Full wwPDB EM Validation Report (i)

Jun 26, 2023 – 12:15 PM EDT

PDB ID	:	8DVE
EMDB ID	:	EMD-27736
Title	:	RyR1 in presence of IpCa-T26E phosphomimetic and activating ligands
Authors	:	Haji-Ghassemi, O.; Van Petegm, F.
Deposited on	:	2022-07-28
Resolution	:	3.84 Å(reported)
Based on initial model	:	6M2W

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

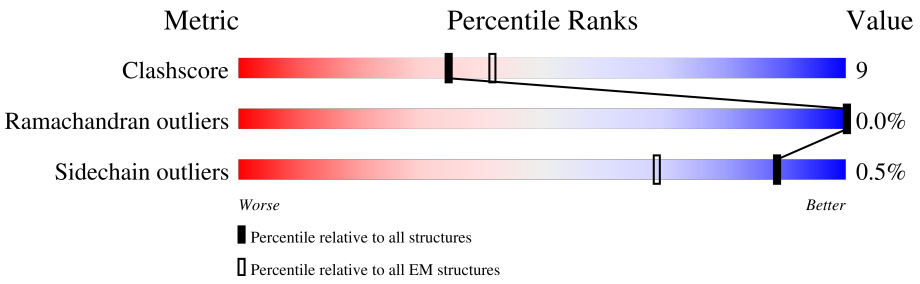
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

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 3.84 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	5037	6% 66% 12% 22%
1	D	5037	10% 64% 14% 22%
1	G	5037	7% 65% 13% 22%
1	J	5037	11% 64% 15% 22%
2	B	107	81% 19%
2	E	107	79% 21%
2	H	107	79% 21%
2	K	107	71% 29%

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Mol	Chain	Length	Quality of chain
3	C	149	27% 91% • 7%
3	F	149	58% 89% • 7%
3	I	149	30% 84% 9% 7%
3	L	149	44% 88% • 8%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 114229 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	D	3942	26818	17244	4812	4614	148	0	0
1	A	3943	27274	17556	4883	4676	159	0	0
1	G	3944	27137	17456	4860	4662	159	0	0
1	J	3943	26962	17331	4814	4668	149	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	E	107	743	475	132	133	3	0	0
2	B	107	743	473	134	132	4	0	0
2	H	107	745	474	134	134	3	0	0
2	K	107	728	466	128	131	3	0	0

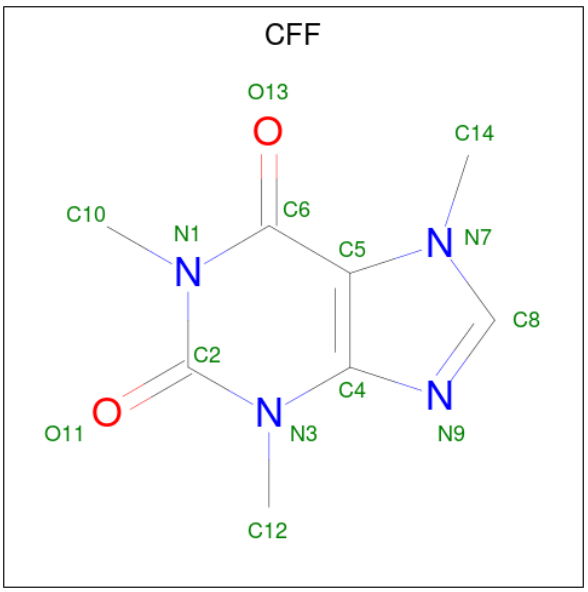
- Molecule 3 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	F	138	715	437	138	139	1	0	0
3	C	138	720	437	139	142	2	0	0
3	I	138	730	447	140	142	1	0	0
3	L	137	726	443	138	141	4	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	32	ALA	GLU	engineered mutation	UNP P0DP23
F	68	ALA	GLU	engineered mutation	UNP P0DP23
F	105	ALA	GLU	engineered mutation	UNP P0DP23
F	141	ALA	GLU	engineered mutation	UNP P0DP23
C	32	ALA	GLU	engineered mutation	UNP P0DP23
C	68	ALA	GLU	engineered mutation	UNP P0DP23
C	105	ALA	GLU	engineered mutation	UNP P0DP23
C	141	ALA	GLU	engineered mutation	UNP P0DP23
I	32	ALA	GLU	engineered mutation	UNP P0DP23
I	68	ALA	GLU	engineered mutation	UNP P0DP23
I	105	ALA	GLU	engineered mutation	UNP P0DP23
I	141	ALA	GLU	engineered mutation	UNP P0DP23
L	32	ALA	GLU	engineered mutation	UNP P0DP23
L	68	ALA	GLU	engineered mutation	UNP P0DP23
L	105	ALA	GLU	engineered mutation	UNP P0DP23
L	141	ALA	GLU	engineered mutation	UNP P0DP23

- Molecule 4 is CAFFEINE (three-letter code: CFF) (formula: $C_8H_{10}N_4O_2$).

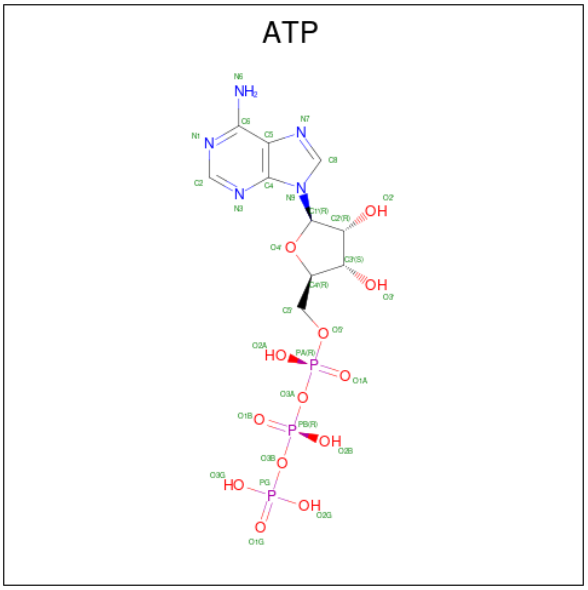


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
4	D	1	14	8	4	2	0
4	A	1	14	8	4	2	0
4	G	1	14	8	4	2	0
4	J	1	14	8	4	2	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
5	D	1	1	1	0
5	A	1	1	1	0
5	G	1	1	1	0
5	J	1	1	1	0

- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

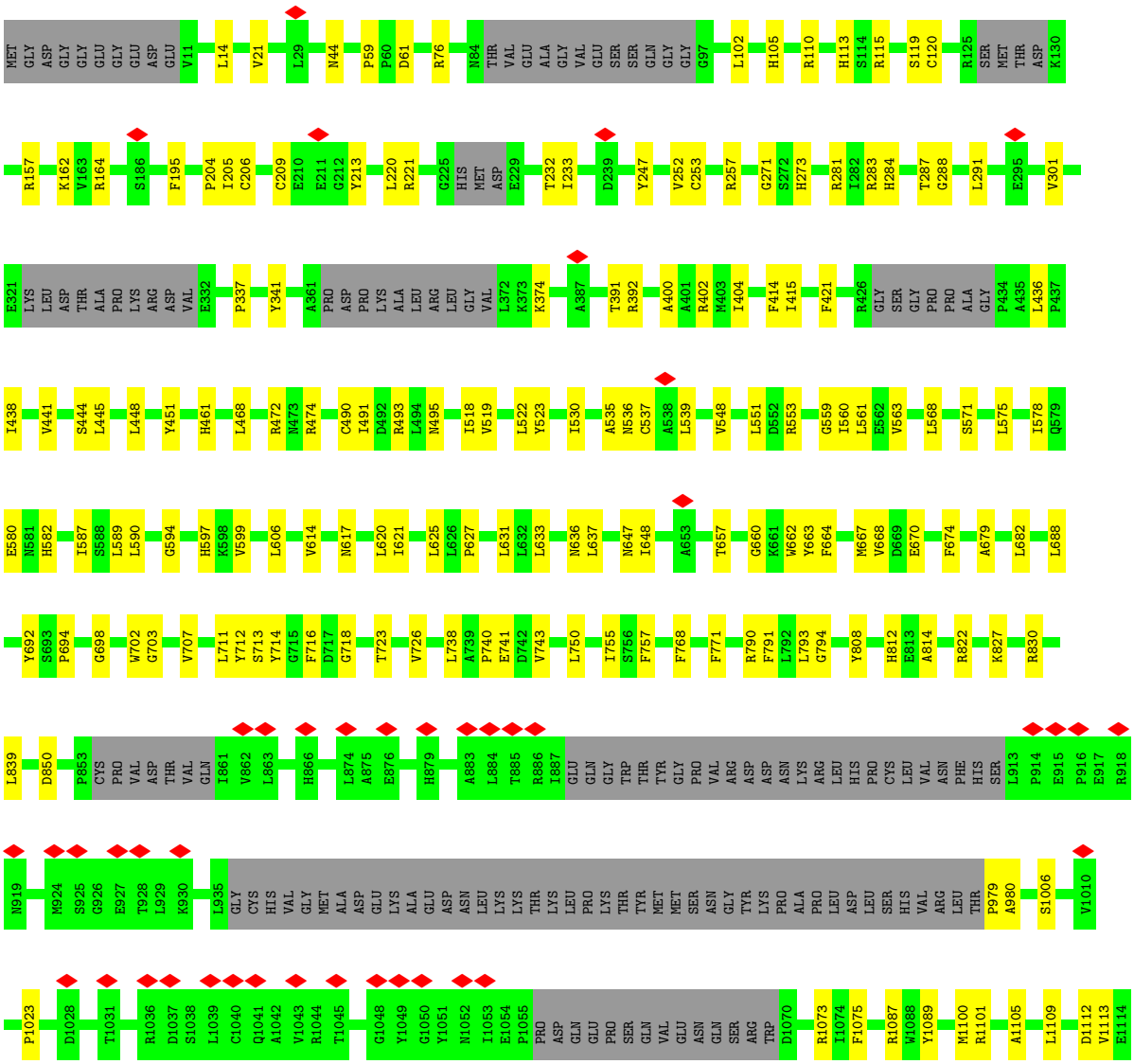
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
7	D	1	1	1	0
7	A	1	1	1	0
7	G	1	1	1	0
7	J	1	1	1	0

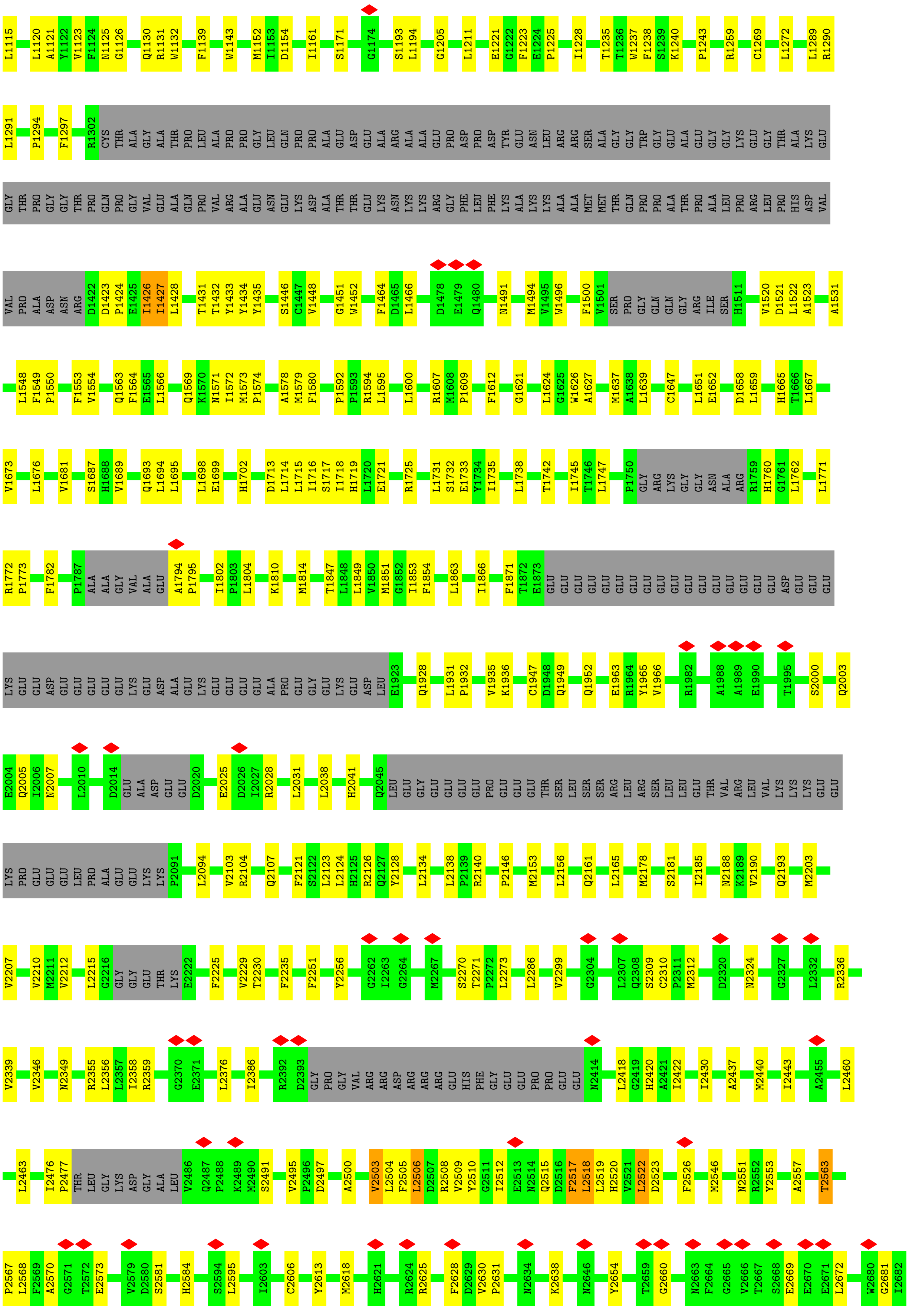
3 Residue-property plots (i)

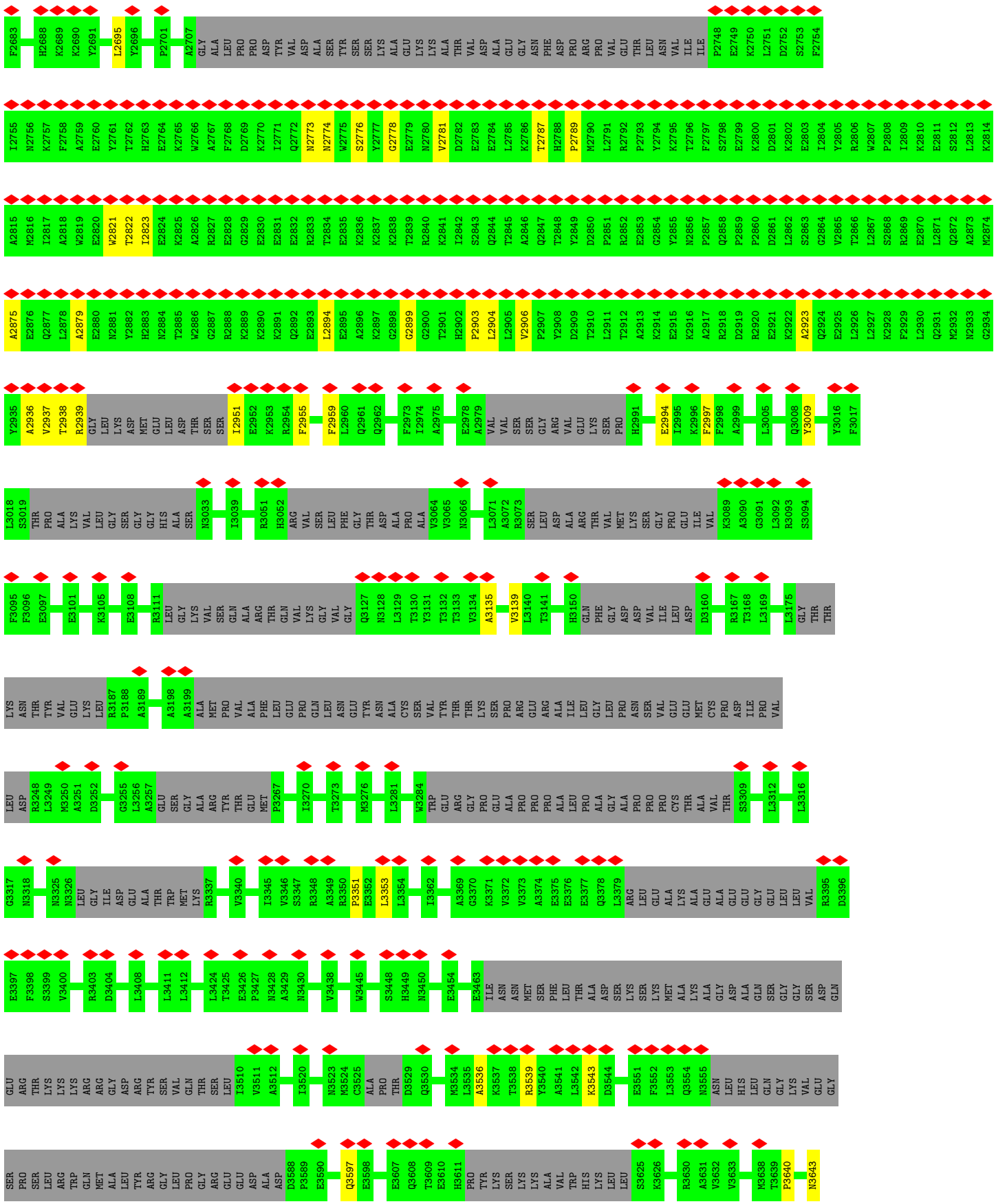
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 D: 10% 64% 14% 22%




L1115 L1120 A1121 Y1122 V1123 F1124 N1125 G1126 Q1130 R1131 W1132 F1139 W1143 M1152 I1153 D1154 I1161 S1171 G1174 S1193 L1194 G1205 L1211 E1221 G1222 F1223 E1224 P1225 I1228 T1235 T1236 W1237 F1238 S1239 K1240 P1243 R1259 C1269 L1272 L1289 R1290
L1291 P1294 F1297 R1302 CYS THR ALA GLY ALA THR PRO LEU ALA PRO PRO GLY LEU GLN PRO PRO ALA GLU ASP GLU ALA ARG ALA ALA GLU PRO ASP PRO ASP TYR GLU ASN LEU ARG ARG SER ALA GLY GLY TRP GLY GLU ALA GLU GLY GLY LYS GLU GLY THR ALA LYS GLU
GLY THR PRO GLY GLY THR PRO GLN PRO GLY VAL GLU ALA GLN PRO VAL ARG ALA 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 ASN ARG D1422 D1423 P1424 E1425 I1426 I1427 L1428 T1431 T1432 Y1433 Y1434 Y1435 S1446 C1447 V1448 G1451 W1452 F1464 D1465 L1466 D1478 E1479 Q1480 N1491 M1494 V1495 W1496 F1500 V1501 SER PRO GLY GLN GLN GLN GLY ARG ILE SER H1511 V1520 D1521 L1522 A1523 A1531
L1548 F1549 P1550 F1553 V1554 Q1563 F1564 E1565 L1566 Q1569 K1570 N1571 I1572 M1573 P1574 A1578 M1579 F1580 P1592 P1593 R1594 L1595 L1600 R1607 M1608 P1609 F1612 G1621 L1624 G1625 W1626 A1627 M1637 A1638 L1639 C1647 L1651 E1652 D1658 L1659 H1665 T1666 L1667
V1673 L1676 V1681 S1687 H1688 V1689 Q1693 L1694 L1695 L1698 E1699 H1702 D1713 L1714 L1715 I1716 S1717 I1718 H1719 L1720 E1721 R1725 L1731 S1732 E1733 Y1734 I1735 L1738 T1742 I1745 T1746 L1747 P1750 GLY ARG LYS GLY GLY ASN ALA ARG R1759 H1760 G1761 L1762 L1771
R1772 P1773 F1782 P1787 ALA ALA GLY VAL ALA GLU A1794 P1795 I1802 P1803 L1804 K1810 M1814 T1847 L1848 L1849 V1850 M1851 G1852 I1853 F1854 L1863 I1866 F1871 T1872 E1873 GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU ASP GLU GLU GLU
LYS GLU GLU ASP GLU GLU GLU GLU GLU LYS GLU ASP ALA GLU LYS GLU GLU GLU GLU ALA PRO GLU GLY GLU LYS GLU ASP LEU E1923 Q1928 L1931 P1932 V1935 K1936 C1947 D1948 Q1949 Q1952 E1963 R1964 Y1965 V1966 R1982 A1988 A1989 E1990 T1995 S2000 Q2003
E2004 Q2005 I2006 N2007 L2010 D2014 GLU ALA ASP GLU GLU D2020 E2025 D2026 I2027 R2028 L2031 L2038 H2041 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 LYS LYS P2091 L2094 V2103 R2104 Q2107 F2121 S2122 L2123 L2124 H2125 R2126 Q2127 Y2128 L2134 L2138 P2139 R2140 P2146 M2153 L2156 Q2161 L2165 M2178 S2181 I2185 N2188 K2189 V2190 Q2193 M2203
V2207 V2210 M2211 V2212 L2215 G2216 GLY GLY GLU THR LYS E2222 F2225 V2229 T2230 F2235 F2251 Y2256 G2262 I2263 G2264 M2267 S2270 T2271 P2272 L2273 L2286 V2299 G2304 L2307 Q2308 S2309 C2310 P2311 M2312 D2320 N2324 G2327 L2332 R2336
V2339 V2346 N2349 R2355 L2356 L2357 I2358 R2359 G2370 E2371 L2376 I2386 R2392 D2393 GLY PRO GLY VAL ARG ARG ASP ARG ARG ARG GLU HIS PHE GLY GLU GLU PRO PRO GLU GLU N2414 L2418 G2419 H2420 A2421 I2422 I2430 A2437 M2440 I2443 A2455 L2460
L2463 I2476 P2477 THR LEU GLY LYS ASP GLY ALA LEU V2486 Q2487 P2488 K2489 M2490 S2491 V2495 P2496 D2497 A2500 V2503 L2504 F2505 L2506 D2507 R2508 V2509 Y2510 G2511 I2512 E2513 N2514 Q2515 D2516 F2517 L2518 L2519 H2520 V2521 L2522 D2523 F2526 M2546 N2551 R2552 Y2553 A2557 T2563
P2567 L2568 F2569 A2570 G2571 T2572 E2573 V2579 D2580 S2581 H2584 S2594 L2595 I2603 C2606 Y2613 M2618 H2621 R2624 R2625 F2628 D2629 V2630 P2631 N2634 K2638 N2646 Y2654 T2659 G2660 N2663 F2664 G2665 V2666 T2667 S2668 E2669 E2670 E2671 L2672 W2680 G2681 I2682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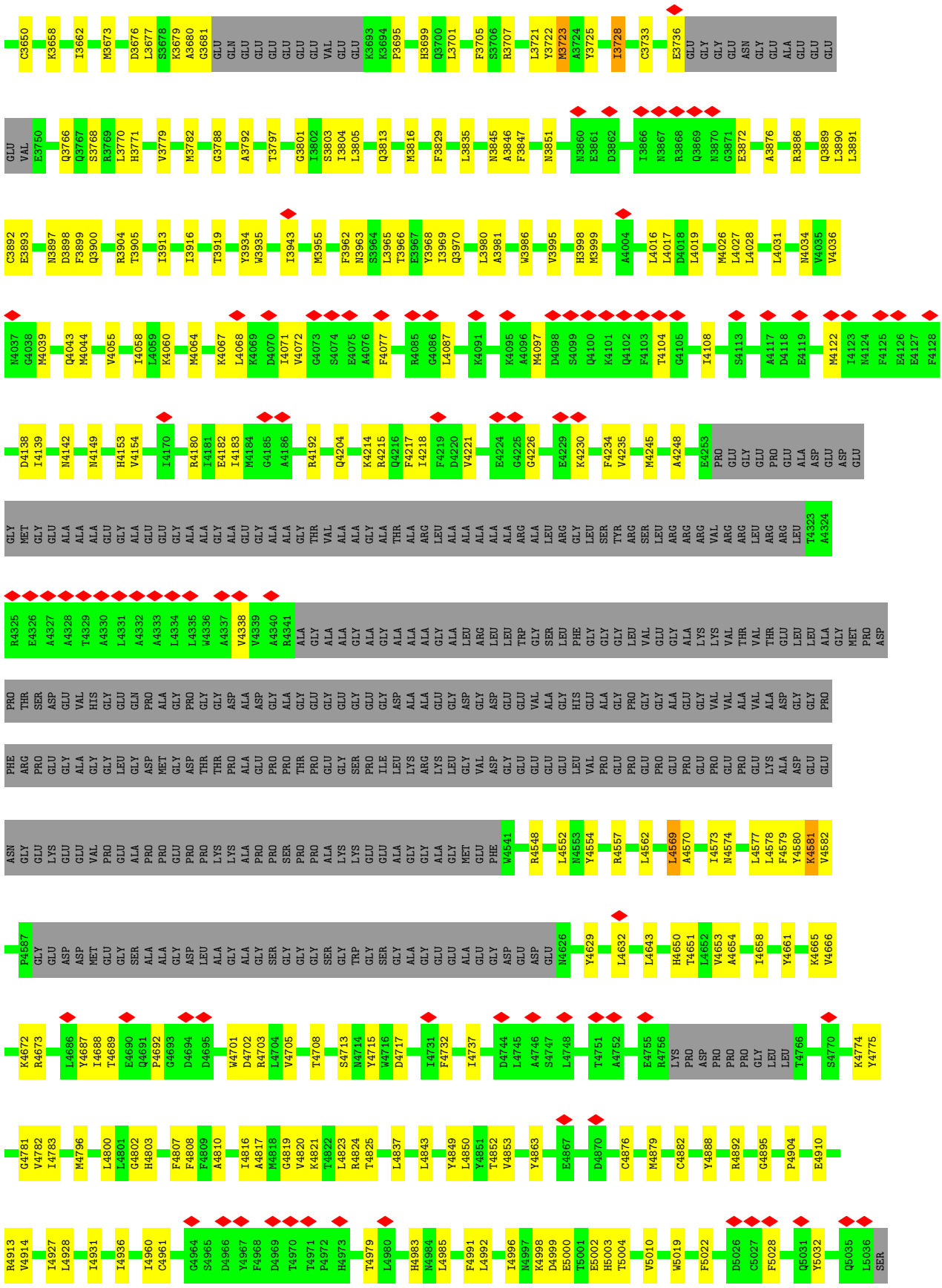
I2755 N2756 K2757 F2758 A2759 E2760 Y2761 T2762 H2763 E2764 K2765 W2766 A2767 F2768 D2769 K2770 I2771 Q2772 N2773 N2774 W2775 S2776 Y2777 G2778 E2779 N2780 V2781 D2782 E2783 E2784 L2785 K2786 T2787 H2788 P2789 M2790 L2791 R2792 P2793 Y2794 K2795 T2796 F2797 S2798 E2799 K2800 D2801 K2802 E2803 I2804 Y2805 R2806 W2807 P2808 I2809 K2810 E2811 S2812 L2813 K2814
A2815 M2816 I2817 A2818 W2819 E2820 W2821 T2822 I2823 E2824 K2825 A2826 R2827 E2828 G2829 E2830 E2831 E2832 R2833 T2834 E2835 K2836 K2837 K2838 T2839 R2840 K2841 I2842 S2843 Q2844 T2845 A2846 Q2847 T2848 Y2849 D2850 P2851 R2852 E2853 G2854 Y2855 N2856 P2857 Q2858 P2859 P2860 D2861 L2862 S2863 G2864 V2865 T2866 L2867 S2868 R2869 E2870 L2871 Q2872 A2873 M2874
A2875 E2876 Q2877 L2878 A2879 E2880 N2881 Y2882 H2883 N2884 T2885 W2886 G2887 R2888 K2889 K2890 K2891 Q2892 E2893 L2894 E2895 A2896 K2897 G2898 G2899 G2900 T2901 H2902 P2903 L2904 L2905 V2906 P2907 Y2908 D2909 T2910 L2911 T2912 A2913 K2914 E2915 K2916 A2917 R2918 D2919 R2920 E2921 K2922 A2923 Q2924 E2925 L2926 L2927 K2928 F2929 L2930 Q2931 M2932 N2933 G2934
Y2935 A2936 V2937 T2938 R2939 GLY LEU LYS ASP MET GLU LEU ASP THR SER SER I2951 E2952 K2953 R2954 F2955 F2959 L2960 Q2961 Q2962 F2973 I2974 A2975 E2978 A2979 VAL VAL SER SER GLY ARG VAL GLU LYS SER PRO H2991 E2994 I2995 K2996 F2997 F2998 A2999 L3005 Q3008 Y3009 Y3016 F3017
L3018 S3019 THR PRO ALA LYS VAL LEU GLY SER GLY GLY HIS ALA SER N3033 I3039 R3051 H3052 ARG VAL SER LEU PHE GLY THR ASP ALA PRO ALA V3064 V3065 N3066 L3071 A3072 R3073 SER LEU ASP ALA ARG THR VAL MET LYS SER GLY PRO GLU ILE VAL K3089 A3090 G3091 L3092 R3093 S3094
F3095 F3096 E3097 E3101 K3105 E3108 R3111 LEU GLY LYS VAL SER GLN ALA ARG THR GLN VAL LYS GLY VAL GLY Q3127 N3128 L3129 T3130 Y3131 T3132 T3133 V3134 A3135 V3139 L3140 T3141 H3150 GLN PHE GLY ASP ASP VAL ILE LEU ASP D3160 R3167 T3168 L3169 L3175 GLY THR THR
LYS ASN THR TYR VAL GLU LYS LEU R3187 P3188 A3189 A3198 A3199 ALA MET PRO VAL ALA PHE LEU GLU PRO GLN LEU ASN GLU TYR ASN ALA CYS SER VAL TYR THR THR LYS SER PRO ARG GLU ARG ALA ILE LEU GLY LEU PRO ASN SER VAL GLU GLU MET CYS PRO ASP ILE PRO VAL
LEU ASP R3248 L3249 M3250 A3251 D3252 G3255 L3256 A3257 GLU SER GLY ALA ARG TYR THR GLU MET P3267 T3270 T3273 M3276 L3281 W3284 TRP GLU ARG GLY PRO GLU ALA PRO PRO PRO ALA LEU PRO ALA GLY ALA PRO PRO PRO CYS THR ALA VAL THR S3309 L3312 L3316
G3317 N3318 N3325 N3326 LEU GLY ILE ASP GLU ALA THR TRP MET LYS R3337 V3340 I3345 V3346 S3347 R3348 A3349 R3350 P3351 E3352 L3353 L3354 I3362 A3369 G3370 K3371 V3372 V3373 A3374 E3375 E3376 E3377 Q3378 L3379 ARG LEU GLU ALA LYS ALA GLU ALA GLU GLU GLY GLU LEU LEU VAL R3395 D3396
E3397 F3398 S3399 V3400 R3403 D3404 L3408 L3411 L3412 L3424 T3425 E3426 P3427 N3428 A3429 N3430 V3438 W3445 S3448 H3449 N3450 E3454 E3463 ILE ASN ASN MET SER PHE LEU THR ALA ASP SER 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 SER VAL GLN THR SER LEU I3510 V3511 A3512 I3520 N3523 M3524 C3525 ALA PRO THR D3529 Q3530 M3534 L3535 A3536 K3537 T3538 R3539 Y3540 A3541 L3542 K3543 D3544 E3551 F3552 L3553 Q3554 N3555 ASN LEU HIS LEU GLN GLY LYS VAL GLU GLY
SER PRO SER LEU ARG TRP GLN MET ALA LEU TYR ARG GLY LEU PRO GLY ARG GLU GLU ASP ALA ASP D3588 P3589 E3590 Q3597 E3598 E3607 Q3608 T3609 E3610 H3611 PRO TYR LYS SER LYS LYS ALA VAL TRP HIS LYS LEU LEU S3625 K3626 R3630 A3631 V3632 V3633 M3638 T3639 P3640 N3643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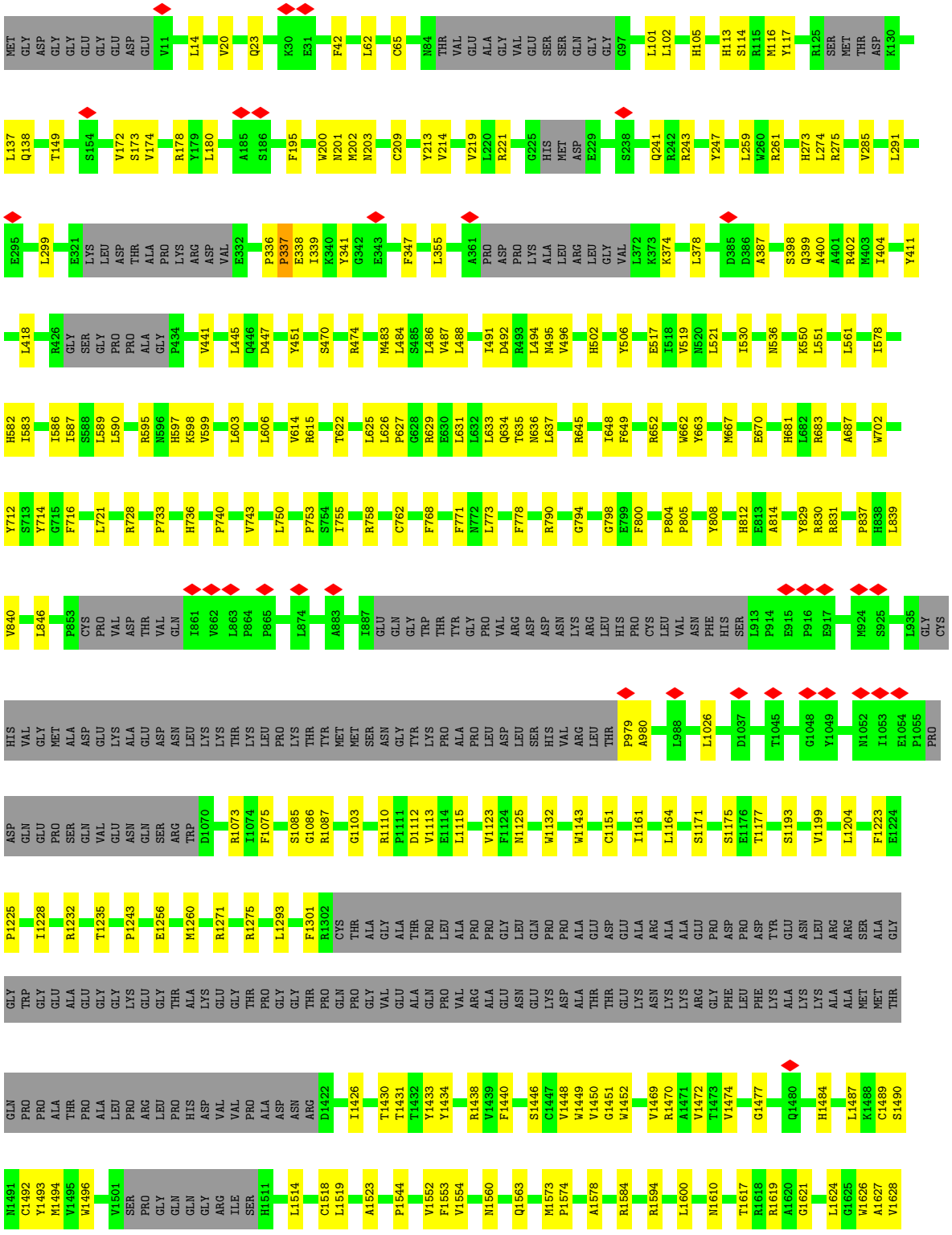
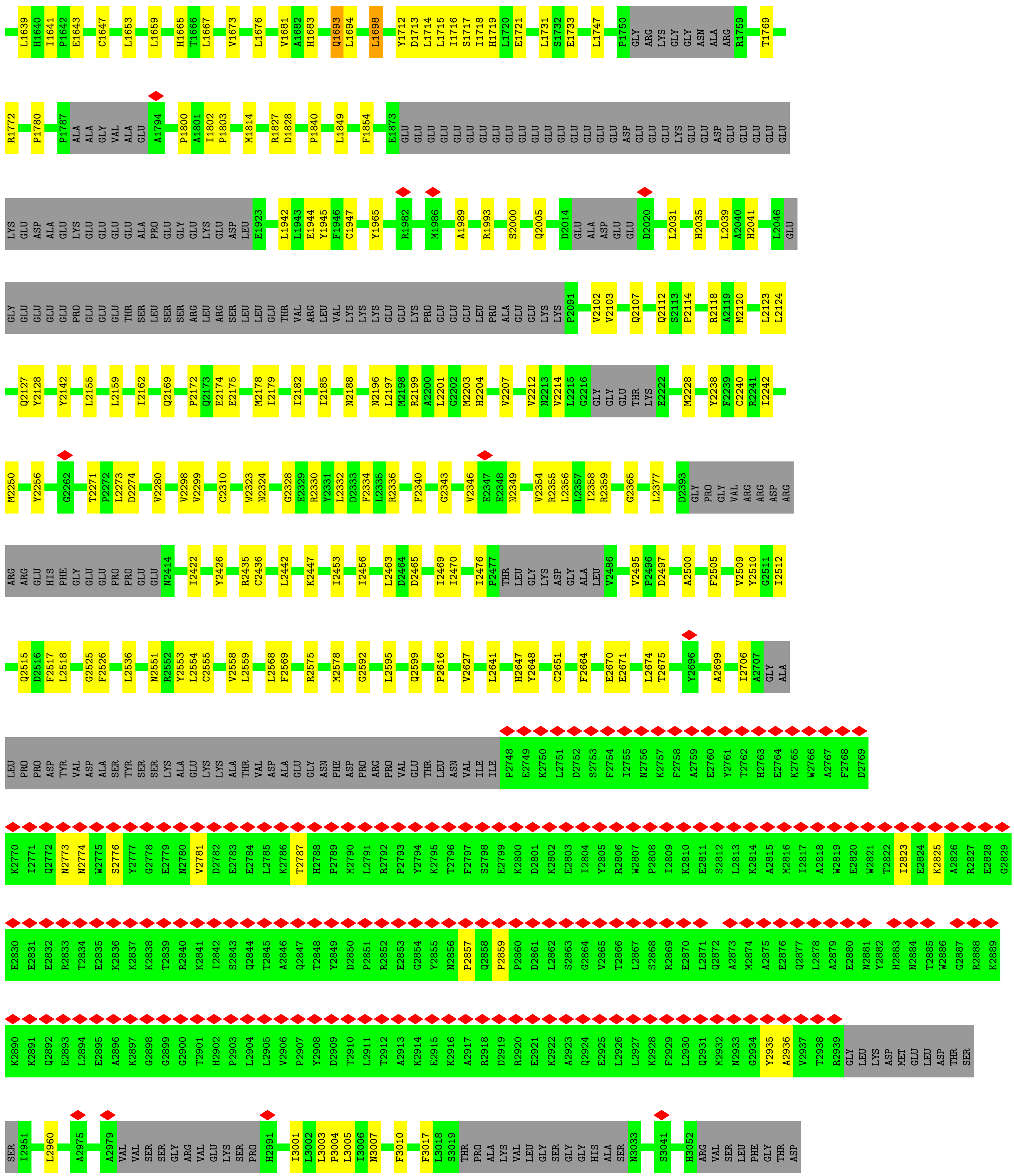
GLU VAL E3750 Q3766 Q3767 S3768 R3769 L3770 H3771 V3779 M3782 G3788 A3792 T3797 G3801 I3802 S3803 I3804 L3805 Q3813 M3816 F3829 L3835 N3845 A3846 F3847 N3851 N3860 E3861 D3862 I3866 N3867 R3868 Q3869 N3870 G3871 E3872 A3876 R3886 Q3889 L3890 L3891
C3892 E3893 N3897 D3898 F3899 Q3900 R3904 T3905 I3913 I3916 T3919 Y3934 W3935 I3943 M3955 F3962 N3963 S3964 L3965 T3966 E3967 Y3968 I3969 Q3970 L3980 A3981 W3986 V3995 H3998 M3999 A4004 L4016 L4017 D4018 L4019 M4026 L4027 L4028 L4031 N4034 V4035 V4036
N4037 G4038 M4039 Q4043 M4044 V4055 I4058 L4059 K4060 M4064 K4067 L4068 K4069 D4070 I4071 V4072 G4073 S4074 E4075 A4076 F4077 R4085 G4086 L4087 K4091 K4095 A4096 M4097 D4098 S4099 Q4100 K4101 Q4102 F4103 T4104 G4105 I4108 S4113 A4117 D4118 E4119 M4122 I4123 M4124 F4125 E4126 E4127 F4128
D4138 I4139 N4142 N4149 H4153 V4154 I4170 R4180 I4181 E4182 I4183 M4184 G4185 A4186 R4192 Q4204 K4214 R4215 Q4216 F4217 I4218 F4219 D4220 V4221 E4224 G4225 G4226 E4229 K4230 F4234 V4235 M4245 A4248 E4253 PRO GLU GLY GLU PRO GLU ALA ASP GLU ASP GLU
GLY MET GLY GLU ALA ALA ALA GLU GLU GLY ALA GLU GLU GLY ALA ALA GLU GLY ALA ALA ALA GLY GLY THR VAL ALA ALA ALA GLY ALA THR ALA ARG LEU ALA ALA ALA ALA ALA ARG ALA LEU LEU GLY SER TYR ARG SER LEU ARG ARG ARG VAL ARG ARG LEU ARG ARG LEU T4323 A4324
R4325 E4326 A4327 A4328 T4329 A4330 L4331 A4332 A4333 L4334 L4335 W4336 A4337 V4338 V4339 A4340 R4341 ALA GLY ALA ALA GLY ALA GLY ALA ALA ALA ALA GLY ALA ALA LEU ARG GLY HIS GLU ALA GLY PRO GLU VAL GLU GLY ALA LYS LYS VAL ALA ALA 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 PRO GLY GLY ASP ALA ASP GLY ALA GLY GLU GLU GLY GLU GLY ALA ALA ALA GLU GLY ASP GLY ASP GLU GLU VAL ALA GLY GLY GLU GLY ALA GLY GLY ALA ALA GLU GLY GLY GLU ALA ALA GLU GLU GLY PRO
PHE ARG PRO GLU GLY ALA LEU GLY ASP MET GLY ASP THR THR PRO ALA GLU PRO PRO THR THR GLU GLY SER PRO ILE LEU LYS ARG LYS LEU GLY VAL ASP GLY GLU GLU GLU GLU LEU VAL PRO GLU PRO GLU PRO GLU GLU PRO GLU PRO GLU ALA ASP GLU GLU
ASN GLY GLU LYS GLU GLU VAL PRO GLU ALA PRO PRO GLU LYS LYS ALA PRO PRO SER PRO PRO ALA LYS LYS GLU GLU ALA GLY GLY ALA GLY MET GLU PHE W4541 R4548 L4552 N4553 Y4554 R4557 L4562 L4569 A4570 I4573 N4574 L4577 L4578 F4579 Y4580 K4581 V4582
P4587 GLY GLU ASP ASP MET GLU GLY SER ALA ALA GLY ASP GLY ALA GLY SER GLY GLY GLY SER GLY TRP GLY SER GLY ALA GLY GLU GLU ALA GLU GLY ASP GLU GLU M4626 Y4629 L4632 L4643 H4650 T4651 L4652 V4653 A4654 I4658 Y4661 K4665 V4666
K4672 R4673 L4686 Y4687 I4688 T4689 E4690 Q4691 P4692 G4693 D4694 D4695 W4701 D4702 R4703 L4704 V4705 T4708 S4713 N4714 Y4715 W4716 D4717 I4731 F4732 I4737 D4744 L4745 A4746 S4747 L4748 T4751 A4752 E4755 R4756 LYS PRO ASP PRO PRO PRO GLY LEU LEU T4766 S4770 K4774 Y4775
G4781 V4782 I4783 M4796 L4800 L4801 G4802 H4803 F4807 F4808 F4809 A4810 I4816 A4817 M4818 G4819 V4820 K4821 T4822 L4823 R4824 T4825 L4837 L4843 Y4849 L4850 Y4851 T4852 V4853 Y4863 E4867 D4870 C4876 M4879 C4882 Y4888 R4892 G4895 P4904 E4910
R4913 V4914 I4927 L4928 I4931 I4936 I4960 C4961 G4964 S4965 D4966 Y4967 F4968 D4969 T4970 T4971 P4972 H4973 T4979 L4980 H4983 N4984 L4985 F4991 L4992 I4996 K4997 K4998 D4999 E5000 T5001 E5002 H5003 T5004 V5010 W5019 F5022 D5026 C5027 F5028 Q5031 Y5032 Q5035 L5036 SER

- Molecule 1: Ryanodine receptor 1

Chain A:

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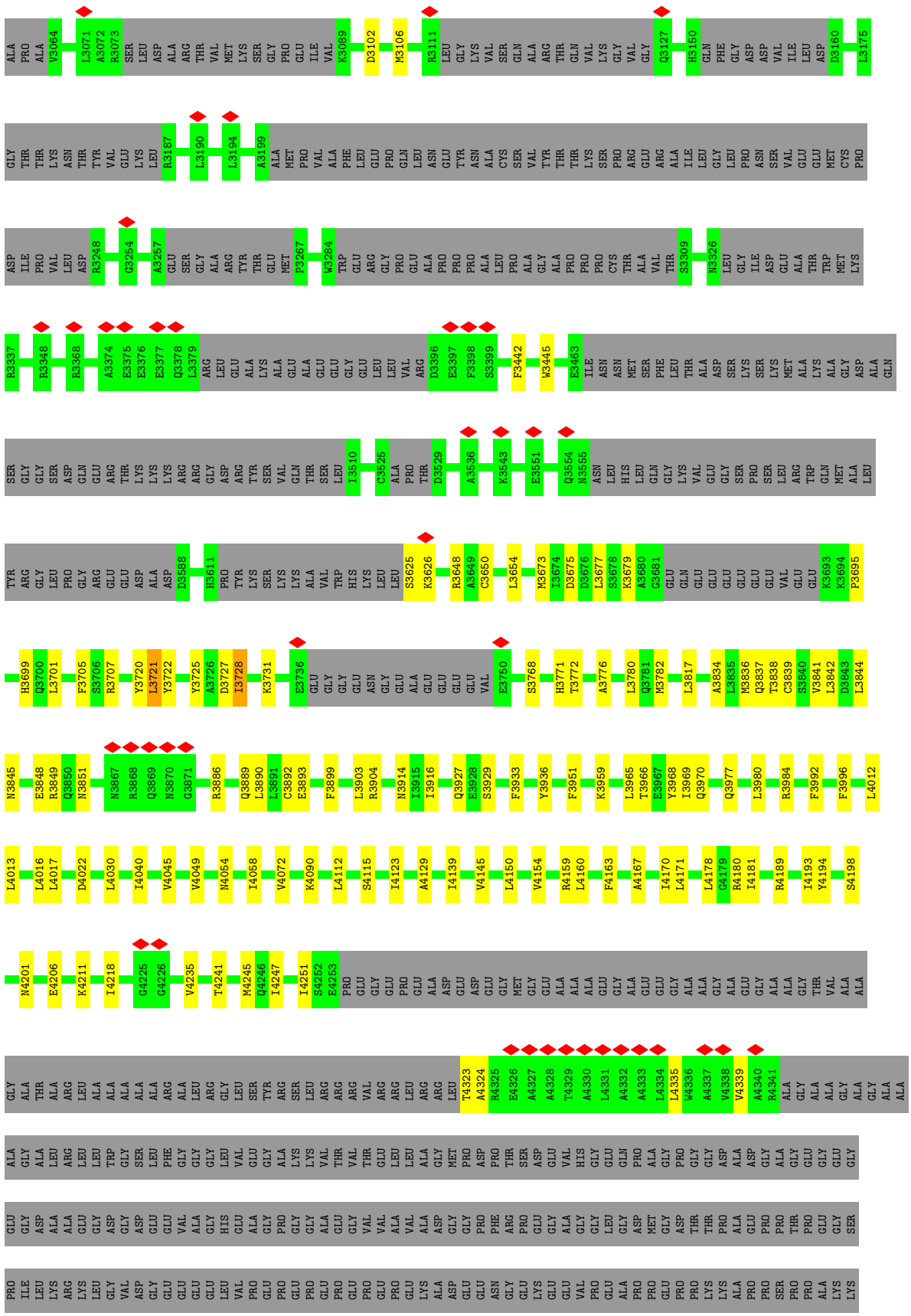
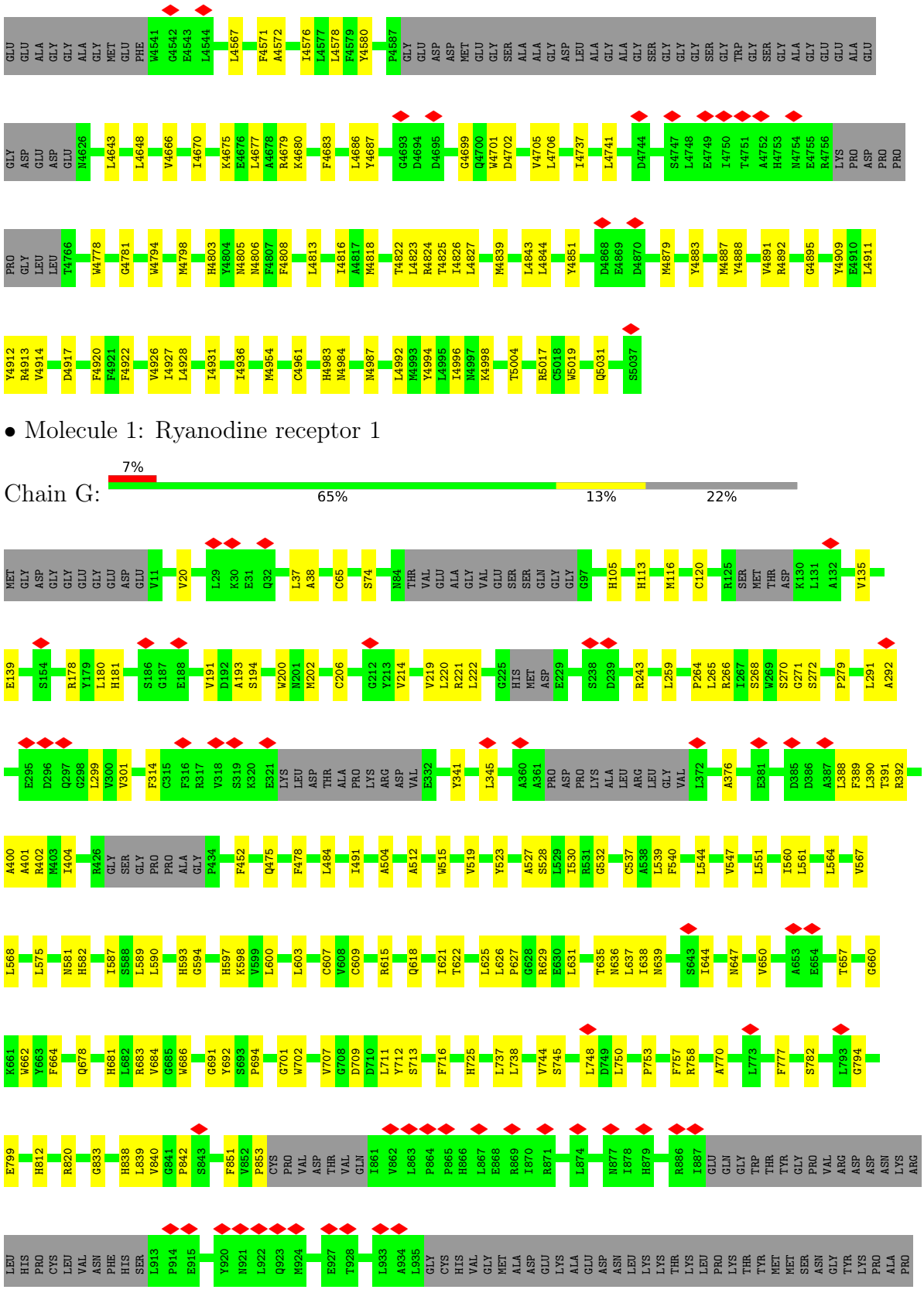
R1772 P1780 P1787 ALA ALA GLY VAL ALA GLU A1794 P1800 A1801 I1802 P1803 M1814 R1827 D1828 P1840 L1849 F1854 E1873 GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU ASP GLU GLU GLU LYS GLU GLU ASP GLU GLU GLU GLU GLU
LYS GLU ASP ALA GLU LYS GLU GLU GLU GLU ALA PRO GLU GLY GLU LYS GLU ASP LEU E1923 L1942 L1943 E1944 Y1945 F1946 C1947 Y1965 R1982 M1986 A1989 R1993 S2000 Q2005 D2014 GLU ALA ASP GLU GLU D2020 L2031 H2035 L2039 A2040 H2041 L2046 GLU
GLY GLU GLU GLU GLU PRO GLU GLU GLU THR SER LEU SER SER ARG LEU ARG SER LEU LEU GLU THR VAL ARG LEU VAL LYS LYS LYS GLU GLU LYS PRO GLU GLU GLU LEU PRO ALA GLU GLU LYS LYS P2091 V2102 V2103 Q2107 Q2112 S2113 P2114 R2118 A2119 M2120 L2123 L2124
Q2127 Y2128 Y2142 L2155 L2159 I2162 Q2169 P2172 Q2173 E2174 E2175 M2178 I2179 I2182 I2185 N2188 N2196 L2197 M2198 R2199 A2200 L2201 G2202 M2203 H2204 V2207 V2212 N2213 V2214 L2215 G2216 GLY GLY GLU THR LYS E2222 M2228 Y2238 F2239 C2240 R2241 I2242
M2250 Y2256 G2262 T2271 P2272 L2273 D2274 V2280 V2298 V2299 C2310 W2323 N2324 G2328 E2329 R2330 Y2331 L2332 D2333 F2334 L2335 R2336 F2340 G2343 V2346 E2347 E2348 N2349 V2354 R2355 L2356 L2357 I2358 R2359 G2365 L2377 D2393 GLY PRO GLY VAL ARG ARG ASP ARG
ARG ARG GLU HIS PHE GLY GLU GLU PRO PRO GLU GLU N2414 I2422 Y2426 R2435 C2436 L2442 K2447 I2453 I2456 L2463 D2464 D2465 I2469 I2470 I2476 P2477 THR LEU GLY LYS ASP GLY ALA LEU V2486 V2495 P2496 D2497 A2500 F2505 V2509 Y2510 G2511 I2512
Q2515 D2516 F2517 L2518 G2525 F2526 L2536 N2551 R2552 Y2553 L2554 C2555 V2558 L2559 L2568 F2569 R2575 M2578 G2592 L2595 Q2599 P2616 V2627 L2641 H2647 Y2648 C2651 F2664 E2670 E2671 L2674 T2675 Y2696 A2699 I2706 A2707 GLY ALA
LEU PRO PRO ASP TYR VAL ASP ALA SER TYR SER SER LYS ALA GLU LYS LYS ALA THR VAL ASP ALA GLU GLY ASN PHE ASP PRO ARG PRO VAL GLU THR LEU ASN VAL ILE ILE P2748 E2749 K2750 L2751 D2752 S2753 F2754 I2755 N2756 K2757 F2758 A2759 E2760 Y2761 T2762 H2763 E2764 K2765 W2766 A2767 F2768 D2769
K2770 I2771 Q2772 N2773 N2774 W2775 S2776 Y2777 G2778 E2779 N2780 V2781 D2782 E2783 E2784 L2785 K2786 T2787 H2788 P2789 M2790 L2791 R2792 P2793 Y2794 K2795 T2796 F2797 S2798 E2799 K2800 D2801 K2802 E2803 I2804 Y2805 R2806 W2807 P2808 I2809 K2810 E2811 S2812 L2813 K2814 A2815 M2816 I2817 A2818 W2819 E2820 W2821 T2822 I2823 E2824 K2825 A2826 R2827 E2828 G2829
E2830 E2831 E2832 R2833 T2834 E2835 K2836 K2837 K2838 T2839 R2840 K2841 I2842 S2843 Q2844 T2845 A2846 Q2847 T2848 Y2849 D2850 P2851 R2852 E2853 G2854 Y2855 N2856 P2857 Q2858 P2859 P2860 D2861 L2862 S2863 G2864 V2865 T2866 L2867 S2868 R2869 E2870 L2871 Q2872 A2873 M2874 A2875 E2876 Q2877 L2878 A2879 E2880 N2881 Y2882 H2883 N2884 T2885 W2886 G2887 R2888 K2889
K2890 K2891 Q2892 E2893 L2894 E2895 A2896 K2897 G2898 G2899 G2900 T2901 H2902 P2903 L2904 L2905 V2906 P2907 Y2908 D2909 T2910 L2911 T2912 A2913 K2914 E2915 K2916 A2917 R2918 D2919 R2920 E2921 K2922 A2923 Q2924 E2925 L2926 L2927 K2928 F2929 L2930 Q2931 M2932 N2933 G2934 Y2935 A2936 V2937 T2938 R2939 GLY LEU LYS ASP MET GLU LEU ASP THR SER
SER I2951 L2960 A2975 A2979 VAL VAL SER SER GLY ARG VAL GLU LYS SER PRO H2991 I3001 L3002 L3003 P3004 L3005 I3006 N3007 F3010 F3017 L3018 S3019 THR PRO ALA LYS VAL LEU GLY SER GLY GLY HIS ALA SER N3033 S3041 H3052 ARG VAL SER LEU PHE GLY THR ASP


ALA PRO ALA V3064 L3071 A3072 R3073 SER LEU ASP ALA ARG THR VAL MET LYS SER GLY PRO GLU ILE VAL K3089 D3102 M3106 R3111 LEU GLY LYS VAL SER GLN ALA ARG THR GLN VAL LYS GLY VAL GLY Q3127 H3150 GLN PHE GLY ASP ASP VAL ILE LEU ASP D3160 L3175
GLY THR THR LYS ASN THR TYR VAL GLU LYS LEU R3187 L3190 L3194 A3199 ALA MET PRO VAL ALA ALA PHE LEU GLU PRO GLN LEU ASN GLU TYR ASN ALA CYS SER VAL TYR THR THR LYS SER PRO ARG GLU ARG ALA ILE LEU GLY LEU PRO ASN SER VAL GLU GLU MET CYS PRO
ASP ILE PRO VAL LEU ASP R3248 G3254 A3257 GLU SER GLY ALA ARG TYR THR GLU MET P3267 W3284 TRP GLU ARG GLY PRO GLU ALA PRO PRO PRO ALA LEU PRO ALA GLY ALA PRO PRO PRO CYS THR ALA VAL THR S3309 N3326 LEU GLY ILE ASP GLU ALA THR TRP MET LYS
R3337 R3348 R3368 A3374 E3375 E3376 E3377 Q3378 L3379 ARG LEU GLU ALA LYS ALA GLU ALA GLU GLU GLY GLU LEU LEU VAL ARG D3396 E3397 F3398 S3399 F3442 W3445 E3463 ILE ASN ASN MET SER PHE LEU THR ALA ASP SER 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 SER VAL GLN THR SER LEU I3510 C3525 ALA PRO THR D3529 A3536 K3543 E3551 Q3554 N3555 ASN LEU HIS LEU GLN GLY LYS VAL GLU GLY SER PRO SER LEU ARG TRP GLN MET ALA LEU
TYR ARG GLY LEU PRO GLY ARG GLU GLU ASP ALA ASP D3588 H3611 PRO TYR LYS SER LYS LYS ALA VAL TRP HIS LYS LEU LEU S3625 K3626 R3648 A3649 C3650 L3654 M3673 I3674 D3675 D3676 L3677 S3678 K3679 A3680 G3681 GLU GLN GLU GLU GLU GLU GLU GLU GLU VAL GLU GLU K3693 K3694 P3695
H3699 Q3700 L3701 F3705 S3706 R3707 Y3720 L3721 Y3722 Y3725 A3726 D3727 I3728 K3731 E3736 GLU GLY GLY GLU ASN GLY GLU ALA GLU GLU GLU GLU VAL E3750 S3768 H3771 T3772 A3776 L3780 Q3781 M3782 L3817 A3834 L3835 M3836 Q3837 T3838 C3839 S3840 V3841 L3842 D3843 L3844
N3845 E3848 R3849 Q3850 N3851 N3867 R3868 Q3869 N3870 G3871 R3886 Q3889 L3890 L3891 C3892 E3893 F3899 L3903 R3904 N3914 I3915 I3916 Q3927 E3928 S3929 F3933 Y3936 F3951 K3959 L3965 T3966 E3967 Y3968 I3969 Q3970 Q3977 L3980 R3984 F3992 F3996 L4012
L4013 L4016 L4017 D4022 L4030 I4040 V4045 V4049 N4054 I4058 V4072 K4090 L4112 S4115 I4123 A4129 I4139 V4145 L4150 V4154 R4159 L4160 F4163 A4167 I4170 L4171 L4178 G4179 R4180 I4181 R4189 I4193 Y4194 S4198
N4201 E4206 K4211 I4218 G4225 G4226 V4235 T4241 M4245 Q4246 I4247 I4251 S4252 E4253 PRO GLU GLY GLU PRO GLU ALA ASP GLU GLU GLU GLY MET GLY GLU ALA ALA ALA GLU GLY ALA GLU GLU GLU GLY ALA GLU GLU GLY ALA ALA ALA GLY ALA GLU GLY ALA ALA ALA GLY THR VAL THR ALA
GLY ALA THR ALA ARG LEU ALA ALA ALA ALA ARG ALA LEU ARG GLY LEU SER TYR ARG SER LEU ARG ARG ARG VAL ARG ARG ARG LEU T4323 A4324 R4325 E4326 A4327 A4328 T4329 A4330 L4331 A4332 A4333 L4334 L4335 W4336 A4337 V4338 V4339 A4340 R4341 ALA GLY ALA ALA GLY ALA GLY ALA ALA
ALA GLY ALA LEU ARG LEU LEU TRP GLY SER LEU PHE GLY GLY GLY LEU VAL GLU GLY ALA LYS LYS VAL THR VAL THR GLU LEU LEU ALA GLY MET PRO ASP PRO THR SER ASP GLU VAL HIS GLY GLU GLN PRO ALA GLY PRO GLY GLY ASP ALA ASP GLY GLU GLU GLY
GLU GLY ASP ALA ALA GLU GLY GLU VAL ASP GLU GLU VAL ALA GLY HIS GLU ALA GLY PRO GLY GLY ALA GLU GLY VAL VAL ALA ALA ASP GLY GLY PRO PHE ARG PRO GLU GLY ALA GLY LEU GLY ASP MET GLY ASP THR THR PRO ALA GLU PRO PRO THR PRO GLU GLU
PRO ILE LEU LYS ARG LYS LEU GLY VAL ASP GLY GLU GLU GLU LEU VAL PRO GLU PRO GLU PRO GLU PRO GLU PRO GLU LYS ALA ASP GLU GLU ASN GLY GLU LYS GLU GLU VAL PRO GLU ALA PRO PRO GLU PRO PRO LYS LYS ALA PRO PRO SER PRO PRO ALA LYS LYS



• Molecule 1: Ryanodine receptor 1

Chain G: 7% 65% 13% 22%

LEU ASP LEU SER HIS VAL ARG LEU THR P979 A980 Q981 R1000 Q1003 G1004 V1010 P1023 K1032 R1036 D1037 S1038 L1039 C1040 Q1041 A1042 V1043 R1044 T1045 L1046 L1047 G1048 Y1049 G1050 Y1051 N1052 I1053 E1054 P1055 PRO ASP GLN GLU PRO SER GLN VAL GLU ASN GLN SER ARG TRP D1070 R1071

V1072 R1073 I1074 F1075 R1076 R1087 E1099 P1111 L1115 V1123 F1124 N1125 G1126 H1127 Q1130 R1131 W1132 F1139 W1143 M1152 I1153 D1154 L1155 N1158 T1159 I1160 T1163 L1164 V1168 S1173 G1174 S1175 A1178 F1179 I1182 E1183 I1184 L1194 V1199 G1200 H1201 F1214

F1223 E1224 P1225 I1228 W1237 P1243 Q1244 F1245 E1246 P1247 R1259 V1264 C1269 L1270 L1287 F1288 L1289 R1290 L1291 F1297 R1302 CYS THR ALA GLY ALA THR PRO LEU ALA PRO PRO GLY LEU GLN PRO PRO ALA GLU ASP GLU ALA ARG ALA ALA GLU PRO ASP PRO ASP

TYR GLU ASN LEU ARG ARG SER ALA GLY GLY TRP GLY GLU ALA GLU GLY GLY LYS GLU GLY THR ALA LYS GLU GLY THR PRO GLY GLY THR PRO GLN PRO GLY VAL GLU ALA GLN PRO VAL ARG ALA GLU ASN GLU LYS ASP ALA THR THR GLU LYS ASN LYS LYS ARG GLY PHE LEU PHE

LYS ALA LYS LYS ALA ALA MET MET THR GLN PRO PRO ALA THR PRO ALA LEU PRO ARG LEU PRO HIS ASP VAL VAL PRO ALA ASP ASN ARG D1422 I1426 T1430 T1431 T1432 Y1433 Y1434 R1438 V1439 F1440 W1449 V1450 G1451 T1454 P1455 D1456 H1460 V1469 R1470 M1476 E1479

Q1480 N1491 C1492 Y1493 M1494 V1501 SER PRO GLY GLN GLN GLY ARG ILE SER H1511 T1512 D1513 L1514 V1515 I1516 G1517 V1520 D1521 L1522 M1527 N1537 P1544 P1550 A1551 V1552 F1553 N1560 Q1563 M1573 P1574 A1578 M1579 F1580 R1584 P1592 P1593 R1594 L1595 E1596 V1597 Q1598

M1599 L1600 V1603 A1620 R1623 V1628 T1635 M1636 M1637 A1638 L1639 H1640 E1643 C1647 L1651 E1652 L1653 D1658 H1663 S1664 H1665 R1671 A1672 V1673 N1678 V1681 S1687 L1698 H1702 L1707 R1708 A1709 G1710 Y1711 Y1712 D1713 L1714 L1715 I1716 S1717 I1718 H1719

E1733 P1750 GLY ARG LYS GLY GLY ASN ALA ARG R1759 H1760 P1763 R1772 F1782 V1783 A1784 P1787 ALA ALA GLY VAL ALA GLU A1794 I1802 P1803 L1804 L1807 L1815 V1830 F1836 Q1837 F1838 V1839 P1840 V1845 L1848 I1853 F1854 V1859 I1862 L1863 I1866

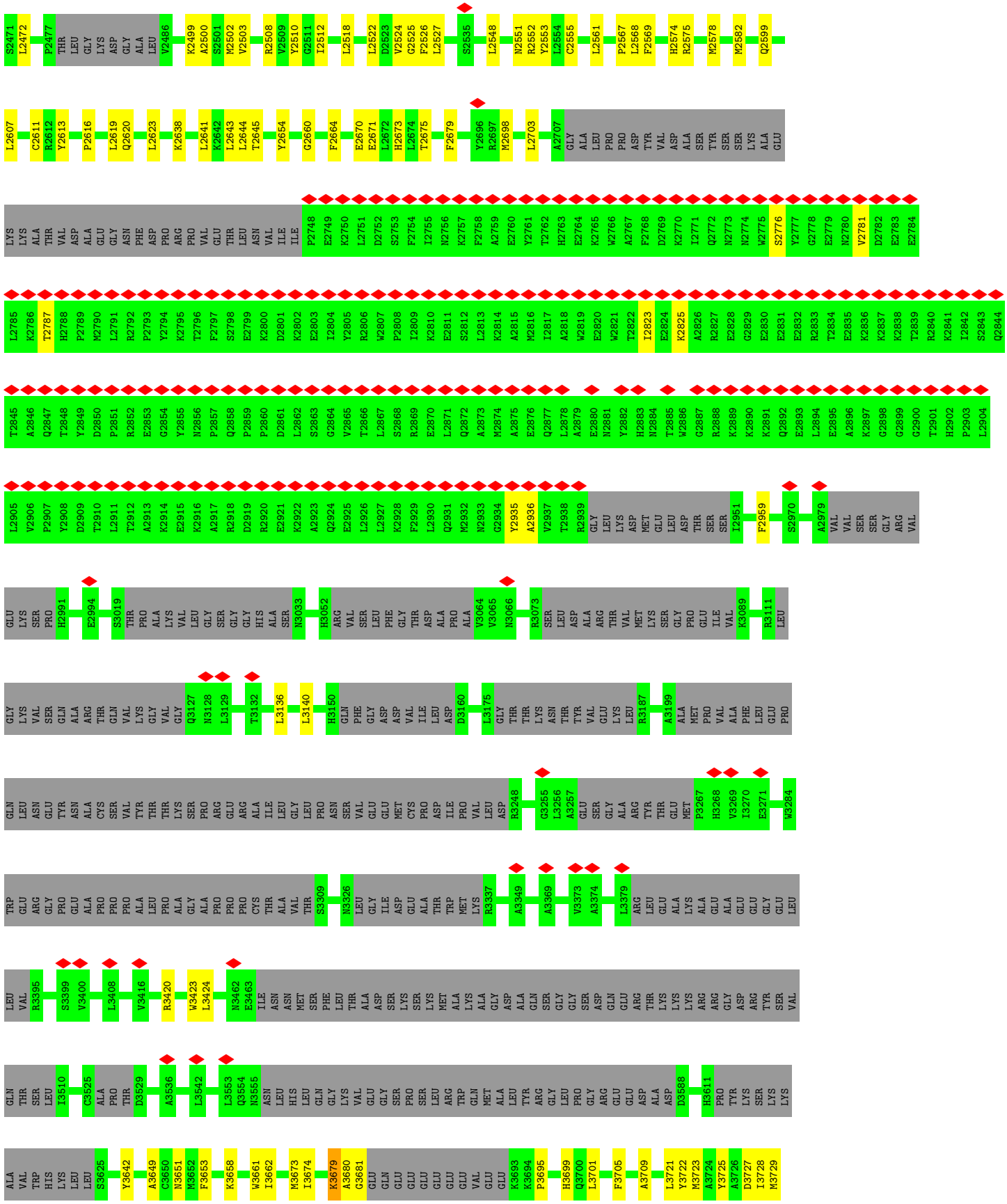
E1873 GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU ASP GLU GLU GLU LYS GLU GLU ASP GLU GLU GLU GLU GLU LYS GLU ASP ALA GLU LYS GLU GLU GLU GLU ALA PRO GLU GLY GLU LYS GLU ASP LEU E1923 E1933 K1936 L1937 Q1938 E1944

C1947 Q1952 Y1965 V1966 L1969 Q1970 R1982 M1986 S1987 P2002 I2006 L2009 L2010 H2011 F2012 K2013 D2014 GLU ALA ASP GLU GLU D2020 L2031 Q2032 Q2036 L2039 A2040 H2041 I2044 Q2045 L2046 GLU GLY GLU GLU GLU GLU PRO GLU GLU GLU THR SER LEU SER SER

ARG LEU ARG SER LEU LEU GLU THR VAL ARG LEU VAL LYS LYS LYS GLU GLU LYS PRO GLU GLU GLU LEU PRO ALA GLU GLU LYS LYS P2091 S2099 V2102 A2119 M2120 F2121 S2122 L2123 L2124 H2125 R2126 Q2127 Y2128 Y2142 L2155 Q2161 L2165 V2168 G2171 P2172 Q2173 E2174

E2175 N2176 L2177 M2178 I2179 I2182 I2185 M2186 K2189 Y2192 Q2193 H2194 P2195 R2199 A2200 L2201 M2211 V2212 N2213 V2214 L2215 G2216 GLY GLY GLU THR LYS E2222 M2228 Y2238 F2239 C2240 R2241 I2242 N2246 M2250 F2251 Y2256 L2257 N2260 L2286 A2287 C2305 G2306 L2307

Y2331 L2332 R2336 V2346 N2349 V2354 I2358 F2364 E2371 G2372 G2373 L2377 D2393 GLY PRO GLY VAL ARG ARG ASP ARG ARG ARG GLU HIS PHE GLY GLU GLU PRO PRO GLU GLU N2414 L2429 I2430 R2435 C2436 E2439 L2463 D2464 D2465 L2466 V2467 G2468 I2469 I2470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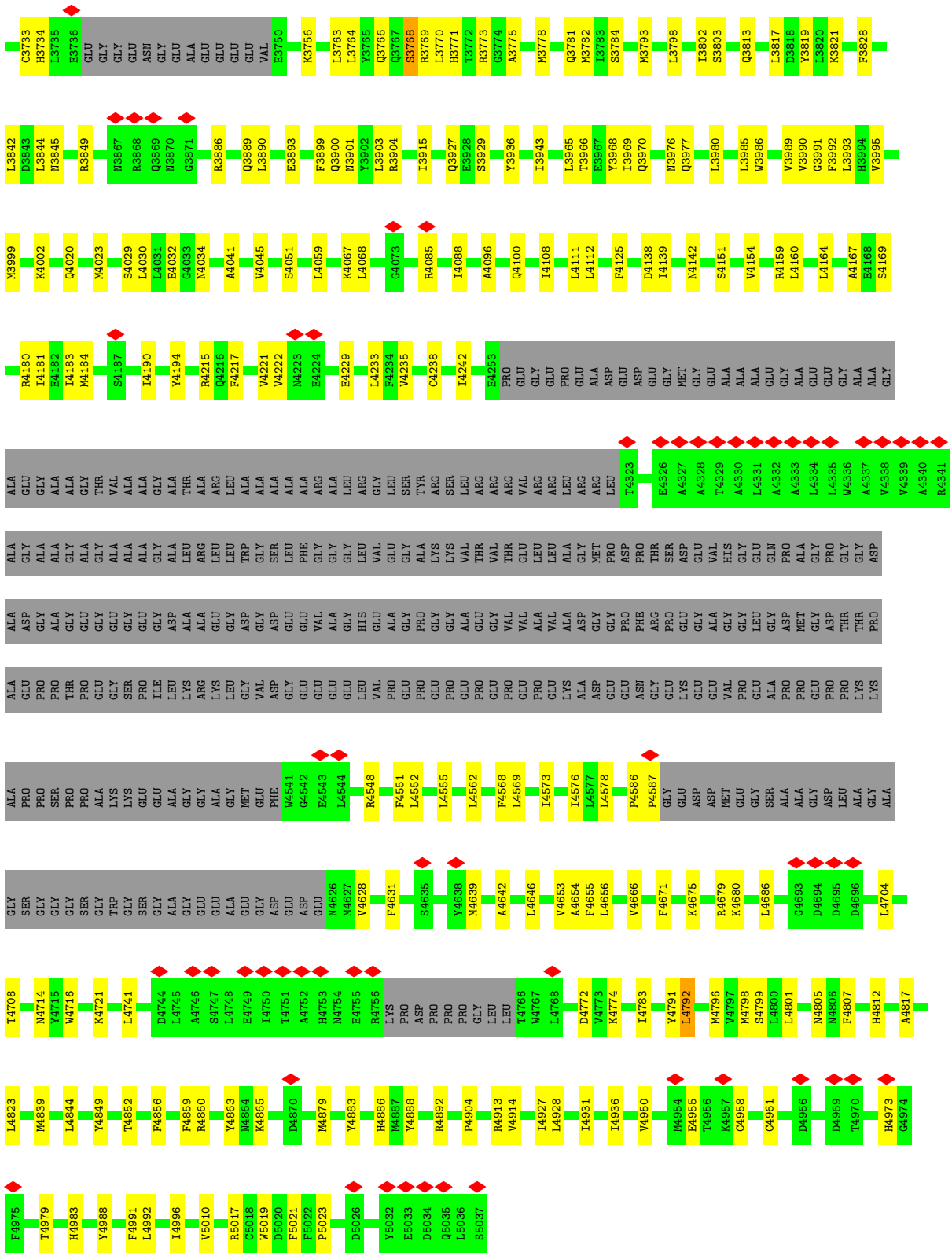
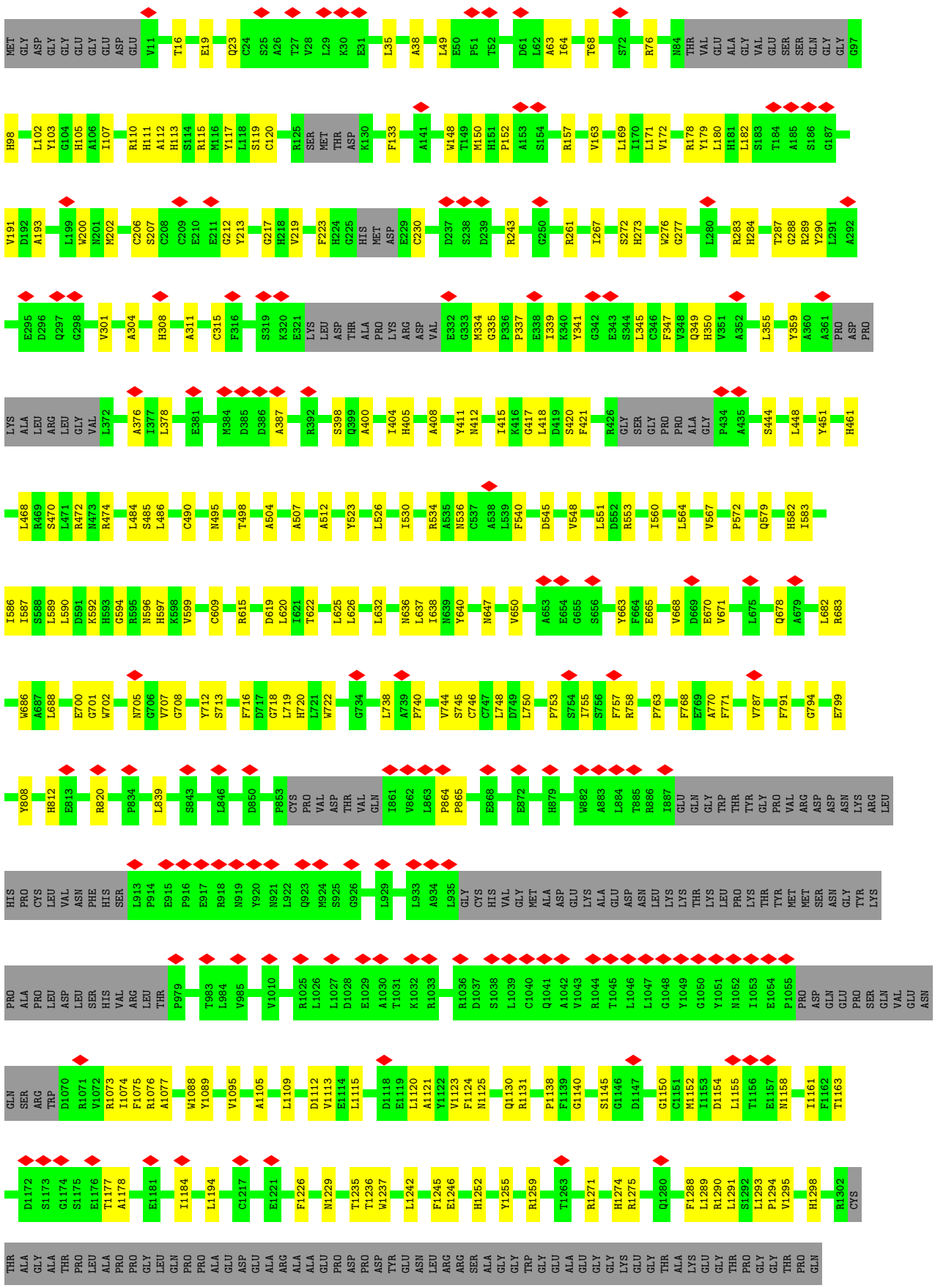
L2607 C2611 R2612 Y2613 P2616 L2619 Q2620 L2623 K2638 L2641 K2642 L2643 L2644 T2645 Y2654 G2660 F2664 E2670 E2671 L2672 H2673 L2674 T2675 F2679 Y2696 R2697 M2698 L2703 A2707 GLY ALA LEU PRO PRO ASP TYR VAL ASP ALA SER TYR SER SER LYS ALA GLU
LYS LYS ALA THR VAL ASP ALA GLU GLY ASN PHE ASP PRO ARG PRO VAL GLU THR LEU ASN VAL ILE ILE P2748 E2749 K2750 L2751 D2752 S2753 F2754 I2755 N2756 K2757 F2758 A2759 E2760 Y2761 T2762 H2763 E2764 K2765 W2766 A2767 F2768 D2769 K2770 I2771 Q2772 N2773 N2774 W2775 S2776 Y2777 G2778 E2779 N2780 V2781 D2782 E2783 E2784
L2785 K2786 T2787 H2788 P2789 M2790 L2791 R2792 P2793 Y2794 K2795 T2796 F2797 S2798 E2799 K2800 D2801 K2802 E2803 I2804 Y2805 R2806 W2807 P2808 I2809 K2810 E2811 S2812 L2813 K2814 A2815 M2816 I2817 A2818 W2819 E2820 W2821 T2822 I2823 E2824 K2825 A2826 R2827 E2828 G2829 E2830 E2831 E2832 R2833 T2834 E2835 K2836 K2837 K2838 T2839 R2840 K2841 I2842 S2843 Q2844
T2845 A2846 Q2847 T2848 Y2849 D2850 P2851 R2852 E2853 G2854 Y2855 N2856 P2857 Q2858 P2859 P2860 D2861 L2862 S2863 G2864 V2865 T2866 L2867 S2868 R2869 E2870 L2871 Q2872 A2873 M2874 A2875 E2876 Q2877 L2878 A2879 E2880 N2881 Y2882 H2883 N2884 T2885 W2886 G2887 R2888 K2889 K2890 K2891 Q2892 E2893 L2894 E2895 A2896 K2897 G2898 G2899 G2900 T2901 H2902 P2903 L2904
L2905 V2906 P2907 Y2908 D2909 T2910 L2911 T2912 A2913 K2914 E2915 K2916 A2917 R2918 D2919 R2920 E2921 K2922 A2923 Q2924 E2925 L2926 L2927 K2928 F2929 L2930 Q2931 M2932 N2933 G2934 Y2935 A2936 V2937 T2938 R2939 GLY LEU LYS ASP MET GLU LEU ASP THR SER SER I2951 F2959 S2970 A2979 VAL VAL SER SER GLY ARG VAL
GLU LYS SER PRO H2991 E2994 S3019 THR PRO ALA LYS VAL LEU GLY SER GLY GLY HIS ALA SER N3033 H3052 ARG VAL SER LEU PHE GLY THR ASP ALA PRO ALA V3064 V3065 N3066 R3073 SER SER LEU ASP ALA ARG THR VAL MET LYS SER GLY PRO GLU ILE VAL K3089 R3111 LEU
GLY LYS VAL SER GLN ALA ARG THR GLN VAL LYS GLY VAL GLY Q3127 N3128 L3129 T3132 L3136 L3140 H3150 GLN PHE GLY ASP ASP VAL ILE LEU ASP D3160 L3175 GLY THR THR LYS ASN THR TYR VAL GLU LYS LEU R3187 A3199 ALA MET PRO VAL ALA PHE LEU GLU PRO
GLN LEU ASN GLU TYR ASN ALA CYS SER VAL TYR THR THR LYS SER PRO ARG GLU ARG ALA ILE LEU GLY LEU PRO ASN SER VAL GLU GLU MET CYS PRO ASP ILE PRO VAL LEU ASP R3248 G3255 L3256 A3257 GLU SER GLY ALA ARG TYR THR GLU MET P3267 H3268 V3269 I3270 E3271 W3284
TRP GLU ARG GLY PRO GLU ALA PRO PRO PRO ALA LEU PRO ALA GLY ALA PRO PRO PRO CYS THR ALA VAL THR S3309 N3326 LEU GLY ILE ASP GLU ALA THR TRP MET LYS R3337 A3349 A3369 V3373 A3374 L3379 ARG LEU GLU ALA LYS ALA GLU ALA GLU GLU GLY GLU LEU
LEU VAL R3395 S3399 V3400 L3408 V3416 R3420 W3423 L3424 N3462 E3463 ILE ASN ASN MET SER PHE LEU THR ALA ASP SER 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 SER VAL
GLN THR SER LEU I3510 C3525 ALA PRO THR D3529 A3536 L3542 L3553 Q3554 N3555 ASN LEU HIS LEU GLN GLY LYS VAL GLU GLY SER PRO SER LEU ARG TRP GLN MET ALA LEU TYR ARG GLY LEU PRO GLY ARG GLU GLU ASP ALA ASP D3588 H3611 PRO TYR LYS SER LYS LYS
ALA VAL TRP HIS LYS LEU LEU S3625 Y3642 A3649 C3650 N3651 M3652 F3653 K3658 W3661 I3662 M3673 I3674 K3679 A3680 G3681 GLU GLN GLU GLU GLU GLU GLU GLU GLU VAL GLU GLU K3693 K3694 P3695 H3699 Q3700 L3701 F3705 A3709 L3721 Y3722 M3723 A3724 Y3725 A3726 D3727 I3728 M3729



- Molecule 1: Ryanodine receptor 1

Chain J: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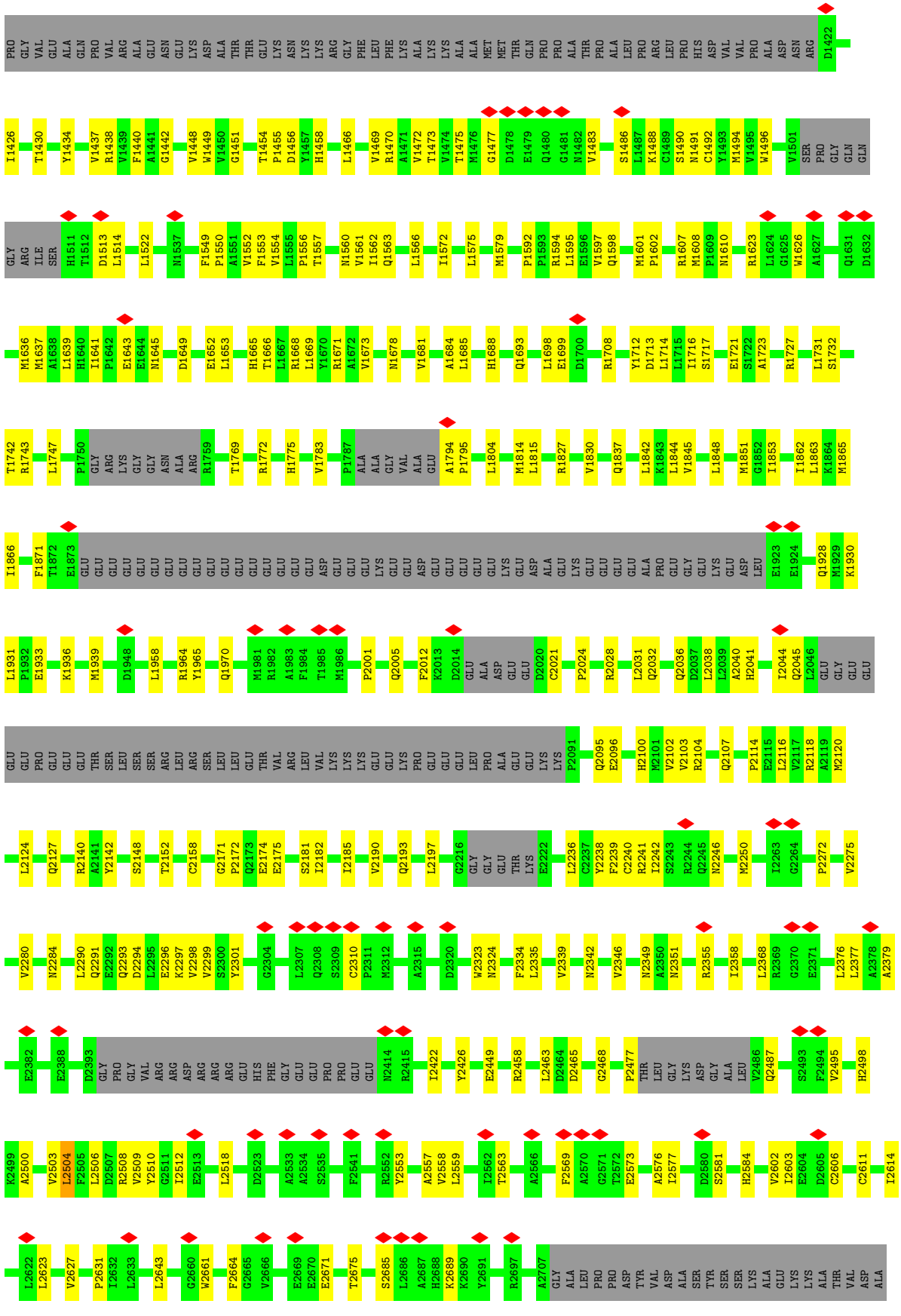
H98 L102 Y103 G104 H105 A106 I107 R110 H111 A112 H113 S114 R115 M116 Y117 L118 S119 C120 R125 SER MET THR ASP K130 F133 A141 W148 T149 M150 H151 P152 A153 S154 R157 V163 L169 I170 L171 V172 R178 Y179 L180 H181 L182 S183 T184 A185 S186 G187
V191 D192 A193 L199 W200 N201 M202 C206 S207 C208 C209 E210 E211 G212 Y213 G217 H218 V219 F223 H224 G225 HIS MET ASP E229 C230 D237 S238 D239 R243 G250 R261 I267 S272 H273 W276 G277 L280 R283 H284 T287 G288 R289 Y290 L291 A292
E295 D296 Q297 G298 V301 A304 H308 A311 C315 F316 S319 K320 E321 LYS LEU ASP THR ALA PRO LYS ARG ASP VAL E332 G333 M334 G335 P336 P337 E338 I339 K340 Y341 G342 E343 S344 L345 C346 F347 V348 Q349 H350 V351 A352 L355 Y359 A360 A361 PRO ASP PRO
LYS ALA LEU ARG LEU GLY VAL L372 A376 I377 L378 E381 M384 D385 D386 A387 R392 S398 Q399 A400 I404 H405 A408 Y411 N412 I415 K416 G417 L418 D419 S420 F421 R426 GLY SER GLY PRO PRO ALA GLY P434 A435 S444 L448 Y451 H461
L468 R469 S470 L471 R472 N473 R474 L484 S485 L486 C490 N495 T498 A504 A507 A512 Y523 L526 I530 R534 A535 N536 C537 A538 L539 F540 D545 V548 L551 D552 R553 I560 L564 V567 P572 Q579 H582 I583
I586 I587 S588 L589 L590 D591 K592 H593 G594 R595 N596 H597 K598 V599 C609 R615 D619 L620 I621 T622 L625 L626 L632 N636 L637 I638 N639 Y640 N647 V650 A653 E654 G655 S656 Y663 F664 E665 V668 D669 E670 V671 L675 Q678 A679 L682 R683
W686 A687 L688 E700 G701 W702 N705 G706 V707 G708 Y712 S713 F716 D717 G718 L719 H720 L721 W722 G734 L738 A739 P740 V744 S745 C746 C747 L748 D749 L750 P753 S754 I755 S756 F757 R758 P763 F768 E769 A770 F771 V787 F791 G794 E799
Y808 H812 E813 R820 P834 L839 S843 L846 D850 P853 CYS PRO VAL ASP THR VAL GLN I861 V862 L863 P864 P865 E868 E872 H879 W882 A883 L884 T885 R886 I887 GLU GLN GLY TRP TYR GLY PRO VAL ARG ASP ASP ASN LYS ARG LEU
HIS PRO CYS LEU VAL ASN PHE HIS SER L913 P914 E915 P916 E917 R918 N919 Y920 N921 L922 Q923 M924 S925 G926 L929 L933 A934 L935 GLY CYS HIS VAL GLY MET ALA ASP GLU LYS ALA GLU ASP ASN LEU LYS LYS THR LYS LEU PRO LYS THR TYR MET MET SER ASN GLY TYR LYS
PRO ALA PRO LEU ASP LEU SER HIS VAL ARG LEU THR P979 T983 L984 V985 V1010 R1025 L1026 L1027 D1028 E1029 A1030 T1031 K1032 R1033 R1036 D1037 S1038 L1039 C1040 Q1041 A1042 V1043 R1044 T1045 L1046 L1047 G1048 Y1049 G1050 Y1051 N1052 I1053 E1054 P1055 PRO ASP GLN GLU PRO SER GLN VAL GLU ASN
GLN SER ARG TRP D1070 R1071 V1072 R1073 I1074 F1075 R1076 A1077 W1088 Y1089 V1095 A1105 L1109 D1112 V1113 E1114 L1115 D1118 E1119 L1120 A1121 Y1122 V1123 F1124 N1125 Q1130 R1131 P1138 F1139 G1140 S1145 G1146 D1147 G1150 C1151 M1152 I1153 D1154 L1155 T1156 E1157 N1158 I1161 F1162 T1163
D1172 S1173 G1174 S1175 E1176 T1177 A1178 E1181 I1184 L1194 C1217 E1221 F1226 N1229 T1235 T1236 W1237 L1242 F1245 E1246 H1252 Y1255 R1259 T1263 R1271 H1274 R1275 Q1280 F1288 L1289 R1290 L1291 S1292 L1293 P1294 V1295 H1298 R1302 CYS
THR ALA GLY ALA THR PRO LEU ALA PRO PRO GLY LEU GLN PRO PRO ALA GLU ASP GLU ALA ARG ALA ALA GLU PRO ASP PRO ASP TYR GLU ASN LEU ARG ARG SER ALA GLY GLY TRP GLY GLU ALA GLU GLY GLY LYS GLU GLY THR ALA LYS GLU GLY THR PRO GLY GLY THR PRO GLN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I1426 T1430 Y1434 V1437 R1438 V1439 F1440 A1441 G1442 V1448 W1449 V1450 G1451 T1454 P1455 D1456 Y1457 H1458 L1466 V1469 R1470 A1471 V1472 T1473 V1474 T1475 M1476 G1477 D1478 E1479 Q1480 G1481 N1482 V1483 S1486 L1487 K1488 C1489 S1490 N1491 C1492 Y1493 M1494 V1495 W1496 V1501 SER PRO GLY GLN GLN
GLY ARG ILE SER H1511 T1512 D1513 L1514 L1522 M1537 F1549 P1550 A1551 V1552 F1553 V1554 L1555 P1556 T1557 N1560 V1561 I1562 Q1563 L1566 I1572 L1575 M1579 P1592 P1593 R1594 L1595 E1596 V1597 Q1598 M1601 P1602 R1607 M1608 P1609 N1610 R1623 L1624 G1625 W1626 A1627 Q1631 D1632
M1636 M1637 A1638 L1639 H1640 I1641 P1642 E1643 E1644 N1645 D1649 E1652 L1653 H1665 T1666 L1667 R1668 L1669 Y1670 R1671 A1672 V1673 N1678 V1681 A1684 L1685 H1688 Q1693 L1698 E1699 D1700 R1708 Y1712 D1713 L1714 L1715 I1716 S1717 E1721 S1722 A1723 R1727 L1731 S1732
T1742 R1743 L1747 P1750 GLY ARG LYS GLY GLY ASN ALA ARG R1759 T1769 R1772 H1775 V1783 P1787 ALA ALA GLY VAL ALA GLU A1794 P1795 L1804 M1814 L1815 R1827 V1830 Q1837 L1842 K1843 L1844 V1845 L1848 M1851 G1852 I1853 I1862 L1863 K1864 M1865
I1866 F1871 T1872 E1873 GLU GLU GLU

GLU GLY ASN PHE ASP PRO ARG PRO VAL GLU THR LEU ASN VAL ILE ILE P2748 E2749 K2750 L2751 D2752 S2753 F2754 I2755 N2756 K2757 F2758 A2759 E2760 Y2761 T2762 H2763 E2764 K2765 W2766 A2767 F2768 D2769 K2770 I2771 Q2772 N2773 N2774 W2775 S2776 Y2777 G2778 E2779 N2780 V2781 D2782 E2783 E2784 L2785 K2786 T2787 H2788 P2789 M2790 L2791

R2792 P2793 Y2794 K2795 T2796 F2797 S2798 E2799 K2800 D2801 K2802 E2803 I2804 Y2805 R2806 W2807 P2808 I2809 K2810 E2811 S2812 L2813 K2814 A2815 M2816 I2817 A2818 W2819 E2820 W2821 T2822 I2823 E2824 K2825 A2826 R2827 E2828 G2829 E2830 E2831 E2832 R2833 T2834 E2835 K2836 K2837 K2838 T2839 R2840 K2841 I2842 S2843 Q2844 T2845 A2846 Q2847 T2848 Y2849 D2850 P2851

R2852 E2853 G2854 Y2855 N2856 P2857 Q2858 P2859 P2860 D2861 L2862 S2863 G2864 V2865 T2866 L2867 S2868 R2869 E2870 L2871 Q2872 A2873 M2874 A2875 E2876 Q2877 L2878 A2879 E2880 N2881 Y2882 H2883 N2884 T2885 W2886 G2887 R2888 K2889 K2890 K2891 Q2892 E2893 L2894 E2895 A2896 K2897 G2898 G2899 G2900 T2901 H2902 P2903 L2904 L2905 V2906 P2907 Y2908 D2909 T2910 L2911

T2912 A2913 K2914 E2915 K2916 A2917 R2918 D2919 R2920 E2921 K2922 A2923 Q2924 E2925 L2926 L2927 K2928 F2929 L2930 Q2931 M2932 N2933 G2934 Y2935 A2936 V2937 T2938 R2939 GLY LEU LYS ASP MET GLU LEU ASP THR SER SER I2951 E2952 K2953 W2966 S2970 Q2971 E2972 F2973 A2979 VAL VAL SER SER GLY ARG VAL GLU LYS

SER PRO H2991 E2992 Q2993 E2994 I3001 L3002 L3003 P3004 N3007 F3010 S3019 THR PRO ALA LYS VAL LEU GLY SER GLY GLY HIS ALA SER N3033 K3034 E3035 I3039 H3052 ARG VAL SER LEU PHE GLY THR ASP ALA PRO ALA V3064 V3065 N3066 R3073 SER LEU ASP ALA ARG THR VAL

MET LYS SER GLY PRO GLU ILE VAL K3089 L3092 F3095 E3101 D3102 K3105 M3106 R3111 LEU GLY LYS VAL SER GLN ALA ARG THR GLN VAL LYS GLY VAL GLY Q3127 N3128 L3129 T3130 Y3131 T3132 T3133 V3134 L3137 H3150 GLN PHE GLY ASP ASP VAL ILE LEU ASP D3160 Y3173

S3174 L3175 GLY THR THR LYS ASN THR TYR VAL GLU LYS LEU R3187 L3190 A3199 ALA MET PRO VAL ALA PHE LEU GLU PRO GLN LEU ASN GLU TYR ASN ALA CYS SER VAL TYR THR THR LYS SER PRO ARG GLU ARG ALA ILE LEU GLY LEU PRO ASN SER VAL GLU GLU MET CYS PRO

ASP ILE PRO VAL LEU ASP R3248 A3257 GLU SER GLY ALA ARG TYR THR GLU MET P3267 M3276 W3284 TRP GLU ARG GLY PRO GLU ALA PRO PRO PRO ALA LEU PRO ALA GLY ALA PRO PRO PRO CYS THR ALA VAL THR S3309 M3326 LEU GLY ILE ASP GLU ALA THR TRP MET LYS

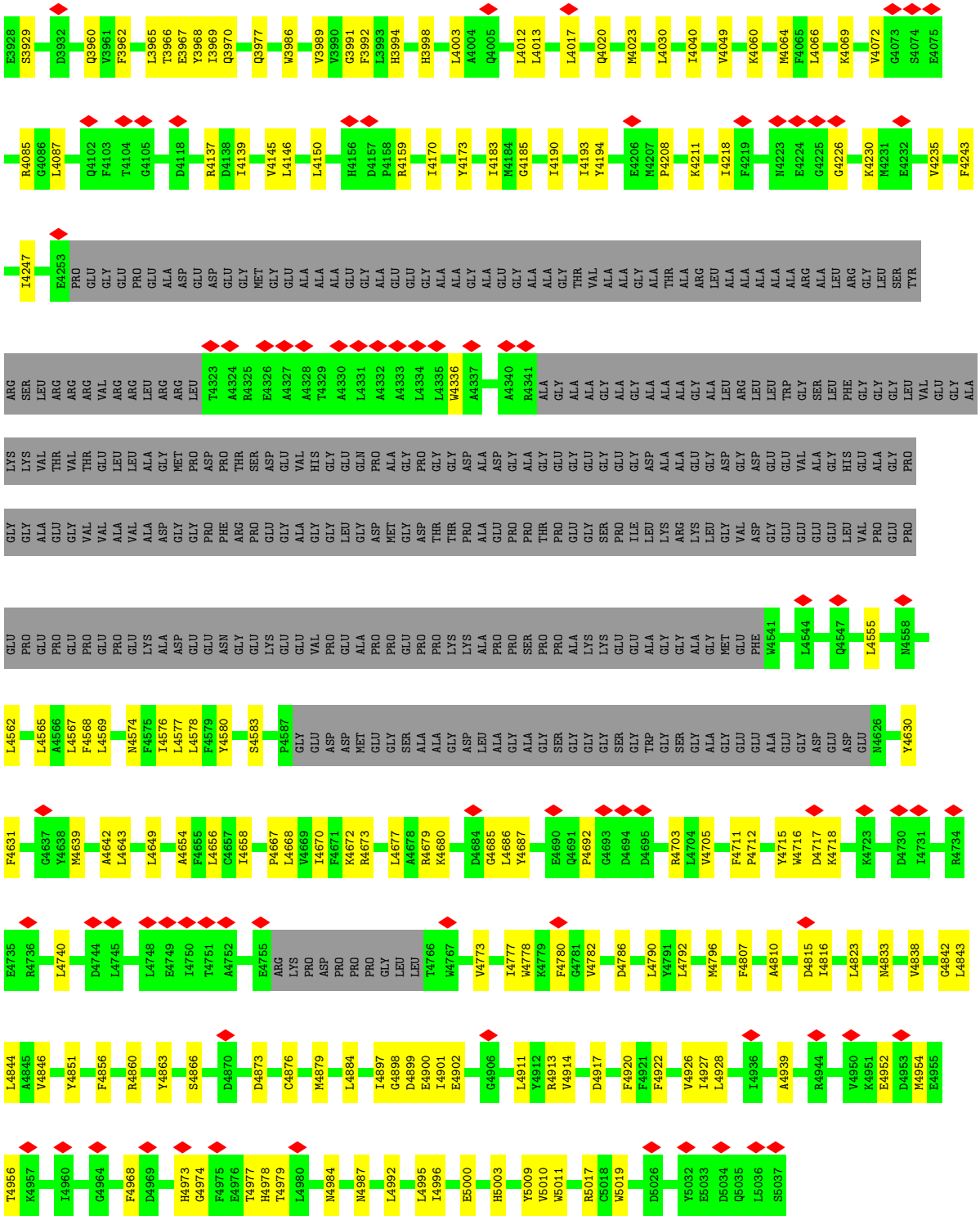
R3337 Q3343 P3344 A3349 R3350 P3351 E3375 E3376 E3377 Q3378 L3379 ARG LEU GLU ALA LYS ALA GLU ALA GLU GLU GLY GLU LEU LEU VAL R3395 D3396 S3399 R3403 L3412 W3423 W3445 F3451 K3452 Q3461 N3462 E3463 ILE ASN ASN MET SER PHE LEU THR ALA ASP SER LYS

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 SER VAL GLN THR SER LEU I3510 V3511 A3512 C3525 ALA PRO THR D3529 A3536 R3539 K3543 E3551 F3552 L3553 Q3554 N3555 ASN LEU HIS LEU GLN

GLY LYS VAL GLU GLY SER PRO SER LEU ARG TRP GLN MET ALA LEU TYR ARG GLY LEU PRO GLY ARG GLU GLU ASP ALA ASP D3588 P3589 E3590 K3591 H3611 PRO TYR LYS SER LYS LYS ALA VAL TRP HIS LYS LEU LEU S3625 V3633 M3638 Y3642 C3650 L3654 K3658

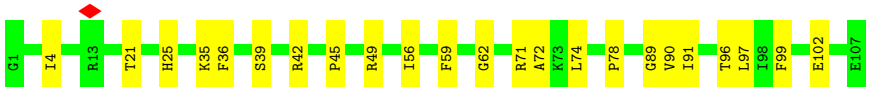
I3662 H3667 E3670 I3674 S3678 G3681 GLU GLN GLU GLU GLU GLU GLU GLU VAL GLU GLU K3693 R3707 L3716 L3721 Y3722 M3723 A3724 Y3725 A3726 D3727 I3728 H3734 L3735 E3736 GLU GLY GLY GLU ASN GLY GLU ALA GLU GLU GLU VAL E3750 V3751 M3758 S3768

H3771 T3772 R3773 G3774 A3775 A3776 E3777 M3778 V3779 L3780 Q3781 A3785 L3805 L3820 K3821 F3829 L3842 N3851 K3852 A3853 L3856 D3862 N3867 R3868 Q3869 N3870 M3875 Q3882 Q3889 L3890 E3893 F3899 Y3902 L3903 R3904 T3905 Q3906 T3907 T3910 T3911 L3923 Q3927



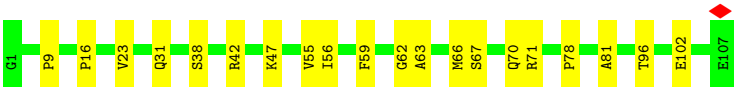
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain E:



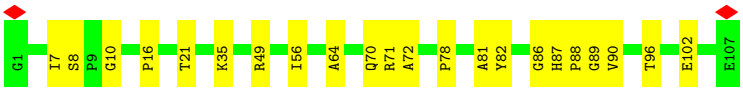
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain B:



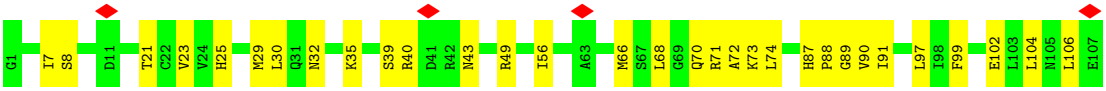
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H:



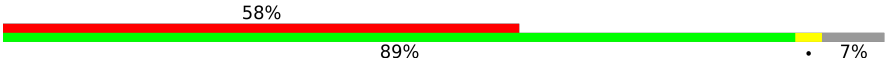
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

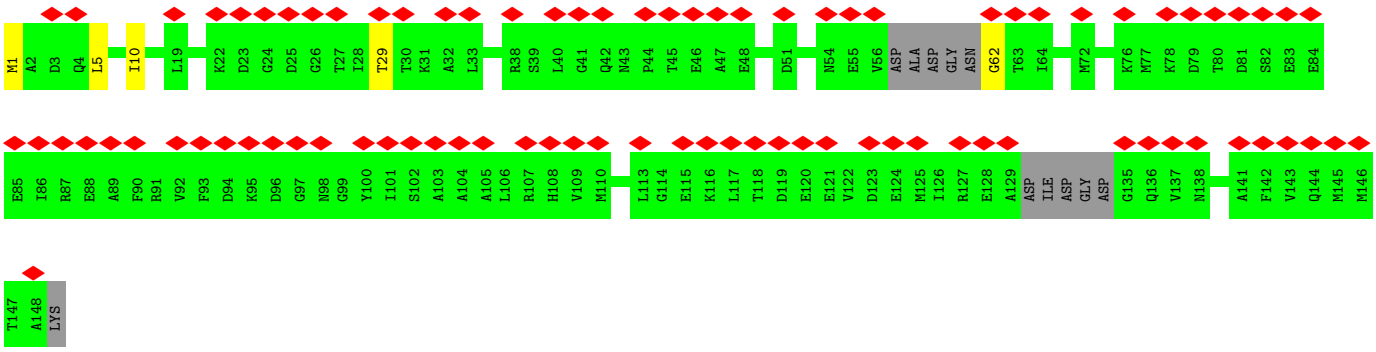
Chain K:



- Molecule 3: Calmodulin-1

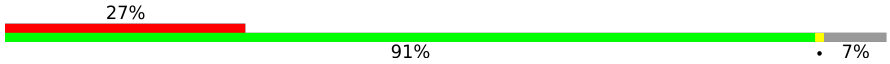
Chain F:

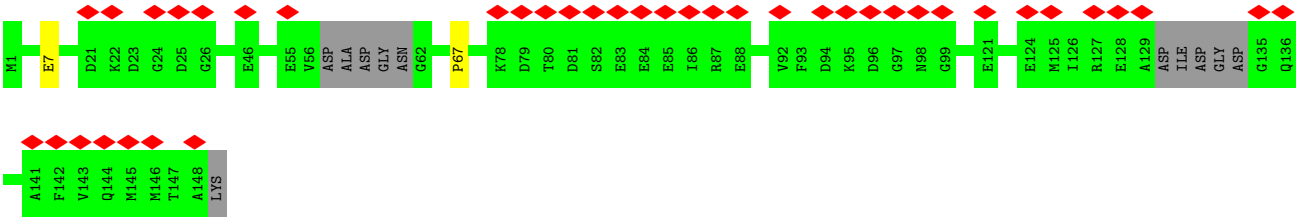




- Molecule 3: Calmodulin-1

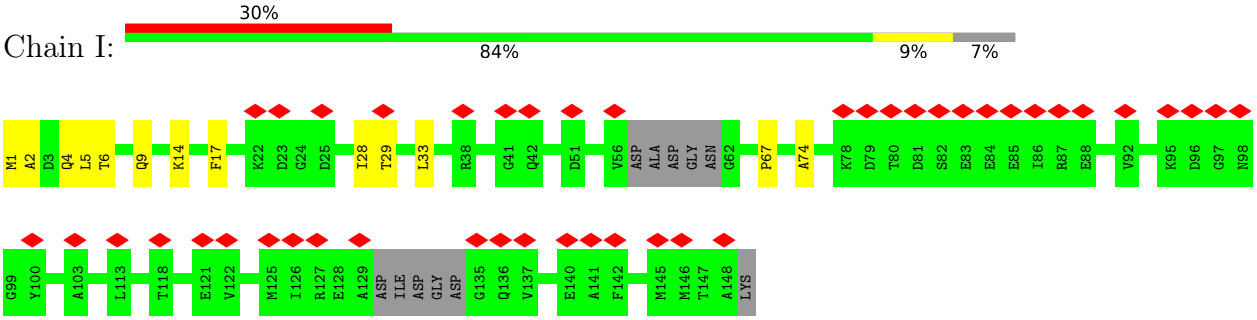
Chain C:





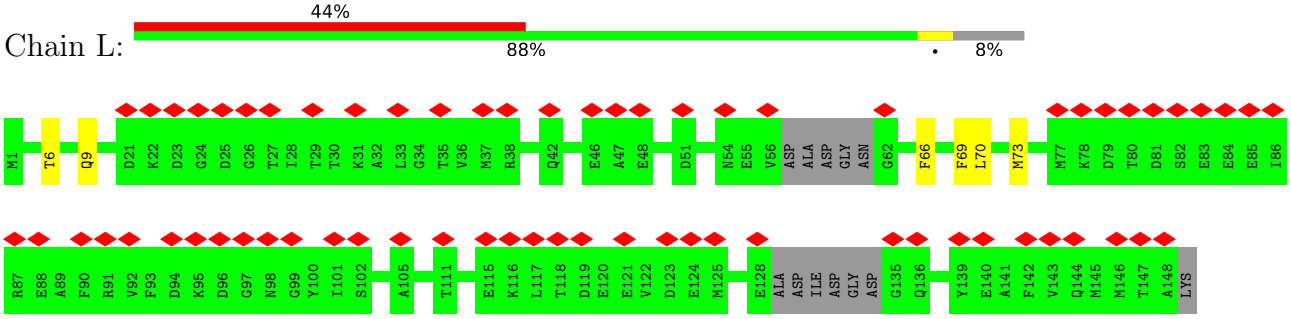
- Molecule 3: Calmodulin-1

Chain I:



- Molecule 3: Calmodulin-1

Chain L:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	41834	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.366	Depositor
Minimum map value	-0.097	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.09	Depositor
Map size (Å)	481.28, 481.28, 481.28	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.94, 0.94, 0.94	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: CA, ZN, ATP, CFF

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.26	0/27849	0.47	0/38070
1	D	0.27	0/27383	0.47	0/37497
1	G	0.26	0/27706	0.47	0/37888
1	J	0.26	0/27526	0.47	0/37679
2	B	0.26	0/758	0.51	0/1032
2	E	0.30	0/758	0.50	0/1033
2	H	0.32	0/761	0.54	0/1036
2	K	0.25	0/744	0.51	0/1018
3	C	0.24	0/720	0.37	0/993
3	F	0.24	0/716	0.37	0/989
3	I	0.24	0/731	0.36	0/1007
3	L	0.24	0/727	0.38	0/1001
All	All	0.26	0/116379	0.47	0/159243

There are no bond length outliers.

There are no bond angle outliers.

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	A	27274	0	23938	406	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	26818	0	23065	467	0
1	G	27137	0	23674	449	0
1	J	26962	0	23301	513	0
2	B	743	0	703	12	0
2	E	743	0	703	17	0
2	H	745	0	694	17	0
2	K	728	0	670	21	0
3	C	720	0	401	2	0
3	F	715	0	391	3	0
3	I	730	0	421	8	0
3	L	726	0	425	3	0
4	A	14	0	10	0	0
4	D	14	0	10	0	0
4	G	14	0	10	1	0
4	J	14	0	10	0	0
5	A	1	0	0	0	0
5	D	1	0	0	0	0
5	G	1	0	0	0	0
5	J	1	0	0	0	0
6	A	31	0	12	0	0
6	D	31	0	12	2	0
6	G	31	0	12	4	0
6	J	31	0	12	2	0
7	A	1	0	0	0	0
7	D	1	0	0	0	0
7	G	1	0	0	0	0
7	J	1	0	0	0	0
All	All	114229	0	98474	1865	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 9.

All (1865) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4577:LEU:HD12	1:D:4580:TYR:HE2	1.12	1.10
1:D:4577:LEU:HD12	1:D:4580:TYR:CE2	1.96	1.00
1:J:4017:LEU:HD12	1:J:4139:ILE:HG21	1.50	0.92
2:H:10:GLY:HA3	2:H:70:GLN:HB2	1.53	0.91
1:D:4577:LEU:CD1	1:D:4580:TYR:HE2	1.85	0.90
1:A:2179:ILE:HD11	1:A:2228:MET:HA	1.54	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:636:ASN:HB3	1:D:702:TRP:HZ2	1.42	0.85
2:E:39:SER:HA	2:E:42:ARG:NH2	1.91	0.85
1:D:2121:PHE:HB3	1:D:3725:TYR:HE2	1.41	0.84
1:G:1712:TYR:HD2	1:G:1840:PRO:HB2	1.43	0.83
1:J:49:LEU:HD11	1:J:191:VAL:HG23	1.61	0.83
1:G:1143:TRP:HB3	1:G:1164:LEU:HD11	1.62	0.82
1:J:103:TYR:CD2	1:J:152:PRO:HB3	2.14	0.82
1:D:1115:LEU:HD21	1:D:1193:SER:HB2	1.61	0.82
1:D:1131:ARG:HB3	1:D:1139:PHE:HE1	1.44	0.82
1:J:2503:VAL:HG21	1:J:2558:VAL:HG12	1.61	0.82
1:A:1440:PHE:HD2	1:A:1560:ASN:HB3	1.45	0.81
1:G:3768:SER:HA	1:G:3771:HIS:CE1	2.16	0.81
1:A:1849:LEU:HD12	1:A:1942:LEU:HD11	1.64	0.80
1:D:2512:ILE:HA	1:D:2517:PHE:HE2	1.45	0.80
1:D:1205:GLY:HA2	1:D:1211:LEU:HD11	1.63	0.80
1:G:3886:ARG:HD2	1:G:3889:GLN:HE21	1.48	0.79
1:D:1651:LEU:HD23	1:D:1702:HIS:HB2	1.64	0.78
1:A:1698:LEU:HA	1:A:1712:TYR:HE1	1.49	0.78
1:J:668:VAL:HG21	1:J:738:LEU:HD21	1.66	0.78
1:J:1743:ARG:HA	1:J:1964:ARG:HH12	1.48	0.77
1:G:3990:VAL:HG23	1:G:4051:SER:HB3	1.66	0.77
1:A:3673:MET:HE3	1:A:3728:ILE:HG21	1.67	0.76
1:G:2670:GLU:HA	1:G:2673:HIS:CE1	2.20	0.76
1:J:594:GLY:HA2	1:J:1594:ARG:HD2	1.68	0.75
1:A:2214:VAL:HG11	1:A:2228:MET:HE1	1.69	0.75
1:J:3969:ILE:HG12	1:J:4030:LEU:HA	1.68	0.75
1:J:63:ALA:HB2	1:J:261:ARG:HH12	1.52	0.74
1:J:2377:LEU:HD21	1:J:2465:ASP:HA	1.68	0.74
1:D:1694:LEU:HB3	1:D:1715:LEU:HD12	1.70	0.74
1:G:2512:ILE:HG21	1:G:2518:LEU:HD12	1.70	0.74
1:A:3817:LEU:HB2	1:A:3899:PHE:HE1	1.53	0.74
1:D:551:LEU:HA	1:D:560:ILE:HG21	1.70	0.73
1:J:2310:CYS:HB2	1:J:2324:ASN:HD22	1.53	0.73
1:J:716:PHE:HD2	1:J:718:GLY:H	1.35	0.73
1:G:2121:PHE:HB3	1:G:3725:TYR:HE2	1.52	0.73
1:G:833:GLY:HA3	1:G:838:HIS:CD2	2.23	0.73
1:J:1289:LEU:HD23	1:J:1597:VAL:HB	1.69	0.73
1:J:2355:ARG:NH1	1:J:2449:GLU:OE2	2.22	0.73
2:H:82:TYR:HB3	2:H:86:GLY:HA2	1.71	0.73
1:G:3817:LEU:HB2	1:G:3899:PHE:HE1	1.51	0.73
1:A:728:ARG:NH2	1:A:1489:CYS:SG	2.62	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1161:ILE:HG13	1:J:1177:THR:HA	1.71	0.72
1:G:3768:SER:HA	1:G:3771:HIS:ND1	2.04	0.72
1:J:682:LEU:HD21	1:J:787:VAL:HG11	1.70	0.72
1:G:1163:THR:HG22	1:G:1168:VAL:HA	1.70	0.72
1:J:4901:ILE:HG21	1:J:4913:ARG:HE	1.55	0.72
1:J:2239:PHE:O	1:J:2246:ASN:ND2	2.23	0.72
1:D:2563:THR:HG23	1:D:2606:CYS:HA	1.71	0.72
1:D:1731:LEU:HD12	1:D:1772:ARG:HH12	1.54	0.72
1:A:411:TYR:HB3	1:A:486:LEU:HD21	1.71	0.72
1:A:1235:THR:HG22	1:A:1610:ASN:HD21	1.53	0.72
1:J:1731:LEU:HG	1:J:1772:ARG:HH22	1.53	0.72
1:D:580:GLU:HA	1:D:620:LEU:HD21	1.72	0.71
1:D:1291:LEU:HD13	1:D:1550:PRO:HB2	1.70	0.71
1:D:1448:VAL:HG22	1:D:1554:VAL:HG23	1.73	0.71
1:G:2781:VAL:HA	1:G:2787:THR:O	1.90	0.71
1:J:708:GLY:HA3	1:J:722:TRP:HB3	1.70	0.71
1:G:4839:MET:HB3	1:J:4823:LEU:HD11	1.71	0.71
1:A:530:ILE:HG22	1:A:536:ASN:HB3	1.72	0.71
1:A:1143:TRP:HB3	1:A:1164:LEU:HD11	1.71	0.71
1:J:1448:VAL:HG22	1:J:1554:VAL:HG23	1.72	0.71
1:D:4215:ARG:NH2	6:D:5103:ATP:O1B	2.23	0.71
1:A:2781:VAL:HA	1:A:2787:THR:O	1.90	0.71
1:A:4911:LEU:HA	1:A:4914:VAL:HG12	1.72	0.71
1:D:4732:PHE:HD2	1:D:4737:ILE:HD11	1.56	0.71
1:G:1969:LEU:HD21	1:G:2009:LEU:HD13	1.73	0.71
1:D:636:ASN:HB3	1:D:702:TRP:CZ2	2.24	0.71
1:G:222:LEU:HD12	1:G:388:LEU:HD13	1.73	0.71
1:A:3969:ILE:HD11	1:A:3980:LEU:HD12	1.70	0.70
1:G:2377:LEU:HA	1:G:2469:ILE:HD11	1.71	0.70
1:D:1115:LEU:HD13	1:D:1123:VAL:HG11	1.73	0.70
1:D:4913:ARG:NH1	1:A:4888:TYR:OH	2.24	0.70
1:A:219:VAL:HG21	1:A:398:SER:HB3	1.71	0.70
1:D:716:PHE:HD2	1:D:718:GLY:H	1.39	0.70
1:A:1673:VAL:HG12	1:A:1681:VAL:HG11	1.73	0.70
1:J:2781:VAL:HA	1:J:2787:THR:O	1.90	0.70
1:G:1430:THR:HG22	1:G:1432:THR:H	1.56	0.70
2:E:78:PRO:HD3	2:E:96:THR:HG22	1.72	0.70
1:A:1161:ILE:HG22	1:A:1177:THR:HA	1.74	0.70
1:D:2271:THR:HG22	1:D:2273:LEU:H	1.56	0.70
1:A:2509:VAL:HG23	1:A:2510:TYR:HD1	1.57	0.69
1:A:2575:ARG:HG3	1:A:2578:MET:HB3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1225:PRO:HG2	1:G:1228:ILE:HB	1.74	0.69
1:A:4913:ARG:NH1	1:A:4917:ASP:OD2	2.26	0.69
1:J:2879:ALA:HB2	1:J:2920:ARG:HA	1.74	0.69
1:J:4677:LEU:HD22	1:J:4711:PHE:CZ	2.27	0.69
1:D:2625:ARG:CB	1:D:2904:LEU:H	2.06	0.69
1:A:14:LEU:HD23	1:A:101:LEU:HD22	1.75	0.69
1:A:2551:ASN:HD21	1:A:2595:LEU:HG	1.57	0.68
1:A:2512:ILE:HD12	1:A:2518:LEU:HD12	1.75	0.68
1:J:2044:ILE:HG13	1:J:3667:HIS:HD2	1.56	0.68
1:D:1269:CYS:SG	1:D:1563:GLN:NE2	2.66	0.68
1:J:720:HIS:HE1	1:J:722:TRP:HE1	1.38	0.68
1:A:3977:GLN:NE2	1:A:4030:LEU:O	2.26	0.68
1:D:1851:MET:HB3	1:D:1853:ILE:HG13	1.76	0.68
1:D:2376:LEU:HD11	1:D:2430:ILE:HD11	1.76	0.68
1:G:220:LEU:HD23	1:G:390:LEU:HB3	1.75	0.68
1:A:2518:LEU:HD13	1:A:2568:LEU:HD23	1.75	0.67
1:D:4577:LEU:CD1	1:D:4580:TYR:CE2	2.69	0.67
1:G:341:TYR:OH	1:G:392:ARG:N	2.26	0.67
1:D:2522:LEU:HA	1:D:2526:PHE:HB2	1.77	0.67
1:A:3970:GLN:HE22	1:A:5004:THR:HG22	1.59	0.67
1:D:113:HIS:NE2	1:D:402:ARG:HB3	2.10	0.67
1:D:4578:LEU:HD12	1:J:4879:MET:HB3	1.75	0.67
1:J:1863:LEU:HD11	1:J:1871:PHE:HD2	1.59	0.67
1:J:794:GLY:HA3	1:J:812:HIS:HB3	1.76	0.67
1:G:701:GLY:HA3	1:G:725:HIS:NE2	2.10	0.67
1:J:1125:ASN:N	1:J:1130:GLN:O	2.28	0.67
1:J:636:ASN:OD1	1:J:1693:GLN:NE2	2.28	0.67
1:G:1698:LEU:HA	1:G:1712:TYR:HE1	1.60	0.67
1:J:451:TYR:CE2	1:J:474:ARG:HD3	2.30	0.67
1:G:1440:PHE:HD2	1:G:1560:ASN:HB3	1.60	0.66
1:J:647:ASN:ND2	1:J:820:ARG:O	2.28	0.66
1:D:3969:ILE:HD11	1:D:3980:LEU:HD22	1.75	0.66
1:A:2124:LEU:HD21	1:A:3677:LEU:HD11	1.77	0.66
1:A:635:THR:HB	1:A:1693:GLN:HE22	1.60	0.66
1:J:551:LEU:HD21	1:J:589:LEU:HB2	1.77	0.66
1:D:670:GLU:HA	1:D:740:PRO:HB3	1.77	0.66
2:B:71:ARG:HG2	2:B:102:GLU:HB3	1.76	0.66
1:G:180:LEU:O	1:G:200:TRP:NE1	2.27	0.66
1:J:716:PHE:HZ	1:J:744:VAL:HG21	1.59	0.66
1:D:438:ILE:HG23	1:D:518:ILE:HD11	1.77	0.66
1:D:1747:LEU:HD21	1:D:2041:HIS:HB2	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3673:MET:CE	1:A:3728:ILE:HG12	2.25	0.66
1:G:833:GLY:HA3	1:G:838:HIS:HD2	1.60	0.65
1:G:3901:ASN:OD1	1:G:3904:ARG:NH2	2.26	0.65
1:A:4737:ILE:HG23	1:A:4741:LEU:HD23	1.78	0.65
1:J:2661:TRP:CD1	1:J:2664:PHE:HD1	2.14	0.65
1:A:4879:MET:HG3	1:G:4578:LEU:HA	1.77	0.65
1:G:1594:ARG:NH2	1:G:1643:GLU:OE2	2.29	0.65
1:G:1578:ALA:HA	1:G:1584:ARG:HH12	1.62	0.65
2:K:30:LEU:HD23	2:K:32:ASN:H	1.61	0.65
1:D:4816:ILE:HG12	1:D:4823:LEU:HG	1.79	0.64
1:J:171:LEU:HB2	1:J:180:LEU:HD23	1.79	0.64
1:D:4027:LEU:HD22	1:D:4044:MET:HE1	1.79	0.64
2:E:25:HIS:CD2	2:E:45:PRO:HA	2.32	0.64
1:J:102:LEU:HB2	1:J:105:HIS:HE1	1.61	0.64
1:J:758:ARG:HG2	1:J:763:PRO:HA	1.79	0.64
1:J:103:TYR:CE1	1:J:163:VAL:HG13	2.32	0.64
1:J:4085:ARG:HE	1:J:4087:LEU:HD12	1.61	0.64
1:A:3904:ARG:O	1:A:3914:ASN:ND2	2.31	0.64
1:G:1160:ILE:HD11	1:G:1182:ILE:HD13	1.77	0.64
1:G:1639:LEU:HD11	1:G:1653:LEU:HD11	1.80	0.64
1:G:4798:MET:HB3	1:G:4812:HIS:NE2	2.12	0.64
1:J:683:ARG:HH21	1:J:708:GLY:H	1.45	0.64
1:D:2358:ILE:HD11	1:D:2460:LEU:HD11	1.79	0.64
1:D:4578:LEU:O	1:J:4879:MET:HB2	1.97	0.64
1:D:2584:HIS:HA	1:D:2903:PRO:CB	2.28	0.64
1:A:1110:ARG:NH2	1:A:1112:ASP:OD2	2.31	0.64
1:J:4208:PRO:HA	1:J:4211:LYS:HB2	1.78	0.64
1:D:4960:ILE:HD11	1:D:4985:LEU:HA	1.79	0.64
1:A:595:ARG:NH1	1:A:631:LEU:O	2.31	0.64
1:G:3813:GLN:HB3	1:G:3899:PHE:CE2	2.32	0.64
1:J:4673:ARG:HD2	1:J:4782:VAL:HG21	1.79	0.64
1:D:4892:ARG:NH1	1:J:4917:ASP:OD2	2.31	0.63
1:G:618:GLN:O	1:G:621:ILE:HG22	1.98	0.63
1:J:638:ILE:HG22	1:J:678:GLN:HE22	1.63	0.63
1:G:3733:CYS:SG	1:G:3803:SER:HB3	2.38	0.63
1:J:579:GLN:H	1:J:582:HIS:HD2	1.43	0.63
1:J:2293:GLN:OE1	1:J:2293:GLN:N	2.30	0.63
1:D:794:GLY:HA2	1:D:812:HIS:HB3	1.78	0.63
1:D:3676:ASP:HA	1:D:3679:LYS:NZ	2.13	0.63
1:G:4067:LYS:NZ	1:G:4169:SER:OG	2.31	0.63
1:D:3892:CYS:SG	1:D:3900:GLN:NE2	2.72	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:2469:ILE:HA	1:G:2472:LEU:HD23	1.79	0.63
1:J:103:TYR:CG	1:J:152:PRO:HB3	2.32	0.63
1:D:2000:SER:O	1:D:2005:GLN:NE2	2.23	0.63
1:D:221:ARG:N	1:D:391:THR:O	2.30	0.63
1:D:4204:GLN:NE2	1:D:4245:MET:O	2.31	0.63
1:A:2470:ILE:HG22	1:A:2525:GLY:HA3	1.81	0.63
1:J:1293:LEU:HD11	1:J:1594:ARG:HG2	1.79	0.63
1:D:232:THR:HG21	1:D:252:VAL:HG11	1.80	0.63
1:D:627:PRO:HD3	2:E:89:GLY:HA2	1.79	0.63
1:D:648:ILE:HD11	1:D:814:ALA:HB3	1.81	0.63
1:A:4909:TYR:HA	1:A:4912:TYR:HD2	1.64	0.63
2:K:25:HIS:NE2	2:K:102:GLU:OE1	2.32	0.63
1:D:4800:LEU:HA	1:D:4803:HIS:HD2	1.64	0.62
1:D:3886:ARG:HD2	1:D:3889:GLN:HE21	1.64	0.62
1:G:3817:LEU:HB2	1:G:3899:PHE:CE1	2.31	0.62
1:G:4961:CYS:HB3	1:G:5023:PRO:HB2	1.80	0.62
1:J:2661:TRP:HD1	1:J:2664:PHE:H	1.47	0.62
1:A:2592:GLY:HA3	1:A:2595:LEU:HD13	1.82	0.62
1:J:2158:CYS:HG	1:J:2181:SER:HG	1.45	0.62
1:J:1150:GLY:N	1:J:1163:THR:O	2.31	0.62
1:D:1139:PHE:HB2	1:D:1171:SER:HA	1.80	0.62
1:A:2495:VAL:HG12	1:A:2497:ASP:H	1.64	0.62
1:G:4238:CYS:O	1:G:4242:ILE:HG12	1.99	0.62
1:D:3676:ASP:HA	1:D:3679:LYS:HZ2	1.63	0.62
1:G:664:PHE:HE1	1:G:686:TRP:HE1	1.45	0.62
1:G:4992:LEU:O	1:G:4996:ILE:HG12	1.99	0.62
1:J:359:TYR:HA	1:J:376:ALA:HA	1.82	0.62
1:J:2158:CYS:SG	1:J:2181:SER:OG	2.53	0.62
1:J:4705:VAL:HG22	1:J:4711:PHE:HD1	1.65	0.62
1:D:341:TYR:OH	1:D:392:ARG:N	2.24	0.62
1:A:2476:ILE:HB	1:A:2536:LEU:HD11	1.81	0.62
1:G:4068:LEU:HD13	1:G:4111:LEU:HD11	1.82	0.62
1:A:1115:LEU:HD13	1:A:1193:SER:HB2	1.82	0.62
1:J:1237:TRP:HH2	1:J:1652:GLU:HG3	1.65	0.62
1:A:3648:ARG:NH2	3:C:7:GLU:OE2	2.33	0.62
1:J:4060:LYS:O	1:J:4064:MET:HG3	1.99	0.62
1:D:4582:VAL:HB	1:J:4856:PHE:HZ	1.63	0.61
1:J:4003:LEU:HD21	1:J:4012:LEU:HD22	1.82	0.61
1:D:1966:VAL:HG21	1:D:3650:CYS:HA	1.80	0.61
1:A:794:GLY:HA3	1:A:812:HIS:HB3	1.82	0.61
1:G:650:VAL:O	1:G:777:PHE:N	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1454:THR:HG23	1:G:1456:ASP:H	1.64	0.61
1:G:1573:MET:SD	1:G:1574:PRO:HD2	2.39	0.61
1:J:670:GLU:HA	1:J:740:PRO:HB3	1.82	0.61
1:A:1573:MET:SD	1:A:1574:PRO:HD2	2.40	0.61
1:J:1668:ARG:HE	1:J:1671:ARG:NH2	1.97	0.61
1:D:1714:LEU:O	1:D:1718:ILE:HG12	2.01	0.61
1:A:1780:PRO:HG2	2:B:42:ARG:HD3	1.81	0.61
1:J:3724:ALA:O	1:J:3728:ILE:HG13	2.00	0.61
1:D:3847:PHE:O	1:D:3851:ASN:ND2	2.33	0.61
1:A:1698:LEU:HD11	1:A:1814:MET:HE1	1.82	0.61
1:A:1431:THR:HG21	1:A:1523:ALA:HB3	1.82	0.61
1:J:2323:TRP:HH2	1:J:2422:ILE:HG13	1.65	0.61
1:D:1673:VAL:HG12	1:D:1681:VAL:HG11	1.83	0.61
1:J:1732:SER:HB2	1:J:2140:ARG:HH11	1.65	0.61
2:K:29:MET:HA	2:K:35:LYS:HA	1.82	0.61
1:A:839:LEU:HB3	1:A:1075:PHE:HE2	1.65	0.61
1:G:2619:LEU:HD23	1:G:2623:LEU:HB2	1.82	0.61
1:J:418:LEU:HA	1:J:421:PHE:CE1	2.34	0.61
1:A:3837:GLN:OE1	1:A:3837:GLN:HA	2.00	0.61
1:G:2574:HIS:CD2	1:G:2575:ARG:HG2	2.35	0.61
1:J:2495:VAL:HB	1:J:2498:HIS:CG	2.36	0.60
1:G:3977:GLN:NE2	1:G:4030:LEU:O	2.34	0.60
1:J:2518:LEU:HD21	1:J:2569:PHE:CE1	2.35	0.60
1:A:2271:THR:HG23	1:A:2274:ASP:H	1.65	0.60
1:J:284:HIS:ND1	1:J:287:THR:OG1	2.33	0.60
1:J:551:LEU:HA	1:J:560:ILE:HG21	1.82	0.60
1:D:21:VAL:HB	1:D:205:ILE:HD11	1.83	0.60
1:D:2776:SER:O	1:D:2787:THR:HA	2.02	0.60
1:J:1928:GLN:HA	1:J:2104:ARG:HH22	1.66	0.60
1:J:4899:ASP:OD1	1:J:4900:GLU:N	2.34	0.60
2:B:78:PRO:HD3	2:B:96:THR:HG22	1.83	0.60
1:J:223:PHE:HD1	1:J:230:CYS:HB3	1.66	0.60
1:D:157:ARG:HH21	1:D:164:ARG:HG3	1.65	0.60
1:D:1431:THR:HG21	1:D:1523:ALA:HB3	1.84	0.60
1:G:292:ALA:HA	1:G:314:PHE:HZ	1.66	0.60
1:G:4817:ALA:HA	1:G:4823:LEU:HB3	1.83	0.60
1:J:587:ILE:HG12	1:J:625:LEU:HD12	1.83	0.60
1:J:1594:ARG:NH2	1:J:1643:GLU:OE2	2.32	0.60
1:D:4991:PHE:HE2	1:D:5010:VAL:HG11	1.67	0.60
1:D:755:ILE:HG13	1:D:771:PHE:CE2	2.37	0.60
1:A:4895:GLY:O	1:G:4892:ARG:NH1	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1470:ARG:HB2	1:G:1491:ASN:HD21	1.67	0.60
2:H:71:ARG:HB3	2:H:102:GLU:HG3	1.82	0.60
1:J:4979:THR:HG21	6:J:5103:ATP:H2'	1.84	0.60
1:D:2778:GLY:O	1:D:2789:PRO:HA	2.01	0.60
1:D:2994:GLU:HA	1:D:2997:PHE:CE1	2.36	0.60
1:A:1115:LEU:HD21	1:A:1123:VAL:HG11	1.84	0.60
1:A:1639:LEU:HD11	1:A:1653:LEU:HD11	1.84	0.60
1:G:345:LEU:HD23	1:G:389:PHE:HB3	1.82	0.60
1:J:111:HIS:CD2	1:J:113:HIS:HB3	2.37	0.60
1:J:2767:ALA:HB3	1:J:2857:PRO:CB	2.32	0.60
1:D:1427:ILE:HD11	1:D:1571:ASN:HA	1.83	0.60
1:J:1742:THR:HG23	1:J:1769:THR:HG21	1.83	0.60
1:A:830:ARG:HE	1:A:837:PRO:HB3	1.67	0.59
1:D:4927:ILE:HG13	1:A:4936:ILE:HG21	1.84	0.59
1:A:495:ASN:HD22	1:A:550:LYS:HD3	1.67	0.59
1:A:1434:TYR:HB3	1:A:1519:LEU:HD23	1.82	0.59
1:G:4576:ILE:HD11	1:G:4639:MET:HG3	1.84	0.59
1:J:619:ASP:OD1	1:J:620:LEU:N	2.35	0.59
1:D:3845:ASN:OD1	1:D:3846:ALA:N	2.34	0.59
1:G:2165:LEU:HD22	1:G:2177:LEU:HD23	1.84	0.59
1:G:4856:PHE:O	1:G:4860:ARG:NH1	2.34	0.59
1:G:1440:PHE:CD2	1:G:1560:ASN:HB3	2.36	0.59
1:J:2581:SER:HA	1:J:2584:HIS:CE1	2.37	0.59
1:J:3007:ASN:HA	1:J:3010:PHE:CE2	2.38	0.59
1:D:4581:LYS:HB2	1:D:4632:LEU:HD23	1.85	0.59
1:A:1440:PHE:CD2	1:A:1560:ASN:HB3	2.34	0.59
1:J:3977:GLN:NE2	1:J:4030:LEU:O	2.36	0.59
1:J:4992:LEU:O	1:J:4996:ILE:HG12	2.03	0.59
1:D:220:LEU:HA	1:D:392:ARG:HA	1.83	0.59
1:G:1733:GLU:HG2	1:G:2201:LEU:HD12	1.85	0.59
1:D:548:VAL:HG11	1:D:582:HIS:HD2	1.68	0.59
1:J:3829:PHE:HE2	1:J:3902:TYR:HE2	1.49	0.59
1:D:2781:VAL:HA	1:D:2787:THR:O	2.01	0.59
1:D:4820:VAL:HB	1:D:4823:LEU:HD23	1.85	0.59
1:A:195:PHE:CZ	1:G:2358:ILE:HD11	2.38	0.59
1:A:4680:LYS:HD2	1:A:4686:LEU:HD22	1.85	0.59
1:J:102:LEU:HB2	1:J:105:HIS:CE1	2.37	0.59
1:J:495:ASN:OD1	1:J:553:ARG:NH1	2.35	0.59
1:J:1936:LYS:HB2	1:J:2116:LEU:HD11	1.84	0.59
1:J:2503:VAL:O	1:J:2506:LEU:HG	2.03	0.59
1:J:4816:ILE:HG22	1:J:4823:LEU:HD22	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1259:ARG:NH2	1:D:1595:LEU:O	2.34	0.59
1:A:1438:ARG:HD3	1:A:1563:GLN:HE21	1.68	0.59
1:G:4562:LEU:HD21	1:G:4656:LEU:HB3	1.85	0.59
1:J:590:LEU:HB2	1:J:599:VAL:HG11	1.85	0.59
1:D:1109:LEU:HA	1:D:1120:LEU:HD13	1.85	0.58
1:D:4138:ASP:O	1:D:4142:ASN:ND2	2.32	0.58
2:E:62:GLY:HA3	2:E:74:LEU:HD11	1.85	0.58
1:J:1804:LEU:HD11	1:J:1853:ILE:HG13	1.84	0.58
1:J:2032:GLN:O	1:J:2036:GLN:HG2	2.03	0.58
1:J:2500:ALA:O	1:J:2503:VAL:HG12	2.02	0.58
1:A:1714:LEU:O	1:A:1718:ILE:HG12	2.03	0.58
1:G:622:THR:HA	1:G:626:LEU:HD13	1.85	0.58
1:J:3842:LEU:O	1:J:3929:SER:OG	2.20	0.58
1:G:2518:LEU:HD22	1:G:2569:PHE:HE1	1.67	0.58
1:J:755:ILE:HB	1:J:768:PHE:HB2	1.86	0.58
1:G:794:GLY:HA3	1:G:812:HIS:HB3	1.84	0.58
1:G:1713:ASP:HA	1:G:1716:ILE:HG22	1.85	0.58
1:G:3965:LEU:HA	1:G:3968:TYR:HD2	1.69	0.58
1:J:2044:ILE:HG13	1:J:3667:HIS:CD2	2.37	0.58
1:D:1433:TYR:CZ	1:D:1578:ALA:HB2	2.38	0.58
2:H:8:SER:HB2	2:H:71:ARG:HG2	1.86	0.58
2:H:21:THR:HA	2:H:49:ARG:HA	1.86	0.58
1:J:415:ILE:HD11	1:J:490:CYS:SG	2.44	0.58
1:J:2296:GLU:HA	1:J:2299:VAL:HG22	1.85	0.58
1:D:1573:MET:SD	1:D:1574:PRO:HD2	2.43	0.58
1:D:2476:ILE:HD12	1:D:2477:PRO:HD2	1.85	0.58
1:A:1477:GLY:HA2	1:A:1484:HIS:H	1.69	0.58
1:A:1747:LEU:HD21	1:A:2041:HIS:HB2	1.85	0.58
1:G:2155:LEU:HD12	1:G:2185:ILE:HD11	1.83	0.58
2:B:31:GLN:NE2	2:B:96:THR:OG1	2.28	0.58
1:G:1804:LEU:HD11	1:G:1853:ILE:HG13	1.86	0.58
1:G:4799:SER:HB2	1:G:4812:HIS:HE1	1.69	0.58
1:D:221:ARG:NH1	1:D:253:CYS:O	2.36	0.58
1:D:660:GLY:HA2	1:D:750:LEU:HB2	1.84	0.58
1:A:2647:HIS:CE1	1:A:2651:CYS:HG	2.21	0.58
1:G:637:LEU:HA	1:G:1637:MET:HA	1.86	0.58
1:G:1698:LEU:HA	1:G:1712:TYR:CE1	2.38	0.58
1:G:2121:PHE:HB3	1:G:3725:TYR:CE2	2.37	0.58
1:G:4576:ILE:HD11	1:G:4639:MET:CG	2.34	0.58
1:J:799:GLU:H	1:J:1623:ARG:HA	1.67	0.58
1:D:451:TYR:O	1:D:474:ARG:NH2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:839:LEU:HD13	1:D:1075:PHE:HD2	1.68	0.58
1:J:632:LEU:HD23	1:J:1666:THR:HG23	1.86	0.58
1:D:1434:TYR:HB2	1:D:1572:ILE:HG21	1.85	0.57
1:A:670:GLU:HA	1:A:740:PRO:HB3	1.86	0.57
1:G:716:PHE:HE1	1:G:757:PHE:CD1	2.22	0.57
1:G:1269:CYS:SG	1:G:1563:GLN:HB2	2.44	0.57
1:D:4817:ALA:HA	1:D:4823:LEU:HB3	1.86	0.57
1:G:206:CYS:HB2	1:G:271:GLY:HA3	1.86	0.57
1:D:530:ILE:HG22	1:D:536:ASN:HB3	1.86	0.57
1:A:275:ARG:HB3	1:A:336:PRO:HG3	1.85	0.57
1:A:3673:MET:HE1	1:A:3728:ILE:HG12	1.85	0.57
1:G:2607:LEU:HD21	1:G:2643:LEU:HD22	1.86	0.57
1:D:716:PHE:HE1	1:D:757:PHE:CD1	2.22	0.57
2:H:87:HIS:HD2	2:H:88:PRO:HD2	1.68	0.57
1:D:4016:LEU:O	1:D:4019:LEU:HG	2.05	0.57
2:E:39:SER:HA	2:E:42:ARG:HH21	1.66	0.57
1:A:4045:VAL:O	1:A:4049:VAL:HG23	2.05	0.57
1:G:4708:THR:OG1	1:G:4772:ASP:OD2	2.22	0.57
1:J:1743:ARG:O	1:J:1964:ARG:NH2	2.35	0.57
1:A:1301:PHE:HE2	1:A:1544:PRO:HA	1.70	0.57
1:A:2159:LEU:HD13	1:A:2203:MET:HG2	1.85	0.57
1:G:219:VAL:HG12	1:G:259:LEU:HD12	1.86	0.57
1:D:233:ILE:O	1:D:257:ARG:NH1	2.38	0.57
1:D:1733:GLU:N	1:D:1733:GLU:OE2	2.36	0.57
1:D:2477:PRO:HG3	1:D:2546:MET:HG3	1.86	0.57
1:J:2503:VAL:HG11	1:J:2557:ALA:HB1	1.86	0.57
1:D:3658:LYS:HA	1:D:3662:ILE:HD13	1.85	0.57
1:D:4895:GLY:O	1:A:4892:ARG:NH1	2.38	0.57
1:J:1437:VAL:HG21	1:J:1552:VAL:HG21	1.87	0.57
1:D:830:ARG:HH21	1:D:1612:PHE:HB2	1.69	0.57
1:D:2822:THR:O	1:D:2937:VAL:HA	2.04	0.57
1:G:515:TRP:O	1:G:519:VAL:HG23	2.04	0.57
1:G:4029:SER:O	1:G:4032:GLU:HG3	2.05	0.57
1:J:2879:ALA:CB	1:J:2920:ARG:HA	2.35	0.57
1:A:470:SER:OG	1:A:474:ARG:NH1	2.38	0.57
1:A:4580:TYR:OH	1:A:4806:ASN:ND2	2.34	0.57
1:G:452:PHE:HZ	1:G:478:PHE:HD2	1.53	0.57
1:G:551:LEU:HD21	1:G:589:LEU:HD22	1.86	0.57
1:G:842:PRO:HD3	1:G:1073:ARG:HG2	1.85	0.57
1:G:2039:LEU:HD22	1:G:2044:ILE:HG13	1.87	0.57
1:J:1862:ILE:O	1:J:1866:ILE:HG12	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:2364:PHE:HD1	1:G:2429:LEU:HD21	1.69	0.56
1:J:1477:GLY:HA2	1:J:1483:VAL:HA	1.86	0.56
1:J:1863:LEU:HD11	1:J:1871:PHE:CD2	2.39	0.56
1:D:1112:ASP:OD1	1:D:1113:VAL:N	2.38	0.56
1:A:603:LEU:HD23	1:A:606:LEU:HD12	1.87	0.56
1:J:1109:LEU:HA	1:J:1120:LEU:HD13	1.87	0.56
1:D:468:LEU:O	1:D:472:ARG:HG2	2.04	0.56
1:D:637:LEU:HA	1:D:1637:MET:HA	1.87	0.56
1:D:4097:MET:HG2	1:D:4108:ILE:HG12	1.87	0.56
1:D:4569:LEU:HD23	1:D:4650:HIS:HA	1.86	0.56
1:A:583:ILE:O	1:A:587:ILE:HG12	2.05	0.56
1:G:3927:GLN:HB2	1:G:3992:PHE:CZ	2.40	0.56
1:J:1747:LEU:HD21	1:J:2041:HIS:HB2	1.87	0.56
1:J:2118:ARG:HD2	1:J:3721:LEU:HD22	1.86	0.56
1:D:291:LEU:HD23	1:D:301:VAL:HG12	1.87	0.56
1:G:1802:ILE:HG21	1:G:1807:LEU:HD11	1.87	0.56
1:J:1649:ASP:HB2	1:J:1652:GLU:HB2	1.85	0.56
2:K:90:VAL:HG23	2:K:91:ILE:HG12	1.87	0.56
1:D:4226:GLY:O	1:D:4230:LYS:N	2.38	0.56
1:G:686:TRP:HZ3	1:G:748:LEU:HD22	1.70	0.56
1:D:1932:PRO:O	1:D:1936:LYS:HG2	2.06	0.56
1:G:1130:GLN:HG3	1:G:1132:TRP:HE1	1.71	0.56
1:G:3775:ALA:O	1:G:3778:MET:HG3	2.06	0.56
1:J:1255:TYR:HE1	1:J:1274:HIS:HD2	1.52	0.56
1:J:2152:THR:HG22	1:J:2190:VAL:HG11	1.88	0.56
1:D:2178:MET:SD	1:D:2210:VAL:HG11	2.46	0.56
1:D:2299:VAL:HG21	1:D:2356:LEU:HB3	1.87	0.56
1:G:4654:ALA:C	1:G:4796:MET:HE1	2.26	0.56
1:A:1449:TRP:HB2	1:A:1553:PHE:HB2	1.88	0.56
1:G:840:VAL:HG22	1:G:1199:VAL:HG22	1.88	0.56
1:J:213:TYR:HB3	1:J:337:PRO:HG3	1.88	0.56
1:J:1931:LEU:HD12	1:J:1939:MET:HE1	1.87	0.56
1:D:3904:ARG:HG2	1:D:3905:THR:HG23	1.88	0.56
1:A:2128:TYR:CD2	1:A:3673:MET:HG2	2.40	0.56
1:G:2349:ASN:OD1	1:G:3849:ARG:NH2	2.39	0.56
1:D:1426:ILE:HG23	1:D:1427:ILE:HD13	1.88	0.56
1:A:615:ARG:NH2	1:A:1676:LEU:O	2.38	0.56
1:A:3001:ILE:HG22	1:A:3005:LEU:HD23	1.87	0.56
1:G:1714:LEU:O	1:G:1718:ILE:HG12	2.06	0.56
1:J:2661:TRP:CD1	1:J:2664:PHE:CD1	2.93	0.56
1:A:2515:GLN:NE2	1:A:2568:LEU:O	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4687:TYR:OH	1:A:4699:GLY:O	2.20	0.55
1:A:733:PRO:HG2	1:A:762:CYS:HB3	1.89	0.55
1:A:1446:SER:O	1:A:1496:TRP:NE1	2.30	0.55
1:G:701:GLY:O	1:G:1640:HIS:HD2	1.89	0.55
1:G:839:LEU:HB3	1:G:1075:PHE:HE2	1.71	0.55
1:G:2522:LEU:HA	1:G:2526:PHE:HD2	1.70	0.55
1:G:4151:SER:HB2	1:G:4164:LEU:HD11	1.86	0.55
1:J:2238:TYR:HA	1:J:2241:ARG:HG2	1.87	0.55
1:D:195:PHE:CE1	1:A:2358:ILE:HD11	2.40	0.55
1:A:4218:ILE:HG23	1:A:4954:MET:HE3	1.87	0.55
1:J:1830:VAL:N	1:J:1837:GLN:OE1	2.38	0.55
1:J:2107:GLN:NE2	1:J:3681:GLY:H	2.04	0.55
1:D:59:PRO:HB3	1:D:281:ARG:HH11	1.72	0.55
1:D:830:ARG:NH2	1:D:1612:PHE:HB2	2.21	0.55
1:D:4666:VAL:HG21	1:D:4783:ILE:HG12	1.89	0.55
2:E:71:ARG:HG2	2:E:102:GLU:HB3	1.88	0.55
1:J:564:LEU:HA	1:J:567:VAL:HG12	1.88	0.55
2:K:68:LEU:HD12	2:K:106:LEU:HD23	1.88	0.55
1:D:2821:TRP:HA	1:D:2938:THR:C	2.27	0.55
1:J:2012:PHE:CG	1:J:2028:ARG:HG2	2.42	0.55
1:J:3927:GLN:HE21	1:J:3991:GLY:HA3	1.71	0.55
1:J:4863:TYR:HD2	1:J:4876:CYS:HB2	1.72	0.55
1:D:1446:SER:O	1:D:1496:TRP:NE1	2.31	0.55
1:A:2377:LEU:HA	1:A:2469:ILE:HD11	1.88	0.55
1:G:291:LEU:HA	1:G:301:VAL:HA	1.88	0.55
1:G:1297:PHE:HD2	1:G:1522:LEU:HA	1.72	0.55
1:G:3813:GLN:HB3	1:G:3899:PHE:HE2	1.72	0.55
1:J:1449:TRP:HB2	1:J:1553:PHE:HB2	1.88	0.55
1:D:1871:PHE:HZ	1:D:2094:LEU:HD13	1.72	0.55
1:J:421:PHE:CE2	1:J:507:ALA:HB2	2.42	0.55
1:J:498:THR:O	1:J:553:ARG:NH2	2.40	0.55
1:D:491:ILE:HD11	1:D:519:VAL:HG23	1.88	0.55
1:D:551:LEU:HD21	1:D:589:LEU:HD22	1.88	0.55
1:D:1947:CYS:SG	1:D:2126:ARG:HD2	2.47	0.55
1:D:4837:LEU:HD22	1:D:4936:ILE:HD11	1.88	0.55
1:J:4954:MET:SD	6:J:5103:ATP:H1'	2.46	0.55
1:G:2142:TYR:HE1	1:G:3651:ASN:HD22	1.55	0.54
1:J:4677:LEU:HD22	1:J:4711:PHE:HZ	1.68	0.54
1:D:3916:ILE:O	1:D:3919:THR:OG1	2.22	0.54
1:D:4577:LEU:O	1:J:4879:MET:HG3	2.07	0.54
1:A:633:LEU:HD21	1:A:1659:LEU:HD12	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:523:TYR:CZ	1:G:560:ILE:HD11	2.41	0.54
1:J:4773:VAL:O	1:J:4777:ILE:HD12	2.07	0.54
1:D:2188:ASN:OD1	1:D:2190:VAL:HG12	2.08	0.54
1:D:2823:ILE:HA	1:D:2936:ALA:O	2.07	0.54
1:A:1947:CYS:HB2	1:A:2127:GLN:HE22	1.73	0.54
1:J:579:GLN:H	1:J:582:HIS:CD2	2.23	0.54
1:J:663:TYR:HB2	1:J:808:TYR:HB3	1.89	0.54
1:J:2272:PRO:HA	1:J:2275:VAL:HG12	1.88	0.54
1:J:3889:GLN:HG3	1:J:3967:GLU:HG3	1.88	0.54
1:D:606:LEU:HD22	1:D:621:ILE:HD11	1.89	0.54
1:A:1733:GLU:OE1	1:A:1733:GLU:N	2.41	0.54
1:A:4992:LEU:O	1:A:4996:ILE:HG12	2.06	0.54
1:G:2099:SER:HB3	1:G:2128:TYR:HE1	1.71	0.54
1:G:4655:PHE:N	1:G:4796:MET:HE1	2.23	0.54
1:G:4721:LYS:HD3	1:G:4741:LEU:HD12	1.89	0.54
1:D:206:CYS:HB2	1:D:271:GLY:HA3	1.89	0.54
1:D:633:LEU:HD23	1:D:1639:LEU:HD13	1.88	0.54
1:A:736:HIS:HB2	2:B:9:PRO:HD3	1.89	0.54
1:A:1260:MET:SD	1:A:1271:ARG:NH1	2.80	0.54
1:G:2679:PHE:HE2	1:G:2959:PHE:HE1	1.54	0.54
1:J:4692:PRO:HG2	1:J:4703:ARG:HH21	1.73	0.54
1:D:3673:MET:CE	1:D:3728:ILE:HG12	2.38	0.54
1:D:4992:LEU:O	1:D:4996:ILE:HG12	2.08	0.54
1:A:202:MET:HG3	1:A:202:MET:O	2.06	0.54
1:J:400:ALA:O	1:J:404:ILE:HG12	2.07	0.54
1:D:2121:PHE:HB3	1:D:3725:TYR:CE2	2.33	0.54
1:D:4673:ARG:HD2	1:D:4782:VAL:HG21	1.90	0.54
1:A:2102:VAL:HG13	1:A:2120:MET:HG2	1.88	0.54
1:G:527:ALA:HA	1:G:530:ILE:HG22	1.90	0.54
1:G:638:ILE:HG13	1:G:678:GLN:OE1	2.08	0.54
1:J:2096:GLU:O	1:J:2100:HIS:ND1	2.41	0.54
1:D:2121:PHE:CZ	1:D:3701:LEU:HB2	2.42	0.54
1:D:3963:ASN:O	1:D:3966:THR:OG1	2.24	0.54
1:G:587:ILE:HD12	1:G:625:LEU:HD13	1.89	0.54
1:J:4952:GLU:O	1:J:4956:THR:HG23	2.07	0.54
1:A:4822:THR:O	1:A:4826:ILE:HG12	2.07	0.54
1:J:2012:PHE:HZ	1:J:2031:LEU:HD13	1.72	0.54
1:J:2114:PRO:HG3	1:J:3707:ARG:HH22	1.72	0.54
2:E:4:ILE:HB	2:E:72:ALA:HB1	1.90	0.54
1:A:3844:LEU:HD21	1:A:3936:TYR:HB2	1.88	0.54
2:B:16:PRO:HG2	2:B:63:ALA:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:636:ASN:OD1	2:H:35:LYS:NZ	2.37	0.54
1:G:1426:ILE:O	1:G:1430:THR:OG1	2.20	0.54
1:J:180:LEU:O	1:J:200:TRP:NE1	2.36	0.54
1:J:1454:THR:HG23	1:J:1456:ASP:H	1.73	0.54
1:J:1712:TYR:OH	1:J:1814:MET:SD	2.66	0.54
1:D:2386:ILE:HG21	1:D:2418:LEU:HD22	1.89	0.53
1:A:113:HIS:NE2	1:A:399:GLN:HA	2.22	0.53
1:G:2332:LEU:HD11	1:G:2429:LEU:HA	1.89	0.53
1:D:400:ALA:O	1:D:404:ILE:HG12	2.08	0.53
2:H:78:PRO:HD3	2:H:96:THR:HG22	1.90	0.53
1:A:2505:PHE:O	1:A:2509:VAL:HG22	2.07	0.53
1:G:1794:ALA:O	1:G:2173:GLN:NE2	2.41	0.53
1:J:3445:TRP:HZ3	1:J:3452:LYS:HA	1.73	0.53
1:D:415:ILE:HD11	1:D:493:ARG:HD2	1.90	0.53
1:D:1452:TRP:CE3	1:D:1548:LEU:HB3	2.43	0.53
1:D:4629:TYR:OH	1:J:4860:ARG:NH2	2.42	0.53
1:A:116:MET:HB2	1:A:137:LEU:HD12	1.90	0.53
1:A:4572:ALA:O	1:A:4576:ILE:HG12	2.08	0.53
1:J:355:LEU:HB2	1:J:378:LEU:HD23	1.91	0.53
1:J:1131:ARG:NH1	1:J:1178:ALA:O	2.42	0.53
1:J:2559:LEU:HD23	1:J:2602:VAL:HG12	1.91	0.53
1:D:4055:VAL:HA	1:D:4058:ILE:HG22	1.90	0.53
1:A:62:LEU:HD12	1:A:65:CYS:HB2	1.90	0.53
1:A:561:LEU:HD21	1:A:598:LYS:HB3	1.91	0.53
1:G:3420:ARG:HA	1:G:3423:TRP:HB3	1.89	0.53
1:J:243:ARG:HA	1:J:301:VAL:HB	1.90	0.53
1:A:418:LEU:HD11	1:A:494:LEU:HG	1.89	0.53
1:G:644:ILE:HD11	1:G:1628:VAL:HG11	1.90	0.53
1:G:3842:LEU:O	1:G:3929:SER:OG	2.21	0.53
1:G:4215:ARG:NH2	6:G:5103:ATP:O2G	2.39	0.53
1:G:4879:MET:HG3	1:J:4578:LEU:HD12	1.89	0.53
1:J:150:MET:HB2	1:J:169:LEU:HD21	1.90	0.53
1:J:4911:LEU:HA	1:J:4914:VAL:HG12	1.91	0.53
1:D:4204:GLN:HE21	1:D:4248:ALA:HB3	1.73	0.53
1:A:1293:LEU:HD11	1:A:1594:ARG:HG2	1.91	0.53
1:G:2010:LEU:HD21	1:G:3653:PHE:CE1	2.43	0.53
1:D:2355:ARG:O	1:D:2359:ARG:HG2	2.09	0.53
1:G:684:VAL:HG21	1:G:744:VAL:HG21	1.90	0.53
1:G:1715:LEU:HD12	1:G:1719:HIS:HD2	1.74	0.53
1:G:2124:LEU:HD11	1:G:2128:TYR:CZ	2.44	0.53
1:G:3927:GLN:HE21	1:G:3991:GLY:HA3	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1087:ARG:NE	1:D:1154:ASP:OD1	2.42	0.53
1:D:2025:GLU:HA	1:D:2028:ARG:HG2	1.91	0.53
1:D:3970:GLN:HE22	1:D:5004:THR:HG22	1.73	0.53
1:A:2555:CYS:SG	1:A:2599:GLN:HA	2.49	0.53
1:A:3927:GLN:HB2	1:A:3992:PHE:CZ	2.44	0.53
1:A:4818:MET:O	1:A:4824:ARG:NH2	2.42	0.53
1:J:4583:SER:HB2	1:J:4630:TYR:HE2	1.72	0.53
1:D:657:THR:HB	1:D:1006:SER:HA	1.91	0.53
1:A:2518:LEU:HD21	1:A:2569:PHE:HE1	1.74	0.53
1:G:484:LEU:HD23	1:G:539:LEU:HD22	1.91	0.53
1:J:2500:ALA:N	1:J:2553:TYR:HE1	2.06	0.53
1:D:209:CYS:SG	1:D:273:HIS:NE2	2.77	0.52
1:D:2134:LEU:O	1:D:2138:LEU:HG	2.09	0.52
1:A:2000:SER:O	1:A:2005:GLN:NE2	2.38	0.52
1:A:2142:TYR:CD2	1:A:2197:LEU:HD13	2.44	0.52
1:G:629:ARG:NH1	2:H:90:VAL:O	2.41	0.52
1:G:2638:LYS:HD2	1:G:2698:MET:HG3	1.91	0.52
1:J:1965:TYR:CZ	1:J:2031:LEU:HB2	2.44	0.52
1:A:4813:LEU:O	1:A:4816:ILE:HG22	2.09	0.52
1:G:113:HIS:NE2	1:G:402:ARG:HB3	2.24	0.52
1:G:1947:CYS:SG	1:G:2126:ARG:NH2	2.82	0.52
1:G:2192:TYR:HD1	1:G:2242:ILE:HD13	1.74	0.52
1:G:2567:PRO:HA	1:G:2613:TYR:HD2	1.75	0.52
2:H:10:GLY:HA3	2:H:70:GLN:CB	2.33	0.52
1:G:1289:LEU:HD23	1:G:1597:VAL:HG21	1.92	0.52
1:G:2257:LEU:HA	1:G:2260:ASN:HD22	1.74	0.52
1:G:2641:LEU:O	1:G:2645:THR:HG23	2.08	0.52
1:G:3890:LEU:HA	1:G:3893:GLU:HB2	1.92	0.52
1:J:4777:ILE:HA	1:J:4780:PHE:CE2	2.43	0.52
1:G:3733:CYS:SG	1:G:3734:HIS:N	2.82	0.52
2:H:70:GLN:NE2	2:H:71:ARG:O	2.41	0.52
1:J:133:PHE:O	1:J:193:ALA:N	2.32	0.52
1:D:4843:LEU:HB2	1:A:4823:LEU:HD21	1.90	0.52
1:A:831:ARG:HE	1:A:840:VAL:HG21	1.73	0.52
1:G:1115:LEU:HD13	1:G:1123:VAL:HG11	1.90	0.52
1:D:3813:GLN:HB3	1:D:3899:PHE:CE2	2.45	0.52
1:D:4235:VAL:HG21	1:D:5019:TRP:NE1	2.24	0.52
1:G:707:VAL:HG13	1:G:782:SER:HB2	1.91	0.52
1:G:1291:LEU:HD23	1:G:1550:PRO:HB2	1.90	0.52
1:G:2332:LEU:HD21	1:G:2429:LEU:N	2.24	0.52
1:D:4180:ARG:HG2	1:D:4192:ARG:HH21	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4713:SER:OG	1:D:4775:TYR:OH	2.26	0.52
1:G:181:HIS:HB3	1:G:194:SER:HB3	1.92	0.52
1:G:4034:ASN:HD21	1:G:4041:ALA:HB2	1.74	0.52
1:J:4577:LEU:HD11	1:J:4807:PHE:CD1	2.45	0.52
1:D:3539:ARG:O	1:D:3543:LYS:N	2.43	0.52
1:D:4713:SER:HG	1:D:4775:TYR:HH	1.58	0.52
1:A:622:THR:HG21	1:A:1681:VAL:HG22	1.91	0.52
1:A:629:ARG:HB3	1:A:634:GLN:OE1	2.10	0.52
1:G:2171:GLY:H	1:G:2174:GLU:HB2	1.74	0.52
1:G:2551:ASN:OD1	1:G:2552:ARG:N	2.43	0.52
1:J:597:HIS:HB2	1:J:1665:HIS:ND1	2.25	0.52
1:J:2323:TRP:CH2	1:J:2422:ILE:HG13	2.44	0.52
1:J:4712:PRO:HB2	1:J:4718:LYS:HA	1.92	0.52
2:K:25:HIS:ND1	2:K:25:HIS:O	2.42	0.52
1:D:3680:ALA:O	1:D:3681:GLY:C	2.48	0.52
1:G:4799:SER:HB2	1:G:4812:HIS:CE1	2.45	0.52
1:J:650:VAL:HG12	1:J:750:LEU:HD11	1.92	0.52
1:J:688:LEU:HD22	1:J:712:TYR:HD2	1.75	0.52
1:D:2894:LEU:O	1:D:2899:GLY:N	2.43	0.52
1:G:2287:ALA:O	1:G:2349:ASN:ND2	2.38	0.52
1:J:103:TYR:CE2	1:J:152:PRO:HB3	2.45	0.52
1:J:1475:THR:HG22	1:J:1486:SER:HA	1.92	0.52
1:J:2103:VAL:O	1:J:2107:GLN:HG3	2.10	0.52
1:D:1452:TRP:HE3	1:D:1548:LEU:HB3	1.75	0.51
1:A:830:ARG:NE	1:A:837:PRO:HB3	2.25	0.51
1:A:1944:GLU:HB2	1:A:2123:LEU:HD21	1.92	0.51
1:A:3959:LYS:HG3	1:A:4022:ASP:OD2	2.10	0.51
1:A:4115:SER:HB2	1:A:4123:ILE:HG23	1.92	0.51
1:G:745:SER:N	1:G:758:ARG:O	2.42	0.51
1:J:1130:GLN:HG2	1:J:1138:PRO:HA	1.91	0.51
1:J:2504:LEU:HD11	1:J:2508:ARG:HH12	1.75	0.51
1:D:4580:TYR:OH	1:D:4643:LEU:HD21	2.10	0.51
1:A:1232:ARG:NH2	1:A:1828:ASP:O	2.41	0.51
1:A:4206:GLU:O	1:A:4211:LYS:NZ	2.43	0.51
1:G:1155:LEU:HD12	1:G:1184:ILE:HG22	1.91	0.51
1:G:2128:TYR:HD2	1:G:3673:MET:SD	2.33	0.51
1:G:2189:LYS:HB3	3:I:14:LYS:HG2	1.91	0.51
1:D:1732:SER:O	1:D:2140:ARG:NE	2.42	0.51
1:D:4031:LEU:O	1:D:4034:ASN:ND2	2.43	0.51
1:D:4060:LYS:O	1:D:4064:MET:HG2	2.11	0.51
1:A:578:ILE:HG23	1:A:582:HIS:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1849:LEU:HB3	1:A:1945:TYR:CE2	2.46	0.51
1:G:1494:MET:HE1	1:G:1553:PHE:HD2	1.75	0.51
1:J:1965:TYR:CE1	1:J:2031:LEU:HB2	2.45	0.51
1:J:2012:PHE:CZ	1:J:2031:LEU:HD13	2.45	0.51
1:J:2095:GLN:OE1	1:J:2127:GLN:NE2	2.43	0.51
1:J:3994:HIS:CD2	1:J:3998:HIS:CD2	2.99	0.51
1:D:537:CYS:SG	1:D:571:SER:HB2	2.50	0.51
1:D:791:PHE:N	1:D:1626:TRP:O	2.41	0.51
1:D:4570:ALA:O	1:D:4573:ILE:HG22	2.10	0.51
1:A:840:VAL:HG22	1:A:1199:VAL:HG22	1.93	0.51
1:G:2251:PHE:CD2	1:G:2286:LEU:HD22	2.45	0.51
1:G:3420:ARG:O	1:G:3424:LEU:HG	2.10	0.51
1:J:1607:ARG:NH2	1:J:1610:ASN:OD1	2.43	0.51
1:D:692:TYR:O	1:D:827:LYS:NZ	2.35	0.51
1:D:1297:PHE:HA	1:D:1522:LEU:HD22	1.92	0.51
1:A:113:HIS:NE2	1:A:402:ARG:HB3	2.26	0.51
1:A:451:TYR:CE2	1:A:474:ARG:HD2	2.46	0.51
1:A:3844:LEU:HD13	1:A:3933:PHE:HA	1.92	0.51
2:B:56:ILE:HD11	2:B:81:ALA:HA	1.91	0.51
1:G:711:LEU:HD22	1:G:1491:ASN:HD22	1.74	0.51
1:G:1772:ARG:NH2	1:G:1952:GLN:OE1	2.43	0.51
1:G:4805:ASN:HD21	1:G:4807:PHE:HB2	1.76	0.51
1:J:2559:LEU:HD21	1:J:2603:ILE:HA	1.92	0.51
1:D:1130:GLN:HG3	1:D:1132:TRP:HE1	1.75	0.51
1:D:2515:GLN:HA	1:D:2518:LEU:HD23	1.92	0.51
1:D:3816:MET:SD	1:D:3891:LEU:HD11	2.49	0.51
1:D:59:PRO:HB3	1:D:281:ARG:NH1	2.26	0.51
1:A:173:SER:HB2	1:A:178:ARG:H	1.76	0.51
1:A:1698:LEU:HA	1:A:1712:TYR:CE1	2.38	0.51
1:G:1243:PRO:HB2	1:G:1600:LEU:HD11	1.91	0.51
1:G:1438:ARG:HB3	1:G:1563:GLN:HE21	1.75	0.51
1:G:2238:TYR:CE2	3:I:67:PRO:HB2	2.46	0.51
1:J:35:LEU:HD21	1:J:182:LEU:HD21	1.92	0.51
1:J:468:LEU:O	1:J:472:ARG:HG2	2.10	0.51
3:L:69:PHE:O	3:L:73:MET:HG3	2.10	0.51
1:D:421:PHE:HE1	1:D:436:LEU:HD21	1.75	0.51
1:A:3992:PHE:HB3	1:A:3996:PHE:CE2	2.46	0.51
3:I:1:MET:O	3:I:4:GLN:NE2	2.44	0.51
1:J:290:TYR:HD1	1:J:304:ALA:HA	1.74	0.51
1:A:2155:LEU:HB2	1:A:2188:ASN:ND2	2.26	0.51
1:J:753:PRO:HB2	1:J:770:ALA:H	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1683:HIS:HD2	1:A:1800:PRO:HG3	1.74	0.51
1:A:4839:MET:HB3	1:G:4823:LEU:HD21	1.93	0.51
1:J:719:LEU:HD11	2:K:7:ILE:HA	1.93	0.51
1:D:257:ARG:O	1:D:284:HIS:NE2	2.43	0.50
1:G:799:GLU:N	1:G:1623:ARG:O	2.39	0.50
1:G:1126:GLY:HA3	1:G:1143:TRP:NE1	2.26	0.50
1:J:1115:LEU:HD21	1:J:1123:VAL:HG11	1.93	0.50
1:J:4145:VAL:HG13	1:J:4194:TYR:HD2	1.76	0.50
1:D:14:LEU:HD21	1:D:204:PRO:HB3	1.93	0.50
1:D:1695:LEU:HD12	1:D:1810:LYS:HE3	1.92	0.50
1:D:3722:TYR:CZ	1:D:3782:MET:SD	3.04	0.50
1:G:627:PRO:HD3	2:H:89:GLY:HA2	1.93	0.50
1:A:551:LEU:HD21	1:A:589:LEU:HD22	1.91	0.50
1:A:1621:GLY:HA3	1:A:1624:LEU:HB2	1.92	0.50
1:A:2627:VAL:HG11	1:A:2674:LEU:HD12	1.94	0.50
1:A:3844:LEU:HD21	1:A:3936:TYR:CG	2.46	0.50
1:G:692:TYR:CZ	1:G:694:PRO:HG3	2.46	0.50
1:G:4927:ILE:HG22	1:G:4928:LEU:HD22	1.93	0.50
1:J:217:GLY:HA2	1:J:261:ARG:HD3	1.93	0.50
1:J:1440:PHE:HD2	1:J:1560:ASN:HB3	1.77	0.50
1:D:568:LEU:HD21	1:D:578:ILE:HD11	1.92	0.50
1:D:1928:GLN:HA	1:D:2104:ARG:HH22	1.76	0.50
1:D:2515:GLN:HB2	1:D:2568:LEU:CD1	2.42	0.50
2:E:74:LEU:HB2	2:E:99:PHE:HB2	1.93	0.50
1:A:3442:PHE:O	1:A:3445:TRP:HB3	2.11	0.50
1:G:838:HIS:ND1	1:G:1201:HIS:HB2	2.26	0.50
1:G:4839:MET:HB3	1:J:4823:LEU:CD1	2.39	0.50
1:J:1713:ASP:HA	1:J:1716:ILE:HG22	1.93	0.50
1:J:4069:LYS:HA	1:J:4072:VAL:HG12	1.93	0.50
1:D:2103:VAL:HG12	1:D:2107:GLN:NE2	2.26	0.50
1:A:794:GLY:O	1:A:798:GLY:N	2.36	0.50
1:A:4072:VAL:HG21	1:A:4129:ALA:HB2	1.93	0.50
1:G:1658:ASP:N	1:G:1658:ASP:OD1	2.45	0.50
1:G:2195:PRO:HB2	1:G:2246:ASN:HD21	1.76	0.50
1:G:3844:LEU:HD11	1:G:3936:TYR:CD2	2.46	0.50
1:J:276:TRP:CZ2	1:J:339:ILE:HG13	2.47	0.50
1:J:640:TYR:CZ	1:J:1636:MET:HG2	2.46	0.50
1:D:2251:PHE:CD2	1:D:2286:LEU:HD22	2.46	0.50
1:A:1125:ASN:HB2	1:A:1132:TRP:HD1	1.76	0.50
1:A:4241:THR:O	1:A:4245:MET:HG3	2.11	0.50
1:A:4928:LEU:HD23	1:A:4931:ILE:HD12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1839:VAL:HG13	1:G:1938:GLN:HE21	1.76	0.50
1:J:202:MET:N	1:J:202:MET:SD	2.85	0.50
1:J:2825:LYS:HA	1:J:2935:TYR:HA	1.94	0.50
1:D:667:MET:HA	1:D:743:VAL:HA	1.94	0.50
1:D:4574:ASN:HD21	1:D:4810:ALA:HA	1.77	0.50
1:A:1087:ARG:HB3	1:A:1223:PHE:CD2	2.47	0.50
1:A:4677:LEU:HD22	1:A:4702:ASP:HB3	1.94	0.50
1:G:2465:ASP:O	1:G:2469:ILE:HG12	2.11	0.50
1:G:4666:VAL:HG13	1:G:4783:ILE:HD11	1.93	0.50
1:G:4849:TYR:HA	1:G:4852:THR:HG22	1.94	0.50
1:G:4955:GLU:OE2	6:G:5103:ATP:O2'	2.30	0.50
1:J:4786:ASP:O	1:J:4790:LEU:HD23	2.12	0.50
2:K:8:SER:HB2	2:K:71:ARG:HB2	1.94	0.50
1:D:2638:LYS:NZ	1:D:2695:LEU:HA	2.27	0.50
1:A:2470:ILE:HG21	1:A:2526:PHE:HE1	1.75	0.50
1:G:1259:ARG:NH2	1:G:1595:LEU:O	2.45	0.50
1:G:1862:ILE:O	1:G:1866:ILE:HG12	2.12	0.50
1:G:2102:VAL:HG13	1:G:2120:MET:HG2	1.94	0.50
1:G:3679:LYS:O	1:G:3680:ALA:HB3	2.12	0.50
1:J:4574:ASN:HD21	1:J:4810:ALA:HA	1.77	0.50
1:D:1760:HIS:CE1	1:D:2041:HIS:HA	2.47	0.50
1:D:4104:THR:O	1:D:4108:ILE:HG13	2.12	0.50
1:D:4580:TYR:OH	1:D:4643:LEU:CD2	2.60	0.50
1:A:4643:LEU:HD11	1:A:4806:ASN:HD21	1.76	0.50
1:J:417:GLY:O	1:J:420:SER:OG	2.21	0.50
1:J:1298:HIS:CD2	1:J:1522:LEU:HB3	2.46	0.50
1:D:594:GLY:HA2	1:D:1594:ARG:HD2	1.93	0.49
1:A:273:HIS:CG	1:A:337:PRO:O	2.65	0.49
1:A:625:LEU:HD12	1:A:626:LEU:N	2.27	0.49
1:A:4013:LEU:HD12	1:A:4016:LEU:HD23	1.94	0.49
1:G:2242:ILE:HD12	3:I:2:ALA:HB3	1.94	0.49
1:J:686:TRP:NE1	1:J:746:CYS:SG	2.85	0.49
1:J:2458:ARG:HG2	1:J:2510:TYR:CE1	2.47	0.49
1:J:3805:LEU:HG	1:J:3890:LEU:HB3	1.93	0.49
1:D:1735:ILE:HD11	1:D:2156:LEU:HD11	1.94	0.49
1:A:1452:TRP:HE1	1:A:1518:CYS:HB3	1.76	0.49
1:A:1698:LEU:CA	1:A:1712:TYR:HE1	2.22	0.49
1:G:1451:GLY:HA3	1:G:1494:MET:HA	1.93	0.49
1:G:1678:ASN:HB3	1:G:1681:VAL:HB	1.93	0.49
1:J:4567:LEU:HD21	1:J:4816:ILE:HD11	1.93	0.49
1:J:4667:PRO:HA	1:J:4670:ILE:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1698:LEU:HD11	1:D:1715:LEU:HD13	1.94	0.49
1:D:1719:HIS:CD2	1:D:1802:ILE:HD12	2.47	0.49
1:D:2551:ASN:HD21	1:D:2595:LEU:HD23	1.78	0.49
1:A:597:HIS:HB2	1:A:1665:HIS:ND1	2.26	0.49
1:A:4145:VAL:HG13	1:A:4194:TYR:HD2	1.77	0.49
1:G:2212:VAL:HG22	1:G:2256:TYR:OH	2.13	0.49
1:J:2503:VAL:HA	1:J:2506:LEU:HD21	1.94	0.49
1:J:3965:LEU:HA	1:J:3968:TYR:HD2	1.75	0.49
1:J:3966:THR:O	1:J:3970:GLN:HG3	2.12	0.49
1:D:3788:GLY:HA2	1:D:3835:LEU:HG	1.95	0.49
1:D:4999:ASP:N	1:D:5002:GLU:OE2	2.44	0.49
1:A:800:PHE:HD2	1:A:804:PRO:HG3	1.78	0.49
1:G:709:ASP:HA	1:G:725:HIS:HA	1.94	0.49
1:G:1087:ARG:HB2	1:G:1223:PHE:CD1	2.47	0.49
1:G:4859:PHE:HE2	1:G:4913:ARG:HB2	1.76	0.49
1:J:1470:ARG:O	1:J:1490:SER:OG	2.25	0.49
1:J:2148:SER:O	1:J:2152:THR:HG23	2.12	0.49
1:J:2463:LEU:HD13	1:J:2510:TYR:CD2	2.47	0.49
1:A:291:LEU:HD21	1:A:299:LEU:HD11	1.93	0.49
1:A:1474:VAL:N	1:A:1487:LEU:O	2.31	0.49
1:A:2172:PRO:O	1:A:2175:GLU:HG3	2.11	0.49
1:G:266:ARG:HD2	1:G:268:SER:O	2.12	0.49
1:G:1288:PHE:HB3	1:G:1553:PHE:HE1	1.77	0.49
1:G:2825:LYS:HA	1:G:2935:TYR:HA	1.94	0.49
1:J:347:PHE:HE1	1:J:387:ALA:HA	1.77	0.49
1:D:3770:LEU:HD12	1:D:3804:ILE:HD11	1.94	0.49
1:D:4218:ILE:HA	1:D:4221:VAL:HG12	1.94	0.49
1:A:1448:VAL:HG22	1:A:1554:VAL:HG23	1.93	0.49
1:A:2825:LYS:HA	1:A:2935:TYR:HA	1.94	0.49
1:G:4059:LEU:HD13	1:G:4167:ALA:HB2	1.94	0.49
1:J:534:ARG:HH21	1:J:572:PRO:HD2	1.76	0.49
1:J:4679:ARG:NH2	1:J:4715:TYR:OH	2.45	0.49
1:A:2238:TYR:CE1	3:C:67:PRO:HB2	2.48	0.49
1:G:2182:ILE:O	1:G:2185:ILE:HG22	2.13	0.49
1:G:4183:ILE:O	1:G:4190:ILE:HG13	2.13	0.49
1:D:195:PHE:CZ	1:A:2358:ILE:HD11	2.48	0.49
1:D:2631:PRO:HB3	1:D:2681:GLY:HA2	1.95	0.49
1:A:648:ILE:HG23	1:A:814:ALA:HB3	1.94	0.49
1:A:1594:ARG:NH2	1:A:1643:GLU:OE2	2.41	0.49
1:G:2354:VAL:HG23	1:G:2436:CYS:SG	2.53	0.49
1:J:637:LEU:HA	1:J:1637:MET:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1073:ARG:HG2	1:J:1075:PHE:HE1	1.78	0.49
1:J:1842:LEU:HA	1:J:1845:VAL:HG12	1.95	0.49
1:J:4654:ALA:HB1	1:J:4796:MET:CE	2.43	0.49
1:D:2567:PRO:HA	1:D:2613:TYR:CG	2.47	0.49
1:D:2573:GLU:HA	1:D:2618:MET:HE1	1.95	0.49
1:A:491:ILE:HD11	1:A:519:VAL:HG23	1.94	0.49
1:A:1694:LEU:HD22	1:A:1715:LEU:HB2	1.94	0.49
1:G:1580:PHE:HE2	1:G:1592:PRO:HG2	1.78	0.49
1:G:4573:ILE:HA	1:G:4576:ILE:HG22	1.95	0.49
1:J:2040:ALA:HA	1:J:2045:GLN:HA	1.95	0.49
1:D:3829:PHE:HB3	1:D:3913:ILE:HD11	1.95	0.49
1:G:4991:PHE:HE1	1:G:5010:VAL:HG11	1.78	0.49
1:D:1424:PRO:O	1:D:1428:LEU:HD23	2.13	0.48
1:D:3935:TRP:HB3	1:J:76:ARG:HB3	1.95	0.48
1:D:4892:ARG:HH12	1:J:4898:GLY:HA3	1.77	0.48
1:A:2240:CYS:SG	1:A:2250:MET:HG2	2.53	0.48
1:G:475:GLN:NE2	1:G:528:SER:O	2.45	0.48
1:J:273:HIS:HB3	1:J:337:PRO:HB3	1.94	0.48
1:D:461:HIS:CD2	1:D:3707:ARG:HG3	2.48	0.48
1:D:523:TYR:CZ	1:D:560:ILE:HD11	2.48	0.48
1:D:2654:TYR:HA	1:D:2660:GLY:HA2	1.94	0.48
1:D:2938:THR:O	1:D:2939:ARG:C	2.52	0.48
1:A:829:TYR:HB3	1:A:1073:ARG:HH11	1.78	0.48
1:A:3817:LEU:HB2	1:A:3899:PHE:CE1	2.42	0.48
1:G:214:VAL:HG22	1:G:341:TYR:HD2	1.78	0.48
3:I:6:THR:HG23	3:I:9:GLN:H	1.77	0.48
1:D:162:LYS:HE3	1:A:3984:ARG:HD3	1.95	0.48
1:D:4654:ALA:O	1:D:4658:ILE:HG12	2.12	0.48
1:D:4821:LYS:O	1:D:4825:THR:HG23	2.13	0.48
1:A:484:LEU:O	1:A:488:LEU:HG	2.13	0.48
1:G:3966:THR:O	1:G:3970:GLN:N	2.41	0.48
1:J:1252:HIS:O	1:J:1275:ARG:NE	2.46	0.48
1:J:1958:LEU:HD12	1:J:2038:LEU:HD11	1.95	0.48
1:J:4567:LEU:HD12	1:J:4815:ASP:HB3	1.95	0.48
2:K:21:THR:HA	2:K:49:ARG:HA	1.94	0.48
1:D:4863:TYR:HD2	1:D:4876:CYS:HB2	1.78	0.48
1:J:686:TRP:NE1	1:J:748:LEU:HB2	2.28	0.48
1:J:4235:VAL:HG21	1:J:5019:TRP:NE1	2.29	0.48
1:D:4036:VAL:HB	1:D:5032:TYR:CD1	2.48	0.48
1:A:1639:LEU:O	1:A:1647:CYS:HA	2.14	0.48
1:G:839:LEU:HB3	1:G:1075:PHE:CE2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3889:GLN:HG3	1:G:3890:LEU:HD12	1.94	0.48
1:G:4863:TYR:HH	1:G:4886:HIS:HE2	1.60	0.48
1:J:4577:LEU:HD12	1:J:4580:TYR:CE2	2.48	0.48
1:D:441:VAL:O	1:D:445:LEU:HD23	2.13	0.48
1:D:636:ASN:OD1	1:D:637:LEU:N	2.46	0.48
1:D:1963:GLU:HA	1:D:3650:CYS:SG	2.54	0.48
1:D:2959:PHE:HE2	1:D:3009:TYR:CE1	2.32	0.48
1:A:4170:ILE:HG23	1:A:4171:LEU:HD12	1.96	0.48
1:D:1621:GLY:HA3	1:D:1624:LEU:HB2	1.95	0.48
1:A:2310:CYS:N	1:A:2324:ASN:HB3	2.28	0.48
1:A:3650:CYS:O	1:A:3654:LEU:HG	2.13	0.48
1:J:1154:ASP:O	1:J:1158:ASN:N	2.47	0.48
1:J:1727:ARG:O	1:J:1731:LEU:HB2	2.13	0.48
1:J:4995:LEU:HD21	1:J:5010:VAL:HG13	1.96	0.48
1:D:1294:PRO:HB3	1:D:1549:PHE:CZ	2.49	0.48
1:D:1699:GLU:HA	1:D:1814:MET:HE1	1.96	0.48
1:G:1152:MET:HB3	1:G:1223:PHE:CE1	2.49	0.48
1:J:150:MET:HE2	1:J:163:VAL:HG21	1.96	0.48
1:J:1566:LEU:HD12	1:J:1575:LEU:HB3	1.95	0.48
1:J:1970:GLN:HG2	1:J:3642:TYR:HA	1.96	0.48
1:D:3981:ALA:O	1:D:3986:TRP:NE1	2.41	0.48
1:A:221:ARG:HH21	1:A:259:LEU:HD21	1.79	0.48
1:A:4218:ILE:HG23	1:A:4954:MET:CE	2.44	0.48
1:A:4844:LEU:HD21	1:A:4891:VAL:HG21	1.96	0.48
1:G:400:ALA:HB1	1:G:478:PHE:CE1	2.49	0.48
1:G:1673:VAL:HG12	1:G:1681:VAL:HG11	1.95	0.48
1:G:2527:LEU:HD21	1:G:2582:MET:HB2	1.95	0.48
1:G:3709:ALA:HB2	1:G:3782:MET:HG2	1.95	0.48
1:G:4568:PHE:HD2	1:G:4569:LEU:HD12	1.79	0.48
1:J:2298:VAL:HG21	1:J:2334:PHE:CE2	2.48	0.48
1:D:839:LEU:HB3	1:D:1075:PHE:HE2	1.79	0.48
1:D:2500:ALA:HB2	1:D:2553:TYR:HD1	1.78	0.48
1:A:23:GLN:OE1	1:A:203:ASN:ND2	2.46	0.48
1:A:2349:ASN:OD1	1:A:3849:ARG:NH2	2.35	0.48
1:G:597:HIS:HB2	1:G:1665:HIS:ND1	2.28	0.48
1:G:1708:ARG:NH1	1:G:1836:PHE:O	2.47	0.48
1:J:2171:GLY:N	1:J:2174:GLU:OE2	2.47	0.48
1:J:2284:ASN:ND2	1:J:2342:ASN:HD22	2.12	0.48
1:D:3934:TYR:CZ	1:D:3998:HIS:HB3	2.49	0.47
1:A:102:LEU:HB2	1:A:105:HIS:CD2	2.49	0.47
1:A:712:TYR:HE1	1:A:1470:ARG:HE	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4843:LEU:HB2	1:G:4823:LEU:HD11	1.96	0.47
1:G:2467:VAL:HA	1:G:2470:ILE:HD12	1.96	0.47
1:G:3781:GLN:NE2	1:G:3819:TYR:OH	2.34	0.47
1:J:1245:PHE:CE2	1:J:1290:ARG:HD3	2.49	0.47
1:J:1451:GLY:HA3	1:J:1494:MET:HA	1.94	0.47
1:J:1685:LEU:HD21	1:J:1714:LEU:HD11	1.96	0.47
1:J:1930:LYS:O	1:J:1931:LEU:HD23	2.13	0.47
1:J:2573:GLU:HA	1:J:2576:ALA:HB2	1.96	0.47
1:D:213:TYR:HE2	1:D:337:PRO:HB2	1.79	0.47
1:D:1432:THR:HA	1:D:1520:VAL:O	2.13	0.47
1:D:2185:ILE:HD13	1:D:2203:MET:CE	2.44	0.47
1:A:1433:TYR:CD1	1:A:1573:MET:HB3	2.49	0.47
1:G:647:ASN:ND2	1:G:820:ARG:O	2.44	0.47
1:G:1944:GLU:HA	1:G:2123:LEU:HD11	1.97	0.47
1:G:2670:GLU:HA	1:G:2673:HIS:ND1	2.29	0.47
1:G:3903:LEU:HD22	1:G:3915:ILE:HG21	1.94	0.47
1:J:530:ILE:HG22	1:J:536:ASN:HB3	1.96	0.47
1:J:671:VAL:HG23	1:J:787:VAL:HG22	1.95	0.47
1:J:2611:CYS:CB	1:J:2643:LEU:HD11	2.44	0.47
1:J:2776:SER:O	1:J:2787:THR:HA	2.15	0.47
1:J:4680:LYS:O	1:J:4685:GLY:N	2.47	0.47
1:D:590:LEU:HD22	1:D:631:LEU:HD23	1.97	0.47
1:D:1579:MET:HG2	1:D:1595:LEU:HD11	1.97	0.47
1:A:1617:THR:HA	1:A:1628:VAL:HG12	1.97	0.47
1:A:2776:SER:O	1:A:2787:THR:HA	2.14	0.47
1:A:3842:LEU:O	1:A:3929:SER:HB3	2.15	0.47
1:G:650:VAL:HG11	1:G:662:TRP:CD1	2.48	0.47
1:G:1639:LEU:O	1:G:1647:CYS:HA	2.14	0.47
1:G:3784:SER:HA	1:G:3828:PHE:HA	1.96	0.47
1:G:3986:TRP:HA	1:G:3989:VAL:HG12	1.96	0.47
1:J:1732:SER:HB2	1:J:2140:ARG:NH1	2.29	0.47
1:D:674:PHE:CE1	1:D:679:ALA:HA	2.49	0.47
1:A:839:LEU:HD13	1:A:1075:PHE:HD2	1.79	0.47
1:G:120:CYS:HA	1:G:135:VAL:HA	1.95	0.47
1:G:1131:ARG:NH1	1:G:1178:ALA:O	2.46	0.47
1:G:1287:LEU:HD13	1:G:1289:LEU:CD1	2.44	0.47
1:G:1469:VAL:HG13	1:G:1492:CYS:HB3	1.96	0.47
1:G:1830:VAL:HB	1:G:1837:GLN:HG2	1.95	0.47
1:G:2161:GLN:HE21	1:G:2177:LEU:HD21	1.78	0.47
1:J:3829:PHE:HE2	1:J:3902:TYR:CE2	2.31	0.47
1:D:587:ILE:HG12	1:D:625:LEU:HD12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2124:LEU:HD21	1:D:3677:LEU:HD11	1.97	0.47
1:D:4661:TYR:HE1	1:D:4665:LYS:HD2	1.80	0.47
1:D:4802:GLY:HA2	1:D:4808:PHE:HB2	1.96	0.47
1:D:4904:PRO:HG3	1:D:4913:ARG:HD3	1.97	0.47
1:G:530:ILE:HD11	1:G:537:CYS:HA	1.97	0.47
1:G:1123:VAL:HG23	1:G:1132:TRP:HB2	1.96	0.47
1:G:2239:PHE:O	1:G:2242:ILE:HG22	2.14	0.47
1:G:4680:LYS:HD2	1:G:4686:LEU:HD22	1.97	0.47
1:J:523:TYR:CZ	1:J:560:ILE:HD11	2.49	0.47
1:J:707:VAL:O	1:J:713:SER:HB2	2.13	0.47
1:J:1105:ALA:HA	1:J:1121:ALA:HA	1.95	0.47
1:J:1288:PHE:HB3	1:J:1553:PHE:CE1	2.50	0.47
1:J:1291:LEU:HD12	1:J:1550:PRO:HG2	1.96	0.47
1:J:1933:GLU:HA	1:J:1936:LYS:HD2	1.97	0.47
1:J:2623:LEU:O	1:J:2627:VAL:HG23	2.14	0.47
1:J:3821:LYS:HE2	1:J:3902:TYR:HE1	1.80	0.47
1:J:4866:SER:HB3	1:J:4873:ASP:H	1.79	0.47
1:D:3779:VAL:HG13	1:D:3797:THR:HG22	1.95	0.47
1:D:3966:THR:HG22	1:D:4026:MET:HA	1.96	0.47
1:D:4087:LEU:HB3	1:D:4122:MET:HA	1.97	0.47
1:D:4192:ARG:HG3	1:D:5028:PHE:CD1	2.50	0.47
1:D:4548:ARG:O	1:D:4552:LEU:HD23	2.14	0.47
1:D:4927:ILE:O	1:D:4931:ILE:HG13	2.15	0.47
1:A:213:TYR:CG	1:A:338:GLU:CB	2.98	0.47
1:G:2776:SER:O	1:G:2787:THR:HA	2.15	0.47
1:J:2238:TYR:O	1:J:2242:ILE:HG12	2.14	0.47
1:J:3821:LYS:HE2	1:J:3902:TYR:CE1	2.49	0.47
1:D:4028:LEU:O	1:D:4031:LEU:HG	2.15	0.47
1:A:495:ASN:HB3	1:A:550:LYS:HZ1	1.80	0.47
1:A:614:VAL:HG12	1:A:2169:GLN:HG3	1.97	0.47
1:A:1802:ILE:HG13	1:A:1803:PRO:HD2	1.96	0.47
2:B:62:GLY:O	2:B:66:MET:HG2	2.14	0.47
1:G:299:LEU:HD22	1:G:376:ALA:HB3	1.97	0.47
1:G:589:LEU:HD12	1:G:593:HIS:ND1	2.29	0.47
1:G:1580:PHE:CE2	1:G:1592:PRO:HG2	2.50	0.47
1:G:2199:ARG:NH1	1:G:2246:ASN:OD1	2.47	0.47
1:G:2256:TYR:O	1:G:2260:ASN:ND2	2.48	0.47
1:G:3680:ALA:O	1:G:3681:GLY:C	2.53	0.47
1:G:3995:VAL:O	1:G:3999:MET:HG2	2.14	0.47
1:G:5017:ARG:CZ	1:G:5019:TRP:HH2	2.27	0.47
1:J:103:TYR:CD1	1:J:163:VAL:HG22	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:277:GLY:HA2	1:J:315:CYS:HB2	1.96	0.47
1:J:504:ALA:HB2	1:J:512:ALA:HB2	1.97	0.47
1:J:3768:SER:HA	1:J:3771:HIS:CE1	2.50	0.47
1:J:3962:PHE:HZ	1:J:3992:PHE:CE2	2.32	0.47
1:D:4850:LEU:O	1:D:4853:VAL:HG12	2.14	0.47
1:D:5019:TRP:HD1	1:D:5022:PHE:HE2	1.62	0.47
1:A:2238:TYR:O	1:A:2242:ILE:HG12	2.14	0.47
1:A:3965:LEU:HA	1:A:3968:TYR:HD2	1.78	0.47
1:G:753:PRO:HB2	1:G:770:ALA:H	1.80	0.47
1:G:1269:CYS:SG	1:G:1270:LEU:N	2.87	0.47
1:J:212:GLY:HA2	1:J:341:TYR:CD2	2.49	0.47
1:D:444:SER:O	1:D:448:LEU:HD23	2.15	0.47
1:D:4692:PRO:HB3	1:D:4703:ARG:HH12	1.80	0.47
1:A:492:ASP:O	1:A:496:VAL:HG23	2.15	0.47
1:A:1769:THR:HG22	1:A:1769:THR:O	2.15	0.47
1:A:2346:VAL:HG23	1:A:2349:ASN:HB2	1.97	0.47
1:G:3722:TYR:CD2	1:G:3793:MET:SD	3.08	0.47
1:J:619:ASP:HA	1:J:622:THR:HG22	1.96	0.47
1:J:1561:VAL:HG12	1:J:1562:ILE:H	1.80	0.47
1:D:1289:LEU:HD23	1:D:1564:PHE:CZ	2.50	0.47
1:D:3695:PRO:HB2	1:D:3699:HIS:HB3	1.97	0.47
1:D:3733:CYS:SG	1:D:3803:SER:OG	2.72	0.47
1:A:1719:HIS:CD2	1:A:1802:ILE:HD13	2.50	0.47
1:G:4961:CYS:SG	1:G:4983:HIS:HE1	2.17	0.47
1:J:150:MET:CE	1:J:163:VAL:HG21	2.45	0.47
1:D:1225:PRO:HD2	1:D:1228:ILE:HD13	1.97	0.46
1:D:1609:PRO:HD2	1:D:1612:PHE:CZ	2.50	0.46
1:D:1717:SER:HA	1:D:1721:GLU:HB2	1.96	0.46
1:D:2951:ILE:O	1:D:2955:PHE:N	2.44	0.46
3:F:29:THR:HA	3:F:62:GLY:HA2	1.97	0.46
1:A:716:PHE:HB3	1:A:721:LEU:HG	1.96	0.46
1:A:2196:ASN:OD1	1:A:2199:ARG:NH2	2.44	0.46
1:G:1671:ARG:HH22	1:G:1710:GLY:HA2	1.80	0.46
1:G:2142:TYR:OH	1:G:2194:HIS:ND1	2.46	0.46
1:G:3658:LYS:HG3	1:G:3662:ILE:HD11	1.97	0.46
1:G:3813:GLN:O	1:G:3899:PHE:HZ	1.97	0.46
1:G:4184:MET:HB3	1:G:5021:PHE:HA	1.97	0.46
1:J:1717:SER:HA	1:J:1721:GLU:HB2	1.97	0.46
1:J:3853:ALA:HA	1:J:3856:LEU:HD23	1.96	0.46
1:J:3904:ARG:HG2	1:J:3905:THR:HG22	1.96	0.46
1:J:4673:ARG:HD3	1:J:4778:TRP:CZ2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2567:PRO:HA	1:D:2613:TYR:CB	2.46	0.46
1:D:4708:THR:HB	1:D:4774:LYS:HD2	1.97	0.46
1:D:4888:TYR:CD1	1:J:4914:VAL:HG23	2.50	0.46
1:J:2102:VAL:HG13	1:J:2120:MET:CG	2.45	0.46
1:J:4968:PHE:CE2	1:J:4978:HIS:HB2	2.50	0.46
2:K:23:VAL:HG12	2:K:104:LEU:HB3	1.97	0.46
1:D:1687:SER:OG	2:E:36:PHE:O	2.21	0.46
1:A:687:ALA:HB3	1:A:778:PHE:CE1	2.50	0.46
1:A:2465:ASP:O	1:A:2469:ILE:HG12	2.15	0.46
1:G:214:VAL:HG22	1:G:341:TYR:CD2	2.49	0.46
1:G:1651:LEU:HD23	1:G:1702:HIS:HB2	1.96	0.46
1:G:2499:LYS:O	1:G:2503:VAL:HG12	2.15	0.46
1:G:4108:ILE:O	1:G:4112:LEU:HG	2.15	0.46
1:G:4655:PHE:HA	1:G:4796:MET:HE1	1.97	0.46
1:J:38:ALA:HB1	1:J:64:ILE:HG22	1.96	0.46
1:J:261:ARG:HH21	1:J:283:ARG:HD3	1.80	0.46
1:J:592:LYS:HB3	1:J:1592:PRO:HB3	1.97	0.46
1:J:1246:GLU:O	1:J:1598:GLN:HB2	2.14	0.46
1:J:4658:ILE:CD1	1:J:4792:LEU:HB3	2.45	0.46
1:D:664:PHE:HB2	1:D:793:LEU:HA	1.98	0.46
1:D:2193:GLN:HG2	3:F:10:ILE:HG21	1.97	0.46
1:D:2506:LEU:HD13	1:D:2510:TYR:HD2	1.81	0.46
1:D:2518:LEU:O	1:D:2522:LEU:HB3	2.15	0.46
2:E:39:SER:CA	2:E:42:ARG:NH2	2.70	0.46
1:A:149:THR:HG23	1:A:174:VAL:HG22	1.97	0.46
1:A:663:TYR:HB2	1:A:808:TYR:HB3	1.97	0.46
1:A:755:ILE:HB	1:A:768:PHE:HB2	1.96	0.46
1:A:4167:ALA:O	1:A:4171:LEU:HD13	2.14	0.46
1:A:4843:LEU:HD13	1:G:4823:LEU:HD12	1.98	0.46
1:G:711:LEU:HD13	1:G:1491:ASN:HB3	1.97	0.46
1:G:1247:PRO:HA	1:G:1598:GLN:HG2	1.97	0.46
1:G:4904:PRO:HG3	1:G:4913:ARG:HG2	1.97	0.46
1:G:4973:HIS:ND1	1:G:4973:HIS:O	2.48	0.46
1:J:2182:ILE:O	1:J:2185:ILE:HG22	2.16	0.46
1:D:4687:TYR:HE2	1:D:4703:ARG:HA	1.81	0.46
1:D:4876:CYS:HA	1:D:4882:CYS:HB2	1.97	0.46
1:A:1731:LEU:HD23	1:A:1772:ARG:HH12	1.80	0.46
1:A:3890:LEU:HA	1:A:3893:GLU:HB2	1.97	0.46
1:G:4159:ARG:HD3	1:G:4159:ARG:H	1.81	0.46
1:G:4217:PHE:CE1	1:G:4221:VAL:HG21	2.51	0.46
1:D:2212:VAL:HG22	1:D:2256:TYR:CZ	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3872:GLU:O	1:D:3876:ALA:HB2	2.16	0.46
1:A:241:GLN:O	1:A:243:ARG:NH1	2.49	0.46
1:A:662:TRP:CH2	1:A:814:ALA:HB2	2.49	0.46
1:A:2328:GLY:O	1:A:2332:LEU:HD23	2.15	0.46
1:A:4851:TYR:HD2	1:A:4920:PHE:HD2	1.63	0.46
1:G:607:CYS:SG	1:G:618:GLN:HG3	2.55	0.46
1:G:4704:LEU:O	1:G:4774:LYS:HE2	2.16	0.46
1:J:1124:PHE:HA	1:J:1131:ARG:HA	1.96	0.46
1:J:1673:VAL:HG12	1:J:1681:VAL:HG21	1.97	0.46
1:D:561:LEU:HD11	1:D:599:VAL:HG22	1.98	0.46
1:D:1272:LEU:HD13	1:D:1289:LEU:HD21	1.98	0.46
1:D:1747:LEU:HD11	1:D:2038:LEU:HA	1.98	0.46
1:D:4688:ILE:HG13	1:D:4689:THR:N	2.30	0.46
1:A:1578:ALA:O	1:A:1584:ARG:NH1	2.49	0.46
1:A:2103:VAL:O	1:A:2107:GLN:HG3	2.16	0.46
1:A:3951:PHE:HD2	1:A:4012:LEU:HD11	1.80	0.46
1:A:4994:TYR:OH	1:A:4998:LYS:NZ	2.34	0.46
1:J:206:CYS:SG	1:J:207:SER:N	2.89	0.46
1:J:1669:LEU:O	1:J:1673:VAL:HG23	2.16	0.46
1:J:1815:LEU:HD23	1:J:1862:ILE:HD11	1.96	0.46
1:J:2379:ALA:HB1	1:J:2426:TYR:HE2	1.81	0.46
1:J:4863:TYR:HD2	1:J:4876:CYS:CB	2.27	0.46
1:D:4235:VAL:HG21	1:D:5019:TRP:CD1	2.51	0.46
1:A:2035:HIS:O	1:A:2039:LEU:HD23	2.16	0.46
1:A:4049:VAL:HG21	1:A:4159:ARG:HD2	1.98	0.46
1:G:3679:LYS:HA	1:G:3679:LYS:HD2	1.58	0.46
1:A:114:SER:OG	1:A:116:MET:HG3	2.14	0.46
1:A:652:ARG:NE	1:A:750:LEU:O	2.47	0.46
1:A:1256:GLU:CB	1:A:1275:ARG:HE	2.29	0.46
1:A:2641:LEU:HD21	1:A:2699:ALA:HA	1.98	0.46
1:A:3102:ASP:O	1:A:3106:MET:HG2	2.14	0.46
1:G:544:LEU:HA	1:G:547:VAL:HG12	1.98	0.46
1:G:603:LEU:HB3	1:G:621:ILE:HD11	1.96	0.46
1:G:707:VAL:O	1:G:713:SER:HB2	2.16	0.46
1:G:3943:ILE:HD11	1:G:4002:LYS:NZ	2.29	0.46
2:K:40:ARG:O	2:K:43:ASN:ND2	2.49	0.46
1:D:414:PHE:CD1	1:D:436:LEU:HD12	2.51	0.46
1:A:714:TYR:OH	1:A:1472:VAL:HB	2.16	0.46
1:A:4927:ILE:HD12	1:G:4936:ILE:HG21	1.98	0.46
1:G:1970:GLN:HG3	1:G:3642:TYR:HA	1.97	0.46
1:G:2463:LEU:HB2	1:G:2510:TYR:CE2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:408:ALA:O	1:J:412:ASN:ND2	2.49	0.46
1:J:1473:THR:HA	1:J:1488:LYS:HA	1.97	0.46
1:J:2351:ASN:HB3	1:J:2355:ARG:HH22	1.81	0.46
1:J:2563:THR:HG23	1:J:2606:CYS:HA	1.98	0.46
1:J:3820:LEU:HD21	1:J:3902:TYR:CE2	2.51	0.46
1:D:2336:ARG:HA	1:D:2339:VAL:HG12	1.97	0.45
1:D:3736:GLU:HA	1:D:3766:GLN:HE22	1.80	0.45
1:D:4039:MET:O	1:D:4043:GLN:HG2	2.16	0.45
1:D:4819:GLY:O	1:D:4824:ARG:NH2	2.49	0.45
1:A:149:THR:OG1	1:A:172:VAL:O	2.31	0.45
1:A:634:GLN:HE21	1:A:702:TRP:HH2	1.64	0.45
1:A:2175:GLU:O	1:A:2179:ILE:HG12	2.15	0.45
1:A:2554:LEU:HA	1:A:2558:VAL:HG12	1.99	0.45
1:A:3886:ARG:HD2	1:A:3889:GLN:HE21	1.81	0.45
1:A:4335:LEU:O	1:A:4339:VAL:HG23	2.16	0.45
1:A:4567:LEU:HD11	1:A:4571:PHE:CZ	2.51	0.45
1:A:4679:ARG:HD3	1:A:5017:ARG:CZ	2.46	0.45
1:G:615:ARG:NH2	1:G:2168:VAL:HG11	2.31	0.45
1:G:2620:GLN:HA	1:G:2623:LEU:HB3	1.98	0.45
1:J:665:GLU:HA	1:J:745:SER:HA	1.97	0.45
1:J:2182:ILE:HA	1:J:2185:ILE:HG22	1.98	0.45
1:J:3102:ASP:O	1:J:3106:MET:HG2	2.15	0.45
1:A:180:LEU:HB3	1:A:200:TRP:NE1	2.31	0.45
1:A:551:LEU:HD21	1:A:589:LEU:HB2	1.98	0.45
1:A:1490:SER:HB2	1:A:1493:TYR:CE1	2.52	0.45
1:G:2119:ALA:O	1:G:2123:LEU:HD23	2.16	0.45
1:J:273:HIS:ND1	1:J:335:GLY:O	2.49	0.45
1:J:545:ASP:HA	1:J:548:VAL:HG12	1.97	0.45
1:J:1236:THR:O	1:J:1608:MET:HG3	2.16	0.45
1:J:2021:CYS:SG	1:J:2028:ARG:HD3	2.56	0.45
1:J:2495:VAL:HG12	1:J:2498:HIS:H	1.81	0.45
1:D:575:LEU:HD11	1:D:606:LEU:HA	1.98	0.45
1:D:2628:PHE:CD2	1:D:2906:VAL:CB	3.00	0.45
1:A:180:LEU:HB3	1:A:200:TRP:HE1	1.82	0.45
1:A:4160:LEU:HD12	1:A:4163:PHE:HD2	1.81	0.45
1:G:221:ARG:N	1:G:391:THR:O	2.48	0.45
1:G:3886:ARG:HD2	1:G:3889:GLN:NE2	2.25	0.45
1:J:1295:VAL:HG21	1:J:1575:LEU:HD11	1.98	0.45
1:J:1639:LEU:HD11	1:J:1653:LEU:HD11	1.98	0.45
1:D:1238:PHE:CE2	1:D:1240:LYS:HG3	2.52	0.45
2:E:21:THR:HA	2:E:49:ARG:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:55:VAL:HG11	2:B:59:PHE:HD2	1.82	0.45
1:G:1520:VAL:HG23	1:G:1527:MET:HG2	1.98	0.45
1:J:219:VAL:HG21	1:J:398:SER:HB3	1.97	0.45
1:J:572:PRO:HB3	1:J:609:CYS:SG	2.57	0.45
1:J:716:PHE:CZ	1:J:744:VAL:HG21	2.46	0.45
1:J:2500:ALA:CA	1:J:2553:TYR:HE1	2.29	0.45
1:J:4984:ASN:OD1	1:J:4987:ASN:N	2.41	0.45
1:D:247:TYR:HB2	1:D:374:LYS:HG3	1.98	0.45
1:D:1100:MET:HG2	1:D:1194:LEU:HA	1.97	0.45
1:D:1152:MET:HB3	1:D:1161:ILE:O	2.17	0.45
1:D:2463:LEU:HD13	1:D:2510:TYR:CD2	2.50	0.45
1:D:3673:MET:HE2	1:D:3728:ILE:HG12	1.98	0.45
1:D:3962:PHE:O	1:D:3966:THR:HG23	2.17	0.45
1:D:3965:LEU:HA	1:D:3968:TYR:CD2	2.51	0.45
1:D:4879:MET:HB3	1:A:4578:LEU:O	2.17	0.45
1:D:4927:ILE:HG23	1:D:4928:LEU:N	2.32	0.45
2:E:4:ILE:HG13	2:E:4:ILE:O	2.17	0.45
1:A:1125:ASN:HB2	1:A:1132:TRP:CD1	2.52	0.45
1:A:2204:HIS:HB2	1:A:2250:MET:HE1	1.99	0.45
1:A:2616:PRO:HD2	1:A:2664:PHE:CD2	2.52	0.45
1:A:4180:ARG:HG2	1:A:4194:TYR:CE1	2.51	0.45
1:G:594:GLY:H	1:G:1594:ARG:HB2	1.81	0.45
1:G:2002:PRO:O	1:G:2006:ILE:HG12	2.16	0.45
1:G:2336:ARG:HG3	1:G:2435:ARG:HD2	1.97	0.45
1:J:1088:TRP:HE3	1:J:1226:PHE:HA	1.80	0.45
1:J:2102:VAL:HG11	1:J:2124:LEU:HB2	1.98	0.45
2:K:66:MET:SD	2:K:70:GLN:HB3	2.57	0.45
1:D:2128:TYR:CD2	1:D:3673:MET:HG2	2.52	0.45
1:D:3801:GLY:O	1:D:3805:LEU:HB2	2.17	0.45
1:D:4961:CYS:HB3	1:D:4983:HIS:ND1	2.32	0.45
1:A:1469:VAL:HG13	1:A:1492:CYS:HB3	1.98	0.45
1:A:2118:ARG:HD2	1:A:3721:LEU:HD22	1.99	0.45
1:A:2212:VAL:HG21	1:A:2256:TYR:CE2	2.51	0.45
1:A:2340:PHE:CZ	1:A:2343:GLY:HA2	2.51	0.45
1:A:3966:THR:O	1:A:3970:GLN:HG2	2.16	0.45
1:A:4090:LYS:HG3	1:A:4112:LEU:HD22	1.99	0.45
1:G:1000:ARG:O	1:G:1004:GLY:N	2.49	0.45
1:J:615:ARG:HD3	1:J:1678:ASN:ND2	2.32	0.45
1:J:4654:ALA:HB1	1:J:4796:MET:HE1	1.98	0.45
2:K:91:ILE:HD12	2:K:97:LEU:HD22	1.98	0.45
1:A:790:ARG:HA	1:A:1627:ALA:HA	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1225:PRO:HG2	1:A:1228:ILE:HB	1.99	0.45
1:A:1667:LEU:HD22	1:A:1714:LEU:HD13	1.99	0.45
1:A:2354:VAL:HG23	1:A:2436:CYS:SG	2.57	0.45
2:B:23:VAL:HG12	2:B:47:LYS:HG2	1.98	0.45
1:G:1125:ASN:HD21	1:G:1127:HIS:CE1	2.35	0.45
1:G:1243:PRO:HG3	1:G:1460:HIS:HB2	1.98	0.45
1:G:3766:GLN:HG2	1:G:3769:ARG:HH21	1.81	0.45
1:G:3900:GLN:HB3	1:G:3976:ASN:ND2	2.32	0.45
1:J:152:PRO:HB2	1:J:157:ARG:CB	2.47	0.45
1:J:720:HIS:CE1	1:J:722:TRP:HE1	2.26	0.45
1:J:1426:ILE:O	1:J:1430:THR:N	2.50	0.45
1:J:3923:LEU:HD21	1:J:3962:PHE:CZ	2.52	0.45
1:J:4670:ILE:HD11	1:J:4778:TRP:CZ3	2.52	0.45
1:D:1667:LEU:HD22	1:D:1714:LEU:HD22	1.99	0.45
1:D:2503:VAL:HG11	1:D:2557:ALA:HB1	1.98	0.45
1:D:3725:TYR:HD1	1:D:3725:TYR:HA	1.70	0.45
1:D:4582:VAL:HB	1:J:4856:PHE:CZ	2.49	0.45
1:A:1713:ASP:HA	1:A:1716:ILE:HG22	1.98	0.45
1:G:635:THR:HG22	1:G:1639:LEU:HD23	1.98	0.45
1:G:686:TRP:HE3	1:G:777:PHE:HB3	1.81	0.45
1:G:1434:TYR:HE1	1:G:1517:GLY:HA3	1.81	0.45
1:G:1663:HIS:HD2	1:G:1707:LEU:HD22	1.81	0.45
1:G:3980:LEU:HD11	1:G:3985:LEU:HD22	1.99	0.45
1:J:1723:ALA:HB1	1:J:1775:HIS:CE1	2.52	0.45
1:J:2001:PRO:O	1:J:2005:GLN:HG3	2.16	0.45
1:J:2495:VAL:HB	1:J:2498:HIS:HB2	1.98	0.45
1:J:3986:TRP:HA	1:J:3989:VAL:HG12	1.99	0.45
1:D:636:ASN:HD21	2:E:35:LYS:NZ	2.15	0.45
1:D:3640:PRO:HG2	1:D:3643:ASN:HB2	1.98	0.45
1:D:4031:LEU:HD13	1:D:4149:ASN:ND2	2.32	0.45
1:D:4055:VAL:O	1:D:4058:ILE:HG22	2.16	0.45
1:D:4154:VAL:O	1:D:4154:VAL:HG13	2.17	0.45
1:A:117:TYR:O	1:A:138:GLN:N	2.45	0.45
1:A:4198:SER:HB2	1:A:4201:ASN:ND2	2.32	0.45
1:G:590:LEU:HD22	1:G:631:LEU:HD23	1.99	0.45
1:G:1663:HIS:HD2	1:G:1707:LEU:CD2	2.30	0.45
1:G:1944:GLU:CA	1:G:2123:LEU:HD11	2.47	0.45
1:G:4671:PHE:HB2	1:G:4714:ASN:HB3	1.98	0.45
1:G:4852:THR:HG21	1:G:4883:TYR:HD1	1.82	0.45
1:J:35:LEU:HD13	1:J:49:LEU:HD23	1.99	0.45
1:J:3777:GLU:O	1:J:3781:GLN:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:4631:PHE:CE2	1:J:4639:MET:HG3	2.52	0.45
1:J:4863:TYR:CE1	1:J:4901:ILE:HG12	2.52	0.45
1:D:707:VAL:O	1:D:713:SER:HB2	2.17	0.45
1:D:1432:THR:HA	1:D:1521:ASP:HA	1.99	0.45
1:D:2504:LEU:HD22	1:D:2508:ARG:HG3	1.99	0.45
1:A:2112:GLN:OE1	1:A:2112:GLN:N	2.50	0.45
1:G:1297:PHE:HB2	1:G:1544:PRO:O	2.17	0.45
1:G:2555:CYS:SG	1:G:2599:GLN:HG2	2.57	0.45
1:G:4045:VAL:HG22	1:G:4160:LEU:HD21	1.98	0.45
1:J:753:PRO:HB3	1:J:771:PHE:CE2	2.52	0.45
1:J:1255:TYR:CE1	1:J:1274:HIS:HD2	2.32	0.45
1:J:1561:VAL:HG12	1:J:1562:ILE:N	2.32	0.45
1:D:284:HIS:HB3	1:D:287:THR:HG22	1.99	0.44
1:D:663:TYR:HB2	1:D:808:TYR:HB3	1.99	0.44
1:D:1205:GLY:HA2	1:D:1211:LEU:CD1	2.42	0.44
1:D:2495:VAL:HG12	1:D:2497:ASP:H	1.83	0.44
1:A:209:CYS:SG	1:A:273:HIS:NE2	2.89	0.44
1:A:247:TYR:HB2	1:A:374:LYS:HG3	1.98	0.44
1:A:652:ARG:HD2	1:A:773:LEU:HD22	1.99	0.44
2:B:67:SER:OG	2:B:70:GLN:OE1	2.28	0.44
1:J:110:ARG:HA	1:J:117:TYR:HA	1.97	0.44
1:J:411:TYR:O	1:J:415:ILE:HG12	2.16	0.44
1:J:2346:VAL:HG23	1:J:2349:ASN:HB2	1.99	0.44
1:J:4183:ILE:HG12	1:J:4193:ILE:HD13	1.98	0.44
1:J:4995:LEU:HD23	1:J:5011:TRP:HE3	1.81	0.44
2:K:25:HIS:HB2	2:K:39:SER:HB2	1.97	0.44
1:D:698:GLY:O	1:D:703:GLY:HA2	2.17	0.44
1:D:3897:ASN:OD1	1:D:3898:ASP:N	2.50	0.44
1:A:2114:PRO:HB3	1:A:3707:ARG:HH21	1.82	0.44
1:A:3003:LEU:HB2	1:A:3004:PRO:HD3	2.00	0.44
1:A:4675:LYS:HG3	1:A:4679:ARG:HE	1.82	0.44
1:G:266:ARG:HH21	1:G:272:SER:HB3	1.82	0.44
1:G:491:ILE:HG12	1:G:523:TYR:CE1	2.52	0.44
1:G:2500:ALA:HB2	1:G:2553:TYR:HD1	1.81	0.44
1:G:4154:VAL:O	1:G:4154:VAL:HG13	2.18	0.44
1:J:526:LEU:HD11	1:J:540:PHE:HZ	1.83	0.44
1:J:1469:VAL:HG13	1:J:1492:CYS:HB3	1.99	0.44
1:J:1641:ILE:HG22	1:J:1643:GLU:HG2	2.00	0.44
1:D:790:ARG:HA	1:D:1627:ALA:HA	1.98	0.44
1:D:1101:ARG:HH21	1:D:1125:ASN:HD22	1.65	0.44
1:D:1435:TYR:HE1	1:D:1452:TRP:CZ2	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1676:LEU:HA	1:D:1725:ARG:HH12	1.81	0.44
1:D:2515:GLN:HB2	1:D:2568:LEU:HD11	2.00	0.44
1:D:4149:ASN:ND2	1:D:4153:HIS:HD2	2.14	0.44
1:A:20:VAL:HG21	1:A:202:MET:SD	2.58	0.44
1:A:355:LEU:HB2	1:A:378:LEU:HD23	1.99	0.44
1:A:445:LEU:HB3	1:A:521:LEU:HB3	1.99	0.44
1:A:1641:ILE:HG22	1:A:1643:GLU:HG2	1.99	0.44
1:G:243:ARG:HA	1:G:301:VAL:HG22	1.99	0.44
1:G:2182:ILE:O	1:G:2186:MET:HG2	2.18	0.44
1:G:4548:ARG:HD2	1:G:4552:LEU:HD13	2.00	0.44
1:J:411:TYR:HB3	1:J:486:LEU:HD21	1.99	0.44
1:J:583:ILE:O	1:J:587:ILE:HG13	2.17	0.44
1:J:1271:ARG:HA	1:J:1563:GLN:HB2	1.99	0.44
1:J:1434:TYR:HB3	1:J:1572:ILE:HG21	1.98	0.44
1:J:4226:GLY:O	1:J:4230:LYS:HG3	2.18	0.44
1:J:4687:TYR:HB3	1:J:4740:LEU:HD21	1.98	0.44
1:D:1451:GLY:HA3	1:D:1494:MET:HA	1.98	0.44
1:D:2959:PHE:HE2	1:D:3009:TYR:CZ	2.35	0.44
1:D:4060:LYS:HD2	1:D:4060:LYS:HA	1.83	0.44
1:A:102:LEU:HB2	1:A:105:HIS:HD2	1.82	0.44
1:A:2359:ARG:NE	1:A:2359:ARG:HA	2.33	0.44
1:A:4017:LEU:HD22	1:A:4139:ILE:HG21	1.99	0.44
1:G:37:LEU:HD13	1:G:191:VAL:HG11	1.99	0.44
1:G:551:LEU:HA	1:G:560:ILE:HG21	1.99	0.44
1:G:2439:GLU:OE2	1:G:2508:ARG:NH2	2.50	0.44
1:G:3723:MET:HE3	1:G:3723:MET:HB3	1.76	0.44
1:G:3886:ARG:HG3	1:G:3890:LEU:HD13	1.99	0.44
1:G:4041:ALA:O	1:G:4045:VAL:HG23	2.17	0.44
1:G:4235:VAL:HG21	1:G:5019:TRP:NE1	2.33	0.44
1:J:1601:MET:HE3	1:J:1602:PRO:HD2	1.98	0.44
1:J:2293:GLN:O	1:J:2296:GLU:HG3	2.17	0.44
1:J:3678:SER:HB2	1:J:3773:ARG:HH21	1.82	0.44
1:D:839:LEU:HD13	1:D:1075:PHE:CD2	2.52	0.44
1:D:2959:PHE:CE2	1:D:3009:TYR:CZ	3.05	0.44
1:A:209:CYS:HG	1:A:273:HIS:HE2	1.65	0.44
1:A:2178:MET:O	1:A:2182:ILE:HG12	2.17	0.44
1:A:4323:THR:OG1	1:A:4324:ALA:N	2.50	0.44
1:A:4961:CYS:HB3	1:A:4983:HIS:CE1	2.52	0.44
1:G:20:VAL:HG21	1:G:202:MET:SD	2.57	0.44
1:G:4979:THR:HG21	6:G:5103:ATP:H3'	1.99	0.44
1:J:444:SER:O	1:J:448:LEU:HD23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1438:ARG:NH2	1:J:1513:ASP:OD2	2.50	0.44
1:J:1451:GLY:CA	1:J:1494:MET:HG2	2.48	0.44
1:J:3003:LEU:HB3	1:J:3004:PRO:HD3	1.99	0.44
1:D:4910:GLU:O	1:D:4914:VAL:HG23	2.18	0.44
1:D:4998:LYS:HD3	1:D:5002:GLU:HG2	2.00	0.44
1:G:2518:LEU:HD13	1:G:2568:LEU:HD23	1.99	0.44
1:G:2671:GLU:O	1:G:2675:THR:HG23	2.17	0.44
1:J:2280:VAL:O	1:J:2280:VAL:HG13	2.17	0.44
1:J:2500:ALA:HB2	1:J:2553:TYR:HD1	1.83	0.44
1:J:4562:LEU:HD12	1:J:4565:LEU:HD11	2.00	0.44
1:D:518:ILE:O	1:D:522:LEU:HD23	2.18	0.44
1:D:1126:GLY:HA3	1:D:1143:TRP:CZ3	2.52	0.44
1:D:3955:MET:HB2	1:D:4019:LEU:HD23	2.00	0.44
1:D:4554:TYR:HA	1:D:4557:ARG:HH21	1.82	0.44
1:A:1450:VAL:HG22	1:A:1552:VAL:HG22	2.00	0.44
1:A:4054:ASN:O	1:A:4058:ILE:HG12	2.17	0.44
1:G:452:PHE:HZ	1:G:478:PHE:CD2	2.33	0.44
1:G:657:THR:HB	1:G:851:PHE:CE2	2.53	0.44
1:G:4096:ALA:O	1:G:4100:GLN:HG2	2.17	0.44
1:G:4180:ARG:HG2	1:G:4194:TYR:CE1	2.53	0.44
1:G:4555:LEU:HD13	1:G:4656:LEU:HG	1.99	0.44
1:G:4586:PRO:HB3	1:G:4628:VAL:HG11	1.99	0.44
1:G:4791:TYR:HD1	1:G:4792:LEU:HD23	1.82	0.44
3:I:29:THR:O	3:I:33:LEU:N	2.47	0.44
1:J:671:VAL:HG12	1:J:740:PRO:HD3	2.00	0.44
1:J:2294:ASP:O	1:J:2298:VAL:HG23	2.17	0.44
1:J:3445:TRP:HE3	1:J:3451:PHE:HD2	1.64	0.44
1:J:4667:PRO:O	1:J:4670:ILE:HG22	2.18	0.44
1:D:716:PHE:HD2	1:D:718:GLY:N	2.12	0.44
1:D:1931:LEU:HD22	1:D:1935:VAL:HG11	1.99	0.44
1:D:2420:HIS:CD2	1:D:2491:SER:HA	2.53	0.44
1:D:2875:ALA:HB1	1:D:2923:ALA:C	2.38	0.44
1:D:3135:ALA:O	1:D:3139:VAL:N	2.45	0.44
1:D:4979:THR:HG21	6:D:5103:ATP:H2'	1.99	0.44
1:A:441:VAL:O	1:A:445:LEU:HD23	2.18	0.44
1:A:667:MET:HA	1:A:743:VAL:HA	1.99	0.44
1:A:1085:SER:OG	1:A:1086:GLY:N	2.51	0.44
1:A:2159:LEU:HD22	1:A:2201:LEU:HD23	2.00	0.44
1:A:4823:LEU:O	1:A:4827:LEU:HD23	2.18	0.44
1:G:1245:PHE:CG	1:G:1290:ARG:HD3	2.52	0.44
1:G:1815:LEU:HD22	1:G:1845:VAL:HG21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4642:ALA:O	1:G:4646:LEU:HD23	2.18	0.44
1:G:4675:LYS:HD2	1:G:4679:ARG:HH21	1.83	0.44
1:J:1442:GLY:O	1:J:1557:THR:OG1	2.35	0.44
1:J:4185:GLY:HA3	1:J:5009:TYR:CE2	2.52	0.44
1:D:1580:PHE:CE1	1:D:1592:PRO:HG2	2.53	0.44
1:D:1849:LEU:HG	1:D:1854:PHE:HD2	1.81	0.44
1:A:2298:VAL:HG21	1:A:2334:PHE:CE2	2.53	0.44
1:G:1214:PHE:CE2	1:G:1225:PRO:HD3	2.53	0.44
1:G:2611:CYS:CB	1:G:2643:LEU:HD11	2.48	0.44
1:J:3423:TRP:O	1:J:3423:TRP:CG	2.71	0.44
2:K:71:ARG:HG2	2:K:102:GLU:HG3	1.99	0.44
1:D:1289:LEU:HD23	1:D:1564:PHE:CE2	2.52	0.43
1:D:1742:THR:O	1:D:1745:ILE:HG22	2.18	0.43
1:D:2522:LEU:HG	1:D:2523:ASP:N	2.33	0.43
1:D:2638:LYS:HE2	1:D:2695:LEU:HA	1.99	0.43
1:G:660:GLY:HA2	1:G:750:LEU:HD12	2.00	0.43
1:G:2211:MET:HA	1:G:2214:VAL:HG12	2.00	0.43
1:J:1235:THR:HG21	1:J:1607:ARG:HH21	1.82	0.43
1:J:3445:TRP:CE3	1:J:3451:PHE:HD2	2.36	0.43
1:J:3658:LYS:HG3	1:J:3662:ILE:HD11	2.00	0.43
1:J:3889:GLN:O	1:J:3893:GLU:N	2.51	0.43
1:J:4562:LEU:HD21	1:J:4656:LEU:HB3	1.99	0.43
1:J:4926:VAL:HG13	1:J:4927:ILE:HG13	2.00	0.43
1:D:2225:PHE:O	1:D:2229:VAL:HG23	2.18	0.43
1:A:2365:GLY:HA3	1:A:2426:TYR:HE1	1.82	0.43
1:A:4984:ASN:HB3	1:A:4987:ASN:HB2	2.00	0.43
1:G:561:LEU:HD21	1:G:598:LYS:HB2	2.00	0.43
1:G:581:ASN:OD1	1:G:582:HIS:N	2.51	0.43
1:G:2012:PHE:HB2	1:G:3661:TRP:HZ2	1.84	0.43
1:G:4181:ILE:HB	1:G:4988:TYR:CE1	2.53	0.43
1:J:1076:ARG:O	1:J:1237:TRP:N	2.32	0.43
1:J:1077:ALA:HA	1:J:1236:THR:HA	1.99	0.43
1:D:3536:ALA:HB1	1:D:3597:GLN:HA	2.00	0.43
1:A:214:VAL:HG22	1:A:341:TYR:CE1	2.53	0.43
1:A:582:HIS:O	1:A:586:ILE:HG13	2.18	0.43
1:A:1171:SER:OG	1:A:1175:SER:N	2.52	0.43
1:A:1619:ARG:HA	1:A:1626:TRP:HA	2.00	0.43
1:G:540:PHE:HD2	1:G:567:VAL:HG21	1.83	0.43
1:G:1158:ASN:ND2	1:G:1182:ILE:O	2.51	0.43
1:J:1074:ILE:CD1	1:J:1115:LEU:HD12	2.49	0.43
1:J:1556:PRO:HB3	1:J:1561:VAL:HG21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:2293:GLN:HA	1:J:2296:GLU:HG3	1.99	0.43
1:J:4066:LEU:HD13	1:J:4170:ILE:HA	1.99	0.43
1:D:1427:ILE:CD1	1:D:1571:ASN:HA	2.47	0.43
1:D:1771:LEU:HD11	1:D:2153:MET:SD	2.59	0.43
1:A:2323:TRP:HH2	1:A:2422:ILE:HG13	1.82	0.43
1:A:3836:MET:HA	1:A:3839:CYS:SG	2.58	0.43
1:A:4235:VAL:HG11	1:A:5019:TRP:CZ2	2.54	0.43
1:G:2430:ILE:HG21	1:G:2502:MET:HE3	2.01	0.43
1:G:3136:LEU:O	1:G:3140:LEU:N	2.39	0.43
1:G:3695:PRO:HB2	1:G:3699:HIS:HB3	2.01	0.43
2:H:10:GLY:CA	2:H:70:GLN:HB2	2.38	0.43
1:J:2240:CYS:HB2	1:J:2250:MET:HG2	1.99	0.43
1:J:2297:LYS:HG2	1:J:2301:TYR:CE2	2.54	0.43
1:J:2351:ASN:HB3	1:J:2355:ARG:NH2	2.32	0.43
1:J:4020:GLN:HG3	1:J:4139:ILE:CD1	2.49	0.43
1:D:445:LEU:HD11	1:D:522:LEU:HD13	2.00	0.43
1:D:711:LEU:HD12	1:D:1491:ASN:HB3	1.99	0.43
1:D:723:THR:O	1:D:726:VAL:HG12	2.17	0.43
1:D:850:ASP:O	1:D:1023:PRO:HG3	2.19	0.43
1:D:1651:LEU:HD12	1:D:1651:LEU:H	1.82	0.43
1:D:2346:VAL:HG23	1:D:2349:ASN:HB2	2.00	0.43
1:D:2669:GLU:HA	1:D:2672:LEU:HD12	2.01	0.43
1:A:275:ARG:HB3	1:A:336:PRO:CG	2.48	0.43
1:A:3980:LEU:HD23	1:A:3980:LEU:HA	1.78	0.43
1:J:16:THR:HG22	1:J:98:HIS:HA	1.99	0.43
1:J:1074:ILE:HD11	1:J:1115:LEU:HD12	2.01	0.43
1:J:4576:ILE:HG21	1:J:4643:LEU:HB2	1.99	0.43
1:D:495:ASN:OD1	1:D:553:ARG:NH1	2.52	0.43
1:D:4027:LEU:HD23	1:D:4027:LEU:HA	1.90	0.43
1:D:4149:ASN:HD21	1:D:4153:HIS:HD2	1.66	0.43
1:A:590:LEU:HB2	1:A:599:VAL:HG11	2.00	0.43
1:A:2470:ILE:HG21	1:A:2526:PHE:CE1	2.53	0.43
1:A:4705:VAL:HB	1:A:4778:TRP:CG	2.54	0.43
1:A:4883:TYR:CE1	1:A:4887:MET:HE3	2.54	0.43
1:G:2142:TYR:HE1	1:G:3651:ASN:ND2	2.17	0.43
1:G:4655:PHE:CA	1:G:4796:MET:HE1	2.49	0.43
1:J:626:LEU:HB3	1:J:1688:HIS:NE2	2.33	0.43
1:J:716:PHE:CD1	1:J:757:PHE:CD2	3.07	0.43
1:J:3716:LEU:HD21	1:J:3785:ALA:HB1	2.01	0.43
1:D:633:LEU:HD21	1:D:1659:LEU:HD12	1.99	0.43
1:D:647:ASN:OD1	1:D:822:ARG:N	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3351:PRO:O	1:D:3353:LEU:N	2.51	0.43
1:D:4182:GLU:O	1:D:4183:ILE:HD13	2.19	0.43
1:D:4562:LEU:HG	1:D:4653:VAL:HG13	2.01	0.43
1:A:1989:ALA:O	1:A:1993:ARG:HG2	2.18	0.43
1:A:4687:TYR:CG	1:A:4706:LEU:HD11	2.53	0.43
1:G:3729:MET:HB3	1:G:3770:LEU:HD13	2.00	0.43
1:J:23:GLN:HE22	1:J:267:ILE:HD12	1.82	0.43
1:J:107:ILE:N	1:J:148:TRP:O	2.42	0.43
1:J:272:SER:HB2	1:J:334:MET:HA	2.01	0.43
1:J:625:LEU:HD21	1:J:632:LEU:HD11	2.00	0.43
1:J:1454:THR:OG1	1:J:1455:PRO:HD2	2.19	0.43
1:J:2671:GLU:O	1:J:2675:THR:HG23	2.19	0.43
1:J:2823:ILE:HA	1:J:2936:ALA:O	2.18	0.43
1:J:4842:GLY:O	1:J:4846:VAL:HG23	2.18	0.43
1:J:4973:HIS:O	1:J:4977:THR:HG23	2.18	0.43
1:D:688:LEU:HD13	1:D:712:TYR:O	2.19	0.43
1:D:1464:PHE:CE2	1:D:1553:PHE:HD2	2.37	0.43
1:D:4849:TYR:O	1:D:4852:THR:HG22	2.19	0.43
1:D:5000:GLU:HA	1:D:5003:HIS:CD2	2.54	0.43
1:A:979:PRO:HB2	1:A:980:ALA:H	1.66	0.43
1:A:2500:ALA:N	1:A:2553:TYR:HE1	2.16	0.43
1:A:2554:LEU:O	1:A:2559:LEU:HD23	2.18	0.43
1:G:475:GLN:OE1	1:G:532:GLY:HA3	2.19	0.43
1:G:1933:GLU:HA	1:G:1936:LYS:HD3	2.00	0.43
1:J:701:GLY:HA2	1:J:1645:ASN:OD1	2.18	0.43
1:J:1073:ARG:HG2	1:J:1075:PHE:CE1	2.53	0.43
1:J:1237:TRP:CH2	1:J:1652:GLU:HG3	2.47	0.43
1:J:3722:TYR:CE1	1:J:3726:ALA:HB2	2.53	0.43
1:J:4069:LYS:HA	1:J:4069:LYS:HD3	1.91	0.43
1:J:4190:ILE:H	1:J:4190:ILE:HD12	1.84	0.43
1:D:2161:GLN:HE21	1:D:2165:LEU:HG	1.84	0.43
1:D:4017:LEU:HD12	1:D:4139:ILE:HG21	2.01	0.43
1:A:634:GLN:NE2	1:A:702:TRP:HH2	2.17	0.43
1:A:1228:ILE:CG2	1:A:1827:ARG:HH12	2.31	0.43
1:A:2336:ARG:HD3	1:A:2435:ARG:HD2	2.00	0.43
1:A:2960:LEU:HD11	1:A:3017:PHE:HZ	1.83	0.43
1:A:4805:ASN:HB3	1:A:4808:PHE:HD2	1.83	0.43
1:G:737:LEU:HD23	1:G:738:LEU:N	2.33	0.43
1:G:1131:ARG:HD2	1:G:1179:PHE:CE1	2.53	0.43
1:G:1687:SER:HB3	1:G:1782:PHE:CE2	2.53	0.43
1:J:470:SER:OG	1:J:474:ARG:NH2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1293:LEU:HB2	1:J:1579:MET:CE	2.49	0.43
1:J:2500:ALA:HB2	1:J:2553:TYR:CD1	2.54	0.43
1:J:4066:LEU:HD11	1:J:4173:TYR:HB3	2.01	0.43
1:J:4777:ILE:HA	1:J:4780:PHE:CD2	2.53	0.43
1:D:830:ARG:HH21	1:D:1612:PHE:CB	2.31	0.43
1:D:1089:TYR:O	1:D:1225:PRO:HA	2.19	0.43
1:D:1965:TYR:CZ	1:D:2031:LEU:HB2	2.53	0.43
2:E:91:ILE:HD12	2:E:97:LEU:HD21	2.00	0.43
1:A:753:PRO:HB3	1:A:771:PHE:CZ	2.54	0.43
1:A:846:LEU:HD22	1:A:1026:LEU:HD21	2.01	0.43
1:A:1228:ILE:HG23	1:A:1827:ARG:HH12	1.84	0.43
1:A:1433:TYR:CD1	1:A:1578:ALA:HB2	2.53	0.43
1:G:2305:CYS:HG	1:G:2331:TYR:HE2	1.66	0.43
1:G:4586:PRO:HA	1:G:4587:PRO:HD3	1.88	0.43
1:G:4844:LEU:HD12	1:G:4928:LEU:HB3	2.01	0.43
1:J:19:GLU:HA	1:J:68:THR:HA	2.01	0.43
1:J:213:TYR:HB3	1:J:273:HIS:CD2	2.53	0.43
1:J:791:PHE:N	1:J:1626:TRP:O	2.52	0.43
1:J:1684:ALA:HB1	2:K:89:GLY:HA3	2.01	0.43
1:J:4833:ASN:ND2	1:J:4939:ALA:HB2	2.33	0.43
1:J:5017:ARG:CZ	1:J:5019:TRP:HH2	2.32	0.43
1:D:119:SER:OG	1:D:120:CYS:N	2.51	0.42
1:D:597:HIS:HB2	1:D:1665:HIS:ND1	2.33	0.42
1:D:1073:ARG:HB3	1:D:1075:PHE:CE1	2.54	0.42
1:D:1087:ARG:NH1	1:D:1221:GLU:O	2.52	0.42
1:D:1689:VAL:HA	1:D:1693:GLN:OE1	2.18	0.42
1:D:1713:ASP:O	1:D:1716:ILE:HG22	2.19	0.42
1:D:2638:LYS:HZ1	1:D:2695:LEU:HA	1.83	0.42
1:D:4581:LYS:HE2	1:D:4632:LEU:HB3	2.00	0.42
1:D:4701:TRP:CZ2	1:D:4781:GLY:HA3	2.54	0.42
1:D:4715:TYR:CE2	1:D:4717:ASP:HB2	2.54	0.42
1:A:1426:ILE:O	1:A:1430:THR:N	2.52	0.42
1:A:1849:LEU:CD2	1:A:1854:PHE:HD2	2.32	0.42
1:A:2123:LEU:O	1:A:2127:GLN:HG2	2.19	0.42
1:G:2548:LEU:O	1:G:2552:ARG:HG3	2.19	0.42
1:J:582:HIS:O	1:J:586:ILE:HG13	2.19	0.42
1:J:2518:LEU:HD21	1:J:2569:PHE:HE1	1.79	0.42
1:J:4146:LEU:O	1:J:4150:LEU:HD23	2.19	0.42
1:J:4569:LEU:HD21	1:J:4649:LEU:HG	2.01	0.42
1:D:716:PHE:HE1	1:D:757:PHE:CG	2.36	0.42
1:D:1290:ARG:HD2	1:D:1291:LEU:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2437:ALA:HB3	1:D:2508:ARG:HE	1.84	0.42
1:D:2879:ALA:HB2	1:D:2923:ALA:CB	2.49	0.42
1:A:637:LEU:HD23	1:A:1693:GLN:HA	2.01	0.42
1:A:1717:SER:HA	1:A:1721:GLU:HB2	2.01	0.42
1:A:2355:ARG:HA	1:A:2358:ILE:HG22	2.00	0.42
1:A:3701:LEU:HD11	1:A:3705:PHE:CZ	2.54	0.42
1:A:4154:VAL:O	1:A:4154:VAL:HG13	2.19	0.42
1:A:4683:PHE:HZ	1:A:5017:ARG:HG3	1.84	0.42
1:G:2102:VAL:HG13	1:G:2120:MET:CG	2.49	0.42
1:G:2240:CYS:SG	1:G:2250:MET:HG2	2.59	0.42
1:G:3886:ARG:HE	1:G:3890:LEU:HD11	1.85	0.42
1:G:3966:THR:O	1:G:3970:GLN:HG2	2.18	0.42
1:J:1727:ARG:HG3	1:J:1775:HIS:HE1	1.83	0.42
1:D:76:ARG:CZ	1:A:3844:LEU:HD23	2.49	0.42
1:D:2821:TRP:HA	1:D:2939:ARG:N	2.34	0.42
1:D:4068:LEU:O	1:D:4072:VAL:HG23	2.20	0.42
1:D:4338:VAL:HG11	1:J:4838:VAL:HG11	2.01	0.42
2:E:56:ILE:HG23	2:E:59:PHE:H	1.83	0.42
1:A:517:GLU:O	1:A:521:LEU:HD13	2.19	0.42
1:A:1849:LEU:HD23	1:A:1854:PHE:HD2	1.85	0.42
1:A:2823:ILE:HA	1:A:2936:ALA:O	2.18	0.42
1:A:3007:ASN:HA	1:A:3010:PHE:CE1	2.54	0.42
1:A:4040:ILE:H	1:A:4040:ILE:HD12	1.83	0.42
1:G:1966:VAL:HG21	1:G:3649:ALA:HB1	2.02	0.42
1:G:3722:TYR:CE1	1:G:3782:MET:HE1	2.53	0.42
1:J:345:LEU:HD23	1:J:387:ALA:HB1	2.00	0.42
1:J:3650:CYS:O	1:J:3654:LEU:HG	2.19	0.42
1:J:4851:TYR:HE2	1:J:4920:PHE:HA	1.84	0.42
3:L:66:PHE:O	3:L:70:LEU:HD23	2.19	0.42
1:D:535:ALA:O	1:D:539:LEU:HD23	2.20	0.42
1:D:1466:LEU:HD11	1:D:1496:TRP:HB2	2.02	0.42
1:D:2207:VAL:HG21	1:D:2235:PHE:CE2	2.54	0.42
1:D:2505:PHE:CE1	1:D:2509:VAL:HG21	2.54	0.42
1:D:3890:LEU:HA	1:D:3893:GLU:HB2	2.00	0.42
1:A:261:ARG:HB2	1:A:285:VAL:HG12	2.02	0.42
1:G:116:MET:SD	1:G:139:GLU:HA	2.59	0.42
1:G:575:LEU:HD22	1:G:609:CYS:SG	2.59	0.42
1:G:1072:VAL:HG23	1:G:1194:LEU:O	2.19	0.42
1:G:1099:GLU:HA	1:G:1127:HIS:ND1	2.34	0.42
1:G:2641:LEU:O	1:G:2644:LEU:HG	2.18	0.42
1:G:4180:ARG:HG2	1:G:4194:TYR:HE1	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4184:MET:N	1:G:5021:PHE:O	2.48	0.42
1:J:839:LEU:HB3	1:J:1194:LEU:HD11	2.00	0.42
1:J:1259:ARG:NH1	1:J:1595:LEU:O	2.52	0.42
1:J:2335:LEU:O	1:J:2339:VAL:HG23	2.20	0.42
1:D:1235:THR:HG21	1:D:1607:ARG:HH21	1.85	0.42
1:D:3999:MET:HG3	1:D:4016:LEU:HD21	2.01	0.42
1:A:635:THR:CB	1:A:1693:GLN:HE22	2.29	0.42
1:A:645:ARG:HG3	1:A:778:PHE:CD1	2.54	0.42
1:A:3834:ALA:O	1:A:3838:THR:HG23	2.20	0.42
1:G:504:ALA:HB2	1:G:512:ALA:HB2	2.00	0.42
1:J:2290:LEU:HD23	1:J:2291:GLN:O	2.19	0.42
1:J:4901:ILE:HG22	1:J:4902:GLU:O	2.19	0.42
1:J:4974:GLY:O	1:J:4977:THR:OG1	2.22	0.42
1:D:14:LEU:HD23	1:D:14:LEU:HA	1.77	0.42
1:A:400:ALA:O	1:A:404:ILE:HG12	2.20	0.42
1:A:2273:LEU:HD23	1:A:2330:ARG:HB3	2.02	0.42
1:A:2453:ILE:HA	1:A:2456:ILE:HG22	2.02	0.42
1:A:3848:GLU:HA	1:A:3851:ASN:ND2	2.35	0.42
1:G:615:ARG:HD2	1:G:1678:ASN:HD21	1.84	0.42
1:G:4138:ASP:O	1:G:4142:ASN:ND2	2.44	0.42
1:G:4927:ILE:O	1:G:4931:ILE:HG13	2.18	0.42
1:J:2142:TYR:CD2	1:J:2197:LEU:HD12	2.54	0.42
1:J:3829:PHE:CD2	1:J:3906:GLN:HG2	2.55	0.42
1:J:4218:ILE:HD12	1:J:4218:ILE:HA	1.95	0.42
1:D:110:ARG:HD3	1:D:115:ARG:HH21	1.84	0.42
1:D:283:ARG:HH21	1:D:288:GLY:HA2	1.84	0.42
1:D:1794:ALA:HA	1:D:1795:PRO:HD3	1.93	0.42
1:D:2573:GLU:HA	1:D:2618:MET:CE	2.49	0.42
1:D:4104:THR:O	1:D:4108:ILE:N	2.50	0.42
1:A:1451:GLY:HA3	1:A:1494:MET:HA	2.01	0.42
1:A:2670:GLU:O	1:A:2674:LEU:HD23	2.20	0.42
1:A:4666:VAL:O	1:A:4670:ILE:HG12	2.20	0.42
1:G:638:ILE:HD12	1:G:702:TRP:CD1	2.54	0.42
1:G:716:PHE:HE1	1:G:757:PHE:CG	2.37	0.42
1:G:1130:GLN:HG3	1:G:1132:TRP:NE1	2.35	0.42
1:G:2616:PRO:HG2	1:G:2664:PHE:CE2	2.55	0.42
1:G:2823:ILE:HA	1:G:2936:ALA:O	2.18	0.42
1:G:3798:LEU:O	1:G:3802:ILE:HG23	2.20	0.42
1:G:3889:GLN:O	1:G:3893:GLU:N	2.53	0.42
1:G:3943:ILE:HD11	1:G:4002:LYS:HZ1	1.84	0.42
1:J:1775:HIS:NE2	1:J:1851:MET:SD	2.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1423:ASP:O	1:D:1427:ILE:HG12	2.20	0.42
1:D:1773:PRO:HA	1:D:2153:MET:HE1	2.02	0.42
1:D:3701:LEU:HD11	1:D:3705:PHE:CZ	2.55	0.42
1:A:3625:SER:OG	1:A:3626:LYS:N	2.53	0.42
1:A:4189:ARG:HA	1:A:5031:GLN:HE22	1.85	0.42
1:G:2670:GLU:HA	1:G:2673:HIS:HE1	1.80	0.42
1:G:4631:PHE:HZ	1:G:4639:MET:SD	2.42	0.42
1:G:4716:TRP:HB3	4:G:5101:CFF:H142	2.01	0.42
1:J:1089:TYR:HB2	1:J:1152:MET:HE1	2.02	0.42
1:J:3775:ALA:O	1:J:3779:VAL:HG23	2.20	0.42
1:J:4243:PHE:O	1:J:4247:ILE:HG13	2.20	0.42
1:D:4072:VAL:HA	1:D:4077:PHE:HD2	1.83	0.42
1:A:1243:PRO:HB2	1:A:1600:LEU:HD11	2.02	0.42
1:A:1698:LEU:HD11	1:A:1814:MET:CE	2.50	0.42
1:G:74:SER:HA	1:G:105:HIS:HD2	1.85	0.42
1:G:1763:PRO:HG2	1:G:1863:LEU:HD11	2.01	0.42
1:G:3965:LEU:O	1:G:3969:ILE:HG12	2.20	0.42
1:G:4805:ASN:ND2	1:G:4807:PHE:HB2	2.34	0.42
1:J:349:GLN:NE2	1:J:350:HIS:O	2.53	0.42
1:J:1844:LEU:O	1:J:1848:LEU:HD23	2.20	0.42
1:J:4668:LEU:CD2	1:J:4672:LYS:HE2	2.49	0.42
1:D:3768:SER:HA	1:D:3771:HIS:CE1	2.55	0.42
1:D:3768:SER:HA	1:D:3771:HIS:ND1	2.35	0.42
1:D:4214:LYS:HE2	1:D:4985:LEU:HD22	2.02	0.42
1:A:274:LEU:HB3	1:A:339:ILE:HD11	2.02	0.42
1:A:1103:GLY:HA2	1:A:1151:CYS:SG	2.59	0.42
1:A:2280:VAL:HG13	1:A:2280:VAL:O	2.20	0.42
1:A:4145:VAL:HG22	1:A:4178:LEU:HD13	2.02	0.42
1:A:4822:THR:O	1:A:4825:THR:OG1	2.28	0.42
1:G:1111:PRO:HG2	1:G:1603:VAL:HG13	2.02	0.42
1:G:1772:ARG:NH1	1:G:1952:GLN:HE22	2.18	0.42
1:G:1859:VAL:O	1:G:1863:LEU:HD23	2.20	0.42
1:G:4222:VAL:HG12	1:G:4950:VAL:HG22	2.02	0.42
1:J:119:SER:OG	1:J:120:CYS:N	2.53	0.42
1:J:548:VAL:HG11	1:J:582:HIS:ND1	2.35	0.42
1:J:3670:GLU:O	1:J:3674:ILE:HG12	2.20	0.42
1:J:3966:THR:O	1:J:3970:GLN:N	2.47	0.42
1:J:4686:LEU:HD11	1:J:4692:PRO:HA	2.02	0.42
1:D:530:ILE:HD11	1:D:563:VAL:HG13	2.01	0.41
1:D:714:TYR:HB3	1:D:768:PHE:CE2	2.55	0.41
1:D:2440:MET:HA	1:D:2443:ILE:HG22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:681:HIS:CE1	1:A:683:ARG:HH21	2.37	0.41
1:A:2671:GLU:O	1:A:2675:THR:HG23	2.20	0.41
1:A:3675:ASP:O	1:A:3679:LYS:HG2	2.20	0.41
1:G:2179:ILE:HD11	1:G:2228:MET:HA	2.01	0.41
1:G:3756:LYS:HD2	1:G:3756:LYS:HA	1.89	0.41
1:G:4229:GLU:O	1:G:4233:LEU:HD23	2.20	0.41
1:J:112:ALA:HA	1:J:115:ARG:NH1	2.34	0.41
1:J:636:ASN:HB3	1:J:702:TRP:CZ3	2.54	0.41
1:J:1466:LEU:HD11	1:J:1496:TRP:HB2	2.01	0.41
1:J:1699:GLU:OE1	1:J:1699:GLU:N	2.53	0.41
1:J:2685:SER:O	1:J:2689:LYS:N	2.53	0.41
1:D:1087:ARG:HD3	1:D:1223:PHE:CE1	2.55	0.41
1:D:1863:LEU:HA	1:D:1866:ILE:HG22	2.02	0.41
1:D:2181:SER:O	1:D:2185:ILE:HG13	2.20	0.41
1:A:645:ARG:HD2	1:A:649:PHE:HE1	1.84	0.41
1:A:4181:ILE:HD11	1:A:4193:ILE:HB	2.02	0.41
1:G:1076:ARG:O	1:G:1237:TRP:N	2.35	0.41
1:G:1126:GLY:HA3	1:G:1143:TRP:HE1	1.85	0.41
1:G:2470:ILE:HG22	1:G:2525:GLY:HA3	2.00	0.41
2:H:7:ILE:H	2:H:72:ALA:HA	1.84	0.41
1:J:178:ARG:NH1	1:J:193:ALA:O	2.46	0.41
1:J:461:HIS:CE1	1:J:3707:ARG:HG2	2.55	0.41
1:J:1862:ILE:HD12	1:J:1865:MET:SD	2.60	0.41
1:J:2024:PRO:C	1:J:2028:ARG:HH21	2.24	0.41
1:J:2611:CYS:O	1:J:2614:ILE:HG22	2.21	0.41
1:D:1432:THR:HB	1:D:1572:ILE:HD12	2.02	0.41
1:D:1762:LEU:HD23	1:D:1762:LEU:HA	1.89	0.41
1:D:4658:ILE:HG13	1:D:4796:MET:SD	2.60	0.41
1:A:23:GLN:O	1:A:201:ASN:N	2.46	0.41
1:A:3776:ALA:O	1:A:3780:LEU:HD23	2.21	0.41
1:G:650:VAL:HG11	1:G:662:TRP:NE1	2.36	0.41
1:G:853:PRO:HB3	1:G:1023:PRO:HD3	2.01	0.41
1:G:1154:ASP:O	1:G:1158:ASN:N	2.53	0.41
1:G:2102:VAL:HG11	1:G:2124:LEU:HD22	2.02	0.41
1:J:1242:LEU:HD21	1:J:1458:HIS:CD2	2.55	0.41
1:J:1294:PRO:HB3	1:J:1549:PHE:CE1	2.55	0.41
1:J:1698:LEU:O	1:J:1708:ARG:NH1	2.40	0.41
1:J:2190:VAL:HA	1:J:2193:GLN:HB2	2.02	0.41
1:J:3989:VAL:HG23	1:J:4023:MET:HE2	2.01	0.41
1:J:4013:LEU:O	1:J:4017:LEU:HD23	2.20	0.41
1:J:4844:LEU:HD12	1:J:4928:LEU:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:87:HIS:HD2	2:K:88:PRO:HD2	1.85	0.41
1:D:44:ASN:N	1:D:44:ASN:OD1	2.53	0.41
1:D:102:LEU:HB2	1:D:105:HIS:CE1	2.55	0.41
1:D:2418:LEU:O	1:D:2422:ILE:HG12	2.21	0.41
1:D:3943:ILE:HD12	1:D:3943:ILE:HA	1.93	0.41
1:D:4888:TYR:OH	1:J:4913:ARG:NH1	2.53	0.41
1:A:663:TYR:OH	1:A:758:ARG:NH1	2.50	0.41
1:A:805:PRO:HB2	1:A:808:TYR:CD2	2.54	0.41
1:A:1112:ASP:OD1	1:A:1113:VAL:N	2.53	0.41
1:A:1965:TYR:CE2	1:A:2031:LEU:HB2	2.56	0.41
1:A:2648:TYR:HD2	1:A:2706:ILE:HA	1.86	0.41
1:A:2960:LEU:HD11	1:A:3017:PHE:CZ	2.56	0.41
1:A:3768:SER:O	1:A:3772:THR:HG22	2.20	0.41
1:A:4851:TYR:HD2	1:A:4920:PHE:CD2	2.38	0.41
1:A:4914:VAL:HG23	1:G:4888:TYR:CD1	2.55	0.41
1:G:1290:ARG:HA	1:G:1551:ALA:HA	2.01	0.41
1:G:2172:PRO:O	1:G:2175:GLU:HG3	2.20	0.41
1:G:4085:ARG:HE	1:G:4085:ARG:HB2	1.67	0.41
2:H:16:PRO:HG2	2:H:64:ALA:HA	2.01	0.41
1:J:2172:PRO:O	1:J:2175:GLU:HG3	2.20	0.41
1:J:4863:TYR:HE1	1:J:4901:ILE:HG12	1.85	0.41
1:J:5000:GLU:HA	1:J:5003:HIS:CD2	2.55	0.41
1:D:1433:TYR:CE2	1:D:1578:ALA:HB2	2.55	0.41
1:D:1566:LEU:HD13	1:D:1566:LEU:HA	1.81	0.41
1:D:1658:ASP:N	1:D:1658:ASP:OD1	2.54	0.41
1:D:3805:LEU:HD21	1:D:3891:LEU:HD13	2.02	0.41
1:A:483:MET:O	1:A:487:VAL:HG23	2.20	0.41
1:A:2323:TRP:CH2	1:A:2422:ILE:HG13	2.54	0.41
1:A:2512:ILE:HG13	1:A:2512:ILE:O	2.21	0.41
1:A:4794:TRP:O	1:A:4798:MET:HG2	2.20	0.41
1:A:4922:PHE:HA	1:A:4926:VAL:HG12	2.01	0.41
1:G:839:LEU:HD13	1:G:1075:PHE:HD2	1.85	0.41
1:G:1760:HIS:CE1	1:G:2041:HIS:HA	2.55	0.41
1:G:2032:GLN:O	1:G:2036:GLN:HG2	2.19	0.41
1:G:2512:ILE:HD12	1:G:2561:LEU:HD21	2.01	0.41
1:G:3817:LEU:HD11	1:G:3821:LYS:HE2	2.01	0.41
1:J:700:GLU:H	1:J:705:ASN:HD21	1.68	0.41
1:J:1426:ILE:O	1:J:1430:THR:OG1	2.29	0.41
1:J:2627:VAL:O	1:J:2631:PRO:HD3	2.20	0.41
1:D:682:LEU:HB3	1:D:738:LEU:HD12	2.02	0.41
1:D:1433:TYR:N	1:D:1520:VAL:O	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4702:ASP:O	1:D:4705:VAL:HG12	2.20	0.41
1:A:1514:LEU:HD23	1:A:1514:LEU:H	1.85	0.41
1:A:2203:MET:O	1:A:2207:VAL:HG23	2.21	0.41
1:G:1965:TYR:CE2	1:G:2031:LEU:HB2	2.56	0.41
1:G:4958:CYS:HA	6:G:5103:ATP:N7	2.36	0.41
1:J:287:THR:HB	1:J:289:ARG:HH11	1.85	0.41
1:J:337:PRO:O	1:J:339:ILE:HD12	2.21	0.41
1:J:1229:ASN:HB2	1:J:1827:ARG:NE	2.36	0.41
1:J:3875:MET:N	1:J:3875:MET:SD	2.93	0.41
1:J:3927:GLN:NE2	1:J:3991:GLY:HA3	2.33	0.41
1:J:4040:ILE:HD12	1:J:4040:ILE:H	1.86	0.41
1:J:4922:PHE:HA	1:J:4926:VAL:HG12	2.03	0.41
3:L:6:THR:HG23	3:L:9:GLN:H	1.84	0.41
1:D:1237:TRP:CH2	1:D:1652:GLU:HG3	2.54	0.41
1:D:2215:LEU:HD23	1:D:2215:LEU:HA	1.88	0.41
1:A:3916:ILE:HG13	1:A:3980:LEU:HD21	2.02	0.41
1:G:2039:LEU:HD23	1:G:2039:LEU:HA	1.93	0.41
1:G:2467:VAL:HG22	1:G:2524:VAL:HG11	2.03	0.41
1:J:551:LEU:HD11	1:J:589:LEU:HD22	2.02	0.41
1:J:1095:VAL:O	1:J:1145:SER:OG	2.31	0.41
1:J:1112:ASP:OD1	1:J:1113:VAL:N	2.53	0.41
1:J:1454:THR:HG22	1:J:1491:ASN:O	2.19	0.41
1:J:2500:ALA:N	1:J:2553:TYR:CE1	2.87	0.41
2:K:7:ILE:H	2:K:72:ALA:HA	1.86	0.41
1:D:668:VAL:O	1:D:741:GLU:N	2.51	0.41
1:D:1804:LEU:HD21	1:D:1853:ILE:HD13	2.01	0.41
1:D:2570:ALA:HB2	1:D:2613:TYR:O	2.21	0.41
1:D:3723:MET:SD	1:D:3792:ALA:HB1	2.61	0.41
1:A:626:LEU:N	1:A:627:PRO:HD2	2.36	0.41
1:A:2174:GLU:H	1:A:2174:GLU:CD	2.22	0.41
1:A:2346:VAL:HG21	1:A:2349:ASN:HD22	1.84	0.41
1:A:2463:LEU:HD21	1:A:2517:PHE:CE1	2.55	0.41
1:A:3731:LYS:O	1:A:3731:LYS:HG2	2.21	0.41
1:A:3768:SER:HA	1:A:3771:HIS:CE1	2.55	0.41
1:A:4701:TRP:CZ2	1:A:4781:GLY:HA3	2.56	0.41
2:B:38:SER:H	2:B:42:ARG:HH21	1.69	0.41
1:G:265:LEU:HD22	1:G:279:PRO:O	2.21	0.41
1:G:636:ASN:ND2	1:G:637:LEU:H	2.18	0.41
1:G:1449:TRP:O	1:G:1552:VAL:HG13	2.21	0.41
1:G:1514:LEU:H	1:G:1514:LEU:HD23	1.86	0.41
1:G:2654:TYR:HA	1:G:2660:GLY:HA2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:56:ILE:HD13	2:H:81:ALA:HB1	2.02	0.41
1:J:2355:ARG:HA	1:J:2358:ILE:HG22	2.01	0.41
1:J:2512:ILE:HD12	1:J:2518:LEU:HD12	2.03	0.41
1:D:559:GLY:O	1:D:563:VAL:HG23	2.21	0.41
1:D:1500:PHE:CE2	1:D:1531:ALA:HB3	2.56	0.41
1:D:1569:GLN:CB	1:D:1572:ILE:HB	2.51	0.41
1:D:2309:SER:HA	1:D:2324:ASN:HB3	2.02	0.41
1:D:2638:LYS:CE	1:D:2695:LEU:HA	2.50	0.41
1:D:4823:LEU:HD11	1:J:4843:LEU:HB2	2.02	0.41
1:D:5019:TRP:CD1	1:D:5022:PHE:HE2	2.39	0.41
1:A:337:PRO:HB2	1:A:338:GLU:H	1.77	0.41
1:A:1204:LEU:HD23	1:A:1204:LEU:HA	1.96	0.41
1:A:1301:PHE:HB2	1:A:1523:ALA:O	2.21	0.41
1:A:2442:LEU:HD22	1:A:2447:LYS:HD2	2.03	0.41
1:A:2463:LEU:HB2	1:A:2510:TYR:CE2	2.56	0.41
1:G:401:ALA:O	1:G:404:ILE:HG22	2.21	0.41
1:G:564:LEU:O	1:G:568:LEU:HD23	2.21	0.41
1:G:615:ARG:HD2	1:G:1678:ASN:ND2	2.36	0.41
1:G:691:GLY:HA3	1:G:712:TYR:CG	2.56	0.41
1:G:3699:HIS:HB2	1:G:3773:ARG:HD2	2.02	0.41
1:G:4020:GLN:HG3	1:G:4139:ILE:HD11	2.02	0.41
1:G:4914:VAL:HG11	1:J:4884:LEU:HD11	2.01	0.41
1:J:288:GLY:HA3	1:J:405:HIS:CE1	2.56	0.41
1:J:311:ALA:HA	1:J:350:HIS:NE2	2.36	0.41
1:J:484:LEU:HD12	1:J:485:SER:N	2.36	0.41
1:J:1514:LEU:HD23	1:J:1514:LEU:H	1.85	0.41
1:J:1783:VAL:O	2:K:56:ILE:HG23	2.21	0.41
1:J:2477:PRO:HB3	1:J:2487:GLN:HA	2.02	0.41
1:J:3927:GLN:HB2	1:J:3992:PHE:CE1	2.55	0.41
1:J:3986:TRP:O	1:J:3989:VAL:HG12	2.21	0.41
1:J:4555:LEU:HD21	1:J:4656:LEU:HG	2.02	0.41
1:J:4639:MET:HA	1:J:4642:ALA:HB3	2.03	0.41
2:K:7:ILE:HD11	2:K:73:LYS:HB2	2.02	0.41
1:D:2230:THR:HB	1:D:2270:SER:HB2	2.03	0.41
1:A:1712:TYR:CD2	1:A:1840:PRO:HB2	2.56	0.41
1:A:2159:LEU:CD2	1:A:2201:LEU:HD23	2.50	0.41
1:A:2162:ILE:HD11	1:A:2178:MET:HE1	2.03	0.41
1:G:1130:GLN:HA	1:G:1139:PHE:H	1.86	0.41
1:G:1515:VAL:O	1:G:1515:VAL:HG23	2.21	0.41
1:G:2575:ARG:HH21	1:G:2578:MET:CE	2.34	0.41
1:J:223:PHE:CD1	1:J:230:CYS:HB3	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:308:HIS:HB2	1:J:311:ALA:HB3	2.02	0.41
1:J:2368:LEU:HD21	1:J:2376:LEU:HD12	2.01	0.41
1:J:2377:LEU:HD11	1:J:2468:GLY:HA3	2.02	0.41
1:J:3851:ASN:OD1	1:J:3852:LYS:N	2.54	0.41
1:D:491:ILE:HG12	1:D:523:TYR:CE1	2.55	0.40
1:D:561:LEU:HD21	1:D:599:VAL:HG23	2.03	0.40
1:D:614:VAL:HG23	1:D:617:ASN:HB2	2.02	0.40
1:D:698:GLY:HA3	1:D:1647:CYS:O	2.21	0.40
1:D:3934:TYR:CD2	1:D:3995:VAL:HG23	2.56	0.40
1:D:4661:TYR:CE1	1:D:4665:LYS:HD2	2.56	0.40
3:F:1:MET:O	3:F:5:LEU:HG	2.20	0.40
1:A:2159:LEU:HA	1:A:2162:ILE:HG22	2.03	0.40
1:A:4879:MET:O	1:A:4883:TYR:HB2	2.21	0.40
1:G:178:ARG:HB2	1:G:193:ALA:HB1	2.04	0.40
1:G:681:HIS:NE2	1:G:683:ARG:HG3	2.35	0.40
1:G:725:HIS:O	1:G:725:HIS:CG	2.73	0.40
1:G:3701:LEU:HD11	1:G:3705:PHE:CZ	2.56	0.40
1:G:4088:ILE:HG22	1:G:4125:PHE:HD2	1.86	0.40
1:J:2819:TRP:O	1:J:2820:GLU:CB	2.69	0.40
1:J:3829:PHE:CE2	1:J:3906:GLN:HG3	2.57	0.40
1:J:3906:GLN:N	1:J:3906:GLN:CD	2.74	0.40
1:D:415:ILE:HD13	1:D:490:CYS:HA	2.03	0.40
1:D:662:TRP:CH2	1:D:814:ALA:HB2	2.56	0.40
1:D:1105:ALA:HA	1:D:1121:ALA:HA	2.02	0.40
1:D:1716:ILE:HD11	1:D:1847:THR:OG1	2.21	0.40
1:D:2003:GLN:O	1:D:2007:ASN:ND2	2.43	0.40
1:D:4579:PHE:O	1:D:4632:LEU:HG	2.21	0.40
1:D:4732:PHE:CD2	1:D:4737:ILE:HD11	2.46	0.40
1:A:2155:LEU:HB2	1:A:2188:ASN:HD22	1.85	0.40
1:A:3695:PRO:HB2	1:A:3699:HIS:HB3	2.02	0.40
1:A:4150:LEU:HD23	1:A:4150:LEU:HA	1.96	0.40
1:G:600:LEU:HD23	1:G:1665:HIS:HB3	2.02	0.40
1:G:839:LEU:HD13	1:G:1075:PHE:CD2	2.56	0.40
1:G:1848:LEU:HB3	1:G:1854:PHE:HE2	1.85	0.40
1:G:3993:LEU:HG	1:G:4023:MET:HE1	2.03	0.40
1:J:347:PHE:CE1	1:J:387:ALA:HA	2.56	0.40
1:J:1155:LEU:HD12	1:J:1184:ILE:HG23	2.02	0.40
2:K:74:LEU:O	2:K:99:PHE:N	2.37	0.40
1:D:1243:PRO:HB2	1:D:1600:LEU:HD11	2.02	0.40
1:D:1949:GLN:OE1	1:D:1952:GLN:NE2	2.55	0.40
1:D:2630:VAL:N	1:D:2631:PRO:HD2	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4067:LYS:O	1:D:4071:ILE:HG12	2.20	0.40
1:D:4217:PHE:CZ	1:D:4234:PHE:HA	2.57	0.40
1:D:4651:THR:OG1	1:D:4803:HIS:NE2	2.43	0.40
1:A:42:PHE:HA	1:A:447:ASP:OD2	2.21	0.40
1:A:502:HIS:CE1	1:A:506:TYR:CE2	3.09	0.40
1:A:1449:TRP:N	1:A:1553:PHE:O	2.54	0.40
1:A:2299:VAL:HG21	1:A:2356:LEU:HD13	2.03	0.40
1:A:2773:ASN:O	1:A:2774:ASN:CB	2.70	0.40
1:A:3722:TYR:CZ	1:A:3782:MET:SD	3.14	0.40
1:A:4247:ILE:O	1:A:4251:ILE:HG12	2.21	0.40
1:G:567:VAL:HG13	1:G:568:LEU:HD22	2.03	0.40
1:G:2679:PHE:CE1	1:G:2703:LEU:HA	2.56	0.40
1:G:4551:PHE:CD2	1:G:4552:LEU:HD12	2.56	0.40
1:J:172:VAL:HG22	1:J:179:TYR:CE2	2.56	0.40
1:J:596:ASN:HD21	1:J:599:VAL:HG23	1.86	0.40
1:J:771:PHE:HB3	1:J:1472:VAL:HG23	2.03	0.40
1:J:3962:PHE:CZ	1:J:3992:PHE:CE2	3.09	0.40
1:J:4049:VAL:HG21	1:J:4159:ARG:HD2	2.04	0.40
1:J:4716:TRP:CZ3	1:J:4717:ASP:HB2	2.57	0.40
1:D:692:TYR:CZ	1:D:694:PRO:HG3	2.57	0.40
1:D:979:PRO:HB2	1:D:980:ALA:H	1.66	0.40
1:D:1782:PHE:CE1	2:E:90:VAL:HG21	2.56	0.40
1:D:2310:CYS:SG	1:D:2312:MET:HB3	2.62	0.40
1:D:2773:ASN:O	1:D:2774:ASN:CB	2.70	0.40
1:D:4577:LEU:HD21	1:D:4807:PHE:HA	2.02	0.40
1:A:347:PHE:CZ	1:A:387:ALA:HB2	2.56	0.40
1:A:636:ASN:HB3	1:A:702:TRP:HE1	1.85	0.40
1:A:2182:ILE:HA	1:A:2185:ILE:HG22	2.02	0.40
1:A:4648:LEU:HD22	1:A:4803:HIS:HE1	1.85	0.40
1:G:38:ALA:HB2	1:G:65:CYS:SG	2.61	0.40
1:G:1433:TYR:CE1	1:G:1578:ALA:HB2	2.56	0.40
1:G:2346:VAL:HG23	1:G:2349:ASN:HB2	2.04	0.40
3:I:5:LEU:HD11	3:I:74:ALA:HA	2.04	0.40
1:J:1124:PHE:CE1	1:J:1140:GLY:HA3	2.56	0.40
1:J:2236:LEU:HD23	1:J:2236:LEU:HA	1.94	0.40
1:J:3882:GLN:HG3	1:J:3960:GLN:HG3	2.04	0.40
1:J:4336:TRP:CH2	1:J:4568:PHE:HB2	2.56	0.40
1:J:4692:PRO:HG2	1:J:4703:ARG:NH2	2.36	0.40
1:D:61:ASP:HB3	1:D:283:ARG:HH12	1.87	0.40
1:D:1738:LEU:HB2	1:D:2146:PRO:HG3	2.03	0.40
1:A:3892:CYS:SG	1:A:3903:LEU:HD12	2.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4235:VAL:HG21	1:A:5019:TRP:CE2	2.57	0.40
1:G:264:PRO:HG2	1:G:270:SER:O	2.22	0.40
1:G:639:ASN:HA	1:G:1635:THR:HA	2.03	0.40
1:G:1707:LEU:HD23	1:G:1707:LEU:HA	1.80	0.40
1:G:1784:ALA:O	2:H:82:TYR:OH	2.37	0.40
1:G:3845:ASN:O	1:G:3849:ARG:HG3	2.22	0.40
1:G:4562:LEU:HG	1:G:4653:VAL:HG13	2.03	0.40
3:I:17:PHE:CE1	3:I:28:ILE:HD12	2.57	0.40
1:J:864:PRO:HA	1:J:865:PRO:HD3	1.98	0.40
1:J:1794:ALA:HA	1:J:1795:PRO:HD3	1.94	0.40
1:J:2577:ILE:HD12	1:J:2577:ILE:H	1.86	0.40
1:J:4020:GLN:HG3	1:J:4139:ILE:HD11	2.03	0.40
1:J:4658:ILE:HG13	1:J:4796:MET:SD	2.61	0.40
1:J:4897:ILE:O	1:J:4901:ILE:HG13	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	3853/5037 (76%)	3782 (98%)	68 (2%)	3 (0%)	51 83
1	D	3852/5037 (76%)	3792 (98%)	60 (2%)	0	100 100
1	G	3854/5037 (76%)	3797 (98%)	57 (2%)	0	100 100
1	J	3853/5037 (76%)	3778 (98%)	75 (2%)	0	100 100
2	B	105/107 (98%)	102 (97%)	3 (3%)	0	100 100
2	E	105/107 (98%)	103 (98%)	2 (2%)	0	100 100
2	H	105/107 (98%)	100 (95%)	5 (5%)	0	100 100
2	K	105/107 (98%)	104 (99%)	1 (1%)	0	100 100
3	C	132/149 (89%)	131 (99%)	1 (1%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	F	132/149 (89%)	131 (99%)	1 (1%)	0	100	100
3	I	132/149 (89%)	131 (99%)	1 (1%)	0	100	100
3	L	131/149 (88%)	128 (98%)	3 (2%)	0	100	100
All	All	16359/21172 (77%)	16079 (98%)	277 (2%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	337	PRO
1	A	2859	PRO
1	A	2857	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	A	2211/4276 (52%)	2202 (100%)	9 (0%)	91	95
1	D	2095/4276 (49%)	2077 (99%)	18 (1%)	78	88
1	G	2176/4276 (51%)	2165 (100%)	11 (0%)	88	94
1	J	2139/4276 (50%)	2130 (100%)	9 (0%)	91	95
2	B	68/88 (77%)	68 (100%)	0	100	100
2	E	68/88 (77%)	68 (100%)	0	100	100
2	H	68/88 (77%)	68 (100%)	0	100	100
2	K	65/88 (74%)	65 (100%)	0	100	100
3	C	11/123 (9%)	11 (100%)	0	100	100
3	F	9/123 (7%)	9 (100%)	0	100	100
3	I	13/123 (11%)	13 (100%)	0	100	100
3	L	15/123 (12%)	15 (100%)	0	100	100
All	All	8938/17948 (50%)	8891 (100%)	47 (0%)	89	94

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	1426	ILE
1	D	1427	ILE
1	D	2123	LEU
1	D	2503	VAL
1	D	2506	LEU
1	D	2517	PHE
1	D	2518	LEU
1	D	2519	LEU
1	D	2520	HIS
1	D	2522	LEU
1	D	2563	THR
1	D	2581	SER
1	D	3721	LEU
1	D	3723	MET
1	D	3728	ILE
1	D	4569	LEU
1	D	4581	LYS
1	D	4672	LYS
1	A	1693	GLN
1	A	1698	LEU
1	A	3720	TYR
1	A	3721	LEU
1	A	3725	TYR
1	A	3727	ASP
1	A	3728	ILE
1	A	3841	VAL
1	A	3845	ASN
1	G	3674	ILE
1	G	3679	LYS
1	G	3721	LEU
1	G	3727	ASP
1	G	3728	ILE
1	G	3763	LEU
1	G	3764	LEU
1	G	3768	SER
1	G	4792	LEU
1	G	4801	LEU
1	G	4865	LYS
1	J	2504	LEU
1	J	2509	VAL
1	J	3899	PHE
1	J	3903	LEU

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Mol	Chain	Res	Type
1	J	3905	THR
1	J	3907	THR
1	J	3910	THR
1	J	3911	THR
1	J	4137	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (90) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	105	HIS
1	D	465	GLN
1	D	502	HIS
1	D	533	ASN
1	D	1231	GLN
1	D	1563	GLN
1	D	1590	GLN
1	D	2161	GLN
1	D	2515	GLN
1	D	3647	HIS
1	D	3771	HIS
1	D	3781	GLN
1	D	3901	ASN
1	D	4149	ASN
1	D	4153	HIS
1	D	4204	GLN
1	D	4558	ASN
1	D	4574	ASN
1	D	4978	HIS
1	A	495	ASN
1	A	536	ASN
1	A	617	ASN
1	A	1563	GLN
1	A	1590	GLN
1	A	1683	HIS
1	A	1693	GLN
1	A	2551	ASN
1	A	3647	HIS
1	A	4054	ASN
1	A	4201	ASN
1	A	4574	ASN
1	A	4806	ASN
2	B	25	HIS

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Mol	Chain	Res	Type
2	B	32	ASN
1	G	190	GLN
1	G	838	HIS
1	G	1127	HIS
1	G	1133	HIS
1	G	1158	ASN
1	G	1206	GLN
1	G	1491	ASN
1	G	1563	GLN
1	G	1640	HIS
1	G	1663	HIS
1	G	1678	ASN
1	G	1719	HIS
1	G	1938	GLN
1	G	2005	GLN
1	G	2032	GLN
1	G	2036	GLN
1	G	2161	GLN
1	G	2260	ASN
1	G	2515	GLN
1	G	2574	HIS
1	G	2647	HIS
1	G	3651	ASN
1	G	3833	GLN
1	G	3889	GLN
1	G	3900	GLN
1	G	4009	GLN
1	G	4558	ASN
1	G	4574	ASN
2	H	70	GLN
2	H	87	HIS
1	J	23	GLN
1	J	138	GLN
1	J	151	HIS
1	J	349	GLN
1	J	582	HIS
1	J	618	GLN
1	J	678	GLN
1	J	705	ASN
1	J	720	HIS
1	J	1254	HIS
1	J	1274	HIS

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Mol	Chain	Res	Type
1	J	1678	ASN
1	J	1953	HIS
1	J	2107	GLN
1	J	2127	GLN
1	J	2246	ASN
1	J	2260	ASN
1	J	2284	ASN
1	J	2584	HIS
1	J	2599	GLN
1	J	3771	HIS
1	J	3781	GLN
1	J	3994	HIS
1	J	3998	HIS
1	J	4714	ASN
2	K	43	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	ATP	D	5103	-	26,33,33	0.61	0	31,52,52	0.75	2 (6%)
4	CFF	G	5101	-	8,15,15	1.23	1 (12%)	8,23,23	2.68	3 (37%)
4	CFF	J	5101	-	8,15,15	1.25	1 (12%)	8,23,23	2.69	3 (37%)
6	ATP	G	5103	-	26,33,33	0.61	0	31,52,52	0.79	2 (6%)
6	ATP	J	5103	-	26,33,33	0.60	0	31,52,52	0.80	2 (6%)
4	CFF	D	5101	-	8,15,15	1.24	1 (12%)	8,23,23	2.68	3 (37%)
4	CFF	A	5101	-	8,15,15	1.23	1 (12%)	8,23,23	2.68	3 (37%)
6	ATP	A	5103	-	26,33,33	0.60	0	31,52,52	0.77	2 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ATP	D	5103	-	-	8/18/38/38	0/3/3/3
4	CFF	G	5101	-	-	-	0/2/2/2
6	ATP	J	5103	-	-	9/18/38/38	0/3/3/3
6	ATP	G	5103	-	-	4/18/38/38	0/3/3/3
4	CFF	J	5101	-	-	-	0/2/2/2
4	CFF	D	5101	-	-	-	0/2/2/2
4	CFF	A	5101	-	-	-	0/2/2/2
6	ATP	A	5103	-	-	3/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	5101	CFF	C6-N1	3.08	1.42	1.38
4	D	5101	CFF	C6-N1	3.06	1.42	1.38
4	G	5101	CFF	C6-N1	3.04	1.42	1.38
4	A	5101	CFF	C6-N1	3.02	1.42	1.38

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	J	5101	CFF	C5-C6-N1	-5.33	112.51	118.20
4	D	5101	CFF	C5-C6-N1	-5.25	112.60	118.20
4	A	5101	CFF	C5-C6-N1	-5.25	112.60	118.20
4	G	5101	CFF	C5-C6-N1	-5.21	112.65	118.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	5101	CFF	C4-C5-C6	4.60	122.91	119.96
4	A	5101	CFF	C4-C5-C6	4.51	122.86	119.96
4	G	5101	CFF	C4-C5-C6	4.49	122.84	119.96
4	J	5101	CFF	C4-C5-C6	4.48	122.84	119.96
4	G	5101	CFF	C12-N3-C4	2.61	121.94	118.25
4	J	5101	CFF	C12-N3-C4	2.50	121.79	118.25
4	A	5101	CFF	C12-N3-C4	2.48	121.76	118.25
4	D	5101	CFF	C12-N3-C4	2.35	121.58	118.25
6	G	5103	ATP	C5-C6-N6	2.32	123.88	120.35
6	A	5103	ATP	C5-C6-N6	2.28	123.82	120.35
6	J	5103	ATP	C5-C6-N6	2.28	123.81	120.35
6	D	5103	ATP	C5-C6-N6	2.26	123.79	120.35
6	D	5103	ATP	PB-O3B-PG	2.06	139.89	132.83
6	J	5103	ATP	PB-O3B-PG	2.05	139.87	132.83
6	A	5103	ATP	PB-O3B-PG	2.05	139.86	132.83
6	G	5103	ATP	PB-O3B-PG	2.05	139.86	132.83

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	5103	ATP	PB-O3B-PG-O3G
6	D	5103	ATP	C5'-O5'-PA-O1A
6	D	5103	ATP	C5'-O5'-PA-O3A
6	G	5103	ATP	O4'-C4'-C5'-O5'
6	G	5103	ATP	C3'-C4'-C5'-O5'
6	J	5103	ATP	PB-O3B-PG-O2G
6	J	5103	ATP	C5'-O5'-PA-O3A
6	J	5103	ATP	C3'-C4'-C5'-O5'
6	D	5103	ATP	PB-O3B-PG-O1G
6	G	5103	ATP	C4'-C5'-O5'-PA
6	J	5103	ATP	PB-O3A-PA-O5'
6	J	5103	ATP	PB-O3B-PG-O3G
6	G	5103	ATP	PG-O3B-PB-O2B
6	J	5103	ATP	C5'-O5'-PA-O1A
6	D	5103	ATP	C3'-C4'-C5'-O5'
6	A	5103	ATP	C3'-C4'-C5'-O5'
6	J	5103	ATP	O4'-C4'-C5'-O5'
6	D	5103	ATP	O4'-C4'-C5'-O5'
6	D	5103	ATP	PA-O3A-PB-O2B
6	J	5103	ATP	PB-O3A-PA-O1A
6	D	5103	ATP	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
6	A	5103	ATP	C5'-O5'-PA-O1A
6	J	5103	ATP	PB-O3B-PG-O1G
6	A	5103	ATP	O4'-C4'-C5'-O5'

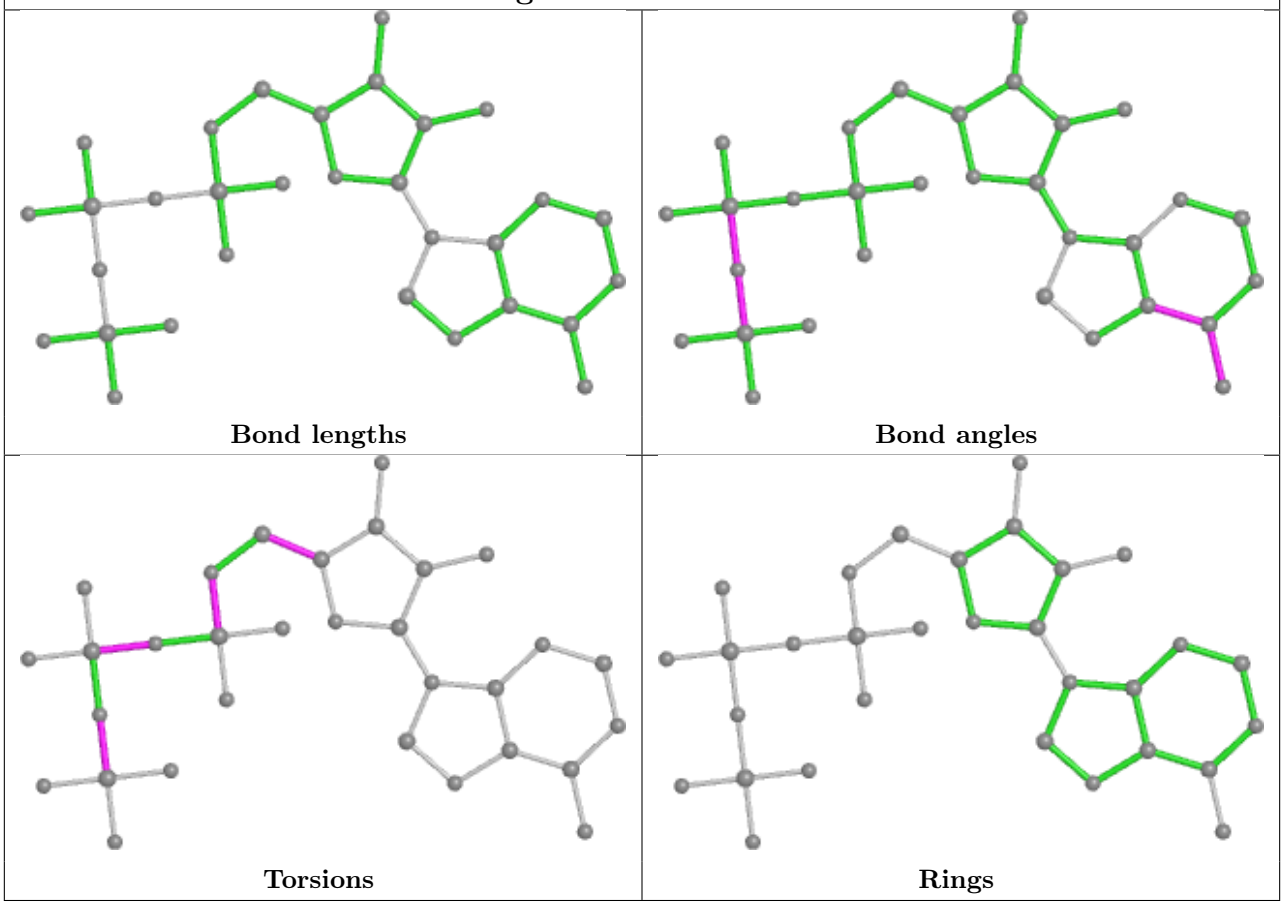
There are no ring outliers.

4 monomers are involved in 9 short contacts:

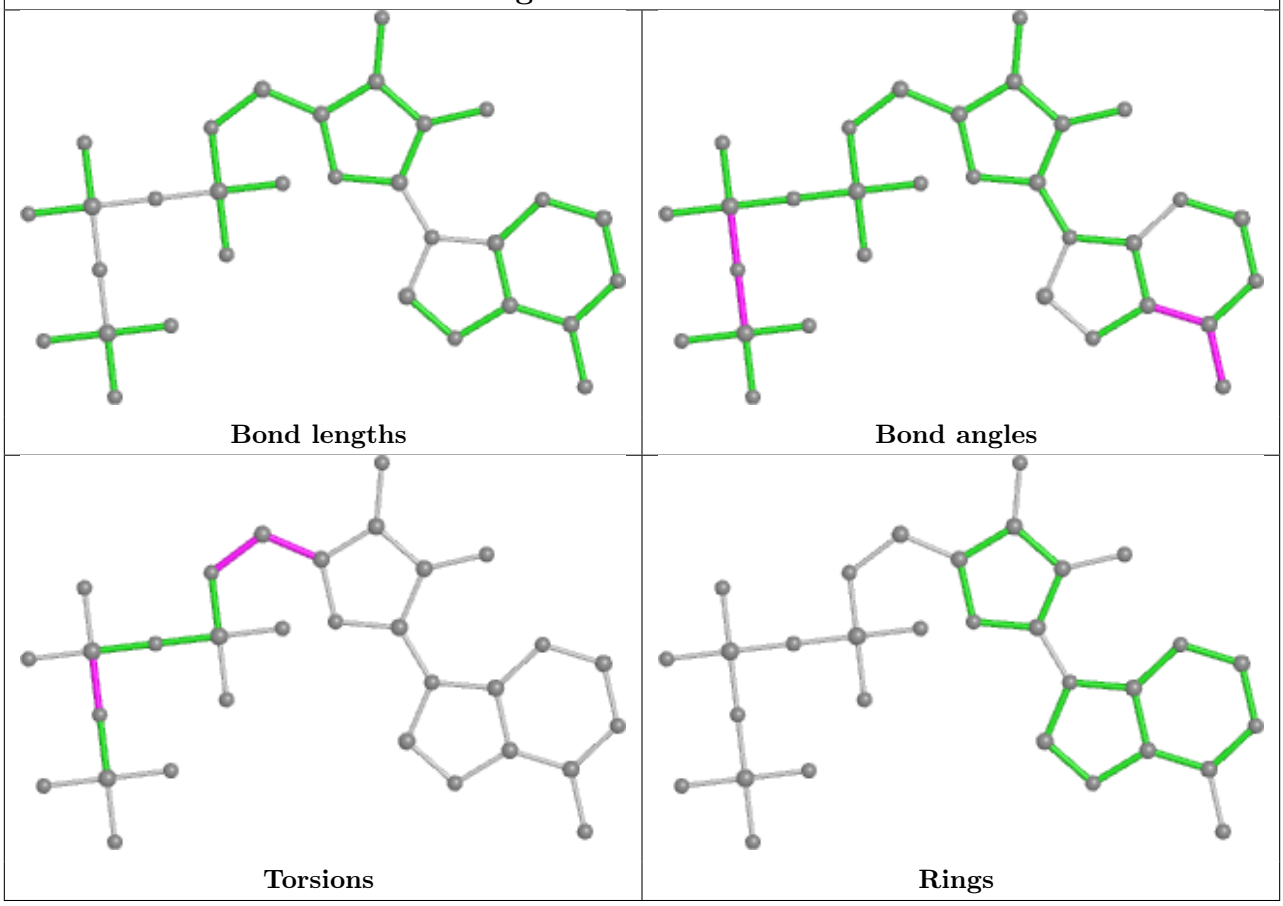
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	5103	ATP	2	0
4	G	5101	CFF	1	0
6	G	5103	ATP	4	0
6	J	5103	ATP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

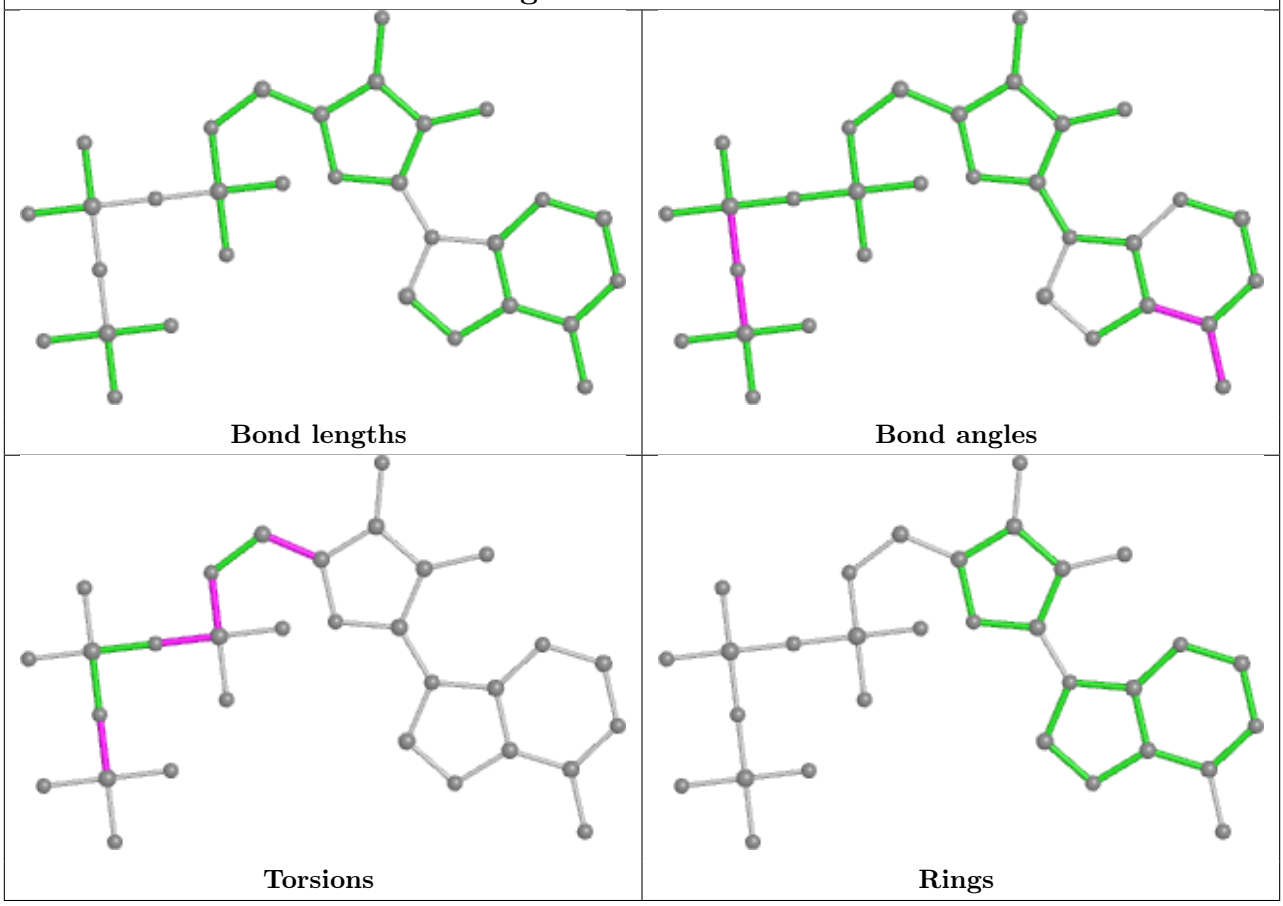
Ligand ATP D 5103



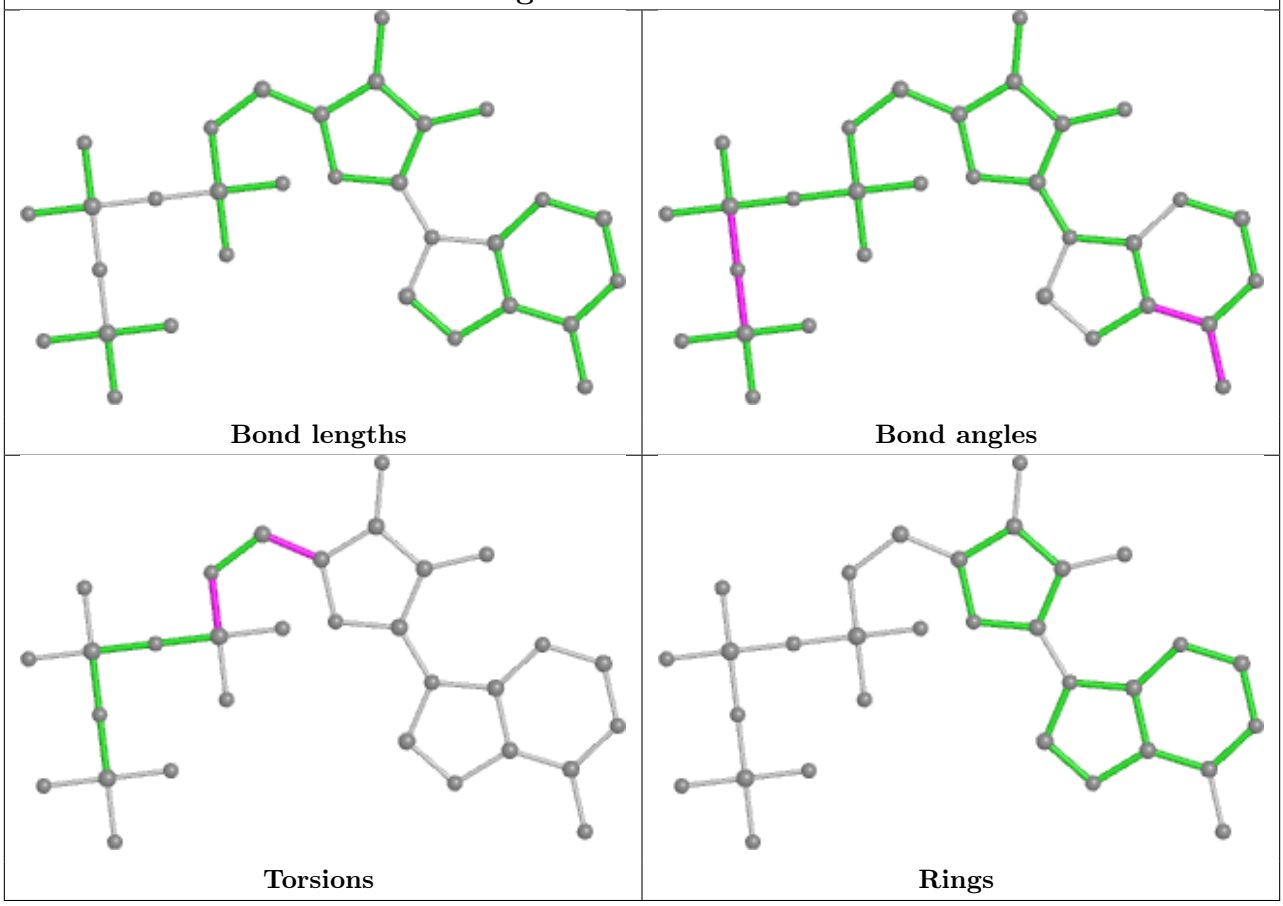
Ligand ATP G 5103



Ligand ATP J 5103



Ligand ATP A 5103



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.

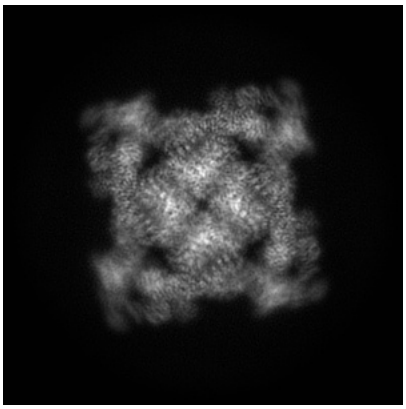
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-27736. These allow visual inspection of the internal detail of the map and identification of artifacts.

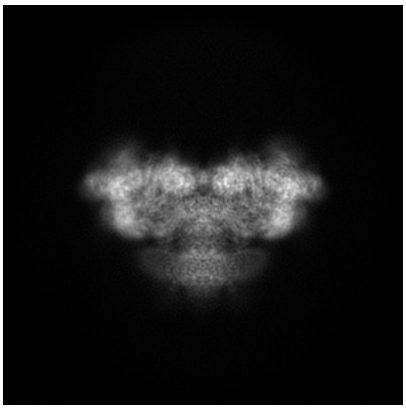
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

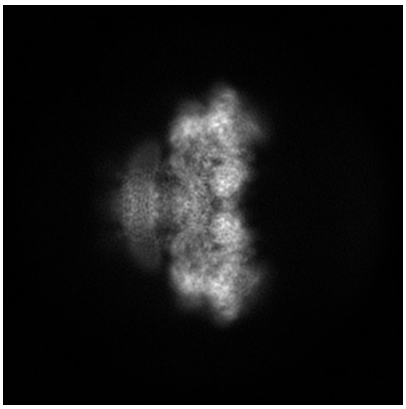
6.1.1 Primary map



X

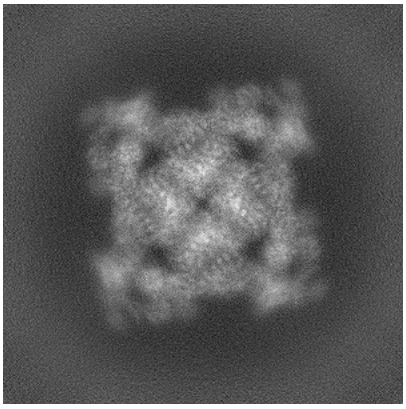


Y

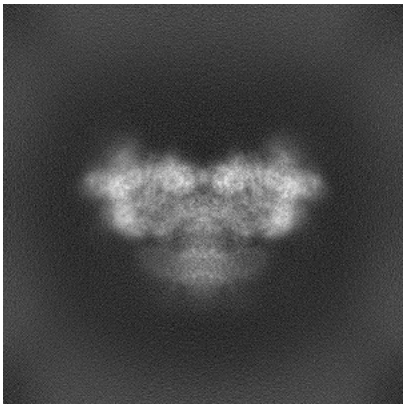


Z

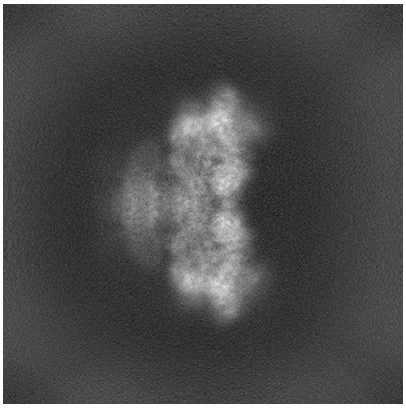
6.1.2 Raw map



X



Y

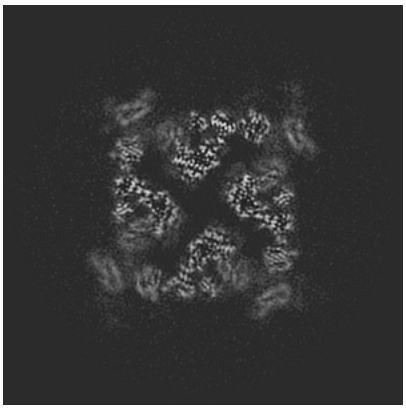


Z

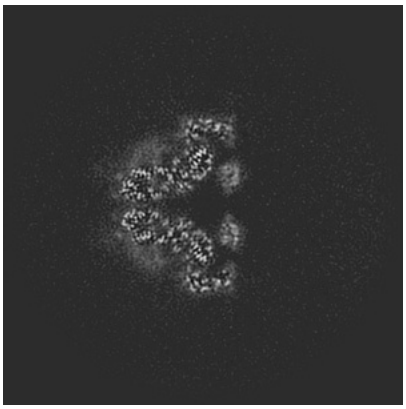
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

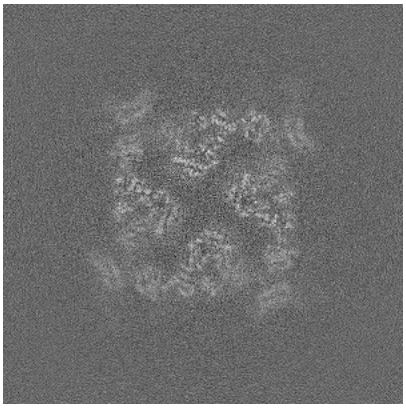
6.2.1 Primary map

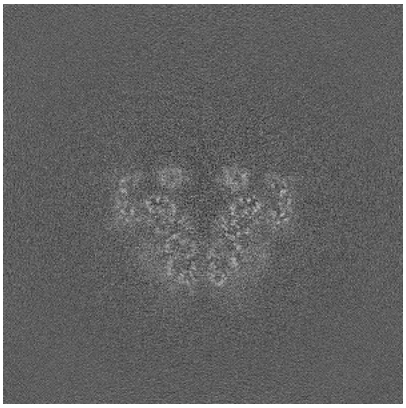

X Index: 256

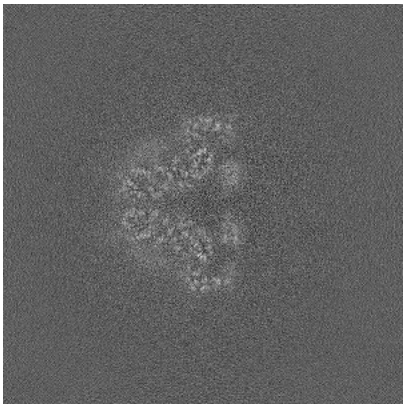
Y Index: 256


Z Index: 256

6.2.2 Raw map


X Index: 256

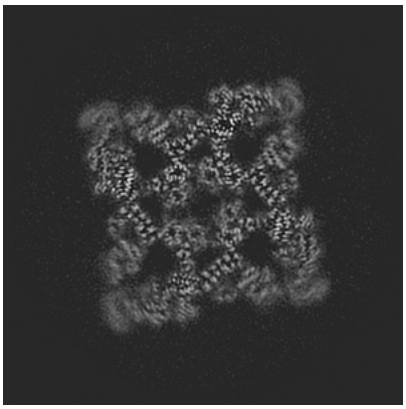

Y Index: 256


Z Index: 256

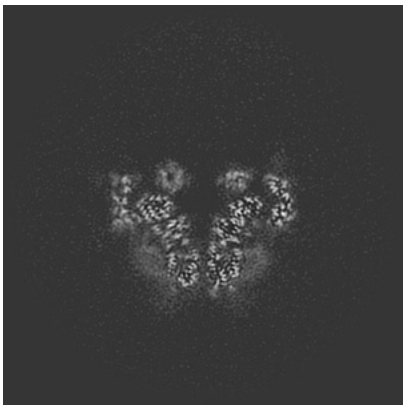
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

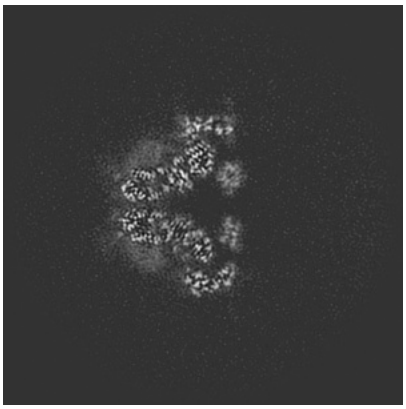
6.3.1 Primary map



X Index: 281

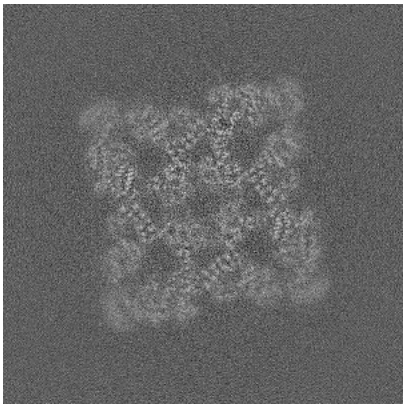


Y Index: 253

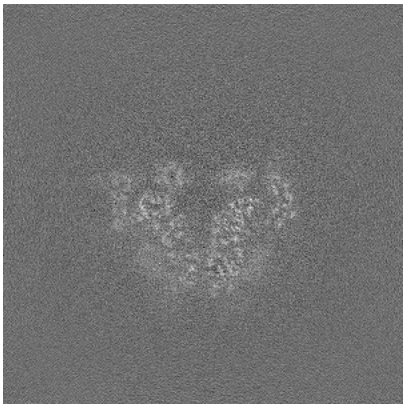


Z Index: 254

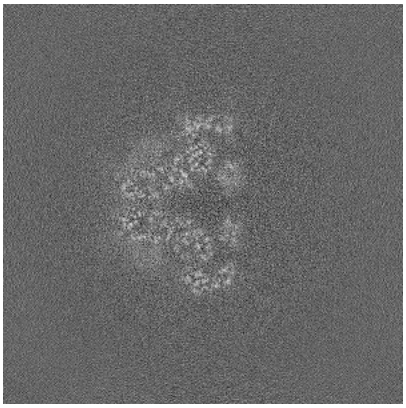
6.3.2 Raw map



X Index: 281



Y Index: 251

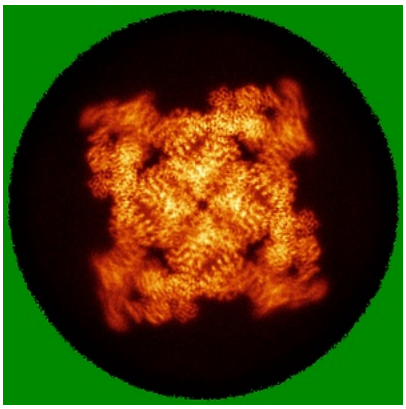


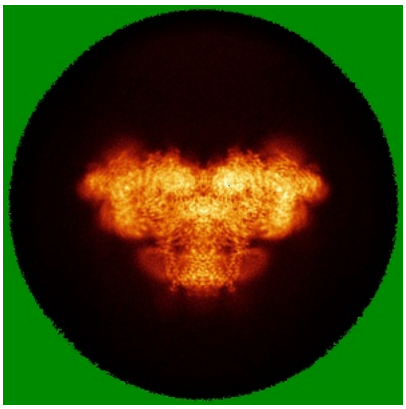
Z Index: 254

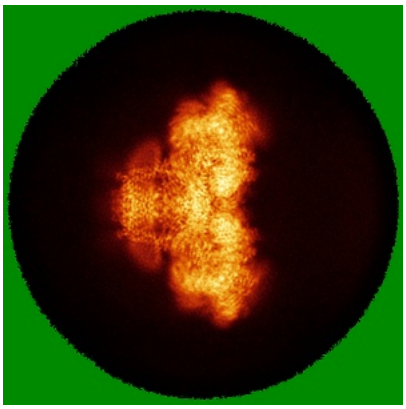
The images above show the largest variance slices of the map in three orthogonal directions.

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

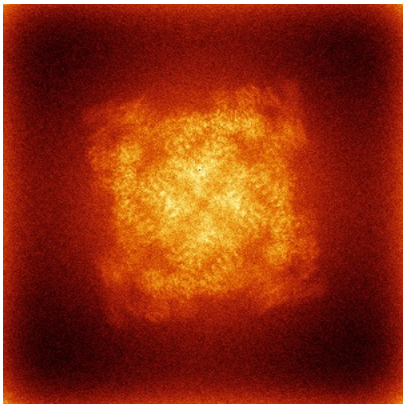
6.4.1 Primary map

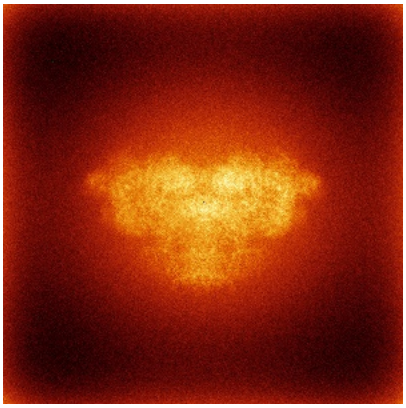

X

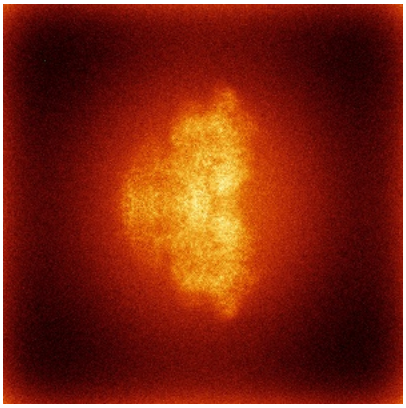

Y


Z

6.4.2 Raw map


X

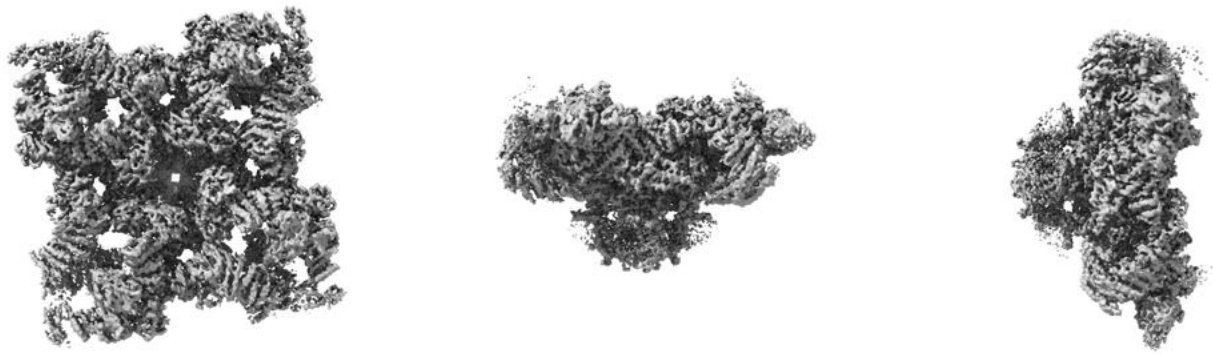

Y


Z

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

6.5 Orthogonal surface views (i)

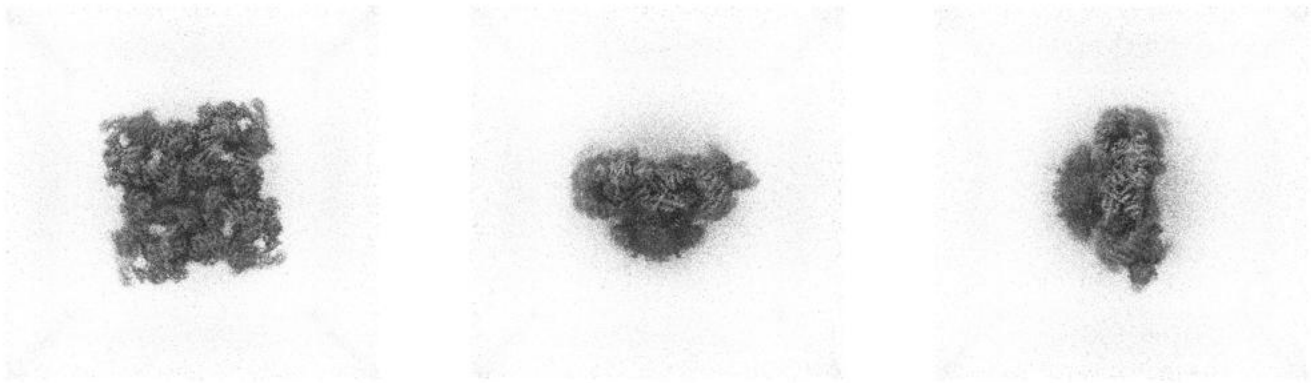
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.09. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

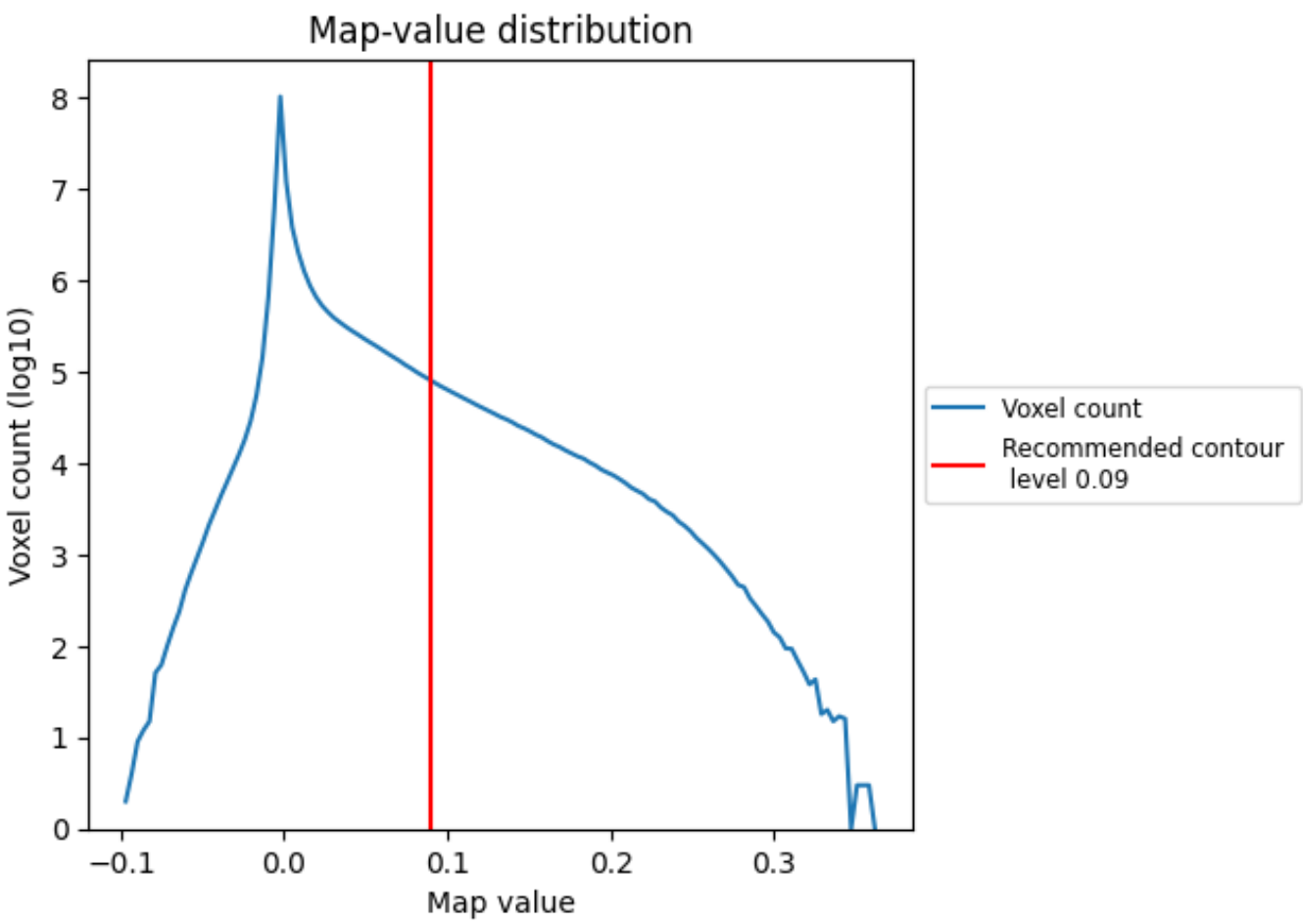
6.6 Mask visualisation (i)

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

7 Map analysis (i)

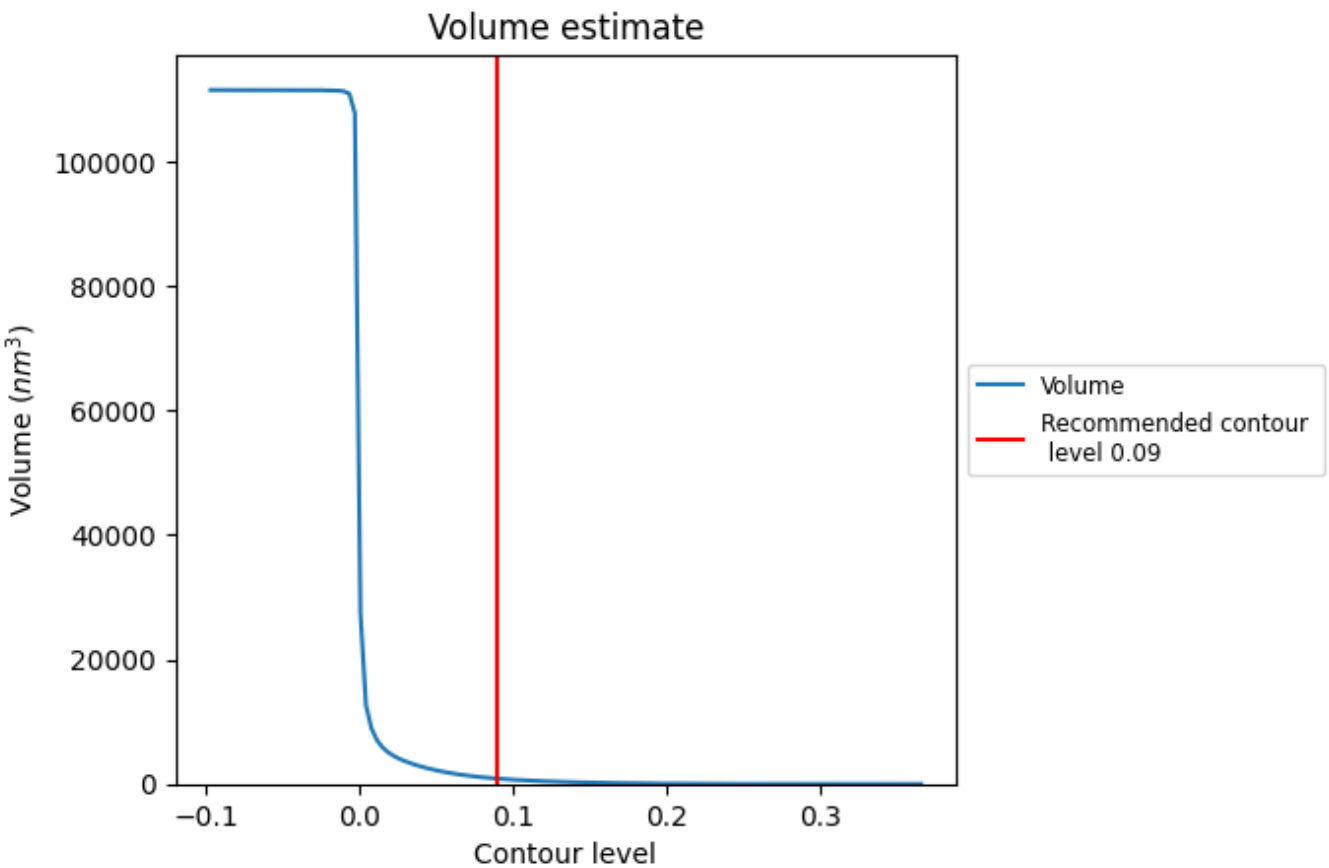
This section contains the results of statistical analysis of the map.

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.

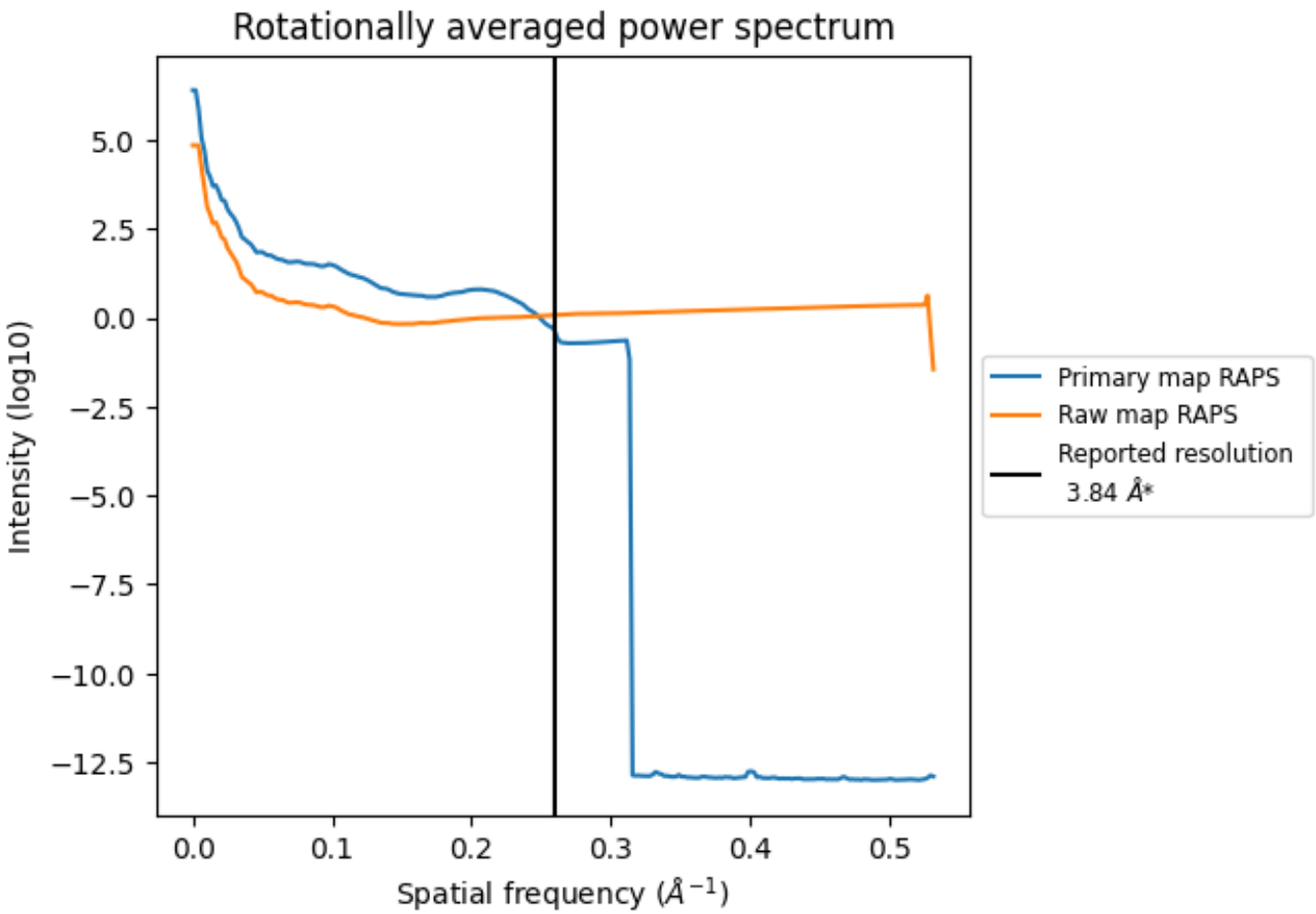
7.2 Volume estimate (i)



The volume at the recommended contour level is 854 nm^3; this corresponds to an approximate mass of 772 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)

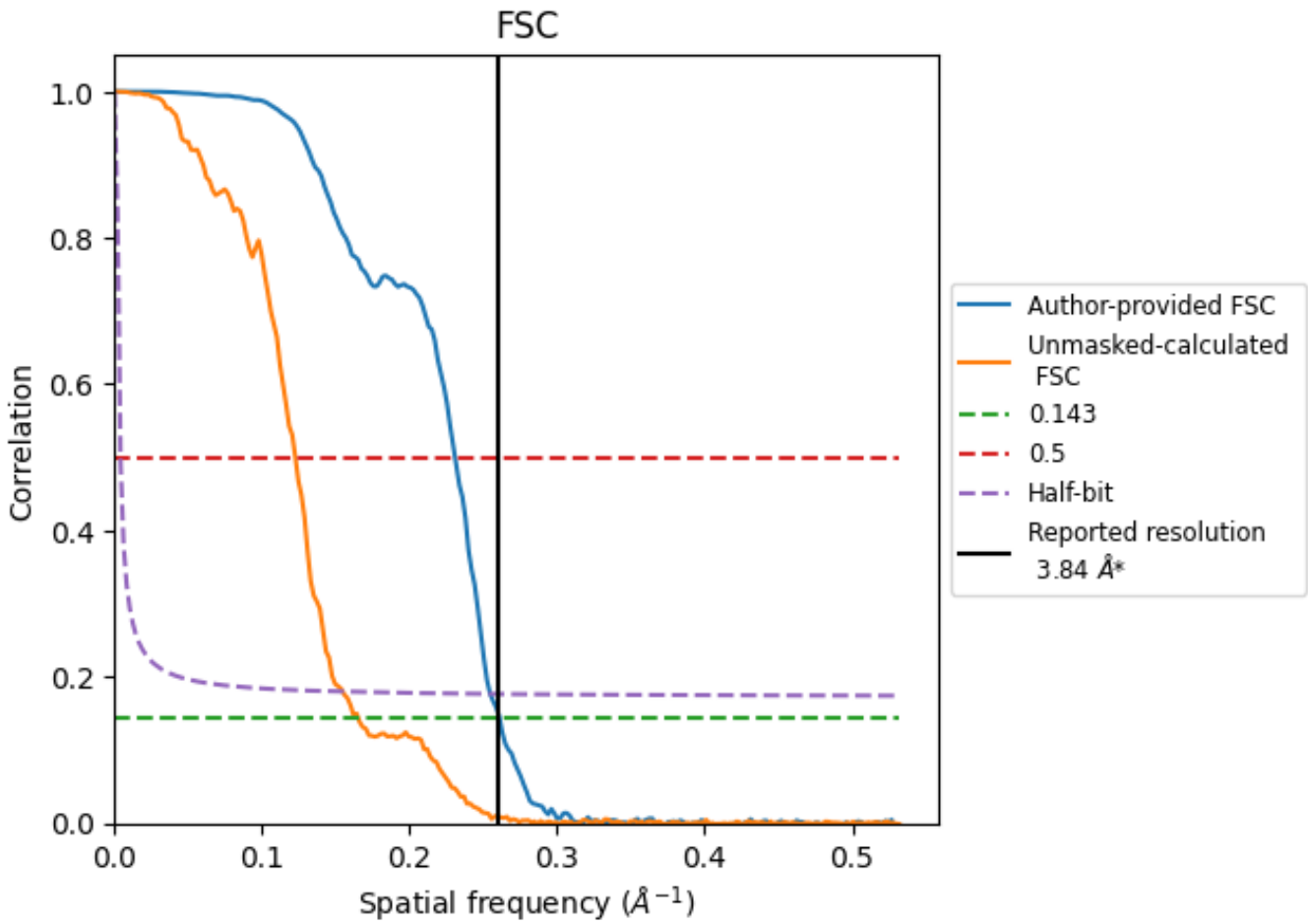


*Reported resolution corresponds to spatial frequency of 0.260 Å^{-1}

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 0.260 Å^{-1}

8.2 Resolution estimates (i)

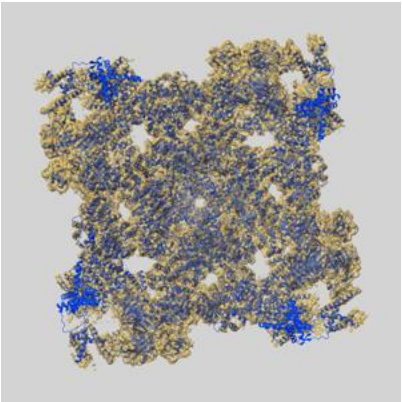
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.84	-	-
Author-provided FSC curve	3.83	4.33	3.93
Unmasked-calculated*	6.05	8.16	6.46

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.05 differs from the reported value 3.84 by more than 10 %

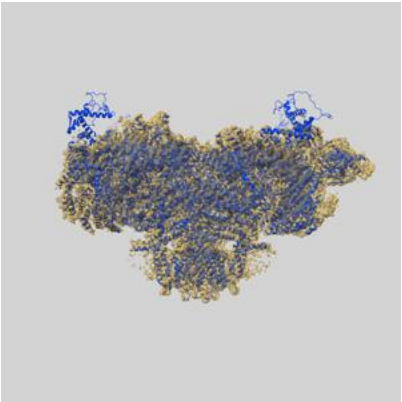
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-27736 and PDB model 8DVE. Per-residue inclusion information can be found in section 3 on page 8.

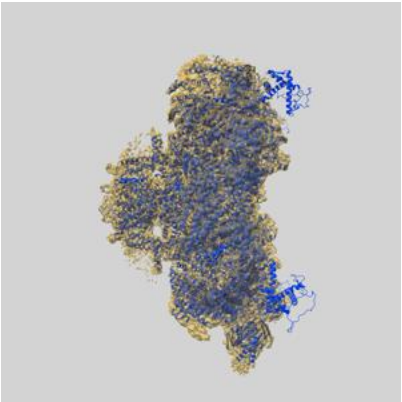
9.1 Map-model overlay (i)



X



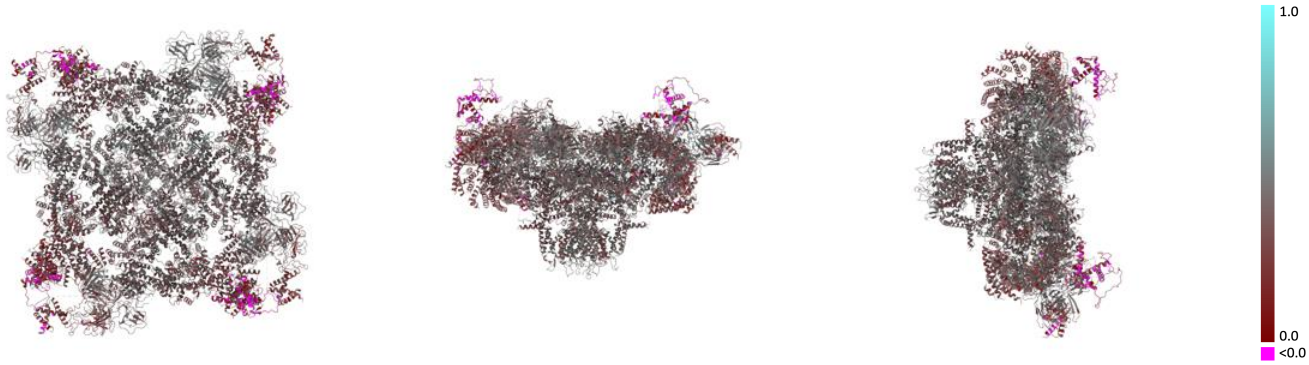
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.09 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

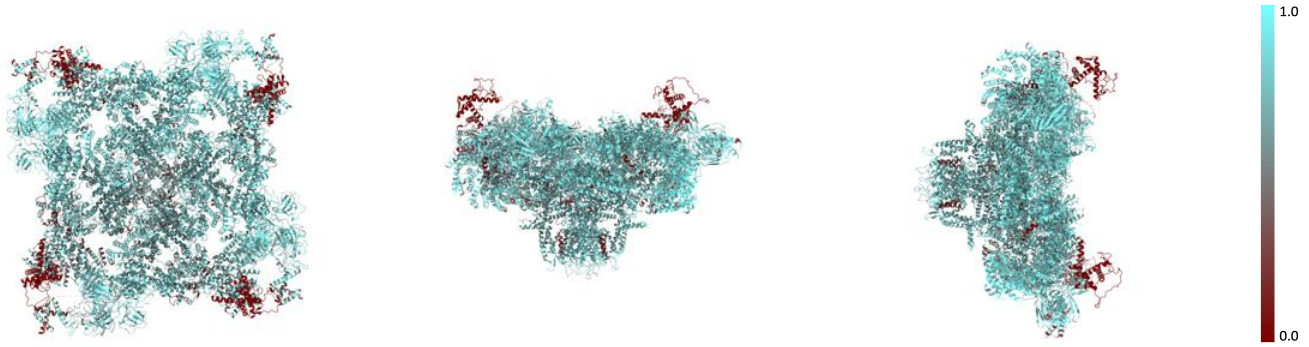
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

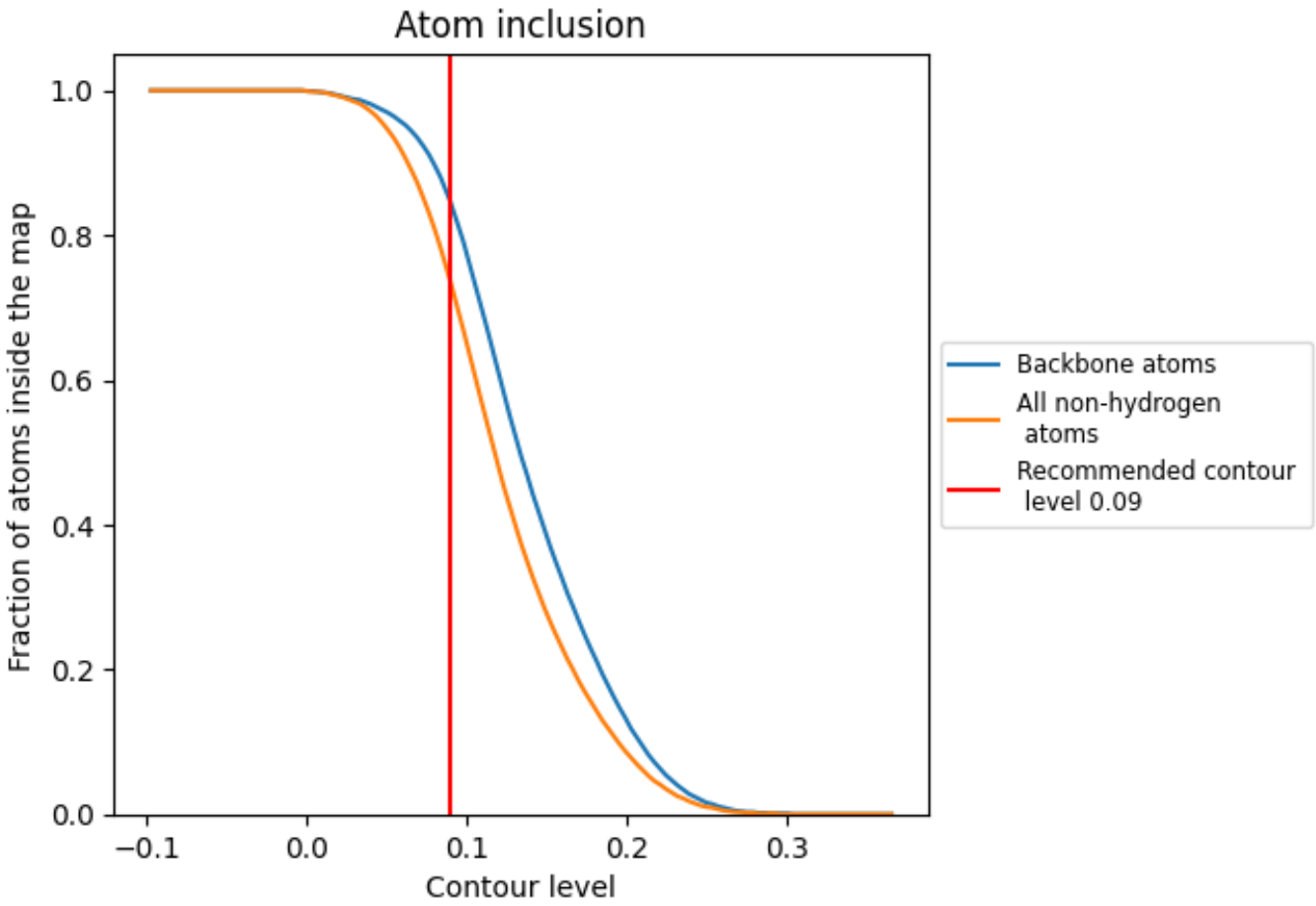
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.09).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 74% 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 (0.09) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7350	0.3920
A	0.7850	0.4170
B	0.8400	0.4640
C	0.6260	0.3710
D	0.7290	0.3920
E	0.8030	0.4430
F	0.3730	0.3380
G	0.7510	0.3940
H	0.7880	0.4340
I	0.5750	0.3400
J	0.6930	0.3630
K	0.7510	0.4140
L	0.4590	0.3390