD23	2:H:36:PHE:HE2	1.75	0.51
2:H:68:LEU:HD13	2:H:106:LEU:HB2	1.92	0.51
3:M:69:ILE:HB	3:M:80:LEU:HD13	1.92	0.51
1:B:758:ARG:HH21	1:B:802:PHE:HB2	1.75	0.51
1:E:758:ARG:HH21	1:E:802:PHE:HB2	1.76	0.51
1:E:3043:PHE:HE2	1:E:3072:ALA:HA	1.76	0.51
1:E:3539:ARG:HB3	1:E:3544:ASP:CG	2.36	0.51
1:G:1000:ARG:NH2	3:M:115:ASP:O	2.43	0.51
1:J:858:THR:HG21	1:J:931:THR:HG23	1.92	0.51
2:A:30:LEU:HD23	2:A:36:PHE:HE2	1.75	0.51
1:B:979:PRO:O	1:B:983:THR:HG23	2.10	0.51
1:B:4069:LYS:HD2	1:B:4133:GLN:HG3	1.91	0.51
1:E:1958:LEU:HD23	1:E:2138:LEU:HD21	1.92	0.51
1:E:2871:LEU:HG	1:E:2927:LEU:HD11	1.91	0.51
1:E:3137:LEU:O	1:E:3141:THR:OG1	2.28	0.51
1:E:3369:ALA:HA	1:E:3401:LEU:HD11	1.91	0.51
1:G:881:LEU:O	1:G:885:THR:HG23	2.10	0.51
1:G:2767:ALA:HB2	1:G:2791:LEU:HD11	1.92	0.51
1:G:3691:GLU:HG2	1:G:3692:GLU:HG3	1.92	0.51
1:J:758:ARG:HH21	1:J:802:PHE:HB2	1.76	0.51
1:J:3293:PRO:HD2	1:J:3296:LEU:HD22	1.92	0.51
1:J:4761:PRO:HB2	1:J:4766:THR:HG21	1.92	0.51
1:B:1623:ARG:NE	1:B:1623:ARG:O	2.43	0.51
1:B:2767:ALA:HB2	1:B:2791:LEU:HD11	1.92	0.51
1:E:4761:PRO:HB2	1:E:4766:THR:HG21	1.92	0.51
1:G:411:TYR:HB2	1:G:486:LEU:HD21	1.92	0.51
1:G:4137:ARG:NH2	1:G:4196:GLU:OE2	2.43	0.51
1:J:266:ARG:HH12	1:J:273:HIS:HE1	1.58	0.51
1:J:3097:GLU:HA	1:J:3167:ARG:HH12	1.76	0.51
1:J:3529:ASP:O	1:J:3533:ILE:HG13	2.11	0.51
3:M:13:GLN:OE1	3:M:13:GLN:N	2.37	0.51
1:E:25:SER:HA	1:E:34:LYS:HA	1.93	0.51
1:E:881:LEU:O	1:E:885:THR:HG23	2.10	0.51
1:E:2751:LEU:O	1:E:2755:ILE:HG12	2.10	0.51
1:E:4936:ILE:HD11	1:J:4931:ILE:HG12	1.92	0.51
1:G:291:LEU:HD11	1:G:299:LEU:HD12	1.93	0.51
1:G:2496:PRO:HG3	1:G:2550:LEU:HD23	1.93	0.51
1:G:2871:LEU:HG	1:G:2927:LEU:HD11	1.91	0.51
1:G:3195:ALA:HA	1:G:3279:SER:HA	1.93	0.51
1:G:3539:ARG:HB3	1:G:3544:ASP:CG	2.35	0.51
1:J:25:SER:HA	1:J:34:LYS:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:291:LEU:HD11	1:J:299:LEU:HD12	1.93	0.51
1:J:411:TYR:HB2	1:J:486:LEU:HD21	1.92	0.51
1:J:3043:PHE:HE2	1:J:3072:ALA:HA	1.76	0.51
1:J:3163:VAL:O	1:J:3167:ARG:HG2	2.11	0.51
1:J:5013:MET:HG2	1:J:5018:CYS:HB2	1.92	0.51
3:K:105:ASN:ND2	3:K:107:TRP:HD1	2.06	0.51
1:B:1110:ARG:NH2	1:B:1112:ASP:OD1	2.44	0.51
1:B:1249:PRO:HG2	1:B:1252:HIS:HB2	1.92	0.51
1:B:1780:PRO:O	2:A:42:ARG:NH1	2.43	0.51
1:B:2686:LEU:HG	1:B:2997:PHE:CE2	2.46	0.51
1:B:3137:LEU:O	1:B:3141:THR:OG1	2.28	0.51
1:E:3753:PHE:HZ	1:E:4718:LYS:HD3	1.76	0.51
1:G:1249:PRO:HG2	1:G:1252:HIS:HB2	1.92	0.51
1:G:3222:LYS:HB3	1:G:3226:GLU:HB2	1.93	0.51
1:G:4069:LYS:HD2	1:G:4133:GLN:HG3	1.91	0.51
1:J:1249:PRO:HG2	1:J:1252:HIS:HB2	1.92	0.51
1:J:3030:HIS:HB2	1:J:3035:GLU:HG2	1.93	0.51
1:J:3446:SER:HA	1:J:3452:LYS:HE3	1.93	0.51
2:D:68:LEU:HD13	2:D:106:LEU:HB2	1.92	0.51
1:B:25:SER:HA	1:B:34:LYS:HA	1.93	0.51
1:B:1011:GLN:OE1	1:B:1020:ARG:NH2	2.35	0.51
1:B:2495:VAL:HG12	1:B:2497:ASP:H	1.76	0.51
1:B:3753:PHE:HZ	1:B:4718:LYS:HD3	1.76	0.51
1:B:4137:ARG:NH2	1:B:4196:GLU:OE2	2.43	0.51
1:E:1110:ARG:NH2	1:E:1112:ASP:OD1	2.44	0.51
1:E:4670:ILE:O	1:E:4674:GLU:HG3	2.10	0.51
1:G:25:SER:HA	1:G:34:LYS:HA	1.93	0.51
1:G:866:HIS:HB3	1:G:929:LEU:HD13	1.93	0.51
1:G:2110:TYR:HB2	1:G:3694:LYS:HA	1.93	0.51
1:G:3293:PRO:HD2	1:G:3296:LEU:HD22	1.92	0.51
1:G:3753:PHE:HZ	1:G:4718:LYS:HD3	1.76	0.51
1:J:1011:GLN:OE1	1:J:1020:ARG:NH2	2.35	0.51
1:J:2710:LEU:HD21	1:J:2955:PHE:HE2	1.75	0.51
1:J:4749:GLU:HG3	1:J:4753:HIS:CE1	2.46	0.51
3:F:69:ILE:HB	3:F:80:LEU:HD13	1.92	0.51
1:B:3893:GLU:HA	1:B:3967:GLU:OE2	2.11	0.51
1:E:2679:PHE:HB2	1:E:2706:ILE:HG21	1.93	0.51
1:E:3529:ASP:O	1:E:3533:ILE:HG13	2.11	0.51
1:E:4749:GLU:HG3	1:E:4753:HIS:CE1	2.46	0.51
1:G:758:ARG:HH21	1:G:802:PHE:HB2	1.75	0.51
1:G:858:THR:HG21	1:G:931:THR:HG23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1110:ARG:NH2	1:G:1112:ASP:OD1	2.44	0.51
1:G:3030:HIS:HB2	1:G:3035:GLU:HG2	1.93	0.51
1:G:5013:MET:HG2	1:G:5018:CYS:HB2	1.92	0.51
1:J:1958:LEU:HD23	1:J:2138:LEU:HD21	1.92	0.51
1:J:2496:PRO:HG3	1:J:2550:LEU:HD23	1.93	0.51
3:M:2:VAL:HG22	3:M:27:SER:H	1.76	0.51
1:B:2679:PHE:HB2	1:B:2706:ILE:HG21	1.93	0.50
1:B:3539:ARG:HB3	1:B:3544:ASP:CG	2.36	0.50
1:E:858:THR:HG21	1:E:931:THR:HG23	1.93	0.50
1:J:2686:LEU:HG	1:J:2997:PHE:CE2	2.46	0.50
1:B:866:HIS:HB3	1:B:929:LEU:HD13	1.93	0.50
1:B:2751:LEU:O	1:B:2755:ILE:HG12	2.10	0.50
1:B:3097:GLU:HA	1:B:3167:ARG:HH12	1.76	0.50
1:B:4670:ILE:O	1:B:4674:GLU:HG3	2.10	0.50
1:E:618:GLN:OE1	1:E:1678:ASN:ND2	2.38	0.50
1:E:867:LEU:HA	1:E:871:ARG:HG2	1.92	0.50
1:E:2686:LEU:HG	1:E:2997:PHE:CE2	2.46	0.50
1:E:2710:LEU:HD21	1:E:2955:PHE:HE2	1.75	0.50
1:E:3030:HIS:HB2	1:E:3035:GLU:HG2	1.93	0.50
1:E:3037:GLU:HG2	1:E:3088:VAL:HG21	1.93	0.50
1:G:2244:ARG:NH2	1:G:2283:ASN:OD1	2.44	0.50
1:G:4761:PRO:HB2	1:G:4766:THR:HG21	1.92	0.50
1:J:2110:TYR:HB2	1:J:3694:LYS:HA	1.93	0.50
2:I:30:LEU:HD23	2:I:36:PHE:HE2	1.75	0.50
3:C:69:ILE:HB	3:C:80:LEU:HD13	1.92	0.50
1:B:2244:ARG:NH2	1:B:2283:ASN:OD1	2.44	0.50
1:E:2495:VAL:HG12	1:E:2497:ASP:H	1.76	0.50
1:E:3097:GLU:HA	1:E:3167:ARG:HH12	1.76	0.50
1:E:3137:LEU:HB3	1:E:3138:PRO:HD3	1.92	0.50
1:E:3222:LYS:HB3	1:E:3226:GLU:HB2	1.93	0.50
1:G:657:THR:HB	1:G:1021:LEU:HD13	1.93	0.50
1:G:2495:VAL:HG12	1:G:2497:ASP:H	1.76	0.50
1:G:3446:SER:HA	1:G:3452:LYS:HE3	1.93	0.50
1:G:3604:TYR:O	1:G:3608:GLN:HG2	2.12	0.50
1:J:2767:ALA:HB2	1:J:2791:LEU:HD11	1.92	0.50
1:J:3037:GLU:HG2	1:J:3088:VAL:HG21	1.93	0.50
1:J:3354:LEU:O	1:J:3358:PHE:HD1	1.94	0.50
1:J:3604:TYR:O	1:J:3608:GLN:HG2	2.12	0.50
1:J:3753:PHE:HZ	1:J:4718:LYS:HD3	1.76	0.50
2:A:16:PRO:HB3	2:A:106:LEU:HD11	1.94	0.50
1:B:3555:ASN:O	1:B:3558:HIS:ND1	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4761:PRO:HB2	1:B:4766:THR:HG21	1.92	0.50
1:E:3435:PHE:CZ	1:E:3602:VAL:HG21	2.47	0.50
1:G:3043:PHE:HE2	1:G:3072:ALA:HA	1.76	0.50
1:J:867:LEU:HA	1:J:871:ARG:HG2	1.92	0.50
1:J:2679:PHE:HB2	1:J:2706:ILE:HG21	1.93	0.50
3:M:101:PRO:HG2	3:M:104:TYR:CE2	2.46	0.50
1:B:3043:PHE:HE2	1:B:3072:ALA:HA	1.76	0.50
1:E:926:GLY:O	1:E:930:LYS:HG3	2.11	0.50
1:G:2336:ARG:HB2	1:G:2435:ARG:HD2	1.93	0.50
1:G:3219:TYR:HA	1:G:3227:ARG:HD3	1.94	0.50
1:G:4749:GLU:HG3	1:G:4753:HIS:CE1	2.46	0.50
1:J:866:HIS:HB3	1:J:929:LEU:HD13	1.93	0.50
1:J:2495:VAL:HG12	1:J:2497:ASP:H	1.76	0.50
1:J:3222:LYS:HB3	1:J:3226:GLU:HB2	1.93	0.50
2:H:16:PRO:HB3	2:H:106:LEU:HD11	1.94	0.50
3:C:105:ASN:ND2	3:C:107:TRP:HD1	2.08	0.50
3:K:69:ILE:HB	3:K:80:LEU:HD13	1.92	0.50
1:B:510:GLU:OE1	1:B:510:GLU:N	2.43	0.50
1:B:2496:PRO:HG3	1:B:2550:LEU:HD23	1.93	0.50
1:B:2970:SER:HA	1:B:2973:PHE:CE2	2.47	0.50
1:B:3529:ASP:O	1:B:3533:ILE:HG13	2.11	0.50
1:B:3547:GLU:O	1:B:3551:GLU:HG2	2.12	0.50
1:B:5013:MET:HG2	1:B:5018:CYS:HB2	1.92	0.50
1:E:231:LEU:O	1:E:260:TRP:NE1	2.41	0.50
1:E:1249:PRO:HG2	1:E:1252:HIS:HB2	1.92	0.50
1:E:3163:VAL:O	1:E:3167:ARG:HG2	2.11	0.50
1:E:3195:ALA:HA	1:E:3279:SER:HA	1.93	0.50
1:E:3229:ILE:H	1:E:3229:ILE:HD12	1.77	0.50
1:E:3604:TYR:O	1:E:3608:GLN:HG2	2.12	0.50
1:G:2679:PHE:HB2	1:G:2706:ILE:HG21	1.93	0.50
1:G:3163:VAL:O	1:G:3167:ARG:HG2	2.11	0.50
1:J:1263:THR:OG1	1:J:1266:THR:OG1	2.26	0.50
1:B:926:GLY:O	1:B:930:LYS:HG3	2.12	0.50
1:B:3354:LEU:O	1:B:3358:PHE:HD1	1.94	0.50
1:B:3427:PRO:HD3	1:B:3579:LEU:HD21	1.94	0.50
1:E:2970:SER:HA	1:E:2973:PHE:CE2	2.47	0.50
1:E:3427:PRO:HD3	1:E:3579:LEU:HD21	1.94	0.50
1:E:4822:THR:HB	1:J:4839:MET:HE1	1.92	0.50
1:G:436:LEU:H	1:G:436:LEU:HD12	1.77	0.50
1:G:2686:LEU:HG	1:G:2997:PHE:CE2	2.46	0.50
1:G:2960:LEU:HB3	1:G:3038:MET:CE	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3097:GLU:HA	1:G:3167:ARG:HH12	1.76	0.50
1:G:3427:PRO:HD3	1:G:3579:LEU:HD21	1.94	0.50
1:G:3529:ASP:O	1:G:3533:ILE:HG13	2.10	0.50
1:J:657:THR:HB	1:J:1021:LEU:HD13	1.93	0.50
1:J:2336:ARG:HB2	1:J:2435:ARG:HD2	1.93	0.50
1:J:2388:GLU:O	1:J:2390:PRO:HD3	2.12	0.50
1:J:3195:ALA:HA	1:J:3279:SER:HA	1.93	0.50
1:J:3280:TYR:HE1	1:J:3283:ARG:HH21	1.60	0.50
2:D:30:LEU:HD23	2:D:36:PHE:HE2	1.75	0.50
1:B:2110:TYR:HB2	1:B:3694:LYS:HA	1.93	0.50
1:B:3222:LYS:HB3	1:B:3226:GLU:HB2	1.93	0.50
1:B:3229:ILE:H	1:B:3229:ILE:HD12	1.77	0.50
1:E:3333:THR:HG22	1:E:3337:ARG:CZ	2.42	0.50
1:G:3137:LEU:HB3	1:G:3138:PRO:HD3	1.92	0.50
1:G:4839:MET:HE1	1:J:4822:THR:HB	1.94	0.50
1:J:3229:ILE:H	1:J:3229:ILE:HD12	1.77	0.50
1:J:4137:ARG:NH2	1:J:4196:GLU:OE2	2.43	0.50
3:F:2:VAL:HG22	3:F:27:SER:H	1.76	0.50
3:M:39:GLN:OE1	3:M:45:ARG:NH2	2.39	0.50
1:B:3163:VAL:O	1:B:3167:ARG:HG2	2.11	0.50
1:B:3959:LYS:HG3	1:B:4022:ASP:OD2	2.11	0.50
1:B:4749:GLU:HG3	1:B:4753:HIS:CE1	2.46	0.50
1:E:657:THR:HB	1:E:1021:LEU:HD13	1.93	0.50
1:G:926:GLY:O	1:G:930:LYS:HG3	2.11	0.50
1:G:4828:SER:O	1:G:4832:HIS:HB3	2.12	0.50
1:J:883:ALA:HA	1:J:886:ARG:HE	1.77	0.50
1:B:3219:TYR:HA	1:B:3227:ARG:HD3	1.94	0.49
1:E:794:GLY:HA3	1:E:812:HIS:HB3	1.94	0.49
1:G:246:TYR:CD1	1:G:373:LYS:HE3	2.47	0.49
1:G:2388:GLU:O	1:G:2390:PRO:HD3	2.12	0.49
1:J:1110:ARG:NH2	1:J:1112:ASP:OD1	2.44	0.49
1:J:2454:ARG:HD2	1:J:2458:ARG:HH21	1.77	0.49
1:J:3427:PRO:HD3	1:J:3579:LEU:HD21	1.94	0.49
1:J:3435:PHE:CZ	1:J:3602:VAL:HG21	2.47	0.49
1:B:436:LEU:H	1:B:436:LEU:HD12	1.77	0.49
1:B:657:THR:HB	1:B:1021:LEU:HD13	1.94	0.49
1:B:4828:SER:O	1:B:4832:HIS:HB3	2.12	0.49
1:E:866:HIS:HB3	1:E:929:LEU:HD13	1.93	0.49
1:E:2110:TYR:HB2	1:E:3694:LYS:HA	1.93	0.49
1:G:3229:ILE:H	1:G:3229:ILE:HD12	1.77	0.49
1:G:3280:TYR:HE1	1:G:3283:ARG:HH21	1.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3547:GLU:O	1:G:3551:GLU:HG2	2.12	0.49
1:J:4731:ILE:HG22	1:J:4732:PHE:CD2	2.48	0.49
1:B:2960:LEU:HB3	1:B:3038:MET:CE	2.42	0.49
1:B:3195:ALA:HA	1:B:3279:SER:HA	1.93	0.49
1:E:510:GLU:N	1:E:510:GLU:OE1	2.43	0.49
1:E:2496:PRO:HG3	1:E:2550:LEU:HD23	1.93	0.49
1:E:2578:MET:SD	1:E:2578:MET:N	2.86	0.49
1:G:710:ASP:OD1	1:G:711:LEU:N	2.46	0.49
1:G:883:ALA:HA	1:G:886:ARG:HE	1.77	0.49
1:G:3354:LEU:O	1:G:3358:PHE:HD1	1.94	0.49
1:G:3688:GLU:N	1:G:3688:GLU:OE1	2.46	0.49
1:G:4744:ASP:HB3	1:G:4747:SER:HB3	1.95	0.49
1:J:794:GLY:HA3	1:J:812:HIS:HB3	1.94	0.49
1:J:4828:SER:O	1:J:4832:HIS:HB3	2.12	0.49
1:B:3604:TYR:O	1:B:3608:GLN:HG2	2.11	0.49
1:B:3688:GLU:N	1:B:3688:GLU:OE1	2.46	0.49
1:B:4097:MET:SD	1:B:4108:ILE:HD12	2.53	0.49
1:B:4202:ARG:O	1:B:4206:GLU:HG2	2.12	0.49
1:E:2244:ARG:NH2	1:E:2283:ASN:OD1	2.44	0.49
1:E:3219:TYR:HA	1:E:3227:ARG:HD3	1.94	0.49
1:E:3446:SER:HA	1:E:3452:LYS:HE3	1.93	0.49
1:G:510:GLU:OE1	1:G:510:GLU:N	2.43	0.49
1:G:4097:MET:SD	1:G:4108:ILE:HD12	2.53	0.49
1:J:4202:ARG:O	1:J:4206:GLU:HG2	2.12	0.49
3:F:90:THR:HG23	3:F:124:THR:HA	1.95	0.49
3:K:2:VAL:HG22	3:K:27:SER:H	1.76	0.49
1:B:883:ALA:HA	1:B:886:ARG:HE	1.78	0.49
1:B:3042:LEU:HD22	1:B:3071:LEU:HD11	1.95	0.49
1:E:883:ALA:HA	1:E:886:ARG:HE	1.78	0.49
1:E:2454:ARG:HD2	1:E:2458:ARG:HH21	1.77	0.49
1:E:3052:HIS:C	1:E:3053:ARG:HD2	2.38	0.49
1:E:4097:MET:SD	1:E:4108:ILE:HD12	2.53	0.49
1:G:210:GLU:HB2	1:G:215:THR:HG22	1.95	0.49
1:G:1037:ASP:O	1:G:1041:GLN:HG2	2.12	0.49
1:G:2970:SER:HA	1:G:2973:PHE:CE2	2.47	0.49
1:G:3052:HIS:C	1:G:3053:ARG:HD2	2.38	0.49
1:G:3097:GLU:O	1:G:3167:ARG:NH2	2.44	0.49
1:J:210:GLU:HB2	1:J:215:THR:HG22	1.95	0.49
1:J:2578:MET:SD	1:J:2578:MET:N	2.86	0.49
1:J:2970:SER:HA	1:J:2973:PHE:CE2	2.47	0.49
1:J:3688:GLU:N	1:J:3688:GLU:OE1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:30:LEU:HD23	2:D:36:PHE:CE2	2.48	0.49
2:I:30:LEU:HD23	2:I:36:PHE:CE2	2.48	0.49
3:C:2:VAL:HG22	3:C:27:SER:H	1.76	0.49
3:M:90:THR:HG23	3:M:124:THR:HA	1.95	0.49
1:B:2336:ARG:HB2	1:B:2435:ARG:HD2	1.93	0.49
1:B:3435:PHE:CZ	1:B:3602:VAL:HG21	2.47	0.49
1:B:3446:SER:HA	1:B:3452:LYS:HE3	1.93	0.49
1:E:3354:LEU:O	1:E:3358:PHE:HD1	1.94	0.49
1:E:3547:GLU:O	1:E:3551:GLU:HG2	2.12	0.49
1:E:4828:SER:O	1:E:4832:HIS:HB3	2.12	0.49
1:G:3333:THR:HG22	1:G:3337:ARG:CZ	2.42	0.49
1:J:371:VAL:HG12	1:J:373:LYS:H	1.78	0.49
1:J:926:GLY:O	1:J:930:LYS:HG3	2.12	0.49
1:J:1037:ASP:O	1:J:1041:GLN:HG2	2.12	0.49
1:J:3547:GLU:O	1:J:3551:GLU:HG2	2.12	0.49
3:C:90:THR:HG23	3:C:124:THR:HA	1.95	0.49
1:B:2970:SER:HA	1:B:2973:PHE:CD2	2.48	0.49
1:B:3315:LEU:HD13	1:B:3341:PHE:HE2	1.77	0.49
1:B:3333:THR:HG22	1:B:3337:ARG:CZ	2.42	0.49
1:B:4876:CYS:HA	1:B:4882:CYS:HB2	1.95	0.49
1:E:359:TYR:HA	1:E:376:ALA:HA	1.95	0.49
1:G:371:VAL:HG12	1:G:373:LYS:H	1.77	0.49
1:G:897:ARG:HD3	1:G:905:PRO:HD3	1.95	0.49
1:G:2578:MET:SD	1:G:2578:MET:N	2.86	0.49
1:J:897:ARG:HD3	1:J:905:PRO:HD3	1.95	0.49
1:J:3219:TYR:HA	1:J:3227:ARG:HD3	1.94	0.49
2:A:4:ILE:HD11	2:A:62:GLY:HA2	1.95	0.49
3:K:90:THR:HG23	3:K:124:THR:HA	1.95	0.49
1:B:4931:ILE:HG12	1:G:4936:ILE:HD11	1.94	0.49
1:E:210:GLU:HB2	1:E:215:THR:HG22	1.95	0.49
1:E:1476:MET:HB2	1:E:1485:SER:HB2	1.95	0.49
1:E:2638:LYS:HB2	1:E:2639:MET:CE	2.43	0.49
1:E:2970:SER:HA	1:E:2973:PHE:CD2	2.48	0.49
1:G:721:LEU:HG	1:G:730:VAL:HG21	1.95	0.49
1:G:4731:ILE:HG22	1:G:4732:PHE:CD2	2.48	0.49
1:G:4931:ILE:HG12	1:J:4936:ILE:HD11	1.94	0.49
1:J:27:THR:HG23	1:J:32:GLN:HG3	1.95	0.49
1:J:246:TYR:CD1	1:J:373:LYS:HE3	2.48	0.49
1:J:1042:ALA:O	1:J:1046:LEU:HG	2.13	0.49
1:J:2638:LYS:HB2	1:J:2639:MET:CE	2.43	0.49
1:J:3052:HIS:C	1:J:3053:ARG:HD2	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:16:PRO:HB3	2:I:106:LEU:HD11	1.94	0.49
1:B:246:TYR:CD1	1:B:373:LYS:HE3	2.48	0.49
1:B:2454:ARG:HD2	1:B:2458:ARG:HH21	1.77	0.49
1:B:2578:MET:SD	1:B:2578:MET:N	2.86	0.49
1:B:4744:ASP:HB3	1:B:4747:SER:HB3	1.95	0.49
1:E:359:TYR:HE1	1:E:385:ASP:HB2	1.77	0.49
1:E:783:PHE:HB2	1:E:787:VAL:HG11	1.94	0.49
1:E:1042:ALA:O	1:E:1046:LEU:HG	2.13	0.49
1:E:2336:ARG:HB2	1:E:2435:ARG:HD2	1.93	0.49
1:G:27:THR:HG23	1:G:32:GLN:HG3	1.95	0.49
1:G:4202:ARG:O	1:G:4206:GLU:HG2	2.12	0.49
1:J:2244:ARG:NH2	1:J:2283:ASN:OD1	2.44	0.49
1:J:2991:HIS:O	1:J:2995:ILE:HG13	2.13	0.49
1:B:27:THR:HG23	1:B:32:GLN:HG3	1.95	0.49
1:B:710:ASP:OD1	1:B:711:LEU:N	2.46	0.49
1:B:1037:ASP:O	1:B:1041:GLN:HG2	2.12	0.49
1:B:2377:LEU:O	1:B:2381:GLU:HG2	2.13	0.49
1:B:3030:HIS:HB2	1:B:3035:GLU:HG2	1.93	0.49
1:B:3443:ILE:O	1:B:3447:LYS:HG3	2.13	0.49
1:B:4936:ILE:HD11	1:E:4931:ILE:HG12	1.93	0.49
1:E:222:LEU:O	1:E:223:PHE:HD1	1.96	0.49
1:E:2325:PRO:HB2	1:E:2421:ALA:HB1	1.95	0.49
1:E:2388:GLU:O	1:E:2390:PRO:HD3	2.12	0.49
1:E:4731:ILE:HG22	1:E:4732:PHE:CD2	2.48	0.49
1:G:251:ALA:O	1:G:255:HIS:ND1	2.40	0.49
1:G:783:PHE:HB2	1:G:787:VAL:HG11	1.94	0.49
1:G:1690:ASP:OD2	1:G:1693:GLN:NE2	2.46	0.49
1:G:4696:ASP:O	1:G:4700:GLN:HG2	2.13	0.49
1:J:251:ALA:O	1:J:255:HIS:ND1	2.40	0.49
1:J:747:CYS:SG	1:J:756:SER:HB2	2.53	0.49
1:J:3315:LEU:HD13	1:J:3341:PHE:HE2	1.77	0.49
2:I:4:ILE:HD11	2:I:62:GLY:HA2	1.95	0.49
1:B:210:GLU:HB2	1:B:215:THR:HG22	1.95	0.48
1:B:2325:PRO:HB2	1:B:2421:ALA:HB1	1.95	0.48
1:B:3052:HIS:C	1:B:3053:ARG:HD2	2.38	0.48
1:B:3183:VAL:O	1:B:3187:ARG:HG3	2.13	0.48
1:B:4235:VAL:HG11	1:B:5019:TRP:CH2	2.48	0.48
1:E:436:LEU:H	1:E:436:LEU:HD12	1.77	0.48
1:E:863:LEU:HD21	1:E:939:VAL:HG21	1.95	0.48
1:E:2960:LEU:HB3	1:E:3038:MET:CE	2.42	0.48
1:E:3183:VAL:O	1:E:3187:ARG:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3280:TYR:HE1	1:E:3283:ARG:HH21	1.60	0.48
1:E:3437:MET:O	1:E:3441:ILE:HG13	2.13	0.48
1:G:2325:PRO:HB2	1:G:2421:ALA:HB1	1.95	0.48
1:G:3435:PHE:CZ	1:G:3602:VAL:HG21	2.47	0.48
1:G:3437:MET:O	1:G:3441:ILE:HG13	2.13	0.48
1:J:222:LEU:O	1:J:223:PHE:HD1	1.96	0.48
1:J:863:LEU:HD21	1:J:939:VAL:HG21	1.95	0.48
1:J:3416:VAL:HB	1:J:3516:LYS:HZ1	1.75	0.48
1:J:3534:MET:O	1:J:3538:THR:HG23	2.13	0.48
1:J:4104:THR:O	1:J:4108:ILE:HG12	2.13	0.48
2:D:4:ILE:HD11	2:D:62:GLY:HA2	1.95	0.48
1:B:897:ARG:HD3	1:B:905:PRO:HD3	1.95	0.48
1:B:2504:LEU:O	1:B:2508:ARG:HG2	2.14	0.48
1:B:2700:MET:CE	1:B:2701:PRO:HD3	2.43	0.48
1:B:4731:ILE:HG22	1:B:4732:PHE:CD2	2.48	0.48
1:B:4943:LEU:O	1:B:4947:GLN:HG2	2.13	0.48
1:E:27:THR:HG23	1:E:32:GLN:HG3	1.95	0.48
1:E:2991:HIS:O	1:E:2995:ILE:HG13	2.13	0.48
1:E:4235:VAL:HG11	1:E:5019:TRP:CH2	2.48	0.48
1:G:794:GLY:HA3	1:G:812:HIS:HB3	1.94	0.48
1:G:3352:GLU:CD	1:G:3352:GLU:H	2.22	0.48
1:G:4104:THR:O	1:G:4108:ILE:HG12	2.13	0.48
1:J:436:LEU:H	1:J:436:LEU:HD12	1.77	0.48
1:J:728:ARG:HE	1:J:1487:LEU:HD12	1.78	0.48
1:J:2960:LEU:HB3	1:J:3038:MET:CE	2.42	0.48
2:D:16:PRO:HB3	2:D:106:LEU:HD11	1.94	0.48
1:B:230:CYS:SG	1:B:231:LEU:HG	2.53	0.48
1:B:728:ARG:HE	1:B:1487:LEU:HD12	1.78	0.48
1:B:747:CYS:SG	1:B:756:SER:HB2	2.53	0.48
1:B:1042:ALA:O	1:B:1046:LEU:HG	2.13	0.48
1:B:2388:GLU:O	1:B:2390:PRO:HD3	2.12	0.48
1:E:747:CYS:SG	1:E:756:SER:HB2	2.53	0.48
1:E:2294:ASP:HA	1:E:2297:LYS:HE2	1.95	0.48
1:E:2504:LEU:O	1:E:2508:ARG:HG2	2.14	0.48
1:E:3206:LEU:H	1:E:3206:LEU:HD12	1.79	0.48
1:G:230:CYS:SG	1:G:231:LEU:HG	2.54	0.48
1:G:1476:MET:HB2	1:G:1485:SER:HB2	1.95	0.48
1:G:2689:LYS:HG2	1:G:2690:LYS:H	1.78	0.48
1:G:3315:LEU:HD13	1:G:3341:PHE:HE2	1.77	0.48
1:G:4876:CYS:HA	1:G:4882:CYS:HB2	1.95	0.48
1:G:4943:LEU:O	1:G:4947:GLN:HG2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:3042:LEU:HD22	1:J:3071:LEU:HD11	1.95	0.48
1:J:3206:LEU:HD12	1:J:3206:LEU:H	1.79	0.48
1:J:4696:ASP:O	1:J:4700:GLN:HG2	2.13	0.48
1:J:4744:ASP:HB3	1:J:4747:SER:HB3	1.95	0.48
2:H:4:ILE:HD11	2:H:62:GLY:HA2	1.95	0.48
3:F:18:LEU:HD21	3:F:85:LEU:HD11	1.95	0.48
3:K:18:LEU:HD21	3:K:85:LEU:HD11	1.96	0.48
1:B:252:VAL:HA	1:B:255:HIS:HB2	1.96	0.48
1:B:266:ARG:HH12	1:B:273:HIS:HE1	1.58	0.48
1:B:1423:ASP:O	1:B:1427:ILE:HG12	2.14	0.48
1:B:1973:GLN:NE2	1:B:2005:GLN:OE1	2.47	0.48
1:E:1037:ASP:O	1:E:1041:GLN:HG2	2.12	0.48
1:E:1423:ASP:O	1:E:1427:ILE:HG12	2.14	0.48
1:E:3443:ILE:O	1:E:3447:LYS:HG3	2.13	0.48
1:E:3688:GLU:OE1	1:E:3688:GLU:N	2.45	0.48
1:E:4696:ASP:O	1:E:4700:GLN:HG2	2.13	0.48
1:G:470:SER:HA	1:G:473:ASN:HD21	1.77	0.48
1:G:747:CYS:SG	1:G:756:SER:HB2	2.53	0.48
1:G:863:LEU:HD21	1:G:939:VAL:HG21	1.95	0.48
1:G:1042:ALA:O	1:G:1046:LEU:HG	2.13	0.48
1:G:3042:LEU:HD22	1:G:3071:LEU:HD11	1.95	0.48
1:J:252:VAL:HA	1:J:255:HIS:HB2	1.96	0.48
1:J:1786:LEU:HD12	1:J:1787:PRO:HD2	1.96	0.48
1:J:2377:LEU:O	1:J:2381:GLU:HG2	2.13	0.48
1:J:4097:MET:SD	1:J:4108:ILE:HD12	2.53	0.48
1:B:213:TYR:HD1	1:B:340:LYS:HA	1.79	0.48
1:B:783:PHE:HB2	1:B:787:VAL:HG11	1.95	0.48
1:B:1476:MET:HB2	1:B:1485:SER:HB2	1.95	0.48
1:B:2689:LYS:HG2	1:B:2690:LYS:H	1.78	0.48
1:B:3352:GLU:CD	1:B:3352:GLU:H	2.21	0.48
1:B:4184:MET:O	1:B:4184:MET:HE3	2.14	0.48
1:E:230:CYS:SG	1:E:231:LEU:HG	2.53	0.48
1:E:299:LEU:CD2	1:E:378:LEU:HG	2.44	0.48
1:E:1786:LEU:HD12	1:E:1787:PRO:HD2	1.96	0.48
1:E:4202:ARG:O	1:E:4206:GLU:HG2	2.12	0.48
1:G:1423:ASP:O	1:G:1427:ILE:HG12	2.14	0.48
1:G:1973:GLN:NE2	1:G:2005:GLN:OE1	2.47	0.48
1:G:3443:ILE:O	1:G:3447:LYS:HG3	2.13	0.48
1:J:2325:PRO:HB2	1:J:2421:ALA:HB1	1.95	0.48
1:J:3097:GLU:O	1:J:3167:ARG:NH2	2.44	0.48
1:J:4109:GLN:HA	1:J:4112:LEU:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:470:SER:HA	1:B:473:ASN:HD21	1.77	0.48
1:B:721:LEU:HG	1:B:730:VAL:HG21	1.95	0.48
1:B:794:GLY:HA3	1:B:812:HIS:HB3	1.94	0.48
1:B:993:HIS:CE1	1:B:1027:LEU:HD11	2.49	0.48
1:B:2328:GLY:HA3	1:B:2425:PHE:HE2	1.79	0.48
1:B:2638:LYS:HB2	1:B:2639:MET:CE	2.43	0.48
1:B:2991:HIS:O	1:B:2995:ILE:HG13	2.13	0.48
1:B:3280:TYR:HE1	1:B:3283:ARG:HH21	1.60	0.48
1:B:3437:MET:O	1:B:3441:ILE:HG13	2.13	0.48
1:B:4696:ASP:O	1:B:4700:GLN:HG2	2.13	0.48
1:E:911:HIS:HB2	1:E:918:ARG:NE	2.29	0.48
1:E:2377:LEU:O	1:E:2381:GLU:HG2	2.13	0.48
1:E:3534:MET:O	1:E:3538:THR:HG23	2.13	0.48
1:G:222:LEU:O	1:G:223:PHE:HD1	1.96	0.48
1:G:252:VAL:HA	1:G:255:HIS:HB2	1.96	0.48
1:G:4235:VAL:HG11	1:G:5019:TRP:CH2	2.48	0.48
1:J:783:PHE:HB2	1:J:787:VAL:HG11	1.94	0.48
1:J:869:ARG:O	1:J:873:LYS:HG3	2.14	0.48
1:J:1423:ASP:O	1:J:1427:ILE:HG12	2.14	0.48
1:J:1476:MET:HB2	1:J:1485:SER:HB2	1.95	0.48
1:J:3352:GLU:HG2	1:J:3353:LEU:H	1.79	0.48
1:J:3850:GLN:HB2	1:J:3873:LYS:HG3	1.96	0.48
1:J:4184:MET:O	1:J:4184:MET:HE3	2.14	0.48
1:J:4235:VAL:HG11	1:J:5019:TRP:CH2	2.49	0.48
2:A:30:LEU:HD23	2:A:36:PHE:CE2	2.48	0.48
3:C:51:ILE:HG23	3:C:71:ARG:HD2	1.96	0.48
3:M:40:ALA:HB3	3:M:43:LYS:HB3	1.96	0.48
1:B:222:LEU:O	1:B:223:PHE:HD1	1.96	0.48
1:B:869:ARG:O	1:B:873:LYS:HG3	2.14	0.48
1:B:1786:LEU:HD12	1:B:1787:PRO:HD2	1.96	0.48
1:B:2294:ASP:HA	1:B:2297:LYS:HE2	1.95	0.48
1:B:4109:GLN:HA	1:B:4112:LEU:HD12	1.96	0.48
1:E:266:ARG:HH12	1:E:273:HIS:HE1	1.58	0.48
1:E:710:ASP:OD1	1:E:711:LEU:N	2.46	0.48
1:G:911:HIS:HB2	1:G:918:ARG:NE	2.29	0.48
1:G:2504:LEU:O	1:G:2508:ARG:HG2	2.14	0.48
1:G:3068:LEU:HA	1:G:3071:LEU:HD12	1.95	0.48
1:G:4184:MET:O	1:G:4184:MET:HE3	2.14	0.48
1:J:470:SER:HA	1:J:473:ASN:HD21	1.77	0.48
1:J:710:ASP:OD1	1:J:711:LEU:N	2.46	0.48
1:J:3183:VAL:O	1:J:3187:ARG:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:4230:LYS:NZ	1:J:4231:MET:SD	2.84	0.48
1:J:4943:LEU:O	1:J:4947:GLN:HG2	2.14	0.48
3:K:104:TYR:C	3:K:104:TYR:CD1	2.92	0.48
1:B:3534:MET:O	1:B:3538:THR:HG23	2.13	0.48
1:E:213:TYR:HD1	1:E:340:LYS:HA	1.79	0.48
1:E:470:SER:HA	1:E:473:ASN:HD21	1.77	0.48
1:E:3537:LYS:HD3	1:E:3600:SER:HB2	1.96	0.48
1:G:2454:ARG:HD2	1:G:2458:ARG:HH21	1.77	0.48
1:G:3352:GLU:HG2	1:G:3353:LEU:H	1.79	0.48
1:G:4109:GLN:HA	1:G:4112:LEU:HD12	1.96	0.48
1:J:993:HIS:CE1	1:J:1027:LEU:HD11	2.49	0.48
1:J:1180:ARG:HG3	1:J:1181:GLU:HG3	1.96	0.48
1:J:2970:SER:HA	1:J:2973:PHE:CD2	2.48	0.48
1:J:3333:THR:HG22	1:J:3337:ARG:CZ	2.42	0.48
1:J:3437:MET:O	1:J:3441:ILE:HG13	2.13	0.48
1:J:3550:ARG:O	1:J:3554:GLN:HG2	2.14	0.48
3:C:18:LEU:HD21	3:C:85:LEU:HD11	1.96	0.48
3:M:18:LEU:HD21	3:M:85:LEU:HD11	1.96	0.48
3:M:100:VAL:HG22	3:M:105:ASN:HB2	1.96	0.48
1:B:1690:ASP:OD2	1:B:1693:GLN:NE2	2.46	0.48
1:B:2751:LEU:HD12	1:B:2754:PHE:HD2	1.79	0.48
1:B:3752:SER:HB2	1:B:3755:GLU:HG3	1.96	0.48
1:B:4574:ASN:ND2	1:B:4813:LEU:HG	2.29	0.48
1:E:266:ARG:NH2	1:E:273:HIS:O	2.47	0.48
1:E:638:ILE:HD11	1:E:1636:MET:HE2	1.96	0.48
1:E:870:ILE:O	1:E:874:LEU:HG	2.14	0.48
1:E:897:ARG:HD3	1:E:905:PRO:HD3	1.95	0.48
1:G:728:ARG:HE	1:G:1487:LEU:HD12	1.78	0.48
1:G:2377:LEU:O	1:G:2381:GLU:HG2	2.13	0.48
1:G:3183:VAL:O	1:G:3187:ARG:HG3	2.13	0.48
1:G:4574:ASN:ND2	1:G:4813:LEU:HG	2.29	0.48
1:J:230:CYS:SG	1:J:231:LEU:HG	2.53	0.48
1:J:2504:LEU:O	1:J:2508:ARG:HG2	2.14	0.48
3:K:40:ALA:HB3	3:K:43:LYS:HB3	1.96	0.48
3:M:51:ILE:HG23	3:M:71:ARG:HD2	1.96	0.48
1:B:2381:GLU:O	1:B:2385:ARG:HG3	2.14	0.48
1:B:3417:ASP:OD1	1:B:3516:LYS:HE2	2.14	0.48
1:E:2689:LYS:HG2	1:E:2690:LYS:H	1.78	0.48
1:E:3834:ALA:O	1:E:3838:THR:HG23	2.14	0.48
1:E:4744:ASP:HB3	1:E:4747:SER:HB3	1.95	0.48
1:G:638:ILE:HD11	1:G:1636:MET:HE2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:2638:LYS:HB2	1:G:2639:MET:CE	2.43	0.48
1:G:3550:ARG:O	1:G:3554:GLN:HG2	2.14	0.48
1:G:3850:GLN:HB2	1:G:3873:LYS:HG3	1.96	0.48
1:J:721:LEU:HG	1:J:730:VAL:HG21	1.95	0.48
1:J:3310:ASP:HA	1:J:3313:ASN:ND2	2.28	0.48
1:J:3352:GLU:CD	1:J:3352:GLU:H	2.22	0.48
1:B:266:ARG:NH2	1:B:273:HIS:O	2.47	0.47
1:B:863:LEU:HD21	1:B:939:VAL:HG21	1.95	0.47
1:B:882:TRP:O	1:B:885:THR:OG1	2.24	0.47
1:B:3537:LYS:HD3	1:B:3600:SER:HB2	1.96	0.47
1:B:4104:THR:O	1:B:4108:ILE:HG12	2.13	0.47
1:E:882:TRP:CD1	1:E:886:ARG:NE	2.82	0.47
1:E:1973:GLN:NE2	1:E:2005:GLN:OE1	2.47	0.47
1:E:3315:LEU:HD13	1:E:3341:PHE:HE2	1.77	0.47
1:E:3550:ARG:O	1:E:3554:GLN:HG2	2.14	0.47
1:E:4104:THR:O	1:E:4108:ILE:HG12	2.13	0.47
1:E:4184:MET:O	1:E:4184:MET:HE3	2.14	0.47
1:E:4876:CYS:HA	1:E:4882:CYS:HB2	1.95	0.47
1:E:4943:LEU:O	1:E:4947:GLN:HG2	2.14	0.47
1:G:869:ARG:O	1:G:873:LYS:HG3	2.14	0.47
1:G:993:HIS:CE1	1:G:1027:LEU:HD11	2.49	0.47
1:G:2991:HIS:O	1:G:2995:ILE:HG13	2.13	0.47
3:K:51:ILE:HG23	3:K:71:ARG:HD2	1.96	0.47
1:B:2011:HIS:O	1:B:2011:HIS:ND1	2.41	0.47
1:E:14:LEU:HD13	1:E:202:MET:HG2	1.96	0.47
1:E:1649:ASP:HB3	1:E:1652:GLU:HG3	1.96	0.47
1:E:1690:ASP:OD2	1:E:1693:GLN:NE2	2.46	0.47
1:E:2328:GLY:HA3	1:E:2425:PHE:HE2	1.79	0.47
1:E:2751:LEU:HD12	1:E:2754:PHE:HD2	1.79	0.47
1:E:3106:MET:HE2	1:E:3106:MET:N	2.29	0.47
1:E:4735:GLU:O	1:E:4739:GLU:HG2	2.14	0.47
1:G:1170:MET:HE1	1:G:1176:GLU:HG2	1.96	0.47
1:G:1180:ARG:HG3	1:G:1181:GLU:HG3	1.96	0.47
1:G:1931:LEU:HD22	1:G:1935:VAL:HG11	1.96	0.47
1:G:2970:SER:HA	1:G:2973:PHE:CD2	2.48	0.47
1:G:3047:ALA:O	1:G:3051:ARG:N	2.47	0.47
1:G:3179:LYS:HG2	1:G:3268:HIS:CE1	2.50	0.47
1:G:3534:MET:O	1:G:3538:THR:HG23	2.13	0.47
1:G:3537:LYS:HD3	1:G:3600:SER:HB2	1.96	0.47
1:J:14:LEU:HD13	1:J:202:MET:HG2	1.96	0.47
1:J:911:HIS:HB2	1:J:918:ARG:NE	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1649:ASP:HB3	1:J:1652:GLU:HG3	1.96	0.47
1:J:3443:ILE:O	1:J:3447:LYS:HG3	2.13	0.47
2:H:30:LEU:HD23	2:H:36:PHE:CE2	2.48	0.47
3:C:40:ALA:HB3	3:C:43:LYS:HB3	1.96	0.47
3:F:40:ALA:HB3	3:F:43:LYS:HB3	1.96	0.47
1:B:3097:GLU:O	1:B:3167:ARG:NH2	2.44	0.47
1:B:3550:ARG:O	1:B:3554:GLN:HG2	2.14	0.47
1:B:3850:GLN:HB2	1:B:3873:LYS:HG3	1.96	0.47
1:E:869:ARG:O	1:E:873:LYS:HG3	2.14	0.47
1:E:3179:LYS:HG2	1:E:3268:HIS:CE1	2.49	0.47
1:E:3310:ASP:HA	1:E:3313:ASN:ND2	2.28	0.47
1:E:3352:GLU:CD	1:E:3352:GLU:H	2.22	0.47
1:E:3352:GLU:HG2	1:E:3353:LEU:H	1.79	0.47
1:E:3850:GLN:HB2	1:E:3873:LYS:HG3	1.96	0.47
1:G:14:LEU:HD13	1:G:202:MET:HG2	1.96	0.47
1:G:2294:ASP:HA	1:G:2297:LYS:HE2	1.95	0.47
1:G:2328:GLY:HA3	1:G:2425:PHE:HE2	1.79	0.47
1:G:2381:GLU:O	1:G:2385:ARG:HG3	2.14	0.47
1:G:3310:ASP:HA	1:G:3313:ASN:ND2	2.28	0.47
1:J:2294:ASP:HA	1:J:2297:LYS:HE2	1.95	0.47
1:J:2689:LYS:HG2	1:J:2690:LYS:H	1.78	0.47
1:J:3068:LEU:HA	1:J:3071:LEU:HD12	1.95	0.47
1:J:3179:LYS:HG2	1:J:3268:HIS:CE1	2.49	0.47
1:J:4735:GLU:O	1:J:4739:GLU:HG2	2.15	0.47
1:B:3106:MET:HE2	1:B:3106:MET:N	2.29	0.47
1:E:252:VAL:HA	1:E:255:HIS:HB2	1.96	0.47
1:E:871:ARG:CZ	1:E:922:LEU:HB3	2.45	0.47
1:E:1620:ALA:HB3	1:E:1624:LEU:HB2	1.97	0.47
1:E:4109:GLN:HA	1:E:4112:LEU:HD12	1.96	0.47
1:G:3417:ASP:OD1	1:G:3516:LYS:HE2	2.14	0.47
1:J:3537:LYS:HD3	1:J:3600:SER:HB2	1.96	0.47
1:J:3713:LYS:NZ	1:J:3715:LYS:O	2.48	0.47
1:J:4090:LYS:HE2	1:J:4123:ILE:HG21	1.97	0.47
1:B:870:ILE:O	1:B:874:LEU:HG	2.14	0.47
1:B:1867:GLU:HG2	1:B:1870:VAL:HG12	1.97	0.47
1:B:3179:LYS:HG2	1:B:3268:HIS:CE1	2.49	0.47
1:B:4822:THR:HB	1:E:4839:MET:HE1	1.95	0.47
1:E:299:LEU:HD22	1:E:378:LEU:HG	1.97	0.47
1:E:728:ARG:HE	1:E:1487:LEU:HD12	1.78	0.47
1:E:882:TRP:O	1:E:885:THR:OG1	2.25	0.47
1:E:993:HIS:CE1	1:E:1027:LEU:HD11	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3417:ASP:OD1	1:E:3516:LYS:HE2	2.14	0.47
1:E:4090:LYS:HE2	1:E:4123:ILE:HG21	1.97	0.47
1:E:4574:ASN:ND2	1:E:4813:LEU:HG	2.29	0.47
1:G:4735:GLU:O	1:G:4739:GLU:HG2	2.15	0.47
1:J:213:TYR:HD1	1:J:340:LYS:HA	1.79	0.47
1:J:871:ARG:CZ	1:J:922:LEU:HB3	2.45	0.47
1:J:1620:ALA:HB3	1:J:1624:LEU:HB2	1.97	0.47
1:J:1690:ASP:OD2	1:J:1693:GLN:NE2	2.46	0.47
2:H:78:PRO:HA	2:H:81:ALA:HB3	1.97	0.47
1:B:882:TRP:CD1	1:B:886:ARG:NE	2.82	0.47
1:B:984:LEU:O	1:B:988:LEU:HD23	2.15	0.47
1:B:3206:LEU:HD12	1:B:3206:LEU:H	1.78	0.47
1:B:3310:ASP:HA	1:B:3313:ASN:ND2	2.28	0.47
1:E:972:LEU:HD12	1:E:976:ARG:HA	1.97	0.47
1:E:3047:ALA:O	1:E:3051:ARG:N	2.47	0.47
1:E:3755:GLU:O	1:E:3758:MET:HG3	2.15	0.47
1:G:213:TYR:HD1	1:G:340:LYS:HA	1.79	0.47
1:G:882:TRP:CD1	1:G:886:ARG:NE	2.83	0.47
1:G:972:LEU:HD12	1:G:976:ARG:HA	1.97	0.47
1:G:3137:LEU:O	1:G:3141:THR:OG1	2.28	0.47
1:G:3206:LEU:HD12	1:G:3206:LEU:H	1.79	0.47
1:G:3752:SER:HB2	1:G:3755:GLU:HG3	1.96	0.47
1:G:4090:LYS:HE2	1:G:4123:ILE:HG21	1.97	0.47
1:J:882:TRP:CD1	1:J:886:ARG:NE	2.83	0.47
1:J:972:LEU:HD12	1:J:976:ARG:HA	1.97	0.47
1:J:4083:ASP:HB3	1:J:4087:LEU:H	1.80	0.47
1:J:4876:CYS:HA	1:J:4882:CYS:HB2	1.95	0.47
1:B:911:HIS:HB2	1:B:918:ARG:NE	2.29	0.47
1:B:972:LEU:HD12	1:B:976:ARG:HA	1.97	0.47
1:B:1649:ASP:HB3	1:B:1652:GLU:HG3	1.96	0.47
1:B:2715:VAL:HG12	1:B:2954:ARG:HA	1.97	0.47
1:B:3018:LEU:HD13	1:B:3150:HIS:HE1	1.80	0.47
1:B:3755:GLU:O	1:B:3758:MET:HG3	2.15	0.47
1:B:4083:ASP:HB3	1:B:4087:LEU:H	1.80	0.47
1:E:365:LYS:O	1:E:369:LEU:HG	2.15	0.47
1:E:721:LEU:HG	1:E:730:VAL:HG21	1.95	0.47
1:E:1170:MET:HE1	1:E:1176:GLU:HG2	1.96	0.47
1:E:1180:ARG:HG3	1:E:1181:GLU:HG3	1.96	0.47
1:E:1867:GLU:HG2	1:E:1870:VAL:HG12	1.97	0.47
1:E:2755:ILE:HD12	1:E:2813:LEU:HD13	1.96	0.47
1:E:2975:ALA:O	1:E:2978:GLU:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3078:ARG:HG3	1:E:3082:LYS:HE3	1.97	0.47
1:E:3752:SER:HB2	1:E:3755:GLU:HG3	1.96	0.47
1:E:5011:TRP:O	1:E:5015:GLN:HG3	2.15	0.47
1:G:1274:HIS:O	1:G:1559:GLN:NE2	2.33	0.47
1:G:2559:LEU:O	1:G:2563:THR:HG23	2.15	0.47
1:G:2751:LEU:HD12	1:G:2754:PHE:HD2	1.79	0.47
1:G:3043:PHE:CE1	1:G:3075:LEU:HD21	2.50	0.47
1:G:3780:LEU:HD11	1:G:3816:MET:HG2	1.97	0.47
1:J:870:ILE:O	1:J:874:LEU:HG	2.14	0.47
1:J:2700:MET:CE	1:J:2701:PRO:HD3	2.43	0.47
1:J:3755:GLU:O	1:J:3758:MET:HG3	2.15	0.47
1:J:3834:ALA:O	1:J:3838:THR:HG23	2.14	0.47
1:J:4574:ASN:ND2	1:J:4813:LEU:HG	2.29	0.47
1:J:5011:TRP:O	1:J:5015:GLN:HG3	2.15	0.47
1:B:1931:LEU:HD22	1:B:1935:VAL:HG11	1.96	0.47
1:B:2975:ALA:O	1:B:2978:GLU:HG2	2.15	0.47
1:B:3047:ALA:O	1:B:3051:ARG:N	2.47	0.47
1:B:3713:LYS:NZ	1:B:3715:LYS:O	2.48	0.47
1:B:3834:ALA:O	1:B:3838:THR:HG23	2.14	0.47
1:B:4091:LYS:NZ	1:B:4092:ASP:OD1	2.48	0.47
1:E:2670:GLU:HG3	1:E:2912:THR:HA	1.97	0.47
1:E:3042:LEU:HD22	1:E:3071:LEU:HD11	1.95	0.47
1:E:3078:ARG:H	1:E:3078:ARG:HD2	1.80	0.47
1:E:4068:LEU:O	1:E:4071:ILE:HG22	2.15	0.47
1:G:20:VAL:HG21	1:G:202:MET:HE3	1.97	0.47
1:G:1620:ALA:HB3	1:G:1624:LEU:HB2	1.97	0.47
1:G:1786:LEU:HD12	1:G:1787:PRO:HD2	1.96	0.47
1:G:2700:MET:N	1:G:2701:PRO:HD2	2.30	0.47
1:G:2715:VAL:HG12	1:G:2954:ARG:HA	1.97	0.47
1:G:3106:MET:HE2	1:G:3106:MET:N	2.29	0.47
1:G:3717:ASP:OD1	1:G:3717:ASP:N	2.48	0.47
1:G:4083:ASP:HB3	1:G:4087:LEU:H	1.80	0.47
1:G:5011:TRP:O	1:G:5015:GLN:HG3	2.15	0.47
1:J:1867:GLU:HG2	1:J:1870:VAL:HG12	1.97	0.47
1:J:2670:GLU:HG3	1:J:2912:THR:HA	1.97	0.47
1:J:3043:PHE:CE1	1:J:3075:LEU:HD21	2.50	0.47
1:B:153:ALA:HB2	1:B:170:ILE:HG13	1.97	0.47
1:B:638:ILE:HD11	1:B:1636:MET:HE2	1.96	0.47
1:B:1620:ALA:HB3	1:B:1624:LEU:HB2	1.97	0.47
1:B:4093:PHE:CD1	1:B:4123:ILE:HD11	2.50	0.47
1:E:3043:PHE:CE1	1:E:3075:LEU:HD21	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:299:LEU:HD23	1:G:376:ALA:O	2.15	0.47
1:G:870:ILE:O	1:G:874:LEU:HG	2.14	0.47
1:G:1436:SER:OG	1:G:1565:GLU:HB2	2.15	0.47
1:G:2755:ILE:HD12	1:G:2813:LEU:HD13	1.96	0.47
1:G:3777:GLU:O	1:G:3781:GLN:HG3	2.15	0.47
1:J:266:ARG:NH2	1:J:273:HIS:O	2.47	0.47
1:J:1931:LEU:HD22	1:J:1935:VAL:HG11	1.96	0.47
3:F:51:ILE:HG23	3:F:71:ARG:HD2	1.96	0.47
1:B:2700:MET:N	1:B:2701:PRO:HD2	2.30	0.47
1:B:3277:LEU:HG	1:B:3341:PHE:CZ	2.50	0.47
1:B:4735:GLU:O	1:B:4739:GLU:HG2	2.15	0.47
1:E:984:LEU:O	1:E:988:LEU:HD23	2.15	0.47
1:E:3018:LEU:HD13	1:E:3150:HIS:HE1	1.80	0.47
1:E:3097:GLU:O	1:E:3167:ARG:NH2	2.44	0.47
1:E:4091:LYS:NZ	1:E:4092:ASP:OD1	2.48	0.47
1:E:4157:ASP:N	1:E:4161:ARG:HH21	2.13	0.47
1:G:153:ALA:HB2	1:G:170:ILE:HG13	1.97	0.47
1:J:20:VAL:HG21	1:J:202:MET:HE3	1.97	0.47
1:J:299:LEU:HD23	1:J:376:ALA:O	2.15	0.47
1:J:551:LEU:HB3	1:J:589:LEU:HD21	1.97	0.47
1:J:638:ILE:HD11	1:J:1636:MET:HE2	1.96	0.47
1:J:1973:GLN:NE2	1:J:2005:GLN:OE1	2.47	0.47
3:F:104:TYR:CD1	3:F:104:TYR:C	2.92	0.47
1:B:871:ARG:CZ	1:B:922:LEU:HB3	2.45	0.46
1:B:3352:GLU:HG2	1:B:3353:LEU:H	1.79	0.46
1:B:4839:MET:HE1	1:G:4822:THR:HB	1.96	0.46
1:E:3713:LYS:NZ	1:E:3715:LYS:O	2.48	0.46
1:E:4093:PHE:CD1	1:E:4123:ILE:HD11	2.50	0.46
1:G:266:ARG:NH2	1:G:273:HIS:O	2.47	0.46
1:G:1079:LYS:HA	1:G:1189:LEU:HD11	1.97	0.46
1:G:1100:MET:HG2	1:G:1194:LEU:HG	1.97	0.46
1:G:1649:ASP:HB3	1:G:1652:GLU:HG3	1.96	0.46
1:G:3078:ARG:H	1:G:3078:ARG:HD2	1.80	0.46
1:G:3834:ALA:O	1:G:3838:THR:HG23	2.14	0.46
1:J:2489:LYS:HE3	1:J:2546:MET:HG2	1.98	0.46
1:J:2751:LEU:HD12	1:J:2754:PHE:HD2	1.79	0.46
1:J:2755:ILE:HD12	1:J:2813:LEU:HD13	1.97	0.46
1:J:2975:ALA:O	1:J:2978:GLU:HG2	2.15	0.46
1:J:3047:ALA:O	1:J:3051:ARG:N	2.47	0.46
1:J:3752:SER:HB2	1:J:3755:GLU:HG3	1.96	0.46
1:J:3780:LEU:HD11	1:J:3816:MET:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:VAL:HG21	1:B:202:MET:HE3	1.97	0.46
1:B:1170:MET:HE1	1:B:1176:GLU:HG2	1.96	0.46
1:B:1617:THR:HG22	1:B:1628:VAL:HG13	1.97	0.46
1:B:2489:LYS:HE3	1:B:2546:MET:HG2	1.98	0.46
1:B:2773:ASN:OD1	1:E:1508:ARG:NH2	2.40	0.46
1:B:3068:LEU:HA	1:B:3071:LEU:HD12	1.96	0.46
1:B:4090:LYS:HE2	1:B:4123:ILE:HG21	1.97	0.46
1:B:4157:ASP:N	1:B:4161:ARG:HH21	2.13	0.46
1:E:20:VAL:HG21	1:E:202:MET:HE3	1.97	0.46
1:E:1436:SER:OG	1:E:1565:GLU:HB2	2.15	0.46
1:E:1617:THR:HG22	1:E:1628:VAL:HG13	1.97	0.46
1:E:3068:LEU:HA	1:E:3071:LEU:HD12	1.96	0.46
1:E:3277:LEU:HG	1:E:3341:PHE:CZ	2.50	0.46
1:J:3144:PHE:CE2	1:J:3197:LEU:HB3	2.51	0.46
1:J:3272:ILE:C	1:J:3275:PRO:HD2	2.41	0.46
1:J:3592:ILE:HA	1:J:3595:ARG:HE	1.80	0.46
1:J:4157:ASP:N	1:J:4161:ARG:HH21	2.13	0.46
1:B:1100:MET:HG2	1:B:1194:LEU:HG	1.97	0.46
1:B:3209:GLN:HG2	1:B:3210:LEU:HG	1.98	0.46
1:B:3780:LEU:HD11	1:B:3816:MET:HG2	1.97	0.46
1:B:4068:LEU:O	1:B:4071:ILE:HG22	2.14	0.46
1:E:153:ALA:HB2	1:E:170:ILE:HG13	1.97	0.46
1:E:1931:LEU:HD22	1:E:1935:VAL:HG11	1.96	0.46
1:E:2381:GLU:O	1:E:2385:ARG:HG3	2.14	0.46
1:E:4083:ASP:HB3	1:E:4087:LEU:H	1.80	0.46
1:G:470:SER:HA	1:G:473:ASN:ND2	2.31	0.46
1:G:1867:GLU:HG2	1:G:1870:VAL:HG12	1.97	0.46
1:J:470:SER:HA	1:J:473:ASN:ND2	2.31	0.46
1:J:981:GLN:O	1:J:985:VAL:HG23	2.15	0.46
1:J:1100:MET:HG2	1:J:1194:LEU:HG	1.97	0.46
1:J:2715:VAL:HG12	1:J:2954:ARG:HA	1.97	0.46
1:J:3417:ASP:OD1	1:J:3516:LYS:HE2	2.14	0.46
1:J:4068:LEU:O	1:J:4071:ILE:HG22	2.15	0.46
1:B:2693:GLN:HB3	1:B:2697:ARG:HH22	1.81	0.46
1:B:3758:MET:O	1:B:3762:ARG:HG2	2.16	0.46
1:B:3927:GLN:NE2	1:B:3991:GLY:HA3	2.31	0.46
1:E:470:SER:HA	1:E:473:ASN:ND2	2.31	0.46
1:E:1079:LYS:HA	1:E:1189:LEU:HD11	1.97	0.46
1:E:2700:MET:N	1:E:2701:PRO:HD2	2.30	0.46
1:E:2973:PHE:CE1	1:E:2995:ILE:HG23	2.51	0.46
1:G:551:LEU:HB3	1:G:589:LEU:HD21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:937:CYS:SG	1:G:984:LEU:HD22	2.56	0.46
1:G:2619:LEU:O	1:G:2623:LEU:HG	2.16	0.46
1:G:3018:LEU:HD13	1:G:3150:HIS:HE1	1.80	0.46
1:G:3713:LYS:NZ	1:G:3715:LYS:O	2.48	0.46
1:J:1727:ARG:NH2	1:J:1773:PRO:O	2.49	0.46
1:J:2765:LYS:HD3	1:J:2765:LYS:HA	1.67	0.46
1:B:14:LEU:HD13	1:B:202:MET:HG2	1.96	0.46
1:B:1180:ARG:HG3	1:B:1181:GLU:HG3	1.96	0.46
1:B:1727:ARG:NH2	1:B:1773:PRO:O	2.48	0.46
1:E:2489:LYS:HE3	1:E:2546:MET:HG2	1.97	0.46
1:E:2619:LEU:O	1:E:2623:LEU:HG	2.16	0.46
1:E:3505:VAL:HG23	1:E:3507:THR:H	1.80	0.46
1:G:2489:LYS:HE3	1:G:2546:MET:HG2	1.98	0.46
1:G:3272:ILE:C	1:G:3275:PRO:HD2	2.41	0.46
1:G:3505:VAL:HG23	1:G:3507:THR:H	1.80	0.46
1:J:1274:HIS:O	1:J:1559:GLN:NE2	2.33	0.46
1:J:2328:GLY:HA3	1:J:2425:PHE:HE2	1.79	0.46
1:J:2381:GLU:O	1:J:2385:ARG:HG3	2.14	0.46
1:J:3106:MET:HE2	1:J:3106:MET:N	2.29	0.46
2:I:78:PRO:HA	2:I:81:ALA:HB3	1.96	0.46
1:B:2559:LEU:O	1:B:2563:THR:HG23	2.15	0.46
1:B:3078:ARG:H	1:B:3078:ARG:HD2	1.80	0.46
1:B:3391:GLU:O	1:B:3395:ARG:HG3	2.16	0.46
1:E:2715:VAL:HG12	1:E:2954:ARG:HA	1.97	0.46
1:E:3144:PHE:CE2	1:E:3197:LEU:HB3	2.51	0.46
1:E:3780:LEU:HD11	1:E:3816:MET:HG2	1.97	0.46
1:G:871:ARG:CZ	1:G:922:LEU:HB3	2.45	0.46
1:G:924:MET:O	1:G:928:THR:HG23	2.16	0.46
1:G:2975:ALA:O	1:G:2978:GLU:HG2	2.15	0.46
1:G:3277:LEU:HG	1:G:3341:PHE:CZ	2.50	0.46
1:G:4097:MET:SD	1:G:4108:ILE:HG23	2.56	0.46
1:J:937:CYS:SG	1:J:984:LEU:HD22	2.56	0.46
1:J:1436:SER:OG	1:J:1565:GLU:HB2	2.15	0.46
1:J:2700:MET:N	1:J:2701:PRO:HD2	2.30	0.46
1:J:3018:LEU:HD13	1:J:3150:HIS:HE1	1.80	0.46
1:J:3078:ARG:H	1:J:3078:ARG:HD2	1.80	0.46
1:J:3078:ARG:HG3	1:J:3082:LYS:HE3	1.97	0.46
1:J:3137:LEU:O	1:J:3141:THR:OG1	2.28	0.46
1:J:3277:LEU:HG	1:J:3341:PHE:CZ	2.50	0.46
1:J:3777:GLU:O	1:J:3781:GLN:HG3	2.15	0.46
3:F:105:ASN:OD1	3:F:111:ASN:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2670:GLU:HG3	1:B:2912:THR:HA	1.97	0.46
1:B:3043:PHE:CE1	1:B:3075:LEU:HD21	2.50	0.46
1:B:3144:PHE:CE2	1:B:3197:LEU:HB3	2.51	0.46
1:B:3272:ILE:C	1:B:3275:PRO:HD2	2.40	0.46
1:B:3777:GLU:O	1:B:3781:GLN:HG3	2.15	0.46
1:E:283:ARG:NH1	1:E:290:TYR:OH	2.49	0.46
1:E:551:LEU:HB3	1:E:589:LEU:HD21	1.98	0.46
1:E:2495:VAL:HB	1:E:2498:HIS:CD2	2.51	0.46
1:E:3272:ILE:C	1:E:3275:PRO:HD2	2.40	0.46
1:E:3717:ASP:OD1	1:E:3717:ASP:N	2.48	0.46
1:E:3777:GLU:O	1:E:3781:GLN:HG3	2.15	0.46
1:G:3209:GLN:HG2	1:G:3210:LEU:HG	1.98	0.46
1:G:3391:GLU:O	1:G:3395:ARG:HG3	2.16	0.46
1:G:4118:ASP:OD1	1:G:4119:GLU:N	2.49	0.46
1:J:2559:LEU:O	1:J:2563:THR:HG23	2.15	0.46
1:J:3051:ARG:NH2	1:J:3098:SER:HB3	2.31	0.46
1:J:3262:ARG:HG3	1:J:3326:ASN:ND2	2.28	0.46
1:J:3540:TYR:HA	1:J:3544:ASP:O	2.16	0.46
2:A:78:PRO:HA	2:A:81:ALA:HB3	1.97	0.46
1:B:171:LEU:HB2	1:B:180:LEU:HD13	1.98	0.46
1:B:921:ASN:O	1:B:924:MET:HB3	2.15	0.46
1:B:1436:SER:OG	1:B:1565:GLU:HB2	2.15	0.46
1:E:251:ALA:O	1:E:255:HIS:ND1	2.40	0.46
1:E:924:MET:CE	3:F:107:TRP:CD1	2.99	0.46
1:E:2559:LEU:O	1:E:2563:THR:HG23	2.15	0.46
1:E:3051:ARG:NH2	1:E:3098:SER:HB3	2.31	0.46
1:G:171:LEU:HB2	1:G:180:LEU:HD13	1.98	0.46
1:G:921:ASN:O	1:G:924:MET:HB3	2.15	0.46
1:G:3051:ARG:NH2	1:G:3098:SER:HB3	2.31	0.46
1:G:3078:ARG:HG3	1:G:3082:LYS:HE3	1.97	0.46
1:G:3755:GLU:O	1:G:3758:MET:HG3	2.15	0.46
1:G:4093:PHE:CD1	1:G:4123:ILE:HD11	2.50	0.46
1:J:984:LEU:O	1:J:988:LEU:HD23	2.15	0.46
1:J:1738:LEU:HD12	1:J:1738:LEU:HA	1.80	0.46
1:J:2639:MET:HE2	1:J:2639:MET:N	2.31	0.46
1:J:3927:GLN:NE2	1:J:3991:GLY:HA3	2.31	0.46
3:C:105:ASN:OD1	3:C:111:ASN:HB2	2.16	0.46
1:B:551:LEU:HB3	1:B:589:LEU:HD21	1.97	0.46
1:B:2639:MET:HE2	1:B:2639:MET:N	2.31	0.46
1:B:2755:ILE:HD12	1:B:2813:LEU:HD13	1.97	0.46
1:B:3078:ARG:HG3	1:B:3082:LYS:HE3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3435:PHE:HZ	1:B:3602:VAL:HG21	1.81	0.46
1:B:3592:ILE:HA	1:B:3595:ARG:HE	1.80	0.46
1:E:861:ILE:HG21	1:E:933:LEU:HD22	1.98	0.46
1:E:924:MET:O	1:E:928:THR:HG23	2.16	0.46
1:E:2693:GLN:HB3	1:E:2697:ARG:HH22	1.81	0.46
1:E:3758:MET:O	1:E:3762:ARG:HG2	2.16	0.46
1:G:661:LYS:HG2	1:G:749:ASP:OD1	2.16	0.46
1:G:887:ILE:HG21	1:G:959:TYR:HA	1.97	0.46
1:G:984:LEU:O	1:G:988:LEU:HD23	2.15	0.46
1:G:1727:ARG:NH2	1:G:1773:PRO:O	2.48	0.46
1:G:2670:GLU:HG3	1:G:2912:THR:HA	1.97	0.46
1:G:3758:MET:O	1:G:3762:ARG:HG2	2.16	0.46
1:J:661:LYS:HG2	1:J:749:ASP:OD1	2.16	0.46
1:J:2619:LEU:O	1:J:2623:LEU:HG	2.16	0.46
1:J:3505:VAL:HG23	1:J:3507:THR:H	1.80	0.46
1:J:4093:PHE:CD1	1:J:4123:ILE:HD11	2.50	0.46
2:D:78:PRO:HA	2:D:81:ALA:HB3	1.97	0.46
3:K:32:ASN:ND2	3:K:101:PRO:HB3	2.31	0.46
3:M:105:ASN:ND2	3:M:107:TRP:HD1	2.12	0.46
1:B:222:LEU:O	1:B:230:CYS:HB3	2.16	0.46
1:B:283:ARG:NH1	1:B:290:TYR:OH	2.49	0.46
1:B:861:ILE:HG21	1:B:933:LEU:HD22	1.98	0.46
1:B:924:MET:O	1:B:928:THR:HG23	2.16	0.46
1:B:1000:ARG:NH2	3:C:115:ASP:O	2.49	0.46
1:B:3051:ARG:NH2	1:B:3098:SER:HB3	2.31	0.46
1:E:222:LEU:O	1:E:230:CYS:HB3	2.16	0.46
1:E:3391:GLU:O	1:E:3395:ARG:HG3	2.16	0.46
1:E:3592:ILE:HA	1:E:3595:ARG:HE	1.80	0.46
1:G:140:ASP:OD1	1:G:140:ASP:N	2.49	0.46
1:G:981:GLN:O	1:G:985:VAL:HG23	2.15	0.46
1:G:2523:ASP:OD1	1:G:2524:VAL:N	2.49	0.46
1:G:2973:PHE:CE1	1:G:2995:ILE:HG23	2.51	0.46
1:G:3445:TRP:HA	1:G:3451:PHE:CD1	2.49	0.46
1:J:1170:MET:HE1	1:J:1176:GLU:HG2	1.96	0.46
1:J:2523:ASP:OD1	1:J:2524:VAL:N	2.49	0.46
1:J:4107:GLU:O	1:J:4111:LEU:HG	2.16	0.46
2:A:17:LYS:N	2:A:20:GLN:OE1	2.49	0.46
3:C:104:TYR:C	3:C:104:TYR:CD1	2.94	0.46
3:K:105:ASN:OD1	3:K:111:ASN:HB2	2.16	0.46
1:B:2495:VAL:HB	1:B:2498:HIS:CD2	2.51	0.45
1:B:2619:LEU:O	1:B:2623:LEU:HG	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2973:PHE:CE1	1:B:2995:ILE:HG23	2.51	0.45
1:B:3505:VAL:HG23	1:B:3507:THR:H	1.80	0.45
1:E:3989:VAL:HG13	1:E:4023:MET:CE	2.46	0.45
1:G:2639:MET:HE2	1:G:2639:MET:N	2.31	0.45
1:G:3144:PHE:CE2	1:G:3197:LEU:HB3	2.51	0.45
1:G:4068:LEU:O	1:G:4071:ILE:HG22	2.15	0.45
1:G:4157:ASP:N	1:G:4161:ARG:HH21	2.13	0.45
1:J:153:ALA:HB2	1:J:170:ILE:HG13	1.97	0.45
1:J:228:ASP:HA	1:J:247:TYR:HE1	1.82	0.45
1:J:1617:THR:HG22	1:J:1628:VAL:HG13	1.97	0.45
1:J:2689:LYS:HG2	1:J:2690:LYS:N	2.31	0.45
1:J:3223:SER:O	1:J:3227:ARG:HG3	2.17	0.45
1:J:3391:GLU:O	1:J:3395:ARG:HG3	2.16	0.45
1:B:77:ALA:O	1:B:81:MET:HG3	2.17	0.45
1:B:470:SER:HA	1:B:473:ASN:ND2	2.31	0.45
1:B:937:CYS:SG	1:B:984:LEU:HD22	2.56	0.45
1:B:1079:LYS:HA	1:B:1189:LEU:HD11	1.97	0.45
1:B:2765:LYS:HD3	1:B:2765:LYS:HA	1.67	0.45
1:B:3717:ASP:N	1:B:3717:ASP:OD1	2.48	0.45
1:E:228:ASP:HA	1:E:247:TYR:HE1	1.82	0.45
1:E:2523:ASP:OD1	1:E:2524:VAL:N	2.49	0.45
1:E:3006:ILE:HD11	1:E:3071:LEU:HD21	1.97	0.45
1:E:3148:ALA:HB2	1:E:3200:ALA:HB2	1.98	0.45
1:G:222:LEU:O	1:G:230:CYS:HB3	2.16	0.45
1:G:2689:LYS:HG2	1:G:2690:LYS:N	2.31	0.45
1:G:3592:ILE:HA	1:G:3595:ARG:HE	1.80	0.45
1:J:921:ASN:O	1:J:924:MET:HB3	2.15	0.45
1:J:1079:LYS:HA	1:J:1189:LEU:HD11	1.97	0.45
1:B:3075:LEU:O	1:B:3146:HIS:HE1	1.99	0.45
1:B:3540:TYR:HA	1:B:3544:ASP:O	2.16	0.45
1:B:4097:MET:SD	1:B:4108:ILE:HG23	2.56	0.45
1:B:4107:GLU:O	1:B:4111:LEU:HG	2.16	0.45
1:B:4230:LYS:NZ	1:B:4231:MET:SD	2.84	0.45
1:B:5011:TRP:O	1:B:5015:GLN:HG3	2.15	0.45
1:E:171:LEU:HB2	1:E:180:LEU:HD13	1.98	0.45
1:E:921:ASN:O	1:E:924:MET:HB3	2.15	0.45
1:E:981:GLN:O	1:E:985:VAL:HG23	2.15	0.45
1:E:4655:PHE:O	1:E:4659:ILE:HG12	2.17	0.45
1:G:861:ILE:HG21	1:G:933:LEU:HD22	1.98	0.45
1:G:1617:THR:HG22	1:G:1628:VAL:HG13	1.97	0.45
1:G:3006:ILE:HD11	1:G:3071:LEU:HD21	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3435:PHE:HZ	1:G:3602:VAL:HG21	1.81	0.45
1:J:861:ILE:HG21	1:J:933:LEU:HD22	1.98	0.45
1:J:1081:TYR:HD1	1:J:1230:MET:HE1	1.82	0.45
1:J:2765:LYS:HZ3	1:J:2857:PRO:HG2	1.80	0.45
1:J:3989:VAL:HG13	1:J:4023:MET:CE	2.46	0.45
1:B:23:GLN:HB3	1:B:34:LYS:HG2	1.99	0.45
1:B:981:GLN:O	1:B:985:VAL:HG23	2.15	0.45
1:B:2978:GLU:HB3	1:B:3056:LEU:HD11	1.99	0.45
1:B:3223:SER:O	1:B:3227:ARG:HG3	2.17	0.45
1:E:1727:ARG:NH2	1:E:1773:PRO:O	2.48	0.45
1:G:228:ASP:HA	1:G:247:TYR:HE1	1.82	0.45
1:G:2495:VAL:HB	1:G:2498:HIS:CD2	2.51	0.45
1:G:2693:GLN:HB3	1:G:2697:ARG:HH22	1.81	0.45
1:G:2978:GLU:HB3	1:G:3056:LEU:HD11	1.99	0.45
1:G:3540:TYR:HA	1:G:3544:ASP:O	2.16	0.45
1:J:2973:PHE:CE1	1:J:2995:ILE:HG23	2.51	0.45
1:J:3018:LEU:HD13	1:J:3150:HIS:CE1	2.51	0.45
1:J:4032:GLU:HG3	1:J:5006:GLN:HE21	1.81	0.45
1:J:4655:PHE:O	1:J:4659:ILE:HG12	2.17	0.45
2:H:25:HIS:HB3	2:H:40:ARG:CZ	2.47	0.45
1:B:601:ASP:OD1	1:B:1668:ARG:NH2	2.49	0.45
1:B:937:CYS:HB3	1:B:1053:ILE:HG22	1.98	0.45
1:B:3018:LEU:HD13	1:B:3150:HIS:CE1	2.51	0.45
1:E:601:ASP:OD1	1:E:1668:ARG:NH2	2.49	0.45
1:E:1081:TYR:HD1	1:E:1230:MET:HE1	1.82	0.45
1:E:2639:MET:HE2	1:E:2639:MET:N	2.31	0.45
1:E:2689:LYS:HG2	1:E:2690:LYS:N	2.31	0.45
1:E:3075:LEU:O	1:E:3146:HIS:HE1	1.99	0.45
1:E:3223:SER:O	1:E:3227:ARG:HG3	2.17	0.45
1:G:4032:GLU:HG3	1:G:5006:GLN:HE21	1.81	0.45
1:G:4085:ARG:HH12	1:G:4122:MET:HE1	1.81	0.45
1:J:77:ALA:O	1:J:81:MET:HG3	2.17	0.45
1:J:222:LEU:O	1:J:230:CYS:HB3	2.16	0.45
1:J:601:ASP:OD1	1:J:1668:ARG:NH2	2.50	0.45
1:J:2208:MET:HE1	1:J:2253:HIS:CG	2.52	0.45
1:J:4085:ARG:HH12	1:J:4122:MET:HE1	1.81	0.45
1:J:4097:MET:SD	1:J:4108:ILE:HG23	2.56	0.45
2:A:25:HIS:HB3	2:A:40:ARG:CZ	2.47	0.45
2:I:17:LYS:N	2:I:20:GLN:OE1	2.49	0.45
1:B:228:ASP:HA	1:B:247:TYR:HE1	1.82	0.45
1:B:3148:ALA:HB2	1:B:3200:ALA:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:871:ARG:HB2	1:E:925:SER:HB3	1.99	0.45
1:E:887:ILE:HG21	1:E:959:TYR:HA	1.97	0.45
1:E:917:GLU:CB	3:F:104:TYR:HE2	2.23	0.45
1:E:2765:LYS:NZ	1:E:2860:PRO:HA	2.32	0.45
1:E:3018:LEU:HD13	1:E:3150:HIS:CE1	2.51	0.45
1:E:3693:LYS:HZ2	1:E:3694:LYS:HD2	1.82	0.45
1:G:871:ARG:HB2	1:G:925:SER:HB3	1.99	0.45
1:G:4230:LYS:NZ	1:G:4231:MET:SD	2.84	0.45
1:J:283:ARG:NH1	1:J:290:TYR:OH	2.49	0.45
1:J:2495:VAL:HB	1:J:2498:HIS:CD2	2.51	0.45
1:J:3075:LEU:O	1:J:3146:HIS:HE1	1.99	0.45
1:J:3327:LEU:HD22	1:J:3368:ARG:CZ	2.47	0.45
1:B:3006:ILE:HD11	1:B:3071:LEU:HD21	1.97	0.45
1:B:4032:GLU:HG3	1:B:5006:GLN:HE21	1.81	0.45
1:B:4093:PHE:CZ	1:B:4097:MET:HE2	2.51	0.45
1:E:487:VAL:O	1:E:491:ILE:HG13	2.17	0.45
1:E:661:LYS:HG2	1:E:749:ASP:OD1	2.16	0.45
1:E:937:CYS:SG	1:E:984:LEU:HD22	2.56	0.45
1:E:1100:MET:HG2	1:E:1194:LEU:HG	1.97	0.45
1:J:140:ASP:OD1	1:J:140:ASP:N	2.49	0.45
1:J:3148:ALA:HB2	1:J:3200:ALA:HB2	1.98	0.45
1:J:3209:GLN:HG2	1:J:3210:LEU:HG	1.98	0.45
1:J:4091:LYS:NZ	1:J:4092:ASP:OD1	2.48	0.45
1:B:487:VAL:O	1:B:491:ILE:HG13	2.17	0.45
1:B:871:ARG:HB2	1:B:925:SER:HB3	1.99	0.45
1:B:887:ILE:HG21	1:B:959:TYR:HA	1.97	0.45
1:B:4085:ARG:HH12	1:B:4122:MET:HE1	1.82	0.45
1:B:4767:TRP:O	1:B:4767:TRP:HD1	1.99	0.45
1:B:5017:ARG:HD3	1:B:5019:TRP:CZ2	2.52	0.45
1:E:127:MET:O	1:E:130:LYS:NZ	2.49	0.45
1:E:2208:MET:HE1	1:E:2253:HIS:CG	2.52	0.45
1:E:2702:CYS:O	1:E:2706:ILE:HD13	2.17	0.45
1:E:3927:GLN:NE2	1:E:3991:GLY:HA3	2.31	0.45
1:E:4107:GLU:O	1:E:4111:LEU:HG	2.16	0.45
1:E:4813:LEU:HD23	1:E:4813:LEU:HA	1.85	0.45
1:G:426:ARG:H	1:G:506:TYR:HA	1.82	0.45
1:G:3927:GLN:NE2	1:G:3991:GLY:HA3	2.31	0.45
1:G:4107:GLU:O	1:G:4111:LEU:HG	2.16	0.45
1:J:171:LEU:HB2	1:J:180:LEU:HD13	1.98	0.45
1:J:887:ILE:HG21	1:J:959:TYR:HA	1.97	0.45
1:J:924:MET:CE	3:K:107:TRP:CD1	3.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:3758:MET:O	1:J:3762:ARG:HG2	2.16	0.45
1:J:4093:PHE:CZ	1:J:4097:MET:HE2	2.51	0.45
2:I:25:HIS:HB3	2:I:40:ARG:CZ	2.47	0.45
3:F:32:ASN:ND2	3:F:101:PRO:HB3	2.32	0.45
3:K:104:TYR:CE1	3:K:106:PRO:HG3	2.46	0.45
1:B:728:ARG:NH2	1:B:1489:CYS:SG	2.90	0.45
1:B:3318:ASN:O	1:B:3322:ILE:HG12	2.17	0.45
1:B:4655:PHE:O	1:B:4659:ILE:HG12	2.16	0.45
1:E:424:LYS:HE2	1:E:424:LYS:HB2	1.85	0.45
1:E:937:CYS:HB3	1:E:1053:ILE:HG22	1.98	0.45
1:E:3327:LEU:HD22	1:E:3368:ARG:CZ	2.47	0.45
1:G:77:ALA:O	1:G:81:MET:HG3	2.17	0.45
1:G:283:ARG:NH1	1:G:290:TYR:OH	2.49	0.45
1:G:553:ARG:NH1	1:G:555:GLU:OE2	2.48	0.45
1:G:960:MET:HE2	1:G:963:ASN:HB2	1.99	0.45
1:G:2208:MET:HE1	1:G:2253:HIS:CG	2.52	0.45
1:G:2283:ASN:HB3	1:G:2286:LEU:HB2	1.99	0.45
1:G:3401:LEU:HD23	1:G:3401:LEU:HA	1.81	0.45
1:J:937:CYS:HB3	1:J:1053:ILE:HG22	1.98	0.45
1:J:3459:VAL:HG11	1:J:3505:VAL:HG11	1.99	0.45
1:B:173:SER:HB2	1:B:176:SER:O	2.17	0.45
1:B:251:ALA:O	1:B:255:HIS:ND1	2.40	0.45
1:B:426:ARG:H	1:B:506:TYR:HA	1.82	0.45
1:B:936:GLY:HA3	1:B:1056:PRO:HB3	1.99	0.45
1:B:2523:ASP:OD1	1:B:2524:VAL:N	2.49	0.45
1:B:2689:LYS:HG2	1:B:2690:LYS:N	2.31	0.45
1:B:2758:PHE:O	1:B:2762:THR:HG23	2.17	0.45
1:E:426:ARG:H	1:E:506:TYR:HA	1.82	0.45
1:E:613:ALA:HB1	1:E:618:GLN:HE22	1.83	0.45
1:E:864:PRO:N	1:E:865:PRO:HD2	2.32	0.45
1:E:3262:ARG:HG3	1:E:3326:ASN:ND2	2.28	0.45
1:E:3540:TYR:HA	1:E:3544:ASP:O	2.16	0.45
1:E:4065:PHE:HA	1:E:4068:LEU:HB2	1.99	0.45
1:E:4069:LYS:O	1:E:4072:VAL:HG12	2.17	0.45
1:E:4767:TRP:O	1:E:4767:TRP:HD1	1.99	0.45
1:G:340:LYS:HB2	1:G:344:SER:HB3	1.99	0.45
1:G:601:ASP:OD1	1:G:1668:ARG:NH2	2.50	0.45
1:G:874:LEU:O	1:G:878:ILE:HG12	2.17	0.45
1:G:2758:PHE:O	1:G:2762:THR:HG23	2.17	0.45
1:G:3075:LEU:O	1:G:3146:HIS:HE1	1.99	0.45
1:G:3223:SER:O	1:G:3227:ARG:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:874:LEU:O	1:J:878:ILE:HG12	2.17	0.45
1:J:924:MET:O	1:J:928:THR:HG23	2.16	0.45
1:J:2693:GLN:HB3	1:J:2697:ARG:HH22	1.81	0.45
1:J:2702:CYS:O	1:J:2706:ILE:HD13	2.17	0.45
1:J:2801:ASP:HA	1:J:2804:ILE:HG12	1.99	0.45
1:J:3006:ILE:HD11	1:J:3071:LEU:HD21	1.97	0.45
1:J:4767:TRP:O	1:J:4767:TRP:HD1	1.99	0.45
1:J:5017:ARG:HD3	1:J:5019:TRP:CZ2	2.52	0.45
3:M:104:TYR:CD1	3:M:104:TYR:C	2.95	0.45
1:B:371:VAL:HG12	1:B:373:LYS:H	1.82	0.44
1:B:2886:TRP:HA	1:B:2889:LYS:HG2	1.99	0.44
1:E:77:ALA:O	1:E:81:MET:HG3	2.17	0.44
1:E:728:ARG:NH2	1:E:1489:CYS:SG	2.90	0.44
1:E:3318:ASN:O	1:E:3322:ILE:HG12	2.17	0.44
1:E:3435:PHE:HZ	1:E:3602:VAL:HG21	1.81	0.44
1:G:487:VAL:O	1:G:491:ILE:HG13	2.17	0.44
1:G:864:PRO:N	1:G:865:PRO:HD2	2.32	0.44
1:G:937:CYS:HB3	1:G:1053:ILE:HG22	1.98	0.44
1:G:1943:LEU:HD13	1:G:2098:VAL:HG22	1.99	0.44
1:G:4093:PHE:CZ	1:G:4097:MET:HE2	2.51	0.44
1:G:4655:PHE:O	1:G:4659:ILE:HG12	2.17	0.44
1:G:5017:ARG:HD3	1:G:5019:TRP:CZ2	2.52	0.44
1:J:861:ILE:HD12	1:J:934:ALA:HA	2.00	0.44
1:J:2758:PHE:O	1:J:2762:THR:HG23	2.17	0.44
1:B:246:TYR:CE1	1:B:373:LYS:HE3	2.52	0.44
1:B:2208:MET:HE1	1:B:2253:HIS:CG	2.52	0.44
1:B:3979:SER:O	1:B:3983:SER:OG	2.31	0.44
1:E:24:CYS:HB2	1:E:200:TRP:CE3	2.53	0.44
1:E:553:ARG:NH1	1:E:555:GLU:OE2	2.48	0.44
1:E:2700:MET:CE	1:E:2701:PRO:HD3	2.43	0.44
1:E:2978:GLU:HB3	1:E:3056:LEU:HD11	1.99	0.44
1:E:4093:PHE:CZ	1:E:4097:MET:HE2	2.52	0.44
1:E:4097:MET:SD	1:E:4108:ILE:HG23	2.56	0.44
1:E:5017:ARG:HD3	1:E:5019:TRP:CZ2	2.52	0.44
1:G:861:ILE:HD12	1:G:934:ALA:HA	2.00	0.44
1:G:913:LEU:HD11	1:G:922:LEU:HD11	2.00	0.44
1:G:936:GLY:HA3	1:G:1056:PRO:HB3	1.99	0.44
1:G:2865:VAL:HG23	1:G:2928:LYS:HZ1	1.81	0.44
1:G:3018:LEU:HD13	1:G:3150:HIS:CE1	2.51	0.44
1:J:426:ARG:H	1:J:506:TYR:HA	1.82	0.44
1:J:1943:LEU:HD13	1:J:2098:VAL:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:3717:ASP:OD1	1:J:3717:ASP:N	2.48	0.44
1:J:4157:ASP:H	1:J:4161:ARG:HH21	1.66	0.44
3:M:101:PRO:HD2	3:M:104:TYR:O	2.17	0.44
1:B:2283:ASN:HB3	1:B:2286:LEU:HB2	1.99	0.44
1:B:2765:LYS:NZ	1:B:2860:PRO:HA	2.32	0.44
1:B:3372:VAL:HG12	1:B:3398:PHE:CZ	2.52	0.44
1:B:4920:PHE:O	1:B:4924:VAL:HG22	2.17	0.44
1:E:2608:MET:HE2	1:E:2608:MET:HB3	1.76	0.44
1:E:2886:TRP:HA	1:E:2889:LYS:HG2	1.99	0.44
1:E:3651:ASN:O	1:E:3655:GLU:HG2	2.18	0.44
1:E:4666:VAL:O	1:E:4670:ILE:HG12	2.18	0.44
1:G:23:GLN:HB3	1:G:34:LYS:HG2	1.99	0.44
1:G:1667:LEU:O	1:G:1671:ARG:HG3	2.18	0.44
1:G:1860:LYS:O	1:G:1864:LYS:HG2	2.18	0.44
1:G:2420:HIS:HB2	1:G:2492:ALA:HA	1.99	0.44
1:G:3148:ALA:HB2	1:G:3200:ALA:HB2	1.98	0.44
1:G:3372:VAL:HG12	1:G:3398:PHE:CZ	2.52	0.44
1:G:4157:ASP:H	1:G:4161:ARG:HH21	1.66	0.44
1:J:871:ARG:HB2	1:J:925:SER:HB3	1.99	0.44
1:J:1667:LEU:O	1:J:1671:ARG:HG3	2.18	0.44
1:J:2978:GLU:HB3	1:J:3056:LEU:HD11	1.99	0.44
1:B:960:MET:HE2	1:B:963:ASN:HB2	1.99	0.44
1:B:1274:HIS:O	1:B:1559:GLN:NE2	2.33	0.44
1:B:3327:LEU:HD22	1:B:3368:ARG:CZ	2.47	0.44
1:E:936:GLY:HA3	1:E:1056:PRO:HB3	2.00	0.44
1:E:2865:VAL:HG23	1:E:2928:LYS:HZ1	1.83	0.44
1:E:3039:ILE:O	1:E:3043:PHE:HD1	2.00	0.44
1:E:3040:THR:OG1	1:E:3080:VAL:HG12	2.18	0.44
1:E:4230:LYS:NZ	1:E:4231:MET:SD	2.84	0.44
1:G:173:SER:HB2	1:G:176:SER:O	2.17	0.44
1:G:728:ARG:NH2	1:G:1489:CYS:SG	2.90	0.44
1:G:1123:VAL:HG12	1:G:1132:TRP:HB3	1.99	0.44
1:G:4920:PHE:O	1:G:4924:VAL:HG22	2.17	0.44
1:J:131:LEU:O	1:J:178:ARG:NH2	2.46	0.44
1:J:340:LYS:HB2	1:J:344:SER:HB3	1.99	0.44
1:J:728:ARG:NH2	1:J:1489:CYS:SG	2.90	0.44
1:J:913:LEU:HD11	1:J:922:LEU:HD11	1.99	0.44
1:J:2765:LYS:NZ	1:J:2860:PRO:HA	2.32	0.44
1:J:3039:ILE:O	1:J:3043:PHE:HD1	2.00	0.44
3:F:104:TYR:CE1	3:F:106:PRO:HG3	2.46	0.44
1:B:613:ALA:HB1	1:B:618:GLN:HE22	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:864:PRO:N	1:B:865:PRO:HD2	2.32	0.44
1:B:874:LEU:O	1:B:878:ILE:HG12	2.17	0.44
1:B:3207:GLU:HG3	1:B:3246:LEU:HD21	1.99	0.44
1:B:4157:ASP:H	1:B:4161:ARG:HH21	1.66	0.44
1:E:3209:GLN:HG2	1:E:3210:LEU:HG	1.98	0.44
1:G:247:TYR:HD2	1:G:372:LEU:HB3	1.80	0.44
1:G:3039:ILE:O	1:G:3043:PHE:HD1	2.00	0.44
1:G:3327:LEU:HD22	1:G:3368:ARG:CZ	2.47	0.44
1:G:3989:VAL:HG13	1:G:4023:MET:CE	2.46	0.44
1:J:24:CYS:HB2	1:J:200:TRP:CE3	2.53	0.44
1:J:3651:ASN:O	1:J:3655:GLU:HG2	2.18	0.44
1:J:4028:LEU:HD23	1:J:4146:LEU:HD13	2.00	0.44
1:B:4118:ASP:OD1	1:B:4119:GLU:N	2.49	0.44
1:B:4157:ASP:HB3	1:B:4160:LEU:HB3	2.00	0.44
1:E:222:LEU:C	1:E:230:CYS:HB3	2.43	0.44
1:E:2686:LEU:HD22	1:E:2696:TYR:CZ	2.52	0.44
1:E:3049:LEU:HB3	1:E:3057:PHE:CE1	2.53	0.44
1:E:4120:ASN:HB2	1:E:4122:MET:HG2	2.00	0.44
1:G:2765:LYS:HA	1:G:2765:LYS:HD3	1.67	0.44
1:G:2765:LYS:NZ	1:G:2860:PRO:HA	2.32	0.44
1:G:2813:LEU:HA	1:G:2816:MET:SD	2.58	0.44
1:G:4666:VAL:O	1:G:4670:ILE:HG12	2.18	0.44
1:G:4767:TRP:O	1:G:4767:TRP:HD1	1.99	0.44
1:J:936:GLY:HA3	1:J:1056:PRO:HB3	1.99	0.44
1:J:2813:LEU:HA	1:J:2816:MET:SD	2.58	0.44
1:J:3318:ASN:O	1:J:3322:ILE:HG12	2.17	0.44
2:D:25:HIS:HB3	2:D:40:ARG:CZ	2.47	0.44
3:M:30:SER:HB3	3:M:99:ARG:CB	2.48	0.44
1:B:81:MET:HE2	1:B:81:MET:HB2	1.94	0.44
1:B:222:LEU:C	1:B:230:CYS:HB3	2.43	0.44
1:B:961:MET:C	1:B:961:MET:HE2	2.43	0.44
1:B:1667:LEU:O	1:B:1671:ARG:HG3	2.18	0.44
1:B:1758:ARG:NH2	1:B:2036:GLN:OE1	2.51	0.44
1:B:1860:LYS:O	1:B:1864:LYS:HG2	2.18	0.44
1:B:3040:THR:OG1	1:B:3080:VAL:HG12	2.18	0.44
1:B:4065:PHE:HA	1:B:4068:LEU:HB2	1.99	0.44
1:B:4069:LYS:O	1:B:4072:VAL:HG12	2.17	0.44
1:B:4666:VAL:O	1:B:4670:ILE:HG12	2.18	0.44
1:E:4032:GLU:HG3	1:E:5006:GLN:HE21	1.81	0.44
1:E:4157:ASP:H	1:E:4161:ARG:HH21	1.65	0.44
1:G:131:LEU:O	1:G:178:ARG:NH2	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:499:THR:HG23	1:G:502:HIS:H	1.83	0.44
1:G:735:GLN:OE1	1:G:735:GLN:HA	2.18	0.44
1:G:2886:TRP:HA	1:G:2889:LYS:HG2	1.99	0.44
1:J:173:SER:HB2	1:J:176:SER:O	2.17	0.44
1:J:487:VAL:O	1:J:491:ILE:HG13	2.17	0.44
1:J:917:GLU:CB	3:K:104:TYR:HE2	2.23	0.44
1:J:1123:VAL:HG12	1:J:1132:TRP:HB3	1.99	0.44
1:J:3249:LEU:HD21	1:J:3276:MET:HE3	2.00	0.44
1:J:4118:ASP:OD1	1:J:4119:GLU:N	2.49	0.44
1:B:1081:TYR:HD1	1:B:1230:MET:HE1	1.82	0.44
1:B:1738:LEU:HD12	1:B:1738:LEU:HA	1.80	0.44
1:B:2010:LEU:HD12	1:B:3656:SER:HB2	2.00	0.44
1:B:2813:LEU:HA	1:B:2816:MET:SD	2.58	0.44
1:B:3039:ILE:O	1:B:3043:PHE:HD1	2.00	0.44
1:B:4945:ASP:O	1:B:4948:GLU:HG3	2.18	0.44
1:E:874:LEU:O	1:E:878:ILE:HG12	2.17	0.44
1:E:1815:LEU:HD22	1:E:1845:VAL:HG21	2.00	0.44
1:E:2801:ASP:HA	1:E:2804:ILE:HG12	1.99	0.44
1:E:3207:GLU:HG3	1:E:3246:LEU:HD21	1.99	0.44
1:E:3459:VAL:HG11	1:E:3505:VAL:HG11	1.99	0.44
1:G:3546:ASP:O	1:G:3550:ARG:HG2	2.18	0.44
1:J:23:GLN:HB3	1:J:34:LYS:HG2	1.99	0.44
1:J:961:MET:C	1:J:961:MET:HE2	2.43	0.44
1:J:2538:THR:O	1:J:2542:SER:N	2.42	0.44
1:J:3040:THR:OG1	1:J:3080:VAL:HG12	2.18	0.44
1:J:3207:GLU:HG3	1:J:3246:LEU:HD21	1.99	0.44
1:J:4120:ASN:HB2	1:J:4122:MET:HG2	2.00	0.44
1:B:298:GLY:HA3	1:B:378:LEU:H	1.83	0.44
1:B:661:LYS:HG2	1:B:749:ASP:OD1	2.16	0.44
1:B:2686:LEU:HD22	1:B:2696:TYR:CZ	2.52	0.44
1:B:2825:LYS:HG3	1:B:2935:TYR:CE1	2.53	0.44
1:B:3844:LEU:HD11	1:E:76:ARG:HH21	1.83	0.44
1:E:913:LEU:HD11	1:E:922:LEU:HD11	1.99	0.44
1:E:2713:ASP:HA	1:E:2954:ARG:HD3	2.00	0.44
1:E:4157:ASP:HB3	1:E:4160:LEU:HB3	2.00	0.44
1:G:917:GLU:CB	3:M:104:TYR:HE2	2.25	0.44
1:G:1081:TYR:HD1	1:G:1230:MET:HE1	1.81	0.44
1:G:2702:CYS:O	1:G:2706:ILE:HD13	2.17	0.44
1:G:3207:GLU:HG3	1:G:3246:LEU:HD21	1.99	0.44
1:G:3318:ASN:O	1:G:3322:ILE:HG12	2.17	0.44
1:G:3969:ILE:HG21	1:G:3980:LEU:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:298:GLY:HA3	1:J:378:LEU:H	1.83	0.44
1:J:613:ALA:HB1	1:J:618:GLN:HE22	1.83	0.44
1:J:2352:VAL:O	1:J:2356:LEU:HG	2.18	0.44
1:J:2865:VAL:HG23	1:J:2928:LYS:HZ1	1.82	0.44
1:J:2886:TRP:HA	1:J:2889:LYS:HG2	1.99	0.44
1:J:3420:ARG:NH1	1:J:3516:LYS:O	2.51	0.44
1:J:4069:LYS:O	1:J:4072:VAL:HG12	2.17	0.44
2:H:17:LYS:N	2:H:20:GLN:OE1	2.49	0.44
1:B:340:LYS:HB2	1:B:344:SER:HB3	1.99	0.43
1:B:1694:LEU:HB3	1:B:1715:LEU:HD12	1.99	0.43
1:B:2420:HIS:HB2	1:B:2492:ALA:HA	1.99	0.43
1:B:3100:SER:HB2	1:B:3167:ARG:NH2	2.33	0.43
1:E:3372:VAL:HG12	1:E:3398:PHE:CZ	2.52	0.43
1:E:4085:ARG:HH12	1:E:4122:MET:HE1	1.82	0.43
1:E:4118:ASP:OD1	1:E:4119:GLU:N	2.49	0.43
1:E:4145:VAL:HG22	1:E:4178:LEU:HD13	2.00	0.43
1:G:961:MET:C	1:G:961:MET:HE2	2.43	0.43
1:G:1758:ARG:NH2	1:G:2036:GLN:OE1	2.51	0.43
1:G:4157:ASP:HB3	1:G:4160:LEU:HB3	2.00	0.43
1:J:133:PHE:HB2	1:J:193:ALA:HB3	2.00	0.43
1:J:864:PRO:N	1:J:865:PRO:HD2	2.32	0.43
1:J:960:MET:HE2	1:J:963:ASN:HB2	1.99	0.43
1:J:1860:LYS:O	1:J:1864:LYS:HG2	2.18	0.43
1:J:3546:ASP:O	1:J:3550:ARG:HG2	2.18	0.43
1:J:4157:ASP:HB3	1:J:4160:LEU:HB3	2.00	0.43
2:D:17:LYS:N	2:D:20:GLN:OE1	2.49	0.43
1:B:861:ILE:HD12	1:B:934:ALA:HA	2.00	0.43
1:B:877:ASN:O	1:B:881:LEU:HG	2.18	0.43
1:B:1123:VAL:HG12	1:B:1132:TRP:HB3	1.99	0.43
1:B:1828:ASP:N	1:B:1828:ASP:OD1	2.51	0.43
1:B:2280:VAL:HG21	1:B:2290:LEU:HD11	2.00	0.43
1:B:3049:LEU:HB3	1:B:3057:PHE:CE1	2.53	0.43
1:B:3366:ARG:NH1	1:B:3437:MET:SD	2.91	0.43
1:E:23:GLN:HB3	1:E:34:LYS:HG2	1.99	0.43
1:E:1758:ARG:NH2	1:E:2036:GLN:OE1	2.51	0.43
1:E:1860:LYS:O	1:E:1864:LYS:HG2	2.18	0.43
1:E:3979:SER:O	1:E:3983:SER:OG	2.31	0.43
1:E:4068:LEU:HD23	1:E:4068:LEU:HA	1.90	0.43
1:E:4920:PHE:O	1:E:4924:VAL:HG22	2.17	0.43
1:G:877:ASN:O	1:G:881:LEU:HG	2.18	0.43
1:G:1694:LEU:HB3	1:G:1715:LEU:HD12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:2700:MET:CE	1:G:2701:PRO:HD3	2.43	0.43
1:G:2825:LYS:HG3	1:G:2935:TYR:CE1	2.53	0.43
1:G:3262:ARG:HB2	1:G:3325:ASN:ND2	2.34	0.43
1:G:4768:LEU:HB3	1:G:4769:MET:HE2	2.00	0.43
1:J:222:LEU:C	1:J:230:CYS:HB3	2.43	0.43
1:J:2686:LEU:HD22	1:J:2696:TYR:CZ	2.52	0.43
1:J:3366:ARG:NH1	1:J:3437:MET:SD	2.91	0.43
1:J:3435:PHE:HZ	1:J:3602:VAL:HG21	1.81	0.43
1:J:4731:ILE:HD13	1:J:4731:ILE:HA	1.88	0.43
1:J:4920:PHE:O	1:J:4924:VAL:HG22	2.17	0.43
1:B:499:THR:HG23	1:B:502:HIS:H	1.83	0.43
1:B:1094:ALA:HB1	1:B:1100:MET:HE1	2.00	0.43
1:B:2702:CYS:O	1:B:2706:ILE:HD13	2.17	0.43
1:B:2801:ASP:HA	1:B:2804:ILE:HG12	1.99	0.43
1:B:3398:PHE:CE1	1:B:3451:PHE:HB2	2.54	0.43
1:B:3651:ASN:O	1:B:3655:GLU:HG2	2.18	0.43
1:B:3836:MET:HE2	1:B:3836:MET:HB2	1.96	0.43
1:E:20:VAL:HG12	1:E:22:LEU:H	1.83	0.43
1:E:173:SER:HB2	1:E:176:SER:O	2.17	0.43
1:E:861:ILE:HD12	1:E:934:ALA:HA	2.00	0.43
1:E:2312:MET:H	1:E:2312:MET:HG3	1.70	0.43
1:E:2758:PHE:O	1:E:2762:THR:HG23	2.17	0.43
1:E:3249:LEU:HD21	1:E:3276:MET:HE3	2.00	0.43
1:E:3546:ASP:O	1:E:3550:ARG:HG2	2.18	0.43
1:E:4768:LEU:C	1:E:4769:MET:HE2	2.43	0.43
1:E:4945:ASP:O	1:E:4948:GLU:HG3	2.18	0.43
1:G:244:LEU:HD23	1:G:375:LYS:HZ2	1.82	0.43
1:G:2325:PRO:HG2	1:G:2422:ILE:HD13	2.00	0.43
1:G:2686:LEU:HD22	1:G:2696:TYR:CZ	2.52	0.43
1:G:3040:THR:OG1	1:G:3080:VAL:HG12	2.18	0.43
1:G:3420:ARG:NH1	1:G:3516:LYS:O	2.51	0.43
1:G:4949:GLN:NE2	1:G:4953:ASP:OD2	2.52	0.43
1:J:20:VAL:HG12	1:J:22:LEU:H	1.83	0.43
1:J:2894:LEU:HD21	1:J:2901:THR:HA	2.00	0.43
1:J:3372:VAL:HG12	1:J:3398:PHE:CZ	2.53	0.43
1:J:3398:PHE:CE1	1:J:3451:PHE:HB2	2.54	0.43
1:J:3944:GLU:HG2	1:J:3946:GLN:H	1.83	0.43
1:J:3969:ILE:HG21	1:J:3980:LEU:HD12	2.00	0.43
1:J:4065:PHE:HA	1:J:4068:LEU:HB2	1.99	0.43
1:J:4768:LEU:C	1:J:4769:MET:HE2	2.43	0.43
1:B:553:ARG:NH1	1:B:555:GLU:OE2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1993:ARG:O	1:B:1997:GLU:HG2	2.19	0.43
1:B:3262:ARG:HB2	1:B:3325:ASN:ND2	2.34	0.43
1:B:3546:ASP:O	1:B:3550:ARG:HG2	2.18	0.43
1:B:3562:LYS:HE2	1:B:3562:LYS:HB2	1.81	0.43
1:B:4077:PHE:HE1	1:B:4088:ILE:HG12	1.84	0.43
1:E:901:LYS:HG2	1:E:901:LYS:O	2.18	0.43
1:E:1094:ALA:HB1	1:E:1100:MET:HE1	2.00	0.43
1:E:1667:LEU:O	1:E:1671:ARG:HG3	2.18	0.43
1:E:1694:LEU:HB3	1:E:1715:LEU:HD12	1.99	0.43
1:E:2283:ASN:HB3	1:E:2286:LEU:HB2	1.99	0.43
1:E:2813:LEU:HA	1:E:2816:MET:SD	2.58	0.43
1:E:4676:GLU:O	1:E:4680:LYS:HG2	2.19	0.43
1:G:2713:ASP:HA	1:G:2954:ARG:HD3	2.00	0.43
1:J:477:LEU:O	1:J:480:GLU:HG3	2.19	0.43
1:J:901:LYS:O	1:J:901:LYS:HG2	2.18	0.43
1:J:1694:LEU:HB3	1:J:1715:LEU:HD12	1.99	0.43
1:J:4666:VAL:O	1:J:4670:ILE:HG12	2.18	0.43
1:B:2431:ASP:HB2	1:B:2501:SER:HB2	2.01	0.43
1:B:3249:LEU:HD21	1:B:3276:MET:HE3	2.00	0.43
1:B:3406:TYR:HE1	1:B:3509:LEU:HG	1.83	0.43
1:E:877:ASN:O	1:E:881:LEU:HG	2.18	0.43
1:E:2568:LEU:HD12	1:E:2568:LEU:O	2.19	0.43
1:E:2765:LYS:HD3	1:E:2765:LYS:HA	1.67	0.43
1:E:2773:ASN:OD1	1:J:1508:ARG:NH2	2.39	0.43
1:E:2894:LEU:HD21	1:E:2901:THR:HA	2.01	0.43
1:E:3060:ASP:O	1:E:3064:VAL:HG23	2.19	0.43
1:E:3350:ARG:NE	1:E:3350:ARG:HA	2.34	0.43
1:E:3366:ARG:NH1	1:E:3437:MET:SD	2.91	0.43
1:E:3398:PHE:CE1	1:E:3451:PHE:HB2	2.53	0.43
1:E:3408:LEU:HD12	1:E:3408:LEU:HA	1.81	0.43
1:E:4574:ASN:ND2	1:E:4810:ALA:HA	2.29	0.43
1:G:24:CYS:HB2	1:G:200:TRP:CE3	2.53	0.43
1:G:1828:ASP:OD1	1:G:1828:ASP:N	2.51	0.43
1:G:3944:GLU:HG2	1:G:3946:GLN:H	1.83	0.43
1:J:247:TYR:HD2	1:J:372:LEU:O	2.01	0.43
1:J:365:LYS:O	1:J:369:LEU:HG	2.18	0.43
1:J:2283:ASN:HB3	1:J:2286:LEU:HB2	1.99	0.43
1:J:3408:LEU:HA	1:J:3408:LEU:HD12	1.81	0.43
1:J:4026:MET:HE3	1:J:4026:MET:HB3	1.94	0.43
1:B:1032:LYS:HB3	1:B:1036:ARG:NH2	2.33	0.43
1:B:2764:GLU:HG3	1:B:2857:PRO:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4949:GLN:NE2	1:B:4953:ASP:OD2	2.52	0.43
1:E:246:TYR:HE1	1:E:375:LYS:HZ3	1.66	0.43
1:E:735:GLN:HA	1:E:735:GLN:OE1	2.18	0.43
1:E:960:MET:HE2	1:E:963:ASN:HB2	1.99	0.43
1:E:961:MET:HE2	1:E:961:MET:C	2.43	0.43
1:E:1559:GLN:NE2	1:E:1559:GLN:O	2.52	0.43
1:E:2452:ARG:O	1:E:2456:ILE:HG13	2.19	0.43
1:E:2825:LYS:HG3	1:E:2935:TYR:CE1	2.53	0.43
1:E:2867:LEU:HD12	1:E:2867:LEU:HA	1.82	0.43
1:E:4077:PHE:HE1	1:E:4088:ILE:HG12	1.84	0.43
1:G:20:VAL:HG12	1:G:22:LEU:H	1.83	0.43
1:G:133:PHE:HB2	1:G:193:ALA:HB3	2.00	0.43
1:G:1032:LYS:HB3	1:G:1036:ARG:NH2	2.33	0.43
1:G:1993:ARG:O	1:G:1997:GLU:HG2	2.19	0.43
1:G:3350:ARG:NE	1:G:3350:ARG:HA	2.34	0.43
1:G:3366:ARG:NH1	1:G:3437:MET:SD	2.91	0.43
1:G:4028:LEU:HD23	1:G:4146:LEU:HD13	2.00	0.43
1:G:4069:LYS:O	1:G:4072:VAL:HG12	2.17	0.43
1:G:4768:LEU:C	1:G:4769:MET:HE2	2.43	0.43
1:G:4945:ASP:O	1:G:4948:GLU:HG3	2.18	0.43
1:J:1559:GLN:NE2	1:J:1559:GLN:O	2.52	0.43
1:J:2431:ASP:HB2	1:J:2501:SER:HB2	2.01	0.43
1:J:2568:LEU:HD12	1:J:2568:LEU:O	2.19	0.43
1:J:4077:PHE:HE1	1:J:4088:ILE:HG12	1.84	0.43
1:B:20:VAL:HG12	1:B:22:LEU:H	1.83	0.43
1:B:24:CYS:HB2	1:B:200:TRP:CE3	2.53	0.43
1:B:913:LEU:HD11	1:B:922:LEU:HD11	1.99	0.43
1:B:1815:LEU:HD22	1:B:1845:VAL:HG21	2.00	0.43
1:B:2352:VAL:O	1:B:2356:LEU:HG	2.18	0.43
1:B:2713:ASP:HA	1:B:2954:ARG:HD3	2.00	0.43
1:B:3459:VAL:HG11	1:B:3505:VAL:HG11	1.99	0.43
1:B:3962:PHE:O	1:B:3966:THR:HG23	2.19	0.43
1:B:4120:ASN:HB2	1:B:4122:MET:HG2	2.00	0.43
1:B:4768:LEU:C	1:B:4769:MET:HE2	2.43	0.43
1:E:1032:LYS:HB3	1:E:1036:ARG:NH2	2.33	0.43
1:E:1993:ARG:O	1:E:1997:GLU:HG2	2.19	0.43
1:E:2352:VAL:O	1:E:2356:LEU:HG	2.18	0.43
1:E:2969:ILE:O	1:E:2972:GLU:HG3	2.19	0.43
1:E:3100:SER:HB2	1:E:3167:ARG:NH2	2.33	0.43
1:E:4184:MET:HA	1:E:4190:ILE:HD13	2.01	0.43
1:G:298:GLY:HA3	1:G:378:LEU:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:365:LYS:O	1:G:369:LEU:HG	2.19	0.43
1:G:901:LYS:O	1:G:901:LYS:HG2	2.18	0.43
1:G:1094:ALA:HB1	1:G:1100:MET:HE1	2.01	0.43
1:G:2264:GLY:O	1:G:2268:GLN:HG2	2.19	0.43
1:G:2431:ASP:HB2	1:G:2501:SER:HB2	2.01	0.43
1:G:2452:ARG:O	1:G:2456:ILE:HG13	2.19	0.43
1:G:2894:LEU:HD21	1:G:2901:THR:HA	2.01	0.43
1:G:3249:LEU:HD21	1:G:3276:MET:HE3	2.00	0.43
1:G:4152:GLU:OE1	1:G:4194:TYR:OH	2.28	0.43
1:J:735:GLN:OE1	1:J:735:GLN:HA	2.18	0.43
1:J:1032:LYS:HB3	1:J:1036:ARG:NH2	2.33	0.43
1:J:3049:LEU:HB3	1:J:3057:PHE:CE1	2.53	0.43
1:J:3060:ASP:O	1:J:3064:VAL:HG23	2.19	0.43
1:J:3401:LEU:HD23	1:J:3401:LEU:HA	1.80	0.43
1:J:4768:LEU:HB3	1:J:4769:MET:HE2	2.00	0.43
3:K:32:ASN:OD1	3:K:33:SER:N	2.52	0.43
1:B:882:TRP:NE1	1:B:886:ARG:CZ	2.82	0.43
1:B:3969:ILE:HG21	1:B:3980:LEU:HD12	2.01	0.43
1:B:3989:VAL:HG13	1:B:4023:MET:CE	2.47	0.43
1:B:4028:LEU:HD23	1:B:4146:LEU:HD13	1.99	0.43
1:E:133:PHE:HB2	1:E:193:ALA:HB3	2.00	0.43
1:E:477:LEU:O	1:E:480:GLU:HG3	2.19	0.43
1:E:996:TRP:HA	1:E:999:ASP:OD2	2.19	0.43
1:E:1123:VAL:HG12	1:E:1132:TRP:HB3	1.99	0.43
1:E:1943:LEU:HD13	1:E:2098:VAL:HG22	2.00	0.43
1:E:2431:ASP:HB2	1:E:2501:SER:HB2	2.01	0.43
1:E:3268:HIS:CE1	1:E:3272:ILE:HG13	2.54	0.43
1:G:477:LEU:O	1:G:480:GLU:HG3	2.19	0.43
1:G:882:TRP:NE1	1:G:886:ARG:CZ	2.82	0.43
1:G:2655:TYR:OH	1:G:2671:GLU:OE2	2.31	0.43
1:G:3100:SER:HB2	1:G:3167:ARG:NH2	2.33	0.43
1:G:3651:ASN:O	1:G:3655:GLU:HG2	2.18	0.43
1:J:1815:LEU:HD22	1:J:1845:VAL:HG21	2.00	0.43
1:J:2420:HIS:HB2	1:J:2492:ALA:HA	1.99	0.43
1:J:3262:ARG:HB2	1:J:3325:ASN:ND2	2.34	0.43
1:J:3292:PRO:HA	1:J:3293:PRO:HD3	1.91	0.43
1:J:4676:GLU:O	1:J:4680:LYS:HG2	2.19	0.43
1:J:4945:ASP:O	1:J:4948:GLU:HG3	2.18	0.43
3:C:92:VAL:HG12	3:C:122:GLN:OE1	2.19	0.43
3:K:39:GLN:OE1	3:K:45:ARG:NH2	2.39	0.43
1:B:863:LEU:O	1:B:867:LEU:HG	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:917:GLU:CB	3:C:104:TYR:HE2	2.25	0.43
1:B:1559:GLN:NE2	1:B:1559:GLN:O	2.52	0.43
1:B:1943:LEU:HD13	1:B:2098:VAL:HG22	2.00	0.43
1:B:2264:GLY:O	1:B:2268:GLN:HG2	2.19	0.43
1:B:4184:MET:HA	1:B:4190:ILE:HD13	2.01	0.43
1:B:4813:LEU:HD23	1:B:4813:LEU:HA	1.85	0.43
1:B:4998:LYS:HB2	1:B:4998:LYS:HE3	1.72	0.43
1:E:623:GLU:HG2	2:D:88:PRO:HB3	2.00	0.43
1:E:882:TRP:NE1	1:E:886:ARG:CZ	2.82	0.43
1:G:70:GLU:HG2	1:G:71:GLN:HG3	2.01	0.43
1:G:222:LEU:C	1:G:230:CYS:HB3	2.43	0.43
1:G:451:TYR:CZ	1:G:474:ARG:HD2	2.54	0.43
1:G:623:GLU:HG2	2:H:88:PRO:HB3	2.01	0.43
1:G:1012:ASP:HB3	1:G:1015:ALA:HB3	2.01	0.43
1:G:3039:ILE:O	1:G:3043:PHE:CD1	2.72	0.43
1:G:3060:ASP:O	1:G:3064:VAL:HG23	2.19	0.43
1:G:3266:MET:O	1:G:3270:ILE:HG12	2.19	0.43
1:G:4060:LYS:HA	1:G:4063:ASP:OD2	2.19	0.43
1:G:4077:PHE:HE1	1:G:4088:ILE:HG12	1.84	0.43
1:G:4676:GLU:O	1:G:4680:LYS:HG2	2.19	0.43
1:J:1537:ASN:OD1	1:J:1537:ASN:N	2.47	0.43
1:J:2264:GLY:O	1:J:2268:GLN:HG2	2.19	0.43
1:J:2924:GLN:O	1:J:2928:LYS:HG2	2.19	0.43
1:J:4687:TYR:OH	1:J:4699:GLY:O	2.36	0.43
3:F:13:GLN:OE1	3:F:13:GLN:N	2.37	0.43
3:M:32:ASN:OD1	3:M:33:SER:N	2.52	0.43
1:B:133:PHE:HB2	1:B:193:ALA:HB3	2.00	0.43
1:B:745:SER:HB2	1:B:758:ARG:HG2	2.01	0.43
1:B:3039:ILE:O	1:B:3043:PHE:CD1	2.72	0.43
1:B:3060:ASP:O	1:B:3064:VAL:HG23	2.19	0.43
1:B:3268:HIS:CE1	1:B:3272:ILE:HG13	2.54	0.43
1:B:3350:ARG:NE	1:B:3350:ARG:HA	2.34	0.43
1:B:3722:TYR:OH	1:B:3782:MET:HG3	2.19	0.43
1:E:1601:MET:HE3	1:E:1601:MET:HB3	1.89	0.43
1:E:2420:HIS:HB2	1:E:2492:ALA:HA	1.99	0.43
1:E:3207:GLU:HG3	1:E:3246:LEU:CD2	2.49	0.43
1:G:1559:GLN:NE2	1:G:1559:GLN:O	2.52	0.43
1:G:1708:ARG:O	1:G:1712:TYR:HD1	2.02	0.43
1:G:1964:ARG:O	1:G:1968:LYS:NZ	2.46	0.43
1:G:2352:VAL:O	1:G:2356:LEU:HG	2.18	0.43
1:G:3722:TYR:OH	1:G:3782:MET:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3987:ASP:N	1:G:3987:ASP:OD1	2.52	0.43
1:G:4120:ASN:HB2	1:G:4122:MET:HG2	2.00	0.43
1:J:1993:ARG:O	1:J:1997:GLU:HG2	2.19	0.43
1:J:2010:LEU:HD12	1:J:3656:SER:HB2	2.00	0.43
1:J:2713:ASP:HA	1:J:2954:ARG:HD3	2.00	0.43
1:J:2825:LYS:HG3	1:J:2935:TYR:CE1	2.53	0.43
1:J:2909:ASP:N	1:J:2909:ASP:OD1	2.52	0.43
1:J:3100:SER:HB2	1:J:3167:ARG:NH2	2.33	0.43
1:J:3546:ASP:OD1	1:J:3546:ASP:N	2.52	0.43
1:J:4145:VAL:HG22	1:J:4178:LEU:HD13	2.00	0.43
1:J:4949:GLN:NE2	1:J:4953:ASP:OD2	2.52	0.43
3:F:30:SER:HB3	3:F:99:ARG:CB	2.49	0.43
1:B:2924:GLN:O	1:B:2928:LYS:HG2	2.19	0.42
1:B:3207:GLU:HG3	1:B:3246:LEU:CD2	2.49	0.42
1:B:3266:MET:O	1:B:3270:ILE:HG12	2.19	0.42
1:B:4071:ILE:O	1:B:4074:SER:OG	2.36	0.42
1:B:4768:LEU:HB3	1:B:4769:MET:HE2	2.00	0.42
1:E:340:LYS:HB2	1:E:344:SER:HB3	1.99	0.42
1:E:377:ILE:HG22	1:E:378:LEU:N	2.34	0.42
1:E:3183:VAL:HG23	1:E:3187:ARG:HE	1.84	0.42
1:E:3266:MET:O	1:E:3270:ILE:HG12	2.19	0.42
1:E:3315:LEU:O	1:E:3319:ILE:HG13	2.19	0.42
1:E:3760:LYS:O	1:E:3764:LEU:HG	2.19	0.42
1:E:3944:GLU:HG2	1:E:3946:GLN:H	1.83	0.42
1:G:280:LEU:N	1:G:314:PHE:O	2.49	0.42
1:G:2280:VAL:HG21	1:G:2290:LEU:HD11	2.00	0.42
1:G:3398:PHE:CE1	1:G:3451:PHE:HB2	2.54	0.42
1:G:3459:VAL:HG11	1:G:3505:VAL:HG11	1.99	0.42
1:G:3546:ASP:HA	1:G:3549:VAL:HG22	2.00	0.42
1:G:4772:ASP:O	1:G:4776:GLN:HG2	2.19	0.42
1:J:499:THR:HG23	1:J:502:HIS:H	1.83	0.42
1:J:882:TRP:NE1	1:J:886:ARG:CZ	2.82	0.42
1:J:1101:ARG:HG3	1:J:1125:ASN:HB2	2.01	0.42
1:J:2280:VAL:HG21	1:J:2290:LEU:HD11	2.00	0.42
1:J:3722:TYR:OH	1:J:3782:MET:HG3	2.19	0.42
2:D:36:PHE:HZ	2:D:97:LEU:HD22	1.84	0.42
1:B:901:LYS:O	1:B:901:LYS:HG2	2.18	0.42
1:B:2894:LEU:HD21	1:B:2901:THR:HA	2.00	0.42
1:B:3034:LYS:O	1:B:3038:MET:HG3	2.19	0.42
1:B:3315:LEU:O	1:B:3319:ILE:HG13	2.19	0.42
1:B:4209:GLN:H	1:B:4209:GLN:HG3	1.65	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:140:ASP:OD1	1:E:140:ASP:N	2.49	0.42
1:E:2764:GLU:HG3	1:E:2857:PRO:HG3	2.01	0.42
1:E:3034:LYS:O	1:E:3038:MET:HG3	2.19	0.42
1:E:3262:ARG:HB2	1:E:3325:ASN:ND2	2.34	0.42
1:G:1561:VAL:HG23	1:G:1562:ILE:H	1.85	0.42
1:G:2010:LEU:HD12	1:G:3656:SER:HB2	2.00	0.42
1:G:2615:ARG:HB3	1:G:2618:MET:SD	2.59	0.42
1:G:2909:ASP:OD1	1:G:2909:ASP:N	2.52	0.42
1:G:2924:GLN:O	1:G:2928:LYS:HG2	2.19	0.42
1:G:3268:HIS:CE1	1:G:3272:ILE:HG13	2.54	0.42
1:G:4184:MET:HA	1:G:4190:ILE:HD13	2.01	0.42
1:J:280:LEU:N	1:J:314:PHE:O	2.49	0.42
1:J:745:SER:HB2	1:J:758:ARG:HG2	2.01	0.42
1:J:2452:ARG:O	1:J:2456:ILE:HG13	2.19	0.42
1:J:2514:ASN:HB3	1:J:2517:PHE:HB3	2.01	0.42
1:J:2878:LEU:HG	1:J:2882:TYR:CE2	2.55	0.42
1:J:3039:ILE:O	1:J:3043:PHE:CD1	2.72	0.42
1:J:3183:VAL:HG23	1:J:3187:ARG:HE	1.84	0.42
1:J:4772:ASP:O	1:J:4776:GLN:HG2	2.19	0.42
1:J:4813:LEU:HD23	1:J:4813:LEU:HA	1.85	0.42
3:C:105:ASN:CG	3:C:111:ASN:HB2	2.44	0.42
3:F:92:VAL:HG12	3:F:122:GLN:OE1	2.19	0.42
3:K:28:ILE:HD12	3:K:28:ILE:HA	1.89	0.42
3:K:92:VAL:HG12	3:K:122:GLN:OE1	2.19	0.42
1:B:477:LEU:O	1:B:480:GLU:HG3	2.19	0.42
1:B:1668:ARG:HG3	1:B:1671:ARG:HH12	1.84	0.42
1:B:2538:THR:O	1:B:2542:SER:N	2.42	0.42
1:B:3334:TRP:HA	1:B:3337:ARG:HE	1.85	0.42
1:B:3546:ASP:OD1	1:B:3546:ASP:N	2.52	0.42
1:B:3944:GLU:HG2	1:B:3946:GLN:H	1.83	0.42
1:B:4676:GLU:O	1:B:4680:LYS:HG2	2.19	0.42
1:E:2280:VAL:HG21	1:E:2290:LEU:HD11	2.00	0.42
1:E:3406:TYR:HE1	1:E:3509:LEU:HG	1.83	0.42
1:E:3722:TYR:OH	1:E:3782:MET:HG3	2.19	0.42
1:E:3969:ILE:HG21	1:E:3980:LEU:HD12	2.00	0.42
1:E:4090:LYS:N	1:E:4121:GLU:O	2.53	0.42
1:G:863:LEU:O	1:G:867:LEU:HG	2.19	0.42
1:G:996:TRP:HA	1:G:999:ASP:OD2	2.19	0.42
1:G:1668:ARG:HG3	1:G:1671:ARG:HH12	1.84	0.42
1:G:1738:LEU:HD12	1:G:1738:LEU:HA	1.80	0.42
1:G:2514:ASN:HB3	1:G:2517:PHE:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:2801:ASP:HA	1:G:2804:ILE:HG12	2.00	0.42
1:G:3050:VAL:HB	1:G:3054:VAL:HG12	2.01	0.42
1:G:4698:LYS:HE3	1:G:4698:LYS:HB2	1.88	0.42
1:J:244:LEU:HD23	1:J:375:LYS:HZ2	1.84	0.42
1:J:877:ASN:O	1:J:881:LEU:HG	2.18	0.42
1:J:882:TRP:O	1:J:885:THR:OG1	2.25	0.42
1:J:1012:ASP:HB3	1:J:1015:ALA:HB3	2.01	0.42
1:J:1561:VAL:HG23	1:J:1562:ILE:H	1.85	0.42
1:J:2969:ILE:O	1:J:2972:GLU:HG3	2.19	0.42
1:J:3546:ASP:HA	1:J:3549:VAL:HG22	2.00	0.42
3:F:32:ASN:OD1	3:F:33:SER:N	2.52	0.42
1:B:735:GLN:OE1	1:B:735:GLN:HA	2.18	0.42
1:B:955:LEU:HD11	1:B:965:TYR:HA	2.00	0.42
1:B:996:TRP:HA	1:B:999:ASP:OD2	2.19	0.42
1:B:2615:ARG:HB3	1:B:2618:MET:SD	2.59	0.42
1:B:5011:TRP:NE1	1:B:5015:GLN:HE21	2.18	0.42
1:E:246:TYR:HE1	1:E:375:LYS:NZ	2.17	0.42
1:E:1668:ARG:HG3	1:E:1671:ARG:HH12	1.84	0.42
1:E:1708:ARG:O	1:E:1712:TYR:HD1	2.02	0.42
1:E:2264:GLY:O	1:E:2268:GLN:HG2	2.19	0.42
1:E:2799:GLU:O	1:E:2803:GLU:HG2	2.20	0.42
1:E:3530:GLN:OE1	1:E:3530:GLN:N	2.52	0.42
1:E:4026:MET:HE3	1:E:4026:MET:HB3	1.94	0.42
1:G:951:LYS:HE2	1:G:951:LYS:HB3	1.84	0.42
1:G:955:LEU:HD11	1:G:965:TYR:HA	2.00	0.42
1:G:2656:CYS:SG	1:G:2658:PRO:HD2	2.60	0.42
1:G:3034:LYS:O	1:G:3038:MET:HG3	2.19	0.42
1:G:3760:LYS:O	1:G:3764:LEU:HG	2.19	0.42
1:G:4065:PHE:HA	1:G:4068:LEU:HB2	1.99	0.42
1:J:883:ALA:O	1:J:887:ILE:HG13	2.20	0.42
1:J:955:LEU:HD11	1:J:965:TYR:HA	2.00	0.42
1:J:996:TRP:HA	1:J:999:ASP:OD2	2.19	0.42
1:J:1668:ARG:HG3	1:J:1671:ARG:HH12	1.84	0.42
1:J:2312:MET:H	1:J:2312:MET:HG3	1.69	0.42
1:J:2519:LEU:HD22	1:J:2575:ARG:HG3	2.02	0.42
1:J:3266:MET:O	1:J:3270:ILE:HG12	2.19	0.42
1:J:3443:ILE:HG22	1:J:3605:HIS:CG	2.55	0.42
1:J:3678:SER:HA	1:J:3696:ASP:OD2	2.20	0.42
1:J:3916:ILE:O	1:J:3920:VAL:HG23	2.20	0.42
1:J:4160:LEU:O	1:J:4164:LEU:HG	2.20	0.42
1:J:4184:MET:HA	1:J:4190:ILE:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:22:CYS:HB2	2:H:48:PHE:CE1	2.54	0.42
3:F:39:GLN:OE1	3:F:45:ARG:NH2	2.39	0.42
1:B:1864:LYS:HE3	1:B:1872:THR:HA	2.02	0.42
1:B:1870:VAL:HG11	1:B:2097:LEU:HD22	2.02	0.42
1:B:3704:HIS:O	1:B:3708:THR:HG23	2.20	0.42
1:B:4090:LYS:N	1:B:4121:GLU:O	2.53	0.42
1:B:4145:VAL:HG22	1:B:4178:LEU:HD13	2.00	0.42
1:E:499:THR:HG23	1:E:502:HIS:H	1.83	0.42
1:E:924:MET:HE1	3:F:106:PRO:CB	2.50	0.42
1:E:2325:PRO:HG2	1:E:2422:ILE:HD13	2.00	0.42
1:E:2639:MET:HE2	1:E:2639:MET:H	1.85	0.42
1:E:2965:ARG:HE	1:E:2965:ARG:HB3	1.57	0.42
1:E:3443:ILE:HG22	1:E:3605:HIS:CG	2.55	0.42
1:E:3987:ASP:N	1:E:3987:ASP:OD1	2.52	0.42
1:E:4028:LEU:HD23	1:E:4146:LEU:HD13	2.00	0.42
1:E:4725:LEU:HA	1:E:4737:ILE:HG21	2.02	0.42
1:G:613:ALA:HB1	1:G:618:GLN:HE22	1.83	0.42
1:G:745:SER:HB2	1:G:758:ARG:HG2	2.01	0.42
1:G:1815:LEU:HD22	1:G:1845:VAL:HG21	2.00	0.42
1:G:2568:LEU:HD12	1:G:2568:LEU:O	2.19	0.42
1:G:2799:GLU:O	1:G:2803:GLU:HG2	2.20	0.42
1:G:3406:TYR:HE1	1:G:3509:LEU:HG	1.83	0.42
1:G:3916:ILE:O	1:G:3920:VAL:HG23	2.20	0.42
1:J:372:LEU:O	1:J:373:LYS:C	2.62	0.42
1:J:2325:PRO:HG2	1:J:2422:ILE:HD13	2.00	0.42
1:J:2656:CYS:SG	1:J:2658:PRO:HD2	2.60	0.42
1:J:2765:LYS:HZ2	1:J:2860:PRO:HA	1.84	0.42
1:J:3050:VAL:HB	1:J:3054:VAL:HG12	2.01	0.42
1:J:3970:GLN:NE2	1:J:5004:THR:HA	2.33	0.42
1:B:70:GLU:HG2	1:B:71:GLN:HG3	2.01	0.42
1:B:131:LEU:O	1:B:178:ARG:NH2	2.46	0.42
1:B:1101:ARG:HG3	1:B:1125:ASN:HB2	2.02	0.42
1:B:2519:LEU:HD22	1:B:2575:ARG:HG3	2.02	0.42
1:B:2656:CYS:SG	1:B:2658:PRO:HD2	2.60	0.42
1:B:3043:PHE:HZ	1:B:3071:LEU:O	2.03	0.42
1:B:3050:VAL:HB	1:B:3054:VAL:HG12	2.01	0.42
1:B:3443:ILE:HG22	1:B:3605:HIS:CG	2.55	0.42
1:B:3518:LEU:N	1:B:3519:PRO:HD2	2.35	0.42
1:B:3678:SER:HA	1:B:3696:ASP:OD2	2.20	0.42
1:B:3762:ARG:NH2	1:B:4755:GLU:O	2.53	0.42
1:B:3987:ASP:OD1	1:B:3987:ASP:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:372:LEU:O	1:E:374:LYS:HG3	2.20	0.42
1:E:745:SER:HB2	1:E:758:ARG:HG2	2.01	0.42
1:E:863:LEU:O	1:E:867:LEU:HG	2.19	0.42
1:E:2010:LEU:HD12	1:E:3656:SER:HB2	2.00	0.42
1:E:2815:ALA:HB1	1:E:2881:ASN:ND2	2.34	0.42
1:E:2878:LEU:HG	1:E:2882:TYR:CE2	2.54	0.42
1:E:2924:GLN:O	1:E:2928:LYS:HG2	2.19	0.42
1:E:3518:LEU:N	1:E:3519:PRO:HD2	2.35	0.42
1:E:4209:GLN:H	1:E:4209:GLN:HG3	1.65	0.42
1:G:3443:ILE:HG22	1:G:3605:HIS:CG	2.55	0.42
1:G:3592:ILE:O	1:G:3596:VAL:HG22	2.19	0.42
1:G:3678:SER:HA	1:G:3696:ASP:OD2	2.20	0.42
1:G:4063:ASP:OD1	1:G:4064:MET:N	2.53	0.42
1:J:924:MET:HE1	3:K:106:PRO:CB	2.49	0.42
1:J:1708:ARG:O	1:J:1712:TYR:HD1	2.02	0.42
1:J:2624:ARG:HH11	1:J:2903:PRO:HA	1.84	0.42
1:J:3406:TYR:HE1	1:J:3509:LEU:HG	1.83	0.42
1:J:3760:LYS:O	1:J:3764:LEU:HG	2.19	0.42
1:J:4063:ASP:OD1	1:J:4064:MET:N	2.53	0.42
3:M:82:MET:SD	3:M:83:ASN:N	2.93	0.42
1:B:581:ASN:OD1	1:B:581:ASN:N	2.53	0.42
1:B:2815:ALA:HB1	1:B:2881:ASN:ND2	2.34	0.42
1:B:3183:VAL:HG23	1:B:3187:ARG:HE	1.84	0.42
1:B:3458:PHE:CE2	1:B:3464:ILE:HD11	2.55	0.42
1:B:3592:ILE:O	1:B:3596:VAL:HG22	2.19	0.42
1:B:4060:LYS:HA	1:B:4063:ASP:OD2	2.19	0.42
1:B:4090:LYS:HZ2	1:B:4112:LEU:HD23	1.84	0.42
1:B:4725:LEU:HA	1:B:4737:ILE:HG21	2.02	0.42
1:B:4772:ASP:O	1:B:4776:GLN:HG2	2.19	0.42
1:E:371:VAL:HG12	1:E:373:LYS:H	1.85	0.42
1:E:451:TYR:CZ	1:E:474:ARG:HD2	2.54	0.42
1:E:883:ALA:O	1:E:887:ILE:HG13	2.20	0.42
1:E:3039:ILE:O	1:E:3043:PHE:CD1	2.72	0.42
1:E:3420:ARG:NH1	1:E:3516:LYS:O	2.51	0.42
1:E:3704:HIS:O	1:E:3708:THR:HG23	2.20	0.42
1:E:4949:GLN:NE2	1:E:4953:ASP:OD2	2.52	0.42
1:G:1101:ARG:HG3	1:G:1125:ASN:HB2	2.02	0.42
1:G:2764:GLU:HG3	1:G:2857:PRO:HG3	2.01	0.42
1:G:3049:LEU:HB3	1:G:3057:PHE:CE1	2.53	0.42
1:G:4846:VAL:HG13	1:J:4813:LEU:HD13	2.01	0.42
1:J:863:LEU:O	1:J:867:LEU:HG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1076:ARG:HB3	1:J:1191:VAL:HG23	2.01	0.42
1:J:2615:ARG:HB3	1:J:2618:MET:SD	2.59	0.42
1:J:3034:LYS:O	1:J:3038:MET:HG3	2.19	0.42
1:J:3268:HIS:CE1	1:J:3272:ILE:HG13	2.54	0.42
1:J:3300:ALA:HB3	1:J:3301:PRO:HD3	2.01	0.42
1:J:3315:LEU:O	1:J:3319:ILE:HG13	2.19	0.42
1:J:3350:ARG:NE	1:J:3350:ARG:HA	2.34	0.42
1:J:4698:LYS:HE3	1:J:4698:LYS:HB2	1.88	0.42
1:J:4995:LEU:HD21	1:J:5007:GLU:HB3	2.02	0.42
3:C:32:ASN:OD1	3:C:33:SER:N	2.52	0.42
3:C:100:VAL:HG22	3:C:105:ASN:HB2	2.01	0.42
3:K:30:SER:HB3	3:K:99:ARG:CB	2.48	0.42
3:K:38:ARG:NH1	3:K:89:ASP:OD1	2.52	0.42
3:K:82:MET:SD	3:K:83:ASN:N	2.93	0.42
3:M:105:ASN:CG	3:M:111:ASN:HB2	2.45	0.42
1:B:663:TYR:OH	1:B:758:ARG:NH2	2.53	0.42
1:B:2969:ILE:O	1:B:2972:GLU:HG3	2.19	0.42
1:E:73:LEU:O	1:E:106:ALA:N	2.46	0.42
1:E:955:LEU:HD11	1:E:965:TYR:HA	2.00	0.42
1:E:2627:VAL:HB	1:E:2678:LEU:HD11	2.01	0.42
1:E:2656:CYS:SG	1:E:2658:PRO:HD2	2.60	0.42
1:E:3261:ALA:HB1	1:E:3321:ARG:HB3	2.02	0.42
1:E:3546:ASP:HA	1:E:3549:VAL:HG22	2.00	0.42
1:G:247:TYR:HD2	1:G:372:LEU:O	2.02	0.42
1:G:306:LYS:H	1:G:306:LYS:HG2	1.69	0.42
1:G:1864:LYS:HE3	1:G:1872:THR:HA	2.01	0.42
1:G:3183:VAL:HG23	1:G:3187:ARG:HE	1.85	0.42
1:J:1094:ALA:HB1	1:J:1100:MET:HE1	2.01	0.42
1:J:3043:PHE:HZ	1:J:3071:LEU:O	2.03	0.42
1:J:4090:LYS:N	1:J:4121:GLU:O	2.53	0.42
2:A:36:PHE:HZ	2:A:97:LEU:HD22	1.84	0.42
2:A:41:ASP:OD1	2:A:42:ARG:N	2.53	0.42
3:M:92:VAL:HG12	3:M:122:GLN:OE1	2.19	0.42
1:B:2325:PRO:HG2	1:B:2422:ILE:HD13	2.00	0.42
1:B:2627:VAL:HB	1:B:2678:LEU:HD11	2.01	0.42
1:B:3261:ALA:HB1	1:B:3321:ARG:HB3	2.02	0.42
1:B:4063:ASP:OD1	1:B:4064:MET:N	2.53	0.42
1:B:4759:ASP:OD1	1:B:4759:ASP:N	2.53	0.42
1:E:1683:HIS:NE2	1:E:1798:LEU:O	2.52	0.42
1:E:2485:LEU:HD23	1:E:2485:LEU:HA	1.95	0.42
1:E:3043:PHE:HZ	1:E:3071:LEU:O	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3458:PHE:CE2	1:E:3464:ILE:HD11	2.55	0.42
1:E:4087:LEU:HB3	1:E:4122:MET:HB2	2.01	0.42
1:E:4768:LEU:HB3	1:E:4769:MET:HE2	2.00	0.42
1:G:389:PHE:HD1	1:G:390:LEU:N	2.18	0.42
1:G:1508:ARG:NH2	1:J:2773:ASN:OD1	2.42	0.42
1:G:2815:ALA:HB1	1:G:2881:ASN:ND2	2.34	0.42
1:G:3043:PHE:HZ	1:G:3071:LEU:O	2.03	0.42
1:G:3458:PHE:CE2	1:G:3464:ILE:HD11	2.55	0.42
1:G:4966:ASP:OD1	1:G:4966:ASP:N	2.53	0.42
1:J:389:PHE:HD1	1:J:390:LEU:N	2.18	0.42
1:J:2815:ALA:HB1	1:J:2881:ASN:ND2	2.34	0.42
1:J:3518:LEU:N	1:J:3519:PRO:HD2	2.35	0.42
3:F:82:MET:SD	3:F:83:ASN:N	2.93	0.42
1:B:794:GLY:HA2	1:B:810:PRO:HB3	2.02	0.42
1:B:1012:ASP:HB3	1:B:1015:ALA:HB3	2.01	0.42
1:B:2452:ARG:O	1:B:2456:ILE:HG13	2.19	0.42
1:B:2568:LEU:HD12	1:B:2568:LEU:O	2.19	0.42
1:B:2799:GLU:O	1:B:2803:GLU:HG2	2.20	0.42
1:B:3077:ALA:HB3	1:B:3078:ARG:NH1	2.35	0.42
1:B:4087:LEU:HB3	1:B:4122:MET:HB2	2.01	0.42
1:E:1973:GLN:OE1	1:E:3641:LEU:HB2	2.20	0.42
1:E:2615:ARG:HB3	1:E:2618:MET:SD	2.59	0.42
1:E:3011:THR:OG1	1:E:3070:ILE:HG12	2.20	0.42
1:E:3016:TYR:HE2	1:E:3030:HIS:HB3	1.84	0.42
1:E:3194:LEU:O	1:E:3197:LEU:HG	2.20	0.42
1:E:3546:ASP:OD1	1:E:3546:ASP:N	2.52	0.42
1:E:3878:ASP:O	1:E:3882:GLN:HG3	2.20	0.42
1:E:4552:LEU:HD22	1:E:4663:CYS:SG	2.60	0.42
1:E:5011:TRP:NE1	1:E:5015:GLN:HE21	2.18	0.42
1:G:883:ALA:O	1:G:887:ILE:HG13	2.20	0.42
1:G:1699:GLU:HG3	1:G:1810:LYS:HE3	2.02	0.42
1:G:1927:LEU:HD13	1:G:2097:LEU:HD11	2.02	0.42
1:G:2380:ILE:O	1:G:2384:ILE:HG13	2.20	0.42
1:G:2624:ARG:HH11	1:G:2903:PRO:HA	1.84	0.42
1:G:2690:LYS:HE3	1:G:2690:LYS:HB2	1.91	0.42
1:G:3062:PRO:HA	1:G:3065:VAL:HG22	2.02	0.42
1:G:3194:LEU:O	1:G:3197:LEU:HG	2.20	0.42
1:G:3261:ALA:HB1	1:G:3321:ARG:HB3	2.02	0.42
1:G:3518:LEU:N	1:G:3519:PRO:HD2	2.35	0.42
1:G:4131:ARG:HG3	1:G:4132:PHE:CD2	2.55	0.42
1:G:4145:VAL:HG22	1:G:4178:LEU:HD13	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:451:TYR:CZ	1:J:474:ARG:HD2	2.54	0.42
1:J:747:CYS:HB2	1:J:808:TYR:CE2	2.55	0.42
1:J:872:GLU:CD	1:J:872:GLU:H	2.28	0.42
1:J:882:TRP:CD1	1:J:882:TRP:C	2.98	0.42
1:J:882:TRP:CD1	1:J:886:ARG:CZ	3.03	0.42
1:J:1445:PRO:HG2	1:J:1501:VAL:HG21	2.02	0.42
1:J:2627:VAL:HB	1:J:2678:LEU:HD11	2.01	0.42
1:J:3207:GLU:HG3	1:J:3246:LEU:CD2	2.49	0.42
1:J:3564:GLU:H	1:J:3564:GLU:HG3	1.73	0.42
1:J:3592:ILE:O	1:J:3596:VAL:HG22	2.19	0.42
1:J:3962:PHE:O	1:J:3966:THR:HG23	2.20	0.42
1:J:4995:LEU:HD23	1:J:4995:LEU:HA	1.83	0.42
2:H:41:ASP:OD1	2:H:42:ARG:N	2.53	0.42
2:I:22:CYS:HB2	2:I:48:PHE:CE1	2.54	0.42
2:I:36:PHE:HZ	2:I:97:LEU:HD22	1.84	0.42
3:C:38:ARG:NH1	3:C:89:ASP:OD1	2.52	0.42
1:B:2328:GLY:HA3	1:B:2425:PHE:CE2	2.55	0.41
1:E:872:GLU:H	1:E:872:GLU:CD	2.28	0.41
1:E:979:PRO:HA	1:E:982:THR:HG22	2.02	0.41
1:E:1302:ARG:H	1:E:1302:ARG:HG2	1.66	0.41
1:E:2519:LEU:HD22	1:E:2575:ARG:HG3	2.02	0.41
1:E:2624:ARG:HH11	1:E:2903:PRO:HA	1.84	0.41
1:E:3075:LEU:H	1:E:3146:HIS:CE1	2.38	0.41
1:E:4060:LYS:HA	1:E:4063:ASP:OD2	2.19	0.41
1:E:4772:ASP:O	1:E:4776:GLN:HG2	2.19	0.41
1:G:663:TYR:CE1	1:G:745:SER:HB3	2.55	0.41
1:G:1445:PRO:HG2	1:G:1501:VAL:HG21	2.02	0.41
1:G:2878:LEU:HG	1:G:2882:TYR:CE2	2.54	0.41
1:G:3016:TYR:HE2	1:G:3030:HIS:HB3	1.84	0.41
1:G:3206:LEU:O	1:G:3208:PRO:HD3	2.20	0.41
1:G:3207:GLU:HG3	1:G:3246:LEU:CD2	2.49	0.41
1:G:3334:TRP:HA	1:G:3337:ARG:HE	1.85	0.41
1:G:3762:ARG:NH2	1:G:4755:GLU:O	2.53	0.41
1:J:81:MET:HE2	1:J:81:MET:HB2	1.94	0.41
1:J:1132:TRP:CE2	1:J:1136:SER:HB2	2.55	0.41
1:J:1934:SER:O	1:J:1938:GLN:HG2	2.20	0.41
1:J:3077:ALA:HB3	1:J:3078:ARG:NH1	2.35	0.41
1:J:3704:HIS:O	1:J:3708:THR:HG23	2.20	0.41
1:J:3762:ARG:NH2	1:J:4755:GLU:O	2.53	0.41
1:J:3987:ASP:OD1	1:J:3987:ASP:N	2.52	0.41
1:J:4060:LYS:HA	1:J:4063:ASP:OD2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:4131:ARG:HG3	1:J:4132:PHE:CD2	2.55	0.41
1:J:4552:LEU:HD22	1:J:4663:CYS:SG	2.60	0.41
1:J:4759:ASP:N	1:J:4759:ASP:OD1	2.53	0.41
2:A:26:TYR:HA	2:A:100:ASP:O	2.20	0.41
2:D:41:ASP:OD1	2:D:42:ARG:N	2.53	0.41
1:B:140:ASP:OD1	1:B:140:ASP:N	2.49	0.41
1:B:365:LYS:HE2	1:B:369:LEU:HD11	2.01	0.41
1:B:979:PRO:HA	1:B:982:THR:HG22	2.02	0.41
1:B:1561:VAL:HG23	1:B:1562:ILE:H	1.85	0.41
1:B:2639:MET:HE2	1:B:2639:MET:H	1.85	0.41
1:B:3010:PHE:O	1:B:3014:CYS:HB2	2.20	0.41
1:B:3850:GLN:HE21	1:B:3870:ASN:H	1.68	0.41
1:E:732:SER:O	1:E:735:GLN:HG2	2.20	0.41
1:E:1101:ARG:HG3	1:E:1125:ASN:HB2	2.02	0.41
1:E:1828:ASP:OD1	1:E:1828:ASP:N	2.51	0.41
1:E:2514:ASN:HB3	1:E:2517:PHE:HB3	2.01	0.41
1:E:3050:VAL:HB	1:E:3054:VAL:HG12	2.01	0.41
1:E:3850:GLN:HE21	1:E:3870:ASN:H	1.68	0.41
1:E:3916:ILE:O	1:E:3920:VAL:HG23	2.20	0.41
1:G:872:GLU:H	1:G:872:GLU:CD	2.28	0.41
1:G:1076:ARG:HB3	1:G:1191:VAL:HG23	2.01	0.41
1:G:1973:GLN:OE1	1:G:3641:LEU:HB2	2.20	0.41
1:G:2519:LEU:HD22	1:G:2575:ARG:HG3	2.02	0.41
1:G:3110:LEU:HD23	1:G:3183:VAL:HG12	2.02	0.41
1:G:3300:ALA:HB3	1:G:3301:PRO:HD3	2.01	0.41
1:G:3315:LEU:O	1:G:3319:ILE:HG13	2.19	0.41
1:G:5011:TRP:NE1	1:G:5015:GLN:HE21	2.18	0.41
1:J:246:TYR:HE1	1:J:375:LYS:NZ	2.16	0.41
1:J:1927:LEU:HD13	1:J:2097:LEU:HD11	2.02	0.41
1:J:2357:LEU:HD23	1:J:2357:LEU:HA	1.92	0.41
1:J:2380:ILE:O	1:J:2384:ILE:HG13	2.20	0.41
1:J:2799:GLU:O	1:J:2803:GLU:HG2	2.20	0.41
1:J:3327:LEU:HD13	1:J:3368:ARG:NH1	2.36	0.41
1:J:3458:PHE:CE2	1:J:3464:ILE:HD11	2.55	0.41
1:J:3526:ALA:HB2	1:J:3576:TYR:CE2	2.56	0.41
1:J:4214:LYS:HE2	1:J:4214:LYS:HB3	1.92	0.41
3:M:105:ASN:OD1	3:M:111:ASN:HB2	2.19	0.41
1:B:1708:ARG:O	1:B:1712:TYR:HD1	2.02	0.41
1:B:2380:ILE:O	1:B:2384:ILE:HG13	2.20	0.41
1:B:2610:LEU:O	1:B:2614:ILE:HG12	2.20	0.41
1:B:2661:TRP:CZ3	1:B:2664:PHE:HD2	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2878:LEU:HG	1:B:2882:TYR:CE2	2.54	0.41
1:B:3206:LEU:O	1:B:3208:PRO:HD3	2.20	0.41
1:B:3760:LYS:O	1:B:3764:LEU:HG	2.19	0.41
1:B:3916:ILE:O	1:B:3920:VAL:HG23	2.20	0.41
1:B:4178:LEU:HD11	1:B:4194:TYR:HB3	2.02	0.41
1:E:50:GLU:HA	1:E:51:PRO:HD3	1.94	0.41
1:E:2610:LEU:O	1:E:2614:ILE:HG12	2.20	0.41
1:E:2909:ASP:OD1	1:E:2909:ASP:N	2.52	0.41
1:E:3334:TRP:HA	1:E:3337:ARG:HE	1.84	0.41
1:E:3526:ALA:HB2	1:E:3576:TYR:CE2	2.56	0.41
1:E:3562:LYS:HB2	1:E:3562:LYS:HE2	1.81	0.41
1:E:3678:SER:HA	1:E:3696:ASP:OD2	2.20	0.41
1:E:3762:ARG:NH2	1:E:4755:GLU:O	2.53	0.41
1:E:4157:ASP:O	1:E:4161:ARG:HG2	2.21	0.41
1:E:4838:VAL:O	1:E:4841:VAL:HG12	2.21	0.41
1:E:4851:TYR:HD1	1:E:4916:PHE:CE1	2.38	0.41
1:G:581:ASN:N	1:G:581:ASN:OD1	2.53	0.41
1:G:1870:VAL:HG11	1:G:2097:LEU:HD22	2.02	0.41
1:G:2463:LEU:O	1:G:2467:VAL:HG23	2.21	0.41
1:G:2633:LEU:HB3	1:G:2689:LYS:HZ1	1.85	0.41
1:G:2639:MET:HE2	1:G:2639:MET:H	1.85	0.41
1:G:3458:PHE:HE2	1:G:3464:ILE:HD11	1.85	0.41
1:G:3850:GLN:NE2	1:G:3870:ASN:H	2.19	0.41
1:G:3878:ASP:O	1:G:3882:GLN:HG3	2.20	0.41
1:G:4091:LYS:NZ	1:G:4092:ASP:OD1	2.48	0.41
1:G:4995:LEU:HD21	1:G:5007:GLU:HB3	2.02	0.41
1:J:794:GLY:HA2	1:J:810:PRO:HB3	2.02	0.41
1:J:1758:ARG:NH2	1:J:2036:GLN:OE1	2.51	0.41
1:J:2608:MET:HE2	1:J:2608:MET:HB3	1.76	0.41
1:J:2639:MET:HE2	1:J:2639:MET:H	1.85	0.41
1:J:3562:LYS:HE2	1:J:3562:LYS:HB2	1.81	0.41
1:J:3639:THR:N	1:J:3640:PRO:HD2	2.36	0.41
1:J:3979:SER:O	1:J:3983:SER:OG	2.31	0.41
1:J:4178:LEU:HD11	1:J:4194:TYR:HB3	2.03	0.41
1:J:4679:ARG:HH21	1:J:5017:ARG:NH1	2.18	0.41
1:J:4966:ASP:OD1	1:J:4966:ASP:N	2.53	0.41
2:A:22:CYS:HB2	2:A:48:PHE:CE1	2.54	0.41
1:B:73:LEU:HD12	1:B:73:LEU:HA	1.92	0.41
1:B:623:GLU:HG2	2:A:88:PRO:HB3	2.01	0.41
1:B:872:GLU:H	1:B:872:GLU:CD	2.28	0.41
1:B:2514:ASN:HB3	1:B:2517:PHE:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2624:ARG:HH11	1:B:2903:PRO:HA	1.84	0.41
1:B:2657:LEU:H	1:B:2711:PRO:HG3	1.85	0.41
1:B:3075:LEU:H	1:B:3146:HIS:CE1	2.38	0.41
1:B:3546:ASP:HA	1:B:3549:VAL:HG22	2.01	0.41
1:B:3850:GLN:NE2	1:B:3870:ASN:H	2.19	0.41
1:E:70:GLU:HG2	1:E:71:GLN:HG3	2.01	0.41
1:E:1934:SER:O	1:E:1938:GLN:HG2	2.20	0.41
1:E:2328:GLY:HA3	1:E:2425:PHE:CE2	2.55	0.41
1:E:2532:ALA:O	1:E:2536:LEU:HD23	2.21	0.41
1:E:3639:THR:N	1:E:3640:PRO:HD2	2.36	0.41
1:E:4160:LEU:O	1:E:4164:LEU:HG	2.20	0.41
1:G:882:TRP:CD1	1:G:882:TRP:C	2.98	0.41
1:G:882:TRP:CD1	1:G:886:ARG:CZ	3.03	0.41
1:G:1132:TRP:CE2	1:G:1136:SER:HB2	2.56	0.41
1:G:1934:SER:O	1:G:1938:GLN:HG2	2.20	0.41
1:G:2610:LEU:O	1:G:2614:ILE:HG12	2.20	0.41
1:G:2627:VAL:HB	1:G:2678:LEU:HD11	2.01	0.41
1:G:2657:LEU:H	1:G:2711:PRO:HG3	1.85	0.41
1:G:3077:ALA:HB3	1:G:3078:ARG:NH1	2.35	0.41
1:G:4068:LEU:HD23	1:G:4068:LEU:HA	1.89	0.41
1:G:4090:LYS:N	1:G:4121:GLU:O	2.53	0.41
1:G:4552:LEU:HD22	1:G:4663:CYS:SG	2.60	0.41
1:J:5011:TRP:NE1	1:J:5015:GLN:HE21	2.18	0.41
3:C:82:MET:SD	3:C:83:ASN:N	2.93	0.41
3:M:104:TYR:CE1	3:M:106:PRO:HG3	2.55	0.41
1:B:451:TYR:CZ	1:B:474:ARG:HD2	2.54	0.41
1:B:1132:TRP:CE2	1:B:1136:SER:HB2	2.56	0.41
1:B:2463:LEU:O	1:B:2467:VAL:HG23	2.21	0.41
1:B:3194:LEU:O	1:B:3197:LEU:HG	2.20	0.41
1:B:4131:ARG:HG3	1:B:4132:PHE:CD2	2.55	0.41
1:B:4160:LEU:O	1:B:4164:LEU:HG	2.20	0.41
1:E:1132:TRP:CE2	1:E:1136:SER:HB2	2.56	0.41
1:E:2661:TRP:CZ3	1:E:2664:PHE:HD2	2.38	0.41
1:E:3420:ARG:HD2	1:E:3519:PRO:HG2	2.03	0.41
1:E:4063:ASP:OD1	1:E:4064:MET:N	2.53	0.41
1:E:4131:ARG:HG3	1:E:4132:PHE:CD2	2.55	0.41
1:G:246:TYR:HE1	1:G:375:LYS:NZ	2.16	0.41
1:G:979:PRO:HA	1:G:982:THR:HG22	2.02	0.41
1:G:3509:LEU:HD23	1:G:3509:LEU:HA	1.88	0.41
1:G:3850:GLN:HE21	1:G:3870:ASN:H	1.68	0.41
1:G:3962:PHE:O	1:G:3966:THR:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4188:ARG:HA	1:G:4188:ARG:NE	2.35	0.41
1:G:4759:ASP:OD1	1:G:4759:ASP:N	2.53	0.41
1:J:247:TYR:HD2	1:J:372:LEU:HB3	1.81	0.41
1:J:663:TYR:CE1	1:J:745:SER:HB3	2.55	0.41
1:J:663:TYR:OH	1:J:758:ARG:NH2	2.53	0.41
1:J:3010:PHE:O	1:J:3014:CYS:HB2	2.20	0.41
1:J:3062:PRO:HA	1:J:3065:VAL:HG22	2.02	0.41
1:J:3765:TYR:CZ	1:J:3769:ARG:HD3	2.56	0.41
1:J:4652:LEU:O	1:J:4656:LEU:HG	2.21	0.41
2:D:22:CYS:HB2	2:D:48:PHE:CE1	2.54	0.41
1:B:110:ARG:HD3	1:B:115:ARG:HE	1.86	0.41
1:B:389:PHE:HD1	1:B:390:LEU:N	2.18	0.41
1:B:732:SER:O	1:B:735:GLN:HG2	2.20	0.41
1:B:1076:ARG:HB3	1:B:1191:VAL:HG23	2.01	0.41
1:B:1302:ARG:H	1:B:1302:ARG:HG2	1.66	0.41
1:B:2867:LEU:HD12	1:B:2867:LEU:HA	1.82	0.41
1:B:3327:LEU:HD22	1:B:3368:ARG:NH1	2.36	0.41
1:B:3878:ASP:O	1:B:3882:GLN:HG3	2.20	0.41
1:B:4552:LEU:HD22	1:B:4663:CYS:SG	2.60	0.41
1:E:355:LEU:HD22	1:E:379:HIS:HA	2.03	0.41
1:E:389:PHE:HD1	1:E:390:LEU:N	2.18	0.41
1:E:1699:GLU:HG3	1:E:1810:LYS:HE3	2.02	0.41
1:E:1870:VAL:HG11	1:E:2097:LEU:HD22	2.02	0.41
1:E:2380:ILE:O	1:E:2384:ILE:HG13	2.20	0.41
1:E:2463:LEU:O	1:E:2467:VAL:HG23	2.21	0.41
1:E:3110:LEU:HD23	1:E:3183:VAL:HG12	2.02	0.41
1:E:3592:ILE:O	1:E:3596:VAL:HG22	2.19	0.41
1:E:4759:ASP:OD1	1:E:4759:ASP:N	2.53	0.41
1:G:568:LEU:HD12	1:G:602:VAL:HG13	2.03	0.41
1:G:1115:LEU:HD23	1:G:1123:VAL:HG21	2.03	0.41
1:G:4087:LEU:HB3	1:G:4122:MET:HB2	2.01	0.41
1:G:4178:LEU:HD11	1:G:4194:TYR:HB3	2.03	0.41
1:J:355:LEU:HD22	1:J:379:HIS:HA	2.03	0.41
1:J:568:LEU:HD12	1:J:602:VAL:HG13	2.03	0.41
1:J:1699:GLU:HG3	1:J:1810:LYS:HE3	2.02	0.41
1:J:1973:GLN:OE1	1:J:3641:LEU:HB2	2.20	0.41
1:J:3334:TRP:HA	1:J:3337:ARG:HE	1.84	0.41
1:J:4666:VAL:HG21	1:J:4783:ILE:HD11	2.03	0.41
1:J:4725:LEU:HA	1:J:4737:ILE:HG21	2.02	0.41
2:I:41:ASP:OD1	2:I:42:ARG:N	2.53	0.41
1:B:882:TRP:CD1	1:B:882:TRP:C	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1927:LEU:HD13	1:B:2097:LEU:HD11	2.02	0.41
1:B:1973:GLN:OE1	1:B:3641:LEU:HB2	2.20	0.41
1:B:2532:ALA:O	1:B:2536:LEU:HD23	2.21	0.41
1:B:3327:LEU:HD13	1:B:3368:ARG:NH1	2.36	0.41
1:B:3526:ALA:HB2	1:B:3576:TYR:CE2	2.56	0.41
1:B:4838:VAL:O	1:B:4841:VAL:HG12	2.21	0.41
1:B:4851:TYR:HD1	1:B:4916:PHE:CE1	2.38	0.41
1:E:1012:ASP:HB3	1:E:1015:ALA:HB3	2.01	0.41
1:E:1076:ARG:HB3	1:E:1191:VAL:HG23	2.01	0.41
1:E:3300:ALA:HB3	1:E:3301:PRO:HD3	2.01	0.41
1:E:4541:TRP:O	1:E:4544:LEU:HG	2.21	0.41
1:G:110:ARG:HD3	1:G:115:ARG:HE	1.86	0.41
1:G:172:VAL:HA	1:G:178:ARG:O	2.21	0.41
1:G:663:TYR:OH	1:G:758:ARG:NH2	2.53	0.41
1:G:1619:ARG:HE	1:G:1619:ARG:HB2	1.72	0.41
1:G:2969:ILE:O	1:G:2972:GLU:HG3	2.19	0.41
1:G:3292:PRO:HA	1:G:3293:PRO:HD3	1.92	0.41
1:G:3562:LYS:HE2	1:G:3562:LYS:HB2	1.81	0.41
1:G:4160:LEU:O	1:G:4164:LEU:HG	2.20	0.41
1:G:4666:VAL:HG21	1:G:4783:ILE:HD11	2.03	0.41
1:J:979:PRO:HA	1:J:982:THR:HG22	2.02	0.41
1:J:2764:GLU:HG3	1:J:2857:PRO:HG3	2.01	0.41
1:J:3261:ALA:HB1	1:J:3321:ARG:HB3	2.02	0.41
1:J:3420:ARG:HD2	1:J:3519:PRO:HG2	2.03	0.41
1:J:3850:GLN:NE2	1:J:3870:ASN:H	2.19	0.41
2:D:26:TYR:HA	2:D:100:ASP:O	2.21	0.41
2:I:26:TYR:HA	2:I:100:ASP:O	2.20	0.41
3:C:104:TYR:CE1	3:C:106:PRO:HG3	2.53	0.41
3:F:28:ILE:HD12	3:F:28:ILE:HA	1.89	0.41
3:K:105:ASN:CG	3:K:111:ASN:HB2	2.45	0.41
1:B:747:CYS:HB2	1:B:808:TYR:CE2	2.55	0.41
1:B:883:ALA:O	1:B:887:ILE:HG13	2.20	0.41
1:B:1115:LEU:HD23	1:B:1123:VAL:HG21	2.03	0.41
1:B:2909:ASP:N	1:B:2909:ASP:OD1	2.52	0.41
1:B:3011:THR:OG1	1:B:3070:ILE:HG12	2.20	0.41
1:B:3016:TYR:HE2	1:B:3030:HIS:HB3	1.84	0.41
1:B:4026:MET:HE3	1:B:4026:MET:HB3	1.94	0.41
1:E:663:TYR:OH	1:E:758:ARG:NH2	2.53	0.41
1:E:882:TRP:CD1	1:E:882:TRP:C	2.98	0.41
1:E:1561:VAL:HG23	1:E:1562:ILE:H	1.84	0.41
1:E:1864:LYS:HE3	1:E:1872:THR:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1964:ARG:O	1:E:1968:LYS:NZ	2.46	0.41
1:E:3010:PHE:O	1:E:3014:CYS:HB2	2.20	0.41
1:E:3765:TYR:CZ	1:E:3769:ARG:HD3	2.56	0.41
1:E:3949:ARG:O	1:E:3953:LYS:HG3	2.21	0.41
1:G:50:GLU:HA	1:G:51:PRO:HD3	1.94	0.41
1:G:127:MET:O	1:G:130:LYS:NZ	2.50	0.41
1:G:747:CYS:HB2	1:G:808:TYR:CE2	2.55	0.41
1:G:3011:THR:OG1	1:G:3070:ILE:HG12	2.20	0.41
1:G:3704:HIS:O	1:G:3708:THR:HG23	2.20	0.41
1:G:4851:TYR:HD1	1:G:4916:PHE:CE1	2.38	0.41
1:J:1939:MET:HB3	1:J:1939:MET:HE2	1.85	0.41
1:J:2670:GLU:OE1	1:J:2673:HIS:HB3	2.21	0.41
1:J:3011:THR:OG1	1:J:3070:ILE:HG12	2.20	0.41
1:J:3016:TYR:HE2	1:J:3030:HIS:HB3	1.84	0.41
1:J:3075:LEU:H	1:J:3146:HIS:CE1	2.38	0.41
1:J:3277:LEU:HG	1:J:3341:PHE:HZ	1.86	0.41
1:J:3327:LEU:HD22	1:J:3368:ARG:NH1	2.36	0.41
1:J:4087:LEU:HB3	1:J:4122:MET:HB2	2.02	0.41
1:J:4157:ASP:O	1:J:4161:ARG:HG2	2.21	0.41
1:J:4890:GLY:HA2	1:J:4900:GLU:OE2	2.21	0.41
2:H:36:PHE:HZ	2:H:97:LEU:HD22	1.84	0.41
3:C:101:PRO:HD2	3:C:104:TYR:O	2.20	0.41
1:B:424:LYS:HE2	1:B:424:LYS:HB2	1.85	0.41
1:B:684:VAL:HG22	1:B:781:VAL:HG12	2.02	0.41
1:B:1934:SER:O	1:B:1938:GLN:HG2	2.20	0.41
1:B:2536:LEU:HA	1:B:2541:PHE:HB3	2.03	0.41
1:B:2787:THR:OG1	1:B:2788:HIS:N	2.54	0.41
1:B:2973:PHE:CD1	1:B:2973:PHE:C	2.99	0.41
1:B:3420:ARG:HD2	1:B:3519:PRO:HG2	2.03	0.41
1:B:3445:TRP:HA	1:B:3451:PHE:CD1	2.49	0.41
1:B:4046:ASP:HA	1:B:4049:VAL:HG22	2.03	0.41
1:B:4157:ASP:O	1:B:4161:ARG:HG2	2.21	0.41
1:B:4188:ARG:HA	1:B:4188:ARG:NE	2.35	0.41
1:B:4995:LEU:HD21	1:B:5007:GLU:HB3	2.02	0.41
1:E:172:VAL:HA	1:E:178:ARG:O	2.21	0.41
1:E:568:LEU:HD12	1:E:602:VAL:HG13	2.03	0.41
1:E:747:CYS:HB2	1:E:808:TYR:CE2	2.55	0.41
1:E:882:TRP:CD1	1:E:886:ARG:CZ	3.03	0.41
1:E:1440:PHE:CD2	1:E:1560:ASN:HB3	2.56	0.41
1:E:1445:PRO:HG2	1:E:1501:VAL:HG21	2.02	0.41
1:E:1939:MET:HE2	1:E:1939:MET:HB3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3077:ALA:HB3	1:E:3078:ARG:NH1	2.35	0.41
1:E:3533:ILE:HG13	1:E:3533:ILE:H	1.74	0.41
1:E:4178:LEU:HD11	1:E:4194:TYR:HB3	2.03	0.41
1:E:4188:ARG:HA	1:E:4188:ARG:NE	2.35	0.41
1:E:4214:LYS:HE2	1:E:4214:LYS:HB3	1.91	0.41
1:E:4553:ASN:O	1:E:4557:ARG:HG3	2.21	0.41
1:E:4652:LEU:O	1:E:4656:LEU:HG	2.21	0.41
1:E:4679:ARG:HH21	1:E:5017:ARG:NH1	2.18	0.41
1:E:4754:ASN:CG	1:E:4756:ARG:HH12	2.29	0.41
1:G:138:GLN:NE2	1:G:140:ASP:O	2.54	0.41
1:G:794:GLY:HA2	1:G:810:PRO:HB3	2.02	0.41
1:G:2532:ALA:O	1:G:2536:LEU:HD23	2.21	0.41
1:G:2661:TRP:CZ3	1:G:2664:PHE:HD2	2.39	0.41
1:G:3420:ARG:HD2	1:G:3519:PRO:HG2	2.03	0.41
1:G:3943:ILE:HD11	1:G:4002:LYS:HE2	2.03	0.41
1:G:4157:ASP:O	1:G:4161:ARG:HG2	2.20	0.41
1:G:4541:TRP:O	1:G:4544:LEU:HG	2.21	0.41
1:G:4890:GLY:HA2	1:G:4900:GLU:OE2	2.21	0.41
1:J:70:GLU:HG2	1:J:71:GLN:HG3	2.01	0.41
1:J:172:VAL:HA	1:J:178:ARG:O	2.21	0.41
1:J:684:VAL:HG22	1:J:781:VAL:HG12	2.02	0.41
1:J:732:SER:O	1:J:735:GLN:HG2	2.20	0.41
1:J:1115:LEU:HD23	1:J:1123:VAL:HG21	2.03	0.41
1:J:1864:LYS:HE3	1:J:1872:THR:HA	2.02	0.41
1:J:2325:PRO:HA	1:J:2425:PHE:CD2	2.56	0.41
1:J:2463:LEU:O	1:J:2467:VAL:HG23	2.21	0.41
1:J:2532:ALA:O	1:J:2536:LEU:HD23	2.21	0.41
1:J:2610:LEU:O	1:J:2614:ILE:HG12	2.20	0.41
1:J:2787:THR:OG1	1:J:2788:HIS:N	2.54	0.41
1:J:3194:LEU:O	1:J:3197:LEU:HG	2.20	0.41
1:J:3530:GLN:OE1	1:J:3530:GLN:N	2.52	0.41
1:J:3943:ILE:HD11	1:J:4002:LYS:HE2	2.03	0.41
1:J:4188:ARG:HA	1:J:4188:ARG:NE	2.35	0.41
1:J:4553:ASN:O	1:J:4557:ARG:HG3	2.21	0.41
1:B:355:LEU:HD22	1:B:379:HIS:HA	2.03	0.41
1:B:1445:PRO:HG2	1:B:1501:VAL:HG21	2.02	0.41
1:B:2325:PRO:HA	1:B:2425:PHE:CD2	2.56	0.41
1:B:2670:GLU:OE1	1:B:2673:HIS:HB3	2.21	0.41
1:B:3509:LEU:HD23	1:B:3509:LEU:HA	1.88	0.41
1:B:3530:GLN:OE1	1:B:3530:GLN:N	2.52	0.41
1:B:3949:ARG:O	1:B:3953:LYS:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1927:LEU:HD13	1:E:2097:LEU:HD11	2.02	0.41
1:E:2973:PHE:CD1	1:E:2973:PHE:C	2.99	0.41
1:E:3016:TYR:CE2	1:E:3030:HIS:HB3	2.56	0.41
1:E:3327:LEU:HD13	1:E:3368:ARG:NH1	2.36	0.41
1:E:3458:PHE:HE2	1:E:3464:ILE:HD11	1.85	0.41
1:E:3568:SER:HA	1:E:3571:TRP:CD1	2.56	0.41
1:E:3844:LEU:HD11	1:J:76:ARG:HH21	1.86	0.41
1:E:4813:LEU:HD13	1:J:4846:VAL:HG13	2.03	0.41
1:E:4890:GLY:HA2	1:E:4900:GLU:OE2	2.21	0.41
1:G:924:MET:CE	3:M:106:PRO:HB2	2.44	0.41
1:G:2325:PRO:HA	1:G:2425:PHE:CD2	2.56	0.41
1:G:2670:GLU:OE1	1:G:2673:HIS:HB3	2.21	0.41
1:G:3775:ALA:O	1:G:3779:VAL:HG13	2.21	0.41
1:J:1440:PHE:CD2	1:J:1560:ASN:HB3	2.56	0.41
1:J:1828:ASP:OD1	1:J:1828:ASP:N	2.51	0.41
1:J:3850:GLN:HE21	1:J:3870:ASN:H	1.68	0.41
1:J:3878:ASP:O	1:J:3882:GLN:HG3	2.20	0.41
1:B:76:ARG:HH21	1:G:3844:LEU:HD11	1.86	0.40
1:B:1032:LYS:HB3	1:B:1036:ARG:HH22	1.86	0.40
1:B:1945:TYR:O	1:B:1949:GLN:HG2	2.21	0.40
1:B:2759:ALA:HB1	1:B:2806:ARG:HB2	2.03	0.40
1:B:3003:LEU:O	1:B:3007:ASN:ND2	2.55	0.40
1:B:3277:LEU:HG	1:B:3341:PHE:HZ	1.86	0.40
1:B:3420:ARG:NH1	1:B:3516:LYS:O	2.51	0.40
1:B:4541:TRP:O	1:B:4544:LEU:HG	2.21	0.40
1:B:4553:ASN:O	1:B:4557:ARG:HG3	2.21	0.40
1:B:4754:ASN:CG	1:B:4756:ARG:HH12	2.29	0.40
1:E:372:LEU:O	1:E:373:LYS:C	2.64	0.40
1:E:684:VAL:HG22	1:E:781:VAL:HG12	2.02	0.40
1:E:2536:LEU:HA	1:E:2541:PHE:HB3	2.03	0.40
1:E:2759:ALA:HB1	1:E:2806:ARG:HB2	2.03	0.40
1:E:3277:LEU:HG	1:E:3341:PHE:HZ	1.86	0.40
1:E:3850:GLN:NE2	1:E:3870:ASN:H	2.19	0.40
1:E:3962:PHE:O	1:E:3966:THR:HG23	2.20	0.40
1:G:355:LEU:HD22	1:G:379:HIS:HA	2.03	0.40
1:G:732:SER:O	1:G:735:GLN:HG2	2.20	0.40
1:G:3075:LEU:H	1:G:3146:HIS:CE1	2.38	0.40
1:G:3327:LEU:HD13	1:G:3368:ARG:NH1	2.36	0.40
1:G:4754:ASN:CG	1:G:4756:ARG:HH12	2.29	0.40
1:G:4838:VAL:O	1:G:4841:VAL:HG12	2.20	0.40
1:J:2645:THR:HG23	1:J:2702:CYS:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:2655:TYR:OH	1:J:2671:GLU:OE2	2.31	0.40
1:J:2657:LEU:H	1:J:2711:PRO:HG3	1.85	0.40
1:J:3110:LEU:HD23	1:J:3183:VAL:HG12	2.02	0.40
1:J:3206:LEU:O	1:J:3208:PRO:HD3	2.20	0.40
1:J:3775:ALA:O	1:J:3779:VAL:HG13	2.21	0.40
1:J:3949:ARG:O	1:J:3953:LYS:HG3	2.21	0.40
1:J:4838:VAL:O	1:J:4841:VAL:HG12	2.21	0.40
3:F:105:ASN:CG	3:F:111:ASN:HB2	2.45	0.40
1:B:78:LEU:HD12	1:B:81:MET:SD	2.61	0.40
1:B:127:MET:O	1:B:130:LYS:NZ	2.50	0.40
1:B:568:LEU:HD12	1:B:602:VAL:HG13	2.03	0.40
1:B:663:TYR:CE1	1:B:745:SER:HB3	2.55	0.40
1:B:3110:LEU:HD23	1:B:3183:VAL:HG12	2.02	0.40
1:B:3300:ALA:HB3	1:B:3301:PRO:HD3	2.01	0.40
1:E:110:ARG:HD3	1:E:115:ARG:HE	1.86	0.40
1:E:2325:PRO:HA	1:E:2425:PHE:CD2	2.56	0.40
1:E:2458:ARG:HG3	1:E:2510:TYR:CE1	2.57	0.40
1:E:2645:THR:HG23	1:E:2702:CYS:HA	2.03	0.40
1:E:2747:ILE:HG21	1:E:2814:LYS:HE3	2.03	0.40
1:E:3046:LEU:HA	1:E:3049:LEU:HG	2.03	0.40
1:E:3292:PRO:HA	1:E:3293:PRO:HD3	1.91	0.40
1:E:4998:LYS:HE3	1:E:4998:LYS:HB2	1.72	0.40
1:G:3264:THR:O	1:G:3267:PRO:HD3	2.21	0.40
1:G:4553:ASN:O	1:G:4557:ARG:HG3	2.21	0.40
1:G:4574:ASN:ND2	1:G:4810:ALA:HA	2.29	0.40
1:J:110:ARG:HD3	1:J:115:ARG:HE	1.86	0.40
1:J:664:PHE:CE1	1:J:746:CYS:HB2	2.57	0.40
1:J:2598:ALA:O	1:J:2602:VAL:HG23	2.21	0.40
1:J:3046:LEU:HA	1:J:3049:LEU:HG	2.03	0.40
1:J:3264:THR:O	1:J:3267:PRO:HD3	2.21	0.40
1:J:4574:ASN:ND2	1:J:4810:ALA:HA	2.29	0.40
1:B:138:GLN:NE2	1:B:140:ASP:O	2.54	0.40
1:B:316:PHE:HD2	1:B:339:ILE:HG21	1.87	0.40
1:B:882:TRP:CD1	1:B:886:ARG:CZ	3.03	0.40
1:B:1699:GLU:HG3	1:B:1810:LYS:HE3	2.02	0.40
1:B:4652:LEU:O	1:B:4656:LEU:HG	2.21	0.40
1:B:4679:ARG:HH21	1:B:5017:ARG:NH1	2.18	0.40
1:E:138:GLN:NE2	1:E:140:ASP:O	2.54	0.40
1:E:1115:LEU:HD23	1:E:1123:VAL:HG21	2.03	0.40
1:E:2911:LEU:HD13	1:E:2915:GLU:HG3	2.04	0.40
1:E:4046:ASP:HA	1:E:4049:VAL:HG22	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1053:ILE:H	1:G:1053:ILE:HG12	1.66	0.40
1:G:1945:TYR:O	1:G:1949:GLN:HG2	2.22	0.40
1:G:3016:TYR:CE2	1:G:3030:HIS:HB3	2.56	0.40
1:G:3398:PHE:HD1	1:G:3451:PHE:CD2	2.40	0.40
1:G:4652:LEU:O	1:G:4656:LEU:HG	2.21	0.40
1:J:73:LEU:O	1:J:106:ALA:N	2.46	0.40
1:J:138:GLN:NE2	1:J:140:ASP:O	2.54	0.40
1:J:553:ARG:NH1	1:J:555:GLU:OE2	2.48	0.40
1:J:1870:VAL:HG11	1:J:2097:LEU:HD22	2.02	0.40
1:J:1964:ARG:O	1:J:1968:LYS:NZ	2.46	0.40
1:J:2012:PHE:CZ	1:J:2031:LEU:HD23	2.57	0.40
1:J:2867:LEU:HD12	1:J:2867:LEU:HA	1.82	0.40
1:J:2911:LEU:HD13	1:J:2915:GLU:HG3	2.04	0.40
1:J:3016:TYR:CE2	1:J:3030:HIS:HB3	2.56	0.40
1:J:3836:MET:HE2	1:J:3836:MET:HB2	1.95	0.40
1:J:4046:ASP:HA	1:J:4049:VAL:HG22	2.04	0.40
2:H:26:TYR:HA	2:H:100:ASP:O	2.20	0.40
2:I:39:SER:OG	2:I:44:LYS:O	2.40	0.40
3:C:30:SER:HB3	3:C:99:ARG:CB	2.49	0.40
3:M:105:ASN:ND2	3:M:107:TRP:H	2.20	0.40
1:B:246:TYR:CD1	1:B:373:LYS:HB2	2.57	0.40
1:B:2965:ARG:HE	1:B:2965:ARG:HB3	1.57	0.40
1:B:3016:TYR:CE2	1:B:3030:HIS:HB3	2.56	0.40
1:B:3568:SER:HA	1:B:3571:TRP:CD1	2.56	0.40
1:B:3639:THR:N	1:B:3640:PRO:HD2	2.35	0.40
1:B:3970:GLN:NE2	1:B:5004:THR:HA	2.32	0.40
1:E:192:ASP:OD1	1:E:192:ASP:N	2.55	0.40
1:E:418:LEU:HD13	1:E:493:ARG:HB3	2.04	0.40
1:E:1738:LEU:HD12	1:E:1738:LEU:HA	1.80	0.40
1:E:2951:ILE:HG13	1:E:2957:PHE:HB3	2.04	0.40
1:E:3264:THR:O	1:E:3267:PRO:HD3	2.21	0.40
1:E:3327:LEU:HD22	1:E:3368:ARG:NH1	2.36	0.40
1:E:3558:HIS:CD2	1:E:3559:LEU:HG	2.57	0.40
1:E:3943:ILE:HD11	1:E:4002:LYS:HE2	2.03	0.40
1:E:4071:ILE:O	1:E:4074:SER:OG	2.36	0.40
1:E:4966:ASP:N	1:E:4966:ASP:OD1	2.53	0.40
1:G:439:GLU:H	1:G:439:GLU:CD	2.29	0.40
1:G:2485:LEU:HD23	1:G:2485:LEU:HA	1.95	0.40
1:G:2536:LEU:HA	1:G:2541:PHE:HB3	2.03	0.40
1:G:2598:ALA:O	1:G:2602:VAL:HG23	2.21	0.40
1:G:2973:PHE:CD1	1:G:2995:ILE:HG12	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3010:PHE:O	1:G:3014:CYS:HB2	2.21	0.40
1:G:3327:LEU:HD22	1:G:3368:ARG:NH1	2.36	0.40
1:G:3965:LEU:HA	1:G:3968:TYR:CD2	2.57	0.40
1:G:4725:LEU:HA	1:G:4737:ILE:HG21	2.02	0.40
1:J:144:GLU:HB2	1:J:174:VAL:HG23	2.04	0.40
1:J:2661:TRP:CZ3	1:J:2664:PHE:HD2	2.38	0.40
1:J:2973:PHE:CD1	1:J:2973:PHE:C	2.99	0.40
1:J:3558:HIS:CD2	1:J:3559:LEU:HG	2.57	0.40
1:J:4114:CYS:O	1:J:4131:ARG:NH2	2.55	0.40
1:J:4754:ASN:CG	1:J:4756:ARG:HH12	2.30	0.40
2:H:5:GLU:HA	2:H:5:GLU:OE1	2.22	0.40
2:H:39:SER:OG	2:H:44:LYS:O	2.40	0.40
2:I:5:GLU:OE1	2:I:5:GLU:HA	2.22	0.40
1:B:172:VAL:HA	1:B:178:ARG:O	2.21	0.40
1:B:664:PHE:CE1	1:B:746:CYS:HB2	2.57	0.40
1:B:906:CYS:O	1:B:908:VAL:HG23	2.21	0.40
1:B:2247:GLN:HG3	1:B:2279:SER:HA	2.04	0.40
1:B:3453:ARG:NH1	1:B:3453:ARG:HA	2.37	0.40
1:B:3965:LEU:HA	1:B:3968:TYR:CD2	2.57	0.40
1:B:4077:PHE:O	1:B:4081:VAL:HG23	2.22	0.40
1:B:4966:ASP:OD1	1:B:4966:ASP:N	2.53	0.40
1:E:1733:GLU:O	1:E:1772:ARG:NH1	2.52	0.40
1:E:2247:GLN:HG3	1:E:2279:SER:HA	2.04	0.40
1:E:2598:ALA:O	1:E:2602:VAL:HG23	2.21	0.40
1:E:2968:ASP:OD1	1:E:2968:ASP:N	2.54	0.40
1:E:3062:PRO:HA	1:E:3065:VAL:HG22	2.02	0.40
1:G:2254:LEU:O	1:G:2258:LEU:HG	2.22	0.40
1:G:2286:LEU:HD23	1:G:2286:LEU:HA	1.93	0.40
1:G:3046:LEU:HA	1:G:3049:LEU:HG	2.03	0.40
1:G:3530:GLN:OE1	1:G:3530:GLN:N	2.52	0.40
1:G:3639:THR:N	1:G:3640:PRO:HD2	2.35	0.40
1:G:4209:GLN:H	1:G:4209:GLN:HG3	1.65	0.40
1:J:192:ASP:N	1:J:192:ASP:OD1	2.55	0.40
1:J:361:ALA:O	1:J:362:PRO:C	2.65	0.40
1:J:581:ASN:OD1	1:J:581:ASN:N	2.53	0.40
1:J:623:GLU:HG2	2:I:88:PRO:HB3	2.02	0.40
1:J:987:ARG:HG3	1:J:987:ARG:H	1.75	0.40
1:J:2247:GLN:HG3	1:J:2279:SER:HA	2.04	0.40
1:J:2263:ILE:O	1:J:2330:ARG:NH1	2.51	0.40
1:J:3398:PHE:HD1	1:J:3451:PHE:CD2	2.40	0.40
1:J:4998:LYS:HB2	1:J:4998:LYS:HE3	1.72	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	B	4247/5037 (84%)	4148 (98%)	96 (2%)	3 (0%)	48	79
1	E	4247/5037 (84%)	4149 (98%)	96 (2%)	2 (0%)	100	100
1	G	4247/5037 (84%)	4148 (98%)	97 (2%)	2 (0%)	100	100
1	J	4247/5037 (84%)	4148 (98%)	97 (2%)	2 (0%)	100	100
2	A	105/107 (98%)	102 (97%)	3 (3%)	0	100	100
2	D	105/107 (98%)	102 (97%)	3 (3%)	0	100	100
2	H	105/107 (98%)	102 (97%)	3 (3%)	0	100	100
2	I	105/107 (98%)	102 (97%)	3 (3%)	0	100	100
3	C	124/137 (90%)	118 (95%)	6 (5%)	0	100	100
3	F	124/137 (90%)	118 (95%)	6 (5%)	0	100	100
3	K	124/137 (90%)	118 (95%)	6 (5%)	0	100	100
3	M	124/137 (90%)	117 (94%)	7 (6%)	0	100	100
All	All	17904/21124 (85%)	17472 (98%)	423 (2%)	9 (0%)	49	79

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	4117	ALA
1	E	4117	ALA
1	G	4117	ALA
1	J	4117	ALA
1	B	375	LYS
1	B	3972	PRO
1	E	3972	PRO
1	G	3972	PRO
1	J	3972	PRO

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	B	3658/4276 (86%)	3653 (100%)	5 (0%)	88	91
1	E	3658/4276 (86%)	3656 (100%)	2 (0%)	88	91
1	G	3658/4276 (86%)	3655 (100%)	3 (0%)	88	91
1	J	3658/4276 (86%)	3656 (100%)	2 (0%)	88	91
2	A	88/88 (100%)	88 (100%)	0	100	100
2	D	88/88 (100%)	88 (100%)	0	100	100
2	H	88/88 (100%)	88 (100%)	0	100	100
2	I	88/88 (100%)	88 (100%)	0	100	100
3	C	104/114 (91%)	104 (100%)	0	100	100
3	F	104/114 (91%)	104 (100%)	0	100	100
3	K	104/114 (91%)	104 (100%)	0	100	100
3	M	104/114 (91%)	104 (100%)	0	100	100
All	All	15400/17912 (86%)	15388 (100%)	12 (0%)	87	91

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1170	MET
1	B	1979	LEU
1	B	3069	HIS
1	B	3516	LYS
1	B	3534	MET
1	E	3069	HIS
1	E	3516	LYS
1	G	3069	HIS
1	G	3516	LYS
1	G	3534	MET
1	J	3069	HIS
1	J	3516	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (137)

such sidechains are listed below:

Mol	Chain	Res	Type
1	B	138	GLN
1	B	461	HIS
1	B	765	GLN
1	B	877	ASN
1	B	1299	GLN
1	B	1640	HIS
1	B	1696	HIS
1	B	1973	GLN
1	B	2005	GLN
1	B	2673	HIS
1	B	2892	GLN
1	B	2924	GLN
1	B	2931	GLN
1	B	2933	ASN
1	B	2991	HIS
1	B	3033	ASN
1	B	3069	HIS
1	B	3127	GLN
1	B	3146	HIS
1	B	3150	HIS
1	B	3180	ASN
1	B	3605	HIS
1	B	3734	HIS
1	B	3771	HIS
1	B	3895	HIS
1	B	3914	ASN
1	B	3970	GLN
1	B	4133	GLN
1	B	4574	ASN
1	B	5015	GLN
1	E	461	HIS
1	E	765	GLN
1	E	877	ASN
1	E	994	ASN
1	E	1133	HIS
1	E	1299	GLN
1	E	1586	ASN
1	E	1640	HIS
1	E	1663	HIS
1	E	1696	HIS
1	E	1973	GLN
1	E	2005	GLN

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Mol	Chain	Res	Type
1	E	2892	GLN
1	E	2924	GLN
1	E	2931	GLN
1	E	2933	ASN
1	E	2991	HIS
1	E	3033	ASN
1	E	3069	HIS
1	E	3146	HIS
1	E	3150	HIS
1	E	3180	ASN
1	E	3605	HIS
1	E	3700	GLN
1	E	3771	HIS
1	E	3895	HIS
1	E	3914	ASN
1	E	3970	GLN
1	E	4133	GLN
1	E	4574	ASN
1	E	5015	GLN
1	G	84	ASN
1	G	461	HIS
1	G	765	GLN
1	G	877	ASN
1	G	1133	HIS
1	G	1274	HIS
1	G	1299	GLN
1	G	1586	ASN
1	G	1640	HIS
1	G	1696	HIS
1	G	1973	GLN
1	G	2005	GLN
1	G	2125	HIS
1	G	2673	HIS
1	G	2892	GLN
1	G	2924	GLN
1	G	2931	GLN
1	G	2933	ASN
1	G	2991	HIS
1	G	3033	ASN
1	G	3069	HIS
1	G	3146	HIS
1	G	3150	HIS

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Mol	Chain	Res	Type
1	G	3180	ASN
1	G	3605	HIS
1	G	3771	HIS
1	G	3895	HIS
1	G	3914	ASN
1	G	3970	GLN
1	G	4133	GLN
1	G	4574	ASN
1	G	5015	GLN
1	G	5035	GLN
1	J	461	HIS
1	J	765	GLN
1	J	877	ASN
1	J	1274	HIS
1	J	1299	GLN
1	J	1586	ASN
1	J	1640	HIS
1	J	1663	HIS
1	J	1696	HIS
1	J	1973	GLN
1	J	2005	GLN
1	J	2892	GLN
1	J	2924	GLN
1	J	2931	GLN
1	J	2933	ASN
1	J	3069	HIS
1	J	3127	GLN
1	J	3146	HIS
1	J	3150	HIS
1	J	3180	ASN
1	J	3605	HIS
1	J	3734	HIS
1	J	3771	HIS
1	J	3895	HIS
1	J	3914	ASN
1	J	3970	GLN
1	J	4133	GLN
1	J	4574	ASN
1	J	5015	GLN
2	A	70	GLN
2	D	31	GLN
2	D	70	GLN

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Mol	Chain	Res	Type
2	H	31	GLN
2	H	70	GLN
2	I	31	GLN
2	I	70	GLN
3	C	3	GLN
3	F	3	GLN
3	F	73	ASN
3	K	3	GLN
3	K	73	ASN
3	M	3	GLN
3	M	105	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

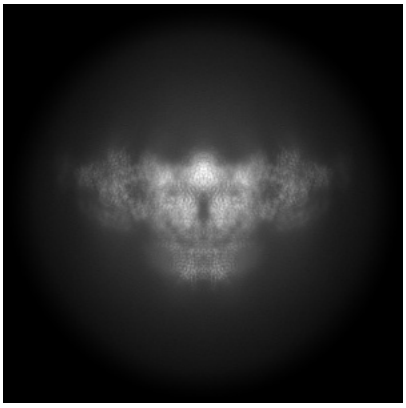
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-19466. These allow visual inspection of the internal detail of the map and identification of artifacts.

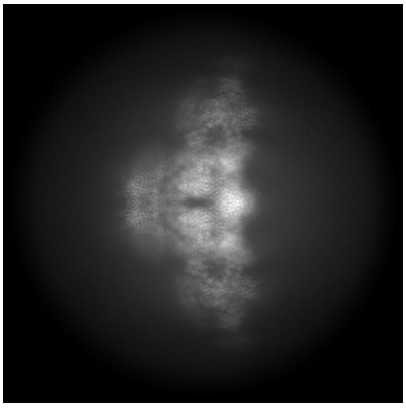
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

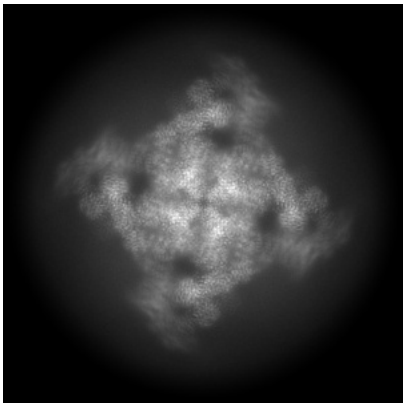
6.1.1 Primary map



X



Y

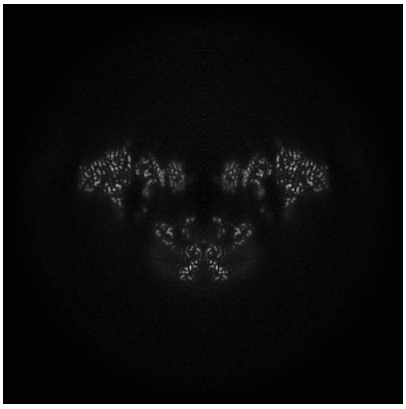


Z

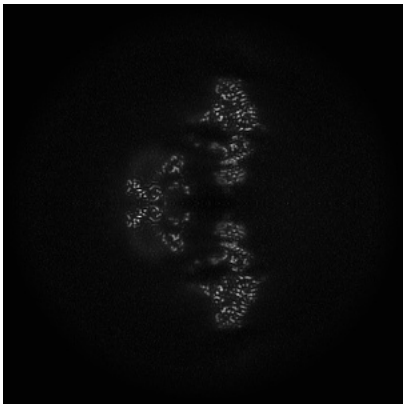
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

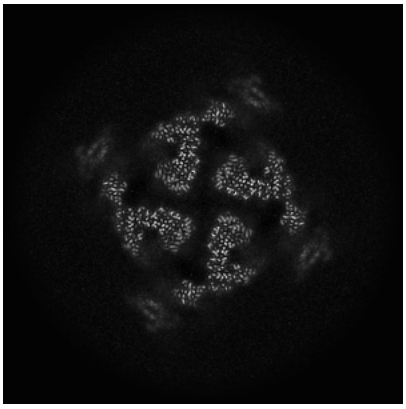
6.2.1 Primary map



X Index: 168



Y Index: 168



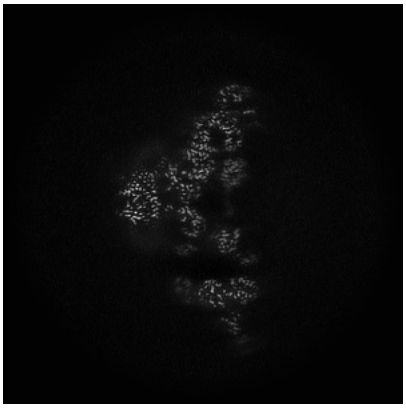
Z Index: 168

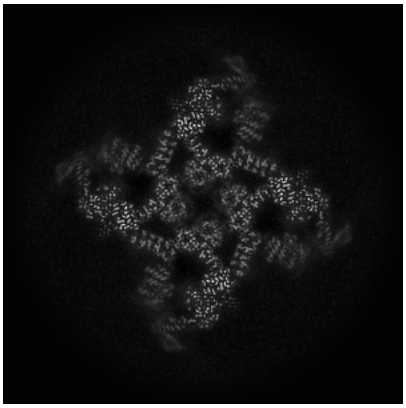
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 178

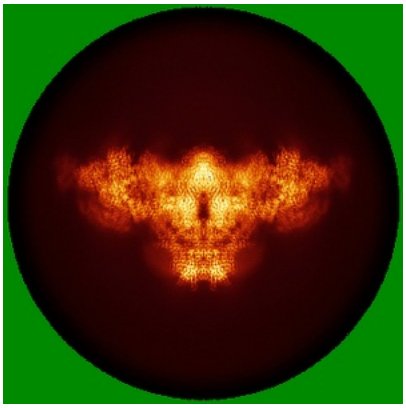

Y Index: 178

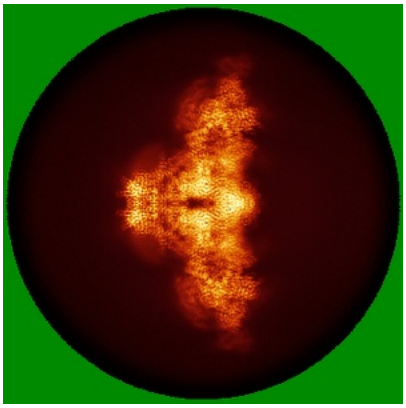

Z Index: 187

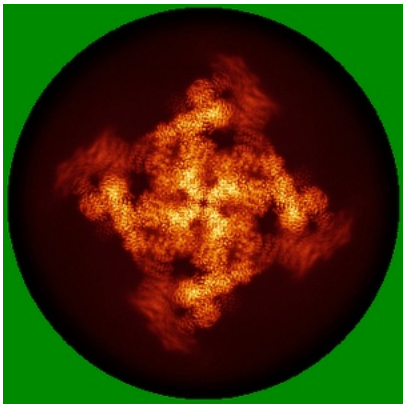
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map


X

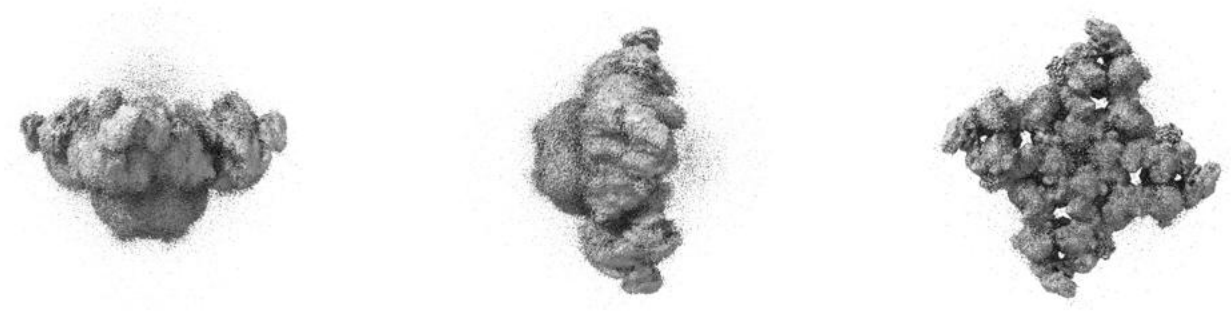

Y


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

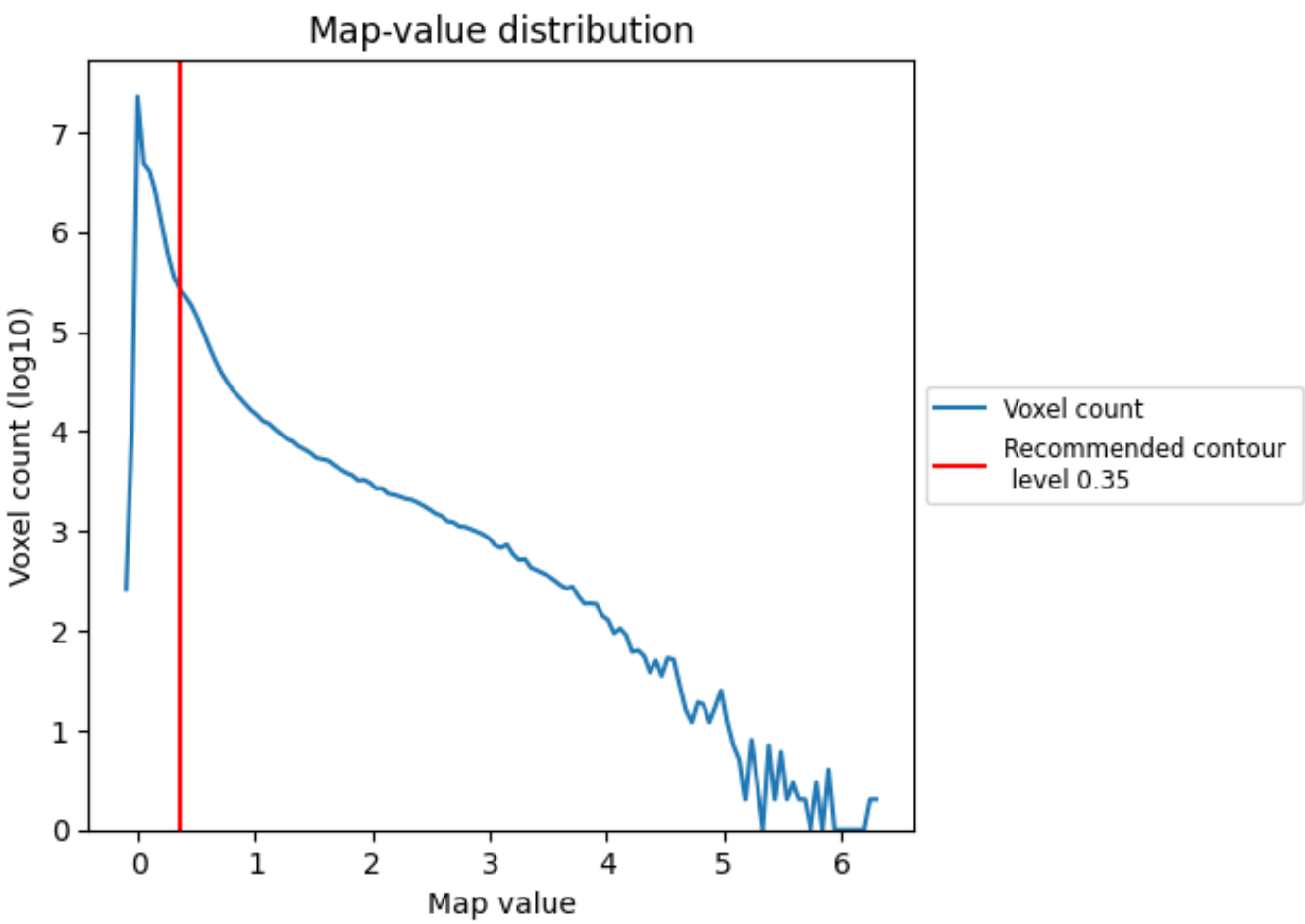
6.6 Mask visualisation (i)

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

7 Map analysis (i)

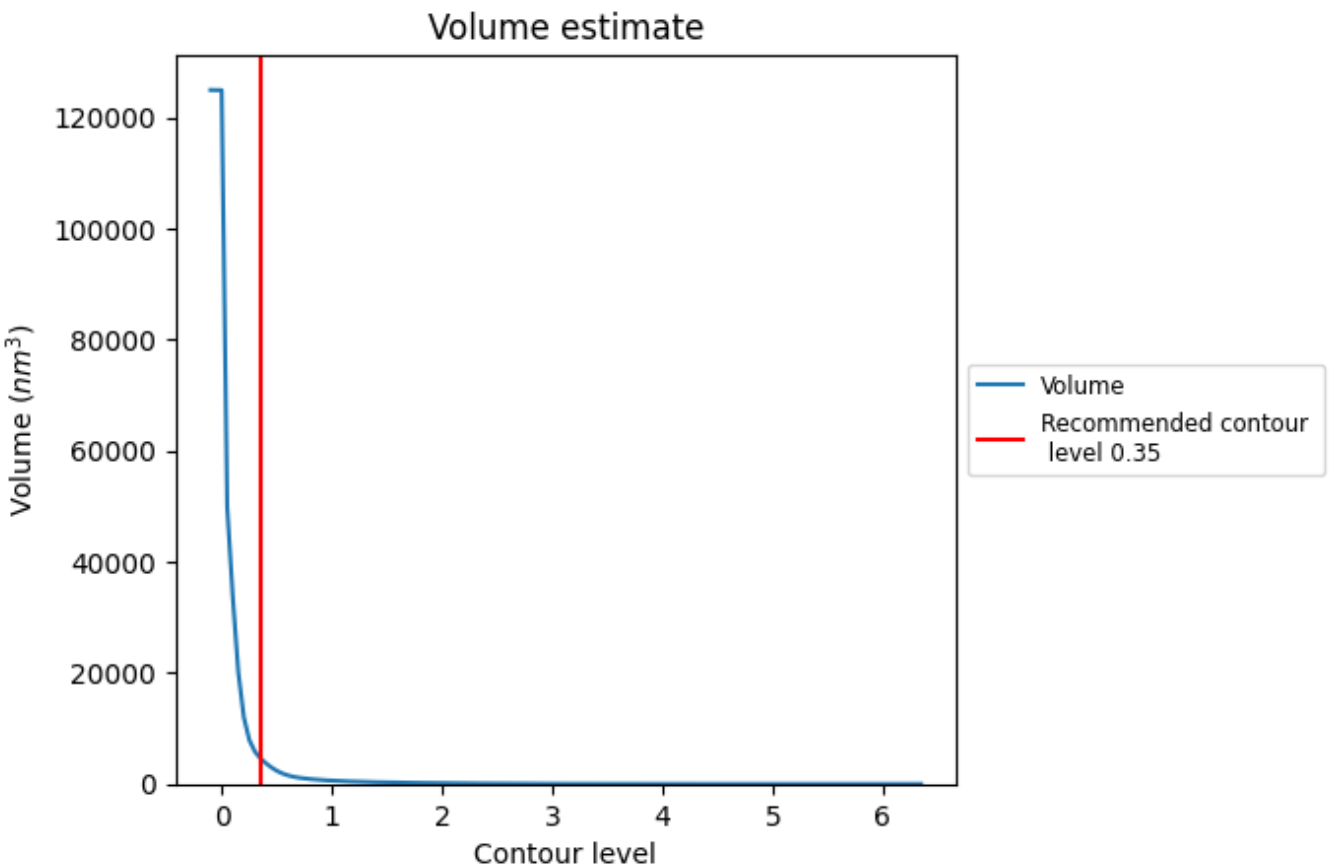
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

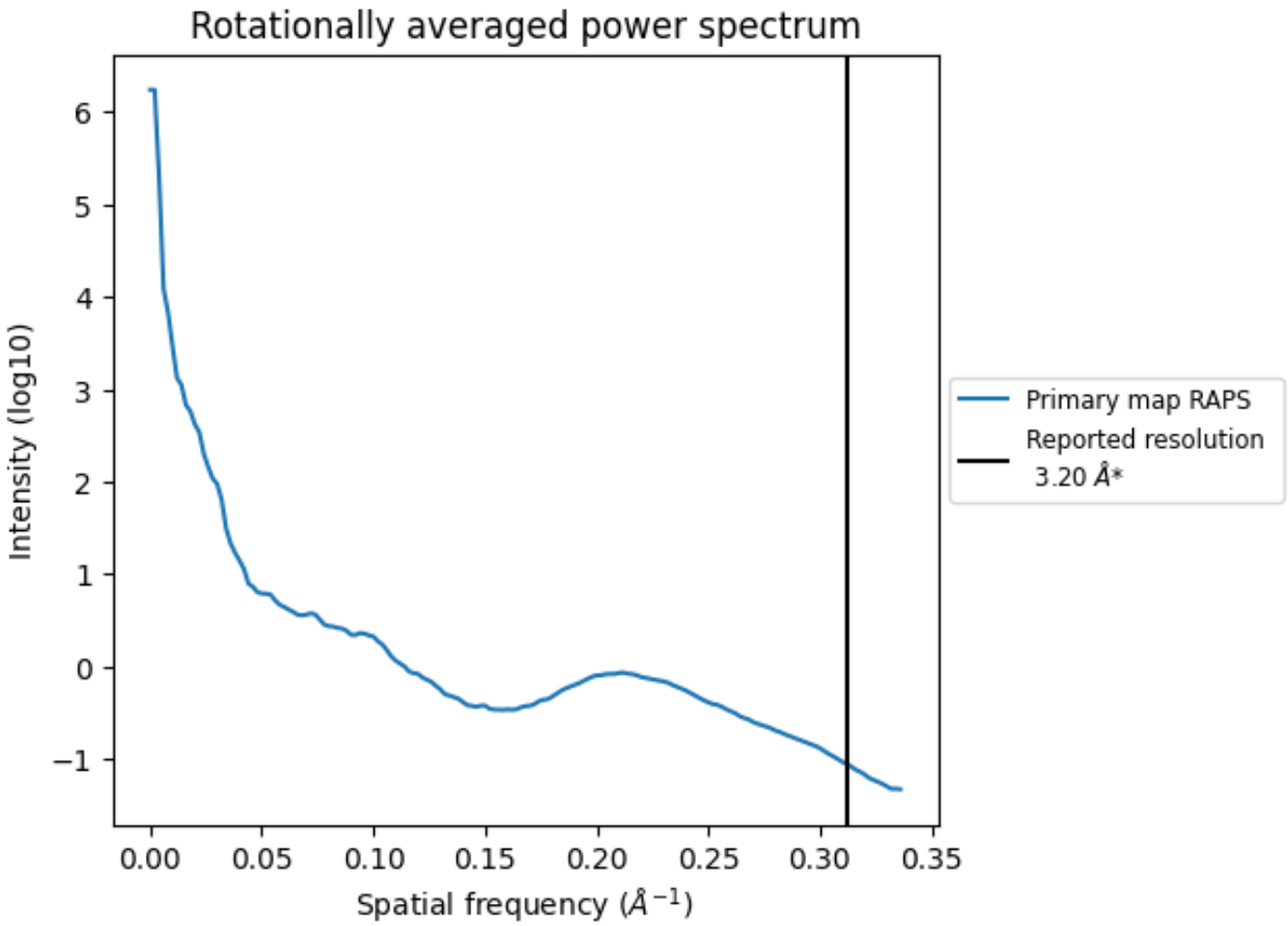
7.2 Volume estimate (i)



The volume at the recommended contour level is 4570 nm^3; this corresponds to an approximate mass of 4129 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)

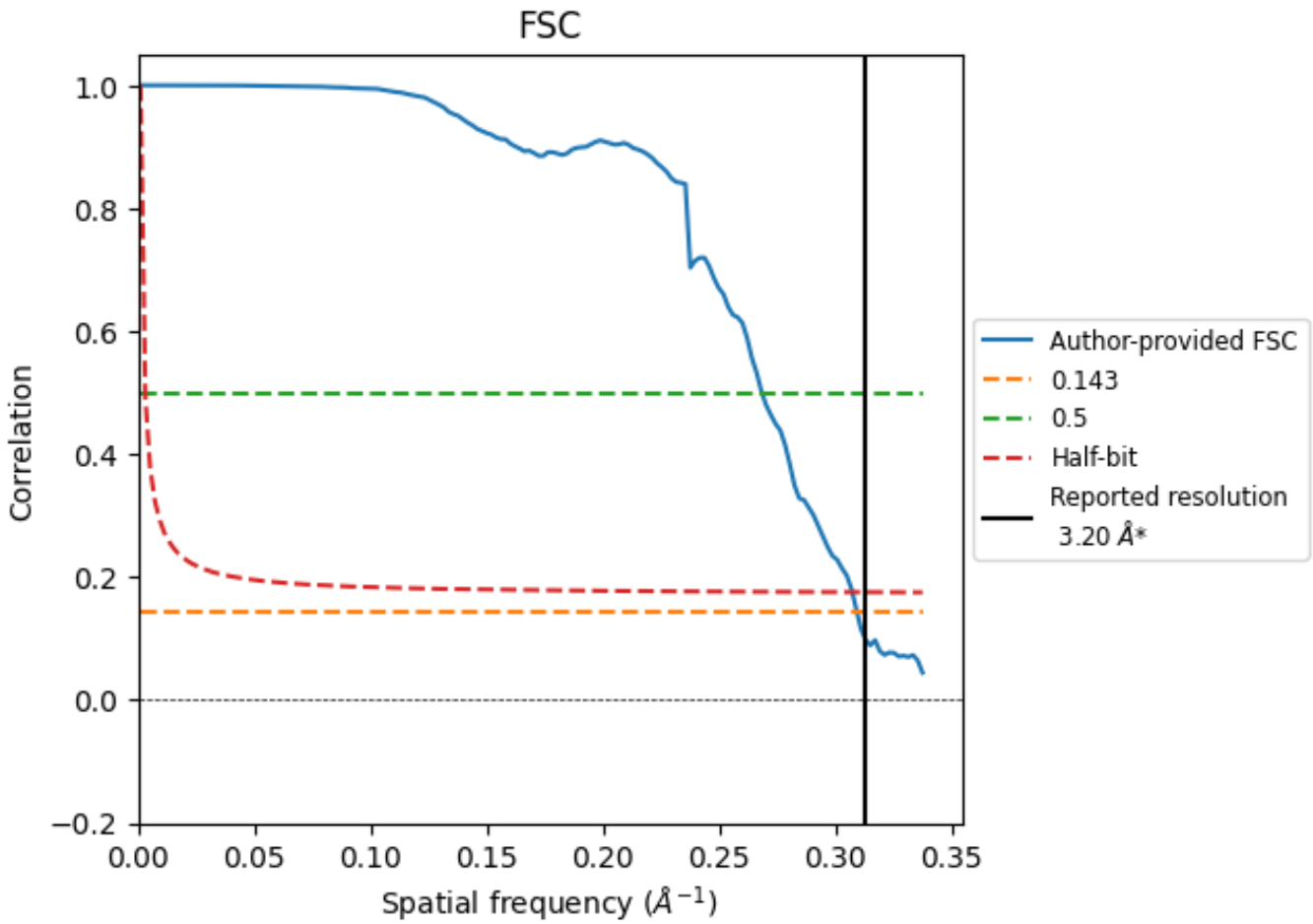


*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8.2 Resolution estimates (i)

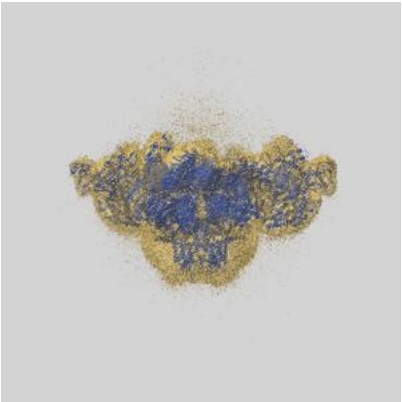
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.23	3.73	3.26
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

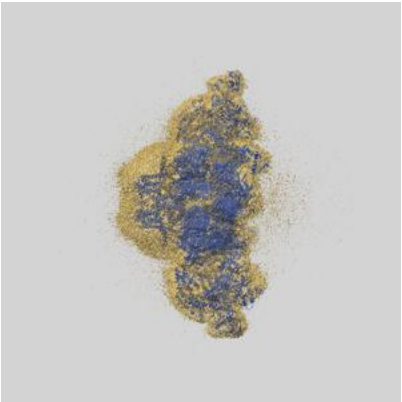
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-19466 and PDB model 8RRV. Per-residue inclusion information can be found in section 3 on page 6.

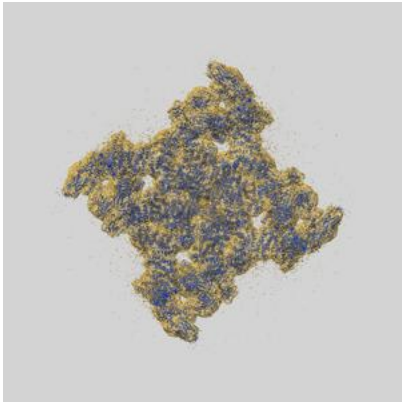
9.1 Map-model overlay (i)



X



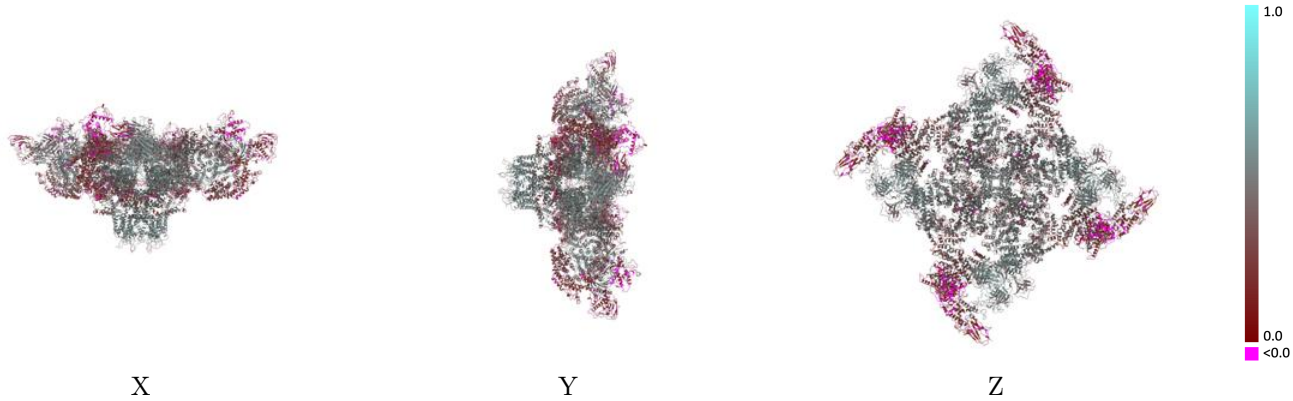
Y



Z

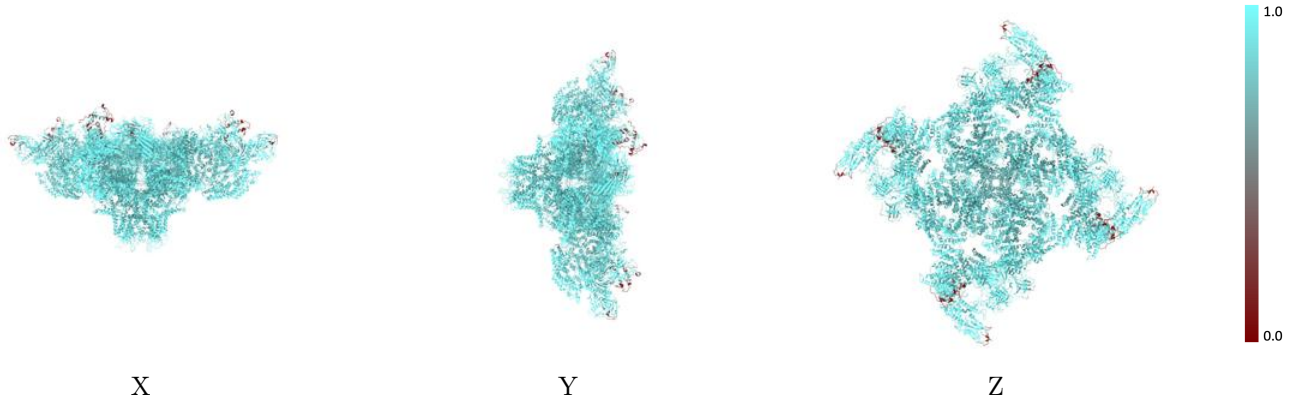
The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



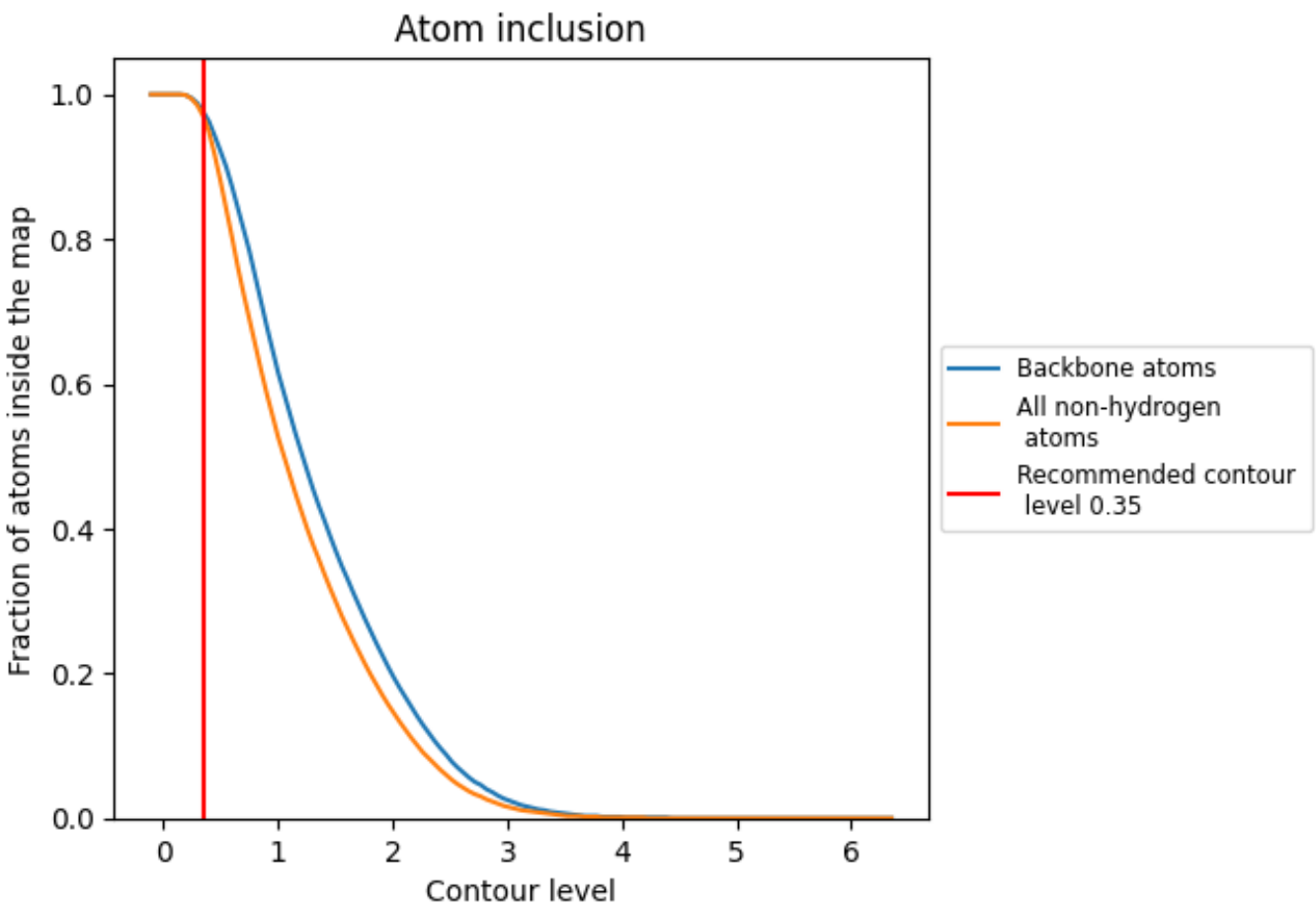
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.35).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 97% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9700	0.3800
A	0.8810	0.4120
B	0.9770	0.3850
C	0.7720	0.1480
D	0.8780	0.4170
E	0.9780	0.3850
F	0.7760	0.1480
G	0.9770	0.3850
H	0.8860	0.4150
I	0.8810	0.4170
J	0.9770	0.3860
K	0.7770	0.1480
M	0.7720	0.1500