Full wwPDB EM Validation Report ⓘ

Jan 25, 2024 – 01:35 PM EST

PDB ID	:	8DVV
EMDB ID	:	EMD-27746
Title	:	Recombinant mouse RyR2 triple phosphomimetic mutant S2807D/S2813D/S2030D in complex with FKBP12.6 and nanodisc under open-state conditions
Authors	:	Iyer, K.A.; Hu, Y.; Murayama, T.; Samso, M.
Deposited on	:	2022-07-29
Resolution	:	3.68 Å(reported)
Based on initial model	:	6WOU

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

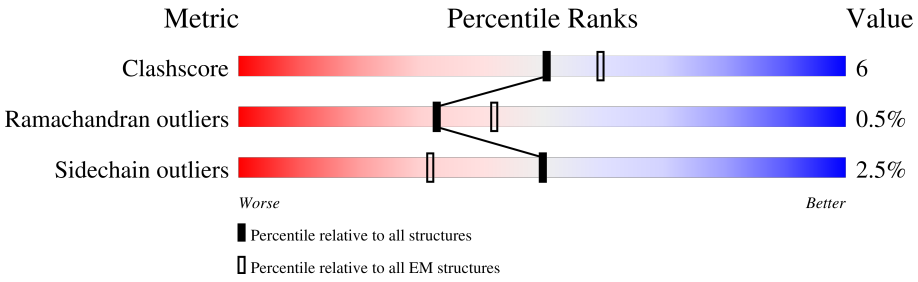
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance

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

The reported resolution of this entry is 3.68 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	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	4966	12% 66% 12% 22%
1	B	4966	12% 65% 12% 22%
1	C	4966	12% 65% 12% 22%
1	D	4966	12% 65% 12% 22%
2	E	107	82% 17%
2	F	107	80% 20%
2	G	107	83% 17%
2	H	107	83% 16%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 119280 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 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3886	Total	C	N	O	S	0	0
			29055	18436	4944	5507	168		
1	B	3886	Total	C	N	O	S	0	0
			29055	18436	4944	5507	168		
1	C	3886	Total	C	N	O	S	0	0
			29055	18436	4944	5507	168		
1	D	3886	Total	C	N	O	S	0	0
			29055	18436	4944	5507	168		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2030	ASP	SER	engineered mutation	UNP E9Q401
A	2807	ASP	SER	engineered mutation	UNP E9Q401
A	2813	ASP	SER	engineered mutation	UNP E9Q401
B	2030	ASP	SER	engineered mutation	UNP E9Q401
B	2807	ASP	SER	engineered mutation	UNP E9Q401
B	2813	ASP	SER	engineered mutation	UNP E9Q401
C	2030	ASP	SER	engineered mutation	UNP E9Q401
C	2807	ASP	SER	engineered mutation	UNP E9Q401
C	2813	ASP	SER	engineered mutation	UNP E9Q401
D	2030	ASP	SER	engineered mutation	UNP E9Q401
D	2807	ASP	SER	engineered mutation	UNP E9Q401
D	2813	ASP	SER	engineered mutation	UNP E9Q401

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	107	Total	C	N	O	S	0	0
			763	480	129	151	3		
2	F	107	Total	C	N	O	S	0	0
			763	480	129	151	3		
2	G	107	Total	C	N	O	S	0	0
			763	480	129	151	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	107	Total	C	N	O	S	0	0
			763	480	129	151	3		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

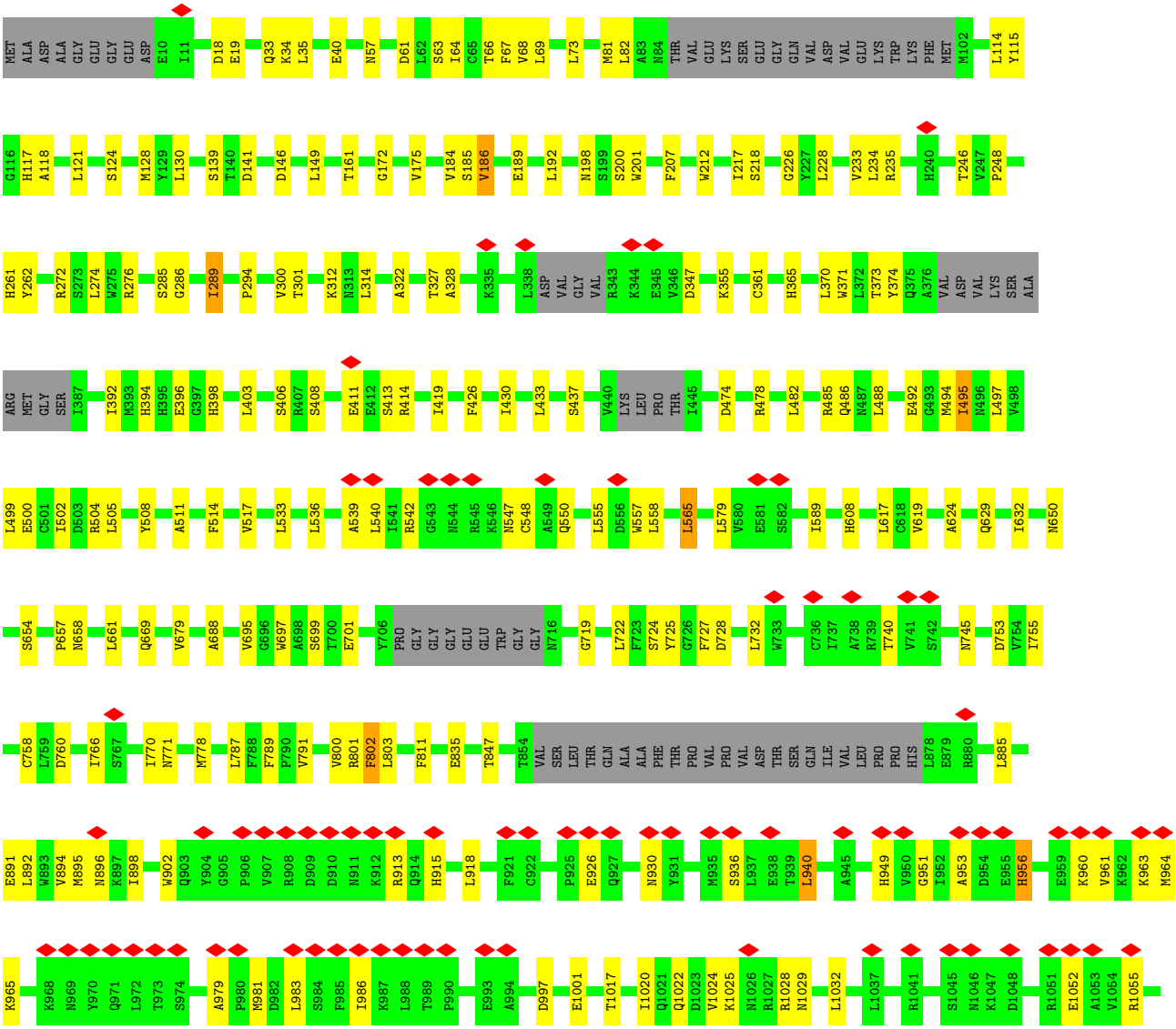
Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Zn	0
			1	1	
4	B	1	Total	Zn	0
			1	1	
4	C	1	Total	Zn	0
			1	1	
4	D	1	Total	Zn	0
			1	1	

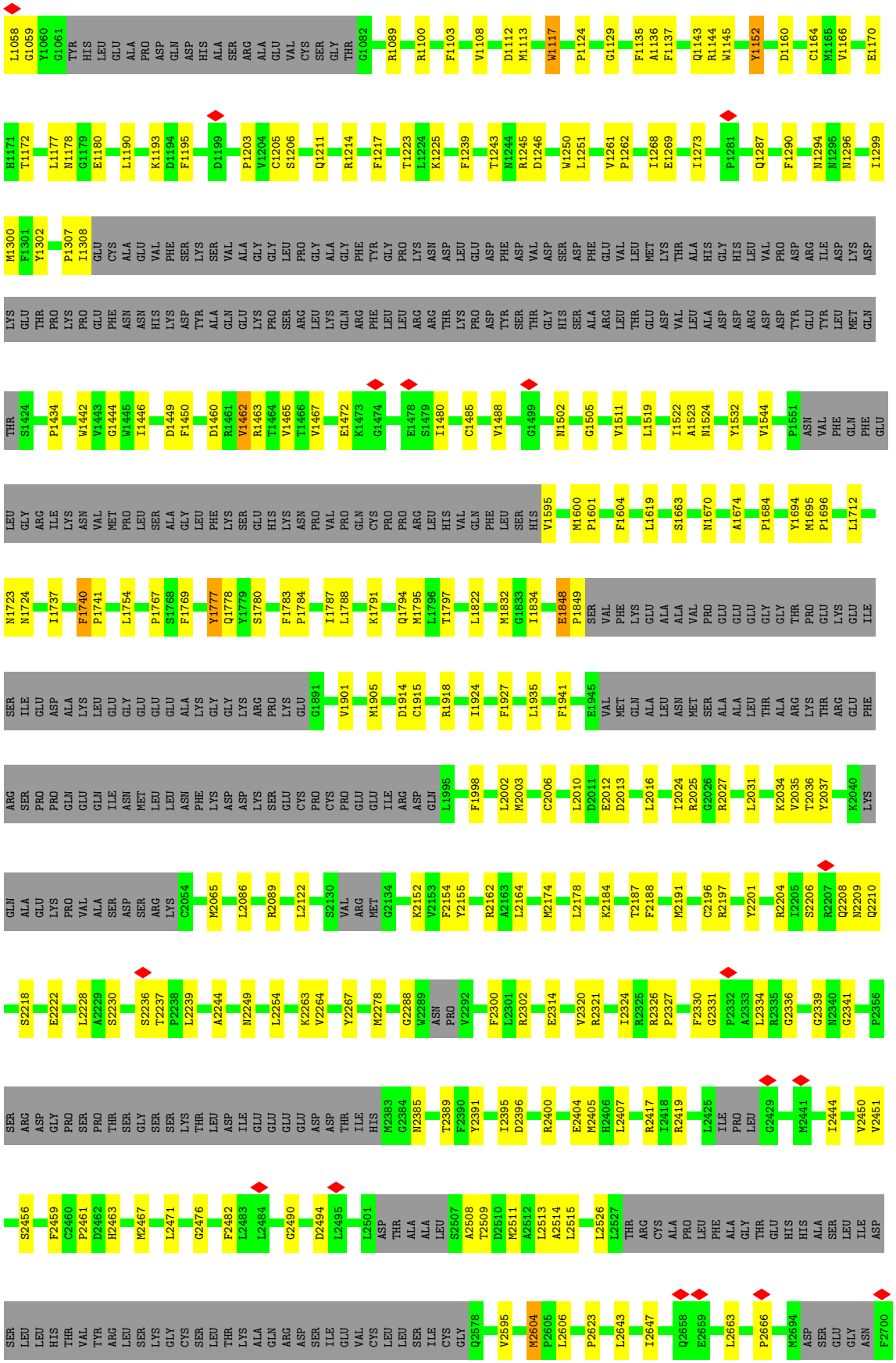
3 Residue-property plots (i)

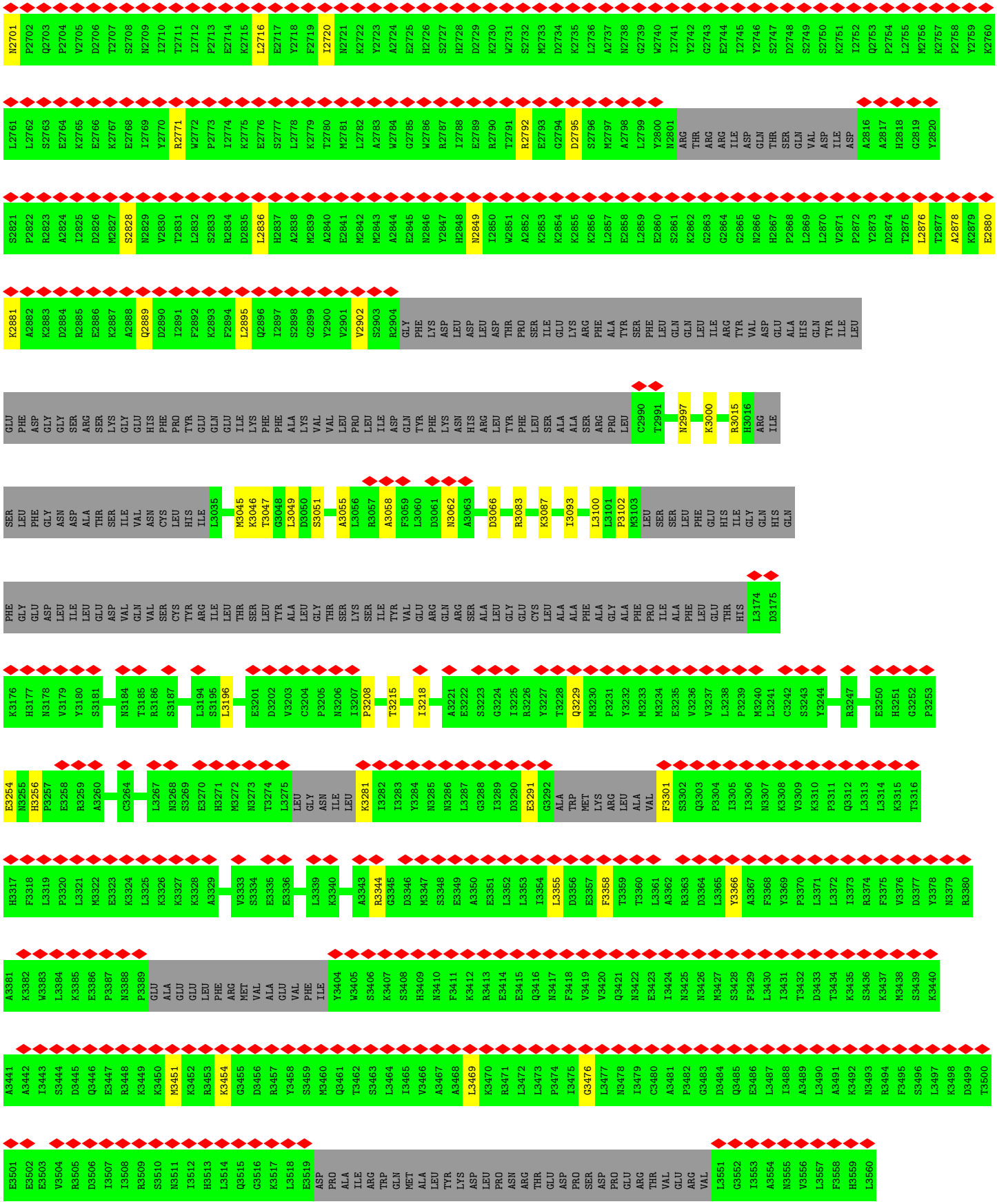
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 2

Chain A:



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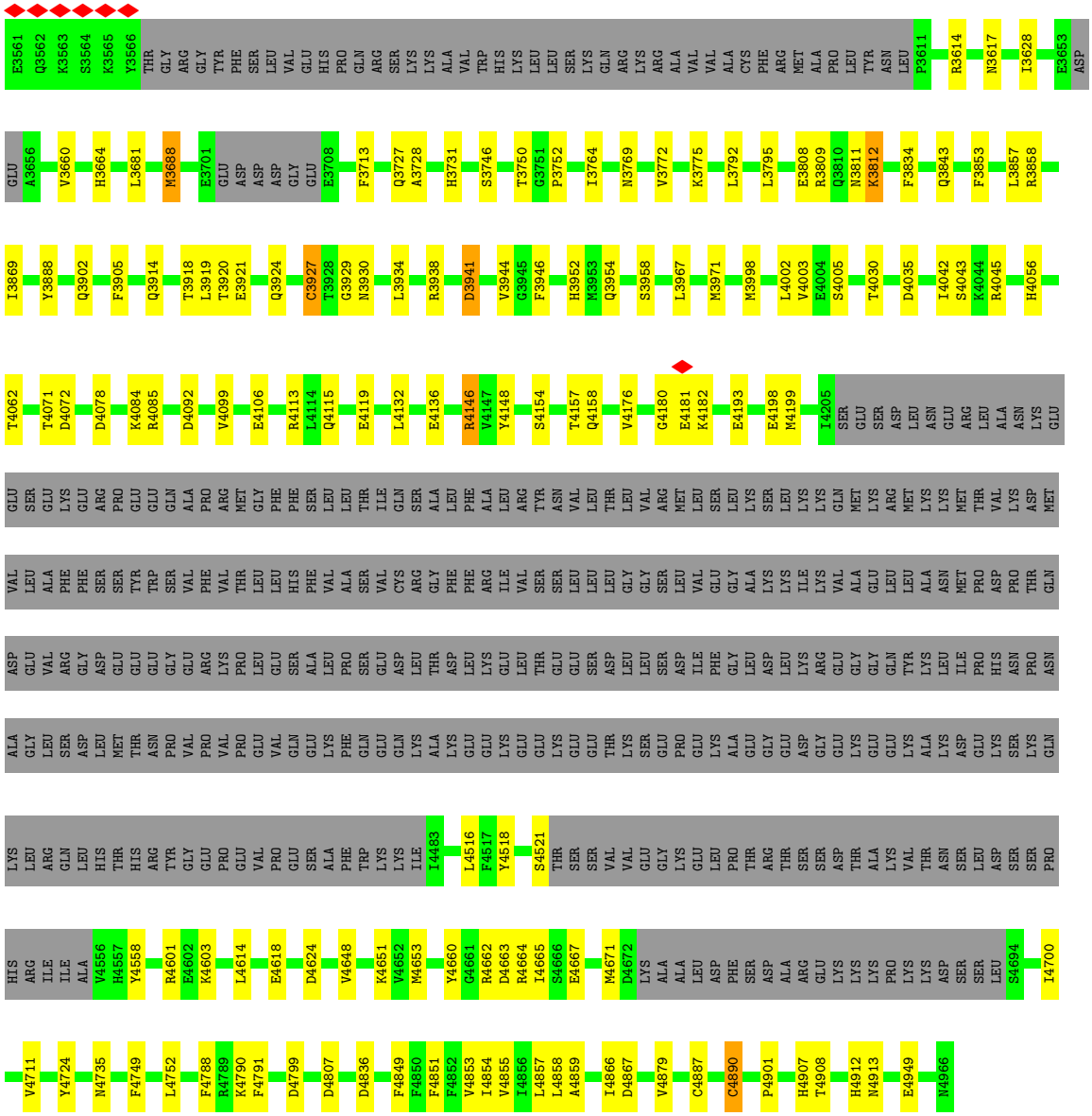
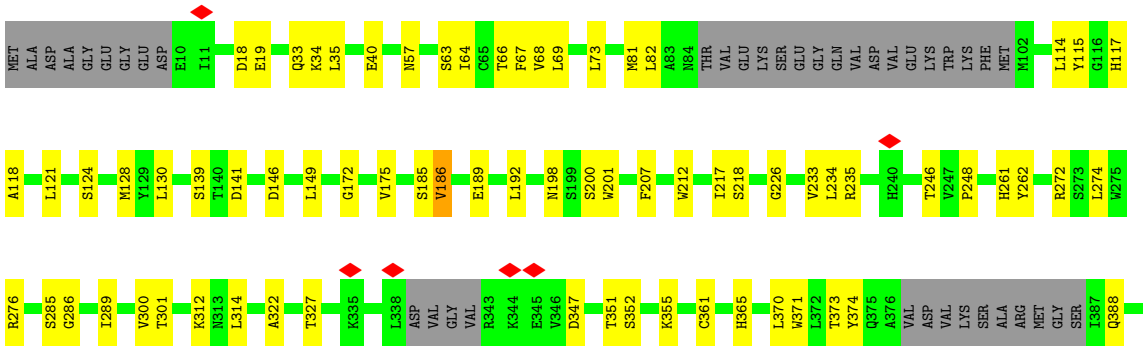
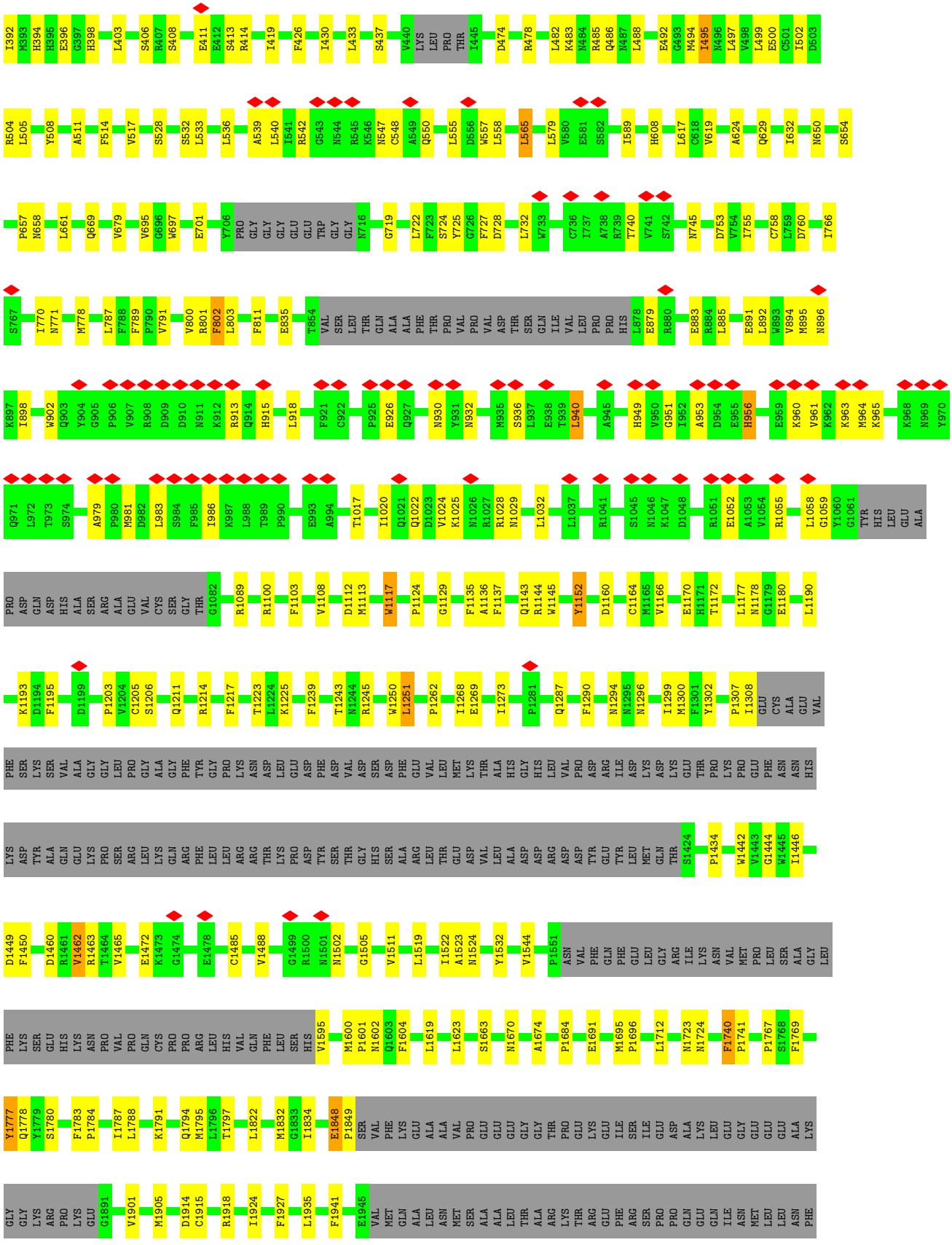
L2761 L2762 S2763 E2764 K2765 E2766 K2767 E2768 I2769 Y2770 R2771 W2772 P2773 I2774 K2775 E2776 S2777 L2778 K2779 T2780 M2781 L2782 A2783 W2784 G2785 W2786 R2787 I2788 E2789 R2790 T2791 R2792 E2793 G2794 D2795 S2796 M2797 A2798 L2799 Y2800 N2801 ARG THR ARG ARG ILE ASP GLN THR SER GLN VAL ASP ILE ASP A2816 A2817 H2818 G2819 Y2820
S2821 P2822 R2823 A2824 I2825 D2826 M2827 S2828 N2829 V2830 T2831 L2832 S2833 R2834 D2835 L2836 H2837 A2838 M2839 A2840 E2841 M2842 M2843 A2844 E2845 N2846 Y2847 H2848 N2849 I2850 W2851 A2852 K2853 K2854 K2855 K2856 L2857 E2858 L2859 E2860 S2861 K2862 G2863 G2864 G2865 N2866 H2867 P2868 L2869 L2870 V2871 P2872 Y2873 D2874 T2875 L2876 T2877 A2878 K2879 E2880
K2881 A2882 K2883 D2884 R2885 E2886 K2887 A2888 Q2889 D2890 I2891 F2892 K2893 F2894 L2895 Q2896 I2897 S2898 G2899 Y2900 V2901 V2902 S2903 R2904 GLY PHE LYS ASP LEU ASP LEU ASP THR PRO SER ILE GLU LYS ARG PHE ALA TYR SER PHE LEU GLN GLN LEU ILE ARG TYR VAL ASP GLU ALA HIS GLN TYR ILE LEU
GLU PHE ASP GLY GLY SER ARG SER LYS GLY GLU HIS PHE PRO TYR GLU GLN GLU ILE LYS PHE PHE ALA ALA LYS VAL VAL LEU PRO LEU ILE ASP GLN TYR PHE LYS ASN HIS ARG LEU TYR PHE LEU SER ALA ALA SER ARG PRO LEU C2990 T2991 N2997 K3000 R3015 H3016 ARG ILE
SER LEU PHE GLY ASN ASP ALA THR SER ILE VAL ASN CYS LEU HIS ILE L3035 M3045 K3046 T3047 G3048 L3049 D3050 S3051 A3055 L3056 R3057 A3058 F3059 L3060 D3061 N3062 A3063 D3066 R3083 K3087 I3093 L3100 L3101 P3102 M3103 LEU SER SER LEU PHE GLU HIS ILE GLY GLN HIS GLN
PHE GLY GLU ASP LEU ILE LEU GLU ASP VAL GLN VAL SER CYS TYR ARG ILE LEU THR SER LEU TYR ALA LEU GLY THR SER LYS SER ILE TYR VAL GLU ARG GLN ARG SER ALA LEU GLY GLU CYS LEU ALA ALA ALA PHE ALA GLY ALA PHE PRO ILE ALA PHE LEU GLU THR HIS L3174 D3175
K3176 H3177 N3178 V3179 Y3180 S3181 N3184 T3185 R3186 S3187 L3194 S3195 L3196 E3201 D3202 V3203 C3204 P3205 N3206 I3207 P3208 T3215 I3218 A3221 E3222 S3223 G3224 I3225 R3226 Y3227 T3228 Q3229 M3230 P3231 Y3232 M3233 M3234 E3235 V3236 V3237 L3238 P3239 M3240 L3241 C3242 S3243 Y3244 R3247 E3250 H3251 G3252 P3253
E3254 N3255 H3256 P3257 E3258 R3259 A3260 C3264 L3267 N3268 S3269 E3270 H3271 H3272 N3273 T3274 L3275 LEU GLY ASN ILE LEU K3281 I3282 I3283 Y3284 N3285 N3286 L3287 G3288 I3289 D3290 E3291 G3292 ALA TRP MET LYS ARG LEU ALA VAL F3301 S3302 Q3303 P3304 I3305 I3306 N3307 K3308 V3309 K3310 P3311 Q3312 L3313 L3314 K3315 T3316
H3317 F3318 L3319 P3320 L3321 M3322 E3323 K3324 L3325 K3326 K3327 K3328 A3329 V3333 S3334 E3335 E3336 L3339 K3340 A3343 R3344 G3345 D3346 M3347 S3348 E3349 A3350 E3351 L3352 L3353 I3354 L3355 D3356 E3357 F3358 T3359 T3360 L3361 A3362 R3363 D3364 L3365 Y3366 A3367 F3368 Y3369 P3370 L3371 L3372 I3373 R3374 F3375 V3376 D3377 Y3378 N3379 R3380
A3381 K3382 W3383 L3384 K3385 E3386 P3387 N3388 P3389 GLU ALA GLU GLU LEU PHE ARG MET VAL ALA GLU VAL PHE ILE Y3404 W3405 S3406 K3407 S3408 H3409 N3410 F3411 K3412 R3413 E3414 E3415 Q3416 N3417 F3418 V3419 V3420 Q3421 N3422 E3423 I3424 N3425 N3426 M3427 S3428 F3429 L3430 I3431 T3432 D3433 T3434 K3435 S3436 K3437 M3438 S3439 K3440
A3441 A3442 I3443 S3444 D3445 Q3446 E3447 R3448 K3449 K3450 M3451 K3452 R3453 K3454 G3455 D3456 R3457 Y3458 S3459 M3460 Q3461 T3462 S3463 L3464 I3465 V3466 A3467 A3468 L3469 K3470 R3471 L3472 L3473 P3474 I3475 G3476 L3477 N3478 I3479 C3480 A3481 P3482 G3483 D3484 Q3485 E3486 L3487 I3488 A3489 L3490 A3491 K3492 N3493 R3494 F3495 S3496 L3497 K3498 D3499 T3500
E3501 E3502 E3503 V3504 R3505 D3506 I3507 I3508 R3509 S3510 N3511 I3512 H3513 L3514 Q3515 G3516 K3517 L3518 E3519 ASP PRO ALA ILE ARG TRP GLN MET ALA LEU TYR LYS ASP LEU PRO ASN ARG THR GLU ASP PRO SER ASP PRO GLU ARG THR VAL GLU ARG VAL L3551 G3552 I3553 A3554 N3555 V3556 L3557 F3558 H3559 L3560

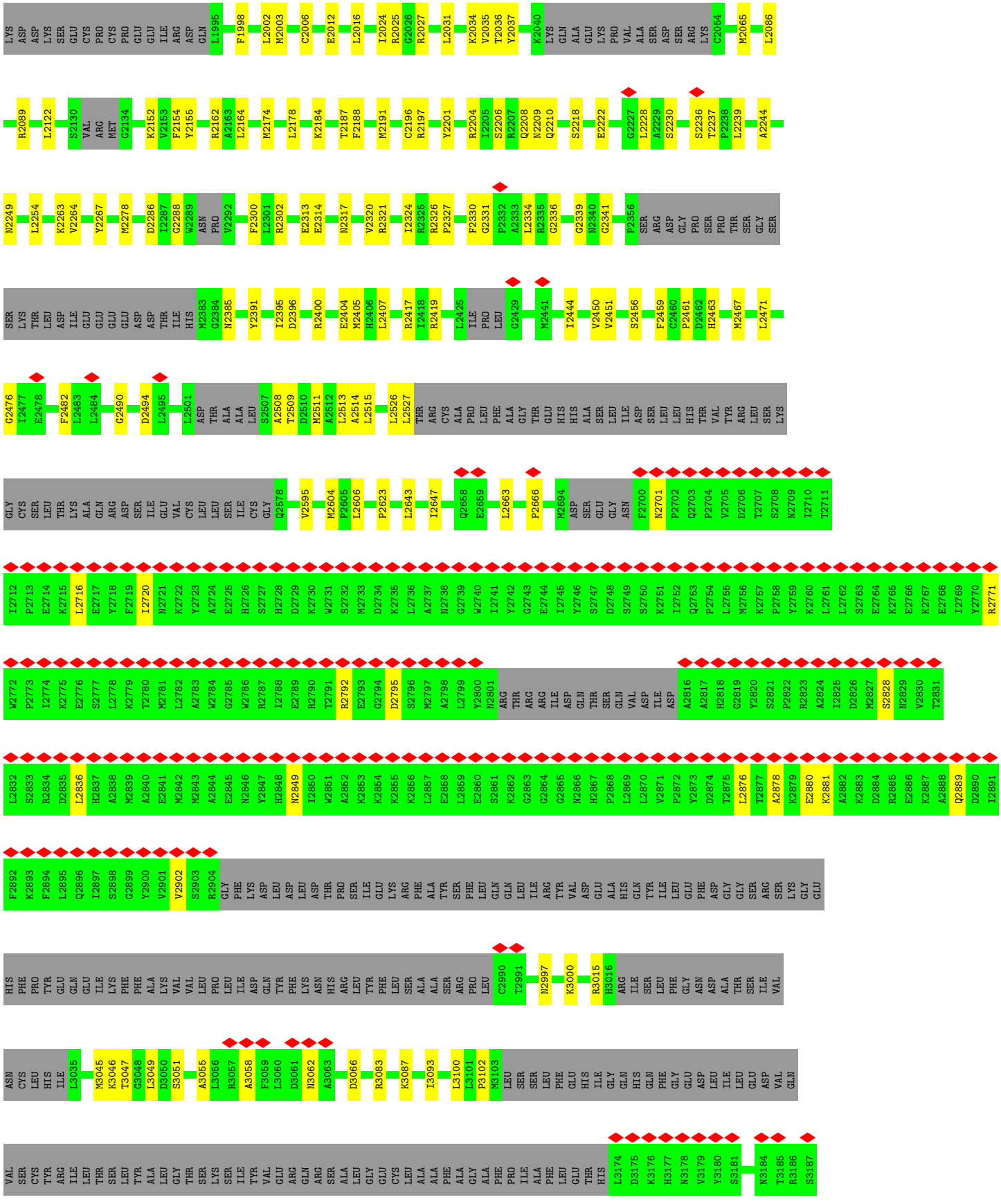


• Molecule 1: Ryanodine receptor 2

Chain B:




I392 M393 H394 H395 E396 G397 H398 L403 S406 R407 S408 E411 E412 S413 R414 I419 F426 I430 L433 S437 V440 LYS LEU PRO THR I445 D474 R478 L482 K483 N484 R485 Q486 N487 L488 E492 G493 M494 I495 N496 L497 V498 L499 E500 C501 I502 D503
R504 L505 Y508 A511 F514 V517 S528 S532 L533 L536 A539 L540 L541 R542 G543 N544 R545 K546 N547 C548 A549 Q550 L555 D556 W557 L558 L565 L579 V580 E581 S582 I589 H608 L617 C618 V619 A624 Q629 I632 N650 S654
P657 N658 L661 Q669 V679 V695 G696 W697 E701 Y706 PRO GLY GLY GLY GLU GLU TRP GLY GLY N716 G719 L722 F723 S724 Y725 G726 F727 D728 L732 W733 C736 I737 A738 R739 T740 V741 S742 N745 D753 W754 I755 C758 L759 D760 I766
S767 I770 N771 M778 L787 F788 F789 P790 V791 V800 R801 F802 L803 F811 E835 T854 VAL SER LEU THR GLN ALA ALA PHE THR PRO VAL PRO VAL ASP THR SER GLN ILE VAL LEU PRO PRO HIS L878 E879 R880 E883 R884 L885 E891 L892 W893 V894 M895 N896
K897 I898 W902 Q903 Y904 G905 P906 V907 R908 D909 D910 N911 K912 R913 Q914 H915 L918 F921 C922 P925 E926 Q927 N930 Y931 N932 M935 S936 L937 E938 T939 L940 A945 H949 V950 G951 I962 A953 D954 E955 H956 E959 K960 V961 K962 K963 M964 K965 K968 N969 Y970
Q971 L972 T973 S974 A979 P980 M981 D982 L983 S984 F985 I986 K987 L988 T989 P990 E993 A994 T1017 I1020 Q1021 Q1022 D1023 V1024 K1025 N1026 R1027 R1028 N1029 L1032 L1037 R1041 S1045 N1046 K1047 D1048 R1051 E1052 A1053 V1054 R1055 L1058 G1059 Y1060 G1061 TYR HIS LEU GLU ALA
PRO ASP GLN ASP HIS ALA SER ARG ALA GLU VAL CYS SER GLY THR G1082 R1089 R1100 F1103 V1108 D1112 M1113 W1117 P1124 G1129 F1135 A1136 F1137 Q1143 R1144 W1145 Y1152 D1160 C1164 M1165 V1166 E1170 H1171 T1172 L1177 N1178 G1179 E1180 L1190
K1193 D1194 F1195 D1199 P1203 V1204 C1205 S1206 Q1211 R1214 F1217 T1223 L1224 K1225 F1239 T1243 N1244 R1245 W1250 L1251 P1262 I1268 E1269 I1273 P1281 Q1287 F1290 N1294 N1295 N1296 I1299 M1300 F1301 Y1302 P1307 I1308 GLU CYS ALA GLU VAL
PHE SER LYS SER VAL ALA GLY GLY LEU PRO GLY ALA GLY PHE TYR GLY PRO LYS ASN ASP LEU GLU ASP PHE ASP VAL ASP SER ASP PHE GLU VAL LEU MET LYS THR ALA HIS GLY HIS LEU VAL PRO ASP ARG ILE ASP LYS ASP LYS GLU VAL PRO LYS GLU PHE ASN ASN HIS
LYS ASP TYR ALA GLN GLU LYS PRO SER ARG LEU LYS GLN ARG PHE LEU LEU ARG ARG THR LYS PRO ASP TYR SER THR GLY HIS SER ALA ARG LEU THR GLU ASP VAL LEU ALA ASP ASP ARG ASP ASP TYR GLU TYR LEU MET GLN THR S1424 P1434 W1442 V1443 G1444 W1445 I1446
D1449 F1450 D1460 R1461 V1462 R1463 T1464 V1465 E1472 K1473 G1474 E1478 C1485 V1488 G1499 R1500 N1501 N1502 G1505 V1511 L1519 I1522 A1523 N1524 Y1532 V1544 P1551 ASN VAL PHE GLN PHE GLU LEU GLY ARG ILE LYS ASN VAL MET PRO LEU SER ALA GLY LEU
PHE LYS SER GLU HIS LYS ASN PRO VAL PRO GLN CYS PRO PRO ARG LEU HIS VAL GLN PHE LEU SER HIS V1595 M1600 P1601 N1602 Q1603 F1604 L1619 L1623 S1663 N1670 A1674 P1684 E1691 M1695 P1696 L1712 N1723 N1724 F1740 P1741 P1767 S1768 F1769
Y1777 Q1778 Y1779 S1780 F1783 P1784 I1787 L1788 K1791 Q1794 M1795 L1796 T1797 L1822 M1832 G1833 I1834 E1848 P1849 SER VAL PHE LYS GLU ALA ALA VAL PRO GLU GLU GLU GLY GLY THR PRO GLU LYS GLU ILE SER ILE GLU ASP ALA LYS LEU GLU GLU GLU GLU ALA LYS
GLY GLY LYS ARG PRO LYS GLU G1891 V1901 M1905 D1914 C1915 R1918 I1924 F1927 L1935 F1941 E1945 VAL MET GLN ALA LEU ASN MET SER ALA ALA LEU THR ALA ARG LYS THR ARG GLU PHE ARG SER PRO PRO GLN GLU GLN ILE ASN MET LEU LEU ASN PHE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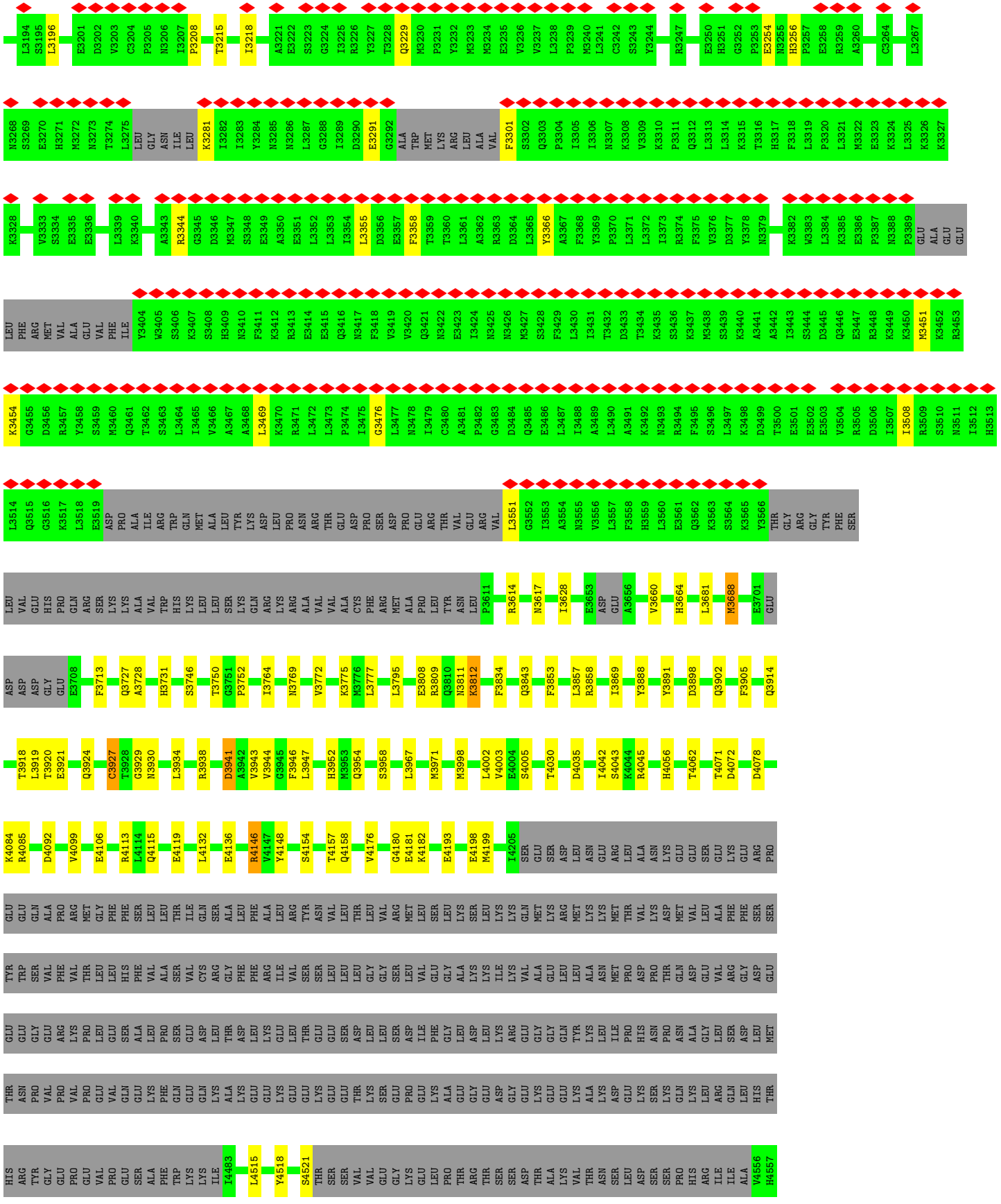
R2089 L2122 S2130 VAL ARG MET G2134 K2152 V2153 F2154 Y2155 R2162 A2163 L2164 M2174 L2178 K2184 T2187 F2188 M2191 C2196 R2197 Y2201 R2204 I2205 S2206 R2207 Q2208 N2209 Q2210 S2218 E2222 G2227 L2228 A2229 S2230 S2236 T2237 P2238 L2239 A2244
N2249 L2254 K2263 V2264 Y2267 M2278 D2286 I2287 G2288 W2289 ASN PRO V2292 F2300 L2301 R2302 E2313 E2314 N2317 V2320 R2321 I2324 R2325 R2326 P2327 F2330 G2331 P2332 A2333 L2334 R2335 G2336 G2339 N2340 G2341 P2356 SER ARG ASP GLY PRO SER PRO THR SER GLY SER
SER LYS THR LEU ASP ILE GLU GLU GLU ASP ASP THR ILE HIS M2383 G2384 N2385 Y2391 I2395 D2396 R2400 E2404 M2405 H2406 L2407 R2417 I2418 R2419 L2425 ILE PRO LEU G2429 M2441 I2444 V2450 V2451 S2456 F2459 C2460 P2461 D2462 H2463 M2467 L2471
G2476 I2477 E2478 F2482 L2483 L2484 G2490 D2494 L2495 L2501 ASP THR ALA ALA LEU S2507 A2508 T2509 D2510 M2511 A2512 L2513 A2514 L2515 L2526 L2527 THR ARG CYS ALA PRO LEU PHE ALA GLY THR GLU HIS HIS ALA SER LEU ILE ASP SER LEU LEU HIS THR VAL TYR ARG LEU SER LYS
GLY CYS SER LEU THR LYS ALA GLN ARG ASP SER ILE GLU VAL CYS LEU LEU SER ILE CYS GLY Q2578 V2595 M2604 P2605 L2606 P2623 L2643 I2647 Q2658 E2659 L2663 P2666 M2694 ASP SER GLU GLY ASN F2700 N2701 P2702 Q2703 P2704 V2705 D2706 T2707 S2708 N2709 I2710 T2711
I2712 P2713 E2714 K2715 L2716 E2717 Y2718 F2719 I2720 W2721 K2722 Y2723 A2724 E2725 H2726 S2727 H2728 D2729 K2730 W2731 S2732 M2733 D2734 K2735 L2736 A2737 N2738 G2739 W2740 I2741 Y2742 G2743 E2744 I2745 Y2746 S2747 D2748 S2749 S2750 K2751 I2752 Q2753 P2754 L2755 M2756 K2757 P2758 S2708 Y2759 K2760 L2761 L2762 S2763 E2764 K2765 E2766 K2767 E2768 I2769 Y2770 R2771
W2772 P2773 I2774 K2775 E2776 S2777 L2778 K2779 T2780 M2781 L2782 A2783 W2784 G2785 W2786 R2787 I2788 E2789 R2790 T2791 R2792 E2793 G2794 D2795 S2796 M2797 A2798 L2799 Y2800 N2801 ARG THR ARG ARG ILE ASP GLN THR SER GLN VAL ASP ILE ASP A2816 A2817 H2818 G2819 Y2820 S2821 P2822 R2823 A2824 I2825 D2826 M2827 S2828 N2829 V2830 T2831
L2832 S2833 R2834 D2835 L2836 H2837 A2838 M2839 A2840 E2841 M2842 M2843 A2844 E2845 N2846 Y2847 H2848 N2849 I2850 W2851 A2852 K2853 K2854 K2855 K2856 L2857 E2858 L2859 E2860 S2861 K2862 G2863 G2864 G2865 N2866 H2867 P2868 L2869 L2870 V2871 P2872 Y2873 D2874 T2875 L2876 T2877 A2878 K2879 E2880 K2881 A2882 K2883 D2884 R2885 E2886 K2887 A2888 Q2889 D2890 I2891
F2892 K2893 F2894 L2895 Q2896 I2897 S2898 G2899 Y2900 V2901 V2902 S2903 R2904 GLY PHE LYS ASP LEU ASP LEU ASP THR PRO SER ILE GLU LYS ARG PHE ALA TYR SER PHE LEU GLN GLN LEU ILE ARG TYR VAL ASP GLU ALA HIS GLN TYR ILE LEU GLU PHE ASP GLY GLY SER ARG SER LYS GLY GLU
HIS PHE PRO TYR GLU GLN GLU ILE LYS PHE PHE ALA LYS VAL VAL LEU PRO LEU ILE ASP GLN TYR PHE LYS ASN HIS ARG LEU TYR PHE LEU SER ALA ALA SER ARG PRO LEU C2990 T2991 N2997 K3000 R3015 H3016 ARG ILE SER LEU PHE GLY ASN ASP ALA THR SER ILE VAL
ASN CYS LEU HIS ILE L3035 M3045 K3046 T3047 G3048 L3049 D3050 S3051 A3055 L3056 R3057 A3058 F3059 L3060 D3061 A3063 D3066 R3083 K3087 I3093 L3100 L3101 P3102 M3103 LEU SER SER LEU PHE GLU HIS ILE GLY GLN HIS GLN PHE GLY GLU ASP LEU ILE LEU GLU ASP VAL GLN
VAL SER CYS TYR ARG ILE LEU THR SER LEU TYR ALA LEU GLY THR SER LYS SER ILE TYR VAL GLU ARG GLN ARG SER ALA LEU GLY GLU CYS LEU ALA ALA PHE ALA GLY ALA PHE PRO ILE ALA PHE LEU GLU THR HIS L3174 D3175 K3176 H3177 N3178 V3179 Y3180 S3181 N3184 T3185 R3186 S3187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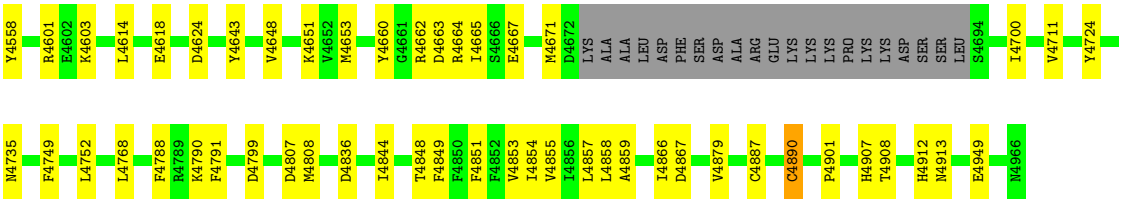
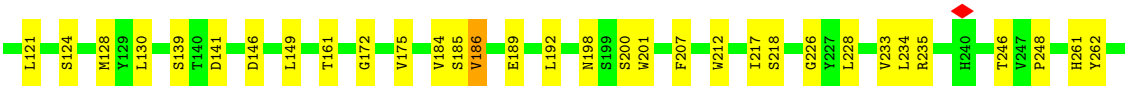
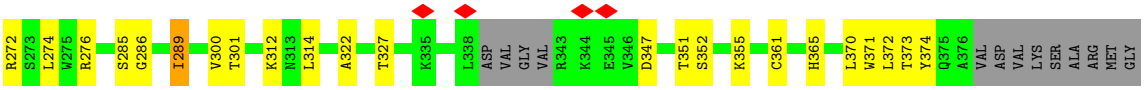
N3268 S3269 E3270 H3271 M3272 N3273 T3274 L3275 LEU GLY ASN ILE LEU K3281 I3282 I3283 Y3284 N3285 N3286 L3287 G3288 I3289 D3290 E3291 G3292 ALA TRP MET LYS ARG LEU ALA VAL F3301 S3302 Q3303 P3304 I3305 I3306 N3307 K3308 V3309 K3310 P3311 Q3312 L3313 L3314 K3315 T3316 H3317 F3318 L3319 P3320 L3321 M3322 E3323 K3324 L3325 K3326 K3327
K3328 V3333 S3334 E3335 E3336 L3339 K3340 A3343 R3344 G3345 D3346 M3347 S3348 E3349 A3350 E3351 L3352 L3353 I3354 L3355 D3356 E3357 F3358 T3359 T3360 L3361 A3362 R3363 D3364 L3365 Y3366 A3367 F3368 Y3369 P3370 L3371 L3372 I3373 R3374 F3375 V3376 D3377 Y3378 N3379 K3382 W3383 L3384 K3385 E3386 P3387 N3388 P3389 GLU ALA GLU GLU
LEU PHE ARG MET VAL ALA GLU VAL PHE ILE Y3404 W3405 S3406 K3407 S3408 H3409 N3410 F3411 K3412 R3413 E3414 E3415 Q3416 N3417 F3418 V3419 V3420 Q3421 N3422 E3423 I3424 N3425 N3426 M3427 S3428 F3429 L3430 I3431 T3432 D3433 T3434 K3435 S3436 K3437 M3438 S3439 K3440 A3441 A3442 I3443 S3444 D3445 Q3446 E3447 R3448 K3449 K3450 M3451 K3452 R3453
K3454 G3455 D3456 R3457 Y3458 S3459 M3460 Q3461 T3462 S3463 L3464 I3465 V3466 A3467 A3468 L3469 K3470 R3471 L3472 L3473 P3474 I3475 G3476 L3477 N3478 I3479 C3480 A3481 P3482 G3483 D3484 Q3485 E3486 L3487 I3488 A3489 L3490 A3491 K3492 N3493 R3494 F3495 S3496 L3497 K3498 D3499 T3500 E3501 E3502 E3503 V3504 R3505 D3506 I3507 I3508 R3509 S3510 N3511 I3512 H3513
L3514 Q3515 G3516 K3517 L3518 E3519 ASP PRO ALA ILE ARG TRP GLN MET ALA LEU TYR LYS ASP LEU PRO ASN ARG THR GLU ASP PRO GLU ARG THR VAL GLU ARG VAL L3551 G3552 I3553 A3554 N3555 V3556 L3557 F3558 H3559 L3560 E3561 Q3562 K3563 S3564 K3565 Y3566 THR GLY ARG GLY TYR PHE SER
LEU VAL GLU HIS PRO GLN ARG SER LYS LYS ALA VAL TRP HIS LYS LEU LEU SER LYS GLN ARG LYS ARG ALA VAL VAL ALA CYS PHE ARG MET ALA PRO LEU TYR ASN LEU P3611 R3614 N3617 I3628 E3653 ASP GLU A3656 V3660 H3664 L3681 M3688 E3701 GLU
ASP ASP ASP GLY GLU E3708 F3713 Q3727 A3728 H3731 S3746 T3750 G3751 P3752 I3764 N3769 V3772 K3775 M3776 L3777 L3795 E3808 R3809 Q3810 N3811 K3812 F3834 Q3843 F3853 L3857 R3858 I3869 Y3888 Y3891 D3898 Q3902 F3905 Q3914
T3918 L3919 T3920 E3921 Q3924 G3927 T3928 G3929 N3930 L3934 R3938 D3941 A3942 V3943 V3944 G3945 F3946 L3947 H3952 K3953 Q3954 S3958 L3967 M3971 M3998 L4002 V4003 E4004 S4005 T4030 D4035 I4042 S4043 K4044 R4045 H4056 T4062 T4071 D4072 D4078
K4084 R4085 D4092 V4099 E4106 R4113 L4114 Q4115 E4119 L4132 E4136 R4146 V4147 Y4148 S4154 T4157 Q4158 V4176 G4180 E4181 K4182 E4193 E4198 M4199 I4205 SER GLU SER ASP LEU ASN GLU ARG LEU ALA ASN LYS GLU GLU SER GLU LYS GLU ARG PRO
GLU GLU GLN ALA PRO ARG MET GLY PHE PHE SER LEU LEU THR ILE GLN SER ALA LEU PHE ALA LEU ARG TYR ASN VAL LEU THR LEU VAL ARG MET LEU SER LEU LYS SER LEU LYS LYS GLN MET LYS ARG MET LYS LYS MET THR VAL LYS ASP MET VAL LEU ALA PHE PHE SER SER
TYR TRP SER VAL PHE VAL THR LEU LEU HIS PHE VAL ALA SER VAL CYS ARG GLY PHE PHE ARG ILE VAL SER SER LEU LEU LEU GLY GLY SER LEU VAL GLU GLY GLY ALA LYS LYS ILE LYS VAL ALA GLU LEU LEU ALA ASN MET PRO ASP PRO THR GLN ASP GLU VAL ARG GLY ASP GLU
GLU GLU GLY GLU ARG LYS PRO LEU GLU SER ALA LEU PRO SER GLU ASP LEU THR ASP LEU LYS GLU LEU THR GLU GLU SER ASP LEU LEU LEU SER ASP ILE PHE GLY LEU ASP LEU LYS ARG GLU GLY GLN TYR LYS LYS LEU ALA LEU ILE PRO HIS ASN PRO ASN ALA GLY LEU SER ASP MET
THR ASN PRO VAL PRO VAL PRO GLU VAL GLN GLU LYS PHE GLN GLU GLN LYS ALA LYS GLU GLU LYS GLU GLU LYS GLU GLU GLU THR LYS SER GLU PRO GLU LYS ALA GLU GLY GLU ASP GLY GLU LYS GLU GLU LYS ALA LYS LEU LEU ARG GLN LEU HIS THR
HIS ARG TYR GLY GLU PRO GLU VAL PRO GLU SER ALA PHE TRP LYS LYS ILE T4483 L4515 Y4518 S4521 THR SER SER VAL VAL GLU GLY LYS GLU LEU PRO THR ARG THR SER SER ASP THR ALA LYS VAL THR ASN SER LEU ASP SER SER PRO HIS ARG ILE ILE ALA V4556 H4557

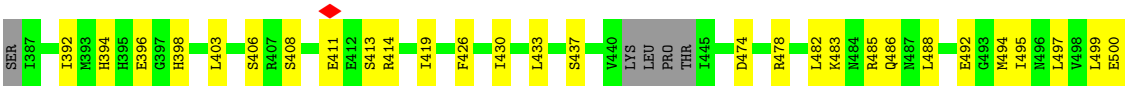


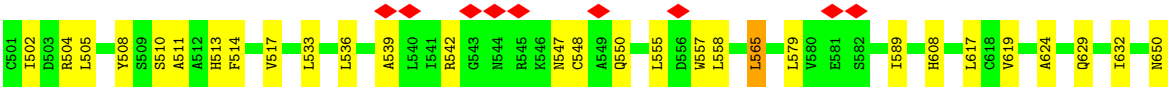
• Molecule 1: Ryanodine receptor 2

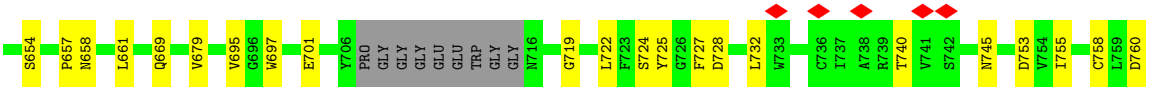
Chain C:

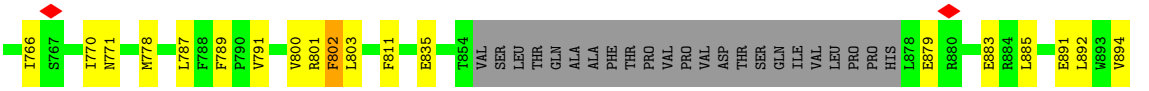


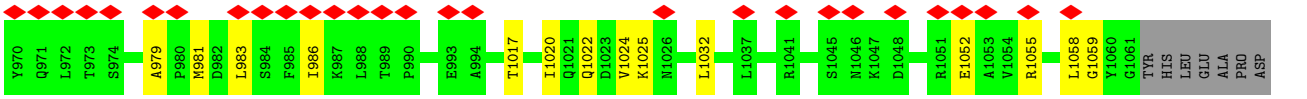


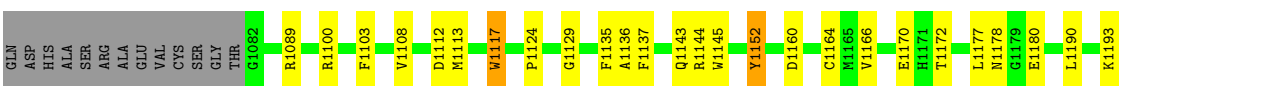


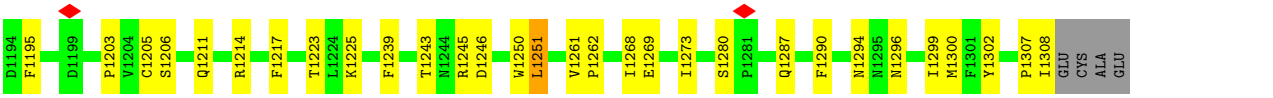


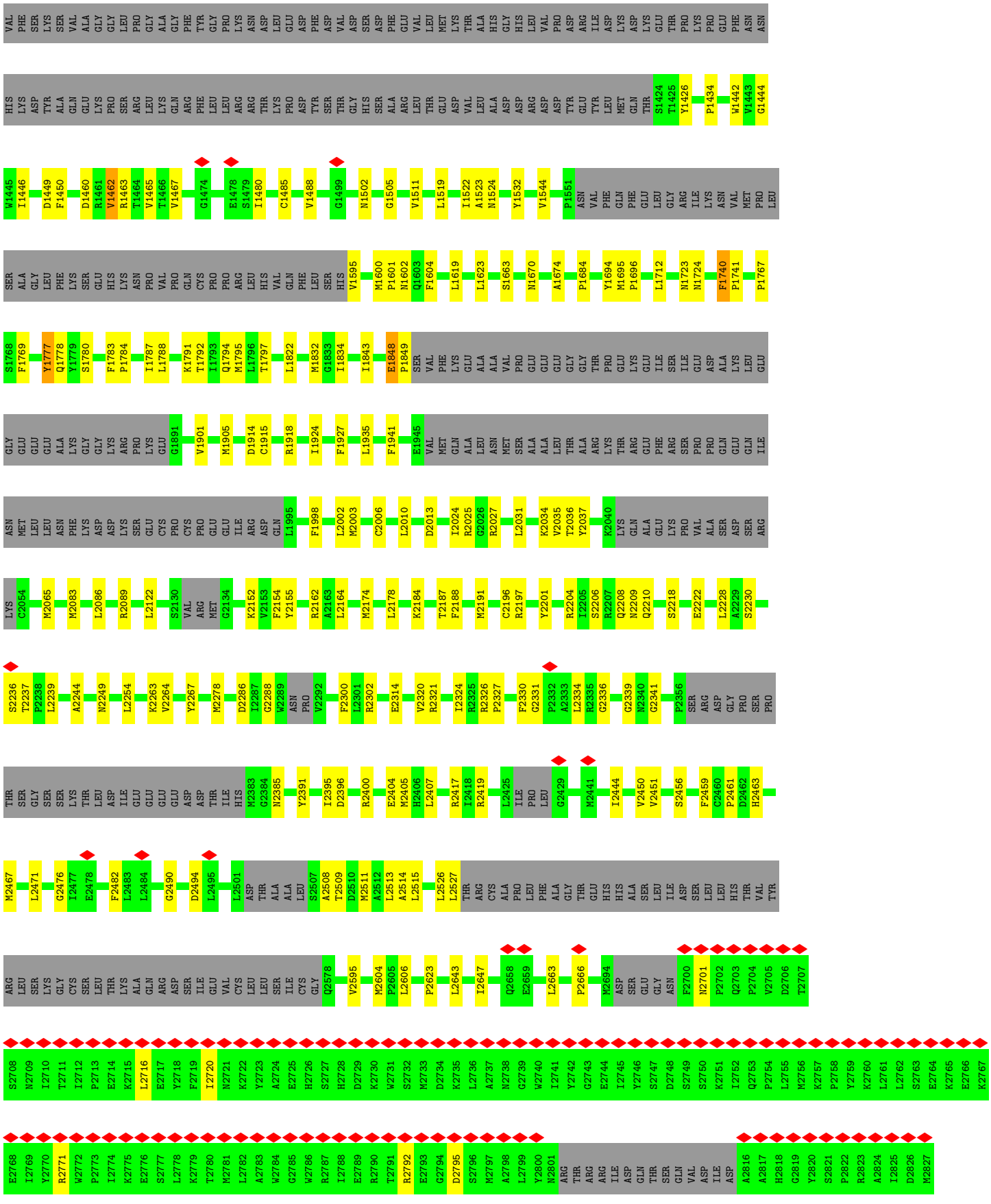








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HIS LYS ASP TYR ALA GLN GLU LYS PRO SER ARG LEU LYS GLN ARG PHE LEU LEU ARG ASN THR LYS PRO ASP TYR SER THR GLY HIS SER ALA ARG LEU THR GLU ASP VAL LEU ALA ASP ASP ARG ASP ASP TYR GLU TYR LEU MET GLN THR S1424 T1425 Y1426 P1434 W1442 V1443 G1444
W1445 I1446 D1449 F1450 D1460 R1461 V1462 R1463 T1464 V1465 T1466 V1467 G1474 E1478 S1479 I1480 C1485 V1488 G1499 N1502 G1505 V1511 L1519 I1522 A1523 N1524 Y1532 V1544 P1551 ASN VAL PHE GLN PHE GLU LEU GLY ARG ILE LYS ASN VAL MET PRO LEU
SER ALA GLY LEU PHE LYS SER GLU HIS LYS ASN PRO VAL PRO GLN CYS PRO PRO ARG LEU HIS VAL GLN PHE LEU SER HIS V1595 M1600 P1601 N1602 Q1603 F1604 L1619 L1623 S1663 N1670 A1674 P1684 Y1694 M1695 P1696 L1712 N1723 N1724 F1740 P1741 P1767
S1768 F1769 Y1777 Q1778 Y1779 S1780 F1783 P1784 I1787 L1788 K1791 T1792 I1793 Q1794 M1795 L1796 T1797 L1822 M1832 G1833 I1834 I1843 E1848 P1849 SER VAL PHE LYS GLU ALA ALA VAL PRO GLU GLU GLU GLY GLY THR PRO GLU LYS GLU ILE SER ILE GLU ASP ALA LYS LEU GLU
GLY GLU GLU GLU ALA LYS GLY GLY LYS ARG PRO LYS GLU G1891 V1901 M1905 D1914 C1915 R1918 I1924 F1927 L1935 F1941 E1945 VAL MET GLN ALA LEU ASN MET SER ALA ALA LEU THR ALA ARG LYS THR ARG GLU PHE ARG SER PRO PRO GLN GLU GLN ILE
ASN MET LEU LEU ASN PHE LYS ASP ASP LYS SER GLU CYS PRO CYS PRO GLU GLU ILE ARG ASP GLN L1995 F1998 L2002 M2003 C2006 L2010 D2013 I2024 R2025 G2026 R2027 L2031 K2034 V2035 T2036 Y2037 K2040 LYS GLN ALA GLU LYS PRO VAL ALA SER ASP SER ARG
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THR SER GLY SER SER LYS THR LEU ASP ILE GLU GLU GLU GLU ASP ASP THR ILE HIS M2383 G2384 N2385 Y2391 I2395 D2396 R2400 E2404 M2405 H2406 L2407 R2417 I2418 R2419 L2425 ILE PRO LEU G2429 M2441 I2444 V2450 V2451 S2456 F2459 C2460 P2461 D2462 H2463
M2467 L2471 G2476 I2477 E2478 F2482 L2483 L2484 G2490 D2494 L2495 L2501 ASP THR ALA ALA LEU S2507 A2508 T2509 D2510 M2511 A2512 L2513 A2514 L2515 L2526 L2527 THR ARG CYS ALA PRO LEU PHE ALA GLY THR GLU HIS HIS ALA SER LEU ILE ASP SER LEU LEU HIS THR VAL TYR
ARG LEU SER LYS GLY CYS SER ILE LEU THR LYS ALA GLN ARG ASP SER ILE GLU VAL CYS LEU LEU SER ILE CYS GLY Q2578 V2595 M2604 P2605 L2606 P2623 L2643 I2647 Q2658 E2659 L2663 P2666 M2694 ASP SER GLU GLY ASN F2700 N2701 P2702 Q2703 P2704 V2705 D2706 T2707
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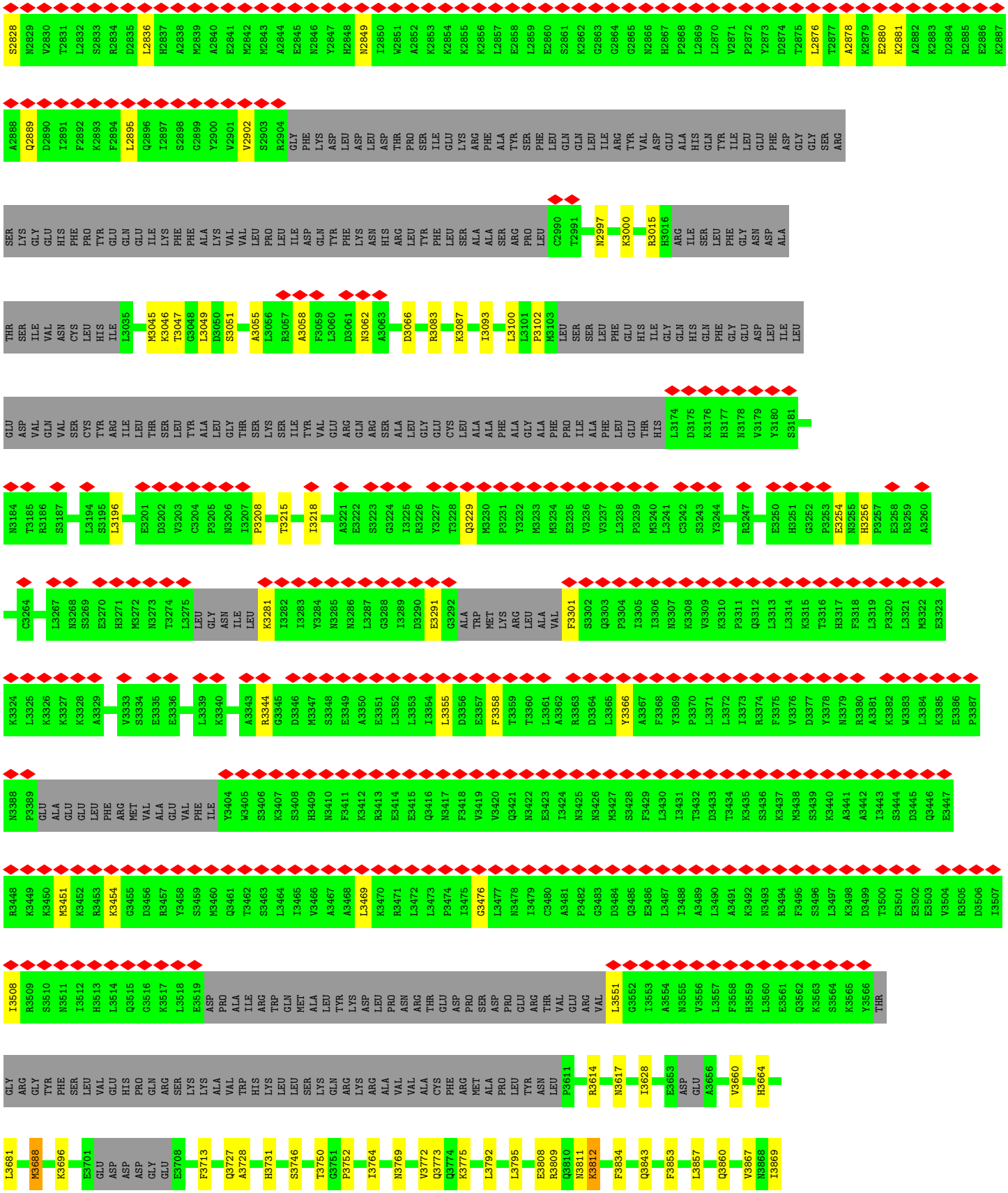
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A2888 Q2889 D2890 I2891 F2892 K2893 F2894 L2895 Q2896 I2897 S2898 G2899 Y2900 V2901 V2902 S2903 R2904 GLY PHE LYS ASP LEU ASP LEU ASP THR PRO SER ILE GLU LYS ARG PHE ALA TYR SER PHE LEU GLN GLN LEU ILE ARG TYR VAL ASP GLU ALA HIS GLN TYR ILE LEU GLU PHE ASP GLY GLY SER ARG
SER LYS GLY GLU HIS PHE PRO TYR GLU GLN GLU ILE LYS PHE PHE ALA ALA LYS VAL VAL LEU PRO LEU ILE ASP GLN TYR PHE LYS ASN HIS ARG LEU TYR PHE LEU SER ALA ALA SER ARG PRO LEU C2990 T2991 N2997 K3000 R3015 H3016 ARG ILE SER LEU PHE GLY ASN ASP ALA
THR SER ILE VAL ASN CYS LEU HIS ILE L3035 M3045 K3046 T3047 G3048 L3049 D3050 S3051 A3055 L3056 R3057 A3058 F3059 L3060 D3061 N3062 A3063 D3066 R3083 K3087 I3093 L3100 L3101 P3102 M3103 LEU SER SER LEU PHE GLU HIS ILE GLY GLN HIS GLN PHE GLY GLU ASP LEU ILE LEU
GLU ASP VAL GLN VAL SER CYS TYR ARG ILE LEU THR SER LEU TYR ALA LEU GLY THR SER LYS SER ILE TYR VAL GLU GLN ARG GLN ARG SER ALA LEU GLY GLU CYS LEU ALA ALA PHE ALA GLY ALA PHE PRO ILE ALA PHE LEU GLU THR HIS L3174 D3175 K3176 H3177 N3178 V3179 Y3180 S3181
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C3264 L3267 N3268 S3269 E3270 H3271 M3272 N3273 T3274 L3275 LEU GLY ASN ILE LEU K3281 I3282 I3283 Y3284 N3285 N3286 L3287 G3288 I3289 D3290 E3291 G3292 ALA TRP MET LYS ARG LEU ALA VAL F3301 S3302 Q3303 P3304 I3305 I3306 N3307 K3308 V3309 K3310 P3311 Q3312 L3313 L3314 K3315 T3316 H3317 F3318 L3319 P3320 L3321 M3322 E3323
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N3388 P3389 GLU ALA GLU GLU LEU PHE ARG MET VAL ALA GLU VAL PHE ILE Y3404 W3405 S3406 K3407 S3408 H3409 N3410 F3411 K3412 R3413 E3414 E3415 Q3416 N3417 F3418 V3419 V3420 Q3421 N3422 E3423 I3424 N3425 N3426 M3427 S3428 F3429 L3430 I3431 T3432 D3433 T3434 K3435 S3436 K3437 M3438 S3439 K3440 A3441 A3442 I3443 S3444 D3445 Q3446 E3447
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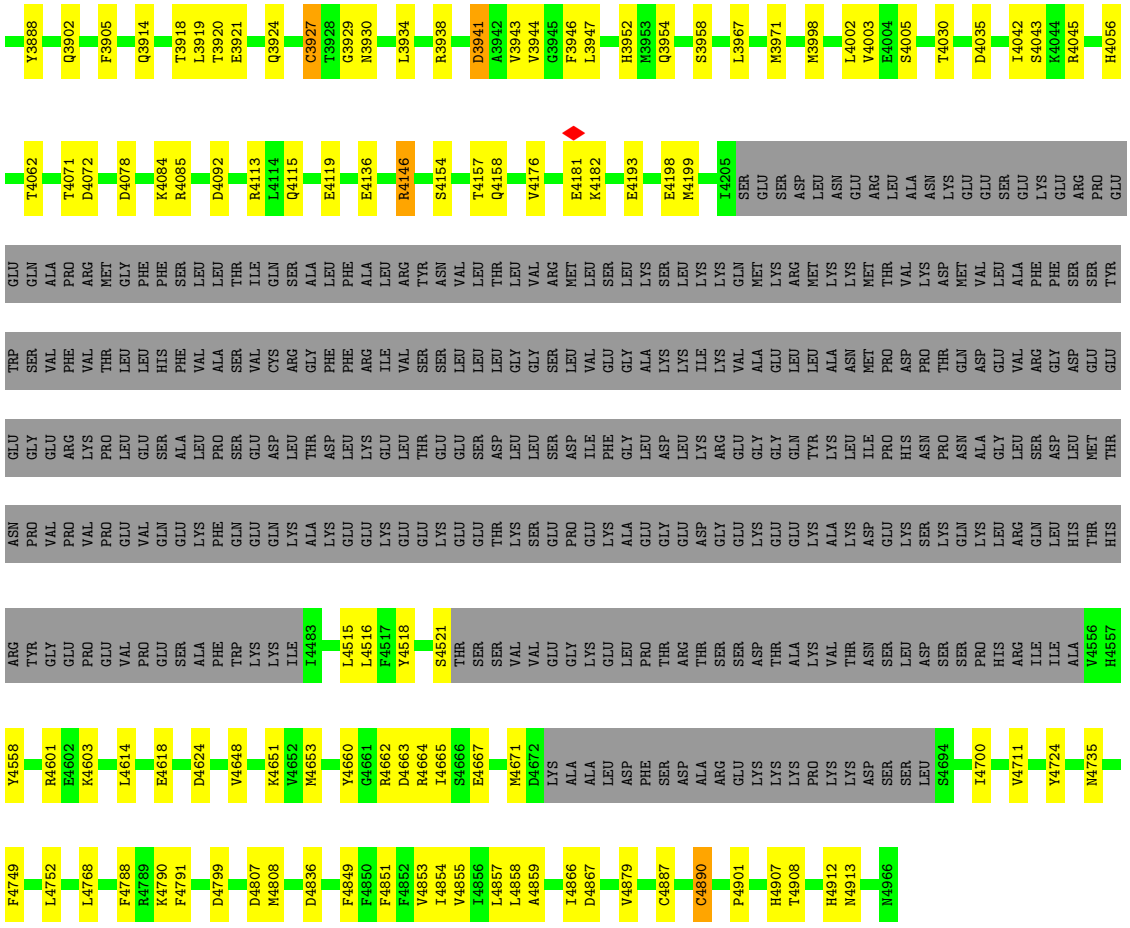
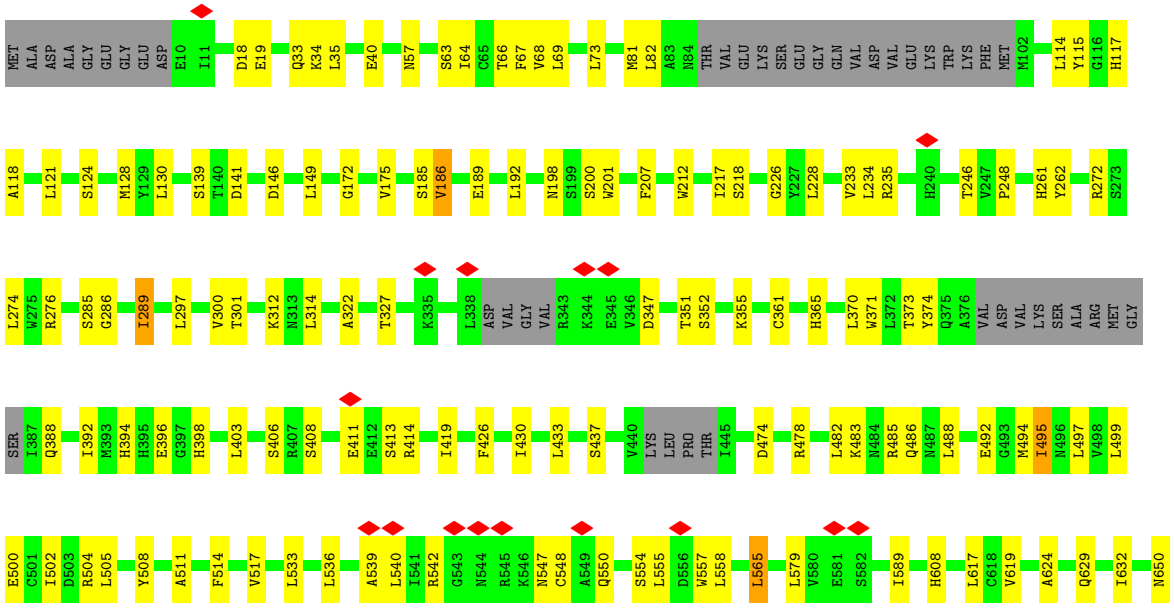
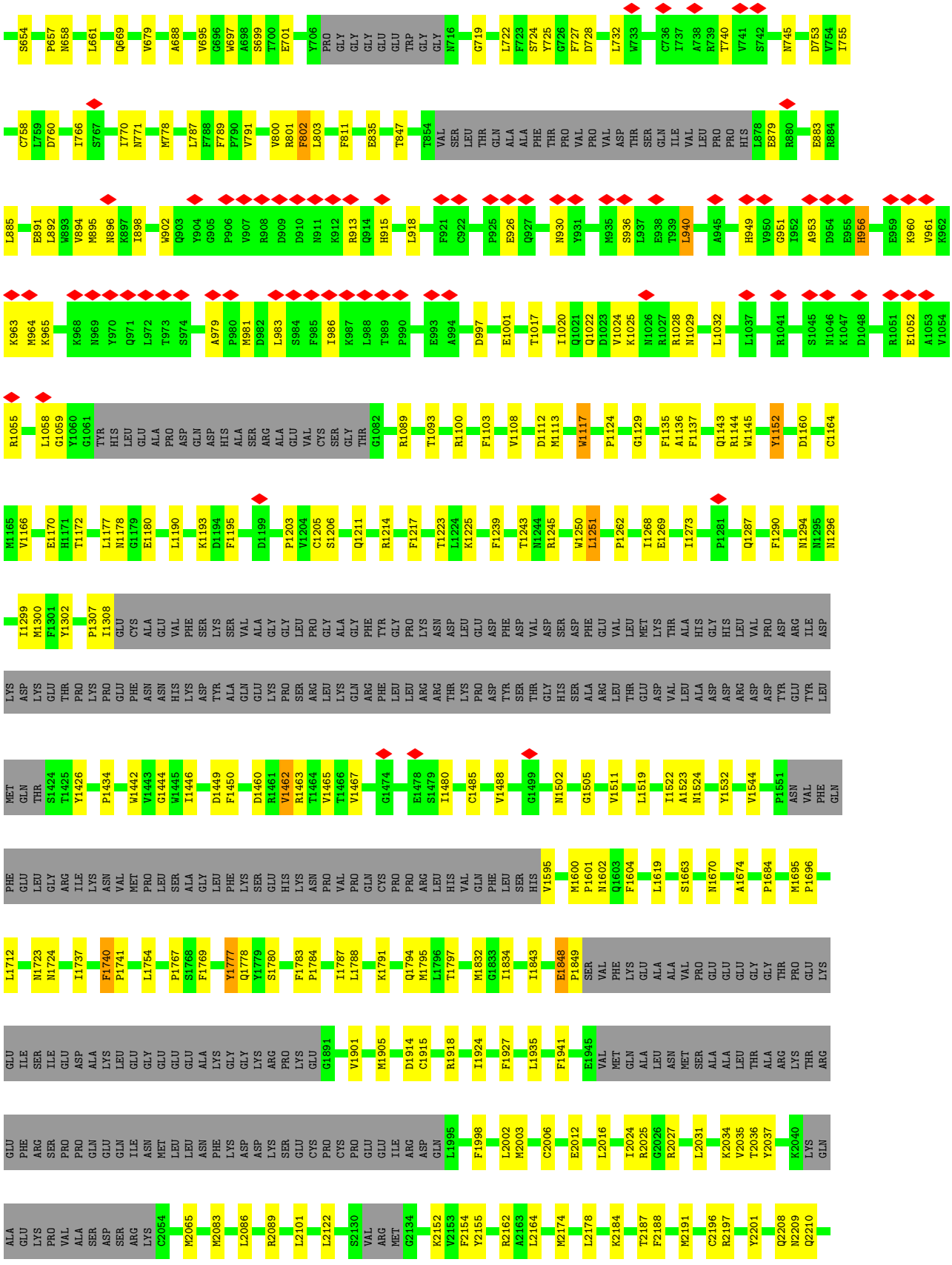
I3508 R3509 S3510 N3511 I3512 H3513 L3514 Q3515 G3516 K3517 L3518 E3519 ASP PRO ALA ILE ARG TRP GLN MET ALA LEU TYR LYS ASP LEU PRO ASN ARG THR GLU ASP PRO SER ASP PRO GLU ARG THR VAL GLU ARG VAL L3551 G3552 I3553 A3554 N3555 V3556 L3557 F3558 H3559 L3560 E3561 Q3562 K3563 S3564 K3565 Y3566 THR
GLY ARG GLY TYR PHE SER LEU VAL GLU HIS PRO GLN ARG SER LYS LYS ALA VAL TRP HIS LYS LEU LEU SER LYS GLN ARG LYS ARG ALA VAL VAL ALA CYS PHE ARG MET ALA PRO LEU TYR ASN LEU P3611 R3614 N3617 I3628 E5653 ASP GLU A3656 V3660 H3664
L3681 M3688 K3696 E3701 GLU ASP ASP ASP GLY GLU E3708 F3713 Q3727 A3728 H3731 S3746 T3750 G3751 P3752 I3764 N3769 V3772 Q3773 Q3774 K3775 L3792 L3795 E3808 R3809 Q3810 N3811 K3812 F3834 Q3843 F3853 L3857 Q3860 V3867 N3868 I3869

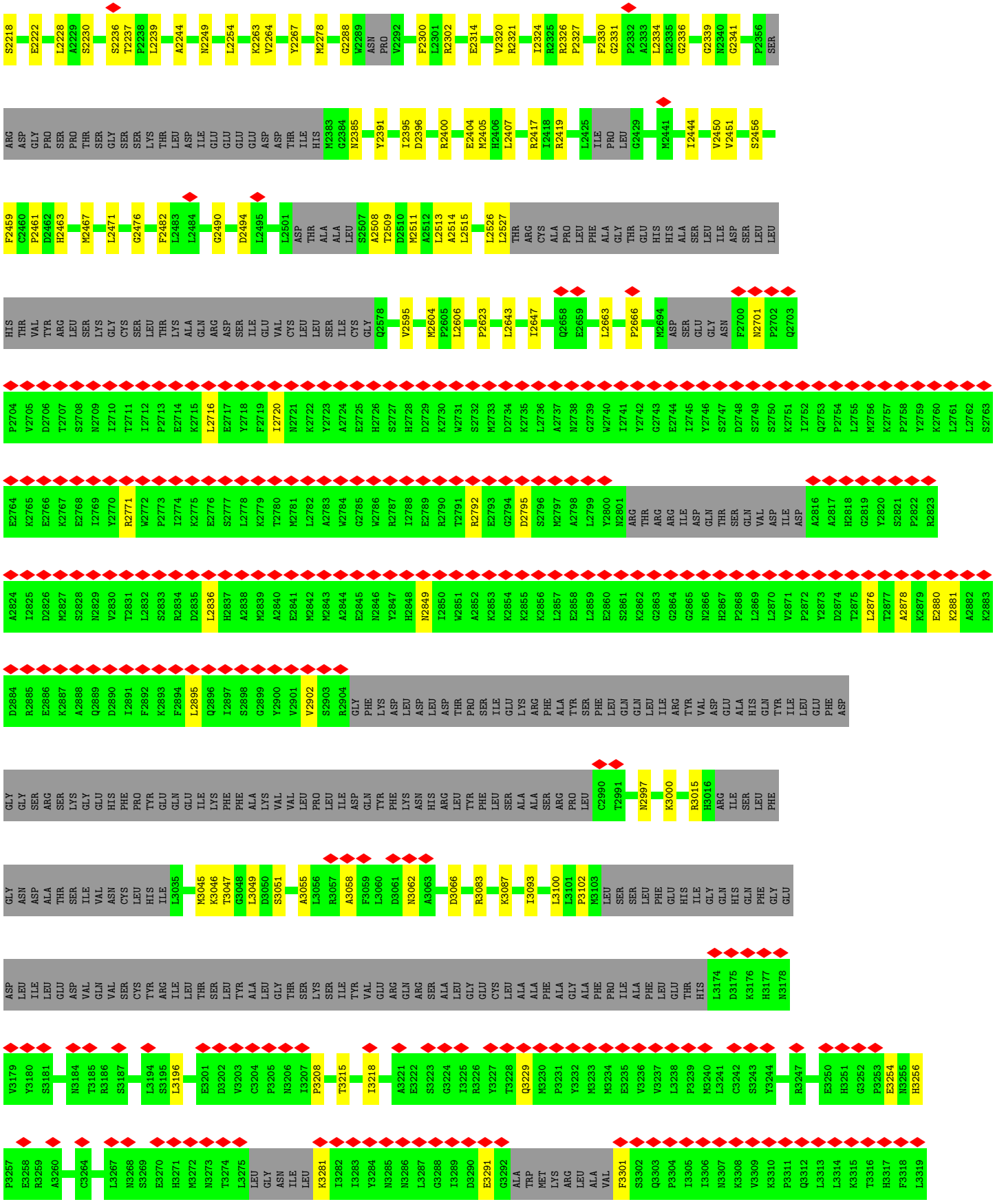


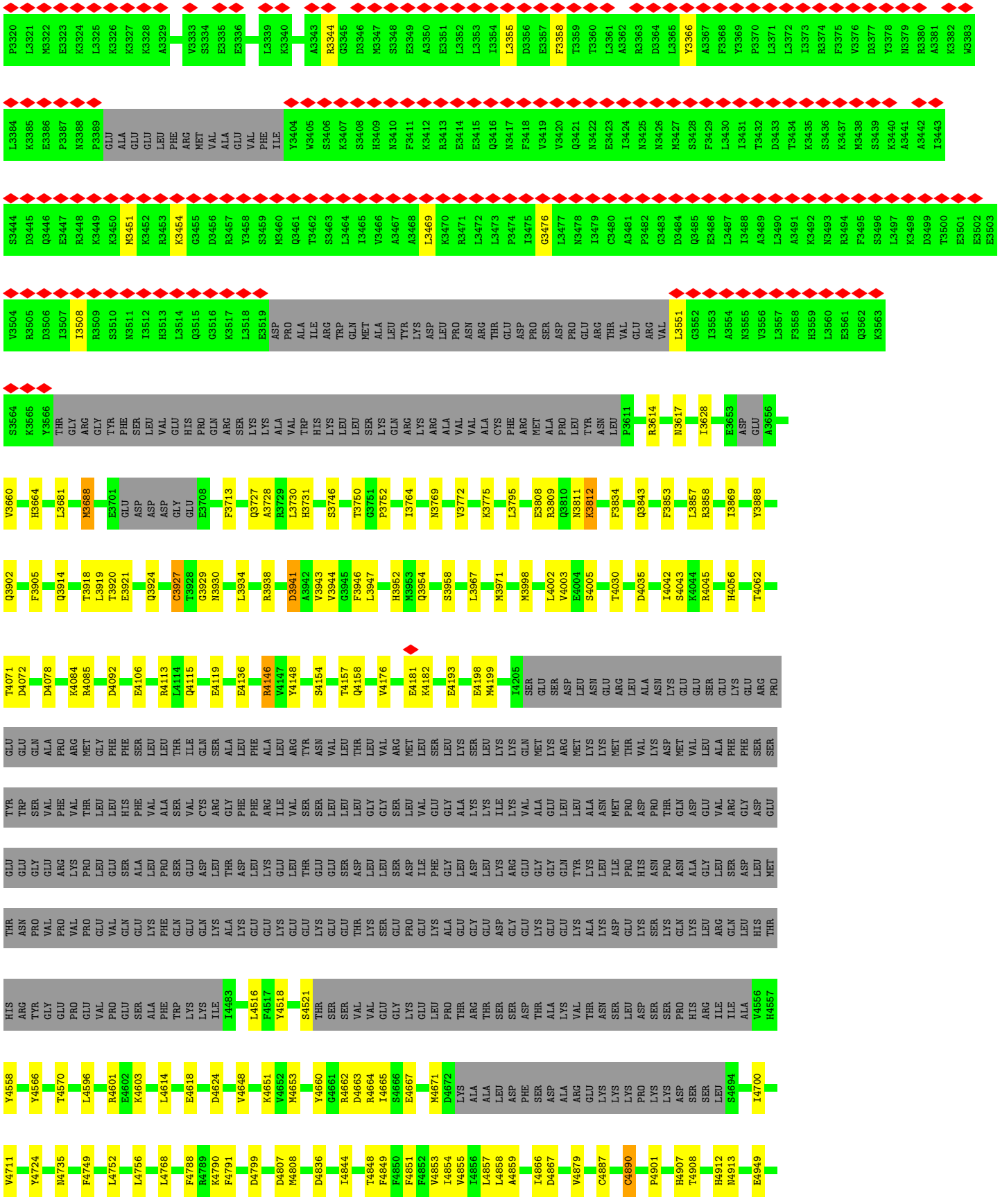
• Molecule 1: Ryanodine receptor 2

Chain D:



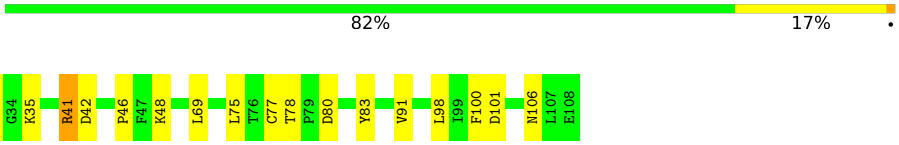

S654 P657 N658 L661 Q669 V679 A688 V695 G696 W697 A698 S699 T700 E701 Y706 PRO GLY GLY GLY GLU GLU TRP GLY GLY N716 G719 L722 F723 S724 Y725 G726 F727 D728 L732 W733 C736 I737 A738 R739 T740 V741 S742 N745 D753 V754 I755
C758 L759 D760 I766 S767 I770 N771 W778 L787 F788 F789 P790 V791 V800 R801 F802 L803 F811 E835 T847 T854 VAL SER LEU THR GLN ALA ALA PHE THR PRO VAL PRO VAL ASP THR SER GLN ILE VAL LEU PRO PRO HIS L878 E879 R880 E883 R884
L885 E891 L892 W893 V894 M895 N896 K897 I898 W902 Q903 Y904 G905 P906 V907 R908 D909 D910 N911 K912 R913 Q914 H915 L918 F921 C922 P925 E926 Q927 N930 Y931 M935 S936 L937 E938 T939 L940 A945 H949 V950 G951 I952 A953 D954 E955 H956 E959 K960 V961 K962
K963 M964 K965 K968 N969 Y970 Q971 L972 T973 S974 A979 P980 H981 D982 L983 S984 F985 I986 K987 L988 T989 P990 E993 A994 D997 E1001 T1017 I1020 Q1021 Q1022 D1023 V1024 K1025 N1026 R1027 R1028 N1029 L1032 L1037 R1041 S1045 N1046 K1047 D1048 R1051 E1052 A1053 V1054
R1055 L1058 G1059 Y1060 G1061 TYR HIS LEU GLU ALA PRO ASP GLN ASP HIS ALA SER ARG ALA GLU VAL CYS SER GLY THR G1082 R1089 T1093 R1100 F1103 V1108 D1112 M1113 W1117 P1124 G1129 F1135 A1136 F1137 Q1143 R1144 W1145 Y1152 D1160 C1164
M1165 V1166 E1170 H1171 T1172 L1177 N1178 G1179 E1180 L1190 K1193 D1194 F1195 D1199 P1203 V1204 C1205 S1206 Q1211 R1214 F1217 T1223 L1224 K1225 F1239 T1243 N1244 R1245 W1250 L1251 P1262 I1268 E1269 I1273 P1281 Q1287 F1290 N1294 N1295 N1296
I1299 M1300 F1301 Y1302 P1307 I1308 GLU CYS ALA GLU VAL PHE SER LYS SER VAL ALA GLY GLY LEU PRO GLY ALA GLY PHE TYR GLY PRO LYS ASN ASP LEU GLU ASP PHE ASP VAL ASP SER ASP PHE GLU VAL LEU MET LYS THR ALA HIS GLY HIS LEU VAL PRO ASP ARG ILE ASP
LYS ASP LYS GLU THR PRO LYS PRO GLU PHE ASN ASN HIS LYS ASP TYR ALA GLN GLU LYS PRO SER ARG LEU LYS GLN ARG PHE LEU LEU ARG ARG THR LYS PRO ASP TYR SER THR GLY HIS SER ALA ARG LEU THR GLU ASP VAL LEU ALA ASP ASP ARG ASP ASP TYR GLU TYR LEU
MET GLN THR S1424 T1425 Y1426 P1434 W1442 V1443 G1444 W1445 I1446 D1449 F1450 D1460 R1461 V1462 R1463 T1464 V1465 T1466 V1467 G1474 E1478 S1479 I1480 C1485 V1488 G1499 N1502 G1505 V1511 L1519 I1522 A1523 N1524 Y1532 V1544 P1551 ASN VAL PHE GLN
PHE GLU LEU GLY ARG ILE LYS ASN VAL MET PRO LEU SER ALA GLY LEU PHE LYS SER GLU HIS LYS ASN PRO VAL PRO GLN CYS PRO PRO ARG LEU HIS VAL GLN PHE LEU SER HIS V1595 M1600 P1601 N1602 Q1603 F1604 L1619 S1663 N1670 A1674 P1684 M1695 P1696
L1712 N1723 N1724 I1737 F1740 P1741 L1754 P1767 S1768 F1769 Y1777 Q1778 Y1779 S1780 F1783 P1784 I1787 L1788 K1791 Q1794 M1795 L1796 T1797 M1832 G1833 I1834 I1843 E1848 P1849 SER VAL PHE LYS GLU ALA ALA VAL PRO GLU GLU GLU GLY GLY THR PRO GLU LYS
GLU ILE SER ILE GLU ASP ALA LYS LEU GLU GLY GLU GLU GLU ALA LYS GLY GLY LYS ARG PRO LYS GLU G1891 V1901 M1905 D1914 C1915 R1918 I1924 F1927 L1935 F1941 E1945 VAL MET GLN ALA LEU ASN MET SER ALA ALA LEU THR ALA ARG LYS THR ARG
GLU PHE ARG SER PRO PRO GLN GLU GLN ILE ASN MET LEU LEU ASN PHE LYS ASP ASP LYS SER GLU CYS PRO CYS PRO GLU GLU ILE ARG ASP GLN L1995 F1998 L2002 M2003 C2006 E2012 L2016 I2024 R2025 G2026 R2027 L2031 K2034 V2035 T2036 Y2037 K2040 LYS GLN
ALA GLU LYS PRO VAL ALA SER ASP SER ARG LYS C2054 M2065 M2083 L2086 R2089 L2101 L2122 S2130 VAL ARG MET C2134 K2152 Y2153 F2154 Y2155 R2162 A2163 L2164 M2174 L2178 K2184 T2187 F2188 M2191 C2196 R2197 Y2201 Q2208 N2209 Q2210


S2218 E2222 L2228 A2229 S2230 S2236 T2237 P2238 L2239 A2244 N2249 L2254 K2263 V2264 Y2267 M2278 G2288 W2289 ASN PRO V2292 F2300 L2301 R2302 E2314 V2320 R2321 I2324 R2325 R2326 P2327 F2330 G2331 P2332 A2333 L2334 H2335 G2336 G2339 N2340 G2341 P2356 SER
ARG ASP GLY PRO SER PRO THR SER GLY SER SER LYS THR LEU ASP ILE GLU GLU GLU GLU ASP ASP THR ILE HIS M2383 G2384 N2385 Y2391 I2395 D2396 R2400 E2404 M2405 H2406 L2407 R2417 I2418 R2419 L2425 ILE PRO LEU G2429 M2441 I2444 V2450 V2451 S2456
F2459 C2460 P2461 D2462 H2463 M2467 L2471 G2476 F2482 L2483 L2484 G2490 D2494 L2495 L2501 ASP THR ALA ALA LEU S2507 A2508 T2509 D2510 M2511 A2512 L2513 A2514 L2515 L2526 L2527 THR ARG CYS ALA PRO LEU PHE ALA GLY THR GLU HIS HIS ALA SER LEU ILE ASP SER LEU LEU
HIS THR VAL TYR ARG LEU SER LYS GLY CYS SER LEU THR LYS ALA GLN ARG ASP SER ILE GLU VAL CYS LEU LEU SER ILE CYS GLY Q2578 V2595 M2604 P2605 L2606 P2623 L2643 I2647 Q2658 E2659 L2663 P2666 M2694 ASP SER GLU GLY ASN F2700 N2701 P2702 Q2703
P2704 V2705 D2706 T2707 S2708 N2709 I2710 T2711 I2712 P2713 E2714 K2715 L2716 E2717 Y2718 F2719 I2720 N2721 K2722 Y2723 A2724 E2725 H2726 S2727 H2728 D2729 K2730 W2731 S2732 M2733 D2734 K2735 L2736 A2737 N2738 G2739 W2740 I2741 Y2742 G2743 E2744 I2745 Y2746 S2747 D2748 S2749 S2750 K2751 I2752 Q2753 P2754 L2755 M2756 K2757 P2758 Y2759 K2760 L2761 L2762 S2763
E2764 K2765 E2766 K2767 E2768 I2769 Y2770 R2771 W2772 P2773 I2774 K2775 E2776 S2777 L2778 K2779 T2780 M2781 L2782 A2783 W2784 G2785 W2786 R2787 I2788 E2789 R2790 T2791 R2792 E2793 G2794 D2795 S2796 M2797 A2798 L2799 Y2800 N2801 ARG THR ARG ARG ILE ASP GLN THR SER GLN VAL ASP ILE ASP A2816 A2817 H2818 G2819 Y2820 S2821 P2822 R2823
A2824 I2825 D2826 M2827 S2828 N2829 V2830 T2831 L2832 S2833 R2834 D2835 L2836 H2837 A2838 M2839 A2840 E2841 M2842 M2843 A2844 E2845 N2846 Y2847 H2848 N2849 I2850 W2851 A2852 K2853 K2854 K2855 K2856 L2857 E2858 L2859 E2860 S2861 K2862 G2863 G2864 G2865 N2866 H2867 P2868 L2869 L2870 V2871 P2872 Y2873 D2874 T2875 L2876 T2877 A2878 K2879 E2880 K2881 A2882 K2883
D2884 R2885 E2886 K2887 A2888 Q2889 D2890 I2891 F2892 K2893 F2894 L2895 Q2896 I2897 S2898 G2899 Y2900 V2901 V2902 S2903 R2904 GLY PHE LYS ASP LEU ASP LEU ASP THR PRO SER ILE GLU LYS ARG PHE ALA TYR SER PHE LEU GLN GLN LEU ILE ARG TYR VAL ASP GLU ALA HIS GLN TYR ILE LEU GLU PHE ASP
GLY GLY SER ARG SER LYS GLY GLU HIS PHE PRO TYR GLU GLN GLU ILE LYS PHE PHE ALA LYS VAL VAL LEU PRO LEU ILE ASP GLN TYR PHE LYS ASN HIS ARG LEU TYR PHE LEU SER ALA ALA SER ARG PRO LEU C2990 T2991 N2997 K3000 R3015 H3016 ARG ILE SER LEU PHE
GLY ASN ASP ALA THR SER ILE VAL ASN CYS LEU HIS ILE L3035 M3045 K3046 T3047 G3048 L3049 D3050 S3051 A3055 L3066 R3067 A3058 F3059 L3060 D3061 N3062 A3063 D3066 R3083 K3087 I3093 L3100 L3101 P3102 M3103 LEU SER SER LEU PHE GLU HIS ILE GLY GLN HIS GLN PHE GLY GLU
ASP LEU ILE LEU GLU ASP VAL GLN VAL SER CYS TYR ARG ILE LEU THR SER LEU TYR ALA LEU GLY THR SER LYS SER ILE TYR VAL GLU ARG GLN ARG SER ALA LEU GLY GLU CYS LEU ALA ALA PHE ALA GLY ALA PHE PRO ILE ALA PHE LEU GLU THR HIS L3174 D3175 K3176 H3177 N3178
V3179 Y3180 S3181 N3184 T3185 R3186 S3187 L3194 S3195 L3196 E3201 D3202 V3203 C3204 P3205 N3206 I3207 P3208 T3215 I3218 A3221 E3222 S3223 G3224 I3225 R3226 Y3227 T3228 Q3229 M3230 P3231 Y3232 M3233 M3234 E3235 V3236 V3237 L3238 P3239 M3240 L3241 C3242 S3243 Y3244 R3247 E3250 H3251 G3252 P3253 E3254 N3255 H3256
P3257 E3258 R3259 A3260 C3264 L3267 N3268 S3269 E3270 H3271 M3272 N3273 T3274 L3275 LEU GLY ASN ILE LEU K3281 I3282 I3283 Y3284 N3285 N3286 L3287 G3288 I3289 D3290 E3291 G3292 ALA TRP MET LYS ARG LEU ALA VAL F3301 S3302 Q3303 P3304 I3305 I3306 N3307 K3308 V3309 K3310 P3311 Q3312 L3313 L3314 K3315 T3316 H3317 F3318 L3319



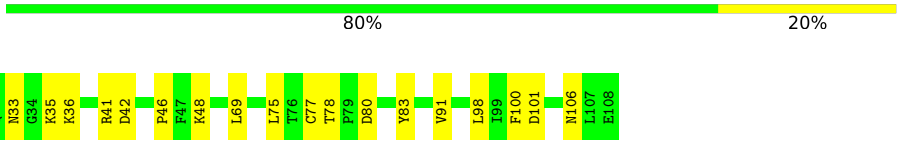
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain E:



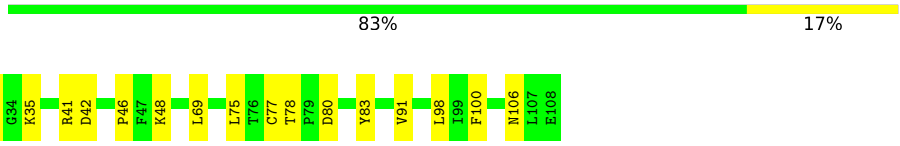
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F:



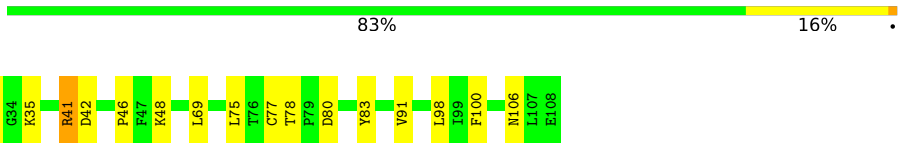
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain G:



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

Chain H:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	73782	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.311	Depositor
Minimum map value	-0.628	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.033	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	496.80002, 496.80002, 496.80002	wwPDB
Map dimensions	460, 460, 460	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	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

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	0.25	0/29611	0.50	4/40214 (0.0%)
1	B	0.25	0/29611	0.50	4/40214 (0.0%)
1	C	0.25	0/29611	0.50	4/40214 (0.0%)
1	D	0.25	0/29611	0.50	4/40214 (0.0%)
2	E	0.25	0/778	0.49	0/1060
2	F	0.25	0/778	0.50	0/1060
2	G	0.25	0/778	0.50	0/1060
2	H	0.25	0/778	0.50	0/1060
All	All	0.25	0/121556	0.50	16/165096 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	565	LEU	CA-CB-CG	6.01	129.12	115.30
1	A	565	LEU	CA-CB-CG	6.01	129.12	115.30
1	C	565	LEU	CA-CB-CG	6.00	129.11	115.30
1	B	565	LEU	CA-CB-CG	6.00	129.09	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	4002	LEU	CA-CB-CG	5.81	128.67	115.30
1	A	4002	LEU	CA-CB-CG	5.81	128.66	115.30
1	D	4002	LEU	CA-CB-CG	5.79	128.62	115.30
1	A	1124	PRO	N-CA-CB	5.78	110.24	103.30
1	D	1124	PRO	N-CA-CB	5.78	110.24	103.30
1	B	4002	LEU	CA-CB-CG	5.78	128.59	115.30
1	C	1124	PRO	N-CA-CB	5.77	110.22	103.30
1	B	1124	PRO	N-CA-CB	5.75	110.19	103.30
1	D	940	LEU	CA-CB-CG	5.15	127.14	115.30
1	A	940	LEU	CA-CB-CG	5.14	127.13	115.30
1	B	940	LEU	CA-CB-CG	5.14	127.11	115.30
1	C	940	LEU	CA-CB-CG	5.12	127.09	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	4181	GLU	Peptide
1	B	4181	GLU	Peptide
1	C	4181	GLU	Peptide
1	D	4181	GLU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	29055	0	27182	342	0
1	B	29055	0	27182	341	0
1	C	29055	0	27182	342	0
1	D	29055	0	27182	352	0
2	E	763	0	709	11	0
2	F	763	0	709	12	0
2	G	763	0	709	10	0
2	H	763	0	709	10	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
All	All	119280	0	111564	1372	0

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

All (1372) 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:C:1205:CYS:SG	1:C:1206:SER:N	2.64	0.71
1:A:189:GLU:OE1	1:B:2417:ARG:NH1	2.24	0.71
1:D:1205:CYS:SG	1:D:1206:SER:N	2.64	0.71
1:A:1205:CYS:SG	1:A:1206:SER:N	2.64	0.71
1:B:1205:CYS:SG	1:B:1206:SER:N	2.64	0.70
1:C:695:VAL:HB	1:C:727:PHE:HB3	1.76	0.67
1:B:695:VAL:HB	1:B:727:PHE:HB3	1.76	0.67
1:A:695:VAL:HB	1:A:727:PHE:HB3	1.76	0.67
1:C:189:GLU:OE1	1:D:2417:ARG:NH1	2.28	0.67
1:D:695:VAL:HB	1:D:727:PHE:HB3	1.76	0.66
1:B:189:GLU:OE1	1:C:2417:ARG:NH1	2.28	0.66
1:A:1450:PHE:HA	1:A:1485:CYS:HB3	1.78	0.66
1:A:2417:ARG:NH1	1:D:189:GLU:OE1	2.29	0.65
1:A:234:LEU:HD12	1:A:408:SER:HB3	1.79	0.65
1:A:3469:LEU:HD11	1:A:3476:GLY:HA3	1.79	0.65
1:D:3469:LEU:HD11	1:D:3476:GLY:HA3	1.79	0.65
1:B:234:LEU:HD12	1:B:408:SER:HB3	1.79	0.65
1:C:234:LEU:HD12	1:C:408:SER:HB3	1.79	0.65
1:C:1450:PHE:HA	1:C:1485:CYS:HB3	1.78	0.65
1:C:1684:PRO:HG3	2:G:42:ASP:HB2	1.78	0.64
1:B:1684:PRO:HG3	2:F:42:ASP:HB2	1.78	0.64
1:D:234:LEU:HD12	1:D:408:SER:HB3	1.79	0.64
1:C:3469:LEU:HD11	1:C:3476:GLY:HA3	1.79	0.64
1:B:1450:PHE:HA	1:B:1485:CYS:HB3	1.77	0.64
1:B:3469:LEU:HD11	1:B:3476:GLY:HA3	1.79	0.64
1:D:1450:PHE:HA	1:D:1485:CYS:HB3	1.78	0.64
1:A:1684:PRO:HG3	2:E:42:ASP:HB2	1.78	0.64
1:A:312:LYS:HG3	1:A:394:HIS:HA	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2196:CYS:SG	1:B:2197:ARG:N	2.71	0.64
1:D:312:LYS:HG3	1:D:394:HIS:HA	1.80	0.64
1:D:1684:PRO:HG3	2:H:42:ASP:HB2	1.78	0.63
1:B:186:VAL:O	1:C:2417:ARG:NH2	2.31	0.63
1:B:312:LYS:HG3	1:B:394:HIS:HA	1.79	0.63
1:C:312:LYS:HG3	1:C:394:HIS:HA	1.80	0.63
1:C:732:LEU:HB2	1:C:740:THR:HA	1.81	0.63
1:C:3769:ASN:HB2	1:C:3772:VAL:HG22	1.81	0.63
1:A:2196:CYS:SG	1:A:2197:ARG:N	2.71	0.63
1:B:732:LEU:HB2	1:B:740:THR:HA	1.81	0.63
1:A:3769:ASN:HB2	1:A:3772:VAL:HG22	1.81	0.62
1:D:732:LEU:HB2	1:D:740:THR:HA	1.81	0.62
1:D:3769:ASN:HB2	1:D:3772:VAL:HG22	1.81	0.62
1:A:732:LEU:HB2	1:A:740:THR:HA	1.81	0.62
1:B:1268:ILE:HD12	1:B:1290:PHE:HZ	1.65	0.62
1:C:1268:ILE:HD12	1:C:1290:PHE:HZ	1.65	0.62
1:D:3451:MET:SD	1:D:3454:LYS:NZ	2.73	0.62
1:B:3769:ASN:HB2	1:B:3772:VAL:HG22	1.81	0.62
1:C:4859:ALA:HB1	1:D:4866:ILE:HD11	1.81	0.62
1:B:189:GLU:OE2	1:C:2321:ARG:NH2	2.32	0.62
1:C:66:THR:HG22	1:C:217:ILE:HG12	1.82	0.62
1:D:66:THR:HG22	1:D:217:ILE:HG12	1.81	0.62
1:A:1268:ILE:HD12	1:A:1290:PHE:HZ	1.65	0.62
1:A:4859:ALA:HB1	1:B:4866:ILE:HD11	1.81	0.62
1:B:3843:GLN:HG3	1:B:3921:GLU:HG3	1.82	0.62
1:D:1268:ILE:HD12	1:D:1290:PHE:HZ	1.64	0.62
1:A:4866:ILE:HD11	1:D:4859:ALA:HB1	1.81	0.62
1:C:3451:MET:SD	1:C:3454:LYS:NZ	2.73	0.61
1:A:3843:GLN:HG3	1:A:3921:GLU:HG3	1.82	0.61
1:C:539:ALA:HA	1:C:542:ARG:HD2	1.82	0.61
1:A:3451:MET:SD	1:A:3454:LYS:NZ	2.73	0.61
1:D:539:ALA:HA	1:D:542:ARG:HD2	1.82	0.61
1:A:186:VAL:O	1:B:2417:ARG:NH2	2.34	0.61
1:A:1914:ASP:OD1	1:A:2089:ARG:NH2	2.34	0.61
1:A:2417:ARG:NH2	1:D:186:VAL:O	2.34	0.61
1:B:3451:MET:SD	1:B:3454:LYS:NZ	2.73	0.61
1:C:1914:ASP:OD1	1:C:2089:ARG:NH2	2.34	0.61
1:C:3049:LEU:HB2	1:C:3093:ILE:HD11	1.83	0.61
1:A:758:CYS:HB3	1:A:766:ILE:HD12	1.82	0.61
1:B:66:THR:HG22	1:B:217:ILE:HG12	1.81	0.61
1:B:758:CYS:HB3	1:B:766:ILE:HD12	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:539:ALA:HA	1:B:542:ARG:HD2	1.82	0.60
1:B:3049:LEU:HB2	1:B:3093:ILE:HD11	1.83	0.60
1:A:701:GLU:HG2	1:A:1462:VAL:HG13	1.83	0.60
1:A:1160:ASP:OD1	1:A:1178:ASN:ND2	2.34	0.60
1:C:758:CYS:HB3	1:C:766:ILE:HD12	1.83	0.60
1:D:1160:ASP:OD1	1:D:1178:ASN:ND2	2.34	0.60
1:A:66:THR:HG22	1:A:217:ILE:HG12	1.82	0.60
1:B:1914:ASP:OD1	1:B:2089:ARG:NH2	2.34	0.60
1:D:1914:ASP:OD1	1:D:2089:ARG:NH2	2.34	0.60
1:C:186:VAL:O	1:D:2417:ARG:NH2	2.34	0.60
1:C:701:GLU:HG2	1:C:1462:VAL:HG13	1.83	0.60
1:C:1160:ASP:OD1	1:C:1178:ASN:ND2	2.34	0.60
1:C:1190:LEU:HD21	1:C:1193:LYS:HG3	1.83	0.60
1:A:539:ALA:HA	1:A:542:ARG:HD2	1.82	0.60
1:B:1160:ASP:OD1	1:B:1178:ASN:ND2	2.34	0.60
1:D:758:CYS:HB3	1:D:766:ILE:HD12	1.83	0.60
1:A:1190:LEU:HD21	1:A:1193:LYS:HG3	1.83	0.60
1:D:3843:GLN:HG3	1:D:3921:GLU:HG3	1.82	0.60
1:C:3843:GLN:HG3	1:C:3921:GLU:HG3	1.82	0.59
1:B:701:GLU:HG2	1:B:1462:VAL:HG13	1.83	0.59
1:C:2196:CYS:SG	1:C:2197:ARG:N	2.71	0.59
1:A:189:GLU:OE2	1:B:2321:ARG:NH2	2.35	0.59
1:A:725:TYR:HD2	1:A:732:LEU:HA	1.68	0.59
1:A:2254:LEU:O	1:A:3809:ARG:NH1	2.36	0.59
1:D:725:TYR:HD2	1:D:732:LEU:HA	1.68	0.59
1:A:2526:LEU:HD22	1:A:2606:LEU:HD22	1.85	0.59
1:A:3049:LEU:HB2	1:A:3093:ILE:HD11	1.82	0.59
1:B:725:TYR:HD2	1:B:732:LEU:HA	1.68	0.59
1:C:725:TYR:HD2	1:C:732:LEU:HA	1.68	0.59
1:D:1190:LEU:HD21	1:D:1193:LYS:HG3	1.83	0.59
1:D:3049:LEU:HB2	1:D:3093:ILE:HD11	1.83	0.59
1:B:81:MET:SD	1:B:81:MET:N	2.76	0.59
1:B:1190:LEU:HD21	1:B:1193:LYS:HG3	1.83	0.59
1:B:2526:LEU:HD22	1:B:2606:LEU:HD22	1.85	0.59
1:D:701:GLU:HG2	1:D:1462:VAL:HG13	1.83	0.59
1:A:81:MET:SD	1:A:81:MET:N	2.76	0.59
1:D:3944:VAL:HG13	1:D:4005:SER:HB3	1.85	0.59
1:B:2254:LEU:O	1:B:3809:ARG:NH1	2.36	0.58
1:B:3215:THR:HA	1:B:3218:ILE:HD12	1.85	0.58
1:C:3215:THR:HA	1:C:3218:ILE:HD12	1.86	0.58
1:C:3944:VAL:HG13	1:C:4005:SER:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2254:LEU:O	1:D:3809:ARG:NH1	2.36	0.58
1:D:2526:LEU:HD22	1:D:2606:LEU:HD22	1.85	0.58
1:B:2184:LYS:O	1:B:2187:THR:OG1	2.20	0.58
1:C:2526:LEU:HD22	1:C:2606:LEU:HD22	1.85	0.58
1:D:81:MET:SD	1:D:81:MET:N	2.76	0.58
1:A:2321:ARG:NH2	1:D:189:GLU:OE2	2.37	0.58
1:A:3215:THR:HA	1:A:3218:ILE:HD12	1.86	0.58
1:C:2254:LEU:O	1:C:3809:ARG:NH1	2.36	0.58
1:D:1294:ASN:O	1:D:1296:ASN:ND2	2.37	0.58
2:G:46:PRO:HG2	2:G:48:LYS:HZ1	1.69	0.58
1:A:1294:ASN:O	1:A:1296:ASN:ND2	2.37	0.57
1:B:3944:VAL:HG13	1:B:4005:SER:HB3	1.85	0.57
1:C:81:MET:SD	1:C:81:MET:N	2.76	0.57
1:C:189:GLU:OE2	1:D:2321:ARG:NH2	2.37	0.57
1:D:2184:LYS:O	1:D:2187:THR:OG1	2.20	0.57
1:C:965:LYS:HE2	1:C:983:LEU:HD13	1.86	0.57
1:C:1794:GLN:O	1:C:1797:THR:OG1	2.21	0.57
1:D:892:LEU:HA	1:D:895:MET:HE3	1.85	0.57
1:D:3215:THR:HA	1:D:3218:ILE:HD12	1.86	0.57
1:C:4907:HIS:HE1	1:C:4912:HIS:ND1	2.03	0.57
1:B:2326:ARG:NH1	1:B:2327:PRO:O	2.38	0.57
1:D:2196:CYS:SG	1:D:2197:ARG:N	2.71	0.57
1:A:3944:VAL:HG13	1:A:4005:SER:HB3	1.85	0.57
1:D:4907:HIS:HE1	1:D:4912:HIS:ND1	2.03	0.57
1:A:1848:GLU:H	1:A:1849:PRO:HD2	1.70	0.57
1:C:2326:ARG:NH1	1:C:2327:PRO:O	2.38	0.57
1:B:1848:GLU:H	1:B:1849:PRO:HD2	1.70	0.57
1:B:4907:HIS:HE1	1:B:4912:HIS:ND1	2.03	0.57
1:B:4859:ALA:HB1	1:C:4866:ILE:HD11	1.86	0.57
1:C:33:GLN:N	1:C:33:GLN:OE1	2.38	0.57
1:D:1848:GLU:H	1:D:1849:PRO:HD2	1.70	0.57
1:C:1294:ASN:O	1:C:1296:ASN:ND2	2.37	0.56
1:D:33:GLN:N	1:D:33:GLN:OE1	2.38	0.56
1:D:965:LYS:HE2	1:D:983:LEU:HD13	1.86	0.56
1:B:965:LYS:HE2	1:B:983:LEU:HD13	1.86	0.56
1:D:2326:ARG:NH1	1:D:2327:PRO:O	2.38	0.56
1:A:965:LYS:HE2	1:A:983:LEU:HD13	1.86	0.56
1:B:1794:GLN:O	1:B:1797:THR:OG1	2.21	0.56
1:C:2236:SER:HB2	1:C:2239:LEU:HB2	1.88	0.56
2:H:46:PRO:HG2	2:H:48:LYS:HZ1	1.69	0.56
1:A:4790:LYS:NZ	1:A:4836:ASP:OD2	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1294:ASN:O	1:B:1296:ASN:ND2	2.37	0.56
1:D:2236:SER:HB2	1:D:2239:LEU:HB2	1.88	0.56
1:C:2002:LEU:HB3	1:C:2006:CYS:HB2	1.88	0.56
1:D:1777:TYR:HD1	1:D:1778:GLN:HG2	1.71	0.56
1:D:2836:LEU:HD21	1:D:2902:VAL:H	1.71	0.56
1:A:33:GLN:OE1	1:A:33:GLN:N	2.38	0.56
1:A:2326:ARG:NH1	1:A:2327:PRO:O	2.38	0.56
1:A:4907:HIS:HE1	1:A:4912:HIS:ND1	2.03	0.56
1:B:1674:ALA:HB1	1:B:1780:SER:HB2	1.88	0.56
1:C:892:LEU:HA	1:C:895:MET:HE3	1.88	0.56
1:B:235:ARG:HB2	1:B:406:SER:HB3	1.88	0.56
1:C:1712:LEU:HB3	1:C:1832:MET:HE1	1.88	0.56
1:C:235:ARG:HB2	1:C:406:SER:HB3	1.88	0.56
1:C:1777:TYR:HD1	1:C:1778:GLN:HG2	1.71	0.56
1:A:1674:ALA:HB1	1:A:1780:SER:HB2	1.88	0.55
1:A:2836:LEU:HD21	1:A:2902:VAL:H	1.71	0.55
1:B:33:GLN:N	1:B:33:GLN:OE1	2.38	0.55
1:B:2236:SER:HB2	1:B:2239:LEU:HB2	1.88	0.55
1:D:1740:PHE:HD1	1:D:1741:PRO:HD2	1.72	0.55
1:D:4003:VAL:HG11	1:D:4113:ARG:HD2	1.88	0.55
2:F:46:PRO:HG2	2:F:48:LYS:HZ1	1.70	0.55
1:A:1112:ASP:O	1:A:1211:GLN:NE2	2.40	0.55
1:B:892:LEU:HA	1:B:895:MET:HE3	1.88	0.55
1:B:1712:LEU:HB3	1:B:1832:MET:HE1	1.89	0.55
1:C:2184:LYS:O	1:C:2187:THR:OG1	2.20	0.55
1:C:3083:ARG:HH12	1:C:3208:PRO:HG3	1.72	0.55
1:D:2002:LEU:HB3	1:D:2006:CYS:HB2	1.88	0.55
1:A:1243:THR:HG22	1:A:1245:ARG:H	1.71	0.55
1:A:3083:ARG:HH12	1:A:3208:PRO:HG3	1.72	0.55
1:B:697:TRP:H	1:B:724:SER:HB2	1.72	0.55
1:C:4003:VAL:HG11	1:C:4113:ARG:HD2	1.89	0.55
1:D:624:ALA:HB1	1:D:629:GLN:HB3	1.89	0.55
1:D:3083:ARG:HH12	1:D:3208:PRO:HG3	1.72	0.55
1:A:1777:TYR:HD1	1:A:1778:GLN:HG2	1.71	0.55
1:B:2002:LEU:HB3	1:B:2006:CYS:HB2	1.88	0.55
1:C:514:PHE:HA	1:C:517:VAL:HG12	1.88	0.55
1:C:2836:LEU:HD21	1:C:2902:VAL:H	1.71	0.55
1:A:3045:MET:HG2	1:A:3093:ILE:HG12	1.89	0.55
1:C:697:TRP:H	1:C:724:SER:HB2	1.72	0.55
1:A:697:TRP:H	1:A:724:SER:HB2	1.72	0.55
1:A:1712:LEU:HB3	1:A:1832:MET:HE1	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2236:SER:HB2	1:A:2239:LEU:HB2	1.88	0.55
1:A:4003:VAL:HG11	1:A:4113:ARG:HD2	1.88	0.55
1:B:1777:TYR:HD1	1:B:1778:GLN:HG2	1.71	0.55
1:B:2836:LEU:HD21	1:B:2902:VAL:H	1.71	0.55
1:D:235:ARG:HB2	1:D:406:SER:HB3	1.88	0.55
1:A:217:ILE:O	1:A:285:SER:N	2.40	0.55
1:A:235:ARG:HB2	1:A:406:SER:HB3	1.88	0.55
1:A:272:ARG:HB2	1:A:492:GLU:HG2	1.89	0.55
1:A:514:PHE:HA	1:A:517:VAL:HG12	1.88	0.55
1:B:2716:LEU:HD13	1:B:2720:ILE:HG21	1.89	0.55
1:B:3083:ARG:HH12	1:B:3208:PRO:HG3	1.72	0.55
1:D:755:ILE:HG22	1:D:770:ILE:HG12	1.89	0.55
1:C:217:ILE:O	1:C:285:SER:N	2.40	0.55
1:C:624:ALA:HB1	1:C:629:GLN:HB3	1.89	0.55
1:D:896:ASN:ND2	1:D:1052:GLU:OE1	2.40	0.55
1:D:1112:ASP:O	1:D:1211:GLN:NE2	2.40	0.55
1:D:3920:THR:O	1:D:3924:GLN:N	2.40	0.55
1:B:272:ARG:HB2	1:B:492:GLU:HG2	1.89	0.55
1:B:3045:MET:HG2	1:B:3093:ILE:HG12	1.89	0.55
1:C:1243:THR:HG22	1:C:1245:ARG:H	1.71	0.55
1:D:1674:ALA:HB1	1:D:1780:SER:HB2	1.88	0.55
1:A:1740:PHE:HD1	1:A:1741:PRO:HD2	1.72	0.55
1:B:1243:THR:HG22	1:B:1245:ARG:H	1.71	0.55
1:C:1112:ASP:O	1:C:1211:GLN:NE2	2.40	0.55
1:C:1740:PHE:HD1	1:C:1741:PRO:HD2	1.72	0.55
1:C:2036:THR:HG21	1:C:3628:ILE:HG21	1.89	0.55
1:D:3045:MET:HG2	1:D:3093:ILE:HG12	1.89	0.55
1:B:3731:HIS:O	1:B:3775:LYS:NZ	2.41	0.54
1:D:697:TRP:H	1:D:724:SER:HB2	1.72	0.54
1:D:1243:THR:HG22	1:D:1245:ARG:H	1.71	0.54
1:D:2331:GLY:HA3	1:D:2341:GLY:H	1.72	0.54
1:A:589:ILE:HG21	1:A:617:LEU:HD21	1.89	0.54
1:A:2331:GLY:HA3	1:A:2341:GLY:H	1.72	0.54
1:A:2716:LEU:HD13	1:A:2720:ILE:HG21	1.89	0.54
1:A:4849:PHE:O	1:A:4853:VAL:HG12	2.07	0.54
1:C:896:ASN:ND2	1:C:1052:GLU:OE1	2.40	0.54
1:C:1674:ALA:HB1	1:C:1780:SER:HB2	1.88	0.54
1:C:1848:GLU:H	1:C:1849:PRO:HD2	1.70	0.54
1:C:3920:THR:O	1:C:3924:GLN:N	2.40	0.54
1:A:547:ASN:HB2	1:A:550:GLN:HB2	1.89	0.54
1:A:892:LEU:HA	1:A:895:MET:HE3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2002:LEU:HB3	1:A:2006:CYS:HB2	1.88	0.54
1:A:3015:ARG:NH1	1:A:3083:ARG:O	2.40	0.54
1:D:272:ARG:HB2	1:D:492:GLU:HG2	1.89	0.54
1:D:514:PHE:HA	1:D:517:VAL:HG12	1.89	0.54
1:B:4849:PHE:O	1:B:4853:VAL:HG12	2.07	0.54
1:C:3015:ARG:NH1	1:C:3083:ARG:O	2.40	0.54
1:D:3731:HIS:O	1:D:3775:LYS:NZ	2.41	0.54
1:A:4648:VAL:HA	1:A:4651:LYS:HD2	1.89	0.54
1:B:217:ILE:O	1:B:285:SER:N	2.40	0.54
1:B:1112:ASP:O	1:B:1211:GLN:NE2	2.40	0.54
1:B:4003:VAL:HG11	1:B:4113:ARG:HD2	1.88	0.54
1:C:547:ASN:HB2	1:C:550:GLN:HB2	1.89	0.54
1:C:3614:ARG:O	1:C:3617:ASN:ND2	2.41	0.54
1:D:217:ILE:O	1:D:285:SER:N	2.40	0.54
1:D:547:ASN:HB2	1:D:550:GLN:HB2	1.90	0.54
1:D:1794:GLN:O	1:D:1797:THR:OG1	2.21	0.54
1:A:679:VAL:HA	1:A:800:VAL:HG12	1.90	0.54
1:A:3731:HIS:O	1:A:3775:LYS:NZ	2.41	0.54
1:B:172:GLY:O	1:C:3938:ARG:NH1	2.41	0.54
1:B:2331:GLY:HA3	1:B:2341:GLY:H	1.72	0.54
1:C:3344:ARG:O	1:C:3366:TYR:OH	2.23	0.54
1:C:4849:PHE:O	1:C:4853:VAL:HG12	2.07	0.54
1:D:322:ALA:HB1	1:D:327:THR:HG21	1.90	0.54
1:D:3015:ARG:NH1	1:D:3083:ARG:O	2.40	0.54
1:D:3614:ARG:O	1:D:3617:ASN:ND2	2.41	0.54
1:A:755:ILE:HG22	1:A:770:ILE:HG12	1.89	0.54
1:A:896:ASN:ND2	1:A:1052:GLU:OE1	2.40	0.54
1:B:3614:ARG:O	1:B:3617:ASN:ND2	2.41	0.54
1:C:4648:VAL:HA	1:C:4651:LYS:HD2	1.89	0.54
1:B:413:SER:OG	1:B:414:ARG:N	2.41	0.54
1:B:624:ALA:HB1	1:B:629:GLN:HB3	1.89	0.54
1:B:896:ASN:ND2	1:B:1052:GLU:OE1	2.40	0.54
1:C:272:ARG:HB2	1:C:492:GLU:HG2	1.89	0.54
1:C:755:ILE:HG22	1:C:770:ILE:HG12	1.89	0.54
1:C:2024:ILE:HA	1:C:2027:ARG:HH12	1.73	0.54
1:D:4849:PHE:O	1:D:4853:VAL:HG12	2.07	0.54
1:A:3920:THR:O	1:A:3924:GLN:N	2.40	0.54
1:B:370:LEU:HD12	1:B:396:GLU:HA	1.90	0.54
1:B:547:ASN:HB2	1:B:550:GLN:HB2	1.89	0.54
1:B:679:VAL:HA	1:B:800:VAL:HG12	1.90	0.54
1:B:1137:PHE:HA	1:B:1144:ARG:HA	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3920:THR:O	1:B:3924:GLN:N	2.40	0.54
1:C:322:ALA:HB1	1:C:327:THR:HG21	1.90	0.54
1:C:679:VAL:HA	1:C:800:VAL:HG12	1.90	0.54
1:C:3045:MET:HG2	1:C:3093:ILE:HG12	1.89	0.54
1:A:1137:PHE:HA	1:A:1144:ARG:HA	1.90	0.54
1:B:322:ALA:HB1	1:B:327:THR:HG21	1.90	0.54
1:B:983:LEU:HD21	1:B:1059:GLY:HA3	1.90	0.54
1:C:192:LEU:O	1:C:212:TRP:NE1	2.39	0.54
1:C:3731:HIS:O	1:C:3775:LYS:NZ	2.40	0.54
1:D:2024:ILE:HA	1:D:2027:ARG:HH12	1.73	0.54
1:D:2036:THR:HG21	1:D:3628:ILE:HG21	1.89	0.54
2:E:46:PRO:HG2	2:E:48:LYS:HZ1	1.72	0.54
1:A:3614:ARG:O	1:A:3617:ASN:ND2	2.41	0.53
1:B:4648:VAL:HA	1:B:4651:LYS:HD2	1.89	0.53
1:C:2716:LEU:HD13	1:C:2720:ILE:HG21	1.89	0.53
1:D:361:CYS:O	1:D:403:LEU:N	2.38	0.53
1:D:2716:LEU:HD13	1:D:2720:ILE:HG21	1.89	0.53
1:A:983:LEU:HD21	1:A:1059:GLY:HA3	1.90	0.53
1:A:3102:PRO:HB2	1:A:3229:GLN:HB3	1.90	0.53
1:A:3938:ARG:NH1	1:D:172:GLY:O	2.41	0.53
1:B:3015:ARG:NH1	1:B:3083:ARG:O	2.40	0.53
1:C:1137:PHE:HA	1:C:1144:ARG:HA	1.90	0.53
1:C:1723:ASN:O	1:C:1918:ARG:NH2	2.42	0.53
1:C:4790:LYS:NZ	1:C:4836:ASP:OD2	2.37	0.53
1:D:370:LEU:HD12	1:D:396:GLU:HA	1.90	0.53
1:D:2210:GLN:NE2	1:D:2244:ALA:O	2.41	0.53
1:A:322:ALA:HB1	1:A:327:THR:HG21	1.90	0.53
1:A:1723:ASN:O	1:A:1918:ARG:NH2	2.42	0.53
1:B:1740:PHE:HD1	1:B:1741:PRO:HD2	1.71	0.53
1:B:3344:ARG:O	1:B:3366:TYR:OH	2.23	0.53
1:C:983:LEU:HD21	1:C:1059:GLY:HA3	1.90	0.53
1:C:2210:GLN:NE2	1:C:2244:ALA:O	2.41	0.53
1:C:2331:GLY:HA3	1:C:2341:GLY:H	1.72	0.53
1:D:589:ILE:HG21	1:D:617:LEU:HD21	1.89	0.53
1:D:1723:ASN:O	1:D:1918:ARG:NH2	2.42	0.53
1:D:4648:VAL:HA	1:D:4651:LYS:HD2	1.89	0.53
1:B:514:PHE:HA	1:B:517:VAL:HG12	1.89	0.53
1:C:986:ILE:HG12	1:C:1058:LEU:HB3	1.90	0.53
1:D:679:VAL:HA	1:D:800:VAL:HG12	1.90	0.53
1:A:3055:ALA:HB3	1:A:3100:LEU:HD13	1.90	0.53
1:B:2036:THR:HG21	1:B:3628:ILE:HG21	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3102:PRO:HB2	1:D:3229:GLN:HB3	1.90	0.53
1:D:4790:LYS:NZ	1:D:4836:ASP:OD2	2.37	0.53
1:A:624:ALA:HB1	1:A:629:GLN:HB3	1.89	0.53
1:B:589:ILE:HG21	1:B:617:LEU:HD21	1.89	0.53
1:B:986:ILE:HG12	1:B:1058:LEU:HB3	1.90	0.53
1:C:3055:ALA:HB3	1:C:3100:LEU:HD13	1.90	0.53
2:E:75:LEU:N	2:E:100:PHE:O	2.42	0.53
1:A:2036:THR:HG21	1:A:3628:ILE:HG21	1.89	0.53
1:B:755:ILE:HG22	1:B:770:ILE:HG12	1.89	0.53
1:B:3055:ALA:HB3	1:B:3100:LEU:HD13	1.90	0.53
1:C:3291:GLU:OE1	1:C:3301:PHE:N	2.42	0.53
1:A:1794:GLN:O	1:A:1797:THR:OG1	2.21	0.53
1:A:2490:GLY:O	1:A:2494:ASP:N	2.39	0.53
1:C:3102:PRO:HB2	1:C:3229:GLN:HB3	1.90	0.53
2:E:24:VAL:HG13	2:E:48:LYS:HE3	1.91	0.53
2:F:75:LEU:N	2:F:100:PHE:O	2.42	0.53
1:C:370:LEU:HD12	1:C:396:GLU:HA	1.90	0.53
1:C:1434:PRO:HB2	1:C:1502:ASN:HB3	1.91	0.53
1:D:413:SER:OG	1:D:414:ARG:N	2.41	0.53
2:G:24:VAL:HG13	2:G:48:LYS:HE3	1.91	0.53
1:A:2184:LYS:O	1:A:2187:THR:OG1	2.20	0.53
1:B:2024:ILE:HA	1:B:2027:ARG:HH12	1.73	0.53
1:B:2396:ASP:OD1	1:B:2400:ARG:NH1	2.42	0.53
1:B:3291:GLU:OE1	1:B:3301:PHE:N	2.42	0.53
1:C:172:GLY:O	1:D:3938:ARG:NH1	2.42	0.53
1:A:3291:GLU:OE1	1:A:3301:PHE:N	2.42	0.52
1:A:4853:VAL:HA	1:A:4857:LEU:HD12	1.91	0.52
1:B:1723:ASN:O	1:B:1918:ARG:NH2	2.42	0.52
1:D:3344:ARG:O	1:D:3366:TYR:OH	2.23	0.52
1:D:3954:GLN:O	1:D:3958:SER:OG	2.28	0.52
1:C:2396:ASP:OD1	1:C:2400:ARG:NH1	2.42	0.52
1:A:2210:GLN:NE2	1:A:2244:ALA:O	2.41	0.52
1:A:3681:LEU:HD22	1:A:3746:SER:HB2	1.91	0.52
1:B:4071:THR:OG1	1:B:4072:ASP:N	2.42	0.52
1:B:4790:LYS:NZ	1:B:4836:ASP:OD2	2.37	0.52
1:C:3681:LEU:HD22	1:C:3746:SER:HB2	1.91	0.52
1:D:2396:ASP:OD1	1:D:2400:ARG:NH1	2.42	0.52
1:C:504:ARG:HD2	1:C:505:LEU:HD13	1.92	0.52
1:D:986:ILE:HG12	1:D:1058:LEU:HB3	1.90	0.52
1:D:3681:LEU:HD22	1:D:3746:SER:HB2	1.91	0.52
1:B:3102:PRO:HB2	1:B:3229:GLN:HB3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1444:GLY:HA3	1:C:1488:VAL:HA	1.92	0.52
1:D:1137:PHE:HA	1:D:1144:ARG:HA	1.90	0.52
1:D:1434:PRO:HB2	1:D:1502:ASN:HB3	1.91	0.52
1:D:3291:GLU:OE1	1:D:3301:PHE:N	2.42	0.52
2:H:75:LEU:N	2:H:100:PHE:O	2.42	0.52
1:A:504:ARG:HD2	1:A:505:LEU:HD13	1.92	0.52
1:B:504:ARG:HD2	1:B:505:LEU:HD13	1.92	0.52
1:B:2210:GLN:NE2	1:B:2244:ALA:O	2.41	0.52
1:C:413:SER:OG	1:C:414:ARG:N	2.41	0.52
1:D:504:ARG:HD2	1:D:505:LEU:HD13	1.92	0.52
2:F:24:VAL:HG13	2:F:48:LYS:HE3	1.90	0.52
2:H:24:VAL:HG13	2:H:48:LYS:HE3	1.90	0.52
1:A:370:LEU:HD12	1:A:396:GLU:HA	1.90	0.52
1:A:2024:ILE:HA	1:A:2027:ARG:HH12	1.73	0.52
1:D:778:MET:SD	1:D:778:MET:N	2.83	0.52
1:D:1444:GLY:HA3	1:D:1488:VAL:HA	1.92	0.52
1:A:218:SER:HA	1:A:286:GLY:H	1.75	0.52
1:B:1723:ASN:ND2	1:B:1914:ASP:OD2	2.41	0.52
1:C:589:ILE:HG21	1:C:617:LEU:HD21	1.89	0.52
1:C:3919:LEU:HD22	1:C:3934:LEU:HD21	1.92	0.52
1:D:983:LEU:HD21	1:D:1059:GLY:HA3	1.90	0.52
1:A:413:SER:OG	1:A:414:ARG:N	2.41	0.52
1:A:2396:ASP:OD1	1:A:2400:ARG:NH1	2.42	0.52
1:C:1100:ARG:HA	1:C:1166:VAL:HG23	1.92	0.52
1:C:3750:THR:HG22	1:C:3795:LEU:HD23	1.92	0.52
1:C:4853:VAL:HA	1:C:4857:LEU:HD12	1.91	0.52
2:G:75:LEU:N	2:G:100:PHE:O	2.42	0.52
1:B:3750:THR:HG22	1:B:3795:LEU:HD23	1.92	0.52
1:A:1434:PRO:HB2	1:A:1502:ASN:HB3	1.91	0.51
1:A:3254:GLU:OE1	1:A:3256:HIS:NE2	2.43	0.51
1:A:4193:GLU:OE1	1:A:4603:LYS:NZ	2.43	0.51
1:B:778:MET:N	1:B:778:MET:SD	2.83	0.51
1:B:1100:ARG:HA	1:B:1166:VAL:HG23	1.92	0.51
1:B:3254:GLU:OE1	1:B:3256:HIS:NE2	2.43	0.51
1:C:361:CYS:O	1:C:403:LEU:N	2.38	0.51
1:C:373:THR:HG21	1:C:398:HIS:H	1.75	0.51
1:A:986:ILE:HG12	1:A:1058:LEU:HB3	1.90	0.51
1:B:218:SER:HA	1:B:286:GLY:H	1.75	0.51
1:B:891:GLU:HA	1:B:894:VAL:HG22	1.93	0.51
1:B:1444:GLY:HA3	1:B:1488:VAL:HA	1.92	0.51
1:B:3681:LEU:HD22	1:B:3746:SER:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2065:MET:HE1	1:D:2086:LEU:HD23	1.91	0.51
1:A:1444:GLY:HA3	1:A:1488:VAL:HA	1.92	0.51
1:C:778:MET:SD	1:C:778:MET:N	2.83	0.51
1:D:3055:ALA:HB3	1:D:3100:LEU:HD13	1.90	0.51
1:D:3919:LEU:HD22	1:D:3934:LEU:HD21	1.92	0.51
1:A:778:MET:SD	1:A:778:MET:N	2.83	0.51
1:A:3919:LEU:HD22	1:A:3934:LEU:HD21	1.92	0.51
1:C:218:SER:HA	1:C:286:GLY:H	1.75	0.51
1:D:218:SER:HA	1:D:286:GLY:H	1.75	0.51
1:D:373:THR:HG21	1:D:398:HIS:H	1.75	0.51
1:B:3058:ALA:HA	1:B:3062:ASN:HB3	1.93	0.51
1:A:3750:THR:HG22	1:A:3795:LEU:HD23	1.92	0.51
1:B:2174:MET:HG2	1:B:2178:LEU:HD23	1.93	0.51
1:B:3919:LEU:HD22	1:B:3934:LEU:HD21	1.92	0.51
1:C:3058:ALA:HA	1:C:3062:ASN:HB3	1.93	0.51
1:D:2162:ARG:NH2	1:D:2208:GLN:OE1	2.44	0.51
1:D:4853:VAL:HA	1:D:4857:LEU:HD12	1.91	0.51
1:A:4071:THR:OG1	1:A:4072:ASP:N	2.42	0.51
1:B:2162:ARG:NH2	1:B:2208:GLN:OE1	2.44	0.51
1:B:4807:ASP:N	1:B:4807:ASP:OD1	2.41	0.51
1:C:891:GLU:HA	1:C:894:VAL:HG22	1.93	0.51
1:C:1723:ASN:ND2	1:C:1914:ASP:OD2	2.41	0.51
1:C:2065:MET:HE1	1:C:2086:LEU:HD23	1.92	0.51
1:D:3750:THR:HG22	1:D:3795:LEU:HD23	1.92	0.51
1:B:207:PHE:CD2	1:C:2324:ILE:HD13	2.46	0.51
1:B:4853:VAL:HA	1:B:4857:LEU:HD12	1.91	0.51
1:C:2162:ARG:NH2	1:C:2208:GLN:OE1	2.44	0.51
1:D:139:SER:O	1:D:198:ASN:ND2	2.44	0.51
1:D:1100:ARG:HA	1:D:1166:VAL:HG23	1.92	0.51
1:D:4158:GLN:NE2	1:D:4199:MET:O	2.44	0.51
1:A:2174:MET:HG2	1:A:2178:LEU:HD23	1.93	0.51
1:B:2878:ALA:HA	1:B:2881:LYS:HB2	1.93	0.51
1:C:139:SER:O	1:C:198:ASN:ND2	2.44	0.51
1:D:1522:ILE:HD11	1:D:1532:TYR:HB2	1.93	0.51
1:A:2162:ARG:NH2	1:A:2208:GLN:OE1	2.44	0.51
1:B:146:ASP:OD1	1:B:146:ASP:N	2.43	0.51
1:B:4115:GLN:O	1:B:4119:GLU:HG2	2.11	0.51
1:C:728:ASP:OD1	1:C:728:ASP:N	2.44	0.51
1:C:4115:GLN:O	1:C:4119:GLU:HG2	2.11	0.51
2:H:31:LEU:N	2:H:35:LYS:O	2.44	0.51
1:A:33:GLN:HE21	1:A:35:LEU:HD11	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:LEU:O	1:A:212:TRP:NE1	2.39	0.50
1:A:373:THR:HG21	1:A:398:HIS:H	1.75	0.50
1:A:891:GLU:HA	1:A:894:VAL:HG22	1.93	0.50
1:A:508:TYR:HD2	1:A:511:ALA:H	1.60	0.50
1:A:1723:ASN:ND2	1:A:1914:ASP:OD2	2.41	0.50
1:A:4158:GLN:NE2	1:A:4199:MET:O	2.44	0.50
1:B:951:GLY:O	1:B:953:ALA:N	2.44	0.50
1:B:4521:SER:HB3	1:B:4558:TYR:HE2	1.76	0.50
1:C:146:ASP:OD1	1:C:146:ASP:N	2.43	0.50
1:D:728:ASP:N	1:D:728:ASP:OD1	2.44	0.50
1:D:1712:LEU:HB3	1:D:1832:MET:HE1	1.93	0.50
1:B:1434:PRO:HB2	1:B:1502:ASN:HB3	1.91	0.50
1:D:3254:GLU:OE1	1:D:3256:HIS:NE2	2.43	0.50
1:D:4071:THR:OG1	1:D:4072:ASP:N	2.42	0.50
1:D:4115:GLN:O	1:D:4119:GLU:HG2	2.11	0.50
1:D:4854:ILE:O	1:D:4858:LEU:HB2	2.12	0.50
1:A:500:GLU:OE1	1:A:557:TRP:NE1	2.45	0.50
1:A:3344:ARG:O	1:A:3366:TYR:OH	2.23	0.50
1:B:4614:LEU:HA	1:B:4618:GLU:HB3	1.94	0.50
1:C:508:TYR:HD2	1:C:511:ALA:H	1.59	0.50
1:C:983:LEU:HD23	1:C:1055:ARG:HD2	1.94	0.50
1:D:3058:ALA:HA	1:D:3062:ASN:HB3	1.93	0.50
1:A:172:GLY:O	1:B:3938:ARG:NH1	2.45	0.50
1:B:500:GLU:OE1	1:B:557:TRP:NE1	2.45	0.50
1:B:508:TYR:HD2	1:B:511:ALA:H	1.60	0.50
1:B:983:LEU:HD23	1:B:1055:ARG:HD2	1.94	0.50
1:B:4158:GLN:NE2	1:B:4199:MET:O	2.44	0.50
1:C:40:GLU:N	1:C:40:GLU:OE1	2.45	0.50
1:C:1522:ILE:HD11	1:C:1532:TYR:HB2	1.94	0.50
1:C:2878:ALA:HA	1:C:2881:LYS:HB2	1.93	0.50
1:C:4071:THR:OG1	1:C:4072:ASP:N	2.42	0.50
1:C:4158:GLN:NE2	1:C:4199:MET:O	2.44	0.50
1:D:2174:MET:HG2	1:D:2178:LEU:HD23	1.92	0.50
1:A:2405:MET:SD	1:A:2419:ARG:NE	2.85	0.50
1:B:33:GLN:HE21	1:B:35:LEU:HD11	1.76	0.50
1:B:139:SER:O	1:B:198:ASN:ND2	2.44	0.50
1:B:373:THR:HG21	1:B:398:HIS:H	1.75	0.50
1:B:1143:GLN:HA	1:B:1152:TYR:H	1.76	0.50
1:C:3254:GLU:OE1	1:C:3256:HIS:NE2	2.43	0.50
1:D:508:TYR:HD2	1:D:511:ALA:H	1.59	0.50
1:A:40:GLU:N	1:A:40:GLU:OE1	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2065:MET:HE1	1:A:2086:LEU:HD23	1.94	0.50
1:B:926:GLU:OE2	1:B:930:ASN:ND2	2.40	0.50
1:B:2405:MET:SD	1:B:2419:ARG:NE	2.85	0.50
1:C:4614:LEU:HA	1:C:4618:GLU:HB3	1.94	0.50
1:D:40:GLU:N	1:D:40:GLU:OE1	2.45	0.50
1:A:1100:ARG:HA	1:A:1166:VAL:HG23	1.92	0.50
1:A:1522:ILE:HD11	1:A:1532:TYR:HB2	1.93	0.50
1:A:3058:ALA:HA	1:A:3062:ASN:HB3	1.93	0.50
1:A:4854:ILE:O	1:A:4858:LEU:HB2	2.12	0.50
1:B:40:GLU:OE1	1:B:40:GLU:N	2.45	0.50
1:C:500:GLU:OE1	1:C:557:TRP:NE1	2.45	0.50
1:C:4854:ILE:O	1:C:4858:LEU:HB2	2.12	0.50
1:D:500:GLU:OE1	1:D:557:TRP:NE1	2.45	0.50
1:D:4807:ASP:OD1	1:D:4807:ASP:N	2.41	0.50
1:A:1143:GLN:HA	1:A:1152:TYR:H	1.76	0.50
1:D:983:LEU:HD23	1:D:1055:ARG:HD2	1.94	0.50
1:A:361:CYS:O	1:A:403:LEU:N	2.38	0.49
1:B:1262:PRO:HG3	1:B:1595:VAL:HG12	1.94	0.49
1:B:4193:GLU:OE1	1:B:4603:LYS:NZ	2.43	0.49
1:D:891:GLU:HA	1:D:894:VAL:HG22	1.93	0.49
1:D:2210:GLN:OE1	1:D:2249:ASN:ND2	2.45	0.49
1:D:4193:GLU:OE1	1:D:4603:LYS:NZ	2.43	0.49
1:A:139:SER:O	1:A:198:ASN:ND2	2.44	0.49
1:A:146:ASP:OD1	1:A:146:ASP:N	2.43	0.49
1:C:951:GLY:O	1:C:953:ALA:N	2.44	0.49
1:C:1791:LYS:O	1:C:1795:MET:HG2	2.13	0.49
1:D:33:GLN:HE21	1:D:35:LEU:HD11	1.76	0.49
1:D:1143:GLN:HA	1:D:1152:TYR:H	1.76	0.49
1:D:4521:SER:HB3	1:D:4558:TYR:HE2	1.76	0.49
1:A:787:LEU:HG	1:A:789:PHE:HE1	1.78	0.49
1:A:983:LEU:HD23	1:A:1055:ARG:HD2	1.94	0.49
1:A:1022:GLN:HG3	1:A:1024:VAL:HG13	1.94	0.49
1:A:1791:LYS:O	1:A:1795:MET:HG2	2.13	0.49
1:A:2210:GLN:OE1	1:A:2249:ASN:ND2	2.46	0.49
1:A:4614:LEU:HA	1:A:4618:GLU:HB3	1.94	0.49
1:B:1791:LYS:O	1:B:1795:MET:HG2	2.13	0.49
1:C:3967:LEU:O	1:C:3971:MET:HG2	2.13	0.49
1:D:548:CYS:HB2	1:D:579:LEU:HD23	1.94	0.49
1:D:915:HIS:HB2	1:D:918:LEU:HB2	1.94	0.49
1:D:3967:LEU:O	1:D:3971:MET:HG2	2.12	0.49
1:A:2471:LEU:O	1:A:2476:GLY:N	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2210:GLN:OE1	1:B:2249:ASN:ND2	2.45	0.49
1:B:2490:GLY:O	1:B:2494:ASP:N	2.39	0.49
1:C:226:GLY:O	1:C:355:LYS:NZ	2.44	0.49
1:C:915:HIS:HB2	1:C:918:LEU:HB2	1.94	0.49
1:C:1767:PRO:O	1:C:1769:PHE:N	2.44	0.49
1:C:4521:SER:HB3	1:C:4558:TYR:HE2	1.77	0.49
1:D:926:GLU:OE2	1:D:930:ASN:ND2	2.40	0.49
1:D:1262:PRO:HG3	1:D:1595:VAL:HG12	1.94	0.49
1:D:3927:CYS:O	1:D:3929:GLY:N	2.46	0.49
1:D:4614:LEU:HA	1:D:4618:GLU:HB3	1.94	0.49
1:A:1262:PRO:HG3	1:A:1595:VAL:HG12	1.94	0.49
1:A:4115:GLN:O	1:A:4119:GLU:HG2	2.11	0.49
1:A:4518:TYR:OH	1:A:4735:ASN:ND2	2.46	0.49
1:B:361:CYS:O	1:B:403:LEU:N	2.38	0.49
1:B:787:LEU:HG	1:B:789:PHE:HE1	1.78	0.49
1:B:3927:CYS:O	1:B:3929:GLY:N	2.46	0.49
1:C:787:LEU:HG	1:C:789:PHE:HE1	1.78	0.49
1:C:2174:MET:HG2	1:C:2178:LEU:HD23	1.93	0.49
1:D:1136:ALA:O	1:D:1145:TRP:N	2.46	0.49
1:D:2878:ALA:HA	1:D:2881:LYS:HB2	1.93	0.49
1:A:548:CYS:HB2	1:A:579:LEU:HD23	1.94	0.49
1:A:915:HIS:HB2	1:A:918:LEU:HB2	1.94	0.49
1:A:2878:ALA:HA	1:A:2881:LYS:HB2	1.93	0.49
1:B:1136:ALA:O	1:B:1145:TRP:N	2.46	0.49
1:C:1143:GLN:HA	1:C:1152:TYR:H	1.76	0.49
2:E:31:LEU:N	2:E:35:LYS:O	2.44	0.49
1:A:2228:LEU:H	1:A:2237:THR:HG22	1.78	0.49
1:A:4030:THR:O	1:A:4035:ASP:N	2.46	0.49
1:B:1522:ILE:HD11	1:B:1532:TYR:HB2	1.94	0.49
1:D:1767:PRO:O	1:D:1769:PHE:N	2.44	0.49
1:D:1791:LYS:O	1:D:1795:MET:HG2	2.13	0.49
1:A:200:SER:OG	1:A:201:TRP:N	2.46	0.49
1:A:1136:ALA:O	1:A:1145:TRP:N	2.46	0.49
1:C:2210:GLN:OE1	1:C:2249:ASN:ND2	2.45	0.49
1:D:192:LEU:O	1:D:212:TRP:NE1	2.39	0.49
1:D:2405:MET:SD	1:D:2419:ARG:NE	2.85	0.49
1:A:246:THR:N	1:A:261:HIS:O	2.44	0.49
1:A:2876:LEU:HD22	1:A:2880:GLU:HG3	1.95	0.49
1:A:3688:MET:HE3	1:A:3752:PRO:HB2	1.95	0.49
1:B:2450:VAL:HG23	1:B:2451:VAL:HG13	1.95	0.49
1:C:801:ARG:NH2	1:C:802:PHE:O	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2395:ILE:HD13	1:A:2467:MET:HE2	1.93	0.49
1:A:2450:VAL:HG23	1:A:2451:VAL:HG13	1.95	0.49
1:B:2876:LEU:HD22	1:B:2880:GLU:HG3	1.95	0.49
1:B:3954:GLN:O	1:B:3958:SER:OG	2.28	0.49
1:B:4518:TYR:OH	1:B:4735:ASN:ND2	2.46	0.49
1:C:33:GLN:HE21	1:C:35:LEU:HD11	1.76	0.49
1:C:1022:GLN:HG3	1:C:1024:VAL:HG13	1.94	0.49
1:C:1262:PRO:HG3	1:C:1595:VAL:HG12	1.95	0.49
1:C:2405:MET:SD	1:C:2419:ARG:NE	2.85	0.49
1:D:2228:LEU:H	1:D:2237:THR:HG22	1.78	0.49
1:D:2471:LEU:O	1:D:2476:GLY:N	2.43	0.49
1:A:69:LEU:H	1:A:69:LEU:HD23	1.78	0.48
1:B:200:SER:OG	1:B:201:TRP:N	2.46	0.48
1:B:915:HIS:HB2	1:B:918:LEU:HB2	1.94	0.48
1:C:1136:ALA:O	1:C:1145:TRP:N	2.46	0.48
1:C:3927:CYS:O	1:C:3929:GLY:N	2.46	0.48
1:D:801:ARG:NH2	1:D:802:PHE:O	2.45	0.48
1:B:1017:THR:HA	1:B:1025:LYS:HD3	1.95	0.48
1:B:2228:LEU:H	1:B:2237:THR:HG22	1.78	0.48
1:B:4030:THR:O	1:B:4035:ASP:N	2.46	0.48
1:C:200:SER:OG	1:C:201:TRP:N	2.46	0.48
1:C:4030:THR:O	1:C:4035:ASP:N	2.46	0.48
1:D:200:SER:OG	1:D:201:TRP:N	2.46	0.48
1:A:728:ASP:OD1	1:A:728:ASP:N	2.45	0.48
1:A:3927:CYS:O	1:A:3929:GLY:N	2.46	0.48
1:A:4521:SER:HB3	1:A:4558:TYR:HE2	1.77	0.48
1:B:4854:ILE:O	1:B:4858:LEU:HB2	2.12	0.48
1:C:1017:THR:HA	1:C:1025:LYS:HD3	1.95	0.48
1:C:1511:VAL:HG23	1:C:1519:LEU:HD12	1.95	0.48
1:C:2228:LEU:H	1:C:2237:THR:HG22	1.78	0.48
1:D:69:LEU:HD23	1:D:69:LEU:H	1.78	0.48
1:D:787:LEU:HG	1:D:789:PHE:HE1	1.78	0.48
1:D:3688:MET:HE3	1:D:3752:PRO:HB2	1.95	0.48
1:A:207:PHE:CD2	1:B:2324:ILE:HD13	2.49	0.48
1:A:1017:THR:HA	1:A:1025:LYS:HD3	1.95	0.48
1:A:2623:PRO:HB3	1:A:2666:PRO:HG3	1.96	0.48
1:C:1505:GLY:O	1:C:1524:ASN:ND2	2.47	0.48
1:C:2450:VAL:HG23	1:C:2451:VAL:HG13	1.95	0.48
1:C:2623:PRO:HB3	1:C:2666:PRO:HG3	1.95	0.48
1:C:4193:GLU:OE1	1:C:4603:LYS:NZ	2.43	0.48
1:D:1511:VAL:HG23	1:D:1519:LEU:HD12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1723:ASN:ND2	1:D:1914:ASP:OD2	2.41	0.48
1:D:2450:VAL:HG23	1:D:2451:VAL:HG13	1.95	0.48
1:D:2623:PRO:HB3	1:D:2666:PRO:HG3	1.95	0.48
1:B:3967:LEU:O	1:B:3971:MET:HG2	2.12	0.48
1:C:4518:TYR:OH	1:C:4735:ASN:ND2	2.46	0.48
1:A:1767:PRO:O	1:A:1769:PHE:N	2.44	0.48
1:A:1769:PHE:O	2:E:83:TYR:OH	2.29	0.48
1:A:3967:LEU:O	1:A:3971:MET:HG2	2.12	0.48
1:B:2471:LEU:O	1:B:2476:GLY:N	2.43	0.48
1:C:926:GLU:OE2	1:C:930:ASN:ND2	2.40	0.48
1:C:2204:ARG:O	1:C:2206:SER:N	2.42	0.48
1:C:2314:GLU:OE2	1:C:3812:LYS:NZ	2.47	0.48
1:D:4078:ASP:OD1	1:D:4078:ASP:N	2.47	0.48
1:A:226:GLY:O	1:A:355:LYS:NZ	2.44	0.48
1:B:192:LEU:O	1:B:212:TRP:NE1	2.39	0.48
1:B:2314:GLU:OE2	1:B:3812:LYS:NZ	2.47	0.48
1:B:4660:TYR:HB3	1:B:4664:ARG:HH12	1.79	0.48
1:C:3954:GLN:O	1:C:3958:SER:OG	2.28	0.48
1:D:619:VAL:HG23	1:D:624:ALA:HB3	1.95	0.48
1:D:1022:GLN:HG3	1:D:1024:VAL:HG13	1.94	0.48
1:D:2314:GLU:OE2	1:D:3812:LYS:NZ	2.47	0.48
1:D:4788:PHE:HB3	1:D:4791:PHE:HD2	1.79	0.48
1:A:2314:GLU:OE2	1:A:3812:LYS:NZ	2.47	0.48
1:A:4136:GLU:OE2	1:A:4146:ARG:NH1	2.47	0.48
1:B:548:CYS:HB2	1:B:579:LEU:HD23	1.94	0.48
1:B:619:VAL:HG23	1:B:624:ALA:HB3	1.95	0.48
1:B:902:TRP:HA	1:B:913:ARG:HB3	1.96	0.48
1:B:1505:GLY:O	1:B:1524:ASN:ND2	2.46	0.48
1:B:1767:PRO:O	1:B:1769:PHE:N	2.44	0.48
1:C:69:LEU:H	1:C:69:LEU:HD23	1.78	0.48
1:C:803:LEU:HD11	1:C:811:PHE:HA	1.96	0.48
1:C:4136:GLU:OE2	1:C:4146:ARG:NH1	2.47	0.48
2:F:31:LEU:N	2:F:35:LYS:O	2.44	0.48
1:B:4078:ASP:OD1	1:B:4078:ASP:N	2.47	0.48
1:B:4136:GLU:OE2	1:B:4146:ARG:NH1	2.47	0.48
1:C:2876:LEU:HD22	1:C:2880:GLU:HG3	1.95	0.48
1:D:1769:PHE:O	2:H:83:TYR:OH	2.29	0.48
1:D:4030:THR:O	1:D:4035:ASP:N	2.46	0.48
1:A:902:TRP:HA	1:A:913:ARG:HB3	1.96	0.48
1:A:4084:LYS:HE2	1:A:4085:ARG:HG2	1.96	0.48
1:B:2623:PRO:HB3	1:B:2666:PRO:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3688:MET:HE3	1:B:3752:PRO:HB2	1.95	0.48
1:C:885:LEU:HD21	1:C:956:HIS:HB2	1.96	0.48
1:C:902:TRP:HA	1:C:913:ARG:HB3	1.96	0.48
1:C:2391:TYR:O	1:C:2395:ILE:HG22	2.13	0.48
1:C:3727:GLN:NE2	1:C:3764:ILE:O	2.32	0.48
1:C:4078:ASP:N	1:C:4078:ASP:OD1	2.47	0.48
1:D:1017:THR:HA	1:D:1025:LYS:HD3	1.95	0.48
1:D:2391:TYR:O	1:D:2395:ILE:HG22	2.13	0.48
2:G:31:LEU:N	2:G:35:LYS:O	2.44	0.48
1:A:482:LEU:HG	1:A:486:GLN:NE2	2.29	0.47
1:A:885:LEU:HD21	1:A:956:HIS:HB2	1.96	0.47
1:A:1505:GLY:O	1:A:1524:ASN:ND2	2.47	0.47
1:A:4660:TYR:HB3	1:A:4664:ARG:HH12	1.79	0.47
1:B:1022:GLN:HG3	1:B:1024:VAL:HG13	1.94	0.47
1:B:3728:ALA:HA	1:B:3731:HIS:CD2	2.49	0.47
1:C:533:LEU:HA	1:C:536:LEU:HB3	1.96	0.47
1:C:2828:SER:OG	1:C:2889:GLN:OE1	2.30	0.47
1:D:803:LEU:HD11	1:D:811:PHE:HA	1.96	0.47
1:D:4136:GLU:OE2	1:D:4146:ARG:NH1	2.47	0.47
1:D:4518:TYR:OH	1:D:4735:ASN:ND2	2.46	0.47
1:B:69:LEU:HD23	1:B:69:LEU:H	1.78	0.47
1:C:548:CYS:HB2	1:C:579:LEU:HD23	1.94	0.47
1:C:4084:LYS:HE2	1:C:4085:ARG:HG2	1.96	0.47
1:C:4788:PHE:HB3	1:C:4791:PHE:HD2	1.79	0.47
1:D:482:LEU:HG	1:D:486:GLN:NE2	2.29	0.47
1:D:2876:LEU:HD22	1:D:2880:GLU:HG3	1.95	0.47
1:D:4056:HIS:O	1:D:4062:THR:OG1	2.29	0.47
1:C:2795:ASP:OD1	1:C:2795:ASP:N	2.47	0.47
1:D:1505:GLY:O	1:D:1524:ASN:ND2	2.47	0.47
1:A:433:LEU:O	1:A:437:SER:N	2.48	0.47
1:A:619:VAL:HG23	1:A:624:ALA:HB3	1.95	0.47
1:A:2391:TYR:O	1:A:2395:ILE:HG22	2.13	0.47
1:A:4890:CYS:SG	1:A:4912:HIS:CE1	3.08	0.47
1:B:2795:ASP:OD1	1:B:2795:ASP:N	2.47	0.47
1:C:3688:MET:HE3	1:C:3752:PRO:HB2	1.95	0.47
1:C:4660:TYR:HB3	1:C:4664:ARG:HH12	1.79	0.47
1:D:902:TRP:HA	1:D:913:ARG:HB3	1.96	0.47
1:D:951:GLY:O	1:D:953:ALA:N	2.44	0.47
1:D:4092:ASP:OD1	1:D:4092:ASP:N	2.47	0.47
1:A:3728:ALA:HA	1:A:3731:HIS:CD2	2.49	0.47
1:D:885:LEU:HD21	1:D:956:HIS:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4084:LYS:HE2	1:D:4085:ARG:HG2	1.96	0.47
1:A:926:GLU:OE2	1:A:930:ASN:ND2	2.40	0.47
1:A:3954:GLN:O	1:A:3958:SER:OG	2.27	0.47
1:A:4788:PHE:HB3	1:A:4791:PHE:HD2	1.79	0.47
1:B:2391:TYR:O	1:B:2395:ILE:HG22	2.13	0.47
1:B:3727:GLN:NE2	1:B:3764:ILE:O	2.32	0.47
1:B:4084:LYS:HE2	1:B:4085:ARG:HG2	1.96	0.47
1:B:4890:CYS:SG	1:B:4912:HIS:CE1	3.08	0.47
1:C:482:LEU:HG	1:C:486:GLN:NE2	2.29	0.47
1:A:803:LEU:HD11	1:A:811:PHE:HA	1.96	0.47
1:A:1511:VAL:HG23	1:A:1519:LEU:HD12	1.95	0.47
1:A:1935:LEU:HD13	1:A:2024:ILE:HD13	1.97	0.47
1:B:482:LEU:HG	1:B:486:GLN:NE2	2.29	0.47
1:B:533:LEU:HA	1:B:536:LEU:HB3	1.96	0.47
1:B:885:LEU:HD21	1:B:956:HIS:HB2	1.96	0.47
1:B:2204:ARG:O	1:B:2206:SER:N	2.42	0.47
1:B:4043:SER:O	1:B:4045:ARG:N	2.48	0.47
1:B:4092:ASP:OD1	1:B:4092:ASP:N	2.47	0.47
1:C:474:ASP:OD2	1:C:478:ARG:NH2	2.48	0.47
1:C:3047:THR:HA	1:C:3051:SER:HB3	1.97	0.47
1:C:3728:ALA:HA	1:C:3731:HIS:CD2	2.49	0.47
1:D:474:ASP:OD2	1:D:478:ARG:NH2	2.48	0.47
1:D:4660:TYR:HB3	1:D:4664:ARG:HH12	1.79	0.47
1:A:533:LEU:HA	1:A:536:LEU:HB3	1.96	0.47
1:B:474:ASP:OD2	1:B:478:ARG:NH2	2.48	0.47
1:B:1129:GLY:HA3	1:B:1145:TRP:HB3	1.96	0.47
1:C:4092:ASP:N	1:C:4092:ASP:OD1	2.47	0.47
1:D:57:ASN:ND2	1:D:322:ALA:O	2.48	0.47
1:A:3727:GLN:NE2	1:A:3764:ILE:O	2.32	0.47
1:B:803:LEU:HD11	1:B:811:PHE:HA	1.96	0.47
1:B:1935:LEU:HD13	1:B:2024:ILE:HD13	1.97	0.47
1:B:4788:PHE:HB3	1:B:4791:PHE:HD2	1.79	0.47
1:C:57:ASN:ND2	1:C:322:ALA:O	2.48	0.47
1:C:1129:GLY:HA3	1:C:1145:TRP:HB3	1.96	0.47
1:C:2471:LEU:O	1:C:2476:GLY:N	2.43	0.47
1:C:4890:CYS:SG	1:C:4912:HIS:CE1	3.08	0.47
1:D:146:ASP:OD1	1:D:146:ASP:N	2.43	0.47
1:D:1129:GLY:HA3	1:D:1145:TRP:HB3	1.96	0.47
1:D:3728:ALA:HA	1:D:3731:HIS:CD2	2.49	0.47
1:A:474:ASP:OD2	1:A:478:ARG:NH2	2.48	0.47
1:C:619:VAL:HG23	1:C:624:ALA:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:ASN:ND2	1:A:322:ALA:O	2.48	0.46
1:A:4653:MET:HA	1:A:4665:ILE:HG21	1.97	0.46
1:B:669:GLN:HB3	1:B:1020:ILE:HG13	1.97	0.46
1:B:1511:VAL:HG23	1:B:1519:LEU:HD12	1.95	0.46
1:D:419:ILE:HG21	1:D:488:LEU:HB3	1.96	0.46
1:D:669:GLN:HB3	1:D:1020:ILE:HG13	1.97	0.46
1:B:728:ASP:OD1	1:B:728:ASP:N	2.44	0.46
1:B:2828:SER:OG	1:B:2889:GLN:OE1	2.30	0.46
1:D:246:THR:N	1:D:261:HIS:O	2.44	0.46
1:D:533:LEU:HA	1:D:536:LEU:HB3	1.96	0.46
1:D:555:LEU:HA	1:D:558:LEU:HD12	1.98	0.46
1:D:1935:LEU:HD13	1:D:2024:ILE:HD13	1.97	0.46
1:D:3047:THR:HA	1:D:3051:SER:HB3	1.97	0.46
1:A:234:LEU:HA	1:A:408:SER:HB3	1.98	0.46
1:B:234:LEU:HA	1:B:408:SER:HB3	1.98	0.46
1:B:2012:GLU:O	1:B:2016:LEU:N	2.41	0.46
1:B:4653:MET:HA	1:B:4665:ILE:HG21	1.98	0.46
1:A:1129:GLY:HA3	1:A:1145:TRP:HB3	1.96	0.46
1:A:4078:ASP:OD1	1:A:4078:ASP:N	2.47	0.46
1:C:1089:ARG:O	1:C:1250:TRP:N	2.48	0.46
1:C:1246:ASP:OD1	1:C:1694:TYR:OH	2.30	0.46
1:D:2795:ASP:N	1:D:2795:ASP:OD1	2.47	0.46
1:D:4890:CYS:SG	1:D:4912:HIS:CE1	3.08	0.46
1:A:419:ILE:HG21	1:A:488:LEU:HB3	1.96	0.46
1:A:4043:SER:O	1:A:4045:ARG:N	2.48	0.46
1:C:555:LEU:HA	1:C:558:LEU:HD12	1.98	0.46
1:C:2509:THR:HA	1:C:2513:LEU:HD11	1.98	0.46
1:A:960:LYS:HG3	1:A:961:VAL:HG23	1.98	0.46
1:A:2795:ASP:OD1	1:A:2795:ASP:N	2.47	0.46
1:B:226:GLY:O	1:B:355:LYS:NZ	2.44	0.46
1:B:801:ARG:NH2	1:B:802:PHE:O	2.45	0.46
1:D:4653:MET:HA	1:D:4665:ILE:HG21	1.97	0.46
1:A:2324:ILE:HD13	1:D:207:PHE:CD2	2.51	0.46
1:B:657:PRO:HD2	1:B:791:VAL:HG12	1.98	0.46
1:B:719:GLY:O	1:B:724:SER:OG	2.34	0.46
1:B:2065:MET:HE1	1:B:2086:LEU:HD23	1.97	0.46
1:C:4043:SER:O	1:C:4045:ARG:N	2.48	0.46
1:D:657:PRO:HD2	1:D:791:VAL:HG12	1.98	0.46
2:H:78:THR:HG23	2:H:80:ASP:HB3	1.98	0.46
1:A:494:MET:HG2	1:A:497:LEU:H	1.81	0.46
1:A:657:PRO:HD2	1:A:791:VAL:HG12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:419:ILE:HG21	1:B:488:LEU:HB3	1.96	0.46
1:B:894:VAL:O	1:B:898:ILE:N	2.47	0.46
1:C:2191:MET:SD	1:C:2191:MET:N	2.89	0.46
1:D:426:PHE:O	1:D:430:ILE:HG12	2.16	0.46
1:D:4566:TYR:O	1:D:4570:THR:OG1	2.26	0.46
2:E:78:THR:HG23	2:E:80:ASP:HB3	1.98	0.46
1:A:3047:THR:HA	1:A:3051:SER:HB3	1.97	0.46
1:C:657:PRO:HD2	1:C:791:VAL:HG12	1.98	0.46
1:C:669:GLN:HB3	1:C:1020:ILE:HG13	1.97	0.46
1:C:1935:LEU:HD13	1:C:2024:ILE:HD13	1.97	0.46
1:D:960:LYS:HG3	1:D:961:VAL:HG23	1.98	0.46
1:A:555:LEU:HA	1:A:558:LEU:HD12	1.98	0.45
1:A:4106:GLU:OE1	1:A:4148:TYR:OH	2.24	0.45
1:B:2509:THR:HA	1:B:2513:LEU:HD11	1.98	0.45
1:B:3808:GLU:HA	1:B:3811:ASN:HD21	1.81	0.45
1:C:419:ILE:HG21	1:C:488:LEU:HB3	1.96	0.45
1:C:2395:ILE:HD13	1:C:2467:MET:HE2	1.97	0.45
1:C:2490:GLY:O	1:C:2494:ASP:N	2.39	0.45
1:C:3808:GLU:HA	1:C:3811:ASN:HD21	1.81	0.45
1:C:3843:GLN:HB2	1:C:3918:THR:HA	1.98	0.45
1:D:902:TRP:HE3	1:D:913:ARG:HG2	1.82	0.45
1:A:426:PHE:O	1:A:430:ILE:HG12	2.16	0.45
1:A:669:GLN:HB3	1:A:1020:ILE:HG13	1.97	0.45
1:A:801:ARG:NH2	1:A:802:PHE:O	2.45	0.45
1:A:1103:PHE:O	1:A:1164:CYS:N	2.49	0.45
1:B:233:VAL:HG12	1:B:274:LEU:HD22	1.99	0.45
1:C:426:PHE:O	1:C:430:ILE:HG12	2.16	0.45
1:D:1108:VAL:HG21	1:D:1214:ARG:HH21	1.82	0.45
1:D:2191:MET:SD	1:D:2191:MET:N	2.89	0.45
1:D:2395:ILE:HD13	1:D:2467:MET:HE2	1.97	0.45
1:D:3808:GLU:HA	1:D:3811:ASN:HD21	1.81	0.45
1:A:1108:VAL:HG21	1:A:1214:ARG:HH21	1.82	0.45
1:A:4092:ASP:OD1	1:A:4092:ASP:N	2.47	0.45
1:B:433:LEU:O	1:B:437:SER:N	2.47	0.45
1:B:2191:MET:SD	1:B:2191:MET:N	2.89	0.45
1:B:3047:THR:HA	1:B:3051:SER:HB3	1.97	0.45
1:C:246:THR:N	1:C:261:HIS:O	2.44	0.45
1:C:494:MET:HG2	1:C:497:LEU:HD22	1.99	0.45
1:C:1103:PHE:O	1:C:1164:CYS:N	2.49	0.45
1:C:4056:HIS:O	1:C:4062:THR:OG1	2.29	0.45
1:D:1089:ARG:HH21	1:D:1601:PRO:HB3	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:LEU:HA	1:C:408:SER:HB3	1.98	0.45
1:C:4653:MET:HA	1:C:4665:ILE:HG21	1.97	0.45
1:D:234:LEU:HA	1:D:408:SER:HB3	1.98	0.45
1:D:494:MET:HG2	1:D:497:LEU:H	1.81	0.45
1:A:1089:ARG:HH21	1:A:1601:PRO:HB3	1.82	0.45
1:A:3808:GLU:HA	1:A:3811:ASN:HD21	1.81	0.45
1:D:347:ASP:N	1:D:347:ASP:OD1	2.50	0.45
1:D:2264:VAL:HG21	1:D:2300:PHE:HE2	1.81	0.45
1:D:3941:ASP:OD1	1:D:3941:ASP:N	2.50	0.45
1:A:347:ASP:N	1:A:347:ASP:OD1	2.50	0.45
1:A:2263:LYS:O	1:A:2267:TYR:HD2	2.00	0.45
1:B:494:MET:HG2	1:B:497:LEU:HD22	1.99	0.45
1:B:555:LEU:HA	1:B:558:LEU:HD12	1.98	0.45
1:B:619:VAL:HA	1:B:624:ALA:HB3	1.99	0.45
1:B:2286:ASP:OD1	1:B:2286:ASP:N	2.48	0.45
1:C:207:PHE:CD2	1:D:2324:ILE:HD13	2.51	0.45
1:C:960:LYS:HG3	1:C:961:VAL:HG23	1.98	0.45
1:C:1108:VAL:HG21	1:C:1214:ARG:HH21	1.82	0.45
1:C:1302:TYR:HB2	1:C:1544:VAL:O	2.17	0.45
1:A:3858:ARG:NH1	1:A:3930:ASN:OD1	2.47	0.45
1:A:4056:HIS:O	1:A:4062:THR:OG1	2.29	0.45
1:A:4154:SER:HA	1:A:4157:THR:HG22	1.99	0.45
1:B:960:LYS:HG3	1:B:961:VAL:HG23	1.98	0.45
1:B:1623:LEU:HD23	1:B:1623:LEU:HA	1.86	0.45
1:B:2263:LYS:O	1:B:2267:TYR:HD2	2.00	0.45
1:B:3355:LEU:HB3	1:B:3358:PHE:HB2	1.99	0.45
1:C:902:TRP:HE3	1:C:913:ARG:HG2	1.82	0.45
1:C:2263:LYS:O	1:C:2267:TYR:HD2	2.00	0.45
1:D:226:GLY:O	1:D:355:LYS:NZ	2.44	0.45
1:D:494:MET:HG2	1:D:497:LEU:HD22	1.99	0.45
1:D:4043:SER:O	1:D:4045:ARG:N	2.48	0.45
1:B:1108:VAL:HG21	1:B:1214:ARG:HH21	1.82	0.45
1:B:1462:VAL:HG12	1:B:1463:ARG:H	1.82	0.45
1:B:1695:MET:HG3	1:B:1696:PRO:HD2	1.99	0.45
1:B:1901:VAL:O	1:B:1905:MET:HG2	2.17	0.45
1:B:2508:ALA:HB2	1:B:2595:VAL:HG21	1.99	0.45
1:B:2876:LEU:HB3	1:B:2880:GLU:HG3	1.99	0.45
1:B:3941:ASP:OD1	1:B:3941:ASP:N	2.50	0.45
1:C:233:VAL:HG12	1:C:274:LEU:HD22	1.99	0.45
1:C:494:MET:HG2	1:C:497:LEU:H	1.81	0.45
1:C:619:VAL:HA	1:C:624:ALA:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2490:GLY:O	1:D:2494:ASP:N	2.39	0.45
1:D:3843:GLN:HB2	1:D:3918:THR:HA	1.98	0.45
1:A:161:THR:OG1	1:A:184:VAL:O	2.32	0.45
1:A:902:TRP:HE3	1:A:913:ARG:HG2	1.82	0.45
1:A:2508:ALA:HB2	1:A:2595:VAL:HG21	1.99	0.45
1:A:3843:GLN:HB2	1:A:3918:THR:HA	1.98	0.45
1:B:2716:LEU:HD21	1:B:2771:ARG:HH22	1.82	0.45
1:B:3888:TYR:OH	1:B:3952:HIS:HB3	2.17	0.45
1:B:4908:THR:O	1:B:4913:ASN:ND2	2.49	0.45
1:C:1695:MET:HG3	1:C:1696:PRO:HD2	1.99	0.45
1:C:2508:ALA:HB2	1:C:2595:VAL:HG21	1.99	0.45
1:C:3941:ASP:N	1:C:3941:ASP:OD1	2.50	0.45
1:D:261:HIS:ND1	1:D:388:GLN:OE1	2.44	0.45
1:D:617:LEU:HG	1:D:632:ILE:HG21	1.99	0.45
1:D:936:SER:O	1:D:940:LEU:HD13	2.17	0.45
1:D:1089:ARG:O	1:D:1250:TRP:N	2.48	0.45
1:D:1302:TYR:HB2	1:D:1544:VAL:O	2.17	0.45
1:D:3858:ARG:NH1	1:D:3930:ASN:OD1	2.47	0.45
1:A:1089:ARG:O	1:A:1250:TRP:N	2.48	0.45
1:A:2320:VAL:O	1:A:2324:ILE:HG13	2.17	0.45
1:A:2716:LEU:HD21	1:A:2771:ARG:HH22	1.82	0.45
1:B:57:ASN:ND2	1:B:322:ALA:O	2.48	0.45
1:B:141:ASP:N	1:B:141:ASP:OD1	2.50	0.45
1:B:1089:ARG:O	1:B:1250:TRP:N	2.48	0.45
1:B:1783:PHE:HE2	1:B:1788:LEU:HD22	1.82	0.45
1:B:2264:VAL:HG21	1:B:2300:PHE:HE2	1.81	0.45
1:B:2320:VAL:O	1:B:2324:ILE:HG13	2.17	0.45
1:B:2331:GLY:H	1:B:2339:GLY:HA2	1.82	0.45
1:B:4154:SER:HA	1:B:4157:THR:HG22	1.99	0.45
1:C:753:ASP:OD1	1:C:753:ASP:N	2.50	0.45
1:C:2228:LEU:HG	1:C:2230:SER:H	1.82	0.45
1:C:2264:VAL:HG21	1:C:2300:PHE:HE2	1.81	0.45
1:C:2716:LEU:HD21	1:C:2771:ARG:HH22	1.82	0.45
1:C:2876:LEU:HB3	1:C:2880:GLU:HG3	1.99	0.45
1:D:619:VAL:HA	1:D:624:ALA:HB3	1.99	0.45
1:D:2263:LYS:O	1:D:2267:TYR:HD2	2.00	0.45
1:A:2331:GLY:H	1:A:2339:GLY:HA2	1.82	0.44
1:A:3857:LEU:HD21	1:A:3869:ILE:HB	2.00	0.44
1:B:73:LEU:O	1:B:118:ALA:N	2.50	0.44
1:B:246:THR:N	1:B:261:HIS:O	2.44	0.44
1:B:4844:ILE:O	1:B:4848:THR:OG1	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:936:SER:O	1:C:940:LEU:HD13	2.17	0.44
1:C:1783:PHE:HE2	1:C:1788:LEU:HD22	1.82	0.44
1:C:1901:VAL:O	1:C:1905:MET:HG2	2.17	0.44
1:D:2228:LEU:HG	1:D:2230:SER:H	1.82	0.44
1:D:3857:LEU:HD21	1:D:3869:ILE:HB	2.00	0.44
1:A:494:MET:HG2	1:A:497:LEU:HD22	1.99	0.44
1:B:753:ASP:OD1	1:B:753:ASP:N	2.50	0.44
1:B:936:SER:O	1:B:940:LEU:HD13	2.17	0.44
1:B:1691:GLU:OE1	1:B:1791:LYS:NZ	2.36	0.44
1:B:4808:MET:HG2	1:C:4516:LEU:HA	1.99	0.44
1:C:1089:ARG:HH21	1:C:1601:PRO:HB3	1.82	0.44
1:C:2461:PRO:HG2	1:C:2514:ALA:HB3	1.99	0.44
1:C:3355:LEU:HB3	1:C:3358:PHE:HB2	1.99	0.44
1:C:4176:VAL:HG13	1:C:4879:VAL:HG22	2.00	0.44
1:D:1901:VAL:O	1:D:1905:MET:HG2	2.17	0.44
1:D:2509:THR:HA	1:D:2513:LEU:HD11	1.98	0.44
1:A:1901:VAL:O	1:A:1905:MET:HG2	2.17	0.44
1:A:2228:LEU:HG	1:A:2230:SER:H	1.82	0.44
1:A:2264:VAL:HG21	1:A:2300:PHE:HE2	1.81	0.44
1:B:494:MET:HG2	1:B:497:LEU:H	1.81	0.44
1:B:1924:ILE:HD11	1:B:2035:VAL:HG21	2.00	0.44
1:D:4176:VAL:HG13	1:D:4879:VAL:HG22	2.00	0.44
2:F:78:THR:HG23	2:F:80:ASP:HB3	1.98	0.44
1:A:617:LEU:HG	1:A:632:ILE:HG21	1.99	0.44
1:A:619:VAL:HA	1:A:624:ALA:HB3	1.99	0.44
1:A:2191:MET:SD	1:A:2191:MET:N	2.89	0.44
1:B:1822:LEU:HD23	1:B:1822:LEU:HA	1.84	0.44
1:B:3843:GLN:HB2	1:B:3918:THR:HA	1.98	0.44
1:C:617:LEU:HG	1:C:632:ILE:HG21	1.99	0.44
1:C:719:GLY:O	1:C:724:SER:OG	2.34	0.44
1:D:2320:VAL:O	1:D:2324:ILE:HG13	2.17	0.44
1:A:1783:PHE:HE2	1:A:1788:LEU:HD22	1.82	0.44
1:A:1924:ILE:HD11	1:A:2035:VAL:HG21	2.00	0.44
1:A:2509:THR:HA	1:A:2513:LEU:HD11	1.98	0.44
1:A:2876:LEU:HB3	1:A:2880:GLU:HG3	1.99	0.44
1:A:4176:VAL:HG13	1:A:4879:VAL:HG22	1.99	0.44
1:A:4182:LYS:HE2	1:B:4901:PRO:HB3	1.99	0.44
1:B:4176:VAL:HG13	1:B:4879:VAL:HG22	1.99	0.44
1:C:4768:LEU:HB3	1:D:4752:LEU:HD21	2.00	0.44
2:G:78:THR:HG23	2:G:80:ASP:HB3	1.98	0.44
1:A:936:SER:O	1:A:940:LEU:HD13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:HIS:ND1	1:B:388:GLN:OE1	2.44	0.44
1:B:1172:THR:HG22	1:B:1193:LYS:HG2	2.00	0.44
1:B:1302:TYR:HB2	1:B:1544:VAL:O	2.17	0.44
1:D:233:VAL:HG12	1:D:274:LEU:HD22	1.99	0.44
1:D:1177:LEU:N	1:D:1180:GLU:O	2.51	0.44
1:D:3355:LEU:HB3	1:D:3358:PHE:HB2	1.99	0.44
1:A:233:VAL:HG12	1:A:274:LEU:HD22	1.99	0.44
1:A:894:VAL:O	1:A:898:ILE:N	2.47	0.44
1:A:1177:LEU:N	1:A:1180:GLU:O	2.51	0.44
1:A:1302:TYR:HB2	1:A:1544:VAL:O	2.17	0.44
1:A:1462:VAL:HG12	1:A:1463:ARG:H	1.82	0.44
1:A:1467:VAL:O	1:A:1480:ILE:N	2.39	0.44
1:A:2152:LYS:HA	1:A:2155:TYR:CZ	2.53	0.44
1:A:3941:ASP:N	1:A:3941:ASP:OD1	2.50	0.44
1:B:426:PHE:O	1:B:430:ILE:HG12	2.16	0.44
1:C:1172:THR:HG22	1:C:1193:LYS:HG2	2.00	0.44
1:C:3857:LEU:HD21	1:C:3869:ILE:HB	2.00	0.44
1:D:1783:PHE:HE2	1:D:1788:LEU:HD22	1.82	0.44
1:D:4154:SER:HA	1:D:4157:THR:HG22	1.99	0.44
1:A:719:GLY:O	1:A:724:SER:OG	2.34	0.44
1:A:951:GLY:O	1:A:953:ALA:N	2.44	0.44
1:A:1695:MET:HG3	1:A:1696:PRO:HD2	1.99	0.44
1:A:4908:THR:O	1:A:4913:ASN:ND2	2.49	0.44
1:B:18:ASP:HB2	1:B:69:LEU:HD21	2.00	0.44
1:B:2228:LEU:HG	1:B:2230:SER:H	1.82	0.44
1:B:4663:ASP:O	1:B:4667:GLU:HG2	2.18	0.44
1:C:161:THR:OG1	1:C:184:VAL:O	2.32	0.44
1:C:433:LEU:O	1:C:437:SER:N	2.47	0.44
1:C:2034:LYS:HA	1:C:2037:TYR:CE2	2.53	0.44
1:C:2320:VAL:O	1:C:2324:ILE:HG13	2.17	0.44
1:C:4154:SER:HA	1:C:4157:THR:HG22	1.99	0.44
1:D:18:ASP:HB2	1:D:69:LEU:HD21	2.00	0.44
1:D:1927:PHE:CD2	1:D:2031:LEU:HD22	2.53	0.44
1:D:2508:ALA:HB2	1:D:2595:VAL:HG21	1.99	0.44
1:A:141:ASP:OD1	1:A:141:ASP:N	2.50	0.44
1:A:1927:PHE:CD2	1:A:2031:LEU:HD22	2.53	0.44
1:B:68:VAL:HG23	1:B:124:SER:HB3	2.00	0.44
1:B:1089:ARG:HH21	1:B:1601:PRO:HB3	1.82	0.44
1:C:347:ASP:OD1	1:C:347:ASP:N	2.50	0.44
1:C:894:VAL:O	1:C:898:ILE:N	2.47	0.44
1:C:3046:LYS:HD3	1:C:3093:ILE:HD13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:73:LEU:O	1:D:118:ALA:N	2.50	0.44
1:D:2716:LEU:HD21	1:D:2771:ARG:HH22	1.82	0.44
1:D:2876:LEU:HB3	1:D:2880:GLU:HG3	1.99	0.44
1:A:949:HIS:NE2	1:A:951:GLY:O	2.51	0.43
1:A:2404:GLU:HB3	1:A:2407:LEU:HB2	2.00	0.43
1:B:347:ASP:OD1	1:B:347:ASP:N	2.50	0.43
1:B:1177:LEU:N	1:B:1180:GLU:O	2.51	0.43
1:B:2511:MET:HB3	1:B:2515:LEU:HD12	2.00	0.43
1:B:3857:LEU:HD21	1:B:3869:ILE:HB	2.00	0.43
1:B:3858:ARG:NH1	1:B:3930:ASN:OD1	2.47	0.43
1:C:1251:LEU:N	1:C:1602:ASN:O	2.47	0.43
1:C:1462:VAL:HG12	1:C:1463:ARG:H	1.82	0.43
1:C:3888:TYR:OH	1:C:3952:HIS:HB3	2.17	0.43
1:D:949:HIS:NE2	1:D:951:GLY:O	2.51	0.43
1:D:2012:GLU:O	1:D:2016:LEU:N	2.41	0.43
1:D:2331:GLY:H	1:D:2339:GLY:HA2	1.82	0.43
1:D:3888:TYR:OH	1:D:3952:HIS:HB3	2.17	0.43
1:D:4663:ASP:O	1:D:4667:GLU:HG2	2.18	0.43
1:A:1784:PRO:HB2	1:A:1787:ILE:HG22	1.99	0.43
1:A:3888:TYR:OH	1:A:3952:HIS:HB3	2.17	0.43
1:A:3930:ASN:O	1:A:3934:LEU:HD12	2.18	0.43
1:B:2313:GLU:OE2	1:B:2317:ASN:ND2	2.48	0.43
1:B:3046:LYS:HD3	1:B:3093:ILE:HD13	2.00	0.43
1:C:248:PRO:HD3	1:C:261:HIS:HD2	1.83	0.43
1:C:949:HIS:NE2	1:C:951:GLY:O	2.51	0.43
1:C:1177:LEU:N	1:C:1180:GLU:O	2.50	0.43
1:C:1927:PHE:CD2	1:C:2031:LEU:HD22	2.53	0.43
1:D:658:ASN:HB2	1:D:835:GLU:N	2.33	0.43
1:D:1695:MET:HG3	1:D:1696:PRO:HD2	1.99	0.43
1:D:2404:GLU:HB3	1:D:2407:LEU:HB2	2.01	0.43
1:D:2511:MET:HB3	1:D:2515:LEU:HD12	2.00	0.43
1:A:19:GLU:O	1:A:217:ILE:HG22	2.18	0.43
1:B:528:SER:O	1:B:532:SER:OG	2.25	0.43
1:B:902:TRP:HE3	1:B:913:ARG:HG2	1.82	0.43
1:B:1927:PHE:CD2	1:B:2031:LEU:HD22	2.53	0.43
1:C:658:ASN:HB2	1:C:835:GLU:N	2.33	0.43
1:C:1307:PRO:HG2	1:C:1308:ILE:HD12	2.01	0.43
1:D:128:MET:HB2	1:D:149:LEU:HD23	2.00	0.43
1:D:1462:VAL:HG12	1:D:1463:ARG:H	1.82	0.43
1:D:1784:PRO:HB2	1:D:1787:ILE:HG22	1.99	0.43
1:A:3000:LYS:HD2	1:A:3066:ASP:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4663:ASP:O	1:A:4667:GLU:HG2	2.18	0.43
1:B:248:PRO:HD3	1:B:261:HIS:HD2	1.83	0.43
1:B:617:LEU:HG	1:B:632:ILE:HG21	1.99	0.43
1:B:1251:LEU:N	1:B:1602:ASN:O	2.47	0.43
1:B:1784:PRO:HB2	1:B:1787:ILE:HG22	1.99	0.43
1:B:2152:LYS:HA	1:B:2155:TYR:CZ	2.53	0.43
1:C:68:VAL:HG23	1:C:124:SER:HB3	2.00	0.43
1:C:1784:PRO:HB2	1:C:1787:ILE:HG22	1.99	0.43
1:D:1769:PHE:HE1	2:H:91:VAL:HG21	1.84	0.43
1:A:18:ASP:HB2	1:A:69:LEU:HD21	2.00	0.43
1:A:658:ASN:HB2	1:A:835:GLU:N	2.33	0.43
1:B:64:ILE:H	1:B:64:ILE:HG12	1.63	0.43
1:C:1261:VAL:HA	1:C:1262:PRO:HD3	1.91	0.43
1:C:4807:ASP:OD1	1:C:4807:ASP:N	2.41	0.43
1:D:115:TYR:CZ	1:D:175:VAL:HG22	2.54	0.43
1:D:753:ASP:OD1	1:D:753:ASP:N	2.50	0.43
1:D:1172:THR:HG22	1:D:1193:LYS:HG2	2.00	0.43
1:D:2152:LYS:HA	1:D:2155:TYR:CZ	2.53	0.43
1:D:3000:LYS:HD2	1:D:3066:ASP:HB3	2.01	0.43
2:F:77:CYS:N	2:F:98:LEU:O	2.49	0.43
1:A:185:SER:OG	1:A:186:VAL:N	2.50	0.43
1:A:1172:THR:HG22	1:A:1193:LYS:HG2	2.00	0.43
1:A:2461:PRO:HG2	1:A:2514:ALA:HB3	2.00	0.43
1:A:2643:LEU:O	1:A:2647:ILE:HG12	2.18	0.43
1:A:4752:LEU:HD21	1:D:4768:LEU:HB3	2.01	0.43
1:A:4807:ASP:OD1	1:A:4807:ASP:N	2.41	0.43
1:B:949:HIS:NE2	1:B:951:GLY:O	2.51	0.43
1:B:1832:MET:HB3	1:B:1834:ILE:HG12	2.01	0.43
1:B:4106:GLU:OE1	1:B:4148:TYR:OH	2.24	0.43
1:C:18:ASP:HB2	1:C:69:LEU:HD21	2.00	0.43
1:C:128:MET:HB2	1:C:149:LEU:HD23	2.00	0.43
1:C:1924:ILE:HD11	1:C:2035:VAL:HG21	2.00	0.43
1:C:3930:ASN:O	1:C:3934:LEU:HD12	2.18	0.43
1:C:4182:LYS:HE2	1:D:4901:PRO:HB3	2.01	0.43
1:D:1251:LEU:N	1:D:1602:ASN:O	2.47	0.43
1:D:2643:LEU:O	1:D:2647:ILE:HG12	2.18	0.43
1:D:3930:ASN:O	1:D:3934:LEU:HD12	2.18	0.43
1:A:73:LEU:O	1:A:118:ALA:N	2.50	0.43
1:A:1832:MET:HB3	1:A:1834:ILE:HG12	2.01	0.43
1:B:19:GLU:O	1:B:217:ILE:HG22	2.18	0.43
1:B:2461:PRO:HG2	1:B:2514:ALA:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:699:SER:OG	1:D:789:PHE:O	2.30	0.43
1:A:115:TYR:CZ	1:A:175:VAL:HG22	2.54	0.43
1:B:128:MET:HB2	1:B:149:LEU:HD23	2.00	0.43
1:B:1307:PRO:HG2	1:B:1308:ILE:HD12	2.01	0.43
1:B:2034:LYS:HA	1:B:2037:TYR:CE2	2.53	0.43
1:B:3930:ASN:O	1:B:3934:LEU:HD12	2.18	0.43
1:B:4749:PHE:HB2	1:B:4752:LEU:HD23	2.01	0.43
1:C:1117:TRP:CD1	1:C:1135:PHE:HB2	2.54	0.43
1:C:1795:MET:HE2	1:C:1822:LEU:HD21	2.00	0.43
1:D:719:GLY:O	1:D:724:SER:OG	2.34	0.43
1:D:1924:ILE:HD11	1:D:2035:VAL:HG21	2.00	0.43
1:D:2034:LYS:HA	1:D:2037:TYR:CE2	2.53	0.43
1:A:4799:ASP:OD1	1:A:4799:ASP:N	2.52	0.43
1:C:73:LEU:O	1:C:118:ALA:N	2.50	0.43
1:C:1769:PHE:HE1	2:G:91:VAL:HG21	1.84	0.43
1:C:2331:GLY:H	1:C:2339:GLY:HA2	1.82	0.43
1:C:4799:ASP:OD1	1:C:4799:ASP:N	2.52	0.43
1:D:4799:ASP:N	1:D:4799:ASP:OD1	2.52	0.43
1:B:1117:TRP:CD1	1:B:1135:PHE:HB2	2.54	0.43
1:B:1769:PHE:HE1	2:F:91:VAL:HG21	1.84	0.43
1:B:2450:VAL:HG23	1:B:2451:VAL:HG22	2.01	0.43
1:C:19:GLU:O	1:C:217:ILE:HG22	2.18	0.43
1:C:2152:LYS:HA	1:C:2155:TYR:CZ	2.53	0.43
1:C:2643:LEU:O	1:C:2647:ILE:HG12	2.18	0.43
1:C:4663:ASP:O	1:C:4667:GLU:HG2	2.18	0.43
1:D:19:GLU:O	1:D:217:ILE:HG22	2.18	0.43
1:D:370:LEU:HD23	1:D:370:LEU:HA	1.93	0.43
1:A:3355:LEU:HB3	1:A:3358:PHE:HB2	1.99	0.42
1:A:4749:PHE:HB2	1:A:4752:LEU:HD23	2.01	0.42
1:B:430:ILE:HB	1:B:502:ILE:HD11	2.01	0.42
1:B:658:ASN:HB2	1:B:835:GLU:N	2.33	0.42
1:B:2643:LEU:O	1:B:2647:ILE:HG12	2.18	0.42
1:B:3000:LYS:HD2	1:B:3066:ASP:HB3	2.01	0.42
1:B:4768:LEU:HB3	1:C:4752:LEU:HD21	2.01	0.42
1:C:115:TYR:CZ	1:C:175:VAL:HG22	2.54	0.42
1:C:2404:GLU:HB3	1:C:2407:LEU:HB2	2.00	0.42
1:C:2511:MET:HB3	1:C:2515:LEU:HD12	2.00	0.42
1:D:433:LEU:O	1:D:437:SER:N	2.48	0.42
1:D:1117:TRP:CD1	1:D:1135:PHE:HB2	2.54	0.42
1:A:68:VAL:HG23	1:A:124:SER:HB3	2.00	0.42
1:A:2034:LYS:HA	1:A:2037:TYR:CE2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2395:ILE:HD13	1:B:2467:MET:HE2	2.00	0.42
1:C:33:GLN:NE2	1:C:35:LEU:HD11	2.34	0.42
1:D:141:ASP:N	1:D:141:ASP:OD1	2.50	0.42
1:D:248:PRO:HD3	1:D:261:HIS:HD2	1.83	0.42
1:D:1307:PRO:HG2	1:D:1308:ILE:HD12	2.01	0.42
1:D:2334:LEU:O	1:D:2336:GLY:N	2.53	0.42
1:D:3046:LYS:HD3	1:D:3093:ILE:HD13	2.00	0.42
1:A:2204:ARG:O	1:A:2206:SER:N	2.42	0.42
1:A:2604:MET:SD	1:A:2604:MET:N	2.85	0.42
1:A:4180:GLY:O	1:A:4182:LYS:N	2.52	0.42
1:A:4901:PRO:HB3	1:D:4182:LYS:HE2	2.01	0.42
1:B:801:ARG:HA	1:B:1619:LEU:HA	2.01	0.42
1:B:963:LYS:O	1:B:964:MET:HG2	2.19	0.42
1:C:141:ASP:OD1	1:C:141:ASP:N	2.50	0.42
1:C:801:ARG:HA	1:C:1619:LEU:HA	2.01	0.42
1:C:4749:PHE:HB2	1:C:4752:LEU:HD23	2.01	0.42
1:D:4596:LEU:HD12	1:D:4596:LEU:HA	1.89	0.42
1:A:963:LYS:O	1:A:964:MET:HG2	2.19	0.42
1:A:1822:LEU:HD23	1:A:1822:LEU:HA	1.84	0.42
1:B:2404:GLU:HB3	1:B:2407:LEU:HB2	2.00	0.42
1:C:1280:SER:O	1:C:1280:SER:OG	2.37	0.42
1:C:2385:ASN:ND2	1:C:2456:SER:O	2.52	0.42
1:C:3000:LYS:HD2	1:C:3066:ASP:HB3	2.01	0.42
1:A:2450:VAL:HG23	1:A:2451:VAL:HG22	2.01	0.42
1:A:3046:LYS:HD3	1:A:3093:ILE:HD13	2.00	0.42
1:B:1103:PHE:O	1:B:1164:CYS:N	2.49	0.42
1:B:3777:LEU:HD12	1:B:3777:LEU:HA	1.92	0.42
1:C:879:GLU:O	1:C:883:GLU:N	2.51	0.42
1:C:2286:ASP:OD1	1:C:2286:ASP:N	2.48	0.42
1:D:185:SER:OG	1:D:186:VAL:N	2.50	0.42
1:D:2461:PRO:HG2	1:D:2514:ALA:HB3	2.00	0.42
1:A:248:PRO:HD3	1:A:261:HIS:HD2	1.83	0.42
1:A:314:LEU:HD11	1:A:365:HIS:HE1	1.85	0.42
1:A:430:ILE:HB	1:A:502:ILE:HD11	2.02	0.42
1:A:2511:MET:HB3	1:A:2515:LEU:HD12	2.00	0.42
1:B:932:ASN:O	1:B:936:SER:OG	2.32	0.42
1:B:4056:HIS:O	1:B:4062:THR:OG1	2.29	0.42
1:C:963:LYS:O	1:C:964:MET:HG2	2.19	0.42
1:C:2450:VAL:HG23	1:C:2451:VAL:HG22	2.01	0.42
1:A:801:ARG:HA	1:A:1619:LEU:HA	2.01	0.42
1:A:2334:LEU:O	1:A:2336:GLY:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2828:SER:OG	1:A:2889:GLN:OE1	2.30	0.42
1:B:67:PHE:HB3	1:B:121:LEU:HD12	2.02	0.42
1:B:185:SER:OG	1:B:186:VAL:N	2.50	0.42
1:B:314:LEU:HD11	1:B:365:HIS:HE1	1.85	0.42
1:B:483:LYS:HD2	1:B:483:LYS:HA	1.86	0.42
1:B:4799:ASP:N	1:B:4799:ASP:OD1	2.52	0.42
1:C:67:PHE:HB3	1:C:121:LEU:HD12	2.02	0.42
1:D:554:SER:O	1:D:554:SER:OG	2.37	0.42
1:D:2385:ASN:ND2	1:D:2456:SER:O	2.52	0.42
1:D:4756:LEU:HD23	1:D:4756:LEU:HA	1.93	0.42
1:A:495:ILE:O	1:A:499:LEU:N	2.48	0.42
1:A:695:VAL:O	1:A:727:PHE:N	2.48	0.42
1:A:847:THR:O	1:A:847:THR:OG1	2.37	0.42
1:A:1307:PRO:HG2	1:A:1308:ILE:HD12	2.01	0.42
1:A:2385:ASN:ND2	1:A:2456:SER:O	2.53	0.42
1:B:114:LEU:HB2	1:B:117:HIS:HD2	1.85	0.42
1:C:1769:PHE:O	2:G:83:TYR:OH	2.29	0.42
1:D:68:VAL:HG23	1:D:124:SER:HB3	2.00	0.42
1:D:3727:GLN:NE2	1:D:3764:ILE:O	2.32	0.42
1:D:4844:ILE:O	1:D:4848:THR:OG1	2.30	0.42
1:A:128:MET:HB2	1:A:149:LEU:HD23	2.00	0.42
1:A:1117:TRP:CD1	1:A:1135:PHE:HB2	2.54	0.42
1:A:1769:PHE:HE1	2:E:91:VAL:HG21	1.84	0.42
1:B:2385:ASN:ND2	1:B:2456:SER:O	2.53	0.42
1:C:488:LEU:HD12	1:C:488:LEU:HA	1.90	0.42
1:C:2334:LEU:O	1:C:2336:GLY:N	2.52	0.42
1:D:64:ILE:H	1:D:64:ILE:HG12	1.63	0.42
1:A:33:GLN:NE2	1:A:35:LEU:HD11	2.34	0.42
1:A:2197:ARG:O	1:A:2201:TYR:HB2	2.20	0.42
1:C:510:SER:OG	1:C:513:HIS:ND1	2.48	0.42
1:D:300:VAL:HG23	1:D:301:THR:HG23	2.02	0.42
1:D:1832:MET:HB3	1:D:1834:ILE:HG12	2.01	0.42
1:D:4908:THR:O	1:D:4913:ASN:ND2	2.49	0.42
1:A:114:LEU:HB2	1:A:117:HIS:HD2	1.85	0.41
1:A:1269:GLU:H	1:A:1290:PHE:HE2	1.68	0.41
1:B:115:TYR:CZ	1:B:175:VAL:HG22	2.54	0.41
1:B:499:LEU:HA	1:B:502:ILE:HD12	2.02	0.41
1:C:430:ILE:HB	1:C:502:ILE:HD11	2.02	0.41
1:C:499:LEU:HA	1:C:502:ILE:HD12	2.02	0.41
1:C:1832:MET:HB3	1:C:1834:ILE:HG12	2.01	0.41
1:C:3792:LEU:HD23	1:C:3792:LEU:HA	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3795:LEU:HD22	1:C:3834:PHE:HZ	1.85	0.41
1:D:63:SER:HB3	1:D:276:ARG:HH12	1.85	0.41
1:D:234:LEU:HD12	1:D:234:LEU:HA	1.94	0.41
1:D:488:LEU:HD12	1:D:488:LEU:HA	1.90	0.41
1:D:963:LYS:O	1:D:964:MET:HG2	2.19	0.41
1:D:1273:ILE:HG13	1:D:1287:GLN:N	2.35	0.41
1:D:1446:ILE:HD11	1:D:1450:PHE:CD2	2.56	0.41
1:D:2197:ARG:O	1:D:2201:TYR:HB2	2.20	0.41
2:F:77:CYS:HB2	2:F:98:LEU:HB2	2.02	0.41
1:A:63:SER:HB3	1:A:276:ARG:HH12	1.85	0.41
1:B:1269:GLU:H	1:B:1290:PHE:HE2	1.68	0.41
1:B:1769:PHE:O	2:F:83:TYR:OH	2.29	0.41
1:C:300:VAL:HG23	1:C:301:THR:HG23	2.02	0.41
1:C:1170:GLU:N	1:C:1170:GLU:OE1	2.53	0.41
1:C:2122:LEU:HD22	1:C:2164:LEU:HD23	2.02	0.41
1:D:297:LEU:HD12	1:D:297:LEU:HA	1.92	0.41
1:D:495:ILE:O	1:D:499:LEU:N	2.48	0.41
1:D:2065:MET:HG3	1:D:2083:MET:HG2	2.03	0.41
1:D:4749:PHE:HB2	1:D:4752:LEU:HD23	2.01	0.41
2:E:77:CYS:HB2	2:E:98:LEU:HB2	2.02	0.41
1:A:2012:GLU:O	1:A:2016:LEU:N	2.41	0.41
1:A:2278:MET:HB3	1:A:2288:GLY:HA2	2.02	0.41
1:B:1170:GLU:N	1:B:1170:GLU:OE1	2.53	0.41
1:B:4182:LYS:HE2	1:C:4901:PRO:HB3	2.02	0.41
1:C:63:SER:HB3	1:C:276:ARG:HH12	1.85	0.41
1:C:2197:ARG:O	1:C:2201:TYR:HB2	2.20	0.41
1:D:33:GLN:NE2	1:D:35:LEU:HD11	2.34	0.41
1:D:430:ILE:HB	1:D:502:ILE:HD11	2.02	0.41
1:D:695:VAL:O	1:D:727:PHE:N	2.48	0.41
1:D:894:VAL:O	1:D:898:ILE:N	2.47	0.41
1:D:1103:PHE:O	1:D:1164:CYS:N	2.49	0.41
1:D:1170:GLU:N	1:D:1170:GLU:OE1	2.53	0.41
1:D:1467:VAL:O	1:D:1480:ILE:N	2.39	0.41
1:D:2836:LEU:HD22	1:D:2895:LEU:HD23	2.02	0.41
1:D:3795:LEU:HD22	1:D:3834:PHE:HZ	1.85	0.41
1:A:67:PHE:HB3	1:A:121:LEU:HD12	2.02	0.41
1:A:1261:VAL:HA	1:A:1262:PRO:HD3	1.91	0.41
1:A:1273:ILE:HG13	1:A:1287:GLN:N	2.35	0.41
1:A:2122:LEU:HD22	1:A:2164:LEU:HD23	2.02	0.41
1:A:4851:PHE:O	1:A:4855:VAL:HB	2.20	0.41
1:B:33:GLN:NE2	1:B:35:LEU:HD11	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:VAL:HG23	1:B:301:THR:HG23	2.02	0.41
1:B:879:GLU:O	1:B:883:GLU:N	2.51	0.41
1:B:2278:MET:HB3	1:B:2288:GLY:HA2	2.02	0.41
1:B:3891:TYR:OH	1:B:3898:ASP:OD1	2.24	0.41
1:C:650:ASN:OD1	1:C:650:ASN:N	2.54	0.41
1:C:1446:ILE:HD11	1:C:1450:PHE:CD2	2.56	0.41
1:D:2122:LEU:HD22	1:D:2164:LEU:HD23	2.02	0.41
1:A:1170:GLU:OE1	1:A:1170:GLU:N	2.53	0.41
1:A:1446:ILE:HD11	1:A:1450:PHE:CD2	2.56	0.41
1:B:63:SER:HB3	1:B:276:ARG:HH12	1.85	0.41
1:B:2334:LEU:O	1:B:2336:GLY:N	2.53	0.41
1:C:1426:TYR:HB2	1:C:1511:VAL:HG12	2.02	0.41
1:D:879:GLU:O	1:D:883:GLU:N	2.51	0.41
1:D:2450:VAL:HG23	1:D:2451:VAL:HG22	2.01	0.41
1:A:499:LEU:HA	1:A:502:ILE:HD12	2.03	0.41
1:A:1223:THR:O	1:A:1225:LYS:NZ	2.54	0.41
1:B:1223:THR:O	1:B:1225:LYS:NZ	2.54	0.41
1:B:2122:LEU:HD22	1:B:2164:LEU:HD23	2.02	0.41
1:B:2701:ASN:O	1:B:2849:ASN:ND2	2.54	0.41
1:B:4601:ARG:HD2	1:B:4711:VAL:HG21	2.02	0.41
1:D:67:PHE:HB3	1:D:121:LEU:HD12	2.02	0.41
2:F:30:MET:HE3	2:F:36:LYS:HG2	2.03	0.41
1:A:370:LEU:HD23	1:A:370:LEU:HA	1.93	0.41
1:A:2701:ASN:O	1:A:2849:ASN:ND2	2.54	0.41
1:B:1217:PHE:HB3	1:B:1239:PHE:HB3	2.03	0.41
1:B:1273:ILE:HG13	1:B:1287:GLN:N	2.35	0.41
1:B:1446:ILE:HD11	1:B:1450:PHE:CD2	2.56	0.41
1:C:185:SER:OG	1:C:186:VAL:N	2.50	0.41
1:D:2101:LEU:HA	1:D:2101:LEU:HD23	1.85	0.41
1:D:2218:SER:O	1:D:2222:GLU:HB2	2.21	0.41
1:D:4106:GLU:OE1	1:D:4148:TYR:OH	2.24	0.41
2:G:77:CYS:HB2	2:G:98:LEU:HB2	2.02	0.41
1:B:650:ASN:OD1	1:B:650:ASN:N	2.54	0.41
1:C:1223:THR:O	1:C:1225:LYS:NZ	2.54	0.41
1:C:2065:MET:HG3	1:C:2083:MET:HG2	2.03	0.41
1:C:3943:VAL:O	1:C:3947:LEU:HD12	2.21	0.41
1:C:4601:ARG:HD2	1:C:4711:VAL:HG21	2.02	0.41
1:D:1217:PHE:HB3	1:D:1239:PHE:HB3	2.03	0.41
1:D:1843:ILE:HD13	1:D:1843:ILE:HA	1.97	0.41
1:D:3943:VAL:O	1:D:3947:LEU:HD12	2.21	0.41
1:A:228:LEU:HG	1:A:289:ILE:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:753:ASP:OD1	1:A:753:ASP:N	2.50	0.41
1:A:1737:ILE:HD13	1:A:1754:LEU:HB3	2.03	0.41
1:A:2385:ASN:O	1:A:2389:THR:OG1	2.29	0.41
1:B:745:ASN:ND2	1:B:771:ASN:O	2.54	0.41
1:B:2197:ARG:O	1:B:2201:TYR:HB2	2.20	0.41
1:B:2218:SER:O	1:B:2222:GLU:HB2	2.21	0.41
1:B:3795:LEU:HD22	1:B:3834:PHE:HZ	1.85	0.41
1:B:3958:SER:O	1:B:4085:ARG:NH1	2.54	0.41
1:B:4180:GLY:O	1:B:4182:LYS:N	2.52	0.41
1:C:1273:ILE:HG13	1:C:1287:GLN:N	2.35	0.41
1:C:2701:ASN:O	1:C:2849:ASN:ND2	2.54	0.41
1:D:228:LEU:HG	1:D:289:ILE:HD12	2.03	0.41
1:D:499:LEU:HA	1:D:502:ILE:HD12	2.03	0.41
1:D:801:ARG:HA	1:D:1619:LEU:HA	2.01	0.41
1:D:1223:THR:O	1:D:1225:LYS:NZ	2.54	0.41
1:D:1426:TYR:HB2	1:D:1511:VAL:HG12	2.02	0.41
1:D:3508:ILE:O	1:D:3551:LEU:N	2.54	0.41
1:D:4735:ASN:OD1	1:D:4735:ASN:N	2.54	0.41
1:D:4851:PHE:O	1:D:4855:VAL:HB	2.21	0.41
2:G:77:CYS:N	2:G:98:LEU:O	2.49	0.41
2:H:77:CYS:HB2	2:H:98:LEU:HB2	2.02	0.41
1:A:488:LEU:HD12	1:A:488:LEU:HA	1.90	0.41
1:B:4603:LYS:HZ3	1:B:4643:TYR:HE1	1.67	0.41
1:C:228:LEU:HG	1:C:289:ILE:HD12	2.03	0.41
1:C:1788:LEU:O	1:C:1792:THR:OG1	2.31	0.41
1:C:2278:MET:HB3	1:C:2288:GLY:HA2	2.02	0.41
1:C:2526:LEU:O	1:C:2527:LEU:HD23	2.21	0.41
1:C:4808:MET:HG2	1:D:4516:LEU:HA	2.03	0.41
1:D:114:LEU:HB2	1:D:117:HIS:HD2	1.85	0.41
1:D:314:LEU:HD11	1:D:365:HIS:HE1	1.85	0.41
1:D:1269:GLU:H	1:D:1290:PHE:HE2	1.68	0.41
1:A:300:VAL:HG23	1:A:301:THR:HG23	2.02	0.40
1:A:688:ALA:HA	2:E:41:ARG:CZ	2.52	0.40
1:A:3795:LEU:HD22	1:A:3834:PHE:HZ	1.85	0.40
1:A:4099:VAL:HG22	1:A:4132:LEU:HD13	2.03	0.40
1:B:3508:ILE:O	1:B:3551:LEU:N	2.54	0.40
1:C:351:THR:OG1	1:C:352:SER:N	2.55	0.40
1:C:745:ASN:ND2	1:C:771:ASN:O	2.54	0.40
1:C:1217:PHE:HB3	1:C:1239:PHE:HB3	2.03	0.40
1:C:1269:GLU:H	1:C:1290:PHE:HE2	1.68	0.40
1:C:2836:LEU:HD22	1:C:2895:LEU:HD23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3696:LYS:HD3	1:C:3696:LYS:HA	1.86	0.40
1:C:3769:ASN:O	1:C:3773:GLN:NE2	2.54	0.40
1:C:4660:TYR:HB3	1:C:4664:ARG:NH1	2.36	0.40
1:C:4851:PHE:O	1:C:4855:VAL:HB	2.21	0.40
1:D:483:LYS:HD2	1:D:483:LYS:HA	1.86	0.40
1:D:745:ASN:ND2	1:D:771:ASN:O	2.54	0.40
1:D:997:ASP:O	1:D:1001:GLU:HG2	2.22	0.40
1:D:2701:ASN:O	1:D:2849:ASN:ND2	2.54	0.40
1:D:3730:LEU:HD23	1:D:3730:LEU:HA	1.87	0.40
1:A:650:ASN:OD1	1:A:650:ASN:N	2.54	0.40
1:A:4516:LEU:HA	1:D:4808:MET:HG2	2.03	0.40
1:A:4601:ARG:HD2	1:A:4711:VAL:HG21	2.02	0.40
1:B:495:ILE:O	1:B:499:LEU:N	2.48	0.40
1:B:4515:LEU:HA	1:B:4518:TYR:CD2	2.56	0.40
1:B:4660:TYR:HB3	1:B:4664:ARG:NH1	2.36	0.40
1:B:4851:PHE:O	1:B:4855:VAL:HB	2.21	0.40
1:C:3958:SER:O	1:C:4085:ARG:NH1	2.54	0.40
1:D:351:THR:OG1	1:D:352:SER:N	2.55	0.40
1:D:540:LEU:HG	1:D:547:ASN:OD1	2.22	0.40
1:D:2526:LEU:O	1:D:2527:LEU:HD23	2.21	0.40
1:A:61:ASP:HB3	1:A:64:ILE:HD11	2.03	0.40
1:A:699:SER:OG	1:A:789:PHE:O	2.30	0.40
1:A:1246:ASP:OD1	1:A:1694:TYR:OH	2.30	0.40
1:A:2010:LEU:HA	1:A:2013:ASP:HB2	2.03	0.40
1:A:3958:SER:O	1:A:4085:ARG:NH1	2.54	0.40
1:A:4735:ASN:OD1	1:A:4735:ASN:N	2.54	0.40
1:B:540:LEU:HG	1:B:547:ASN:OD1	2.22	0.40
1:B:4099:VAL:HG22	1:B:4132:LEU:HD13	2.03	0.40
1:B:4735:ASN:OD1	1:B:4735:ASN:N	2.54	0.40
1:C:483:LYS:HD2	1:C:483:LYS:HA	1.87	0.40
1:C:1467:VAL:O	1:C:1480:ILE:N	2.39	0.40
1:C:1623:LEU:HD23	1:C:1623:LEU:HA	1.86	0.40
1:C:2218:SER:O	1:C:2222:GLU:HB2	2.21	0.40
1:D:1737:ILE:HD13	1:D:1754:LEU:HB3	2.03	0.40
1:D:4601:ARG:HD2	1:D:4711:VAL:HG21	2.02	0.40
2:E:101:ASP:N	2:E:101:ASP:OD1	2.54	0.40
1:A:533:LEU:HD12	1:A:536:LEU:HD22	2.04	0.40
1:A:745:ASN:ND2	1:A:771:ASN:O	2.54	0.40
1:A:1217:PHE:HB3	1:A:1239:PHE:HB3	2.03	0.40
1:A:2836:LEU:HD22	1:A:2895:LEU:HD23	2.02	0.40
1:A:4949:GLU:OE1	1:A:4949:GLU:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2526:LEU:O	1:B:2527:LEU:HD23	2.21	0.40
1:B:4949:GLU:N	1:B:4949:GLU:OE1	2.55	0.40
1:C:1843:ILE:HD13	1:C:1843:ILE:HA	1.97	0.40
1:C:2010:LEU:HA	1:C:2013:ASP:HB2	2.03	0.40
1:C:3508:ILE:O	1:C:3551:LEU:N	2.54	0.40
1:C:4515:LEU:HA	1:C:4518:TYR:CD2	2.56	0.40
1:D:533:LEU:HD12	1:D:536:LEU:HD22	2.04	0.40
1:D:688:ALA:HA	2:H:41:ARG:CZ	2.52	0.40
1:D:1028:ARG:NH2	1:D:1029:ASN:O	2.55	0.40
1:D:3958:SER:O	1:D:4085:ARG:NH1	2.54	0.40
1:D:4663:ASP:N	1:D:4663:ASP:OD1	2.55	0.40
2:F:101:ASP:N	2:F:101:ASP:OD1	2.54	0.40
1:A:294:PRO:HB3	1:A:328:ALA:HB1	2.03	0.40
1:A:540:LEU:HG	1:A:547:ASN:OD1	2.22	0.40
1:A:997:ASP:O	1:A:1001:GLU:HG2	2.22	0.40
1:A:1028:ARG:NH2	1:A:1029:ASN:O	2.55	0.40
1:A:2218:SER:O	1:A:2222:GLU:HB2	2.21	0.40
1:A:3792:LEU:HD23	1:A:3792:LEU:HA	1.93	0.40
1:A:4663:ASP:OD1	1:A:4663:ASP:N	2.55	0.40
1:B:351:THR:OG1	1:B:352:SER:N	2.55	0.40
1:B:1028:ARG:NH2	1:B:1029:ASN:O	2.55	0.40
1:B:3943:VAL:O	1:B:3947:LEU:HD12	2.21	0.40
1:C:114:LEU:HB2	1:C:117:HIS:HD2	1.85	0.40
1:C:314:LEU:HD11	1:C:365:HIS:HE1	1.85	0.40
1:C:370:LEU:O	1:C:372:LEU:N	2.52	0.40
1:C:3860:GLN:HE22	1:C:3867:VAL:HG23	1.87	0.40
1:C:4908:THR:O	1:C:4913:ASN:ND2	2.49	0.40
1:D:650:ASN:OD1	1:D:650:ASN:N	2.54	0.40
1:D:847:THR:O	1:D:847:THR:OG1	2.37	0.40
1:D:2278:MET:HB3	1:D:2288:GLY:HA2	2.02	0.40
1:D:4660:TYR:HB3	1:D:4664:ARG:NH1	2.36	0.40
1:D:4949:GLU:N	1:D:4949:GLU:OE1	2.55	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	3818/4966 (77%)	3361 (88%)	436 (11%)	21 (1%)	25	62
1	B	3818/4966 (77%)	3361 (88%)	436 (11%)	21 (1%)	25	62
1	C	3818/4966 (77%)	3363 (88%)	435 (11%)	20 (0%)	29	66
1	D	3818/4966 (77%)	3362 (88%)	436 (11%)	20 (0%)	29	66
2	E	105/107 (98%)	96 (91%)	9 (9%)	0	100	100
2	F	105/107 (98%)	96 (91%)	9 (9%)	0	100	100
2	G	105/107 (98%)	96 (91%)	9 (9%)	0	100	100
2	H	105/107 (98%)	96 (91%)	9 (9%)	0	100	100
All	All	15692/20292 (77%)	13831 (88%)	1779 (11%)	82 (0%)	32	66

All (82) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1462	VAL
1	B	1462	VAL
1	C	1462	VAL
1	D	1462	VAL
1	A	411	GLU
1	A	654	SER
1	A	1032	LEU
1	A	1523	ALA
1	A	1848	GLU
1	A	3660	VAL
1	A	4042	ILE
1	B	411	GLU
1	B	654	SER
1	B	1032	LEU
1	B	1523	ALA
1	B	1848	GLU
1	B	3660	VAL
1	B	4042	ILE
1	C	411	GLU
1	C	654	SER
1	C	1032	LEU
1	C	1523	ALA
1	C	1848	GLU

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Mol	Chain	Res	Type
1	C	3660	VAL
1	C	4042	ILE
1	D	411	GLU
1	D	654	SER
1	D	1032	LEU
1	D	1523	ALA
1	D	1848	GLU
1	D	3660	VAL
1	D	4042	ILE
1	A	186	VAL
1	A	722	LEU
1	B	186	VAL
1	B	722	LEU
1	C	186	VAL
1	C	722	LEU
1	D	186	VAL
1	D	722	LEU
1	A	289	ILE
1	B	289	ILE
1	C	289	ILE
1	D	289	ILE
1	A	392	ILE
1	A	979	ALA
1	A	1299	ILE
1	A	1465	VAL
1	A	2444	ILE
1	B	392	ILE
1	B	979	ALA
1	B	1299	ILE
1	B	1465	VAL
1	B	2444	ILE
1	C	392	ILE
1	C	979	ALA
1	C	1299	ILE
1	C	1465	VAL
1	C	2444	ILE
1	D	392	ILE
1	D	979	ALA
1	D	1299	ILE
1	D	1465	VAL
1	D	2444	ILE
1	A	82	LEU

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Mol	Chain	Res	Type
1	A	371	TRP
1	A	1472	GLU
1	B	82	LEU
1	B	371	TRP
1	B	1472	GLU
1	C	82	LEU
1	C	371	TRP
1	D	82	LEU
1	D	371	TRP
1	A	4700	ILE
1	B	4700	ILE
1	C	4700	ILE
1	D	4700	ILE
1	A	495	ILE
1	B	495	ILE
1	C	495	ILE
1	D	495	ILE

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	2915/4355 (67%)	2845 (98%)	70 (2%)	49	70
1	B	2915/4355 (67%)	2845 (98%)	70 (2%)	49	70
1	C	2915/4355 (67%)	2845 (98%)	70 (2%)	49	70
1	D	2915/4355 (67%)	2844 (98%)	71 (2%)	49	70
2	E	76/88 (86%)	72 (95%)	4 (5%)	22	54
2	F	76/88 (86%)	72 (95%)	4 (5%)	22	54
2	G	76/88 (86%)	72 (95%)	4 (5%)	22	54
2	H	76/88 (86%)	72 (95%)	4 (5%)	22	54
All	All	11964/17772 (67%)	11667 (98%)	297 (2%)	50	70

All (297) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LYS
1	A	130	LEU
1	A	262	TYR
1	A	374	TYR
1	A	485	ARG
1	A	565	LEU
1	A	608	HIS
1	A	661	LEU
1	A	760	ASP
1	A	802	PHE
1	A	956	HIS
1	A	981	MET
1	A	1113	MET
1	A	1117	TRP
1	A	1152	TYR
1	A	1195	PHE
1	A	1203	PRO
1	A	1251	LEU
1	A	1300	MET
1	A	1442	TRP
1	A	1449	ASP
1	A	1460	ASP
1	A	1600	MET
1	A	1604	PHE
1	A	1663	SER
1	A	1670	ASN
1	A	1724	ASN
1	A	1740	PHE
1	A	1777	TYR
1	A	1915	CYS
1	A	1941	PHE
1	A	1998	PHE
1	A	2003	MET
1	A	2025	ARG
1	A	2154	PHE
1	A	2188	PHE
1	A	2209	ASN
1	A	2302	ARG
1	A	2330	PHE
1	A	2459	PHE
1	A	2463	HIS
1	A	2482	PHE
1	A	2604	MET

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Mol	Chain	Res	Type
1	A	2663	LEU
1	A	2792	ARG
1	A	2997	ASN
1	A	3087	LYS
1	A	3196	LEU
1	A	3281	LYS
1	A	3664	HIS
1	A	3688	MET
1	A	3713	PHE
1	A	3812	LYS
1	A	3853	PHE
1	A	3902	GLN
1	A	3905	PHE
1	A	3914	GLN
1	A	3927	CYS
1	A	3941	ASP
1	A	3946	PHE
1	A	3998	MET
1	A	4146	ARG
1	A	4198	GLU
1	A	4624	ASP
1	A	4662	ARG
1	A	4671	MET
1	A	4724	TYR
1	A	4867	ASP
1	A	4887	CYS
1	A	4890	CYS
1	B	34	LYS
1	B	130	LEU
1	B	262	TYR
1	B	374	TYR
1	B	485	ARG
1	B	565	LEU
1	B	608	HIS
1	B	661	LEU
1	B	760	ASP
1	B	802	PHE
1	B	956	HIS
1	B	981	MET
1	B	1113	MET
1	B	1117	TRP
1	B	1152	TYR

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Mol	Chain	Res	Type
1	B	1195	PHE
1	B	1203	PRO
1	B	1251	LEU
1	B	1300	MET
1	B	1442	TRP
1	B	1449	ASP
1	B	1460	ASP
1	B	1600	MET
1	B	1604	PHE
1	B	1663	SER
1	B	1670	ASN
1	B	1724	ASN
1	B	1740	PHE
1	B	1777	TYR
1	B	1915	CYS
1	B	1941	PHE
1	B	1998	PHE
1	B	2003	MET
1	B	2025	ARG
1	B	2154	PHE
1	B	2188	PHE
1	B	2209	ASN
1	B	2302	ARG
1	B	2330	PHE
1	B	2459	PHE
1	B	2463	HIS
1	B	2482	PHE
1	B	2604	MET
1	B	2663	LEU
1	B	2792	ARG
1	B	2997	ASN
1	B	3087	LYS
1	B	3196	LEU
1	B	3281	LYS
1	B	3664	HIS
1	B	3688	MET
1	B	3713	PHE
1	B	3812	LYS
1	B	3853	PHE
1	B	3902	GLN
1	B	3905	PHE
1	B	3914	GLN

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Mol	Chain	Res	Type
1	B	3927	CYS
1	B	3941	ASP
1	B	3946	PHE
1	B	3998	MET
1	B	4146	ARG
1	B	4198	GLU
1	B	4624	ASP
1	B	4662	ARG
1	B	4671	MET
1	B	4724	TYR
1	B	4867	ASP
1	B	4887	CYS
1	B	4890	CYS
1	C	34	LYS
1	C	130	LEU
1	C	262	TYR
1	C	374	TYR
1	C	485	ARG
1	C	565	LEU
1	C	608	HIS
1	C	661	LEU
1	C	760	ASP
1	C	802	PHE
1	C	956	HIS
1	C	981	MET
1	C	1113	MET
1	C	1117	TRP
1	C	1152	TYR
1	C	1195	PHE
1	C	1203	PRO
1	C	1251	LEU
1	C	1300	MET
1	C	1442	TRP
1	C	1449	ASP
1	C	1460	ASP
1	C	1600	MET
1	C	1604	PHE
1	C	1663	SER
1	C	1670	ASN
1	C	1724	ASN
1	C	1740	PHE
1	C	1777	TYR

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Mol	Chain	Res	Type
1	C	1915	CYS
1	C	1941	PHE
1	C	1998	PHE
1	C	2003	MET
1	C	2025	ARG
1	C	2154	PHE
1	C	2188	PHE
1	C	2209	ASN
1	C	2302	ARG
1	C	2330	PHE
1	C	2459	PHE
1	C	2463	HIS
1	C	2482	PHE
1	C	2604	MET
1	C	2663	LEU
1	C	2792	ARG
1	C	2997	ASN
1	C	3087	LYS
1	C	3196	LEU
1	C	3281	LYS
1	C	3664	HIS
1	C	3688	MET
1	C	3713	PHE
1	C	3812	LYS
1	C	3853	PHE
1	C	3902	GLN
1	C	3905	PHE
1	C	3914	GLN
1	C	3927	CYS
1	C	3941	ASP
1	C	3946	PHE
1	C	3998	MET
1	C	4146	ARG
1	C	4198	GLU
1	C	4624	ASP
1	C	4662	ARG
1	C	4671	MET
1	C	4724	TYR
1	C	4867	ASP
1	C	4887	CYS
1	C	4890	CYS
1	D	34	LYS

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Mol	Chain	Res	Type
1	D	130	LEU
1	D	262	TYR
1	D	374	TYR
1	D	485	ARG
1	D	565	LEU
1	D	608	HIS
1	D	661	LEU
1	D	760	ASP
1	D	802	PHE
1	D	956	HIS
1	D	981	MET
1	D	1093	THR
1	D	1113	MET
1	D	1117	TRP
1	D	1152	TYR
1	D	1195	PHE
1	D	1203	PRO
1	D	1251	LEU
1	D	1300	MET
1	D	1442	TRP
1	D	1449	ASP
1	D	1460	ASP
1	D	1600	MET
1	D	1604	PHE
1	D	1663	SER
1	D	1670	ASN
1	D	1724	ASN
1	D	1740	PHE
1	D	1777	TYR
1	D	1915	CYS
1	D	1941	PHE
1	D	1998	PHE
1	D	2003	MET
1	D	2025	ARG
1	D	2154	PHE
1	D	2188	PHE
1	D	2209	ASN
1	D	2302	ARG
1	D	2330	PHE
1	D	2459	PHE
1	D	2463	HIS
1	D	2482	PHE

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Mol	Chain	Res	Type
1	D	2604	MET
1	D	2663	LEU
1	D	2792	ARG
1	D	2997	ASN
1	D	3087	LYS
1	D	3196	LEU
1	D	3281	LYS
1	D	3664	HIS
1	D	3688	MET
1	D	3713	PHE
1	D	3812	LYS
1	D	3853	PHE
1	D	3902	GLN
1	D	3905	PHE
1	D	3914	GLN
1	D	3927	CYS
1	D	3941	ASP
1	D	3946	PHE
1	D	3998	MET
1	D	4146	ARG
1	D	4198	GLU
1	D	4624	ASP
1	D	4662	ARG
1	D	4671	MET
1	D	4724	TYR
1	D	4867	ASP
1	D	4887	CYS
1	D	4890	CYS
2	E	33	ASN
2	E	41	ARG
2	E	69	LEU
2	E	106	ASN
2	F	33	ASN
2	F	41	ARG
2	F	69	LEU
2	F	106	ASN
2	G	33	ASN
2	G	41	ARG
2	G	69	LEU
2	G	106	ASN
2	H	33	ASN
2	H	41	ARG

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Mol	Chain	Res	Type
2	H	69	LEU
2	H	106	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1147	GLN
1	A	2249	ASN
1	A	3811	ASN
1	B	1147	GLN
1	B	2249	ASN
1	B	3811	ASN
1	C	1147	GLN
1	C	2249	ASN
1	C	3811	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 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

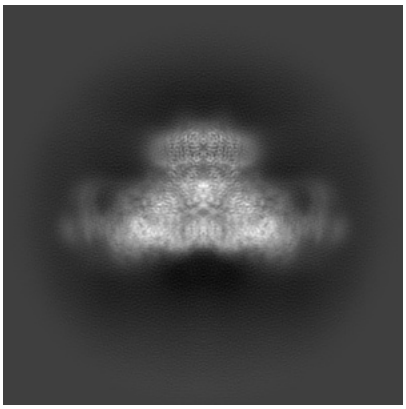
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-27746. These allow visual inspection of the internal detail of the map and identification of artifacts.

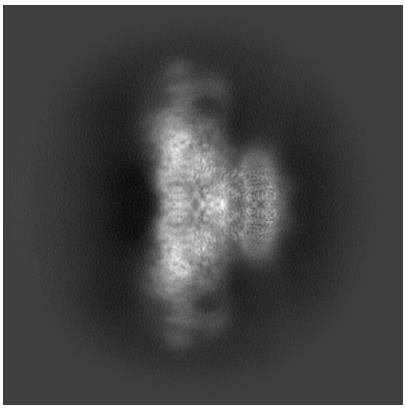
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

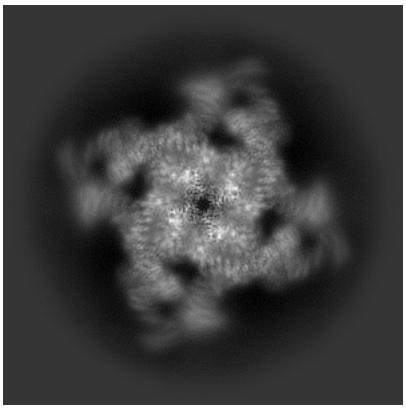
6.1.1 Primary map



X

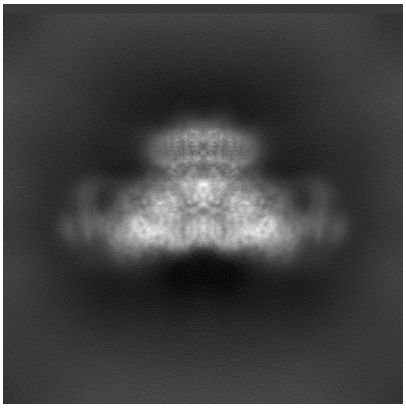


Y

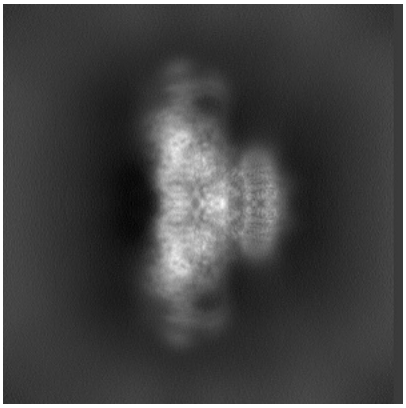


Z

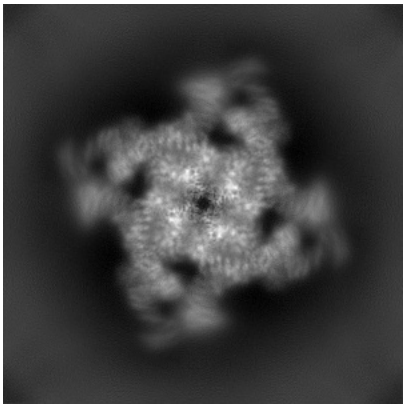
6.1.2 Raw map



X



Y

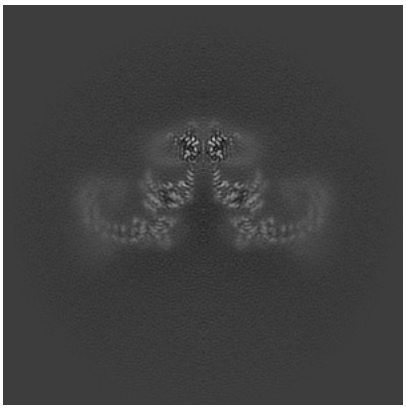


Z

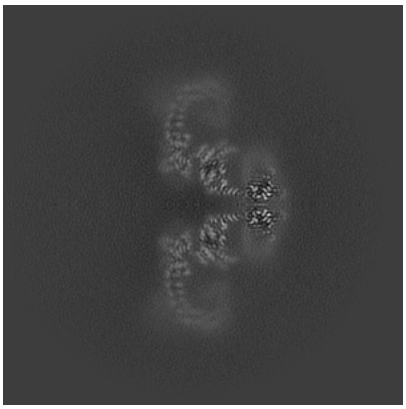
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

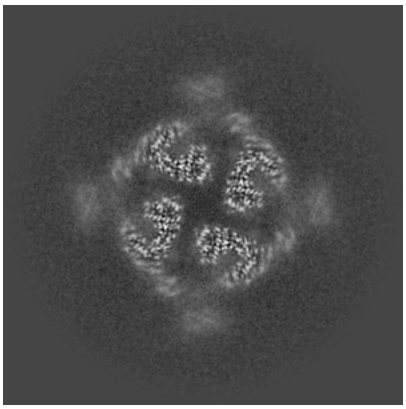
6.2.1 Primary map



X Index: 230

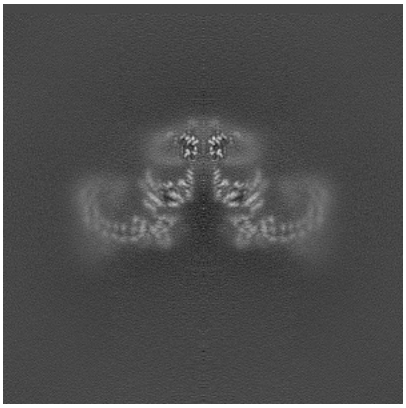


Y Index: 230

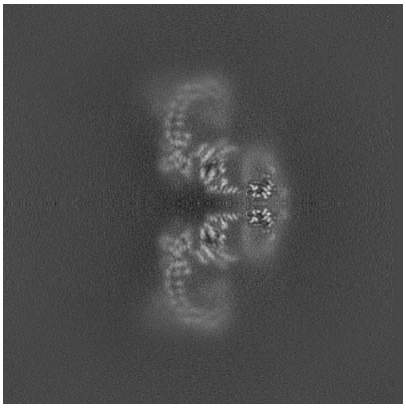


Z Index: 230

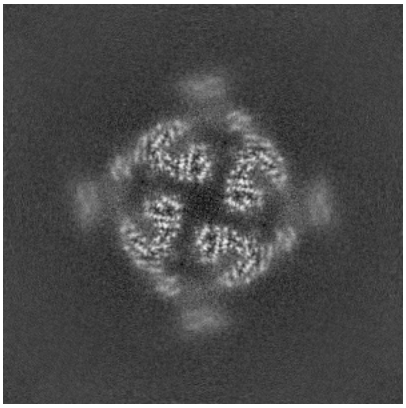
6.2.2 Raw map



X Index: 230



Y Index: 230

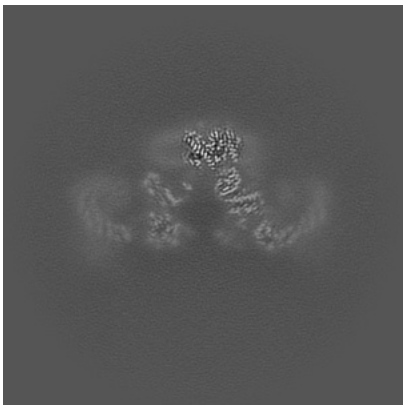


Z Index: 230

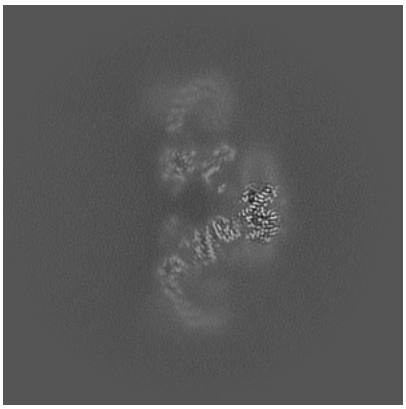
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

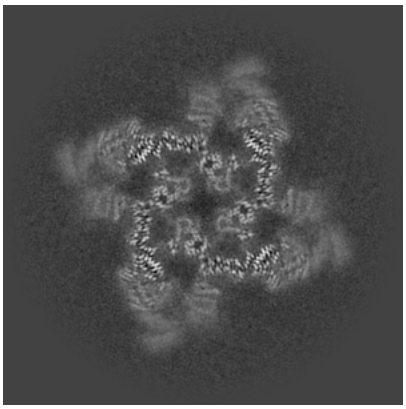
6.3.1 Primary map



X Index: 222

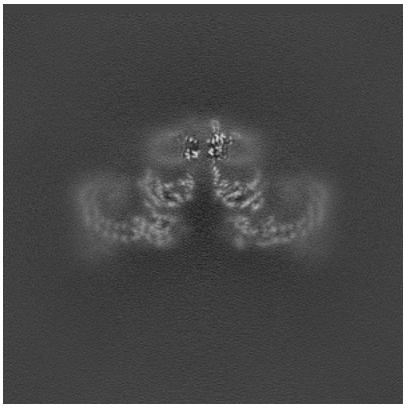


Y Index: 222

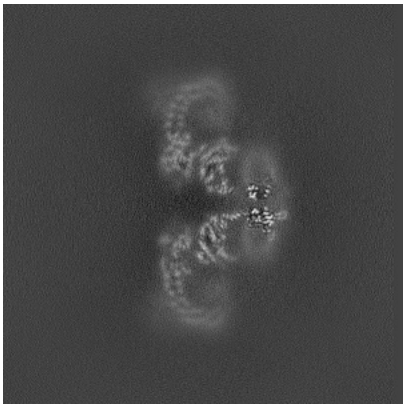


Z Index: 203

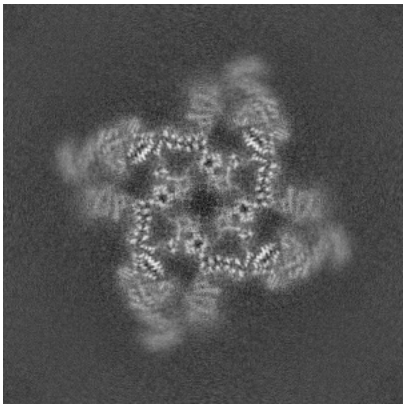
6.3.2 Raw map



X Index: 228



Y Index: 228

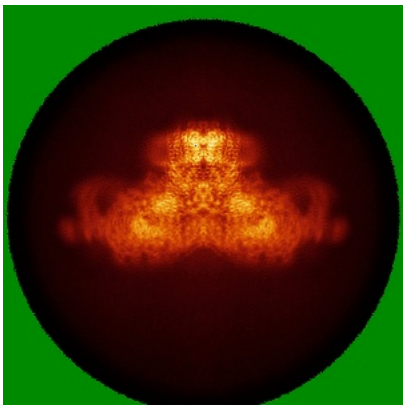


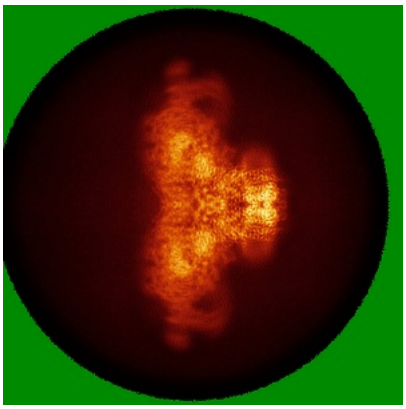
Z Index: 203

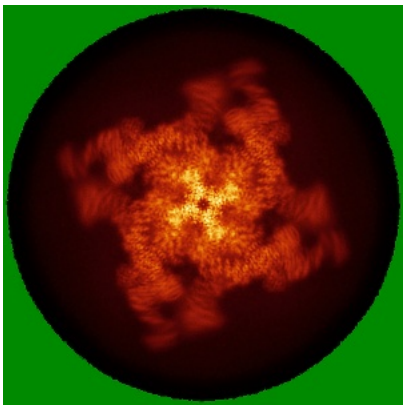
The images above show the largest variance slices of the map in three orthogonal directions.

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

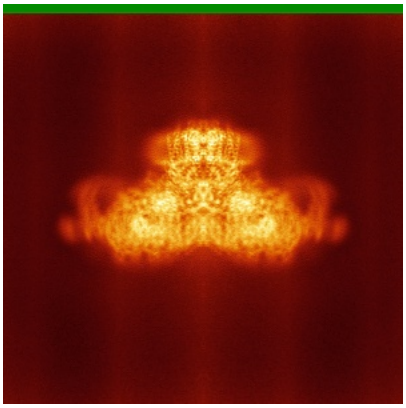
6.4.1 Primary map

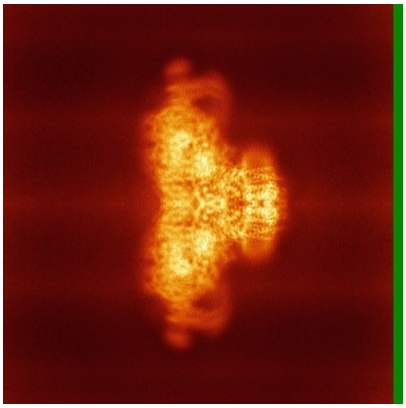

X

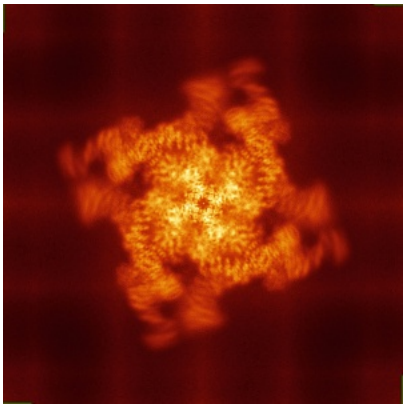

Y


Z

6.4.2 Raw map


X

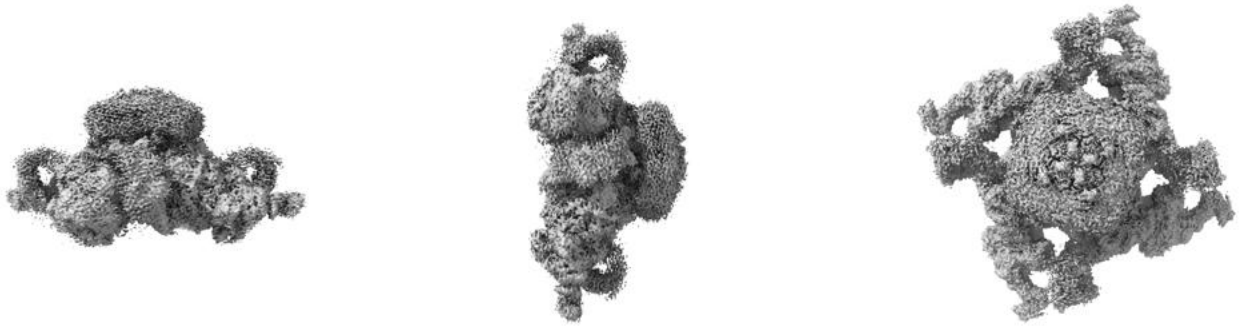

Y


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

6.5.2 Raw map

X Y Z

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

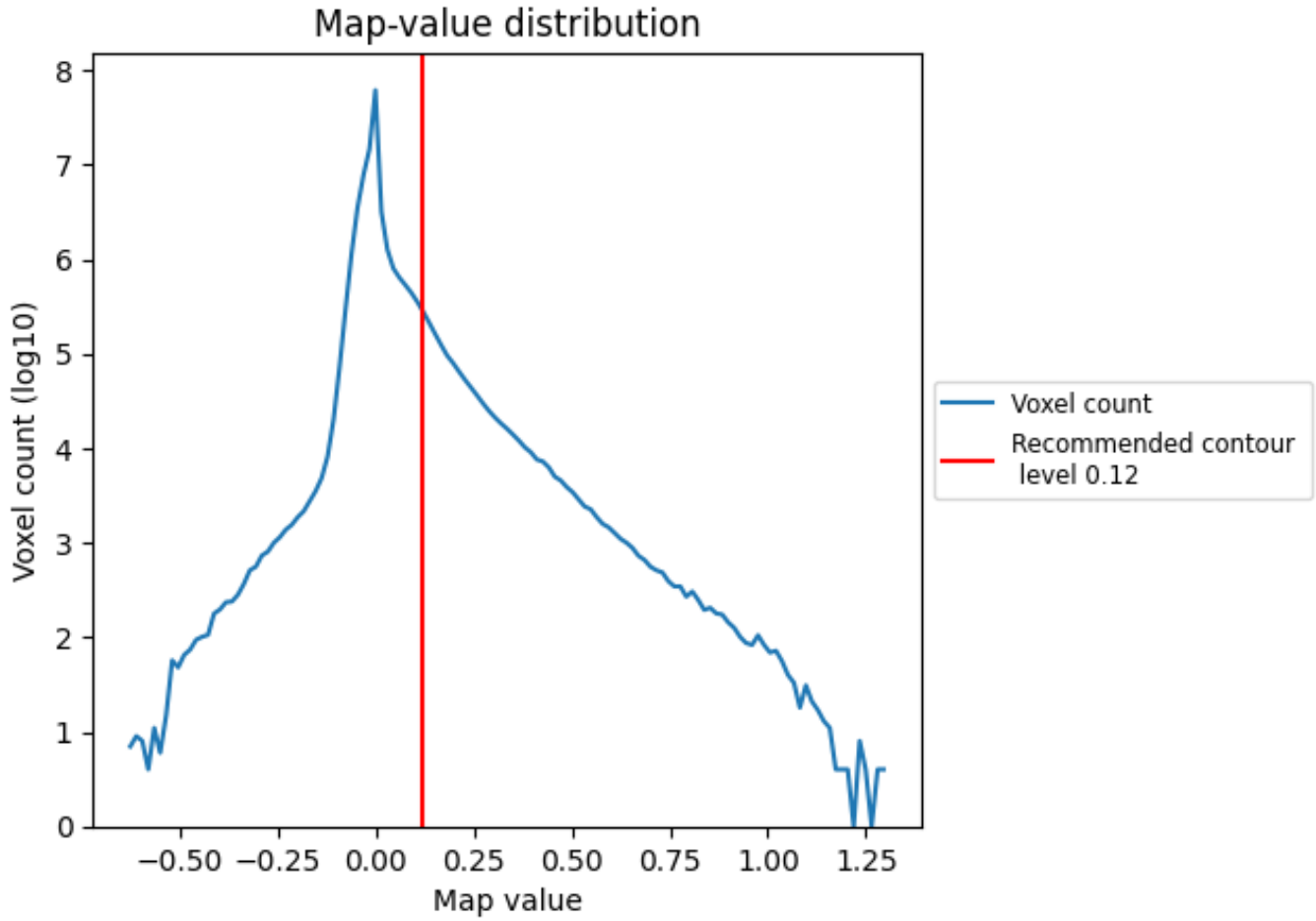
6.6 Mask visualisation (i)

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

7 Map analysis

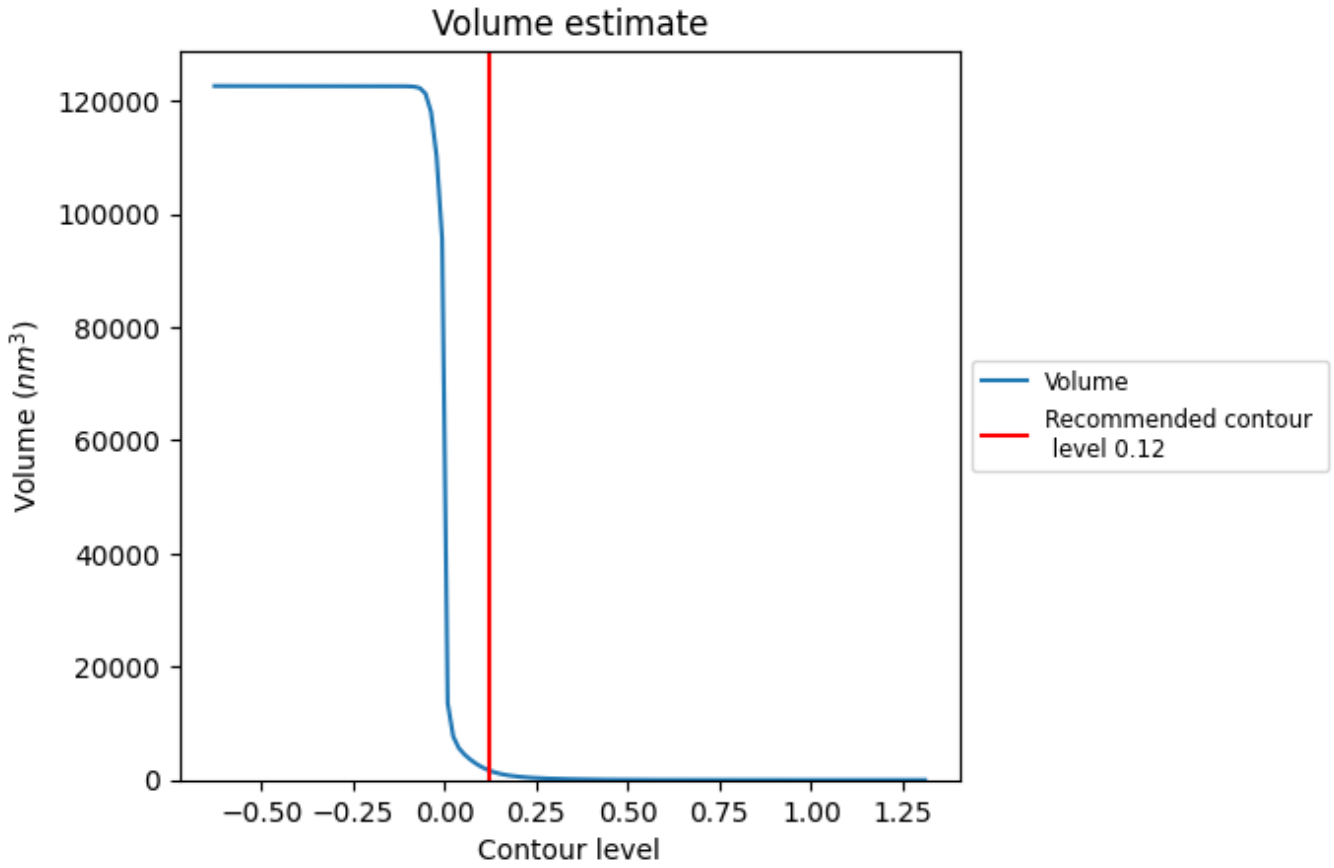
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

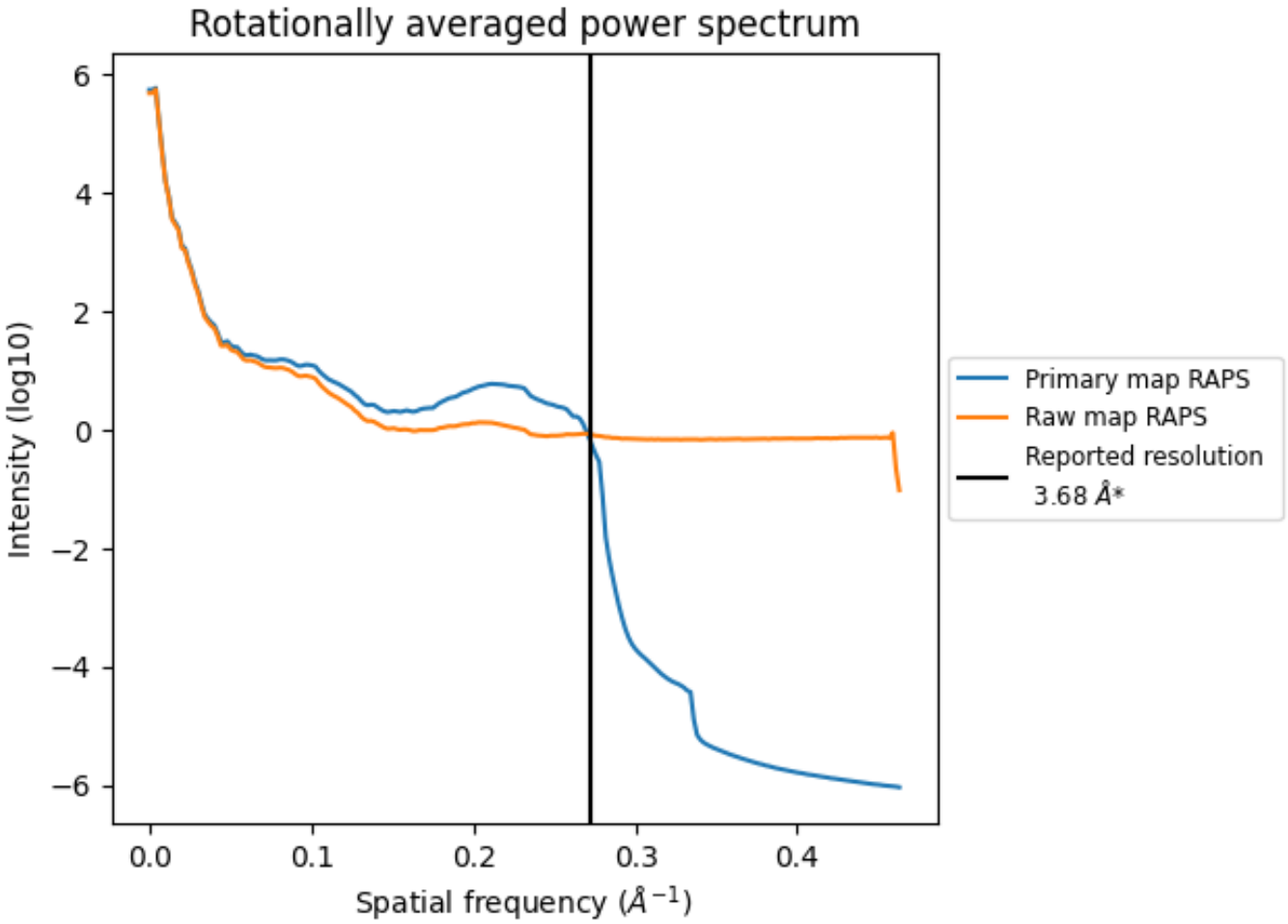
7.2 Volume estimate



The volume at the recommended contour level is 1734 nm^3; this corresponds to an approximate mass of 1567 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)

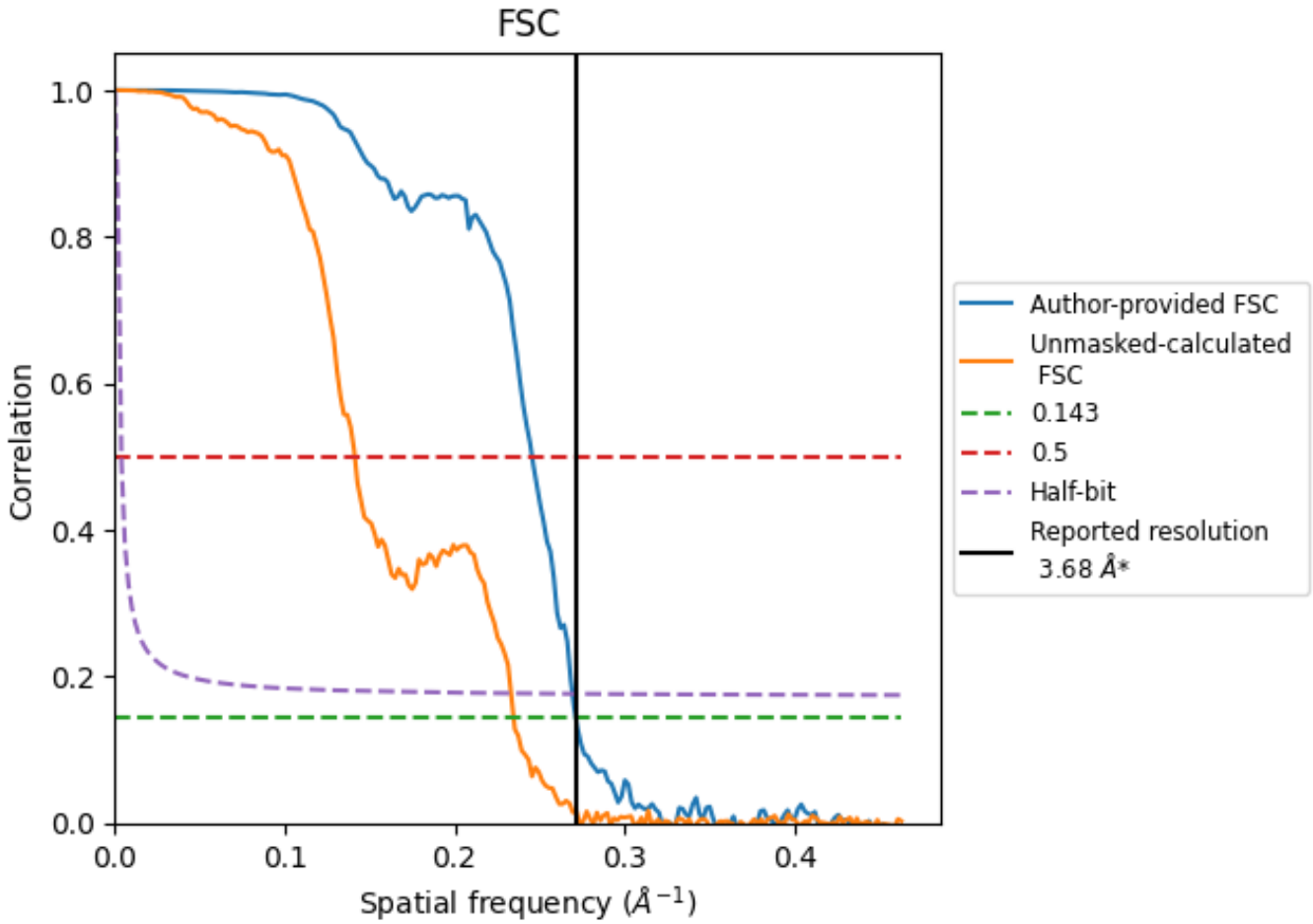


*Reported resolution corresponds to spatial frequency of 0.272 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.272 Å^{-1}

8.2 Resolution estimates (i)

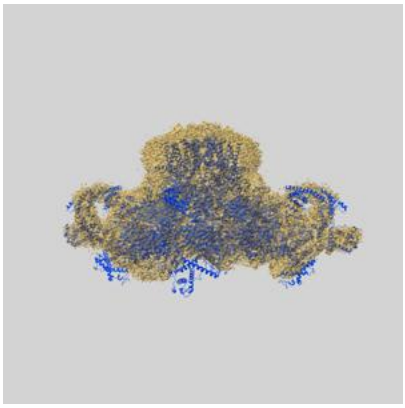
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.68	-	-
Author-provided FSC curve	3.68	4.07	3.71
Unmasked-calculated*	4.26	7.08	4.29

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.26 differs from the reported value 3.68 by more than 10 %

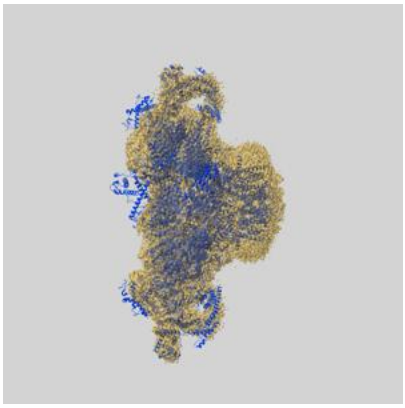
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-27746 and PDB model 8DVV. Per-residue inclusion information can be found in section 3 on page 5.

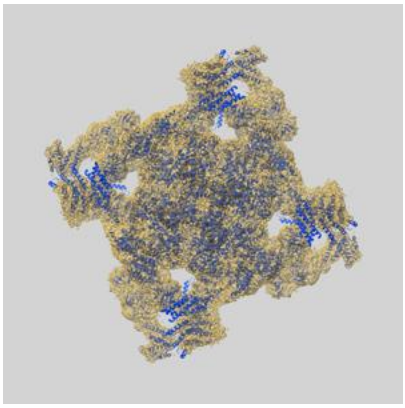
9.1 Map-model overlay



X



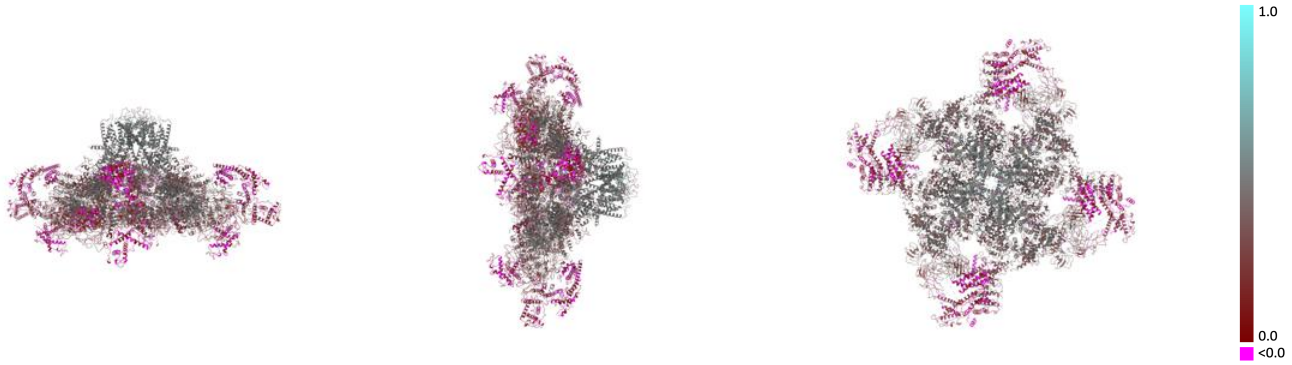
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.12 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.

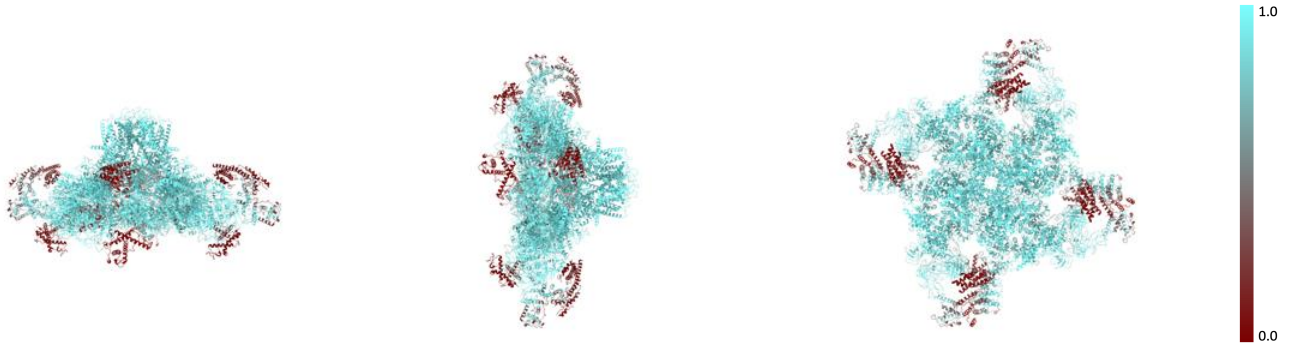
9.2 Q-score mapped to coordinate model (i)



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.

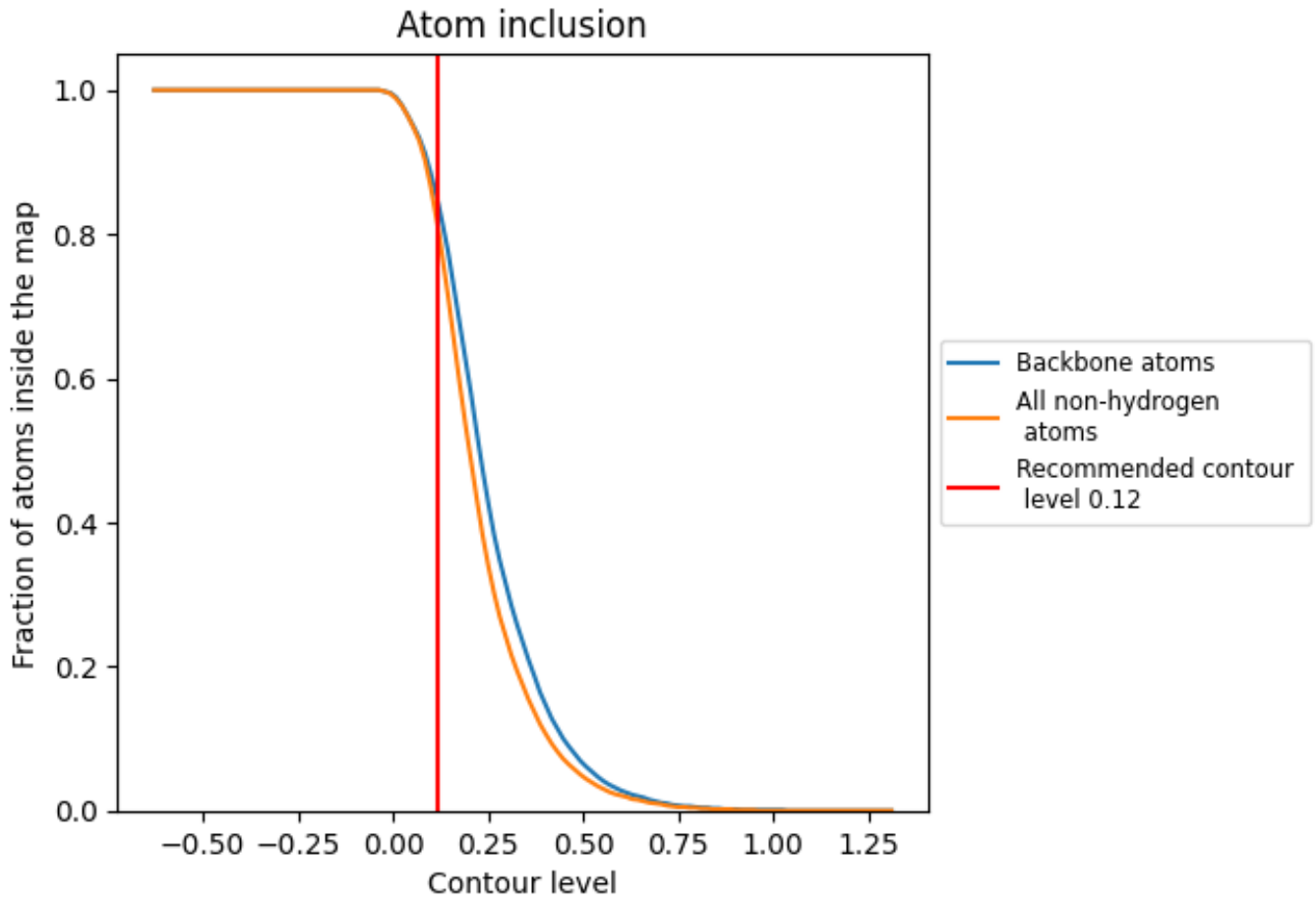
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.12).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8050	0.3180
A	0.8010	0.3150
B	0.8010	0.3160
C	0.8010	0.3160
D	0.8010	0.3160
E	0.9510	0.3910
F	0.9510	0.3940
G	0.9520	0.3930
H	0.9520	0.3910