Full wwPDB EM Validation Report ⓘ

Nov 2, 2022 – 05:02 AM EDT

PDB ID	:	5TAT
EMDB ID	:	EMD-8384
Title	:	Structure of rabbit RyR1 (Caffeine/ATP/EGTA dataset, class 2)
Authors	:	Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.; Frank, J.
Deposited on	:	2016-09-10
Resolution	:	4.80 Å(reported)

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

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

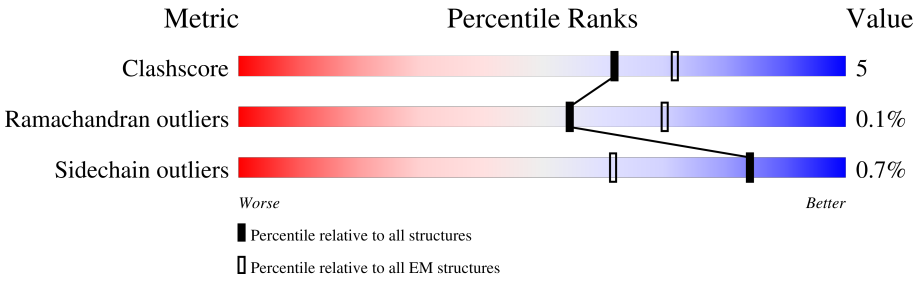
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.80 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	108	36% 84% 15% ·
1	F	108	36% 83% 16% ·
1	H	108	36% 83% 16% ·
1	J	108	37% 85% 14% ·
2	B	4416	39% 84% 11% 5%
2	E	4416	39% 84% 10% 5%
2	G	4416	39% 84% 10% 5%
2	I	4416	39% 84% 10% 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 121452 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.

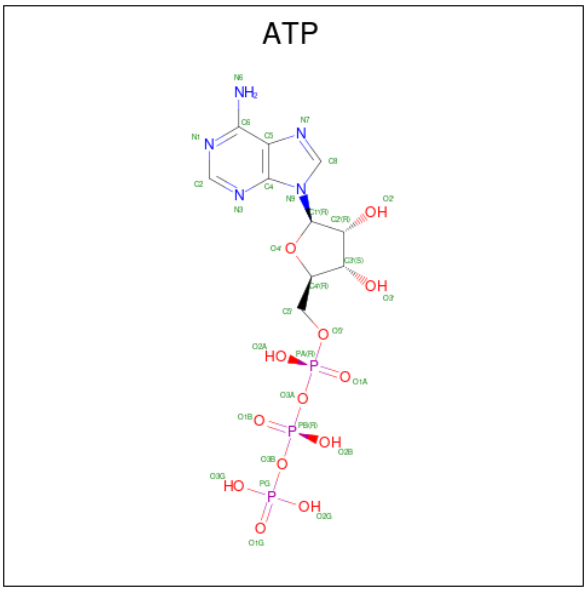
- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	F	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	A	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	H	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	J	107	Total	C	N	O	S	0	0
			818	516	144	154	4		

- Molecule 2 is a protein called Ryanodine receptor 1.

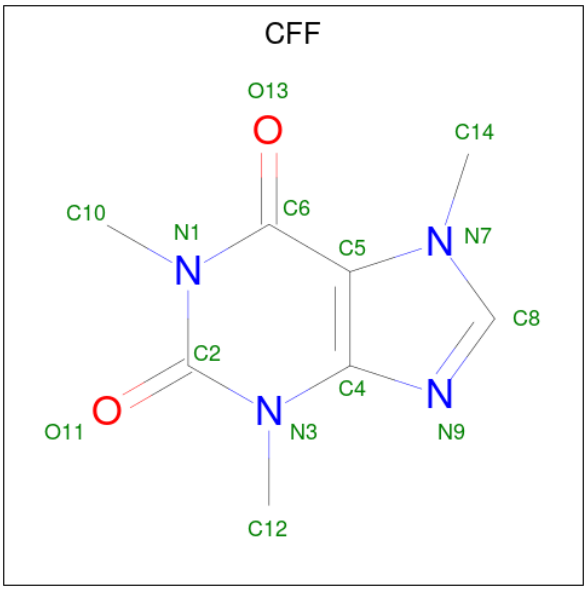
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		

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



Mol	Chain	Residues	Atoms					AltConf
3	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	I	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	E	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	G	1	Total	C	N	O	P	0
			31	10	5	13	3	

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



Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	N	O	0
			14	8	4	2	
4	I	1	Total	C	N	O	0
			14	8	4	2	
4	E	1	Total	C	N	O	0
			14	8	4	2	
4	G	1	Total	C	N	O	0
			14	8	4	2	

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

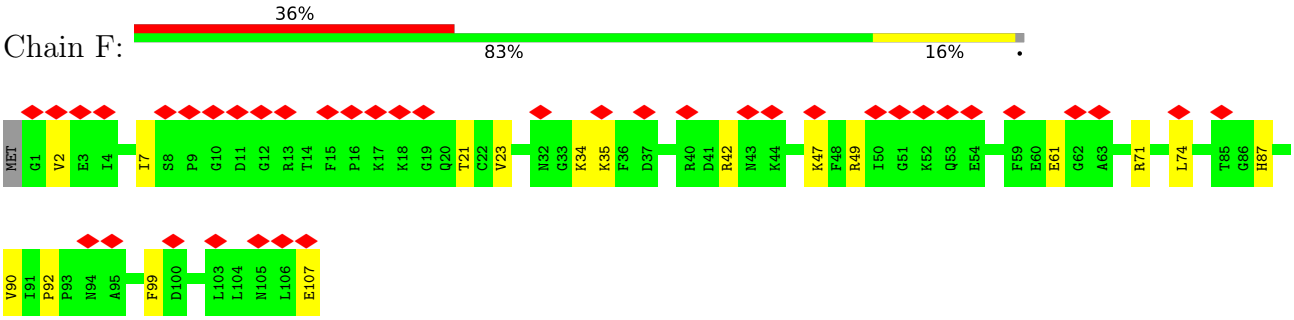
Mol	Chain	Residues	Atoms		AltConf
5	B	1	Total	Zn	0
			1	1	
5	I	1	Total	Zn	0
			1	1	
5	E	1	Total	Zn	0
			1	1	
5	G	1	Total	Zn	0
			1	1	

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.

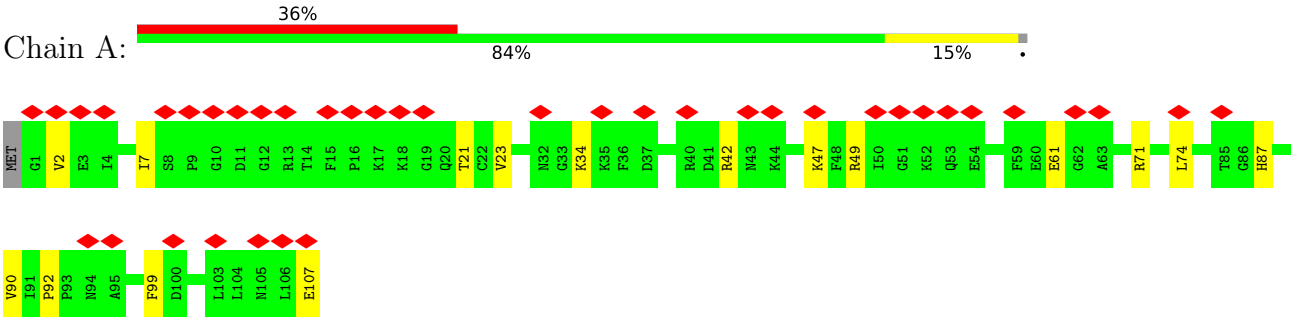
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F:



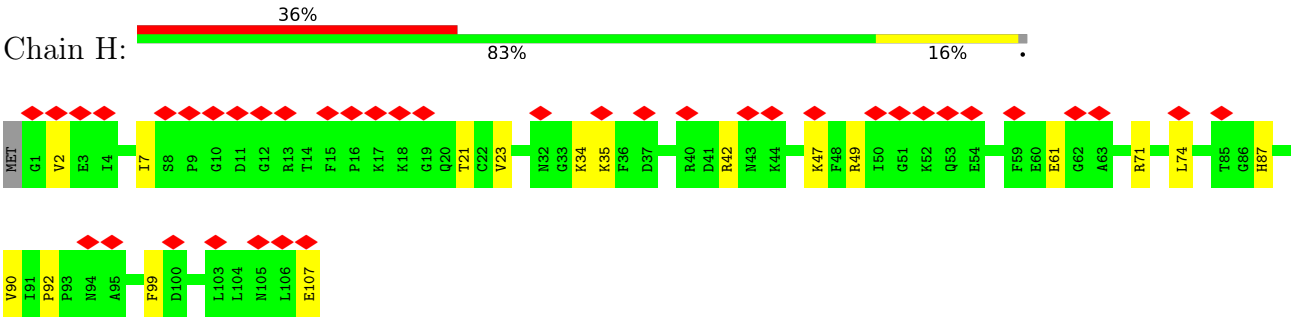
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain A:



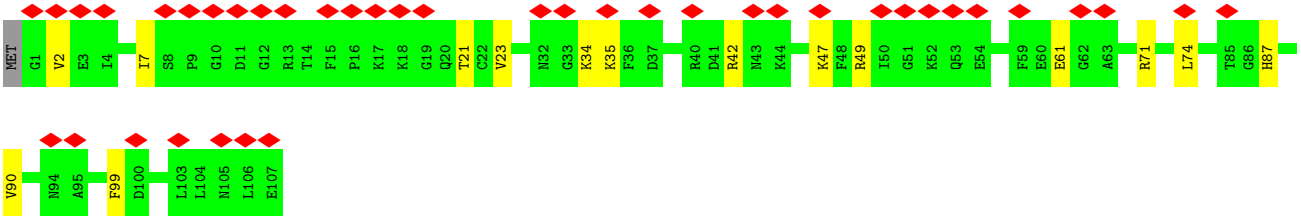
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H:



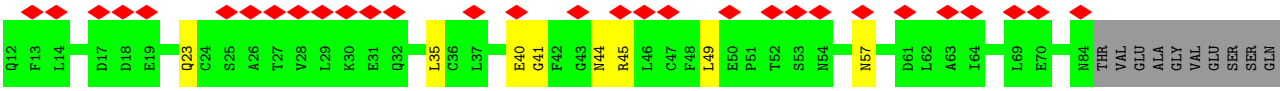
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

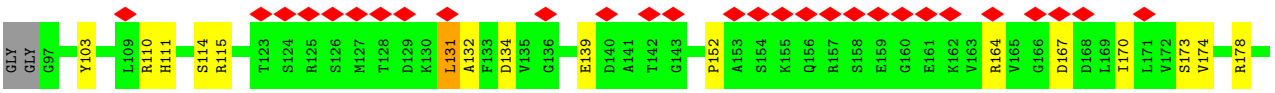
Chain J:

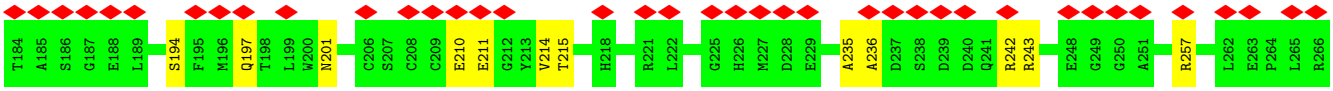


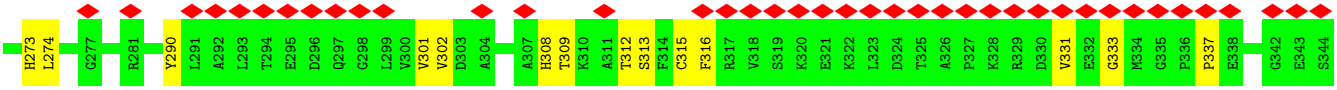
• Molecule 2: Ryanodine receptor 1

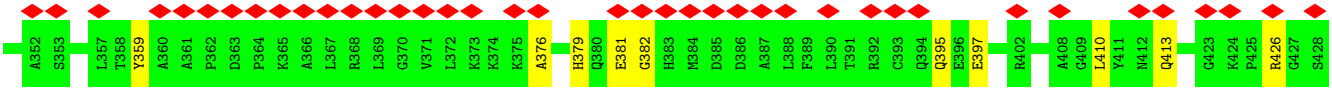
Chain B:

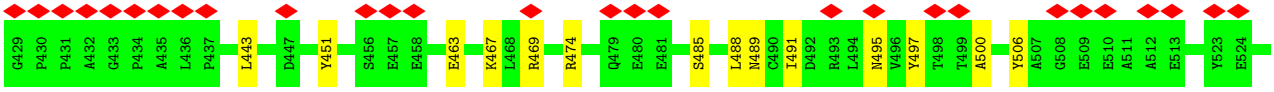


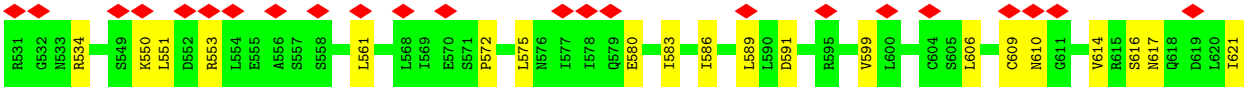


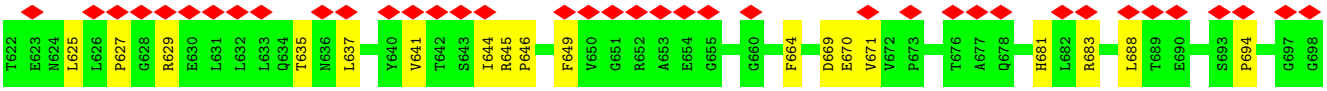


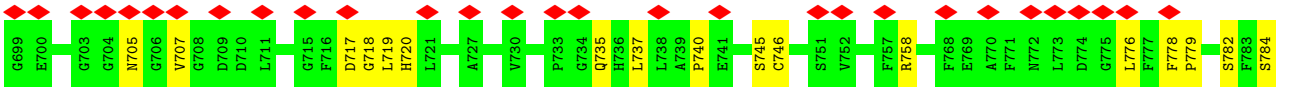


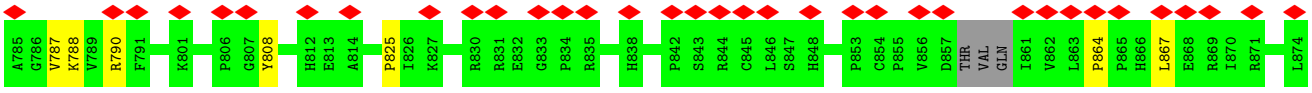


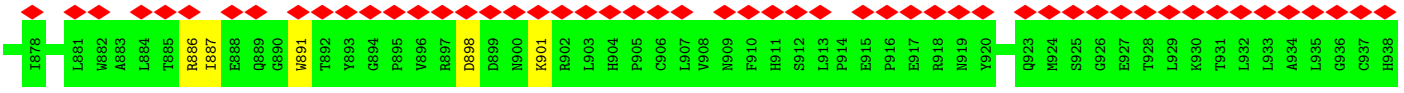


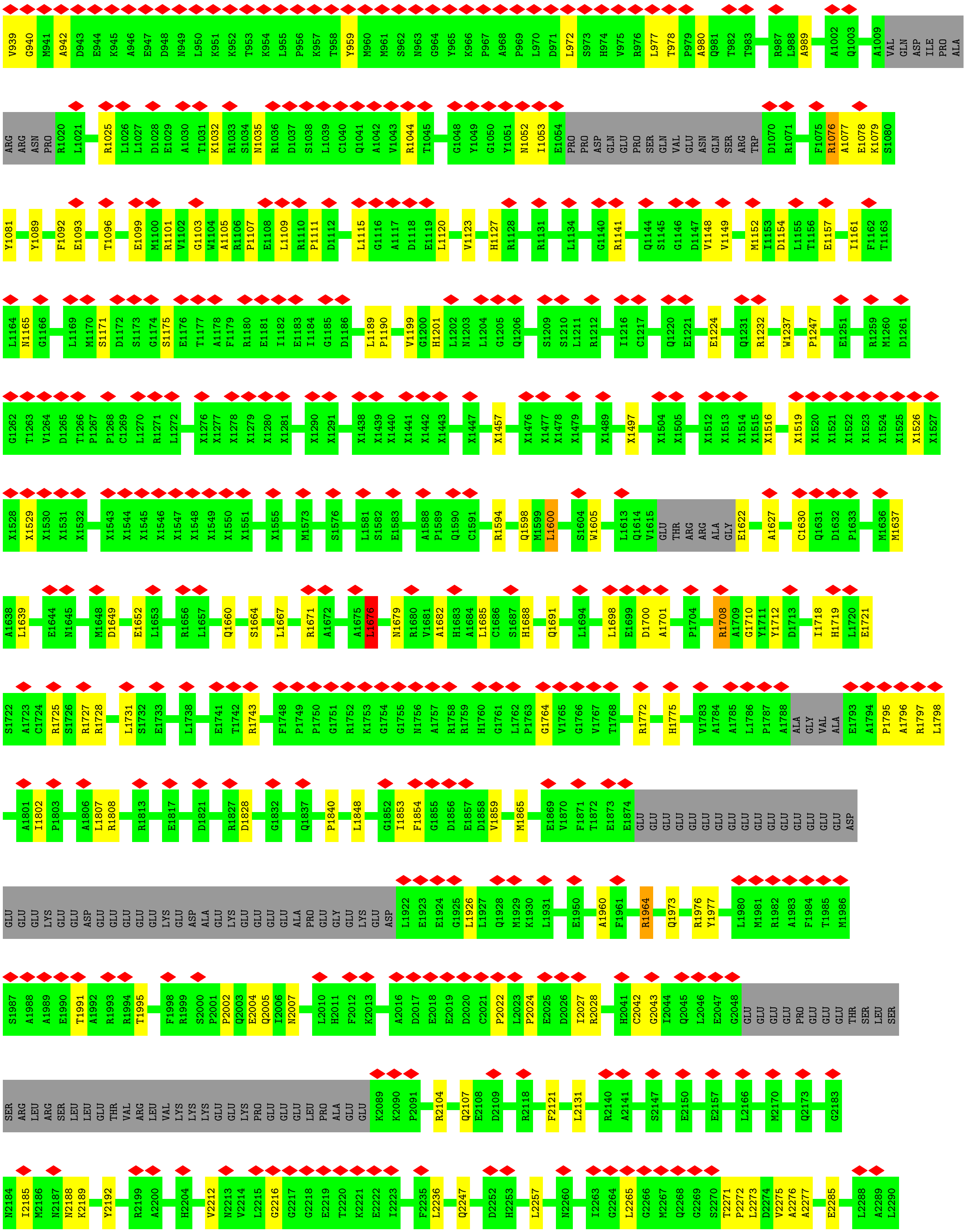








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ARG ARG ASN PRO R1020 L1021 R1025 L1026 L1027 D1028 E1029 A1030 T1031 K1032 R1033 S1034 N1035 R1036 D1037 S1038 L1039 C1040 Q1041 A1042 V1043 R1044 T1045 G1048 Y1049 G1050 Y1051 N1052 I1053 E1054 PRO PRO ASP GLN GLU PRO SER GLN VAL GLU ASN GLN SER ARG TRP D1070 R1071 F1075 R1076 A1077 E1078 K1079 S1080
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L1164 N1165 G1166 L1169 M1170 S1171 D1172 S1173 G1174 S1175 E1176 T1177 A1178 F1179 R1180 E1181 I1182 E1183 I1184 G1185 D1186 L1189 P1190 V1199 G1200 H1201 L1202 N1203 L1204 G1205 Q1206 S1209 S1210 L1211 R1212 I1216 C1217 Q1220 E1221 E1224 Q1231 R1232 W1237 P1247 E1251 R1259 M1260 D1261
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GLU GLU GLU LYS GLU GLU ASP GLU GLU GLU GLU GLU LYS GLU ASP ALA GLU LYS GLU GLU GLU GLU ALA PRO GLU GLY GLU LYS GLU ASP L1922 E1923 E1924 G1925 L1926 L1927 Q1928 M1929 K1930 L1931 E1950 A1960 F1961 R1964 Q1973 R1976 Y1977 L1980 M1981 R1982 A1983 F1984 T1985 M1986
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SER ARG LEU ARG SER LEU LEU GLU THR VAL ARG LEU VAL LYS LYS LYS GLU GLU LYS PRO GLU GLU GLU LEU PRO ALA GLU GLU K2089 K2090 P2091 R2104 Q2107 E2108 D2109 R2118 F2121 L2131 R2140 A2141 S2147 E2150 E2157 L2166 M2170 Q2173 G2183
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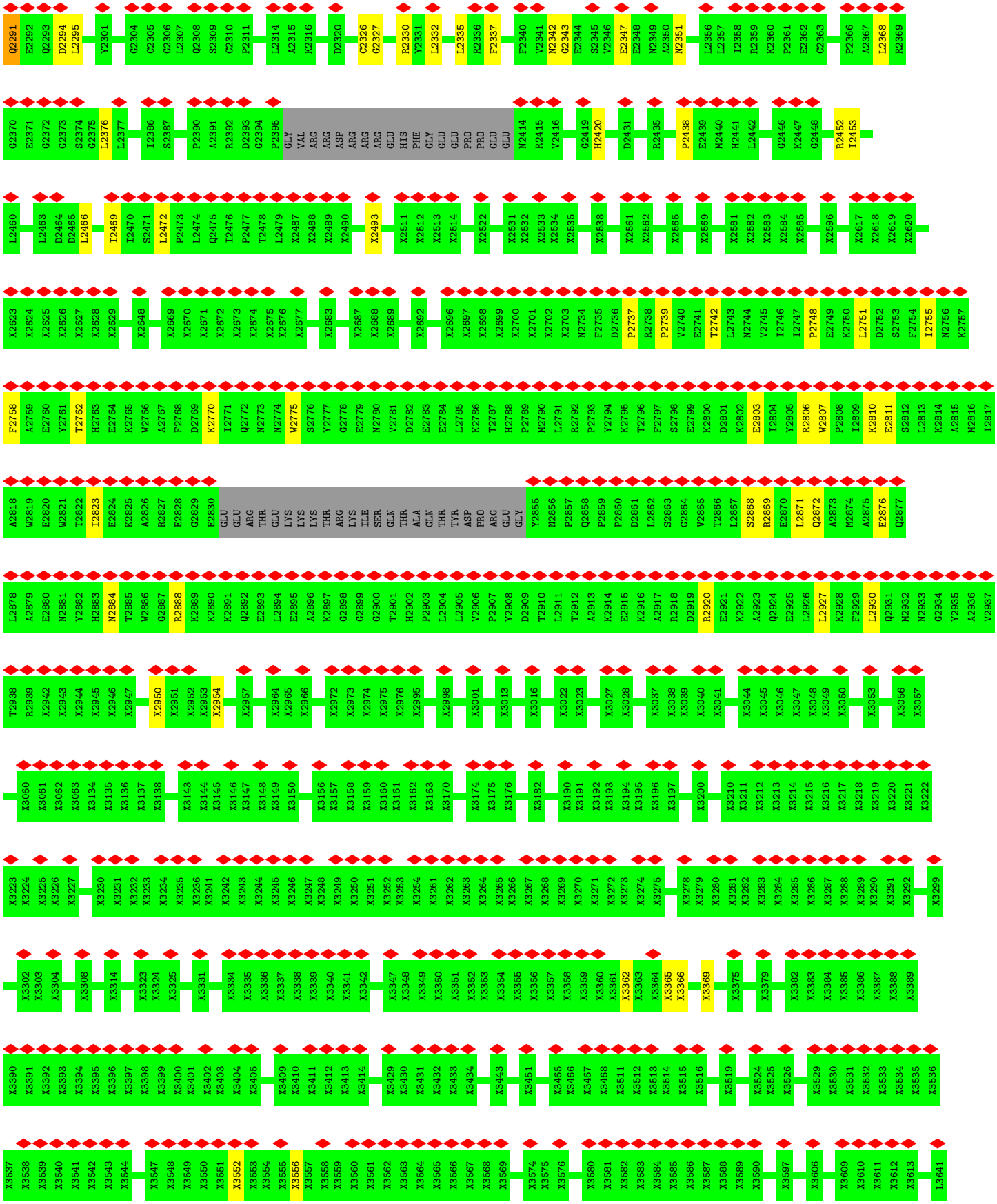
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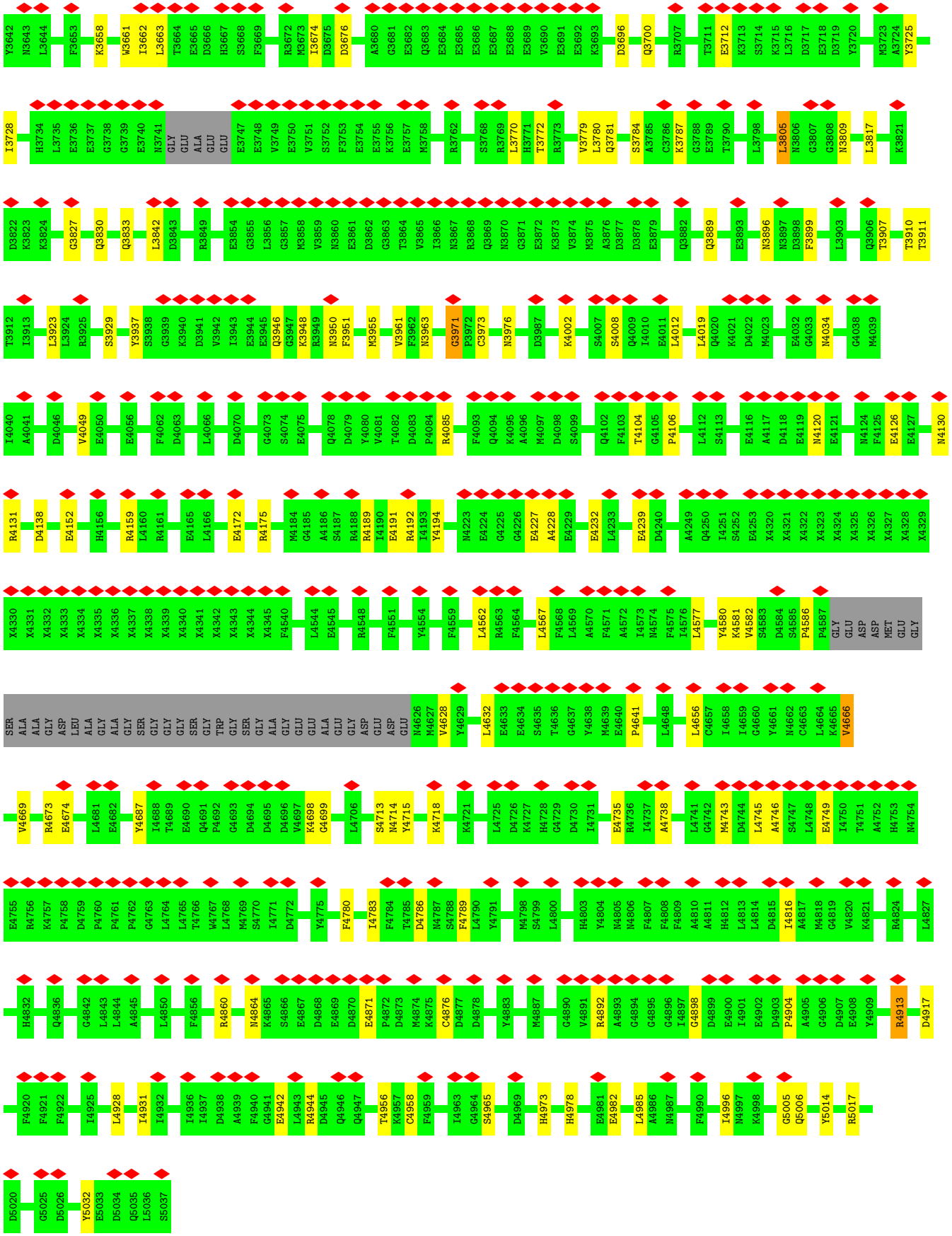
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• Molecule 2: Ryanodine receptor 1

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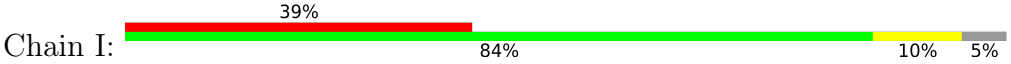

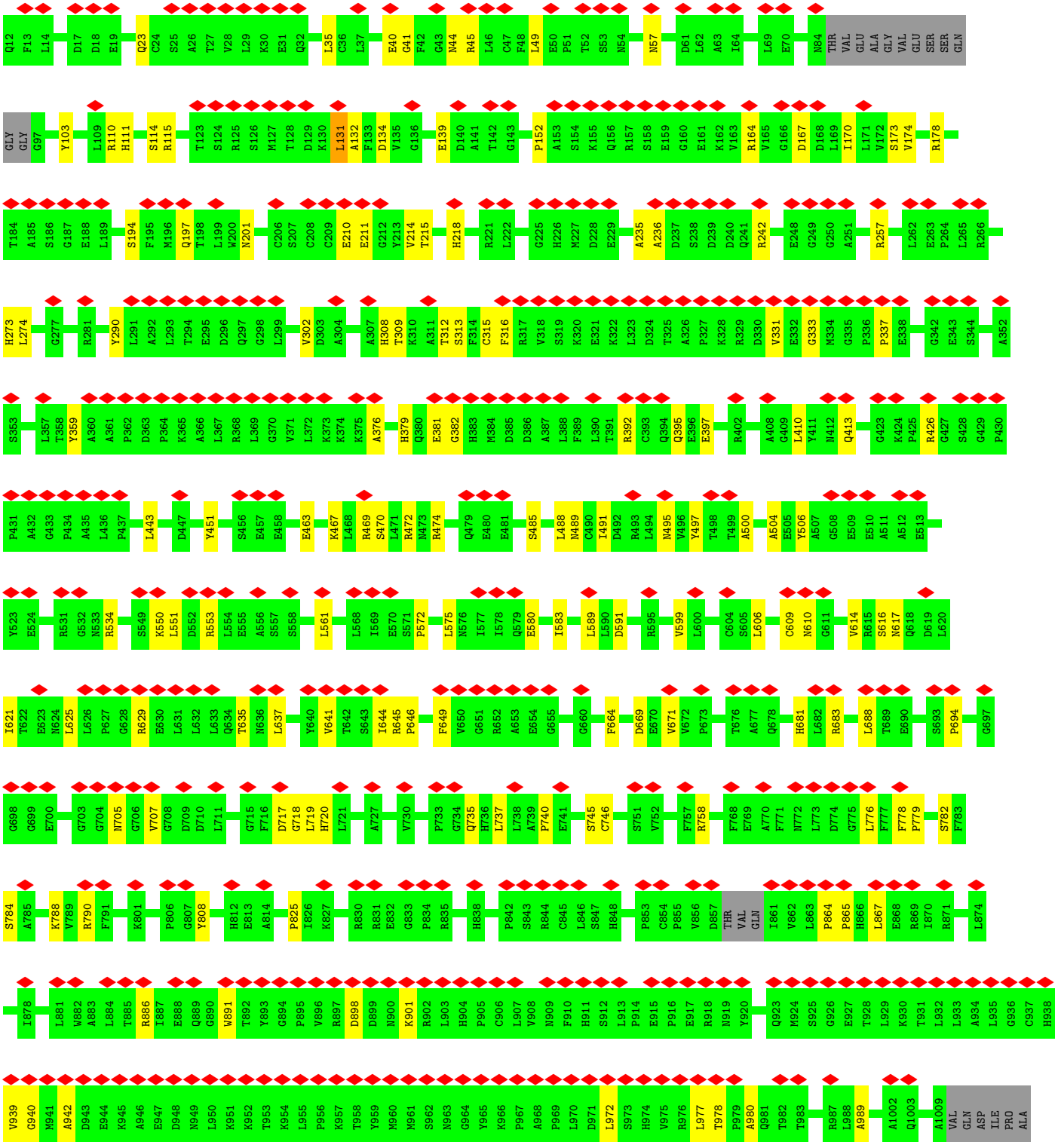

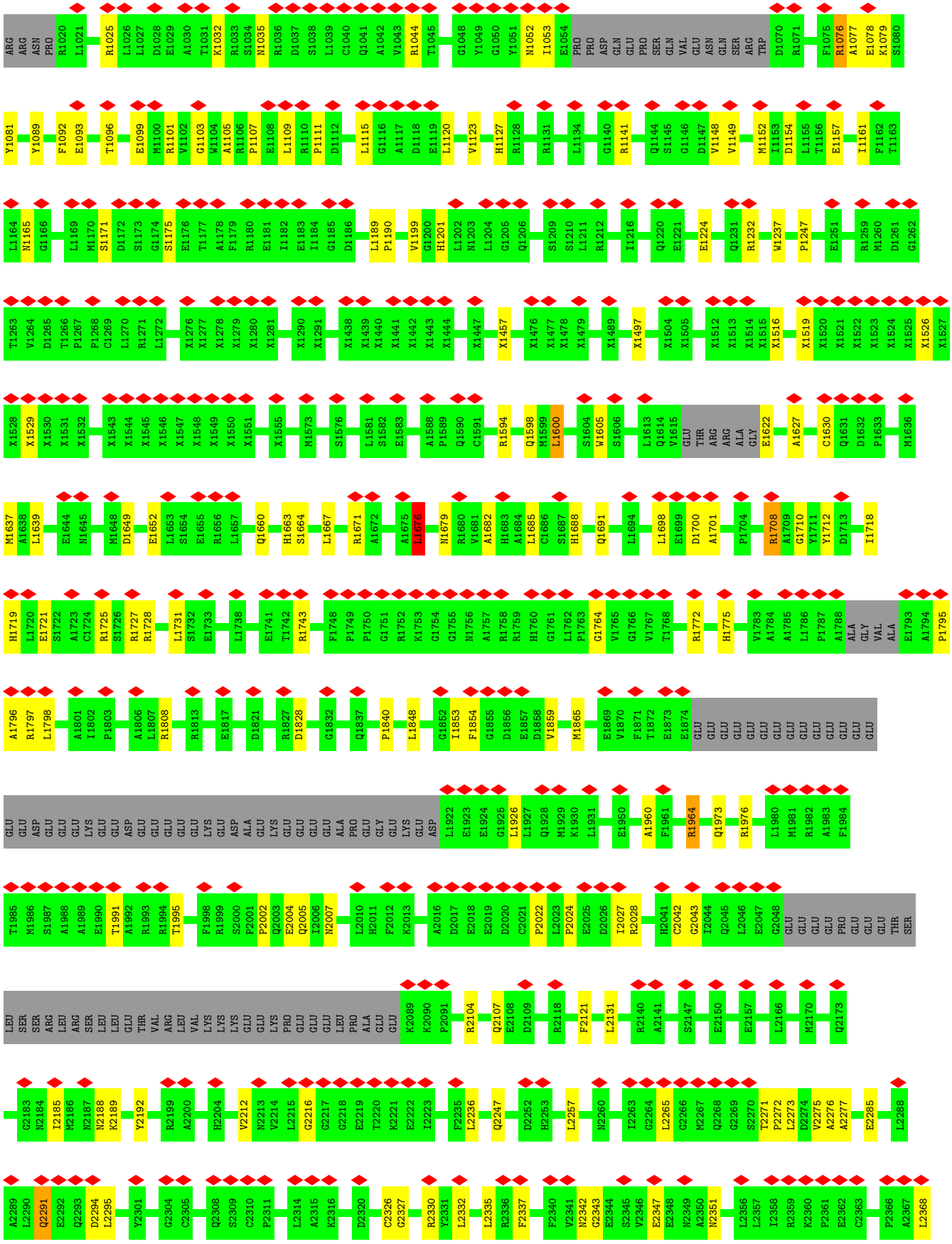
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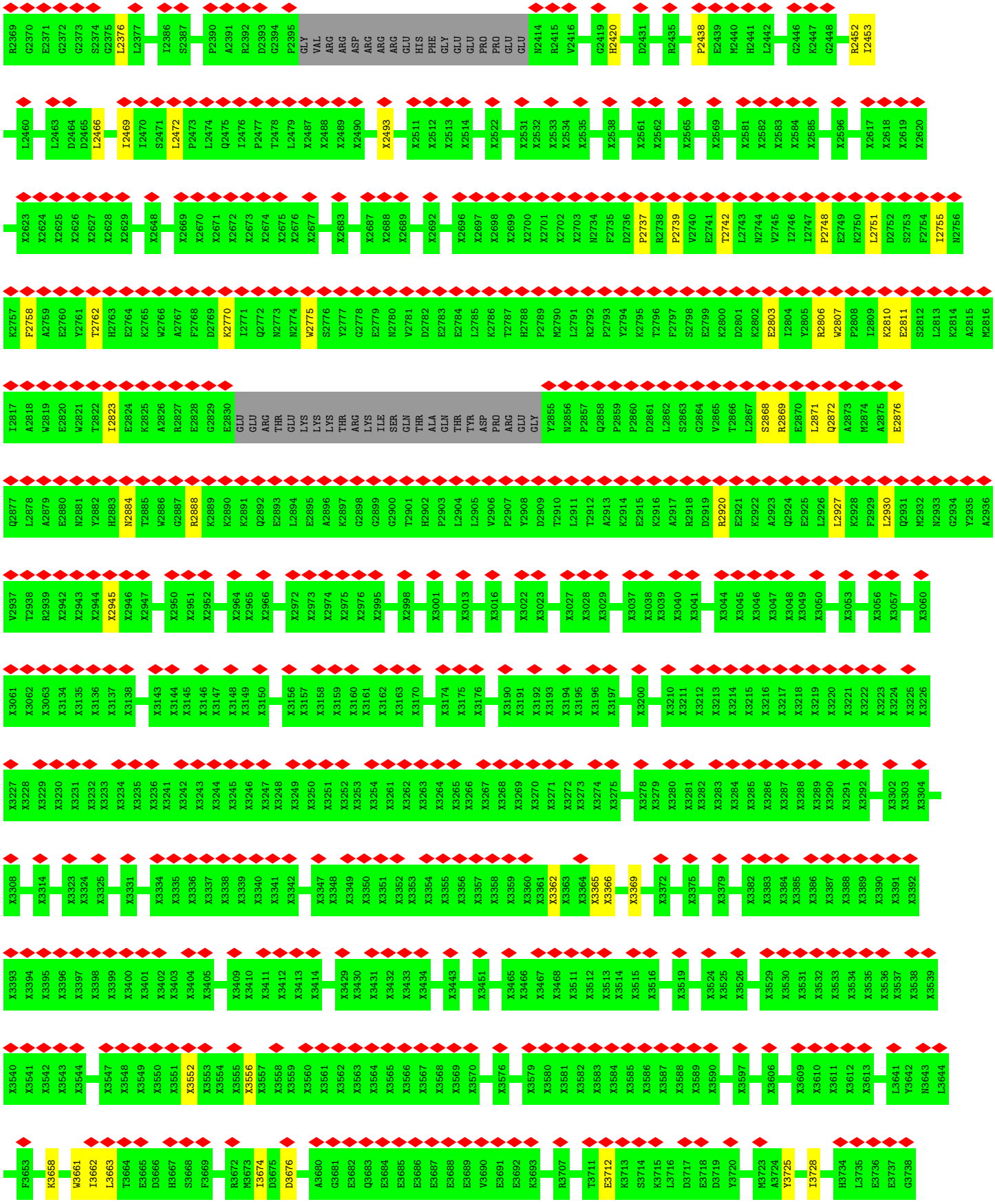
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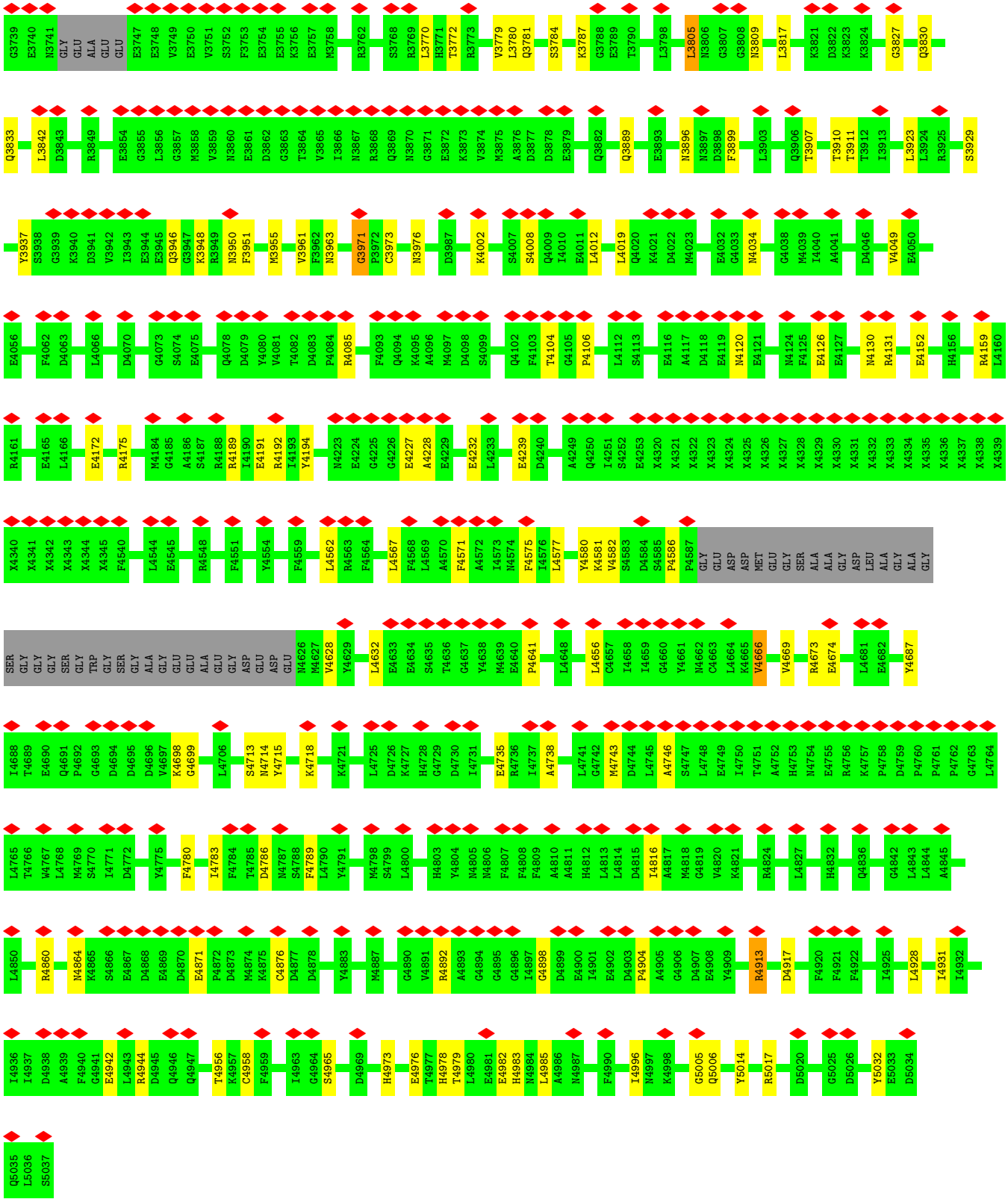
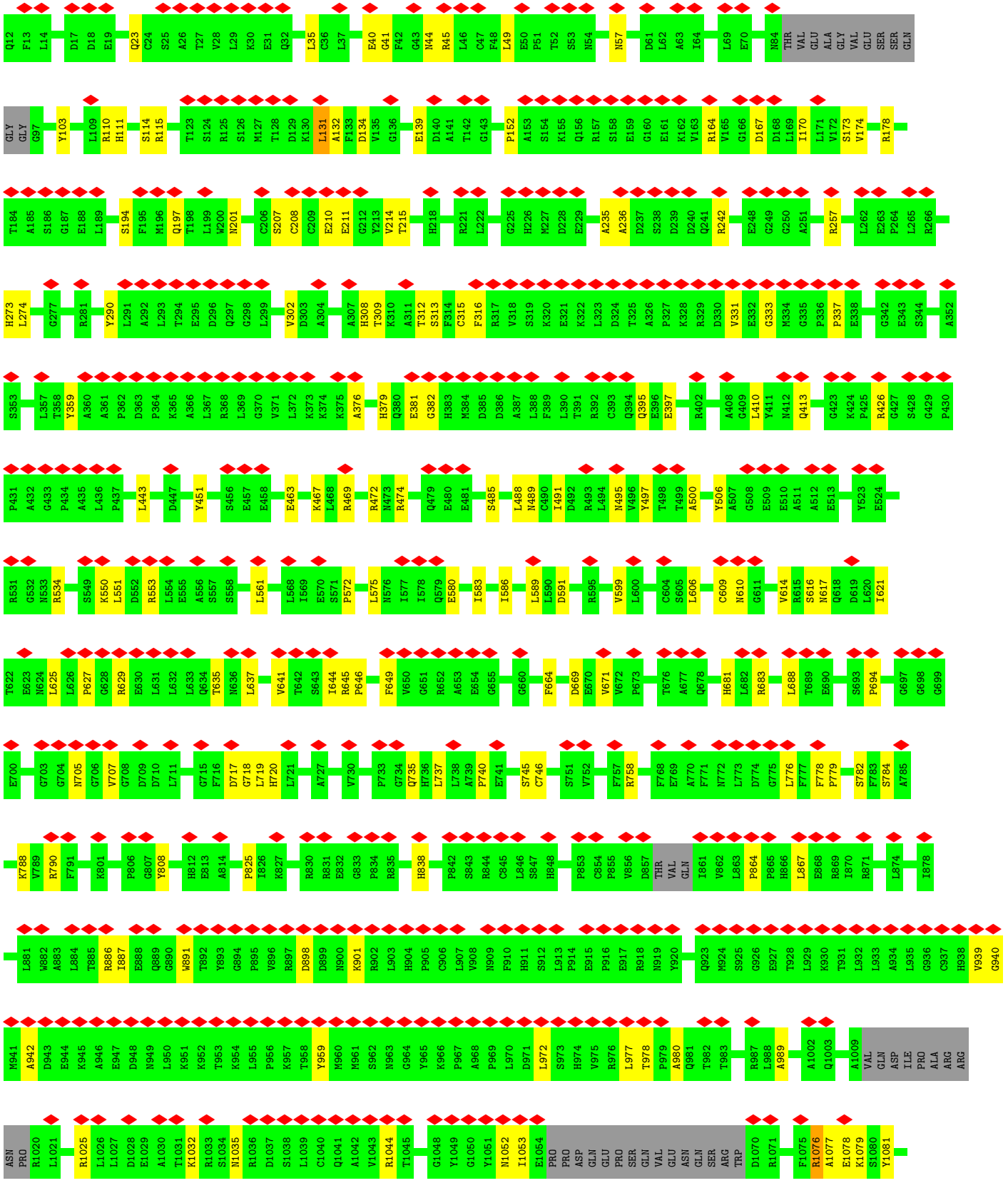


• Molecule 2: Ryanodine receptor 1

Chain E: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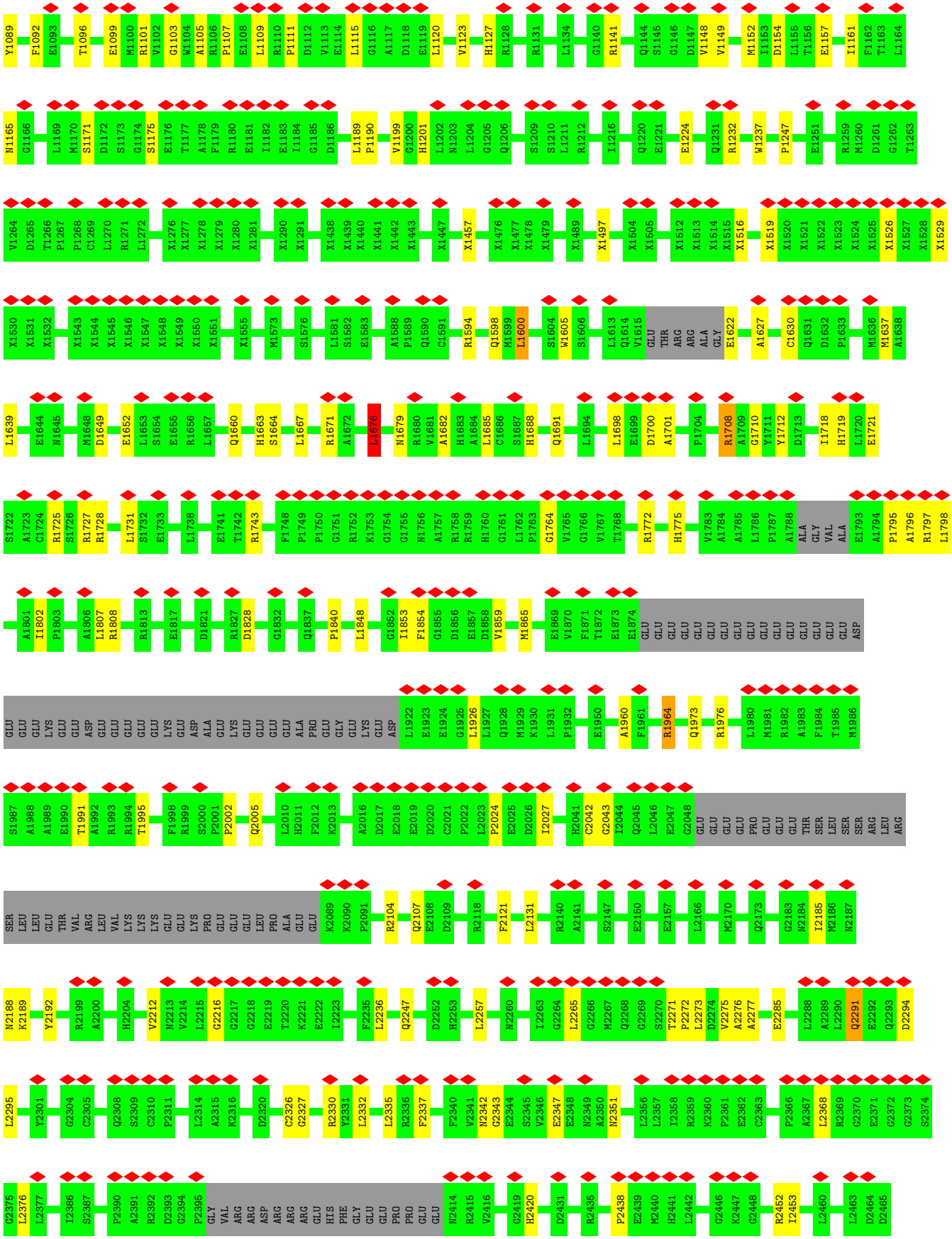
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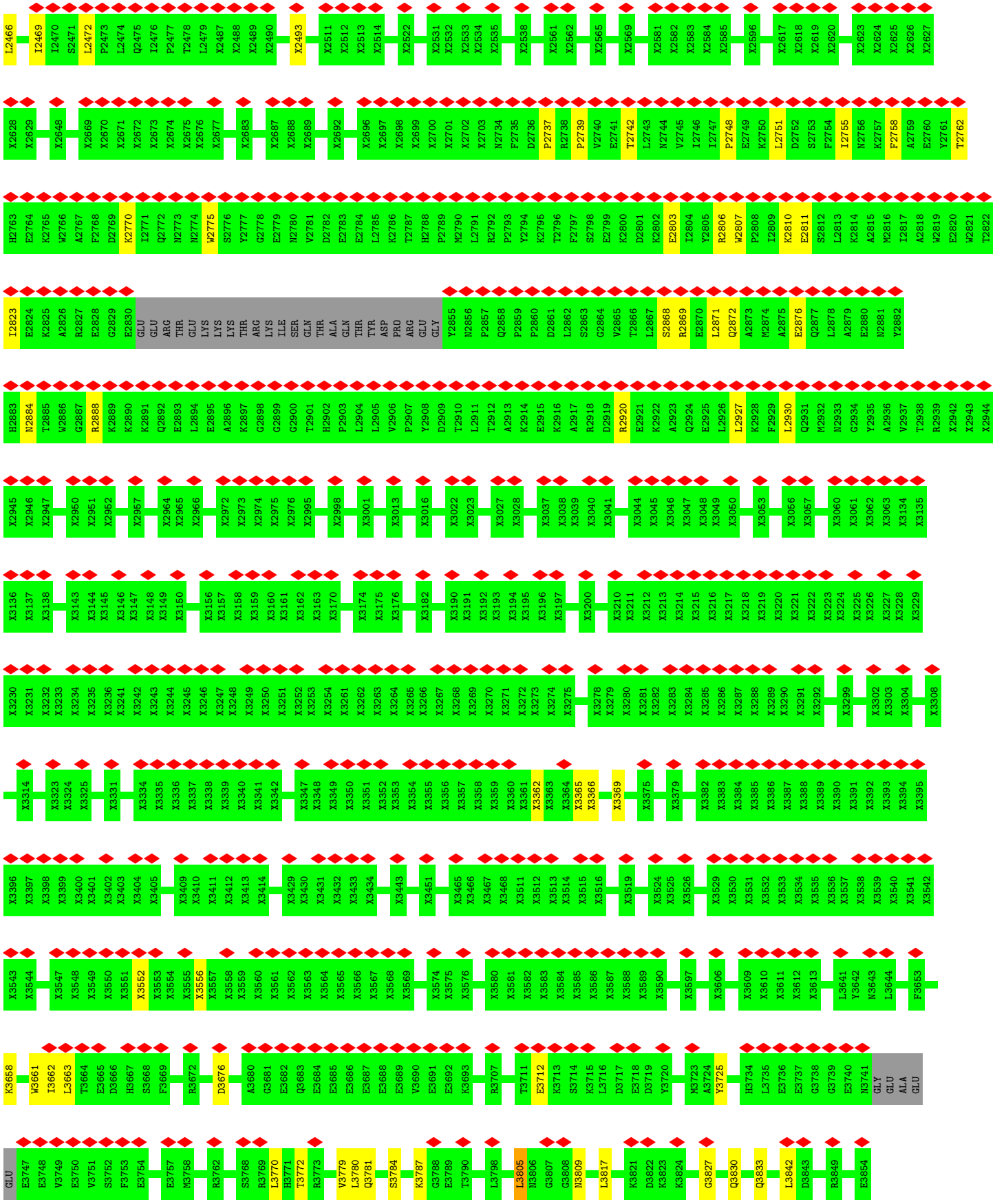
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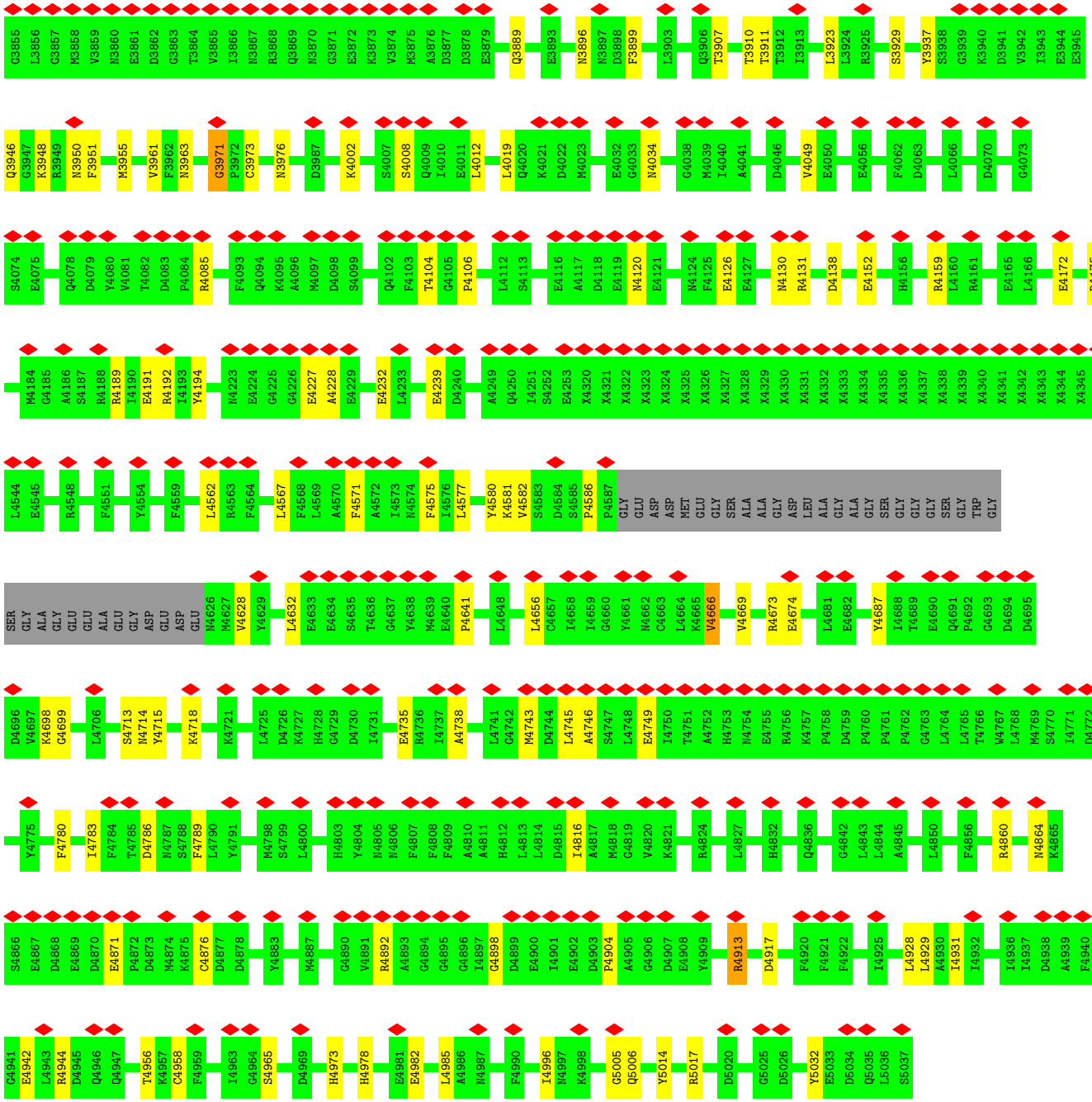
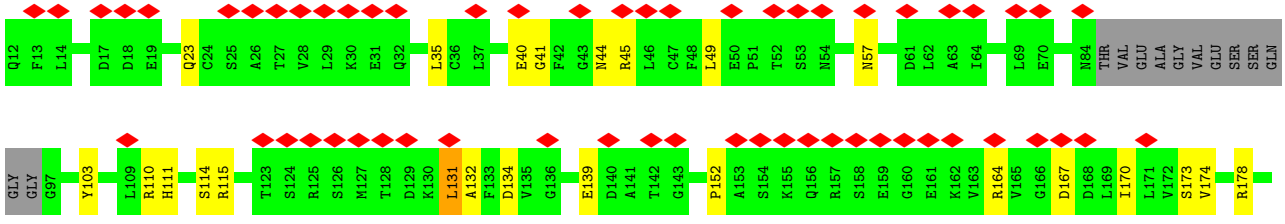
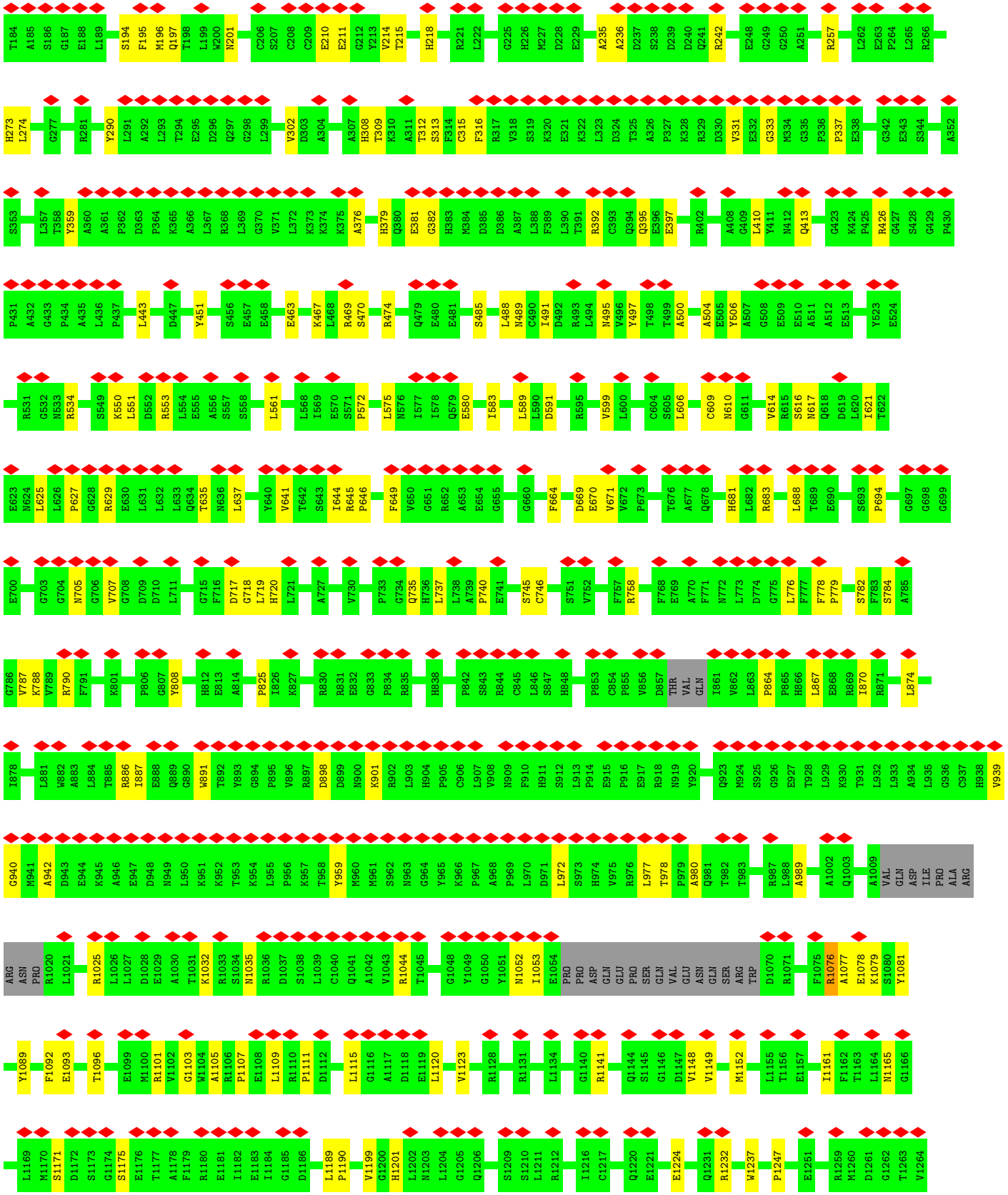


• Molecule 2: Ryanodine receptor 1

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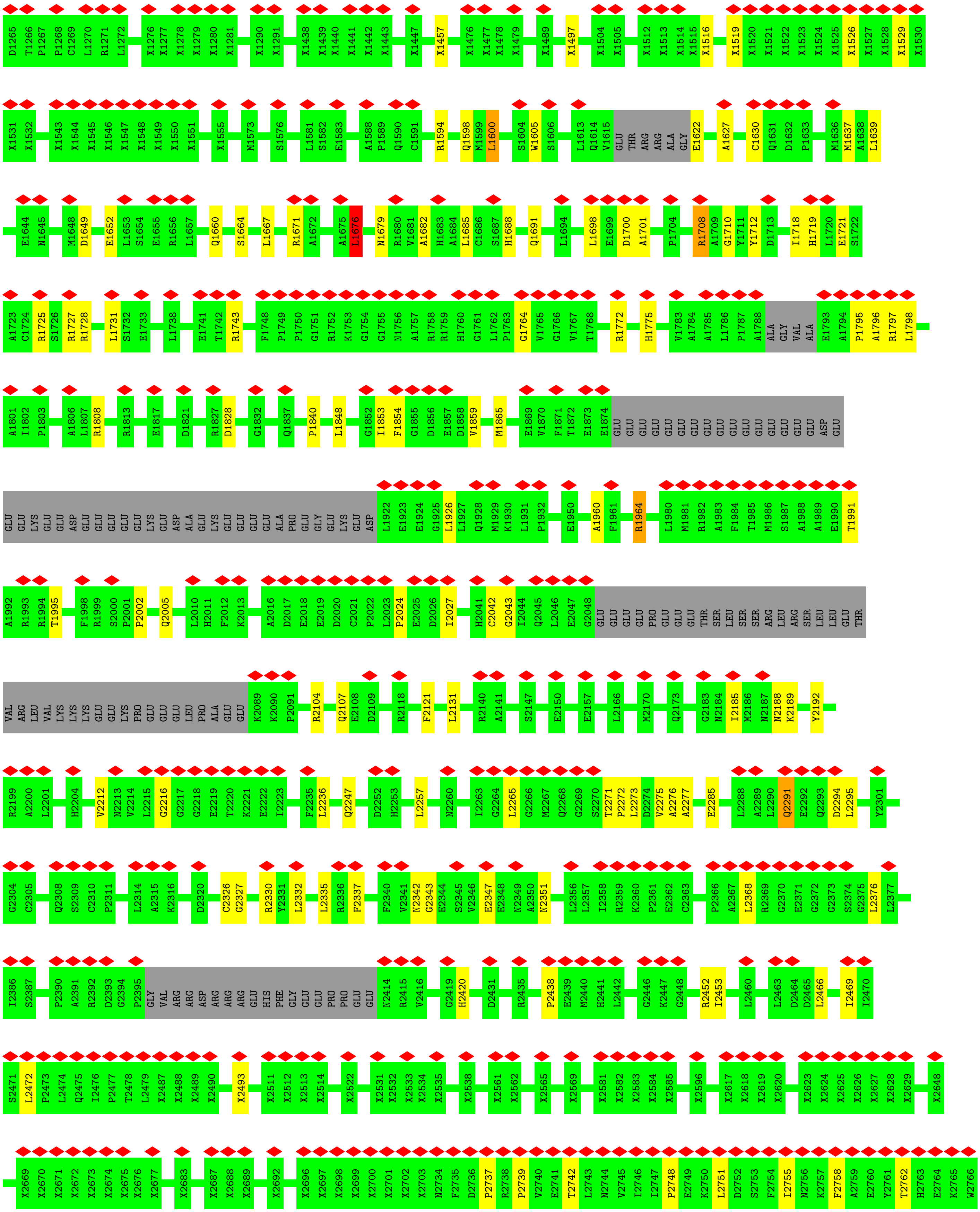
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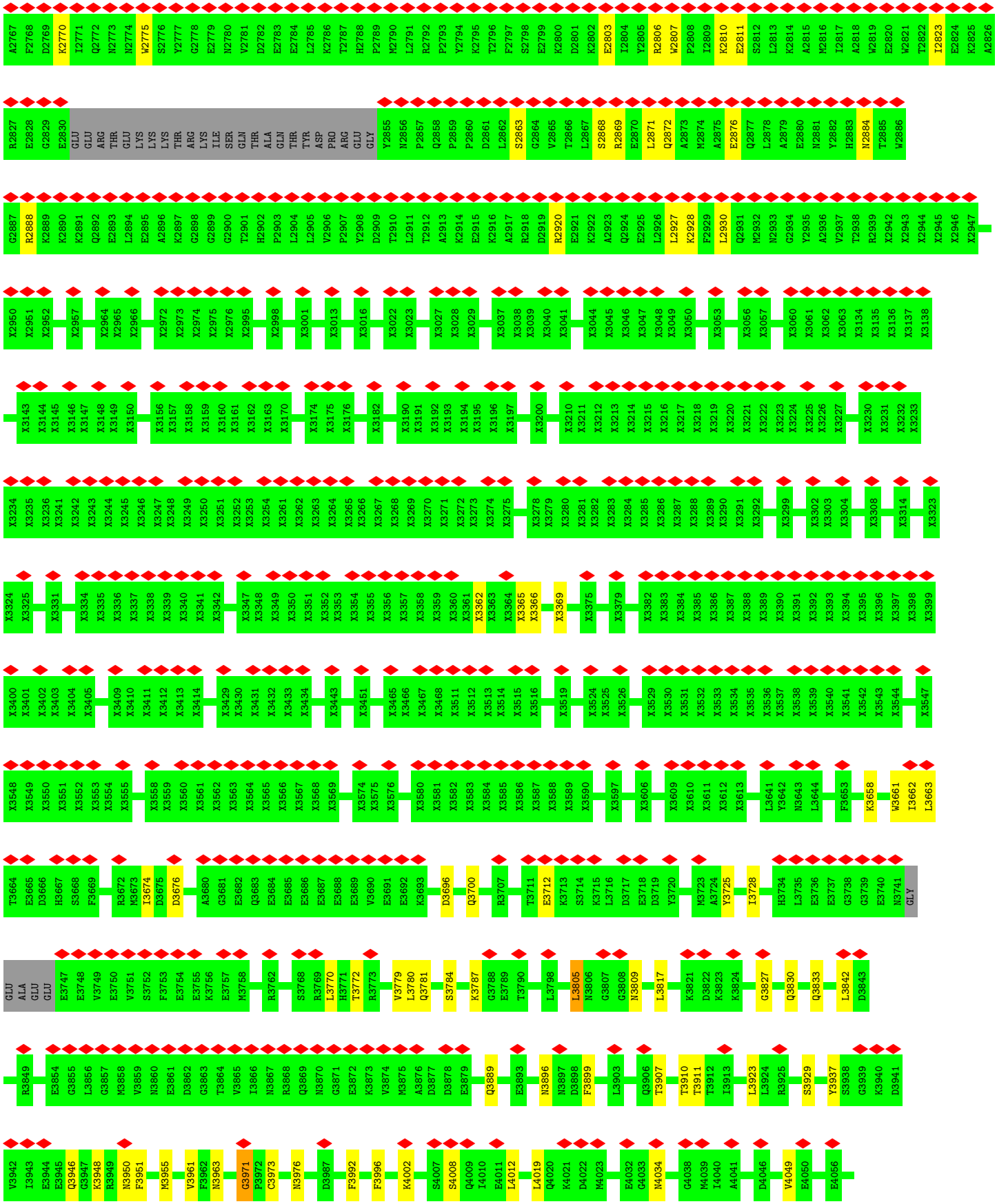
G2304 C2305 Q2308 S2309 C2310 P2311 L2314 A2315 K2316 D2320 C2326 G2327 R2330 Y2331 L2332 L2335 R2336 F2337 F2340 V2341 N2342 G2343 E2344 S2345 V2346 E2347 E2348 N2349 A2350 N2351 L2356 L2357 I2358 R2359 K2360 P2361 E2362 C2363 P2366 A2367 L2368 R2369 G2370 E2371 G2372 G2373 S2374 G2375 L2376 L2377
I2386 S2387 P2390 A2391 R2392 D2393 G2394 P2395 GLY VAL ARG ARG ASP ARG ARG ARG GLU HIS PHE GLY GLU GLU PRO PRO GLU GLU N2414 R2415 V2416 G2419 H2420 D2431 R2435 P2438 E2439 M2440 H2441 L2442 G2446 K2447 G2448 R2452 I2453 L2460 L2463 D2464 D2465 L2466 I2469 I2470
S2471 L2472 P2473 L2474 Q2475 I2476 P2477 T2478 L2479 X2487 X2488 X2489 X2490 X2493 X2511 X2512 X2513 X2514 X2522 X2531 X2532 X2533 X2534 X2535 X2538 X2561 X2562 X2565 X2569 X2581 X2582 X2583 X2584 X2585 X2596 X2617 X2618 X2619 X2620 X2623 X2624 X2625 X2626 X2627 X2628 X2629 X2648
X2669 X2670 X2671 X2672 X2673 X2674 X2675 X2676 X2677 X2683 X2687 X2688 X2689 X2692 X2696 X2697 X2698 X2699 X2700 X2701 X2702 X2703 N2734 F2735 D2736 P2737 R2738 P2739 V2740 E2741 T2742 L2743 N2744 V2745 I2746 I2747 P2748 E2749 K2750 L2751 D2752 S2753 F2754 I2755 N2756 K2757 F2758 A2759 E2760 Y2761 T2762 H2763 E2764 K2765 W2766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R2827 E2828 G2829 E2830 GLU GLU ARG THR GLU LYS LYS LYS THR ARG LYS ILE SER GLN THR ALA GLN THR TYR ASP PRO ARG GLU GLY Y2855 N2856 P2857 Q2858 P2859 P2860 D2861 L2862 S2863 G2864 V2865 T2866 L2867 S2868 R2869 E2870 L2871 Q2872 A2873 M2874 A2875 E2876 Q2877 L2878 A2879 E2880 N2881 Y2882 H2883 N2884 T2885 W2886
G2887 R2888 K2889 K2890 K2891 Q2892 E2893 L2894 E2895 A2896 K2897 G2898 G2899 G2900 T2901 H2902 P2903 L2904 L2905 V2906 P2907 Y2908 D2909 T2910 L2911 T2912 A2913 K2914 E2915 K2916 A2917 R2918 D2919 R2920 E2921 K2922 A2923 Q2924 E2925 L2926 L2927 K2928 F2929 L2930 Q2931 M2932 N2933 G2934 Y2935 A2936 V2937 T2938 R2939 K2940 K2941 K2942 K2943 K2944 K2945 K2946 K2947
X2950 X2951 X2952 X2957 X2964 X2965 X2966 X2972 X2973 X2974 X2975 X2976 X2995 X2998 X3001 X3013 X3016 X3022 X3023 X3027 X3028 X3029 X3037 X3038 X3039 X3040 X3041 X3044 X3045 X3046 X3047 X3048 X3049 X3050 X3053 X3056 X3057 X3060 X3061 X3062 X3063 X3134 X3135 X3136 X3137 X3138
X3143 X3144 X3145 X3146 X3147 X3148 X3149 X3150 X3156 X3157 X3158 X3159 X3160 X3161 X3162 X3163 X3170 X3174 X3175 X3176 X3182 X3190 X3191 X3192 X3193 X3194 X3195 X3196 X3197 X3200 X3210 X3211 X3212 X3213 X3214 X3215 X3216 X3217 X3218 X3219 X3220 X3221 X3222 X3223 X3224 X3225 X3226 X3227 X3230 X3231 X3232 X3233
X3234 X3235 X3236 X3241 X3242 X3243 X3244 X3245 X3246 X3247 X3248 X3249 X3250 X3251 X3252 X3253 X3254 X3261 X3262 X3263 X3264 X3265 X3266 X3267 X3268 X3269 X3270 X3271 X3272 X3273 X3274 X3275 X3278 X3279 X3280 X3281 X3282 X3283 X3284 X3285 X3286 X3287 X3288 X3289 X3290 X3291 X3292 X3299 X3302 X3303 X3304 X3308 X3314 X3323
X3324 X3325 X3331 X3334 X3335 X3336 X3337 X3338 X3339 X3340 X3341 X3342 X3347 X3348 X3349 X3350 X3351 X3352 X3353 X3354 X3355 X3356 X3357 X3358 X3359 X3360 X3361 X3362 X3363 X3364 X3365 X3366 X3369 X3375 X3379 X3382 X3383 X3384 X3385 X3386 X3387 X3388 X3389 X3390 X3391 X3392 X3393 X3394 X3395 X3396 X3397 X3398 X3399
X3400 X3401 X3402 X3403 X3404 X3405 X3409 X3410 X3411 X3412 X3413 X3414 X3429 X3430 X3431 X3432 X3433 X3434 X3443 X3451 X3465 X3466 X3467 X3468 X3511 X3512 X3513 X3514 X3515 X3516 X3519 X3524 X3525 X3526 X3529 X3530 X3531 X3532 X3533 X3534 X3535 X3536 X3537 X3538 X3539 X3540 X3541 X3542 X3543 X3544 X3547
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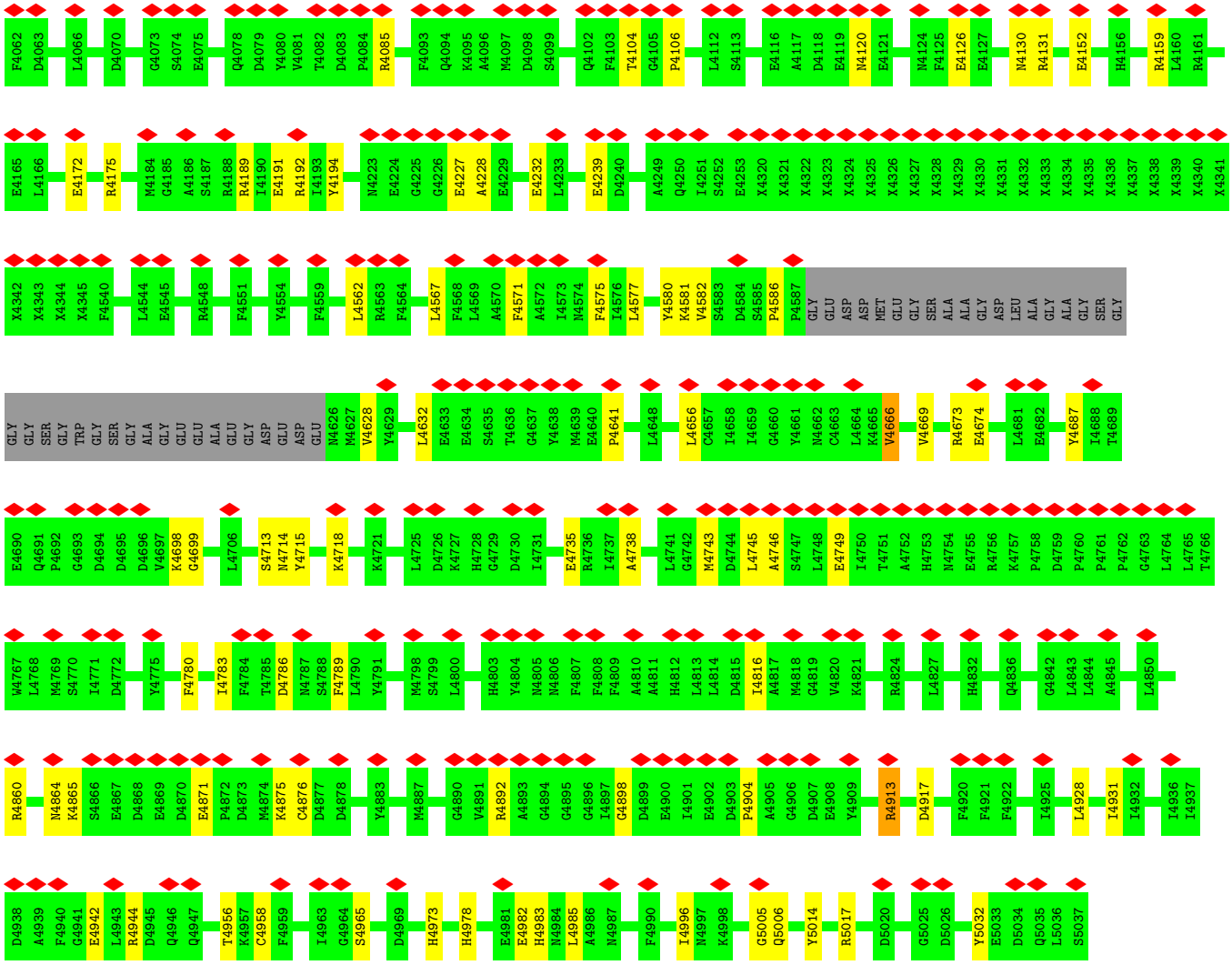
T3664 E3665 D3666 H3667 S3668 F3669 R3672 M3673 I3674 D3675 D3676 A3680 G3681 E3682 Q3683 E3684 E3685 E3686 E3687 E3688 E3689 V3690 E3691 E3692 K3693 D3696 Q3700 R3707 T3711 E3712 K3713 S3714 K3715 L3716 D3717 E3718 D3719 Y3720 M3723 A3724 Y3725 I3728 H3734 L3735 E3736 E3737 G3738 G3739 E3740 N3741 GLY
GLU ALA GLU GLU E3747 E3748 V3749 E3750 V3751 S3752 F3753 E3754 E3755 K3756 E3757 M3758 R3762 S3768 R3769 L3770 H3771 T3772 R3773 V3779 L3780 Q3781 S3784 K3787 G3788 E3789 T3790 L3798 L3805 N3806 G3807 G3808 N3809 L3817 K3821 D3822 K3823 K3824 G3827 Q3830 Q3833 L3842 D3843
R3849 E3854 G3855 L3856 G3857 M3858 V3859 N3860 E3861 D3862 G3863 T3864 V3865 I3866 N3867 R3868 Q3869 N3870 G3871 E3872 K3873 V3874 M3875 A3876 D3877 D3878 E3879 Q3889 E3893 N3896 N3897 D3898 F3899 L3903 Q3906 T3907 T3910 T3911 T3912 I3913 L3923 L3924 R3925 S3929 Y3937 S3938 G3939 K3940 D3941
V3942 I3943 E3944 E3945 Q3946 G3947 K3948 R3949 N3950 F3951 M3955 V3961 F3962 N3963 G3971 P3972 C3973 N3976 D3987 F3992 F3996 K4002 S4007 S4008 Q4009 I4010 E4011 L4012 L4019 Q4020 K4021 D4022 M4023 E4032 G4033 N4034 G4038 M4039 I4040 A4041 D4046 V4049 E4050 E4056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E4165 L4166 E4172 R4175 M4184 G4185 A4186 S4187 R4188 R4189 I4190 E4191 R4192 I4193 Y4194 N4223 E4224 G4225 G4226 E4227 A4228 E4229 E4232 L4233 E4239 D4240 A4249 Q4250 I4251 S4252 E4253 X4320 X4321 X4322 X4323 X4324 X4325 X4326 X4327 X4328 X4329 X4330 X4331 X4332 X4333 X4334 X4335 X4336 X4337 X4338 X4339 X4340 X4341
X4342 X4343 X4344 X4345 F4540 L4544 E4545 R4548 F4551 Y4554 F4559 L4562 R4563 F4564 L4567 F4568 L4569 A4570 F4571 A4572 I4573 N4574 F4575 I4576 L4577 Y4580 K4581 V4582 S4583 D4584 S4585 P4586 P4587 GLY GLU ASP ASP MET GLU GLY SER ALA ALA GLY ASP LEU ALA GLY ALA GLY SER GLY
GLY GLY SER GLY TRP GLY SER GLY ALA GLY GLU GLU ALA GLU GLY ASP GLU ASP GLU N4626 M4627 V4628 Y4629 L4632 E4633 E4634 S4635 T4636 G4637 Y4638 M4639 E4640 P4641 L4648 L4656 C4657 I4658 I4659 G4660 Y4661 N4662 C4663 L4664 K4665 V4666 V4669 R4673 E4674 L4681 E4682 Y4687 I4688 T4689
E4690 Q4691 P4692 G4693 D4694 D4695 D4696 V4697 K4698 G4699 L4706 S4713 N4714 Y4715 K4718 K4721 L4725 D4726 K4727 H4728 G4729 D4730 I4731 E4735 R4736 I4737 A4738 L4741 G4742 M4743 D4744 L4745 A4746 S4747 L4748 E4749 I4750 T4751 A4752 H4753 N4754 E4755 R4756 K4757 P4758 D4759 P4760 P4761 P4762 G4763 L4764 L4765 T4766
W4767 L4768 M4769 S4770 I4771 D4772 Y4775 F4780 I4783 F4784 T4785 D4786 M4787 S4788 F4789 L4790 Y4791 M4798 S4799 L4800 H4803 Y4804 N4805 N4806 F4807 F4808 F4809 A4810 A4811 H4812 L4813 L4814 D4815 I4816 A4817 M4818 G4819 V4820 K4821 R4824 L4827 H4832 Q4836 G4842 L4843 L4844 A4845 L4850
R4860 N4864 K4865 S4866 E4867 D4868 E4869 D4870 E4871 P4872 D4873 M4874 K4875 C4876 D4877 D4878 Y4883 M4887 G4890 V4891 R4892 A4893 G4894 G4895 G4896 I4897 G4898 D4899 E4900 I4901 E4902 D4903 P4904 A4905 G4906 D4907 E4908 Y4909 R4913 D4917 F4920 F4921 F4922 I4925 L4928 I4931 I4932 I4936 I4937
D4938 A4939 F4940 G4941 E4942 L4943 R4944 D4945 Q4946 Q4947 T4956 K4957 C4958 F4959 I4963 G4964 S4965 D4969 H4973 H4978 E4981 E4982 H4983 N4984 L4985 A4986 N4987 F4990 I4996 N4997 K4998 G5005 Q5006 Y5014 R5017 D5020 G5025 D5026 Y5032 E5033 D5034 Q5035 L5036 S5037

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55564	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.095	Depositor
Minimum map value	-0.043	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	502.0, 502.0, 502.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.255, 1.255, 1.255	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, CFF, 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	0.31	0/834	0.52	0/1123
1	F	0.31	0/834	0.52	0/1123
1	H	0.31	0/834	0.52	0/1123
1	J	0.31	0/834	0.52	0/1123
2	B	0.29	0/25428	0.53	6/34534 (0.0%)
2	E	0.29	0/25428	0.53	6/34534 (0.0%)
2	G	0.29	0/25428	0.53	6/34534 (0.0%)
2	I	0.29	0/25428	0.53	6/34534 (0.0%)
All	All	0.29	0/105048	0.53	24/142628 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	14
2	E	0	14
2	G	0	14
2	I	0	14
All	All	0	56

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	131	LEU	CA-CB-CG	8.17	134.09	115.30
2	E	131	LEU	CA-CB-CG	8.17	134.09	115.30
2	I	131	LEU	CA-CB-CG	8.17	134.08	115.30
2	G	131	LEU	CA-CB-CG	8.16	134.08	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	1600	LEU	CA-CB-CG	7.04	131.49	115.30
2	G	1600	LEU	CA-CB-CG	7.04	131.49	115.30
2	B	1600	LEU	CA-CB-CG	7.03	131.47	115.30
2	I	1600	LEU	CA-CB-CG	7.00	131.39	115.30
2	I	1676	LEU	CA-CB-CG	6.44	130.12	115.30
2	G	1676	LEU	CA-CB-CG	6.44	130.11	115.30
2	E	1676	LEU	CA-CB-CG	6.43	130.10	115.30
2	B	1676	LEU	CA-CB-CG	6.42	130.07	115.30
2	G	4985	LEU	CA-CB-CG	6.31	129.82	115.30
2	B	4985	LEU	CA-CB-CG	6.31	129.81	115.30
2	I	4985	LEU	CA-CB-CG	6.30	129.78	115.30
2	E	4985	LEU	CA-CB-CG	6.29	129.76	115.30
2	G	977	LEU	CA-CB-CG	6.18	129.51	115.30
2	I	977	LEU	CA-CB-CG	6.18	129.50	115.30
2	E	977	LEU	CA-CB-CG	6.17	129.50	115.30
2	B	977	LEU	CA-CB-CG	6.17	129.48	115.30
2	B	688	LEU	CA-CB-CG	6.01	129.12	115.30
2	I	688	LEU	CA-CB-CG	6.01	129.11	115.30
2	E	688	LEU	CA-CB-CG	6.00	129.10	115.30
2	G	688	LEU	CA-CB-CG	5.99	129.08	115.30

There are no chirality outliers.

All (56) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	139	GLU	Peptide
2	B	1676	LEU	Peptide
2	B	1795	PRO	Peptide
2	B	1828	ASP	Peptide
2	B	1840	PRO	Peptide
2	B	2291	GLN	Peptide
2	B	2343	GLY	Peptide
2	B	2472	LEU	Peptide
2	B	2807	TRP	Peptide
2	B	312	THR	Peptide
2	B	3971	GLY	Peptide
2	B	4666	VAL	Peptide
2	B	694	PRO	Peptide
2	B	808	TYR	Peptide
2	E	139	GLU	Peptide
2	E	1676	LEU	Peptide
2	E	1795	PRO	Peptide

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Mol	Chain	Res	Type	Group
2	E	1828	ASP	Peptide
2	E	1840	PRO	Peptide
2	E	2291	GLN	Peptide
2	E	2343	GLY	Peptide
2	E	2472	LEU	Peptide
2	E	2807	TRP	Peptide
2	E	312	THR	Peptide
2	E	3971	GLY	Peptide
2	E	4666	VAL	Peptide
2	E	694	PRO	Peptide
2	E	808	TYR	Peptide
2	G	139	GLU	Peptide
2	G	1676	LEU	Peptide
2	G	1795	PRO	Peptide
2	G	1828	ASP	Peptide
2	G	1840	PRO	Peptide
2	G	2291	GLN	Peptide
2	G	2343	GLY	Peptide
2	G	2472	LEU	Peptide
2	G	2807	TRP	Peptide
2	G	312	THR	Peptide
2	G	3971	GLY	Peptide
2	G	4666	VAL	Peptide
2	G	694	PRO	Peptide
2	G	808	TYR	Peptide
2	I	139	GLU	Peptide
2	I	1676	LEU	Peptide
2	I	1795	PRO	Peptide
2	I	1828	ASP	Peptide
2	I	1840	PRO	Peptide
2	I	2291	GLN	Peptide
2	I	2343	GLY	Peptide
2	I	2472	LEU	Peptide
2	I	2807	TRP	Peptide
2	I	312	THR	Peptide
2	I	3971	GLY	Peptide
2	I	4666	VAL	Peptide
2	I	694	PRO	Peptide
2	I	808	TYR	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	818	0	824	10	0
1	F	818	0	824	11	0
1	H	818	0	824	11	0
1	J	818	0	824	9	0
2	B	29499	0	24741	252	0
2	E	29499	0	24741	250	0
2	G	29499	0	24741	251	0
2	I	29499	0	24741	253	0
3	B	31	0	12	1	0
3	E	31	0	12	1	0
3	G	31	0	12	1	0
3	I	31	0	12	1	0
4	B	14	0	10	1	0
4	E	14	0	10	1	0
4	G	14	0	10	1	0
4	I	14	0	10	1	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0
5	I	1	0	0	0	0
All	All	121452	0	102348	1016	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 5.

All (1016) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2291:GLN:HB2	2:E:2295:LEU:HG	1.78	0.66
2:G:2291:GLN:HB2	2:G:2295:LEU:HG	1.78	0.66
2:I:379:HIS:HD2	2:I:382:GLY:H	1.45	0.65
2:B:1743:ARG:O	2:B:1964:ARG:NH2	2.30	0.65
2:I:2291:GLN:HB2	2:I:2295:LEU:HG	1.78	0.65
2:E:4958:CYS:O	3:E:5101:ATP:N6	2.30	0.65
2:B:2291:GLN:HB2	2:B:2295:LEU:HG	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:426:ARG:HB2	2:B:506:TYR:HA	1.79	0.64
2:B:4958:CYS:O	3:B:5101:ATP:N6	2.30	0.64
2:G:1743:ARG:O	2:G:1964:ARG:NH2	2.30	0.64
2:E:788:LYS:HG2	2:E:1630:CYS:H	1.63	0.64
2:G:426:ARG:HB2	2:G:506:TYR:HA	1.79	0.64
2:B:379:HIS:HD2	2:B:382:GLY:H	1.45	0.64
2:G:4958:CYS:O	3:G:5101:ATP:N6	2.30	0.64
2:B:641:VAL:HG21	2:B:705:ASN:HA	1.81	0.63
2:E:379:HIS:HD2	2:E:382:GLY:H	1.45	0.63
2:I:426:ARG:HB2	2:I:506:TYR:HA	1.79	0.63
2:I:1743:ARG:O	2:I:1964:ARG:NH2	2.30	0.63
2:I:4958:CYS:O	3:I:5101:ATP:N6	2.30	0.63
2:I:4582:VAL:HG11	2:G:4860:ARG:HD2	1.81	0.63
2:G:788:LYS:HG2	2:G:1630:CYS:H	1.62	0.63
2:B:4582:VAL:HG11	2:I:4860:ARG:HD2	1.81	0.63
2:E:580:GLU:HG2	2:E:583:ILE:HD11	1.80	0.63
2:E:1743:ARG:O	2:E:1964:ARG:NH2	2.30	0.63
2:E:4860:ARG:HD2	2:G:4582:VAL:HG11	1.80	0.63
2:I:683:ARG:HB2	2:I:782:SER:HB3	1.81	0.63
2:I:580:GLU:HG2	2:I:583:ILE:HD11	1.80	0.63
2:B:788:LYS:HG2	2:B:1630:CYS:H	1.62	0.63
2:I:641:VAL:HG21	2:I:705:ASN:HA	1.81	0.63
2:B:745:SER:HB2	2:B:758:ARG:HB3	1.81	0.62
2:I:745:SER:HB2	2:I:758:ARG:HB3	1.81	0.62
2:E:745:SER:HB2	2:E:758:ARG:HB3	1.81	0.62
2:E:4104:THR:HG22	2:E:4106:PRO:HD2	1.82	0.62
2:G:745:SER:HB2	2:G:758:ARG:HB3	1.81	0.62
2:I:788:LYS:HG2	2:I:1630:CYS:H	1.62	0.62
2:E:426:ARG:HB2	2:E:506:TYR:HA	1.79	0.62
2:E:641:VAL:HG21	2:E:705:ASN:HA	1.81	0.62
2:E:1152:MET:HB2	2:E:1161:ILE:HB	1.82	0.62
2:G:1152:MET:HB2	2:G:1161:ILE:HB	1.82	0.62
2:B:1152:MET:HB2	2:B:1161:ILE:HB	1.82	0.62
2:G:683:ARG:HB2	2:G:782:SER:HB3	1.81	0.62
2:G:580:GLU:HG2	2:G:583:ILE:HD11	1.80	0.62
2:G:641:VAL:HG21	2:G:705:ASN:HA	1.81	0.62
2:B:4104:THR:HG22	2:B:4106:PRO:HD2	1.82	0.62
2:E:683:ARG:HB2	2:E:782:SER:HB3	1.81	0.62
2:B:683:ARG:HB2	2:B:782:SER:HB3	1.81	0.61
2:B:3937:TYR:O	2:B:4002:LYS:NZ	2.34	0.61
2:E:4674:GLU:HG3	2:E:4714:ASN:HB3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:379:HIS:HD2	2:G:382:GLY:H	1.45	0.61
2:B:580:GLU:HG2	2:B:583:ILE:HD11	1.80	0.61
2:G:4674:GLU:HG3	2:G:4714:ASN:HB3	1.83	0.61
2:B:4674:GLU:HG3	2:B:4714:ASN:HB3	1.83	0.61
2:I:1152:MET:HB2	2:I:1161:ILE:HB	1.82	0.61
2:G:4104:THR:HG22	2:G:4106:PRO:HD2	1.82	0.61
2:E:3937:TYR:O	2:E:4002:LYS:NZ	2.34	0.61
2:I:173:SER:HB3	2:I:178:ARG:H	1.66	0.61
2:I:4674:GLU:HG3	2:I:4714:ASN:HB3	1.83	0.61
2:G:173:SER:HB3	2:G:178:ARG:H	1.66	0.61
2:B:4860:ARG:HD2	2:E:4582:VAL:HG11	1.81	0.61
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.34	0.60
2:I:4104:THR:HG22	2:I:4106:PRO:HD2	1.82	0.60
2:B:173:SER:HB3	2:B:178:ARG:H	1.66	0.60
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.34	0.60
2:G:3955:MET:HG3	2:G:4019:LEU:HD22	1.84	0.60
2:B:2291:GLN:HB3	2:B:2294:ASP:H	1.67	0.60
2:I:2291:GLN:HB3	2:I:2294:ASP:H	1.67	0.60
2:I:359:TYR:HA	2:I:376:ALA:HA	1.84	0.59
2:I:3955:MET:HG3	2:I:4019:LEU:HD22	1.84	0.59
2:G:2291:GLN:HB3	2:G:2294:ASP:H	1.67	0.59
2:E:3955:MET:HG3	2:E:4019:LEU:HD22	1.84	0.59
2:E:2291:GLN:HB3	2:E:2294:ASP:H	1.67	0.59
2:E:173:SER:HB3	2:E:178:ARG:H	1.66	0.59
2:E:1685:LEU:HA	2:E:1688:HIS:HD2	1.68	0.59
2:B:359:TYR:HA	2:B:376:ALA:HA	1.84	0.59
2:B:3955:MET:HG3	2:B:4019:LEU:HD22	1.84	0.59
2:B:2347:GLU:O	2:B:2351:ASN:N	2.32	0.59
2:I:2737:PRO:O	2:I:2888:ARG:NH2	2.36	0.59
2:E:4996:ILE:HG12	4:E:5102:CFF:H123	1.85	0.59
2:I:4996:ILE:HG12	4:I:5102:CFF:H123	1.85	0.59
2:B:4996:ILE:HG12	4:B:5102:CFF:H123	1.85	0.59
2:I:1685:LEU:HA	2:I:1688:HIS:HD2	1.68	0.59
2:G:1685:LEU:HA	2:G:1688:HIS:HD2	1.68	0.59
2:I:1519:UNK:HA	2:I:1526:UNK:HA	1.85	0.58
2:G:359:TYR:HA	2:G:376:ALA:HA	1.84	0.58
2:E:2737:PRO:O	2:E:2888:ARG:NH2	2.36	0.58
2:G:2737:PRO:O	2:G:2888:ARG:NH2	2.36	0.58
2:G:1519:UNK:HA	2:G:1526:UNK:HA	1.85	0.58
2:G:4996:ILE:HG12	4:G:5102:CFF:H123	1.85	0.58
2:B:1685:LEU:HA	2:B:1688:HIS:HD2	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2737:PRO:O	2:B:2888:ARG:NH2	2.36	0.58
2:E:359:TYR:HA	2:E:376:ALA:HA	1.84	0.58
2:G:331:VAL:HG12	2:G:333:GLY:H	1.68	0.58
2:G:671:VAL:HG22	2:G:740:PRO:HG3	1.86	0.58
2:G:2347:GLU:O	2:G:2351:ASN:N	2.32	0.58
2:I:671:VAL:HG22	2:I:740:PRO:HG3	1.86	0.58
2:B:609:CYS:SG	2:B:610:ASN:N	2.77	0.58
2:E:174:VAL:O	2:G:2452:ARG:NH1	2.37	0.57
2:E:2770:LYS:HB3	2:E:2775:TRP:HB2	1.86	0.57
2:G:609:CYS:SG	2:G:610:ASN:N	2.77	0.57
2:I:2326:CYS:SG	2:I:2327:GLY:N	2.77	0.57
2:G:683:ARG:NH1	2:G:707:VAL:O	2.37	0.57
2:G:3770:LEU:HD23	2:G:3772:THR:HG22	1.86	0.57
2:B:174:VAL:O	2:E:2452:ARG:NH1	2.37	0.57
2:I:2452:ARG:NH1	2:G:174:VAL:O	2.37	0.57
2:E:1519:UNK:HA	2:E:1526:UNK:HA	1.85	0.57
2:E:3770:LEU:HD23	2:E:3772:THR:HG22	1.86	0.57
2:B:2326:CYS:SG	2:B:2327:GLY:N	2.77	0.57
2:B:3770:LEU:HD23	2:B:3772:THR:HG22	1.86	0.57
2:I:609:CYS:SG	2:I:610:ASN:N	2.77	0.57
2:G:2326:CYS:SG	2:G:2327:GLY:N	2.77	0.57
2:E:110:ARG:HH21	2:E:115:ARG:HB3	1.69	0.57
2:E:2326:CYS:SG	2:E:2327:GLY:N	2.77	0.57
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	1.86	0.57
2:G:463:GLU:OE2	2:G:467:LYS:NZ	2.38	0.57
2:B:614:VAL:HG22	2:B:616:SER:H	1.70	0.57
2:I:110:ARG:HH21	2:I:115:ARG:HB3	1.69	0.57
2:I:614:VAL:HG22	2:I:616:SER:H	1.70	0.57
2:B:1519:UNK:HA	2:B:1526:UNK:HA	1.85	0.57
2:G:110:ARG:HH21	2:G:115:ARG:HB3	1.69	0.57
2:G:2748:PRO:HD2	2:G:2751:LEU:HD12	1.86	0.57
2:B:110:ARG:HH21	2:B:115:ARG:HB3	1.69	0.57
2:B:463:GLU:OE2	2:B:467:LYS:NZ	2.38	0.57
2:I:331:VAL:HG12	2:I:333:GLY:H	1.68	0.57
2:E:671:VAL:HG22	2:E:740:PRO:HG3	1.86	0.57
2:B:1079:LYS:NZ	2:B:1107:PRO:O	2.38	0.57
2:I:1079:LYS:NZ	2:I:1107:PRO:O	2.38	0.57
2:I:2770:LYS:HB3	2:I:2775:TRP:HB2	1.86	0.57
2:I:3770:LEU:HD23	2:I:3772:THR:HG22	1.87	0.57
2:E:609:CYS:SG	2:E:610:ASN:N	2.77	0.57
2:B:671:VAL:HG22	2:B:740:PRO:HG3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2748:PRO:HD2	2:B:2751:LEU:HD12	1.86	0.56
2:I:132:ALA:HA	2:I:194:SER:HB2	1.87	0.56
2:E:463:GLU:OE2	2:E:467:LYS:NZ	2.38	0.56
2:E:331:VAL:HG12	2:E:333:GLY:H	1.68	0.56
2:B:210:GLU:HG3	2:B:337:PRO:HG3	1.87	0.56
2:B:1865:MET:HB3	2:B:1926:LEU:HB2	1.88	0.56
2:I:57:ASN:HD22	2:I:308:HIS:HB2	1.70	0.56
2:I:2347:GLU:O	2:I:2351:ASN:N	2.32	0.56
2:I:2748:PRO:HD2	2:I:2751:LEU:HD12	1.86	0.56
2:E:614:VAL:HG22	2:E:616:SER:H	1.70	0.56
2:G:132:ALA:HA	2:G:194:SER:HB2	1.88	0.56
2:B:2452:ARG:NH1	2:I:174:VAL:O	2.38	0.56
2:G:57:ASN:HD22	2:G:308:HIS:HB2	1.70	0.56
2:G:1079:LYS:NZ	2:G:1107:PRO:O	2.38	0.56
2:I:463:GLU:OE2	2:I:467:LYS:NZ	2.38	0.56
2:G:2770:LYS:HB3	2:G:2775:TRP:HB2	1.86	0.56
2:B:331:VAL:HG12	2:B:333:GLY:H	1.68	0.56
2:I:210:GLU:HG3	2:I:337:PRO:HG3	1.88	0.56
2:I:497:TYR:HB3	2:I:500:ALA:HB2	1.88	0.56
2:E:132:ALA:HA	2:E:194:SER:HB2	1.88	0.56
2:B:4904:PRO:HB3	2:B:4913:ARG:HD2	1.88	0.56
2:E:1865:MET:HB3	2:E:1926:LEU:HB2	1.88	0.56
2:E:57:ASN:HD22	2:E:308:HIS:HB2	1.70	0.56
2:G:1077:ALA:HB3	2:G:1189:LEU:HD11	1.88	0.56
2:B:132:ALA:HA	2:B:194:SER:HB2	1.87	0.56
2:B:497:TYR:HB3	2:B:500:ALA:HB2	1.88	0.56
2:B:664:PHE:HB2	2:B:746:CYS:HB2	1.88	0.56
2:I:683:ARG:NH1	2:I:707:VAL:O	2.37	0.56
2:I:1679:ASN:ND2	2:I:1798:LEU:O	2.39	0.56
2:E:2748:PRO:HD2	2:E:2751:LEU:HD12	1.86	0.56
2:G:614:VAL:HG22	2:G:616:SER:H	1.70	0.56
2:G:1679:ASN:ND2	2:G:1798:LEU:O	2.39	0.56
2:G:1865:MET:HB3	2:G:1926:LEU:HB2	1.88	0.56
2:E:1079:LYS:NZ	2:E:1107:PRO:O	2.38	0.56
2:B:1679:ASN:ND2	2:B:1798:LEU:O	2.39	0.55
2:E:1679:ASN:ND2	2:E:1798:LEU:O	2.39	0.55
2:E:4904:PRO:HB3	2:E:4913:ARG:HD2	1.88	0.55
2:B:57:ASN:HD22	2:B:308:HIS:HB2	1.70	0.55
2:I:1865:MET:HB3	2:I:1926:LEU:HB2	1.88	0.55
2:E:210:GLU:HG3	2:E:337:PRO:HG3	1.88	0.55
2:E:2347:GLU:O	2:E:2351:ASN:N	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:645:ARG:HH11	2:I:778:PHE:HE1	1.55	0.55
2:I:1077:ALA:HB3	2:I:1189:LEU:HD11	1.88	0.55
2:B:683:ARG:NH1	2:B:707:VAL:O	2.37	0.55
2:B:1077:ALA:HB3	2:B:1189:LEU:HD11	1.88	0.55
2:I:4944:ARG:HH22	2:G:4942:GLU:HA	1.72	0.55
2:I:664:PHE:HB2	2:I:746:CYS:HB2	1.88	0.55
2:B:1109:LEU:HA	2:B:1120:LEU:HD21	1.89	0.55
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.89	0.55
2:G:1109:LEU:HA	2:G:1120:LEU:HD21	1.89	0.55
2:B:4944:ARG:HH22	2:I:4942:GLU:HA	1.72	0.55
2:I:4904:PRO:HB3	2:I:4913:ARG:HD2	1.88	0.55
2:E:1077:ALA:HB3	2:E:1189:LEU:HD11	1.88	0.55
2:E:1109:LEU:HA	2:E:1120:LEU:HD21	1.89	0.55
2:G:497:TYR:HB3	2:G:500:ALA:HB2	1.88	0.55
2:B:645:ARG:HH11	2:B:778:PHE:HE1	1.55	0.55
2:E:497:TYR:HB3	2:E:500:ALA:HB2	1.88	0.55
2:G:210:GLU:HG3	2:G:337:PRO:HG3	1.87	0.55
2:G:4743:MET:HB3	2:G:4746:ALA:HB3	1.89	0.55
2:E:683:ARG:NH1	2:E:707:VAL:O	2.37	0.55
2:B:1700:ASP:OD2	2:B:1708:ARG:NH2	2.40	0.54
2:I:646:PRO:HD2	2:I:779:PRO:HB2	1.89	0.54
1:J:34:LYS:HD3	2:I:629:ARG:HD2	1.89	0.54
2:B:2420:HIS:ND1	2:B:2493:UNK:O	2.41	0.54
2:E:664:PHE:HB2	2:E:746:CYS:HB2	1.88	0.54
2:E:719:LEU:HD22	2:E:735:GLN:HG2	1.90	0.54
2:E:1105:ALA:HB1	2:E:1109:LEU:HD21	1.89	0.54
2:G:2420:HIS:ND1	2:G:2493:UNK:O	2.40	0.54
2:G:4904:PRO:HB3	2:G:4913:ARG:HD2	1.88	0.54
2:B:4189:ARG:NH1	2:B:5032:TYR:OH	2.39	0.54
2:B:4942:GLU:HA	2:E:4944:ARG:HH22	1.73	0.54
2:G:645:ARG:HH11	2:G:778:PHE:HE1	1.55	0.54
2:G:1105:ALA:HB1	2:G:1109:LEU:HD21	1.89	0.54
2:B:4743:MET:HB3	2:B:4746:ALA:HB3	1.89	0.54
2:I:2420:HIS:ND1	2:I:2493:UNK:O	2.40	0.54
2:I:3948:LYS:NZ	2:I:4008:SER:O	2.41	0.54
2:E:646:PRO:HD2	2:E:779:PRO:HB2	1.89	0.54
2:B:1092:PHE:HB3	2:B:1149:VAL:HB	1.89	0.54
2:I:103:TYR:HB3	2:I:152:PRO:HD3	1.89	0.54
2:I:1700:ASP:OD2	2:I:1708:ARG:NH2	2.40	0.54
2:E:103:TYR:HB3	2:E:152:PRO:HD3	1.89	0.54
2:I:1109:LEU:HA	2:I:1120:LEU:HD21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1700:ASP:OD2	2:E:1708:ARG:NH2	2.41	0.54
2:E:2420:HIS:ND1	2:E:2493:UNK:O	2.41	0.54
2:I:1105:ALA:HB1	2:I:1109:LEU:HD21	1.89	0.54
2:I:4189:ARG:NH1	2:I:5032:TYR:OH	2.39	0.54
2:E:886:ARG:HB3	2:E:891:TRP:HB2	1.90	0.54
2:E:2131:LEU:HD23	2:E:3662:ILE:HB	1.90	0.54
2:E:4942:GLU:HA	2:G:4944:ARG:HH22	1.72	0.54
2:G:664:PHE:HB2	2:G:746:CYS:HB2	1.88	0.54
2:G:886:ARG:HB3	2:G:891:TRP:HB2	1.90	0.54
2:G:1700:ASP:OD2	2:G:1708:ARG:NH2	2.41	0.54
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.89	0.54
2:B:3948:LYS:NZ	2:B:4008:SER:O	2.41	0.54
2:I:886:ARG:HB3	2:I:891:TRP:HB2	1.90	0.54
2:E:645:ARG:HH11	2:E:778:PHE:HE1	1.55	0.54
2:I:1092:PHE:HB3	2:I:1149:VAL:HB	1.89	0.54
2:E:3948:LYS:NZ	2:E:4008:SER:O	2.41	0.54
2:G:3948:LYS:NZ	2:G:4008:SER:O	2.40	0.54
2:B:886:ARG:HB3	2:B:891:TRP:HB2	1.90	0.54
2:B:1105:ALA:HB1	2:B:1109:LEU:HD21	1.89	0.54
2:I:719:LEU:HD22	2:I:735:GLN:HG2	1.90	0.54
2:E:4126:GLU:O	2:E:4130:ASN:ND2	2.40	0.54
2:B:719:LEU:HD22	2:B:735:GLN:HG2	1.90	0.53
2:B:669:ASP:OD2	2:B:790:ARG:NH2	2.41	0.53
2:B:1103:GLY:HA3	2:B:1123:VAL:HA	1.91	0.53
2:I:4126:GLU:O	2:I:4130:ASN:ND2	2.40	0.53
2:G:1103:GLY:HA3	2:G:1123:VAL:HA	1.91	0.53
2:G:2131:LEU:HD23	2:G:3662:ILE:HB	1.90	0.53
2:G:4189:ARG:NH1	2:G:5032:TYR:OH	2.39	0.53
2:G:4674:GLU:HB3	2:G:4715:TYR:HB2	1.91	0.53
2:I:4743:MET:HB3	2:I:4746:ALA:HB3	1.89	0.53
2:G:103:TYR:HB3	2:G:152:PRO:HD3	1.89	0.53
2:G:4232:GLU:OE2	2:G:5017:ARG:NH1	2.36	0.53
1:H:34:LYS:HD3	2:G:629:ARG:HD2	1.91	0.53
2:E:591:ASP:O	2:E:1594:ARG:NH2	2.42	0.53
2:B:103:TYR:HB3	2:B:152:PRO:HD3	1.89	0.53
2:I:2751:LEU:HD11	2:I:2823:ILE:HG21	1.91	0.53
2:E:1092:PHE:HB3	2:E:1149:VAL:HB	1.89	0.53
2:E:1457:UNK:N	2:E:1497:UNK:O	2.42	0.53
2:G:1092:PHE:HB3	2:G:1149:VAL:HB	1.89	0.53
2:B:591:ASP:O	2:B:1594:ARG:NH2	2.42	0.53
2:I:1103:GLY:HA3	2:I:1123:VAL:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:23:GLN:HB3	2:E:201:ASN:HB2	1.91	0.53
2:E:1103:GLY:HA3	2:E:1123:VAL:HA	1.91	0.53
2:B:2751:LEU:HD11	2:B:2823:ILE:HG21	1.91	0.53
2:I:591:ASP:O	2:I:1594:ARG:NH2	2.42	0.53
2:B:4687:TYR:OH	2:B:4699:GLY:O	2.27	0.53
2:I:1457:UNK:N	2:I:1497:UNK:O	2.42	0.53
2:E:4743:MET:HB3	2:E:4746:ALA:HB3	1.89	0.53
2:B:978:THR:HB	2:B:980:ALA:H	1.74	0.53
2:I:4674:GLU:HB3	2:I:4715:TYR:HB2	1.91	0.53
2:E:978:THR:HB	2:E:980:ALA:H	1.74	0.53
2:G:719:LEU:HD22	2:G:735:GLN:HG2	1.90	0.53
2:B:23:GLN:HB3	2:B:201:ASN:HB2	1.91	0.52
2:B:2042:CYS:SG	2:B:2043:GLY:N	2.82	0.52
2:B:2131:LEU:HD23	2:B:3662:ILE:HB	1.90	0.52
2:G:591:ASP:O	2:G:1594:ARG:NH2	2.42	0.52
2:G:1457:UNK:N	2:G:1497:UNK:O	2.42	0.52
2:G:942:ALA:HB2	2:G:1052:ASN:HB2	1.92	0.52
2:B:4581:LYS:HD2	2:B:4632:LEU:HD22	1.92	0.52
2:I:4581:LYS:HD2	2:I:4632:LEU:HD22	1.92	0.52
2:E:4674:GLU:HB3	2:E:4715:TYR:HB2	1.90	0.52
2:E:942:ALA:HB2	2:E:1052:ASN:HB2	1.92	0.52
2:E:1796:ALA:HB1	2:E:1797:ARG:HH21	1.75	0.52
2:E:4232:GLU:OE2	2:E:5017:ARG:NH1	2.36	0.52
2:G:23:GLN:HB3	2:G:201:ASN:HB2	1.91	0.52
2:I:2042:CYS:SG	2:I:2043:GLY:N	2.82	0.52
2:I:2131:LEU:HD23	2:I:3662:ILE:HB	1.90	0.52
2:I:4232:GLU:OE2	2:I:5017:ARG:NH1	2.36	0.52
2:E:4189:ARG:NH1	2:E:5032:TYR:OH	2.39	0.52
2:B:942:ALA:HB2	2:B:1052:ASN:HB2	1.92	0.52
2:B:1796:ALA:HB1	2:B:1797:ARG:HH21	1.75	0.52
2:I:978:THR:HB	2:I:980:ALA:H	1.74	0.52
2:I:4687:TYR:OH	2:I:4699:GLY:O	2.27	0.52
2:E:2332:LEU:HD13	2:E:2335:LEU:HD12	1.92	0.52
2:G:4860:ARG:HG3	2:G:4876:CYS:HB3	1.92	0.52
2:B:1111:PRO:HD3	2:B:1605:TRP:HE1	1.75	0.52
2:E:4687:TYR:OH	2:E:4699:GLY:O	2.27	0.52
2:E:635:THR:HB	2:E:1639:LEU:HD23	1.92	0.52
2:E:3910:THR:HG23	2:E:3911:THR:HG23	1.92	0.52
2:G:669:ASP:OD2	2:G:790:ARG:NH2	2.41	0.52
2:G:2751:LEU:HD11	2:G:2823:ILE:HG21	1.91	0.52
2:G:4152:GLU:OE1	2:G:4192:ARG:NH2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1457:UNK:N	2:B:1497:UNK:O	2.42	0.52
2:I:4860:ARG:HG3	2:I:4876:CYS:HB3	1.92	0.52
1:A:34:LYS:HD3	2:B:629:ARG:HD2	1.90	0.51
2:B:4674:GLU:HB3	2:B:4715:TYR:HB2	1.91	0.51
2:B:4860:ARG:HG3	2:B:4876:CYS:HB3	1.92	0.51
2:I:4152:GLU:OE1	2:I:4192:ARG:NH2	2.43	0.51
2:G:978:THR:HB	2:G:980:ALA:H	1.74	0.51
2:B:635:THR:HB	2:B:1639:LEU:HD23	1.92	0.51
2:B:1667:LEU:HD23	2:B:1671:ARG:HH12	1.76	0.51
2:I:942:ALA:HB2	2:I:1052:ASN:HB2	1.92	0.51
2:I:1796:ALA:HB1	2:I:1797:ARG:HH21	1.75	0.51
2:I:2257:LEU:HD11	2:I:2276:ALA:HB2	1.93	0.51
2:E:1111:PRO:HD3	2:E:1605:TRP:HE1	1.75	0.51
2:E:2751:LEU:HD11	2:E:2823:ILE:HG21	1.91	0.51
2:G:2332:LEU:HD13	2:G:2335:LEU:HD12	1.92	0.51
2:B:3805:LEU:HA	2:B:3809:ASN:HD22	1.76	0.51
2:B:4152:GLU:OE1	2:B:4192:ARG:NH2	2.43	0.51
2:I:23:GLN:HB3	2:I:201:ASN:HB2	1.91	0.51
2:E:111:HIS:HD2	2:E:114:SER:H	1.59	0.51
2:B:2257:LEU:HD11	2:B:2276:ALA:HB2	1.93	0.51
2:E:4860:ARG:HG3	2:E:4876:CYS:HB3	1.92	0.51
1:F:23:VAL:HG22	1:F:47:LYS:HG2	1.93	0.51
2:I:1111:PRO:HD3	2:I:1605:TRP:HE1	1.75	0.51
2:I:3805:LEU:HA	2:I:3809:ASN:HD22	1.76	0.51
2:E:3805:LEU:HA	2:E:3809:ASN:HD22	1.76	0.51
2:G:3910:THR:HG23	2:G:3911:THR:HG23	1.92	0.51
1:H:23:VAL:HG22	1:H:47:LYS:HG2	1.93	0.51
2:B:4049:VAL:HG21	2:B:4159:ARG:HD2	1.92	0.51
2:G:1796:ALA:HB1	2:G:1797:ARG:HH21	1.75	0.51
2:G:4581:LYS:HD2	2:G:4632:LEU:HD22	1.92	0.51
1:F:42:ARG:HG2	2:E:1691:GLN:HG2	1.93	0.51
2:E:669:ASP:OD2	2:E:790:ARG:NH2	2.41	0.51
2:E:4049:VAL:HG21	2:E:4159:ARG:HD2	1.92	0.51
2:B:717:ASP:OD1	2:B:720:HIS:ND1	2.44	0.51
2:I:717:ASP:OD1	2:I:720:HIS:ND1	2.44	0.51
2:I:1667:LEU:HD23	2:I:1671:ARG:HH12	1.76	0.51
2:E:485:SER:O	2:E:489:ASN:N	2.41	0.51
2:E:4152:GLU:OE1	2:E:4192:ARG:NH2	2.43	0.51
2:G:635:THR:HB	2:G:1639:LEU:HD23	1.92	0.51
2:G:4687:TYR:OH	2:G:4699:GLY:O	2.27	0.51
2:B:236:ALA:HA	2:B:242:ARG:HD2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:3817:LEU:HD13	2:E:3899:PHE:HD1	1.75	0.51
2:E:4581:LYS:HD2	2:E:4632:LEU:HD22	1.92	0.51
2:G:111:HIS:HD2	2:G:114:SER:H	1.59	0.51
2:G:1111:PRO:HD3	2:G:1605:TRP:HE1	1.75	0.51
2:G:3805:LEU:HA	2:G:3809:ASN:HD22	1.76	0.51
1:J:23:VAL:HG22	1:J:47:LYS:HG2	1.93	0.51
2:I:635:THR:HB	2:I:1639:LEU:HD23	1.92	0.51
2:E:717:ASP:OD1	2:E:720:HIS:ND1	2.44	0.51
2:G:972:LEU:O	2:G:1044:ARG:NH2	2.44	0.51
2:E:40:GLU:HB3	2:E:44:ASN:HB3	1.93	0.50
2:E:236:ALA:HA	2:E:242:ARG:HD2	1.93	0.50
1:J:42:ARG:HG2	2:I:1691:GLN:HG2	1.93	0.50
2:B:111:HIS:HD2	2:B:114:SER:H	1.59	0.50
2:B:989:ALA:O	2:B:1035:ASN:ND2	2.44	0.50
2:I:2332:LEU:HD13	2:I:2335:LEU:HD12	1.92	0.50
2:G:898:ASP:HB3	2:G:901:LYS:HB2	1.94	0.50
2:G:2257:LEU:HD11	2:G:2276:ALA:HB2	1.93	0.50
2:B:4126:GLU:O	2:B:4130:ASN:ND2	2.40	0.50
2:I:3910:THR:HG23	2:I:3911:THR:HG23	1.92	0.50
2:E:2257:LEU:HD11	2:E:2276:ALA:HB2	1.93	0.50
2:B:972:LEU:O	2:B:1044:ARG:NH2	2.44	0.50
2:B:2332:LEU:HD13	2:B:2335:LEU:HD12	1.92	0.50
2:B:3779:VAL:HG23	2:B:3780:LEU:HD12	1.94	0.50
2:B:4978:HIS:HA	2:B:4982:GLU:HB2	1.94	0.50
2:E:4978:HIS:HA	2:E:4982:GLU:HB2	1.94	0.50
2:G:40:GLU:HB3	2:G:44:ASN:HB3	1.93	0.50
2:G:3817:LEU:HD13	2:G:3899:PHE:HD1	1.75	0.50
1:F:34:LYS:HD3	2:E:629:ARG:HD2	1.92	0.50
1:H:42:ARG:HG2	2:G:1691:GLN:HG2	1.94	0.50
2:B:3817:LEU:HD13	2:B:3899:PHE:HD1	1.75	0.50
2:B:3910:THR:HG23	2:B:3911:THR:HG23	1.92	0.50
2:I:989:ALA:O	2:I:1035:ASN:ND2	2.44	0.50
2:I:1721:GLU:OE2	2:I:1725:ARG:NH2	2.45	0.50
2:I:3817:LEU:HD13	2:I:3899:PHE:HD1	1.75	0.50
2:E:989:ALA:O	2:E:1035:ASN:ND2	2.44	0.50
2:E:1721:GLU:OE2	2:E:1725:ARG:NH2	2.45	0.50
2:G:1721:GLU:OE2	2:G:1725:ARG:NH2	2.45	0.50
2:B:40:GLU:HB3	2:B:44:ASN:HB3	1.93	0.50
2:I:111:HIS:CD2	2:I:114:SER:H	2.30	0.50
2:I:309:THR:O	2:I:313:SER:OG	2.30	0.50
2:E:972:LEU:O	2:E:1044:ARG:NH2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4786:ASP:OD2	2:E:4789:PHE:N	2.43	0.50
2:G:717:ASP:OD1	2:G:720:HIS:ND1	2.44	0.50
2:B:111:HIS:CD2	2:B:114:SER:H	2.30	0.50
2:B:1698:LEU:N	2:B:1712:TYR:OH	2.45	0.50
2:I:111:HIS:HD2	2:I:114:SER:H	1.59	0.50
2:I:4049:VAL:HG21	2:I:4159:ARG:HD2	1.92	0.50
2:I:4978:HIS:HA	2:I:4982:GLU:HB2	1.94	0.50
2:E:1667:LEU:HD23	2:E:1671:ARG:HH12	1.75	0.50
2:E:2042:CYS:SG	2:E:2043:GLY:N	2.82	0.50
2:E:2868:SER:O	2:E:2872:GLN:N	2.43	0.50
2:E:3779:VAL:HG23	2:E:3780:LEU:HD12	1.94	0.50
2:G:2042:CYS:SG	2:G:2043:GLY:N	2.82	0.50
2:G:4049:VAL:HG21	2:G:4159:ARG:HD2	1.92	0.50
2:G:4126:GLU:O	2:G:4130:ASN:ND2	2.40	0.50
2:B:485:SER:O	2:B:489:ASN:N	2.41	0.50
2:B:2739:PRO:HB3	2:B:2884:ASN:HB3	1.94	0.50
2:E:410:LEU:HD12	2:E:413:GLN:HE21	1.77	0.50
2:E:2466:LEU:HA	2:E:2469:ILE:HD12	1.93	0.50
2:G:111:HIS:CD2	2:G:114:SER:H	2.30	0.50
2:G:1698:LEU:N	2:G:1712:TYR:OH	2.45	0.50
2:B:309:THR:O	2:B:313:SER:OG	2.30	0.50
2:B:410:LEU:HD12	2:B:413:GLN:HE21	1.77	0.50
2:I:40:GLU:HB3	2:I:44:ASN:HB3	1.93	0.50
2:I:1698:LEU:N	2:I:1712:TYR:OH	2.45	0.50
2:I:2739:PRO:HB3	2:I:2884:ASN:HB3	1.94	0.50
2:G:4567:LEU:HD12	2:G:4816:ILE:HD12	1.94	0.50
2:G:4786:ASP:OD2	2:G:4789:PHE:N	2.43	0.50
2:B:940:GLY:O	2:B:1052:ASN:N	2.45	0.49
2:B:2265:LEU:HD22	2:B:2330:ARG:HB3	1.93	0.49
2:I:236:ALA:HA	2:I:242:ARG:HD2	1.93	0.49
2:E:111:HIS:CD2	2:E:114:SER:H	2.30	0.49
2:E:4666:VAL:HG23	2:E:4669:VAL:HB	1.94	0.49
2:G:4666:VAL:HG23	2:G:4669:VAL:HB	1.94	0.49
1:A:23:VAL:HG22	1:A:47:LYS:HG2	1.93	0.49
2:I:972:LEU:O	2:I:1044:ARG:NH2	2.44	0.49
2:I:1247:PRO:HA	2:I:1598:GLN:HA	1.95	0.49
2:I:4567:LEU:HD12	2:I:4816:ILE:HD12	1.94	0.49
2:I:4666:VAL:HG23	2:I:4669:VAL:HB	1.94	0.49
2:G:410:LEU:HD12	2:G:413:GLN:HE21	1.77	0.49
2:G:4978:HIS:HA	2:G:4982:GLU:HB2	1.94	0.49
2:B:1247:PRO:HA	2:B:1598:GLN:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:41:GLY:O	2:I:45:ARG:NH1	2.45	0.49
2:E:2739:PRO:HB3	2:E:2884:ASN:HB3	1.94	0.49
2:G:2466:LEU:HA	2:G:2469:ILE:HD12	1.93	0.49
2:G:3779:VAL:HG23	2:G:3780:LEU:HD12	1.94	0.49
1:A:42:ARG:HG2	2:B:1691:GLN:HG2	1.94	0.49
2:I:3779:VAL:HG23	2:I:3780:LEU:HD12	1.94	0.49
2:E:41:GLY:O	2:E:45:ARG:NH1	2.45	0.49
2:G:236:ALA:HA	2:G:242:ARG:HD2	1.93	0.49
2:G:864:PRO:HD2	2:G:867:LEU:HD12	1.95	0.49
2:G:1667:LEU:HD23	2:G:1671:ARG:HH12	1.76	0.49
2:B:2466:LEU:HA	2:B:2469:ILE:HD12	1.93	0.49
2:I:669:ASP:OD2	2:I:790:ARG:NH2	2.41	0.49
2:E:2265:LEU:HD22	2:E:2330:ARG:HB3	1.93	0.49
2:G:41:GLY:O	2:G:45:ARG:NH1	2.45	0.49
2:G:940:GLY:O	2:G:1052:ASN:N	2.45	0.49
2:G:989:ALA:O	2:G:1035:ASN:ND2	2.44	0.49
2:G:2868:SER:O	2:G:2872:GLN:N	2.43	0.49
1:A:74:LEU:HB2	1:A:99:PHE:HB2	1.95	0.49
2:B:3842:LEU:O	2:B:3929:SER:OG	2.30	0.49
2:I:451:TYR:O	2:I:474:ARG:NH1	2.43	0.49
2:I:898:ASP:HB3	2:I:901:LYS:HB2	1.94	0.49
2:E:309:THR:O	2:E:313:SER:OG	2.30	0.49
2:E:1698:LEU:N	2:E:1712:TYR:OH	2.45	0.49
2:E:3842:LEU:O	2:E:3929:SER:OG	2.30	0.49
2:G:451:TYR:O	2:G:474:ARG:NH1	2.43	0.49
2:G:1960:ALA:O	2:G:1964:ARG:NE	2.46	0.49
2:G:3946:GLN:OE1	2:G:3950:ASN:ND2	2.46	0.49
1:F:74:LEU:HB2	1:F:99:PHE:HB2	1.95	0.49
2:B:898:ASP:HB3	2:B:901:LYS:HB2	1.94	0.49
2:B:4567:LEU:HD12	2:B:4816:ILE:HD12	1.94	0.49
2:I:864:PRO:HD2	2:I:867:LEU:HD12	1.95	0.49
2:I:2265:LEU:HD22	2:I:2330:ARG:HB3	1.93	0.49
2:E:290:TYR:O	2:E:302:VAL:N	2.46	0.49
2:E:940:GLY:O	2:E:1052:ASN:N	2.45	0.49
2:E:4567:LEU:HD12	2:E:4816:ILE:HD12	1.94	0.49
2:G:2265:LEU:HD22	2:G:2330:ARG:HB3	1.93	0.49
2:B:2803:GLU:OE2	2:B:2806:ARG:NH1	2.46	0.49
2:I:410:LEU:HD12	2:I:413:GLN:HE21	1.77	0.49
2:I:2466:LEU:HA	2:I:2469:ILE:HD12	1.93	0.49
2:E:898:ASP:HB3	2:E:901:LYS:HB2	1.94	0.49
2:E:1247:PRO:HA	2:E:1598:GLN:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:THR:HA	1:A:49:ARG:HA	1.95	0.49
2:B:41:GLY:O	2:B:45:ARG:NH1	2.45	0.49
2:B:1721:GLU:OE2	2:B:1725:ARG:NH2	2.45	0.49
2:E:451:TYR:O	2:E:474:ARG:NH1	2.43	0.49
2:E:2803:GLU:OE2	2:E:2806:ARG:NH1	2.46	0.49
2:G:2739:PRO:HB3	2:G:2884:ASN:HB3	1.94	0.49
2:B:1808:ARG:HD2	2:B:1854:PHE:HA	1.95	0.49
2:B:4666:VAL:HG23	2:B:4669:VAL:HB	1.94	0.49
2:G:309:THR:O	2:G:313:SER:OG	2.30	0.49
2:G:2803:GLU:OE2	2:G:2806:ARG:NH1	2.46	0.49
2:B:488:LEU:HD23	2:B:491:ILE:HD12	1.95	0.48
2:I:1808:ARG:HD2	2:I:1854:PHE:HA	1.95	0.48
1:F:21:THR:HA	1:F:49:ARG:HA	1.95	0.48
2:I:488:LEU:HD23	2:I:491:ILE:HD12	1.95	0.48
2:I:681:HIS:HB3	2:I:784:SER:HB3	1.95	0.48
2:E:3946:GLN:OE1	2:E:3950:ASN:ND2	2.46	0.48
2:G:1247:PRO:HA	2:G:1598:GLN:HA	1.95	0.48
2:I:3946:GLN:OE1	2:I:3950:ASN:ND2	2.46	0.48
2:E:864:PRO:HD2	2:E:867:LEU:HD12	1.95	0.48
2:I:2868:SER:O	2:I:2872:GLN:N	2.43	0.48
2:E:1991:THR:O	2:E:1995:THR:OG1	2.32	0.48
2:G:1991:THR:O	2:G:1995:THR:OG1	2.32	0.48
2:B:864:PRO:HD2	2:B:867:LEU:HD12	1.95	0.48
2:B:3946:GLN:OE1	2:B:3950:ASN:ND2	2.46	0.48
2:I:1991:THR:O	2:I:1995:THR:OG1	2.32	0.48
2:B:290:TYR:O	2:B:302:VAL:N	2.46	0.48
2:B:621:ILE:O	2:B:625:LEU:N	2.46	0.48
2:I:2927:LEU:HD23	2:I:2930:LEU:HD12	1.96	0.48
2:G:290:TYR:O	2:G:302:VAL:N	2.46	0.48
2:B:681:HIS:HB3	2:B:784:SER:HB3	1.95	0.48
2:I:606:LEU:HG	2:I:617:ASN:HD22	1.78	0.48
2:I:1960:ALA:O	2:I:1964:ARG:NE	2.46	0.48
2:I:2803:GLU:OE2	2:I:2806:ARG:NH1	2.46	0.48
1:J:21:THR:HA	1:J:49:ARG:HA	1.95	0.48
1:J:74:LEU:HB2	1:J:99:PHE:HB2	1.95	0.48
2:B:4892:ARG:NH2	2:I:4898:GLY:O	2.47	0.48
2:B:4898:GLY:O	2:E:4892:ARG:NH2	2.47	0.48
2:I:551:LEU:HD21	2:I:589:LEU:HD13	1.96	0.48
2:I:940:GLY:O	2:I:1052:ASN:N	2.45	0.48
2:I:1025:ARG:O	2:I:1032:LYS:NZ	2.43	0.48
2:B:551:LEU:HD21	2:B:589:LEU:HD13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2755:ILE:HD13	2:B:2810:LYS:HG2	1.96	0.48
2:I:4973:HIS:ND1	2:G:4227:GLU:OE2	2.47	0.48
2:E:1808:ARG:HD2	2:E:1854:PHE:HA	1.95	0.48
2:B:606:LEU:HG	2:B:617:ASN:HD22	1.78	0.47
2:I:2271:THR:HG22	2:I:2273:LEU:H	1.79	0.47
2:I:2742:THR:OG1	2:I:2811:GLU:OE1	2.31	0.47
2:E:45:ARG:HG2	2:E:443:LEU:HD21	1.95	0.47
2:E:606:LEU:HG	2:E:617:ASN:HD22	1.78	0.47
2:E:681:HIS:HB3	2:E:784:SER:HB3	1.95	0.47
2:E:1731:LEU:HA	2:E:1772:ARG:HH12	1.79	0.47
2:G:488:LEU:HD23	2:G:491:ILE:HD12	1.95	0.47
2:G:681:HIS:HB3	2:G:784:SER:HB3	1.95	0.47
2:G:2755:ILE:HD13	2:G:2810:LYS:HG2	1.96	0.47
1:H:74:LEU:HB2	1:H:99:PHE:HB2	1.95	0.47
2:B:451:TYR:O	2:B:474:ARG:NH1	2.43	0.47
2:B:4973:HIS:ND1	2:I:4227:GLU:OE2	2.47	0.47
2:I:45:ARG:HG2	2:I:443:LEU:HD21	1.95	0.47
2:I:1171:SER:OG	2:I:1175:SER:N	2.47	0.47
2:I:4892:ARG:NH2	2:G:4898:GLY:O	2.47	0.47
2:G:1808:ARG:HD2	2:G:1854:PHE:HA	1.95	0.47
2:G:2758:PHE:O	2:G:2762:THR:N	2.45	0.47
2:I:2755:ILE:HD13	2:I:2810:LYS:HG2	1.96	0.47
2:E:2876:GLU:OE1	2:E:2920:ARG:NH2	2.48	0.47
1:H:21:THR:HA	1:H:49:ARG:HA	1.95	0.47
2:B:2876:GLU:OE1	2:B:2920:ARG:NH2	2.48	0.47
2:I:290:TYR:O	2:I:302:VAL:N	2.46	0.47
2:I:2342:ASN:OD1	2:I:2342:ASN:N	2.47	0.47
2:E:2755:ILE:HD13	2:E:2810:LYS:HG2	1.96	0.47
2:G:1731:LEU:HA	2:G:1772:ARG:HH12	1.78	0.47
2:B:45:ARG:HG2	2:B:443:LEU:HD21	1.95	0.47
2:I:2876:GLU:OE1	2:I:2920:ARG:NH2	2.48	0.47
2:E:683:ARG:HG2	2:E:717:ASP:HB3	1.97	0.47
2:E:1171:SER:OG	2:E:1175:SER:N	2.47	0.47
2:E:1232:ARG:HH21	2:E:1701:ALA:HB1	1.80	0.47
2:G:1171:SER:OG	2:G:1175:SER:N	2.47	0.47
2:G:1232:ARG:HH21	2:G:1701:ALA:HB1	1.80	0.47
2:B:2271:THR:HG22	2:B:2273:LEU:H	1.79	0.47
2:B:2342:ASN:OD1	2:B:2342:ASN:N	2.47	0.47
2:B:4232:GLU:OE2	2:B:5017:ARG:NH1	2.36	0.47
2:I:1731:LEU:HA	2:I:1772:ARG:HH12	1.79	0.47
2:E:488:LEU:HD23	2:E:491:ILE:HD12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2271:THR:HG22	2:E:2273:LEU:H	1.79	0.47
2:G:45:ARG:HG2	2:G:443:LEU:HD21	1.95	0.47
2:B:4227:GLU:OE2	2:E:4973:HIS:ND1	2.48	0.47
2:E:621:ILE:O	2:E:625:LEU:N	2.45	0.47
2:E:1960:ALA:O	2:E:1964:ARG:NE	2.46	0.47
2:G:211:GLU:OE2	2:G:3907:THR:OG1	2.33	0.47
2:G:2271:THR:HG22	2:G:2273:LEU:H	1.79	0.47
2:G:2927:LEU:HD23	2:G:2930:LEU:HD12	1.96	0.47
2:B:683:ARG:HG2	2:B:717:ASP:HB3	1.97	0.47
2:B:1991:THR:O	2:B:1995:THR:OG1	2.32	0.47
2:B:2868:SER:O	2:B:2872:GLN:N	2.43	0.47
2:E:4227:GLU:OE2	2:G:4973:HIS:ND1	2.48	0.47
2:G:683:ARG:HG2	2:G:717:ASP:HB3	1.97	0.47
2:B:1232:ARG:HH21	2:B:1701:ALA:HB1	1.80	0.47
2:I:485:SER:O	2:I:489:ASN:N	2.40	0.47
2:I:683:ARG:HG2	2:I:717:ASP:HB3	1.97	0.47
2:E:211:GLU:OE2	2:E:3907:THR:OG1	2.33	0.47
2:E:1727:ARG:HH21	2:E:1775:HIS:CE1	2.33	0.47
2:G:606:LEU:HG	2:G:617:ASN:HD22	1.78	0.47
2:G:2876:GLU:OE1	2:G:2920:ARG:NH2	2.48	0.47
2:B:1731:LEU:HA	2:B:1772:ARG:HH12	1.78	0.46
2:I:1727:ARG:HH21	2:I:1775:HIS:CE1	2.33	0.46
2:E:379:HIS:CD2	2:E:381:GLU:H	2.34	0.46
2:G:214:VAL:HG12	2:G:274:LEU:HD12	1.98	0.46
2:G:551:LEU:HD21	2:G:589:LEU:HD13	1.96	0.46
2:B:379:HIS:CD2	2:B:381:GLU:H	2.34	0.46
2:B:1727:ARG:HH21	2:B:1775:HIS:CE1	2.33	0.46
2:I:2758:PHE:O	2:I:2762:THR:N	2.45	0.46
2:G:621:ILE:O	2:G:625:LEU:N	2.45	0.46
2:G:1727:ARG:HH21	2:G:1775:HIS:CE1	2.33	0.46
2:B:1171:SER:OG	2:B:1175:SER:N	2.47	0.46
2:B:2189:LYS:HA	2:B:2192:TYR:HD2	1.81	0.46
2:E:35:LEU:HD13	2:E:49:LEU:HD13	1.97	0.46
2:E:2002:PRO:HA	2:E:2005:GLN:HB3	1.97	0.46
2:E:2189:LYS:HA	2:E:2192:TYR:HD2	1.81	0.46
2:G:4673:ARG:HH12	2:G:4698:LYS:HE3	1.79	0.46
2:B:211:GLU:OE2	2:B:3907:THR:OG1	2.33	0.46
2:B:214:VAL:HG12	2:B:274:LEU:HD12	1.98	0.46
2:B:4673:ARG:HH12	2:B:4698:LYS:HE3	1.79	0.46
2:I:211:GLU:OE2	2:I:3907:THR:OG1	2.33	0.46
2:G:379:HIS:CD2	2:G:381:GLU:H	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:572:PRO:HA	2:B:575:LEU:HD13	1.97	0.46
2:B:2871:LEU:HD22	2:B:2927:LEU:HD22	1.97	0.46
2:E:2927:LEU:HD23	2:E:2930:LEU:HD12	1.96	0.46
2:I:379:HIS:CD2	2:I:381:GLU:H	2.33	0.46
2:I:2871:LEU:HD22	2:I:2927:LEU:HD22	1.97	0.46
2:I:4673:ARG:HH12	2:I:4698:LYS:HE3	1.79	0.46
2:E:551:LEU:HD21	2:E:589:LEU:HD13	1.96	0.46
2:E:1725:ARG:HA	2:E:1728:ARG:HG2	1.97	0.46
2:G:485:SER:O	2:G:489:ASN:N	2.40	0.46
2:B:2368:LEU:HD13	2:B:2376:LEU:HD23	1.98	0.46
2:B:4745:LEU:O	2:B:4749:GLU:N	2.46	0.46
2:E:4673:ARG:HH12	2:E:4698:LYS:HE3	1.79	0.46
2:E:4898:GLY:O	2:G:4892:ARG:NH2	2.48	0.46
2:E:4928:LEU:HD13	2:E:4931:ILE:HD12	1.98	0.46
2:G:35:LEU:HD13	2:G:49:LEU:HD13	1.97	0.46
2:G:1649:ASP:HB3	2:G:1652:GLU:HG2	1.98	0.46
2:B:2002:PRO:HA	2:B:2005:GLN:HB3	1.97	0.46
2:I:2212:VAL:O	2:I:2216:GLY:N	2.48	0.46
2:I:3781:GLN:HA	2:I:3784:SER:HB3	1.98	0.46
2:G:2212:VAL:O	2:G:2216:GLY:N	2.48	0.46
2:G:2342:ASN:OD1	2:G:2342:ASN:N	2.47	0.46
1:F:34:LYS:NZ	1:F:35:LYS:O	2.44	0.46
2:B:1025:ARG:O	2:B:1032:LYS:NZ	2.43	0.46
2:I:1725:ARG:HA	2:I:1728:ARG:HG2	1.98	0.46
2:E:2368:LEU:HD13	2:E:2376:LEU:HD23	1.98	0.46
2:E:2742:THR:OG1	2:E:2811:GLU:OE1	2.31	0.46
2:G:4928:LEU:HA	2:G:4931:ILE:HD12	1.97	0.46
1:F:92:PRO:HD3	2:E:627:PRO:HB2	1.98	0.46
2:B:2927:LEU:HD23	2:B:2930:LEU:HD12	1.96	0.46
2:I:214:VAL:HG12	2:I:274:LEU:HD12	1.97	0.46
2:I:2002:PRO:HA	2:I:2005:GLN:HB3	1.97	0.46
2:I:2247:GLN:NE2	2:I:2285:GLU:OE2	2.49	0.46
2:E:3781:GLN:HA	2:E:3784:SER:HB3	1.98	0.46
2:E:4928:LEU:HA	2:E:4931:ILE:HD12	1.97	0.46
2:G:2277:ALA:HB1	2:G:2337:PHE:HD2	1.81	0.46
2:B:1960:ALA:O	2:B:1964:ARG:NE	2.46	0.45
2:I:35:LEU:HD13	2:I:49:LEU:HD13	1.97	0.45
2:I:572:PRO:HA	2:I:575:LEU:HD13	1.98	0.45
2:I:1232:ARG:HH21	2:I:1701:ALA:HB1	1.80	0.45
2:I:2189:LYS:HA	2:I:2192:TYR:HD2	1.81	0.45
2:I:2277:ALA:HB1	2:I:2337:PHE:HD2	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:3973:CYS:SG	2:I:3976:ASN:ND2	2.90	0.45
2:G:3973:CYS:SG	2:G:3976:ASN:ND2	2.90	0.45
2:G:4928:LEU:HD13	2:G:4931:ILE:HD12	1.98	0.45
2:B:2742:THR:OG1	2:B:2811:GLU:OE1	2.31	0.45
2:B:3973:CYS:SG	2:B:3976:ASN:ND2	2.90	0.45
2:B:4239:GLU:OE2	2:B:5014:TYR:OH	2.30	0.45
2:E:649:PHE:HB3	2:E:776:LEU:HB3	1.99	0.45
2:E:2871:LEU:HD22	2:E:2927:LEU:HD22	1.97	0.45
2:G:572:PRO:HA	2:G:575:LEU:HD13	1.97	0.45
2:G:3923:LEU:HD13	2:G:3961:VAL:HG11	1.98	0.45
1:F:7:ILE:HB	1:F:71:ARG:HB3	1.99	0.45
2:I:718:GLY:HA3	2:I:737:LEU:HA	1.98	0.45
2:I:1649:ASP:HB3	2:I:1652:GLU:HG2	1.98	0.45
2:I:2368:LEU:HD13	2:I:2376:LEU:HD23	1.98	0.45
2:E:1649:ASP:HB3	2:E:1652:GLU:HG2	1.98	0.45
2:E:3923:LEU:HD13	2:E:3961:VAL:HG11	1.98	0.45
2:G:4152:GLU:OE1	2:G:4194:TYR:OH	2.35	0.45
2:G:2189:LYS:HA	2:G:2192:TYR:HD2	1.81	0.45
2:G:2368:LEU:HD13	2:G:2376:LEU:HD23	1.98	0.45
2:G:2871:LEU:HD22	2:G:2927:LEU:HD22	1.97	0.45
2:B:35:LEU:HD13	2:B:49:LEU:HD13	1.97	0.45
2:B:1649:ASP:HB3	2:B:1652:GLU:HG2	1.98	0.45
2:E:572:PRO:HA	2:E:575:LEU:HD13	1.97	0.45
2:E:718:GLY:HA3	2:E:737:LEU:HA	1.98	0.45
2:E:1025:ARG:O	2:E:1032:LYS:NZ	2.43	0.45
2:E:3973:CYS:SG	2:E:3976:ASN:ND2	2.90	0.45
2:G:2247:GLN:NE2	2:G:2285:GLU:OE2	2.49	0.45
2:B:649:PHE:HB3	2:B:776:LEU:HB3	1.99	0.45
2:B:2121:PHE:O	2:B:3725:TYR:OH	2.34	0.45
2:I:621:ILE:O	2:I:625:LEU:N	2.45	0.45
2:I:4928:LEU:HD13	2:I:4931:ILE:HD12	1.98	0.45
2:E:2247:GLN:NE2	2:E:2285:GLU:OE2	2.49	0.45
2:G:1725:ARG:HA	2:G:1728:ARG:HG2	1.98	0.45
2:B:2247:GLN:NE2	2:B:2285:GLU:OE2	2.49	0.45
2:I:2104:ARG:HA	2:I:2107:GLN:HB3	1.99	0.45
2:I:4152:GLU:OE1	2:I:4194:TYR:OH	2.35	0.45
2:I:4586:PRO:HA	2:I:4628:VAL:HG11	1.98	0.45
2:I:4928:LEU:HA	2:I:4931:ILE:HD12	1.97	0.45
2:I:4956:THR:O	2:I:4965:SER:N	2.50	0.45
2:E:214:VAL:HG12	2:E:274:LEU:HD12	1.97	0.45
2:E:4586:PRO:HA	2:E:4628:VAL:HG11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2002:PRO:HA	2:G:2005:GLN:HB3	1.97	0.45
2:G:3781:GLN:HA	2:G:3784:SER:HB3	1.98	0.45
2:B:1725:ARG:HA	2:B:1728:ARG:HG2	1.97	0.45
2:B:4928:LEU:HA	2:B:4931:ILE:HD12	1.97	0.45
2:E:2277:ALA:HB1	2:E:2337:PHE:HD2	1.81	0.45
2:E:2342:ASN:N	2:E:2342:ASN:OD1	2.47	0.45
2:E:4956:THR:O	2:E:4965:SER:N	2.50	0.45
2:B:718:GLY:HA3	2:B:737:LEU:HA	1.98	0.45
2:B:3781:GLN:HA	2:B:3784:SER:HB3	1.98	0.45
2:E:1718:ILE:HG13	2:E:1719:HIS:CD2	2.52	0.45
2:G:134:ASP:OD1	2:G:134:ASP:N	2.50	0.45
2:G:2104:ARG:HA	2:G:2107:GLN:HB3	1.99	0.45
2:B:1105:ALA:N	2:B:1189:LEU:O	2.50	0.45
2:I:495:ASN:HD21	2:I:550:LYS:HG3	1.82	0.45
2:I:649:PHE:HB3	2:I:776:LEU:HB3	1.99	0.45
2:G:4239:GLU:OE2	2:G:5014:TYR:OH	2.30	0.45
2:G:4982:GLU:HB3	2:G:4983:HIS:H	1.65	0.45
2:G:495:ASN:HD21	2:G:550:LYS:HG3	1.82	0.44
2:G:1516:UNK:N	2:G:1529:UNK:O	2.50	0.44
1:H:7:ILE:HB	1:H:71:ARG:HB3	1.99	0.44
2:B:1718:ILE:HG13	2:B:1719:HIS:CD2	2.52	0.44
2:I:134:ASP:OD1	2:I:134:ASP:N	2.50	0.44
2:I:1099:GLU:OE2	2:I:1127:HIS:ND1	2.41	0.44
2:I:3923:LEU:HD13	2:I:3961:VAL:HG11	1.98	0.44
1:J:2:VAL:HG21	1:J:61:GLU:HB2	1.99	0.44
2:B:495:ASN:HD21	2:B:550:LYS:HG3	1.82	0.44
2:B:1516:UNK:N	2:B:1529:UNK:O	2.50	0.44
2:B:2277:ALA:HB1	2:B:2337:PHE:HD2	1.81	0.44
2:B:4864:ASN:ND2	2:B:4871:GLU:OE1	2.43	0.44
2:G:1718:ILE:HG13	2:G:1719:HIS:CD2	2.52	0.44
2:G:4586:PRO:HA	2:G:4628:VAL:HG11	1.98	0.44
2:B:1660:GLN:O	2:B:1664:SER:N	2.49	0.44
2:B:2758:PHE:O	2:B:2762:THR:N	2.45	0.44
2:B:4562:LEU:HD13	2:B:4656:LEU:HB3	2.00	0.44
2:B:4586:PRO:HA	2:B:4628:VAL:HG11	1.98	0.44
2:E:395:GLN:NE2	2:E:397:GLU:OE1	2.51	0.44
2:E:4152:GLU:OE1	2:E:4194:TYR:OH	2.35	0.44
2:G:235:ALA:HA	2:G:257:ARG:HD3	2.00	0.44
2:B:243:ARG:NH1	2:B:301:VAL:O	2.43	0.44
2:B:3923:LEU:HD13	2:B:3961:VAL:HG11	1.98	0.44
2:B:4928:LEU:HD13	2:B:4931:ILE:HD12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1516:UNK:N	2:I:1529:UNK:O	2.50	0.44
2:I:1718:ILE:HG13	2:I:1719:HIS:CD2	2.52	0.44
2:E:134:ASP:N	2:E:134:ASP:OD1	2.50	0.44
2:E:1516:UNK:N	2:E:1529:UNK:O	2.50	0.44
2:G:649:PHE:HB3	2:G:776:LEU:HB3	1.99	0.44
2:G:718:GLY:HA3	2:G:737:LEU:HA	1.98	0.44
2:G:1660:GLN:O	2:G:1664:SER:N	2.49	0.44
2:B:395:GLN:NE2	2:B:397:GLU:OE1	2.51	0.44
2:B:583:ILE:H	2:B:583:ILE:HG13	1.65	0.44
2:B:4152:GLU:OE1	2:B:4194:TYR:OH	2.35	0.44
2:I:3842:LEU:O	2:I:3929:SER:OG	2.30	0.44
2:E:495:ASN:HD21	2:E:550:LYS:HG3	1.82	0.44
1:F:2:VAL:HG21	1:F:61:GLU:HB2	1.99	0.44
2:B:3676:ASP:OD1	2:B:3676:ASP:N	2.51	0.44
2:I:4786:ASP:OD2	2:I:4789:PHE:N	2.43	0.44
2:E:235:ALA:HA	2:E:257:ARG:HD3	2.00	0.44
2:E:2758:PHE:O	2:E:2762:THR:N	2.45	0.44
1:A:2:VAL:HG21	1:A:61:GLU:HB2	1.99	0.44
2:B:1078:GLU:HB3	2:B:1081:TYR:HD2	1.83	0.44
2:B:2104:ARG:HA	2:B:2107:GLN:HB3	1.99	0.44
2:B:3951:PHE:HD2	2:B:4012:LEU:HD11	1.83	0.44
2:E:3951:PHE:HD2	2:E:4012:LEU:HD11	1.83	0.44
2:G:3971:GLY:H	2:G:5005:GLY:HA3	1.83	0.44
2:G:4956:THR:O	2:G:4965:SER:N	2.50	0.44
1:H:87:HIS:HD2	1:H:90:VAL:HB	1.83	0.44
2:B:4956:THR:O	2:B:4965:SER:N	2.50	0.44
2:I:4571:PHE:O	2:I:4575:PHE:N	2.51	0.44
2:I:4864:ASN:ND2	2:I:4871:GLU:OE1	2.43	0.44
2:E:1848:LEU:HD22	2:E:1853:ILE:HG13	2.00	0.44
2:E:4864:ASN:ND2	2:E:4871:GLU:OE1	2.43	0.44
2:G:395:GLN:HG3	2:G:397:GLU:H	1.83	0.44
2:G:4571:PHE:O	2:G:4575:PHE:N	2.51	0.44
1:J:7:ILE:HB	1:J:71:ARG:HB3	1.99	0.43
2:I:4227:GLU:HG3	2:I:4228:ALA:H	1.83	0.43
2:E:3971:GLY:H	2:E:5005:GLY:HA3	1.83	0.43
2:E:4562:LEU:HD13	2:E:4656:LEU:HB3	2.00	0.43
2:G:1025:ARG:O	2:G:1032:LYS:NZ	2.43	0.43
1:A:7:ILE:HB	1:A:71:ARG:HB3	1.99	0.43
2:B:395:GLN:HG3	2:B:397:GLU:H	1.83	0.43
2:B:1099:GLU:OE2	2:B:1127:HIS:ND1	2.41	0.43
2:I:1679:ASN:HA	2:I:1682:ALA:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4562:LEU:HD13	2:I:4656:LEU:HB3	2.00	0.43
2:E:2104:ARG:HA	2:E:2107:GLN:HB3	1.99	0.43
2:G:2121:PHE:O	2:G:3725:TYR:OH	2.34	0.43
2:G:4864:ASN:ND2	2:G:4871:GLU:OE1	2.43	0.43
1:A:92:PRO:HD3	2:B:627:PRO:HB2	2.00	0.43
2:B:3971:GLY:H	2:B:5005:GLY:HA3	1.83	0.43
2:B:4913:ARG:O	2:B:4917:ASP:N	2.46	0.43
2:I:1105:ALA:N	2:I:1189:LEU:O	2.50	0.43
2:I:4982:GLU:HB3	2:I:4983:HIS:H	1.65	0.43
2:E:3676:ASP:N	2:E:3676:ASP:OD1	2.51	0.43
2:G:395:GLN:NE2	2:G:397:GLU:OE1	2.51	0.43
2:G:2863:SER:HG	2:G:2928:LYS:HZ3	1.63	0.43
2:G:3951:PHE:HD2	2:G:4012:LEU:HD11	1.83	0.43
2:B:1622:GLU:N	2:B:1627:ALA:O	2.51	0.43
2:I:1148:VAL:HB	2:I:1165:ASN:HA	2.01	0.43
2:I:1622:GLU:N	2:I:1627:ALA:O	2.51	0.43
2:E:1679:ASN:HA	2:E:1682:ALA:HB3	2.01	0.43
2:G:1679:ASN:HA	2:G:1682:ALA:HB3	2.01	0.43
1:F:87:HIS:HD2	1:F:90:VAL:HB	1.84	0.43
2:B:1679:ASN:HA	2:B:1682:ALA:HB3	2.01	0.43
2:B:4227:GLU:HG3	2:B:4228:ALA:H	1.83	0.43
2:B:4780:PHE:HD1	2:B:4783:ILE:HD12	1.84	0.43
2:G:3827:GLY:HA2	2:G:3830:GLN:HE21	1.84	0.43
2:G:3842:LEU:O	2:G:3929:SER:OG	2.30	0.43
2:B:1096:THR:HG23	2:B:1199:VAL:HG22	2.01	0.43
2:I:395:GLN:NE2	2:I:397:GLU:OE1	2.51	0.43
2:E:2212:VAL:O	2:E:2216:GLY:N	2.48	0.43
2:G:1105:ALA:N	2:G:1189:LEU:O	2.50	0.43
2:G:2742:THR:OG1	2:G:2811:GLU:OE1	2.31	0.43
2:G:4191:GLU:OE1	2:G:5006:GLN:NE2	2.51	0.43
1:H:2:VAL:HG21	1:H:61:GLU:HB2	1.99	0.43
1:H:21:THR:N	1:H:107:GLU:OE1	2.43	0.43
2:B:235:ALA:HA	2:B:257:ARG:HD3	2.00	0.43
2:B:3827:GLY:HA2	2:B:3830:GLN:HE21	1.83	0.43
2:I:235:ALA:HA	2:I:257:ARG:HD3	2.00	0.43
2:I:3830:GLN:HA	2:I:3833:GLN:HG2	2.00	0.43
2:I:3951:PHE:HD2	2:I:4012:LEU:HD11	1.83	0.43
2:E:1078:GLU:HB3	2:E:1081:TYR:HD2	1.83	0.43
2:E:4780:PHE:HD1	2:E:4783:ILE:HD12	1.84	0.43
2:G:1096:THR:HG23	2:G:1199:VAL:HG22	2.01	0.43
2:G:1848:LEU:HD22	2:G:1853:ILE:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:34:LYS:NZ	1:H:35:LYS:O	2.44	0.43
2:I:315:CYS:SG	2:I:316:PHE:N	2.92	0.43
2:I:395:GLN:HG3	2:I:397:GLU:H	1.83	0.43
2:I:3971:GLY:H	2:I:5005:GLY:HA3	1.83	0.43
2:E:1660:GLN:O	2:E:1664:SER:N	2.49	0.43
2:E:3827:GLY:HA2	2:E:3830:GLN:HE21	1.84	0.43
2:E:3830:GLN:HA	2:E:3833:GLN:HG2	2.00	0.43
2:B:3830:GLN:HA	2:B:3833:GLN:HG2	2.00	0.43
2:B:4577:LEU:HG	2:B:4580:TYR:HE2	1.84	0.43
2:E:4191:GLU:OE1	2:E:5006:GLN:NE2	2.51	0.43
2:E:4227:GLU:HG3	2:E:4228:ALA:H	1.83	0.43
2:E:4577:LEU:HG	2:E:4580:TYR:HE2	1.84	0.43
2:G:1078:GLU:HB3	2:G:1081:TYR:HD2	1.83	0.43
2:G:4562:LEU:HD13	2:G:4656:LEU:HB3	2.00	0.43
1:A:87:HIS:HD2	1:A:90:VAL:HB	1.83	0.42
1:J:87:HIS:HD2	1:J:90:VAL:HB	1.84	0.42
2:I:1096:THR:HG23	2:I:1199:VAL:HG22	2.01	0.42
2:E:395:GLN:HG3	2:E:397:GLU:H	1.83	0.42
2:E:1105:ALA:N	2:E:1189:LEU:O	2.50	0.42
2:E:1622:GLU:N	2:E:1627:ALA:O	2.51	0.42
2:G:315:CYS:SG	2:G:316:PHE:N	2.92	0.42
2:B:2212:VAL:O	2:B:2216:GLY:N	2.48	0.42
2:B:3889:GLN:HE22	2:B:3963:ASN:HB3	1.84	0.42
2:B:4735:GLU:HA	2:B:4738:ALA:HB3	2.01	0.42
2:I:1078:GLU:HB3	2:I:1081:TYR:HD2	1.83	0.42
2:I:3889:GLN:HE22	2:I:3963:ASN:HB3	1.84	0.42
2:I:4191:GLU:OE1	2:I:5006:GLN:NE2	2.51	0.42
2:I:4780:PHE:HD1	2:I:4783:ILE:HD12	1.84	0.42
2:E:1096:THR:HG23	2:E:1199:VAL:HG22	2.01	0.42
2:E:1101:ARG:HH21	2:E:1115:LEU:HB3	1.84	0.42
2:G:3830:GLN:HA	2:G:3833:GLN:HG2	2.00	0.42
2:B:4191:GLU:OE1	2:B:5006:GLN:NE2	2.51	0.42
2:B:4786:ASP:OD2	2:B:4789:PHE:N	2.43	0.42
2:G:1148:VAL:HB	2:G:1165:ASN:HA	2.01	0.42
1:H:92:PRO:HD3	2:G:627:PRO:HB2	2.00	0.42
2:B:1848:LEU:HD22	2:B:1853:ILE:HG13	2.00	0.42
2:I:1189:LEU:HD12	2:I:1190:PRO:HD2	2.02	0.42
2:I:2022:PRO:O	2:I:2028:ARG:NH2	2.42	0.42
2:I:4735:GLU:HA	2:I:4738:ALA:HB3	2.01	0.42
2:G:1622:GLU:N	2:G:1627:ALA:O	2.51	0.42
2:G:3365:UNK:O	2:G:3369:UNK:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4913:ARG:O	2:G:4917:ASP:N	2.46	0.42
2:B:3362:UNK:O	2:B:3366:UNK:N	2.52	0.42
2:I:2121:PHE:O	2:I:3725:TYR:OH	2.34	0.42
2:I:3676:ASP:OD1	2:I:3676:ASP:N	2.51	0.42
2:E:1099:GLU:OE2	2:E:1127:HIS:ND1	2.41	0.42
2:G:4227:GLU:HG3	2:G:4228:ALA:H	1.83	0.42
1:F:21:THR:N	1:F:107:GLU:OE1	2.43	0.42
2:B:164:ARG:N	2:B:167:ASP:OD2	2.53	0.42
2:B:315:CYS:SG	2:B:316:PHE:N	2.92	0.42
2:B:1101:ARG:HH21	2:B:1115:LEU:HB3	1.84	0.42
2:B:1148:VAL:HB	2:B:1165:ASN:HA	2.01	0.42
2:I:644:ILE:HA	2:I:825:PRO:HA	2.02	0.42
2:I:1660:GLN:O	2:I:1664:SER:N	2.49	0.42
2:I:2236:LEU:HD23	2:I:2275:VAL:HG21	2.02	0.42
2:I:2869:ARG:HA	2:I:2872:GLN:HB3	2.01	0.42
2:I:3362:UNK:O	2:I:3366:UNK:N	2.52	0.42
2:E:3362:UNK:O	2:E:3366:UNK:N	2.52	0.42
2:G:4745:LEU:O	2:G:4749:GLU:N	2.46	0.42
2:I:1663:HIS:O	2:I:1667:LEU:N	2.52	0.42
2:I:1848:LEU:HD22	2:I:1853:ILE:HG13	2.00	0.42
2:E:1189:LEU:HD12	2:E:1190:PRO:HD2	2.02	0.42
2:G:164:ARG:N	2:G:167:ASP:OD2	2.53	0.42
2:G:583:ILE:H	2:G:583:ILE:HG13	1.66	0.42
2:G:1101:ARG:HH21	2:G:1115:LEU:HB3	1.84	0.42
2:G:4780:PHE:HD1	2:G:4783:ILE:HD12	1.84	0.42
2:B:1189:LEU:HD12	2:B:1190:PRO:HD2	2.02	0.42
2:E:315:CYS:SG	2:E:316:PHE:N	2.92	0.42
2:E:4713:SER:HA	2:E:4718:LYS:HE2	2.02	0.42
2:G:1764:GLY:HA3	2:G:1859:VAL:HG11	2.02	0.42
2:I:561:LEU:HD11	2:I:599:VAL:HG12	2.02	0.42
2:E:4239:GLU:OE2	2:E:5014:TYR:OH	2.30	0.42
2:G:170:ILE:HD12	2:G:197:GLN:HB3	2.02	0.42
1:J:34:LYS:NZ	1:J:35:LYS:O	2.44	0.42
2:I:164:ARG:N	2:I:167:ASP:OD2	2.53	0.42
2:I:3827:GLY:HA2	2:I:3830:GLN:HE21	1.83	0.42
2:E:170:ILE:HD12	2:E:197:GLN:HB3	2.02	0.42
2:E:1076:ARG:HD3	2:E:1237:TRP:HB2	2.02	0.42
2:E:3365:UNK:O	2:E:3369:UNK:N	2.53	0.42
2:E:4735:GLU:HA	2:E:4738:ALA:HB3	2.01	0.42
2:G:644:ILE:HA	2:G:825:PRO:HA	2.02	0.42
2:G:1685:LEU:HD22	2:G:1718:ILE:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:3362:UNK:O	2:G:3366:UNK:N	2.52	0.42
2:G:4713:SER:HA	2:G:4718:LYS:HE2	2.02	0.42
2:I:3365:UNK:O	2:I:3369:UNK:N	2.53	0.41
2:I:4577:LEU:HG	2:I:4580:TYR:HE2	1.84	0.41
2:E:561:LEU:HD11	2:E:599:VAL:HG12	2.02	0.41
2:E:1148:VAL:HB	2:E:1165:ASN:HA	2.01	0.41
2:E:2236:LEU:HD23	2:E:2275:VAL:HG21	2.02	0.41
2:G:3676:ASP:OD1	2:G:3676:ASP:N	2.51	0.41
2:G:4577:LEU:HG	2:G:4580:TYR:HE2	1.84	0.41
2:B:644:ILE:HA	2:B:825:PRO:HA	2.02	0.41
2:B:3365:UNK:O	2:B:3369:UNK:N	2.53	0.41
2:I:1101:ARG:HH21	2:I:1115:LEU:HB3	1.84	0.41
2:E:164:ARG:N	2:E:167:ASP:OD2	2.53	0.41
2:E:2024:PRO:HB2	2:E:2027:ILE:HG12	2.02	0.41
2:E:2185:ILE:HA	2:E:2188:ASN:ND2	2.35	0.41
2:E:2272:PRO:HA	2:E:2275:VAL:HG12	2.02	0.41
2:E:2438:PRO:HB3	2:E:2453:ILE:HB	2.03	0.41
2:G:561:LEU:HD11	2:G:599:VAL:HG12	2.02	0.41
2:G:2024:PRO:HB2	2:G:2027:ILE:HG12	2.02	0.41
2:G:2272:PRO:HA	2:G:2275:VAL:HG12	2.02	0.41
2:I:3674:ILE:HD11	2:I:3728:ILE:HG22	2.02	0.41
2:E:1764:GLY:HA3	2:E:1859:VAL:HG11	2.02	0.41
2:E:2869:ARG:HA	2:E:2872:GLN:HB3	2.01	0.41
2:G:4735:GLU:HA	2:G:4738:ALA:HB3	2.01	0.41
1:A:21:THR:N	1:A:107:GLU:OE1	2.43	0.41
2:B:170:ILE:HD12	2:B:197:GLN:HB3	2.02	0.41
2:B:2438:PRO:HB3	2:B:2453:ILE:HB	2.03	0.41
2:I:3552:UNK:O	2:I:3556:UNK:N	2.54	0.41
2:G:1189:LEU:HD12	2:G:1190:PRO:HD2	2.02	0.41
2:G:1671:ARG:NH2	2:G:1710:GLY:O	2.53	0.41
2:G:3889:GLN:HE22	2:G:3963:ASN:HB3	1.84	0.41
2:B:215:THR:HG22	2:B:273:HIS:HA	2.02	0.41
2:B:1973:GLN:O	2:B:1977:TYR:N	2.47	0.41
2:B:3552:UNK:O	2:B:3556:UNK:N	2.54	0.41
2:I:4172:GLU:HA	2:I:4175:ARG:HB2	2.02	0.41
2:E:644:ILE:HA	2:E:825:PRO:HA	2.02	0.41
2:E:3889:GLN:HE22	2:E:3963:ASN:HB3	1.84	0.41
2:B:561:LEU:HD11	2:B:599:VAL:HG12	2.02	0.41
2:B:637:LEU:HD23	2:B:1637:MET:HB3	2.02	0.41
2:B:939:VAL:HG22	2:B:1053:ILE:HG12	2.03	0.41
2:B:1671:ARG:NH2	2:B:1710:GLY:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1764:GLY:HA3	2:B:1859:VAL:HG11	2.02	0.41
2:B:2272:PRO:HA	2:B:2275:VAL:HG12	2.02	0.41
2:B:3674:ILE:HD11	2:B:3728:ILE:HG22	2.02	0.41
2:B:4713:SER:HA	2:B:4718:LYS:HE2	2.02	0.41
2:I:469:ARG:HH21	2:I:3712:GLU:HB3	1.86	0.41
2:E:1663:HIS:O	2:E:1667:LEU:N	2.52	0.41
2:E:4745:LEU:O	2:E:4749:GLU:N	2.46	0.41
2:G:469:ARG:HH21	2:G:3712:GLU:HB3	1.86	0.41
2:G:939:VAL:HG22	2:G:1053:ILE:HG12	2.02	0.41
2:G:2438:PRO:HB3	2:G:2453:ILE:HB	2.03	0.41
2:G:3992:PHE:O	2:G:3996:PHE:N	2.44	0.41
2:B:1076:ARG:HD3	2:B:1237:TRP:HB2	2.02	0.41
2:I:2185:ILE:HA	2:I:2188:ASN:ND2	2.35	0.41
2:I:2869:ARG:HH12	2:I:2945:UNK:C	2.34	0.41
2:E:637:LEU:HD23	2:E:1637:MET:HB3	2.02	0.41
2:E:939:VAL:HG22	2:E:1053:ILE:HG12	2.03	0.41
2:E:1685:LEU:HD22	2:E:1718:ILE:HG21	2.02	0.41
2:E:3552:UNK:O	2:E:3556:UNK:N	2.54	0.41
2:G:470:SER:O	2:G:474:ARG:NE	2.53	0.41
2:G:2185:ILE:HA	2:G:2188:ASN:ND2	2.35	0.41
2:G:2236:LEU:HD23	2:G:2275:VAL:HG21	2.02	0.41
2:G:3696:ASP:O	2:G:3700:GLN:N	2.50	0.41
2:B:1802:ILE:HG21	2:B:1807:LEU:HD22	2.03	0.41
2:B:3658:LYS:HA	2:B:3661:TRP:CE2	2.56	0.41
2:I:472:ARG:NH2	2:I:3712:GLU:OE2	2.54	0.41
2:I:1764:GLY:HA3	2:I:1859:VAL:HG11	2.02	0.41
2:I:2438:PRO:HB3	2:I:2453:ILE:HB	2.03	0.41
2:I:4713:SER:HA	2:I:4718:LYS:HE2	2.02	0.41
2:I:4913:ARG:O	2:I:4917:ASP:N	2.46	0.41
2:E:3658:LYS:HA	2:E:3661:TRP:CE2	2.56	0.41
2:G:2869:ARG:HA	2:G:2872:GLN:HB3	2.01	0.41
2:B:134:ASP:OD1	2:B:134:ASP:N	2.50	0.41
2:B:670:GLU:HG3	2:B:787:VAL:HG13	2.03	0.41
2:B:2236:LEU:HD23	2:B:2275:VAL:HG21	2.02	0.41
2:B:4172:GLU:HA	2:B:4175:ARG:HB2	2.02	0.41
2:I:470:SER:O	2:I:474:ARG:NE	2.53	0.41
2:I:583:ILE:H	2:I:583:ILE:HG13	1.65	0.41
2:I:864:PRO:HA	2:I:865:PRO:HD3	1.96	0.41
2:I:1671:ARG:NH2	2:I:1710:GLY:O	2.53	0.41
2:I:1685:LEU:HD22	2:I:1718:ILE:HG21	2.02	0.41
2:I:1973:GLN:HA	2:I:1976:ARG:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2024:PRO:HB2	2:I:2027:ILE:HG12	2.02	0.41
2:E:215:THR:HG22	2:E:273:HIS:HA	2.02	0.41
2:E:1671:ARG:NH2	2:E:1710:GLY:O	2.53	0.41
2:E:1802:ILE:HG21	2:E:1807:LEU:HD22	2.03	0.41
2:E:2121:PHE:O	2:E:3725:TYR:OH	2.34	0.41
2:G:637:LEU:HD23	2:G:1637:MET:HB3	2.02	0.41
2:G:870:ILE:O	2:G:874:LEU:N	2.45	0.41
2:G:3674:ILE:HD11	2:G:3728:ILE:HG22	2.02	0.41
2:G:4172:GLU:HA	2:G:4175:ARG:HB2	2.02	0.41
2:B:1093:GLU:OE1	2:B:1201:HIS:NE2	2.53	0.41
2:B:2869:ARG:HA	2:B:2872:GLN:HB3	2.01	0.41
2:I:170:ILE:HD12	2:I:197:GLN:HB3	2.02	0.41
2:I:637:LEU:HD23	2:I:1637:MET:HB3	2.02	0.41
2:I:2004:GLU:HA	2:I:2007:ASN:HB2	2.03	0.41
2:E:469:ARG:HH21	2:E:3712:GLU:HB3	1.86	0.41
2:E:1089:TYR:N	2:E:1224:GLU:O	2.54	0.41
2:G:218:HIS:HB3	2:G:392:ARG:HE	1.86	0.41
2:G:500:ALA:HB1	2:G:504:ALA:HB2	2.04	0.41
2:G:670:GLU:HG3	2:G:787:VAL:HG13	2.03	0.41
2:B:1089:TYR:N	2:B:1224:GLU:O	2.54	0.40
2:B:1154:ASP:HB3	2:B:1157:GLU:HB3	2.03	0.40
2:B:2185:ILE:HA	2:B:2188:ASN:ND2	2.35	0.40
2:B:3696:ASP:O	2:B:3700:GLN:N	2.50	0.40
2:I:4239:GLU:OE2	2:I:5014:TYR:OH	2.30	0.40
2:E:583:ILE:HA	2:E:586:ILE:HD12	2.03	0.40
2:E:1154:ASP:HB3	2:E:1157:GLU:HB3	2.03	0.40
2:E:1973:GLN:HA	2:E:1976:ARG:HB3	2.03	0.40
2:G:4865:LYS:HG3	2:G:4875:LYS:HZ3	1.85	0.40
2:B:469:ARG:HH21	2:B:3712:GLU:HB3	1.86	0.40
2:I:500:ALA:HB1	2:I:504:ALA:HB2	2.03	0.40
2:I:1865:MET:SD	2:I:1865:MET:N	2.95	0.40
2:I:3658:LYS:HA	2:I:3661:TRP:CE2	2.56	0.40
2:E:838:HIS:CE1	2:E:1201:HIS:HD2	2.40	0.40
2:E:4913:ARG:O	2:E:4917:ASP:N	2.46	0.40
2:G:215:THR:HG22	2:G:273:HIS:HA	2.02	0.40
2:G:887:ILE:HG21	2:G:959:TYR:HA	2.03	0.40
2:G:1089:TYR:N	2:G:1224:GLU:O	2.54	0.40
2:G:1093:GLU:OE1	2:G:1201:HIS:NE2	2.53	0.40
2:B:583:ILE:HA	2:B:586:ILE:HD12	2.03	0.40
2:B:1973:GLN:HA	2:B:1976:ARG:HB3	2.03	0.40
2:B:2004:GLU:HA	2:B:2007:ASN:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:218:HIS:HB3	2:I:392:ARG:HE	1.86	0.40
2:I:1089:TYR:N	2:I:1224:GLU:O	2.54	0.40
2:I:2272:PRO:HA	2:I:2275:VAL:HG12	2.02	0.40
2:I:4976:GLU:O	2:I:4979:THR:OG1	2.37	0.40
2:E:472:ARG:NH2	2:E:3712:GLU:OE2	2.54	0.40
2:E:583:ILE:H	2:E:583:ILE:HG13	1.66	0.40
2:E:4172:GLU:HA	2:E:4175:ARG:HB2	2.02	0.40
2:E:4929:LEU:HD13	2:E:4929:LEU:HA	1.97	0.40
2:G:1076:ARG:HD3	2:G:1237:TRP:HB2	2.02	0.40
2:G:3658:LYS:HA	2:G:3661:TRP:CE2	2.56	0.40
2:B:2022:PRO:O	2:B:2028:ARG:NH2	2.42	0.40
2:I:939:VAL:HG22	2:I:1053:ILE:HG12	2.03	0.40
2:I:1154:ASP:HB3	2:I:1157:GLU:HB3	2.03	0.40
2:E:4571:PHE:O	2:E:4575:PHE:N	2.51	0.40
2:B:887:ILE:HG21	2:B:959:TYR:HA	2.03	0.40
2:B:2024:PRO:HB2	2:B:2027:ILE:HG12	2.02	0.40
2:B:2950:UNK:O	2:B:2954:UNK:N	2.55	0.40
2:B:4138:ASP:OD1	2:B:4138:ASP:N	2.54	0.40
2:I:215:THR:HG22	2:I:273:HIS:HA	2.02	0.40
2:I:1076:ARG:HD3	2:I:1237:TRP:HB2	2.02	0.40
2:I:1093:GLU:OE1	2:I:1201:HIS:NE2	2.53	0.40
2:E:207:SER:OG	2:E:208:CYS:N	2.55	0.40
2:E:887:ILE:HG21	2:E:959:TYR:HA	2.03	0.40
2:E:4138:ASP:N	2:E:4138:ASP:OD1	2.54	0.40
2:G:195:PHE:HB3	2:G:196:MET:HG2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	105/108 (97%)	94 (90%)	11 (10%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
1	H	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
1	J	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
2	B	3235/4416 (73%)	2929 (90%)	304 (9%)	2 (0%)	51	85
2	E	3235/4416 (73%)	2931 (91%)	302 (9%)	2 (0%)	51	85
2	G	3235/4416 (73%)	2930 (91%)	303 (9%)	2 (0%)	51	85
2	I	3235/4416 (73%)	2930 (91%)	303 (9%)	2 (0%)	51	85
All	All	13360/18096 (74%)	12093 (90%)	1259 (9%)	8 (0%)	54	85

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1708	ARG
2	I	1708	ARG
2	E	1708	ARG
2	G	1708	ARG
2	B	4641	PRO
2	I	4641	PRO
2	E	4641	PRO
2	G	4641	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	88/89 (99%)	88 (100%)	0	100	100
1	F	88/89 (99%)	88 (100%)	0	100	100
1	H	88/89 (99%)	88 (100%)	0	100	100
1	J	88/89 (99%)	88 (100%)	0	100	100
2	B	2493/3022 (82%)	2476 (99%)	17 (1%)	84	90
2	E	2493/3022 (82%)	2476 (99%)	17 (1%)	84	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	G	2493/3022 (82%)	2476 (99%)	17 (1%)	84 90
2	I	2493/3022 (82%)	2476 (99%)	17 (1%)	84 90
All	All	10324/12444 (83%)	10256 (99%)	68 (1%)	84 90

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	131	LEU
2	B	534	ARG
2	B	553	ARG
2	B	1076	ARG
2	B	1141	ARG
2	B	1600	LEU
2	B	1676	LEU
2	B	1964	ARG
2	B	3663	LEU
2	B	3787	LYS
2	B	3805	LEU
2	B	3896	ASN
2	B	4034	ASN
2	B	4085	ARG
2	B	4120	ASN
2	B	4131	ARG
2	B	4913	ARG
2	I	131	LEU
2	I	534	ARG
2	I	553	ARG
2	I	1076	ARG
2	I	1141	ARG
2	I	1600	LEU
2	I	1676	LEU
2	I	1964	ARG
2	I	3663	LEU
2	I	3787	LYS
2	I	3805	LEU
2	I	3896	ASN
2	I	4034	ASN
2	I	4085	ARG
2	I	4120	ASN
2	I	4131	ARG
2	I	4913	ARG

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Mol	Chain	Res	Type
2	E	131	LEU
2	E	534	ARG
2	E	553	ARG
2	E	1076	ARG
2	E	1141	ARG
2	E	1600	LEU
2	E	1676	LEU
2	E	1964	ARG
2	E	3663	LEU
2	E	3787	LYS
2	E	3805	LEU
2	E	3896	ASN
2	E	4034	ASN
2	E	4085	ARG
2	E	4120	ASN
2	E	4131	ARG
2	E	4913	ARG
2	G	131	LEU
2	G	534	ARG
2	G	553	ARG
2	G	1076	ARG
2	G	1141	ARG
2	G	1600	LEU
2	G	1676	LEU
2	G	1964	ARG
2	G	3663	LEU
2	G	3787	LYS
2	G	3805	LEU
2	G	3896	ASN
2	G	4034	ASN
2	G	4085	ARG
2	G	4120	ASN
2	G	4131	ARG
2	G	4913	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (135) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	87	HIS
1	A	87	HIS
1	H	87	HIS
1	J	87	HIS

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Mol	Chain	Res	Type
2	B	57	ASN
2	B	71	GLN
2	B	111	HIS
2	B	379	HIS
2	B	383	HIS
2	B	395	GLN
2	B	413	GLN
2	B	495	ASN
2	B	582	HIS
2	B	838	HIS
2	B	1158	ASN
2	B	1598	GLN
2	B	1679	ASN
2	B	1688	HIS
2	B	1691	GLN
2	B	1719	HIS
2	B	1775	HIS
2	B	2127	GLN
2	B	3809	ASN
2	B	3889	GLN
2	B	3896	ASN
2	B	3946	GLN
2	B	3950	ASN
2	B	3960	GLN
2	B	3976	ASN
2	B	4034	ASN
2	B	4120	ASN
2	B	4728	HIS
2	B	4806	ASN
2	B	4946	GLN
2	B	5003	HIS
2	I	57	ASN
2	I	71	GLN
2	I	111	HIS
2	I	156	GLN
2	I	379	HIS
2	I	383	HIS
2	I	395	GLN
2	I	413	GLN
2	I	582	HIS
2	I	797	HIS
2	I	838	HIS

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Mol	Chain	Res	Type
2	I	1158	ASN
2	I	1598	GLN
2	I	1679	ASN
2	I	1688	HIS
2	I	1691	GLN
2	I	1719	HIS
2	I	1775	HIS
2	I	2127	GLN
2	I	3809	ASN
2	I	3830	GLN
2	I	3889	GLN
2	I	3896	ASN
2	I	3946	GLN
2	I	3950	ASN
2	I	3960	GLN
2	I	3976	ASN
2	I	4034	ASN
2	I	4120	ASN
2	I	4728	HIS
2	I	4806	ASN
2	I	4946	GLN
2	I	5003	HIS
2	E	57	ASN
2	E	71	GLN
2	E	111	HIS
2	E	156	GLN
2	E	379	HIS
2	E	383	HIS
2	E	395	GLN
2	E	413	GLN
2	E	582	HIS
2	E	765	GLN
2	E	838	HIS
2	E	1158	ASN
2	E	1598	GLN
2	E	1679	ASN
2	E	1688	HIS
2	E	1691	GLN
2	E	1719	HIS
2	E	1775	HIS
2	E	2127	GLN
2	E	3809	ASN

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Mol	Chain	Res	Type
2	E	3830	GLN
2	E	3889	GLN
2	E	3896	ASN
2	E	3946	GLN
2	E	3950	ASN
2	E	3960	GLN
2	E	3976	ASN
2	E	4034	ASN
2	E	4120	ASN
2	E	4553	ASN
2	E	4728	HIS
2	E	4806	ASN
2	E	4946	GLN
2	E	5003	HIS
2	G	57	ASN
2	G	71	GLN
2	G	111	HIS
2	G	379	HIS
2	G	383	HIS
2	G	395	GLN
2	G	413	GLN
2	G	582	HIS
2	G	797	HIS
2	G	838	HIS
2	G	1158	ASN
2	G	1598	GLN
2	G	1679	ASN
2	G	1688	HIS
2	G	1691	GLN
2	G	1719	HIS
2	G	1775	HIS
2	G	2127	GLN
2	G	3809	ASN
2	G	3830	GLN
2	G	3889	GLN
2	G	3896	ASN
2	G	3946	GLN
2	G	3950	ASN
2	G	3960	GLN
2	G	3976	ASN
2	G	4034	ASN
2	G	4120	ASN

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Mol	Chain	Res	Type
2	G	4553	ASN
2	G	4728	HIS
2	G	4806	ASN
2	G	4946	GLN
2	G	5003	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	ATP	E	5101	-	26,33,33	0.88	1 (3%)	31,52,52	1.43	5 (16%)
3	ATP	B	5101	-	26,33,33	0.88	1 (3%)	31,52,52	1.43	5 (16%)
3	ATP	G	5101	-	26,33,33	0.88	1 (3%)	31,52,52	1.43	5 (16%)
4	CFF	G	5102	-	8,15,15	2.39	3 (37%)	8,23,23	1.32	1 (12%)
4	CFF	E	5102	-	8,15,15	2.38	3 (37%)	8,23,23	1.30	1 (12%)
3	ATP	I	5101	-	26,33,33	0.88	1 (3%)	31,52,52	1.43	5 (16%)
4	CFF	B	5102	-	8,15,15	2.38	3 (37%)	8,23,23	1.32	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	CFF	I	5102	-	8,15,15	2.37	3 (37%)	8,23,23	1.31	1 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	E	5101	-	-	6/18/38/38	0/3/3/3
3	ATP	B	5101	-	-	6/18/38/38	0/3/3/3
3	ATP	G	5101	-	-	6/18/38/38	0/3/3/3
4	CFF	G	5102	-	-	-	0/2/2/2
4	CFF	E	5102	-	-	-	0/2/2/2
3	ATP	I	5101	-	-	6/18/38/38	0/3/3/3
4	CFF	B	5102	-	-	-	0/2/2/2
4	CFF	I	5102	-	-	-	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	5102	CFF	C5-C4	-4.42	1.33	1.39
4	G	5102	CFF	C5-C4	-4.42	1.33	1.39
4	I	5102	CFF	C5-C4	-4.42	1.33	1.39
4	B	5102	CFF	C5-C4	-4.36	1.33	1.39
4	B	5102	CFF	C6-N1	-3.90	1.32	1.38
4	G	5102	CFF	C6-N1	-3.90	1.32	1.38
4	E	5102	CFF	C6-N1	-3.87	1.32	1.38
4	I	5102	CFF	C6-N1	-3.81	1.32	1.38
4	B	5102	CFF	O13-C6	-2.36	1.18	1.24
4	I	5102	CFF	O13-C6	-2.36	1.18	1.24
4	E	5102	CFF	O13-C6	-2.36	1.18	1.24
4	G	5102	CFF	O13-C6	-2.32	1.18	1.24
3	B	5101	ATP	C5-C4	2.24	1.46	1.40
3	I	5101	ATP	C5-C4	2.22	1.46	1.40
3	G	5101	ATP	C5-C4	2.21	1.46	1.40
3	E	5101	ATP	C5-C4	2.20	1.46	1.40

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	5101	ATP	PB-O3B-PG	-3.51	120.77	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	5101	ATP	PB-O3B-PG	-3.51	120.78	132.83
3	B	5101	ATP	PB-O3B-PG	-3.50	120.81	132.83
3	I	5101	ATP	PB-O3B-PG	-3.50	120.81	132.83
3	E	5101	ATP	C3'-C2'-C1'	3.14	105.71	100.98
3	I	5101	ATP	C3'-C2'-C1'	3.13	105.69	100.98
3	G	5101	ATP	C3'-C2'-C1'	3.12	105.68	100.98
3	B	5101	ATP	C3'-C2'-C1'	3.11	105.66	100.98
3	E	5101	ATP	N3-C2-N1	-3.04	123.93	128.68
3	G	5101	ATP	N3-C2-N1	-3.03	123.94	128.68
3	I	5101	ATP	N3-C2-N1	-3.02	123.96	128.68
3	B	5101	ATP	N3-C2-N1	-3.01	123.98	128.68
4	B	5102	CFF	C14-N7-C8	-2.87	111.63	125.43
4	G	5102	CFF	C14-N7-C8	-2.86	111.67	125.43
4	E	5102	CFF	C14-N7-C8	-2.85	111.70	125.43
4	I	5102	CFF	C14-N7-C8	-2.85	111.72	125.43
3	B	5101	ATP	PA-O3A-PB	-2.59	123.95	132.83
3	E	5101	ATP	PA-O3A-PB	-2.59	123.95	132.83
3	G	5101	ATP	PA-O3A-PB	-2.58	123.98	132.83
3	I	5101	ATP	PA-O3A-PB	-2.58	123.99	132.83
3	I	5101	ATP	C4-C5-N7	-2.21	107.10	109.40
3	B	5101	ATP	C4-C5-N7	-2.20	107.11	109.40
3	G	5101	ATP	C4-C5-N7	-2.19	107.11	109.40
3	E	5101	ATP	C4-C5-N7	-2.16	107.15	109.40

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	5101	ATP	C5'-O5'-PA-O1A
3	B	5101	ATP	C5'-O5'-PA-O2A
3	I	5101	ATP	C5'-O5'-PA-O1A
3	I	5101	ATP	C5'-O5'-PA-O2A
3	E	5101	ATP	C5'-O5'-PA-O1A
3	E	5101	ATP	C5'-O5'-PA-O2A
3	G	5101	ATP	C5'-O5'-PA-O1A
3	G	5101	ATP	C5'-O5'-PA-O2A
3	B	5101	ATP	PB-O3A-PA-O5'
3	I	5101	ATP	PB-O3A-PA-O5'
3	E	5101	ATP	PB-O3A-PA-O5'
3	G	5101	ATP	PB-O3A-PA-O5'
3	B	5101	ATP	C4'-C5'-O5'-PA
3	I	5101	ATP	C4'-C5'-O5'-PA

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Mol	Chain	Res	Type	Atoms
3	E	5101	ATP	C4'-C5'-O5'-PA
3	G	5101	ATP	C4'-C5'-O5'-PA
3	B	5101	ATP	O4'-C4'-C5'-O5'
3	I	5101	ATP	O4'-C4'-C5'-O5'
3	E	5101	ATP	O4'-C4'-C5'-O5'
3	G	5101	ATP	O4'-C4'-C5'-O5'
3	B	5101	ATP	C5'-O5'-PA-O3A
3	I	5101	ATP	C5'-O5'-PA-O3A
3	E	5101	ATP	C5'-O5'-PA-O3A
3	G	5101	ATP	C5'-O5'-PA-O3A

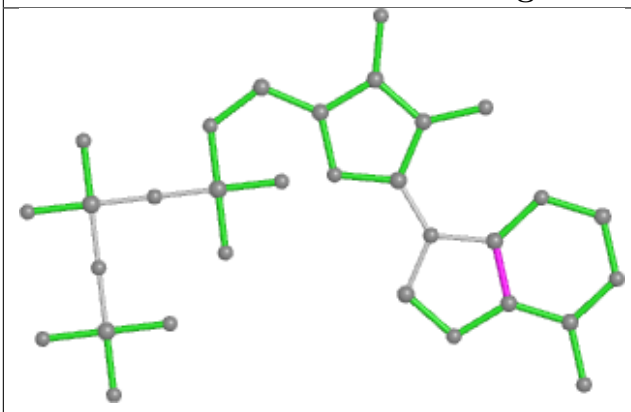
There are no ring outliers.

8 monomers are involved in 8 short contacts:

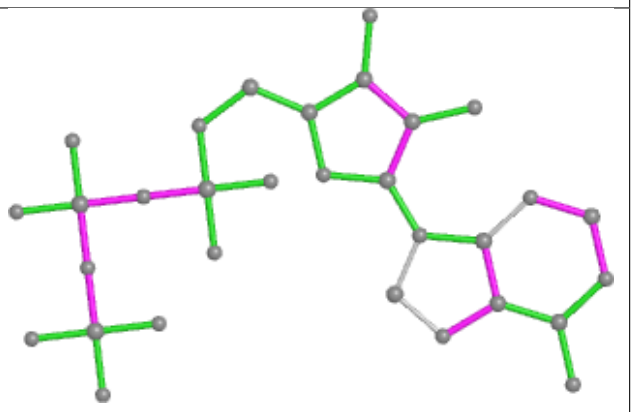
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	5101	ATP	1	0
3	B	5101	ATP	1	0
3	G	5101	ATP	1	0
4	G	5102	CFF	1	0
4	E	5102	CFF	1	0
3	I	5101	ATP	1	0
4	B	5102	CFF	1	0
4	I	5102	CFF	1	0

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

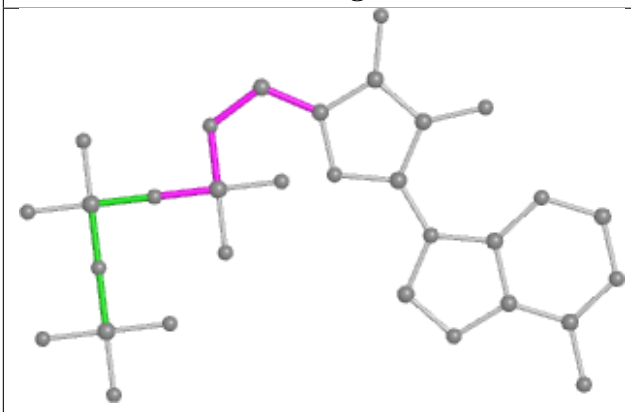
Ligand ATP E 5101



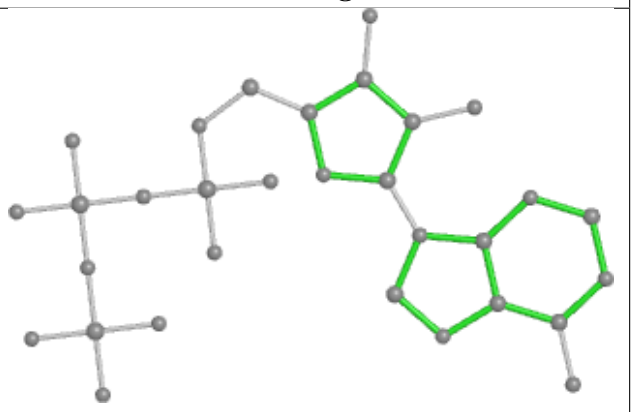
Bond lengths



Bond angles

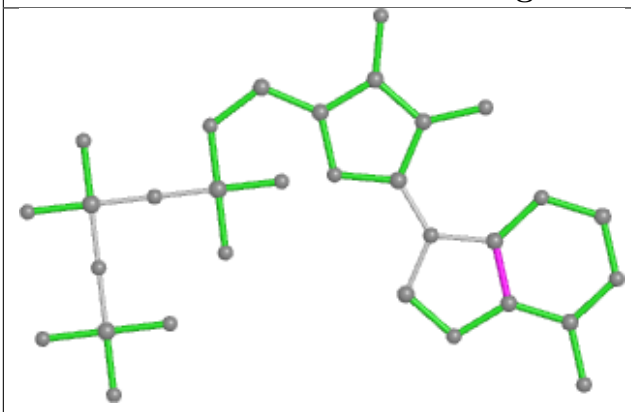


Torsions

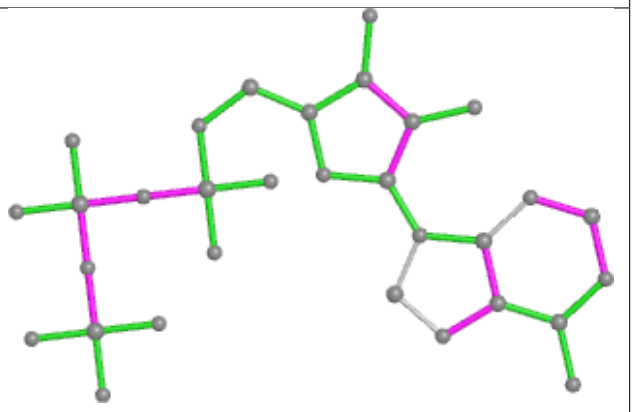


Rings

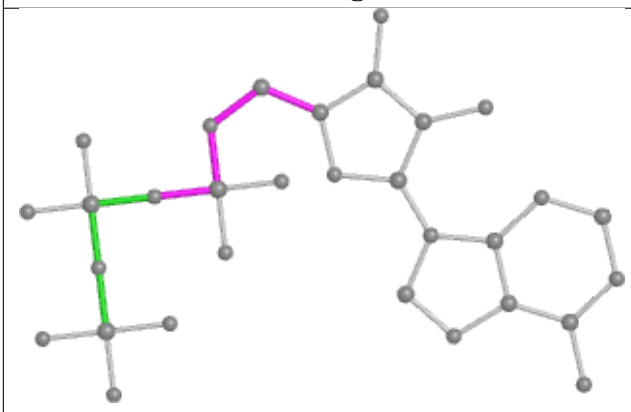
Ligand ATP B 5101



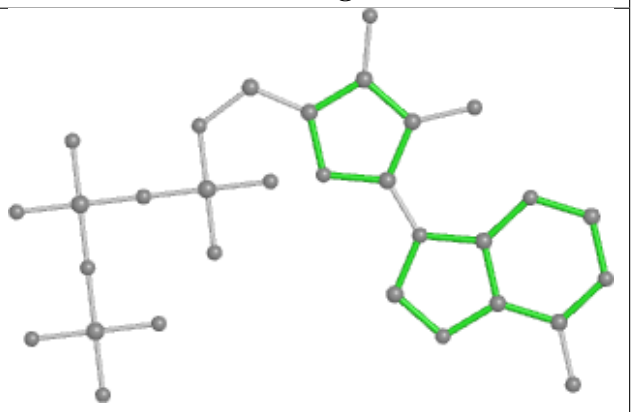
Bond lengths



Bond angles

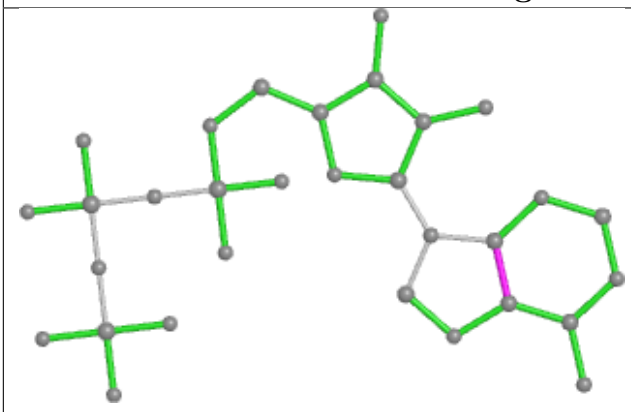


Torsions

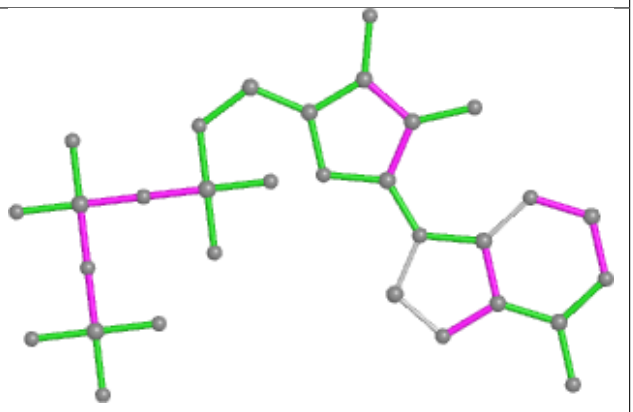


Rings

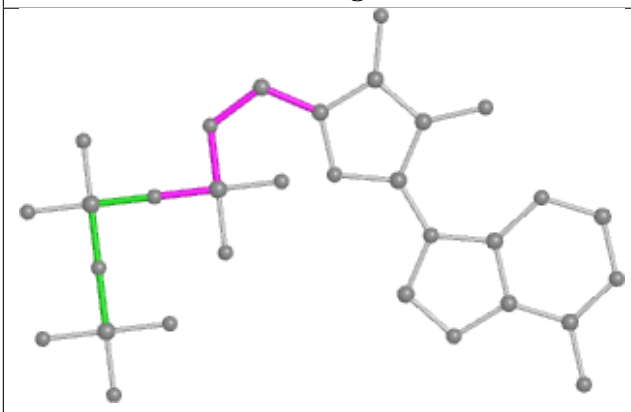
Ligand ATP G 5101



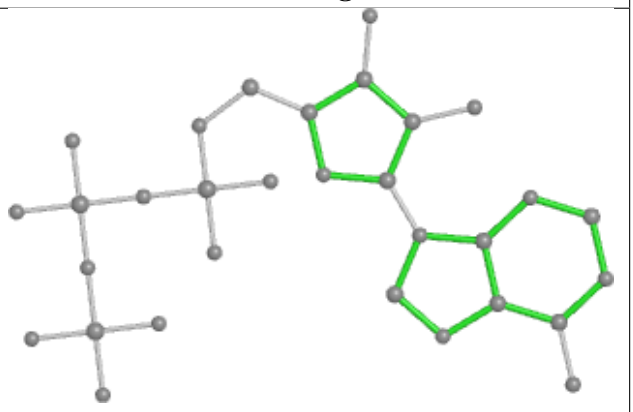
Bond lengths



Bond angles

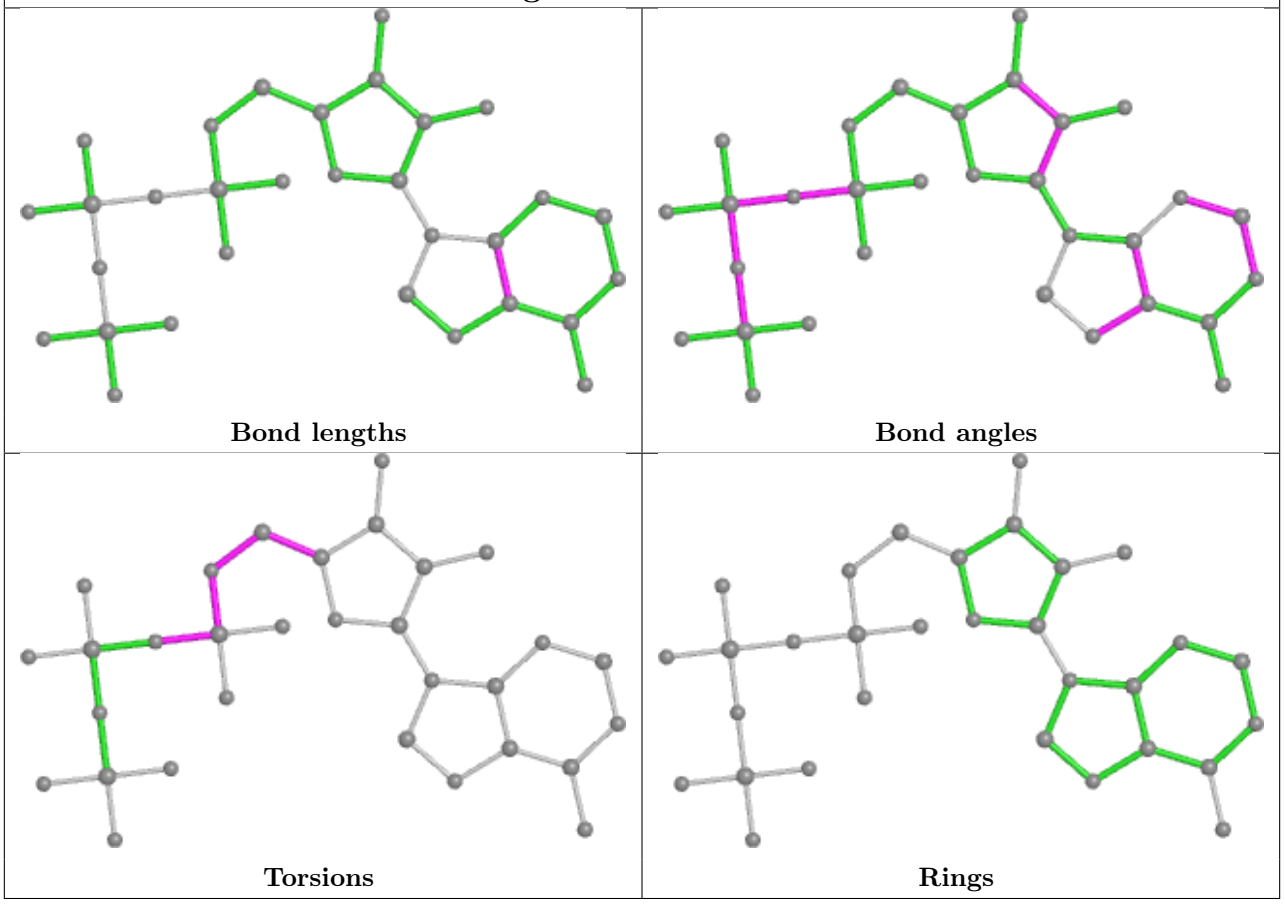


Torsions



Rings

Ligand ATP I 5101



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	14
2	E	14
2	I	14
2	G	14

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	4345:UNK	C	4540:PHE	N	74.23
1	E	4345:UNK	C	4540:PHE	N	74.23

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	4345:UNK	C	4540:PHE	N	74.22
1	G	4345:UNK	C	4540:PHE	N	74.22
1	I	3613:UNK	C	3639:THR	N	43.91
1	B	3613:UNK	C	3639:THR	N	43.90
1	G	3613:UNK	C	3639:THR	N	43.90
1	E	3613:UNK	C	3639:THR	N	43.89
1	B	4253:GLU	C	4320:UNK	N	26.88
1	I	4253:GLU	C	4320:UNK	N	26.88
1	E	4253:GLU	C	4320:UNK	N	26.88
1	G	4253:GLU	C	4320:UNK	N	26.88
1	I	3163:UNK	C	3170:UNK	N	16.01
1	G	3163:UNK	C	3170:UNK	N	16.01
1	B	3163:UNK	C	3170:UNK	N	16.00
1	E	3163:UNK	C	3170:UNK	N	16.00
1	B	3063:UNK	C	3134:UNK	N	14.82
1	I	3063:UNK	C	3134:UNK	N	14.82
1	E	3063:UNK	C	3134:UNK	N	14.82
1	G	3063:UNK	C	3134:UNK	N	14.82
1	B	3468:UNK	C	3511:UNK	N	14.51
1	I	3468:UNK	C	3511:UNK	N	14.51
1	E	3468:UNK	C	3511:UNK	N	14.51
1	G	3468:UNK	C	3511:UNK	N	14.51
1	E	2703:UNK	C	2734:ASN	N	14.06
1	B	2703:UNK	C	2734:ASN	N	14.05
1	I	2703:UNK	C	2734:ASN	N	14.05
1	G	2703:UNK	C	2734:ASN	N	14.05
1	B	3236:UNK	C	3241:UNK	N	13.47
1	I	3236:UNK	C	3241:UNK	N	13.47
1	E	3236:UNK	C	3241:UNK	N	13.47
1	G	3236:UNK	C	3241:UNK	N	13.47
1	B	2976:UNK	C	2995:UNK	N	12.24
1	I	2976:UNK	C	2995:UNK	N	12.24
1	E	2976:UNK	C	2995:UNK	N	12.24
1	G	2976:UNK	C	2995:UNK	N	12.24
1	E	1564:UNK	C	1573:MET	N	12.12
1	G	1564:UNK	C	1573:MET	N	12.12
1	B	1564:UNK	C	1573:MET	N	12.11
1	I	1564:UNK	C	1573:MET	N	12.11
1	B	3254:UNK	C	3261:UNK	N	8.26
1	I	3254:UNK	C	3261:UNK	N	8.26
1	E	3254:UNK	C	3261:UNK	N	8.26
1	G	3254:UNK	C	3261:UNK	N	8.26

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	1297:UNK	C	1430:UNK	N	5.81
1	I	1297:UNK	C	1430:UNK	N	5.81
1	E	1297:UNK	C	1430:UNK	N	5.81
1	G	1297:UNK	C	1430:UNK	N	5.81
1	E	2939:ARG	C	2942:UNK	N	3.53
1	G	2939:ARG	C	2942:UNK	N	3.53
1	B	2939:ARG	C	2942:UNK	N	3.52
1	I	2939:ARG	C	2942:UNK	N	3.52
1	I	2479:LEU	C	2487:UNK	N	3.25
1	B	2479:LEU	C	2487:UNK	N	3.24
1	E	2479:LEU	C	2487:UNK	N	3.24
1	G	2479:LEU	C	2487:UNK	N	3.24

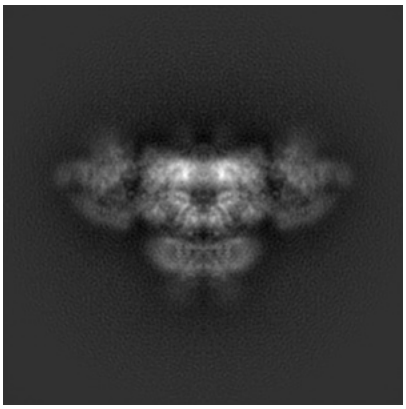
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8384. These allow visual inspection of the internal detail of the map and identification of artifacts.

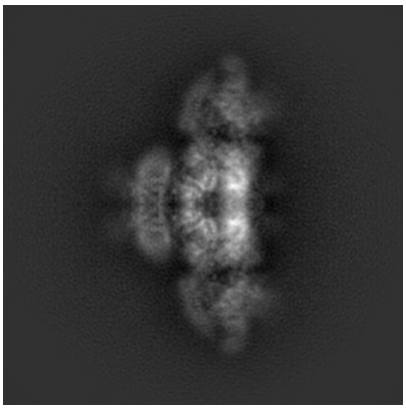
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

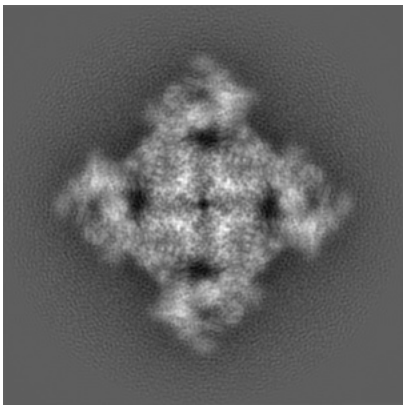
6.1.1 Primary map



X

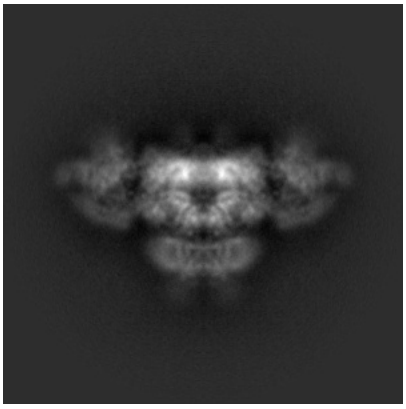


Y

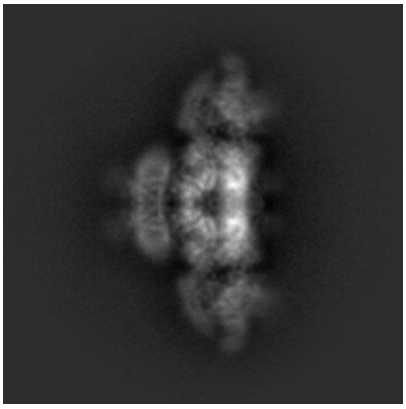


Z

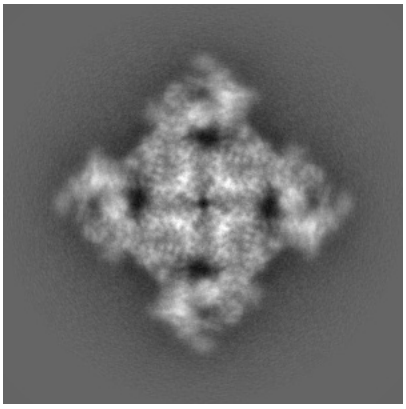
6.1.2 Raw map



X



Y

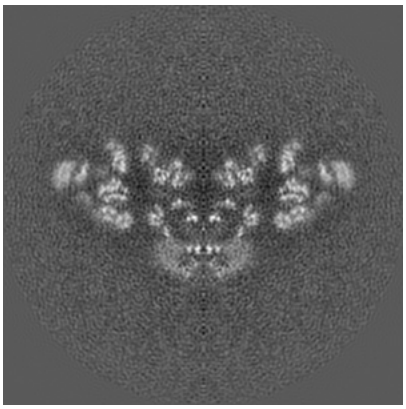


Z

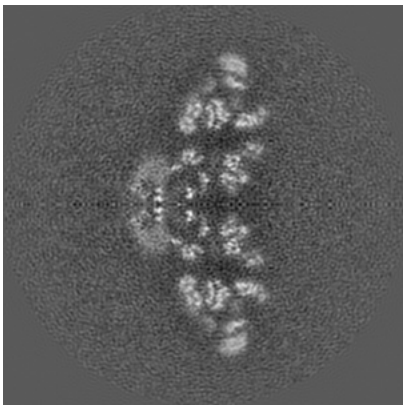
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

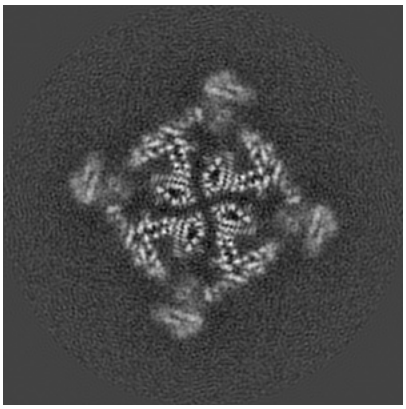
6.2.1 Primary map



X Index: 200

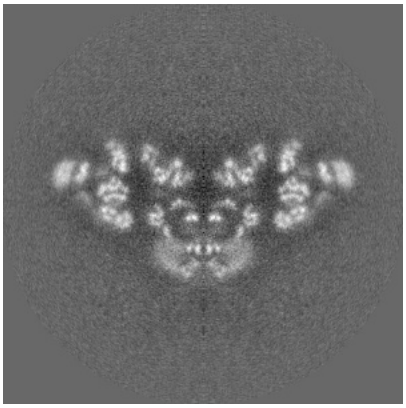


Y Index: 200

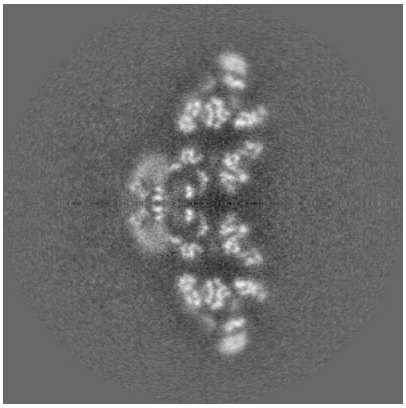


Z Index: 200

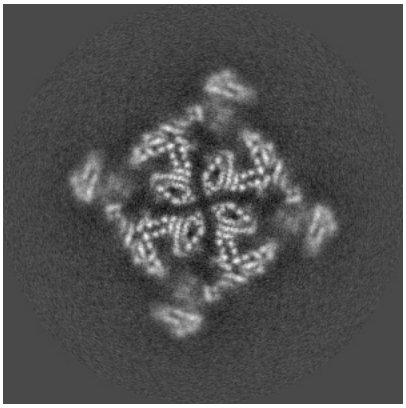
6.2.2 Raw map



X Index: 200



Y Index: 200

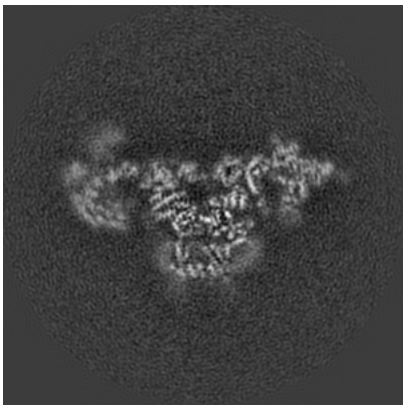


Z Index: 200

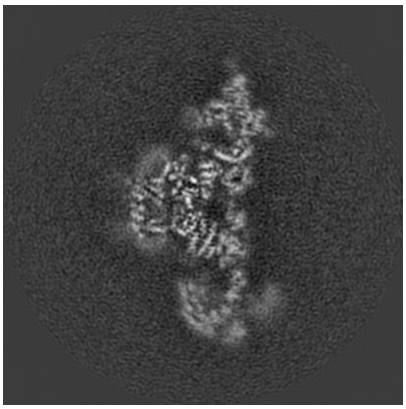
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

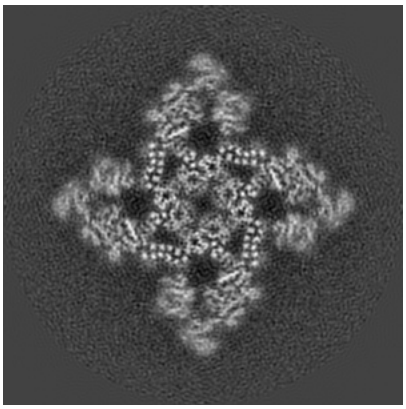
6.3.1 Primary map



X Index: 184

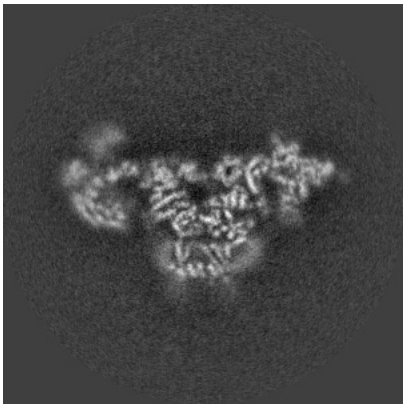


Y Index: 216

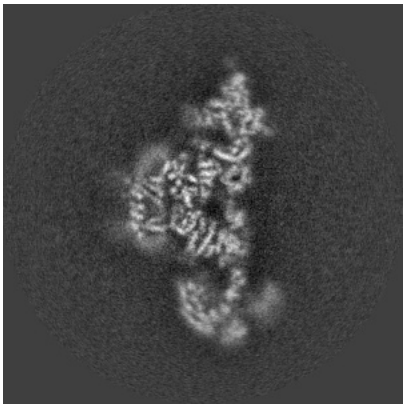


Z Index: 227

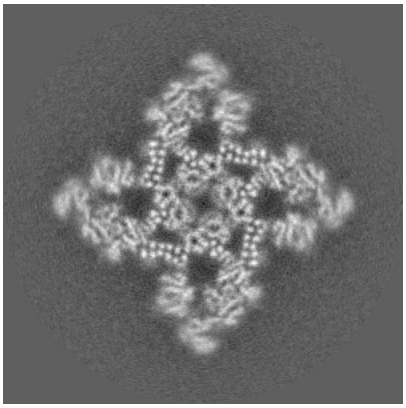
6.3.2 Raw map



X Index: 184



Y Index: 216

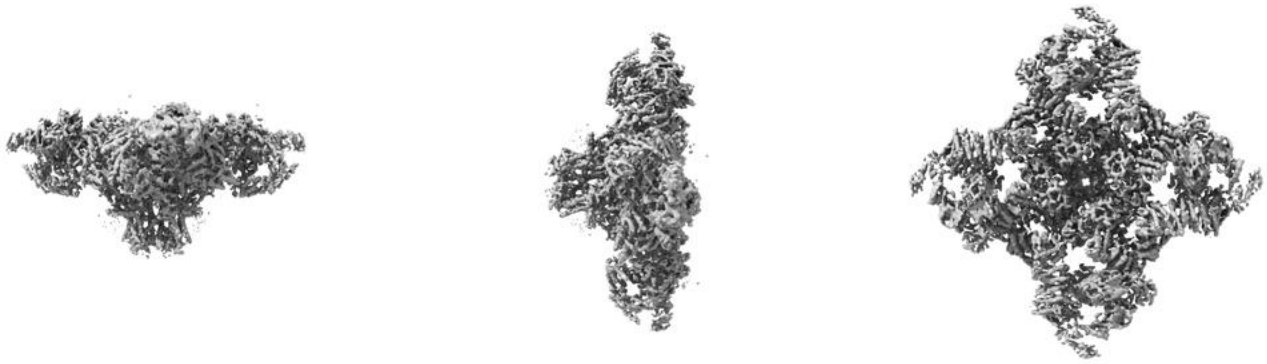


Z Index: 227

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

6.4 Orthogonal surface views (i)

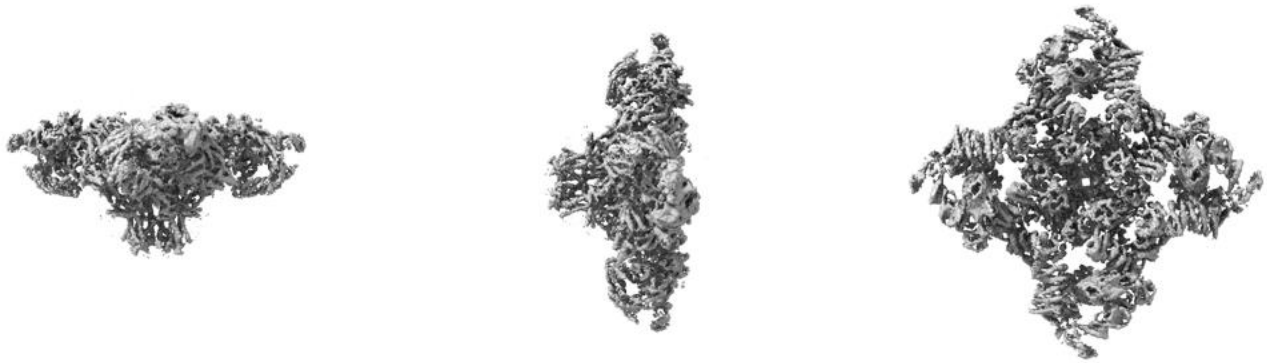
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

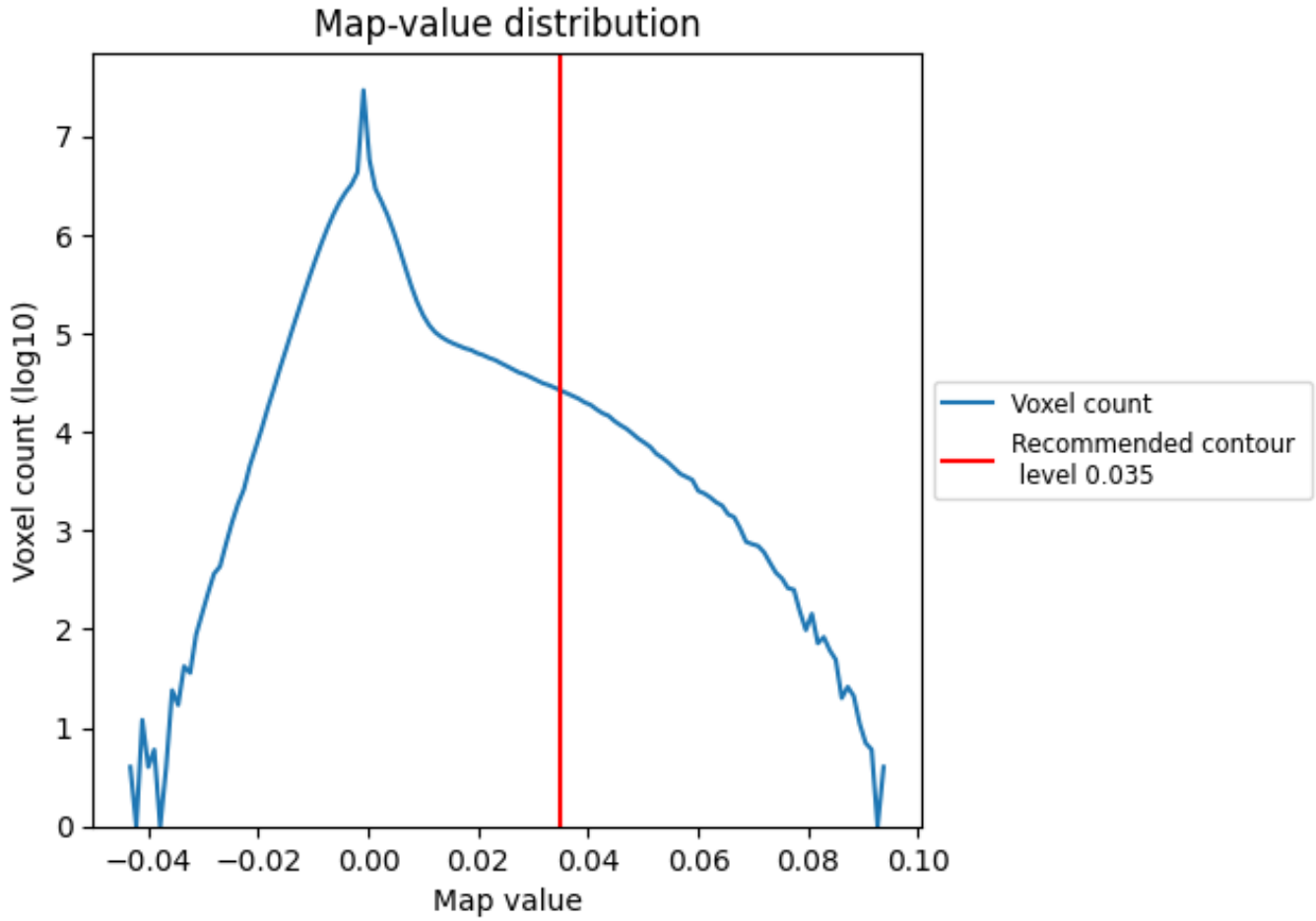
6.5 Mask visualisation (i)

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

7 Map analysis

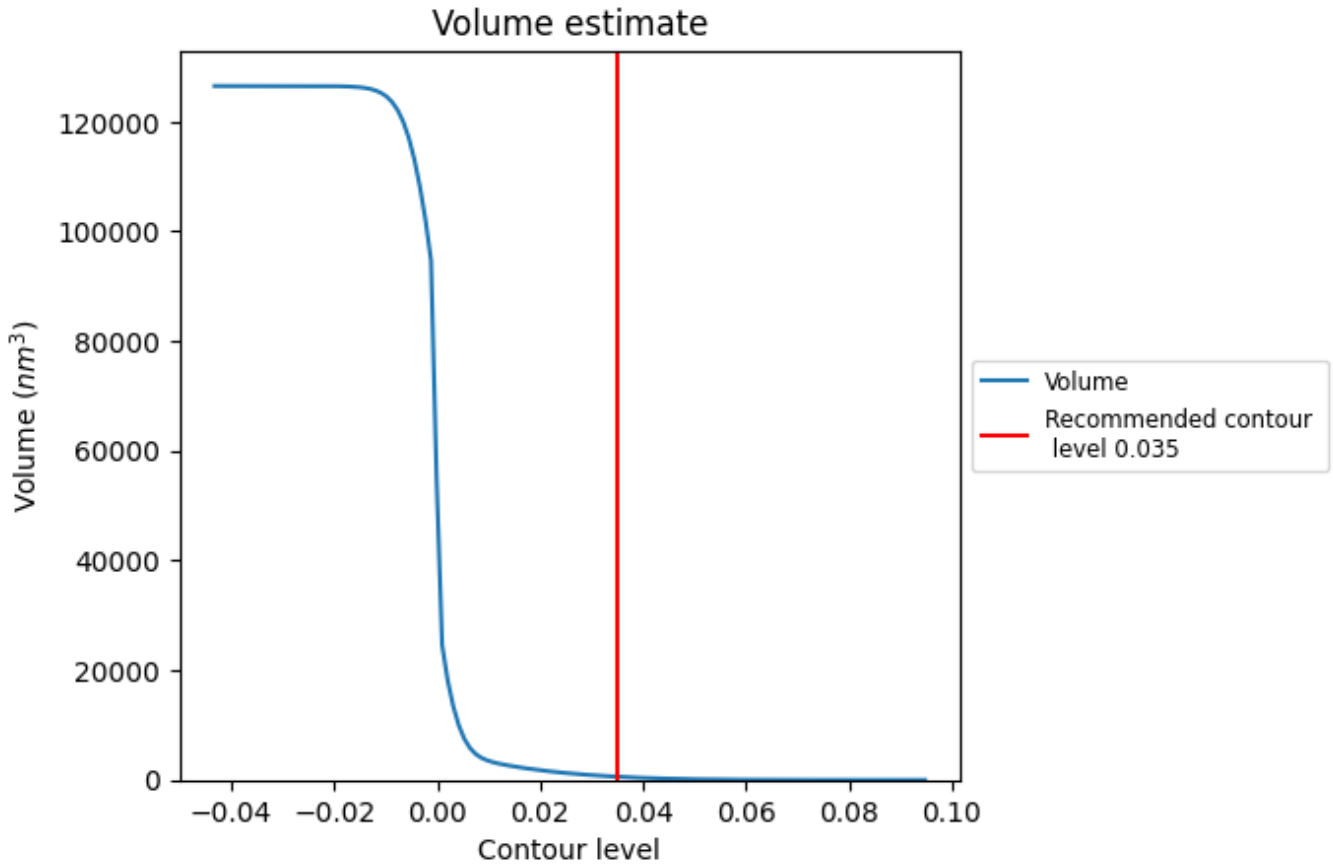
This section contains the results of statistical analysis of the map.

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.

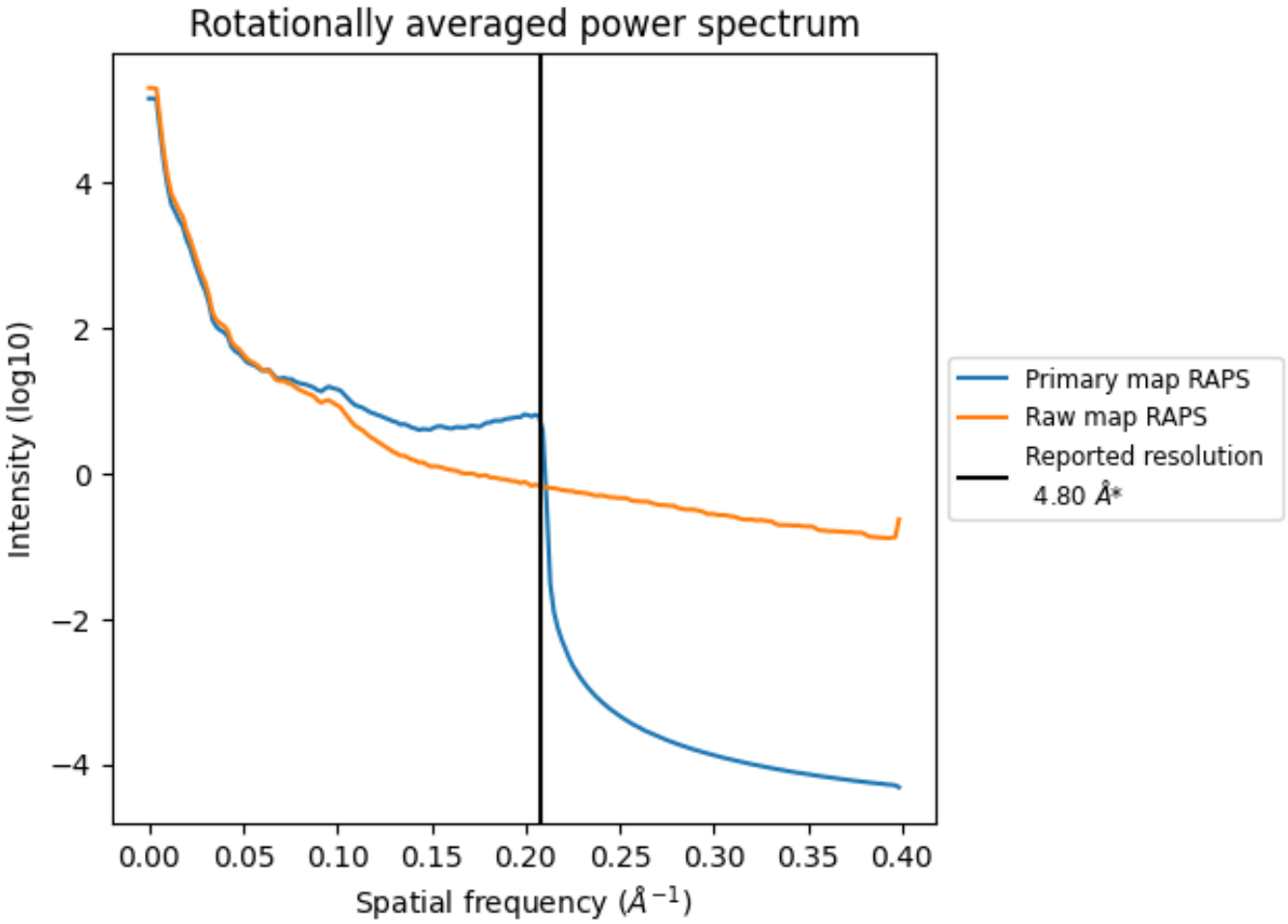
7.2 Volume estimate



The volume at the recommended contour level is 596 nm^3; this corresponds to an approximate mass of 539 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)

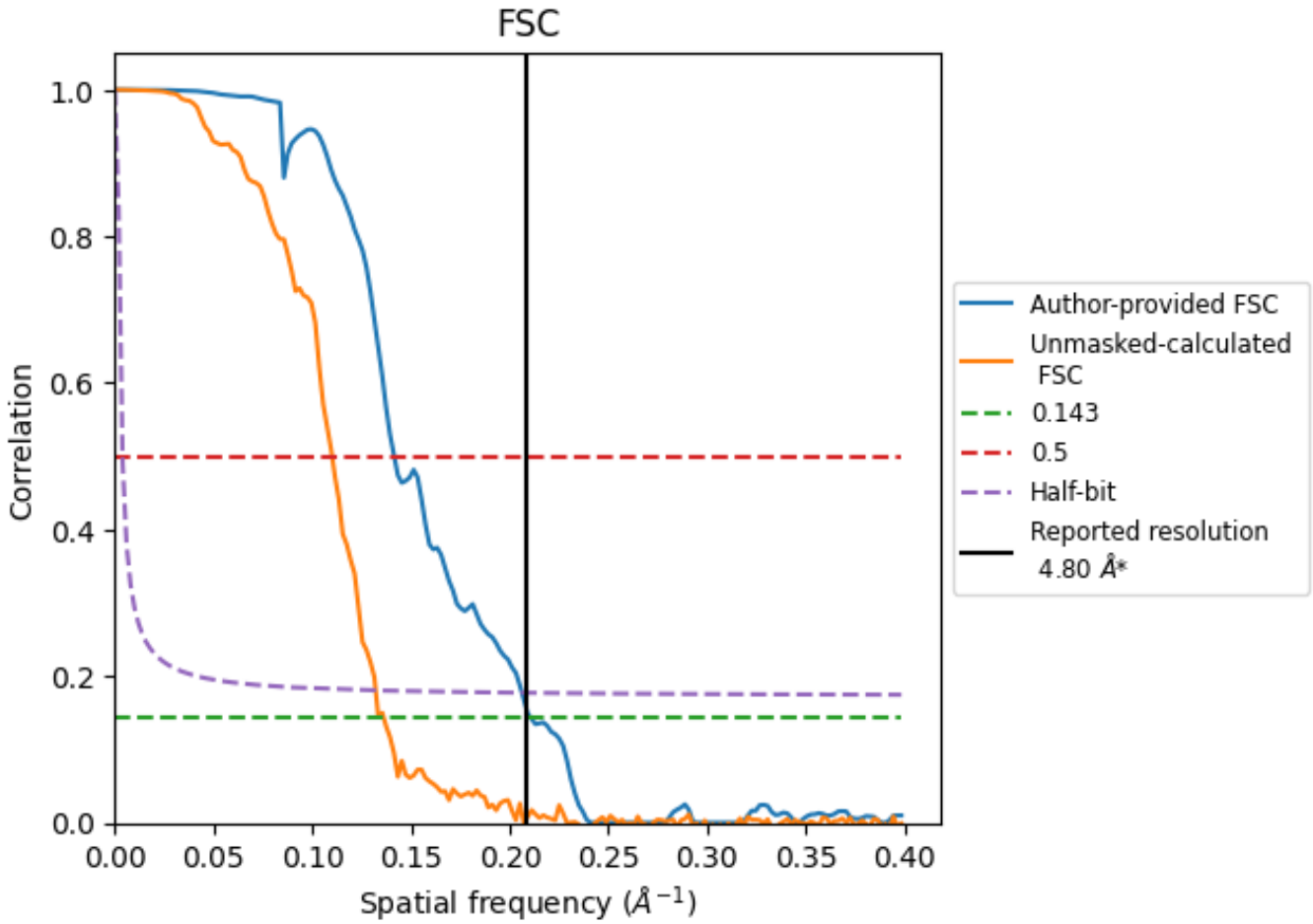


*Reported resolution corresponds to spatial frequency of 0.208 Å^{-1}

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 0.208 Å^{-1}

8.2 Resolution estimates (i)

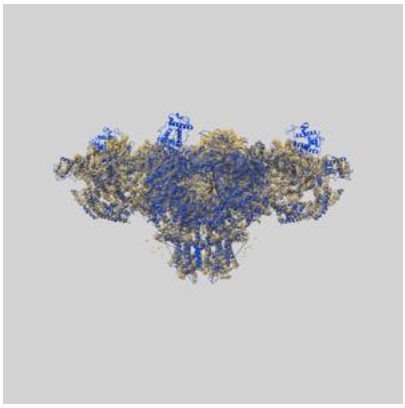
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.80	-	-
Author-provided FSC curve	4.75	7.07	4.85
Unmasked-calculated*	7.34	9.09	7.57

*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 7.34 differs from the reported value 4.8 by more than 10 %

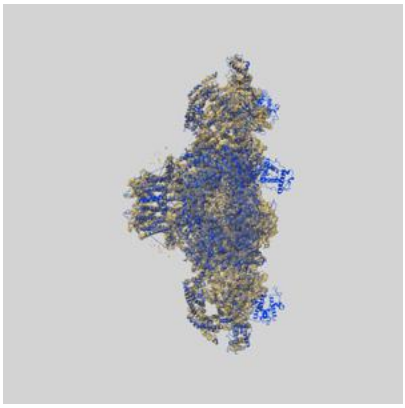
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-8384 and PDB model 5TAT. Per-residue inclusion information can be found in section 3 on page 6.

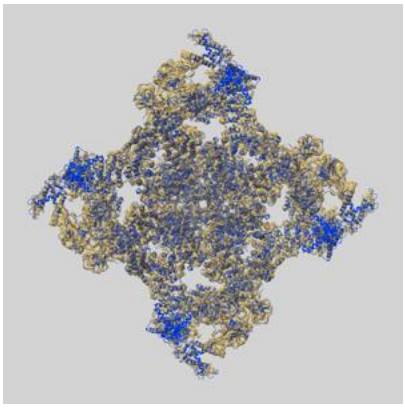
9.1 Map-model overlay



X



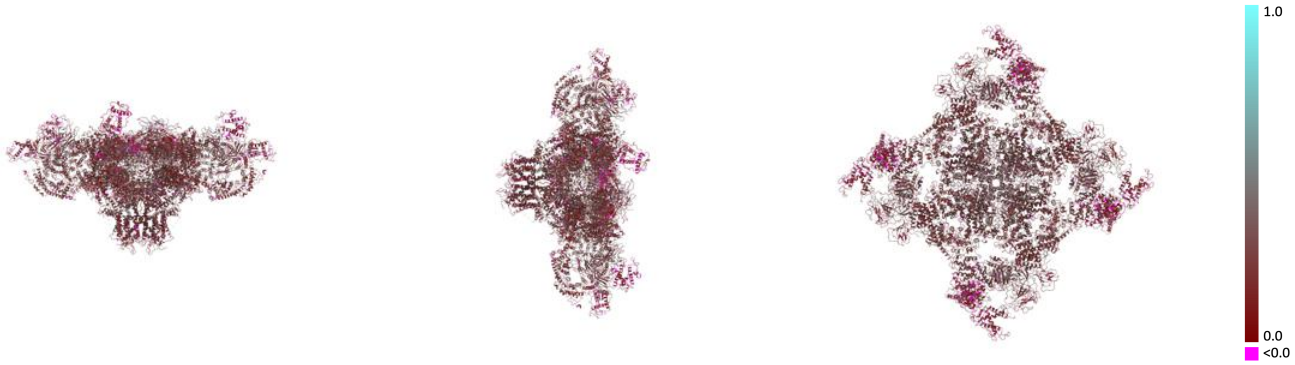
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.035 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.

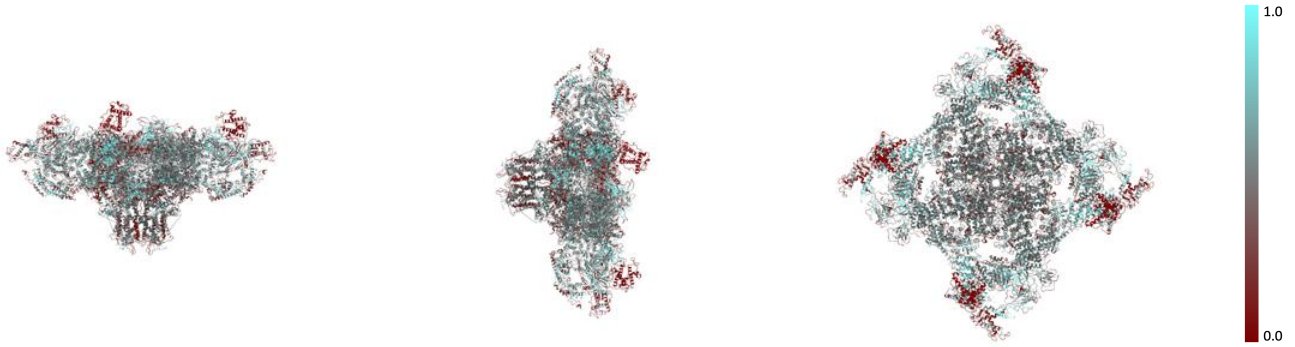
9.2 Q-score mapped to coordinate model (i)



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.

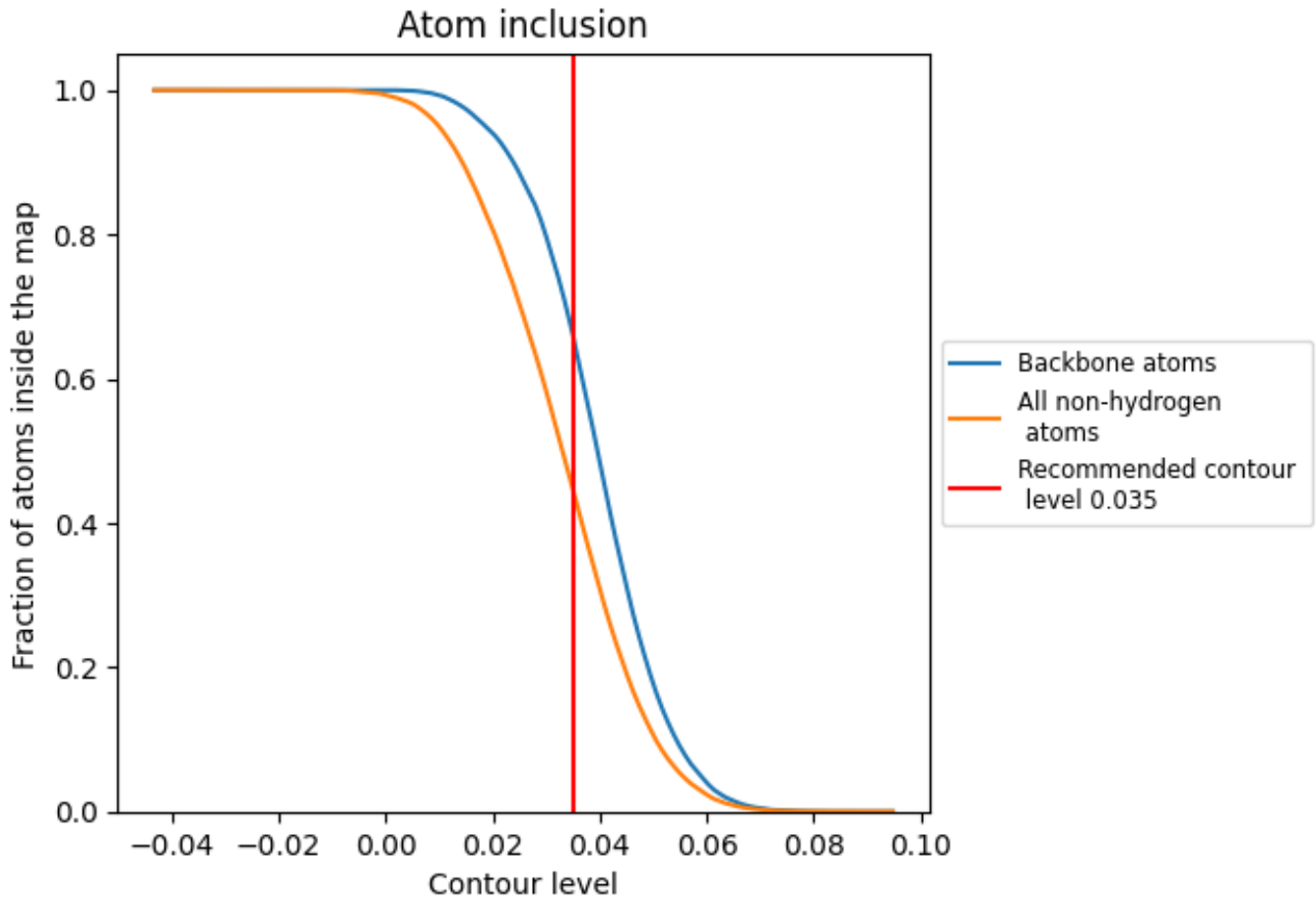
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.035).

9.4 Atom inclusion (i)



At the recommended contour level, 66% of all backbone atoms, 45% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4471	0.2510
A	0.4491	0.2490
B	0.4473	0.2510
E	0.4469	0.2510
F	0.4491	0.2530
G	0.4468	0.2510
H	0.4454	0.2510
I	0.4476	0.2520
J	0.4442	0.2510