Full wwPDB EM Validation Report ⓘ

Jul 10, 2023 – 12:36 PM EDT

PDB ID	:	8SET
EMDB ID	:	EMD-40428
Title	:	Cryo-EM Structure of RyR1 + cAMP
Authors	:	Cholak, S.; Saville, J.W.; Zhu, X.; Berezuk, A.M.; Tuttle, K.S.; Haji-Ghassemi, O.; Van Petegem, F.; Subramaniam, S.
Deposited on	:	2023-04-10
Resolution	:	3.42 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:

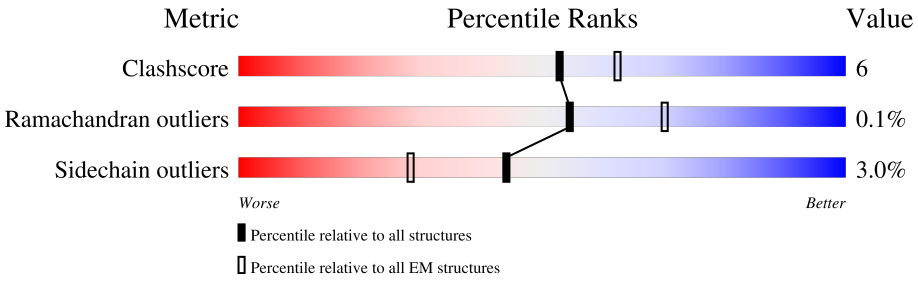
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

1 Overall quality at a glance

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

The reported resolution of this entry is 3.42 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	5037	17% 72% 15% • 13%
1	B	5037	17% 71% 15% 13%
1	C	5037	17% 71% 15% • 13%
1	D	5037	17% 72% 15% • 13%
2	E	350	• 25% 6% 69%
2	F	350	• 24% 7% 69%
2	G	350	• 24% 7% 69%
2	H	350	• 23% 7% 69%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 143048 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4378	Total	C	N	O	S	9	0
			34921	22219	6024	6442	236		
1	B	4378	Total	C	N	O	S	9	0
			34921	22219	6024	6442	236		
1	C	4378	Total	C	N	O	S	9	0
			34921	22219	6024	6442	236		
1	D	4378	Total	C	N	O	S	9	0
			34921	22219	6024	6442	236		

- Molecule 2 is a protein called Glutathione S-transferase class-mu 26 kDa isozyme,Peptidyl-prolyl cis-trans isomerase FKBP1B.

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

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-242	MET	-	expression tag	UNP P08515
E	-241	LYS	-	expression tag	UNP P08515
E	-240	SER	-	expression tag	UNP P08515
E	-239	SER	-	expression tag	UNP P08515
E	-238	HIS	-	expression tag	UNP P08515
E	-237	HIS	-	expression tag	UNP P08515
E	-236	HIS	-	expression tag	UNP P08515
E	-235	HIS	-	expression tag	UNP P08515

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-234	HIS	-	expression tag	UNP P08515
E	-233	HIS	-	expression tag	UNP P08515
E	-232	GLY	-	expression tag	UNP P08515
E	-231	SER	-	expression tag	UNP P08515
E	-230	SER	-	expression tag	UNP P08515
E	-11	GLY	-	linker	UNP P08515
E	-10	ILE	-	linker	UNP P08515
E	-9	GLU	-	linker	UNP P08515
E	-8	GLU	-	linker	UNP P08515
E	-7	ASN	-	linker	UNP P08515
E	-6	LEU	-	linker	UNP P08515
E	-5	TYR	-	linker	UNP P08515
E	-4	PHE	-	linker	UNP P08515
E	-3	GLN	-	linker	UNP P08515
E	-2	SER	-	linker	UNP P08515
E	-1	ASN	-	linker	UNP P08515
E	0	ALA	-	linker	UNP P08515
F	-242	MET	-	expression tag	UNP P08515
F	-241	LYS	-	expression tag	UNP P08515
F	-240	SER	-	expression tag	UNP P08515
F	-239	SER	-	expression tag	UNP P08515
F	-238	HIS	-	expression tag	UNP P08515
F	-237	HIS	-	expression tag	UNP P08515
F	-236	HIS	-	expression tag	UNP P08515
F	-235	HIS	-	expression tag	UNP P08515
F	-234	HIS	-	expression tag	UNP P08515
F	-233	HIS	-	expression tag	UNP P08515
F	-232	GLY	-	expression tag	UNP P08515
F	-231	SER	-	expression tag	UNP P08515
F	-230	SER	-	expression tag	UNP P08515
F	-11	GLY	-	linker	UNP P08515
F	-10	ILE	-	linker	UNP P08515
F	-9	GLU	-	linker	UNP P08515
F	-8	GLU	-	linker	UNP P08515
F	-7	ASN	-	linker	UNP P08515
F	-6	LEU	-	linker	UNP P08515
F	-5	TYR	-	linker	UNP P08515
F	-4	PHE	-	linker	UNP P08515
F	-3	GLN	-	linker	UNP P08515
F	-2	SER	-	linker	UNP P08515
F	-1	ASN	-	linker	UNP P08515
F	0	ALA	-	linker	UNP P08515

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-242	MET	-	expression tag	UNP P08515
G	-241	LYS	-	expression tag	UNP P08515
G	-240	SER	-	expression tag	UNP P08515
G	-239	SER	-	expression tag	UNP P08515
G	-238	HIS	-	expression tag	UNP P08515
G	-237	HIS	-	expression tag	UNP P08515
G	-236	HIS	-	expression tag	UNP P08515
G	-235	HIS	-	expression tag	UNP P08515
G	-234	HIS	-	expression tag	UNP P08515
G	-233	HIS	-	expression tag	UNP P08515
G	-232	GLY	-	expression tag	UNP P08515
G	-231	SER	-	expression tag	UNP P08515
G	-230	SER	-	expression tag	UNP P08515
G	-11	GLY	-	linker	UNP P08515
G	-10	ILE	-	linker	UNP P08515
G	-9	GLU	-	linker	UNP P08515
G	-8	GLU	-	linker	UNP P08515
G	-7	ASN	-	linker	UNP P08515
G	-6	LEU	-	linker	UNP P08515
G	-5	TYR	-	linker	UNP P08515
G	-4	PHE	-	linker	UNP P08515
G	-3	GLN	-	linker	UNP P08515
G	-2	SER	-	linker	UNP P08515
G	-1	ASN	-	linker	UNP P08515
G	0	ALA	-	linker	UNP P08515
H	-242	MET	-	expression tag	UNP P08515
H	-241	LYS	-	expression tag	UNP P08515
H	-240	SER	-	expression tag	UNP P08515
H	-239	SER	-	expression tag	UNP P08515
H	-238	HIS	-	expression tag	UNP P08515
H	-237	HIS	-	expression tag	UNP P08515
H	-236	HIS	-	expression tag	UNP P08515
H	-235	HIS	-	expression tag	UNP P08515
H	-234	HIS	-	expression tag	UNP P08515
H	-233	HIS	-	expression tag	UNP P08515
H	-232	GLY	-	expression tag	UNP P08515
H	-231	SER	-	expression tag	UNP P08515
H	-230	SER	-	expression tag	UNP P08515
H	-11	GLY	-	linker	UNP P08515
H	-10	ILE	-	linker	UNP P08515
H	-9	GLU	-	linker	UNP P08515
H	-8	GLU	-	linker	UNP P08515

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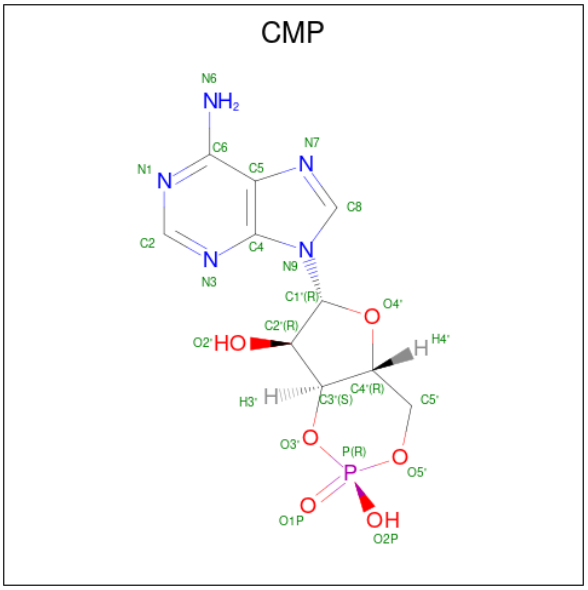
Chain	Residue	Modelled	Actual	Comment	Reference
H	-7	ASN	-	linker	UNP P08515
H	-6	LEU	-	linker	UNP P08515
H	-5	TYR	-	linker	UNP P08515
H	-4	PHE	-	linker	UNP P08515
H	-3	GLN	-	linker	UNP P08515
H	-2	SER	-	linker	UNP P08515
H	-1	ASN	-	linker	UNP P08515
H	0	ALA	-	linker	UNP P08515

- Molecule 3 is ADENOSINE-3',5'-CYCLIC-MONOPHOSPHATE (three-letter code: CMP) (formula: $C_{10}H_{12}N_5O_6P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			22	10	5	6	1	
3	B	1	Total	C	N	O	P	0
			22	10	5	6	1	
3	C	1	Total	C	N	O	P	0
			22	10	5	6	1	
3	D	1	Total	C	N	O	P	0
			22	10	5	6	1	

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

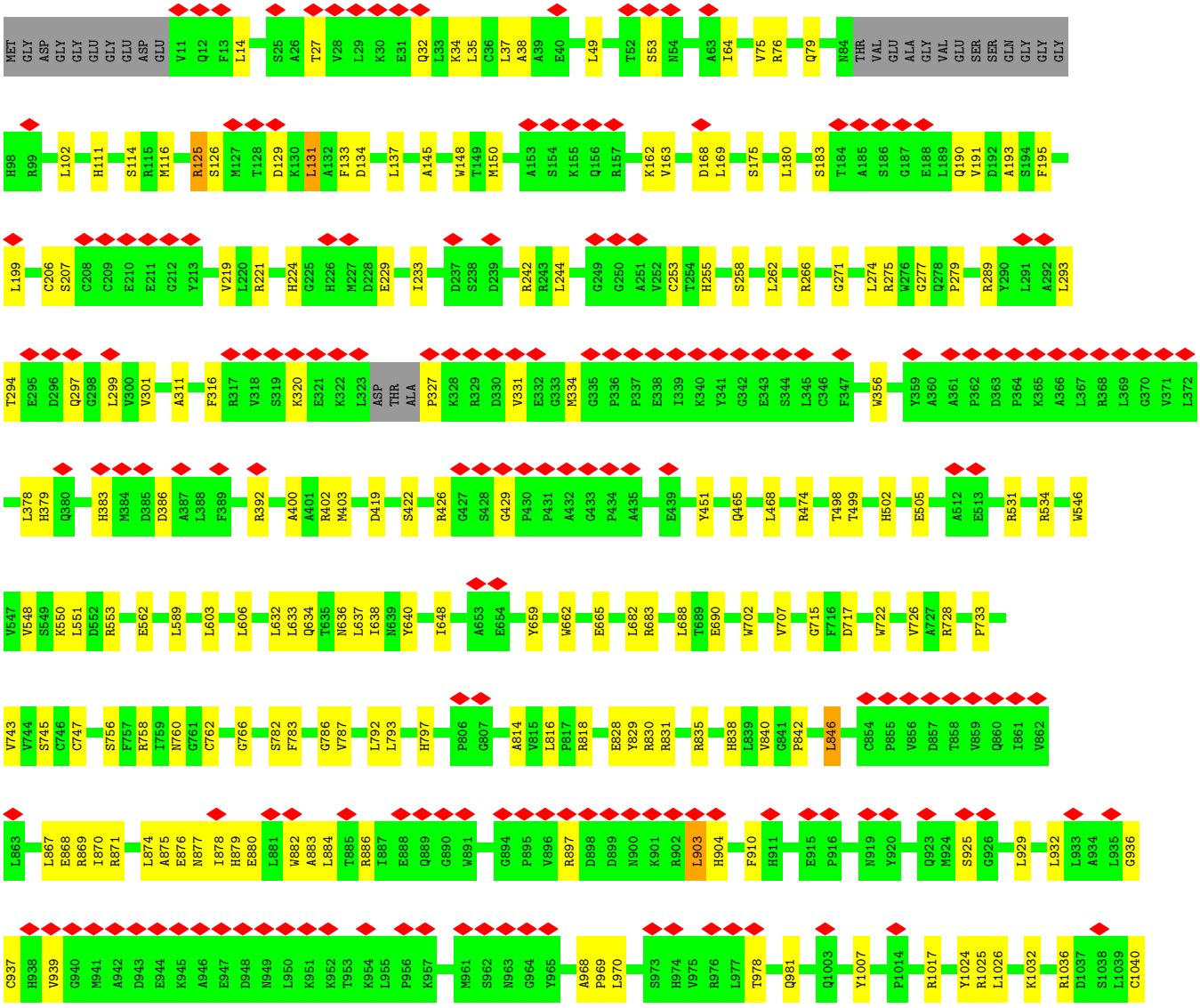
Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total Zn 1 1	0
4	B	1	Total Zn 1 1	0
4	C	1	Total Zn 1 1	0
4	D	1	Total Zn 1 1	0

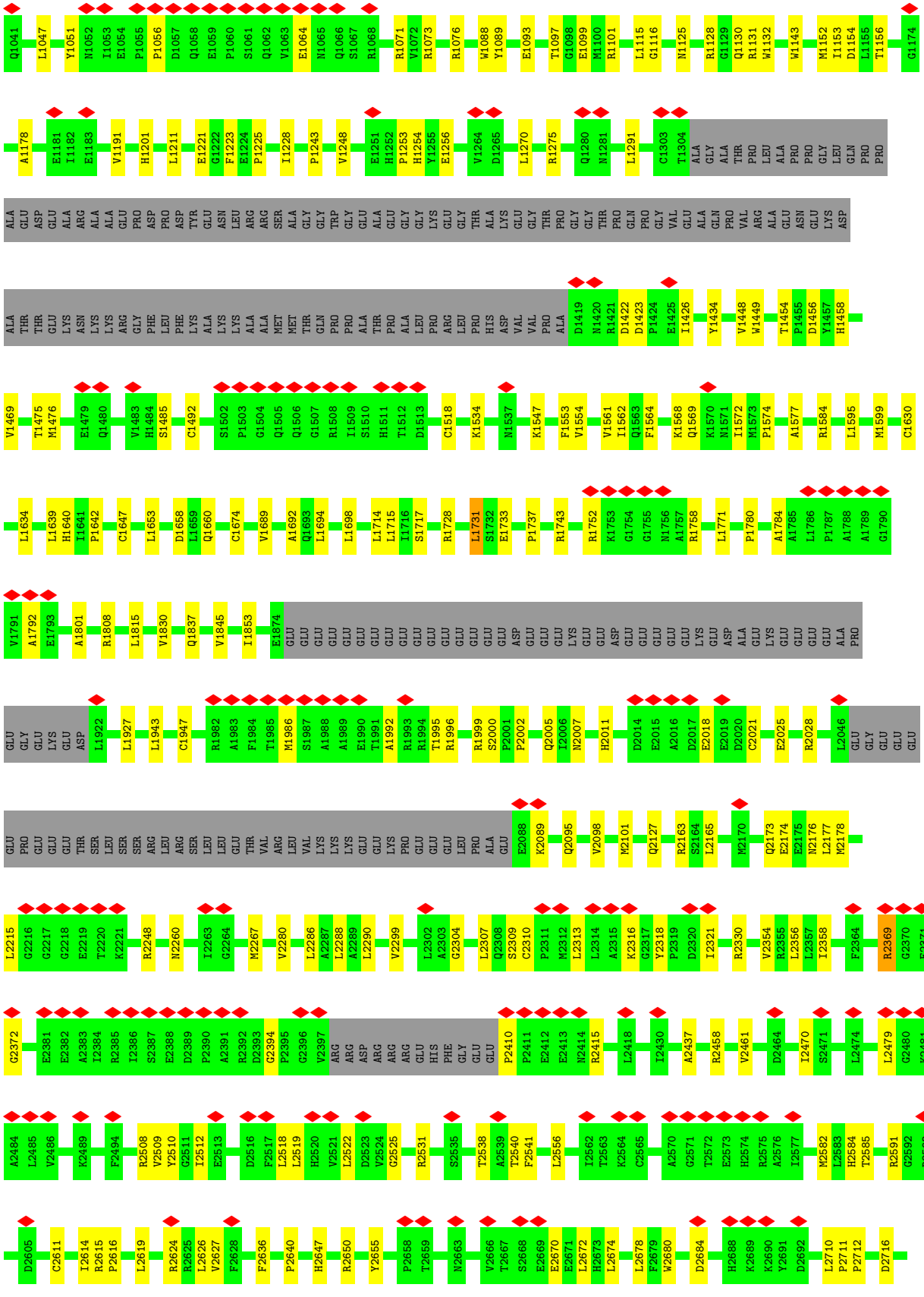
3 Residue-property plots (i)

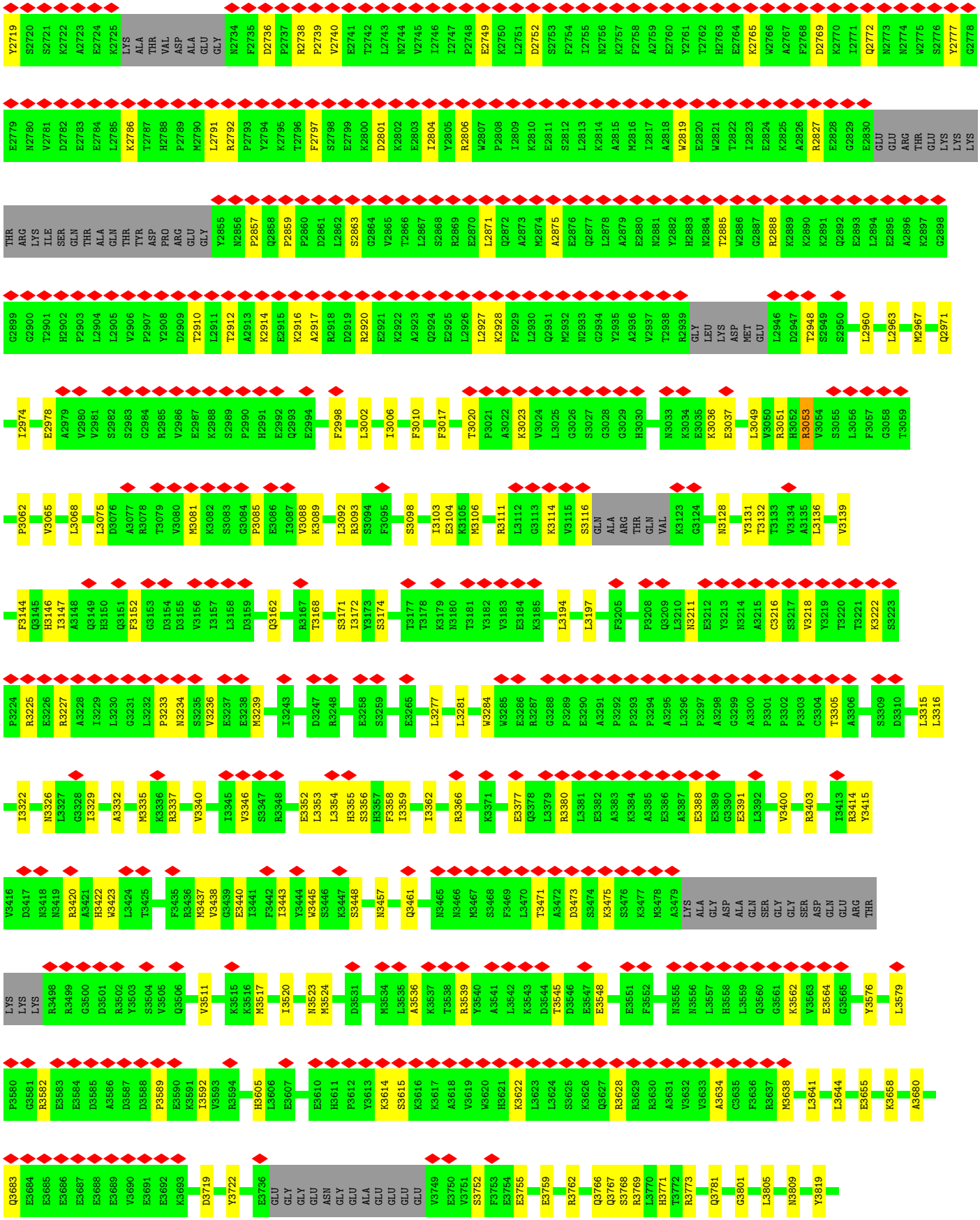
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

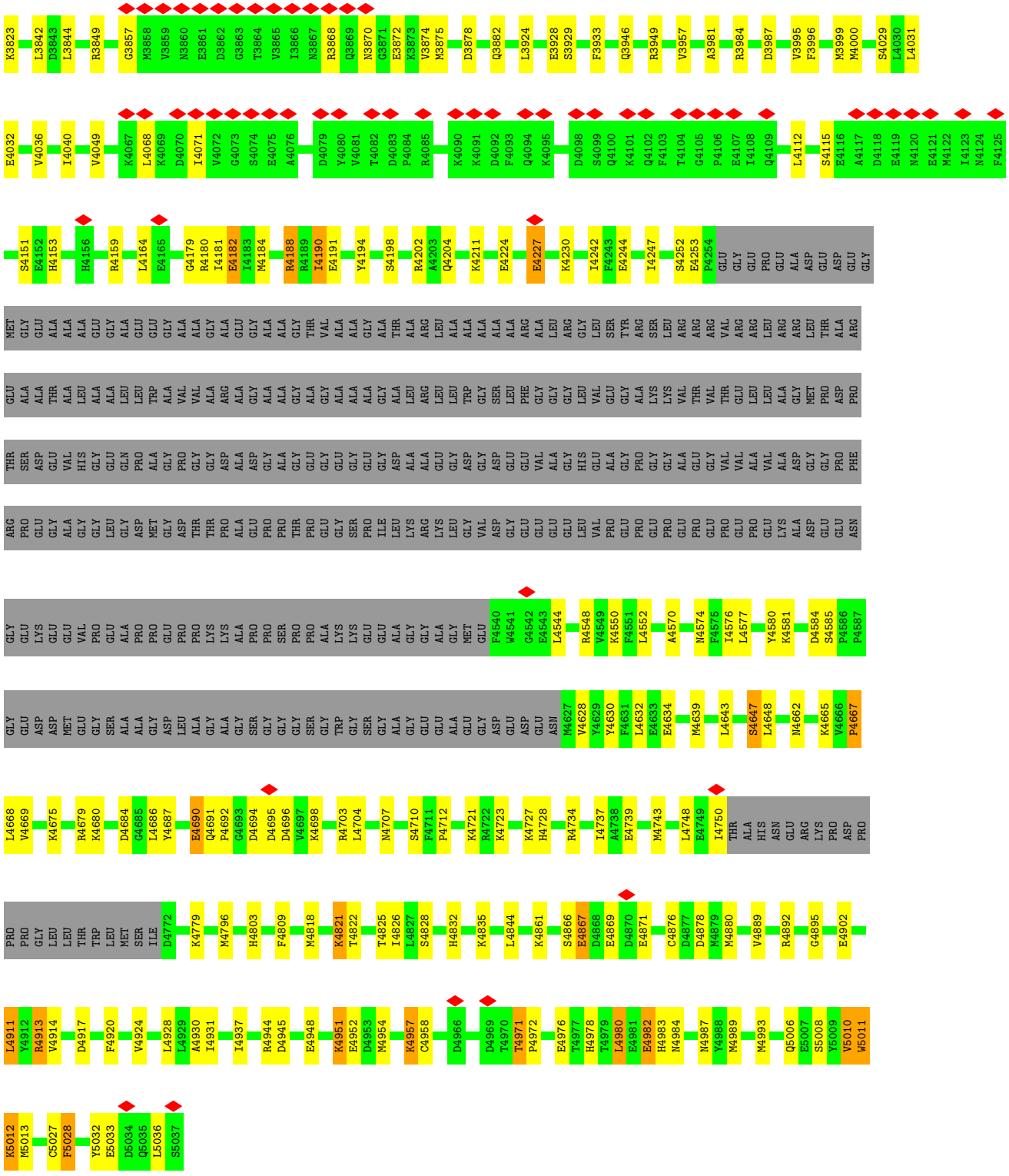
- Molecule 1: Ryanodine receptor 1

Chain A:



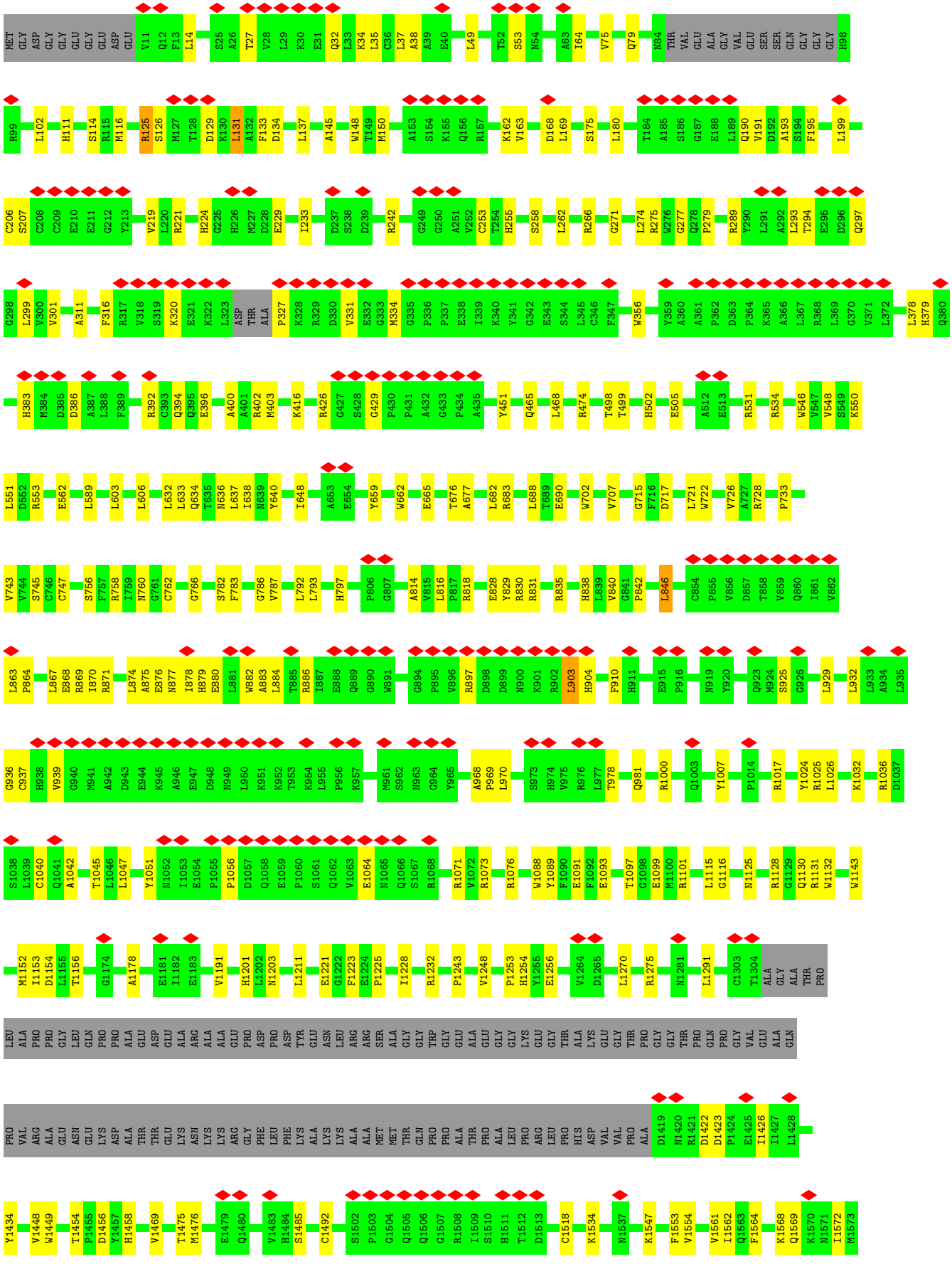



Y2719 S2720 S2721 K2722 A2723 E2724 K2725 LYS ALA THR VAL ASP ALA GLU GLY N2734 F2735 D2736 P2737 R2738 P2739 V2740 E2741 T2742 L2743 N2744 V2745 I2746 I2747 P2748 E2749 K2750 L2751 D2752 S2753 F2754 I2755 N2756 K2757 P2758 A2759 E2760 Y2761 T2762 H2763 E2764 K2765 W2766 A2767 F2768 D2769 K2770 I2771 Q2772 N2773 N2774 W2775 S2776 Y2777 G2778
E2779 N2780 V2781 D2782 E2783 E2784 L2785 K2786 T2787 H2788 P2789 M2790 L2791 R2792 P2793 Y2794 K2795 T2796 F2797 S2798 E2799 K2800 D2801 K2802 E2803 I2804 Y2805 R2806 W2807 P2808 I2809 K2810 E2811 S2812 L2813 K2814 A2815 M2816 I2817 A2818 W2819 E2820 W2821 T2822 I2823 E2824 K2825 A2826 R2827 E2828 G2829 E2830 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 GLY LEU LYS ASP MET GLU L2946 D2947 T2948 S2949 S2950 L2960 L2963 M2967 Q2971
I2974 E2978 A2979 V2980 V2981 S2982 S2983 G2984 R2985 V2986 E2987 K2988 S2989 P2990 H2991 E2992 Q2993 E2994 F2998 L3002 I3006 F3010 F3017 T3020 P3021 A3022 K3023 V3024 L3025 G3026 S3027 G3028 G3029 H3030 N3033 K3034 E3035 K3036 E3037 L3049 V3050 R3051 H3052 R3053 V3054 S3055 L3056 F3057 G3058 T3059
P3062 V3065 L3068 L3075 D3076 A3077 R3078 T3079 V3080 M3081 K3082 S3083 G3084 P3085 E3086 I3087 V3088 K3089 L3092 R3093 S3094 F3095 S3098 I3103 E3104 K3105 M3106 R3111 L3112 G3113 K3114 V3115 S3116 GLN ALA ARG THR GLN VAL K3123 G3124 N3128 Y3131 T3132 T3133 V3134 A3135 L3136 V3139
F3144 Q3145 H3146 I3147 A3148 Q3149 H3150 Q3151 F3152 G3153 D3154 D3155 V3156 I3157 L3158 D3159 Q3162 R3167 T3168 S3171 I3172 Y3173 S3174 T3177 T3178 K3179 N3180 T3181 Y3182 V3183 E3184 K3185 L3194 L3197 F3205 P3208 Q3209 L3210 N3211 E3212 Y3213 N3214 A3215 C3216 S3217 V3218 Y3219 T3220 T3221 K3222 S3223
P3224 R3225 E3226 R3227 A3228 I3229 L3230 G3231 L3232 P3233 N3234 S3235 V3236 E3237 E3238 M3239 I3243 D3247 R3248 E3258 S3259 E3265 L3277 L3281 W3284 W3285 E3286 R3287 G3288 P3289 E3290 A3291 P3292 P3293 P3294 A3295 L3296 P3297 A3298 G3299 A3300 P3301 P3302 P3303 C3304 T3305 A3306 S3309 D3310 L3315 L3316
I3322 N3326 L3327 G3328 I3329 A3332 M3335 K3336 R3337 V3340 I3345 V3346 S3347 R3348 E3352 L3353 L3364 H3355 S3356 H3357 F3358 I3359 I3362 R3366 K3371 E3377 Q3378 L3379 R3380 L3381 E3382 A3383 K3384 A3385 E3386 A3387 E3388 E3389 G3390 E3391 L3392 V3400 R3403 I3413 R3414 Y3415
V3416 D3417 N3418 N3419 R3420 A3421 H3422 W3423 L3424 T3425 F3435 R3436 M3437 V3438 G3439 E3440 I3441 F3442 I3443 Y3444 W3445 S3446 K3447 S3448 N3457 Q3461 N3465 N3466 M3467 S3468 F3469 L3470 T3471 A3472 D3473 S3474 K3475 S3476 K3477 M3478 A3479 LYS ALA GLY ASP ALA GLN SER GLY GLY SER ASP GLN GLU ARG THR
LYS LYS LYS R3498 R3499 G3500 D3501 R3502 Y3503 S3504 V3505 Q3506 V3511 K3515 K3516 M3517 I3520 N3523 M3524 D3531 M3534 L3535 A3536 K3537 T3538 R3539 Y3540 A3541 L3542 K3543 D3544 T3545 D3546 E3547 E3548 E3551 F3552 N3555 N3556 L3557 H3558 L3559 Q3560 G3561 K3562 V3563 E3564 G3565 Y3576 L3579
P3580 G3581 R3582 E3583 E3584 D3585 A3586 D3587 D3588 P3589 E3590 K3591 I3592 V3593 R3594 H3605 L3606 E3607 E3610 H3611 P3612 Y3613 K3614 S3615 K3616 K3617 A3618 V3619 W3620 H3621 K3622 L3623 L3624 S3625 K3626 Q3627 R3628 R3629 R3630 A3631 V3632 V3633 A3634 C3635 F3636 R3637 M3638 L3641 L3644 E3655 K3658 A3680
Q3683 E3684 E3685 E3686 E3687 E3688 E3689 V3690 E3691 E3692 K3693 D3719 Y3722 E3736 GLU GLY GLY GLU ASN GLY GLU ALA GLU GLU GLU GLU V3749 E3750 V3751 S3752 F3753 E3754 E3755 E3759 R3762 Q3766 Q3767 S3768 R3769 L3770 H3771 T3772 R3773 Q3781 G3801 L3805 N3809 Y3819



• Molecule 1: Ryanodine receptor 1

Chain B:


MET GLY ASP GLY GLY GLU GLY GLU ASP GLU V11 Q12 F13 L14 S25 A26 T27 V28 L29 K30 E31 Q32 L33 K34 L35 C36 L37 A38 A39 E40 L49 T52 S53 N54 A63 I64 V75 Q79 N84 THR VAL GLU GLU ALA GLY VAL GLU SER SER GLN GLY GLY GLY H98
R99 L102 H111 S114 R115 M116 R125 S126 M127 T128 D129 K130 L131 A132 F133 D134 L137 A145 W148 T149 M150 A153 S154 K155 Q156 R157 K162 V163 D168 L169 S175 L180 T184 A185 S186 G187 E188 L189 Q190 V191 D192 A193 S194 F195 L199
C206 S207 C208 C209 E210 E211 G212 Y213 V219 L220 R221 H224 G225 H226 M227 D228 E229 I233 D237 S238 D239 R242 G249 G250 A251 V252 C253 T254 H255 S258 L262 R266 G271 L274 R275 W276 G277 Q278 P279 R289 Y290 L291 A292 L293 T294 E295 D296 Q297
G298 L299 V300 V301 A311 F316 R317 V318 S319 K320 E321 K322 L323 ASP THR ALA P327 K328 R329 D330 V331 E332 G333 M334 G335 P336 P337 E338 I339 K340 Y341 G342 E343 S344 L345 C346 F347 W356 Y359 A360 A361 P362 D363 P364 K365 A366 L367 R368 L369 G370 V371 L372 L378 H379 Q380
H383 M384 D385 D386 A387 L388 F389 R392 C393 Q394 Q395 E396 A400 A401 R402 M403 K416 R426 G427 S428 G429 P430 P431 A432 G433 P434 A435 Y451 Q465 L468 R474 T498 T499 H502 E505 A512 E513 R531 R534 W646 V647 V648 S649 K650
L551 D552 R553 E562 L589 L603 L606 L632 L633 Q634 T635 N636 L637 I638 N639 Y640 I648 A653 E654 Y659 W662 E665 T676 A677 L682 R683 L688 T689 E690 W702 V707 G715 F716 D717 L721 W722 V726 A727 R728 P733
V743 V744 S745 C746 C747 S756 F757 R758 I759 N760 G761 C762 G766 S782 F783 G786 V787 L792 L793 H797 P806 G807 A814 V815 L816 P817 R818 E828 Y829 R830 R831 R835 H838 L839 V840 G841 P842 L846 C854 P855 V856 D857 T858 V859 Q860 I861 V862
L863 P864 L867 E868 R869 I870 R871 L874 A875 E876 N877 I878 H879 E880 L881 W882 A883 L884 T885 R886 I887 E888 Q889 G890 W891 G894 P895 V896 R897 D898 D899 N900 K901 R902 L903 H904 F910 H911 E915 P916 N919 Y920 Q923 M924 S925 G926 L929 L932 L933 A934 L935
G936 C937 H938 V939 G940 M941 A942 D943 E944 K945 A946 E947 D948 N949 L950 K951 K952 T953 K954 L955 P956 K957 M961 S962 N963 G964 Y965 A968 P969 L970 S973 H974 V975 R976 L977 T978 Q981 R1000 Q1003 Y1007 P1014 R1017 Y1024 R1025 L1026 K1032 R1036 D1037
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LEU ALA PRO PRO GLY LEU GLN PRO PRO ALA GLU ASP GLU ALA ARG ALA ALA GLU PRO ASP PRO ASP TYR GLU ASN LEU ARG ARG SER ALA GLY GLY TRP GLY GLU ALA GLU GLY GLY LYS GLU GLY THR ALA LYS GLU GLY THR PRO GLY GLY THR PRO GLN PRO GLY VAL GLU ALA ALA GLN
PRO VAL ARG ALA GLU ASN GLU LYS ASP ALA THR THR GLU LYS ASN LYS LYS ARG GLY PHE LEU PHE LYS ALA LYS LYS ALA ALA MET MET THR GLN PRO PRO ALA ALA THR PRO ALA LEU PRO ARG LEU PRO HIS ASP VAL VAL PRO ALA D1419 N1420 R1421 D1422 D1423 P1424 E1425 I1426 I1427 L1428
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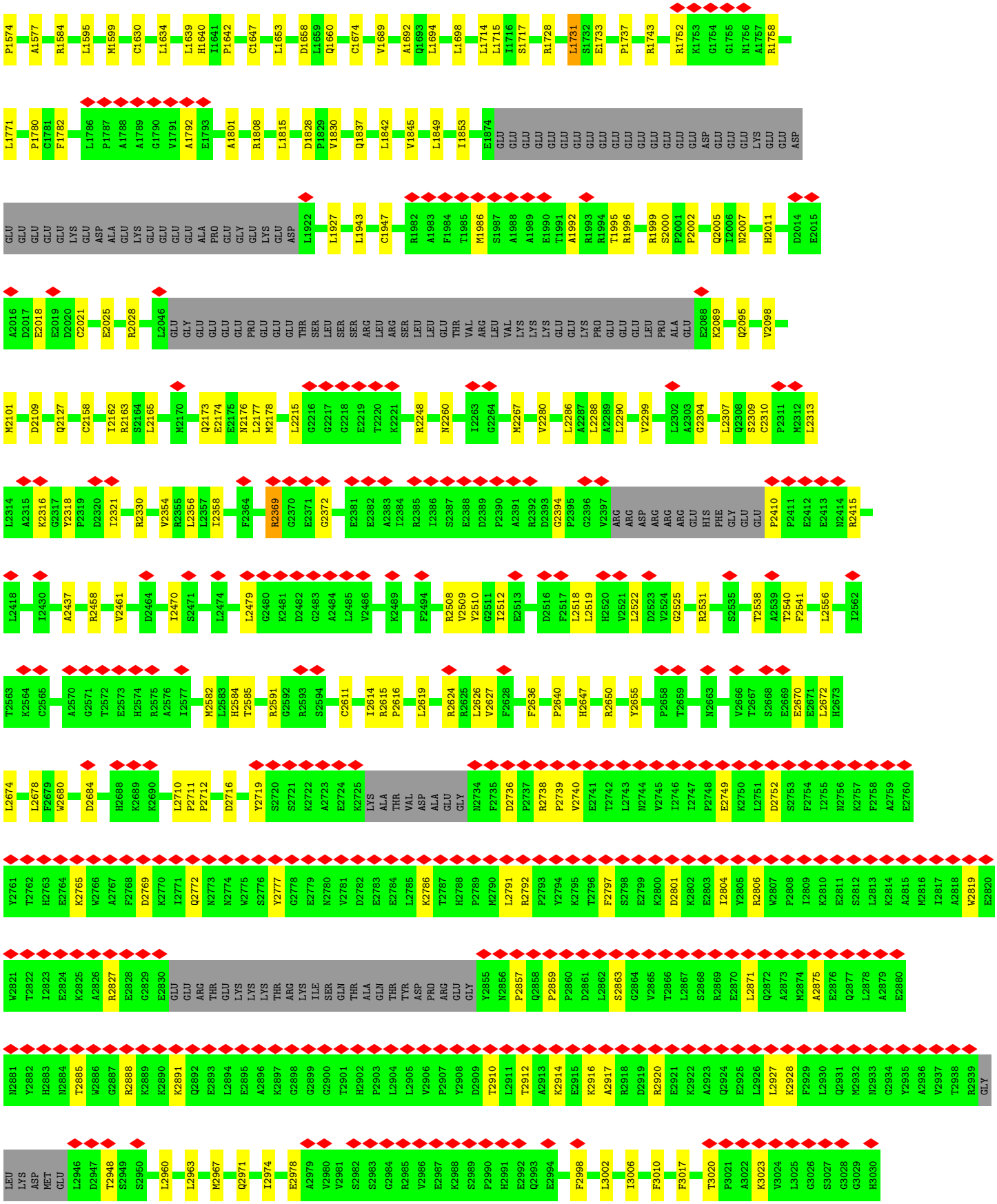
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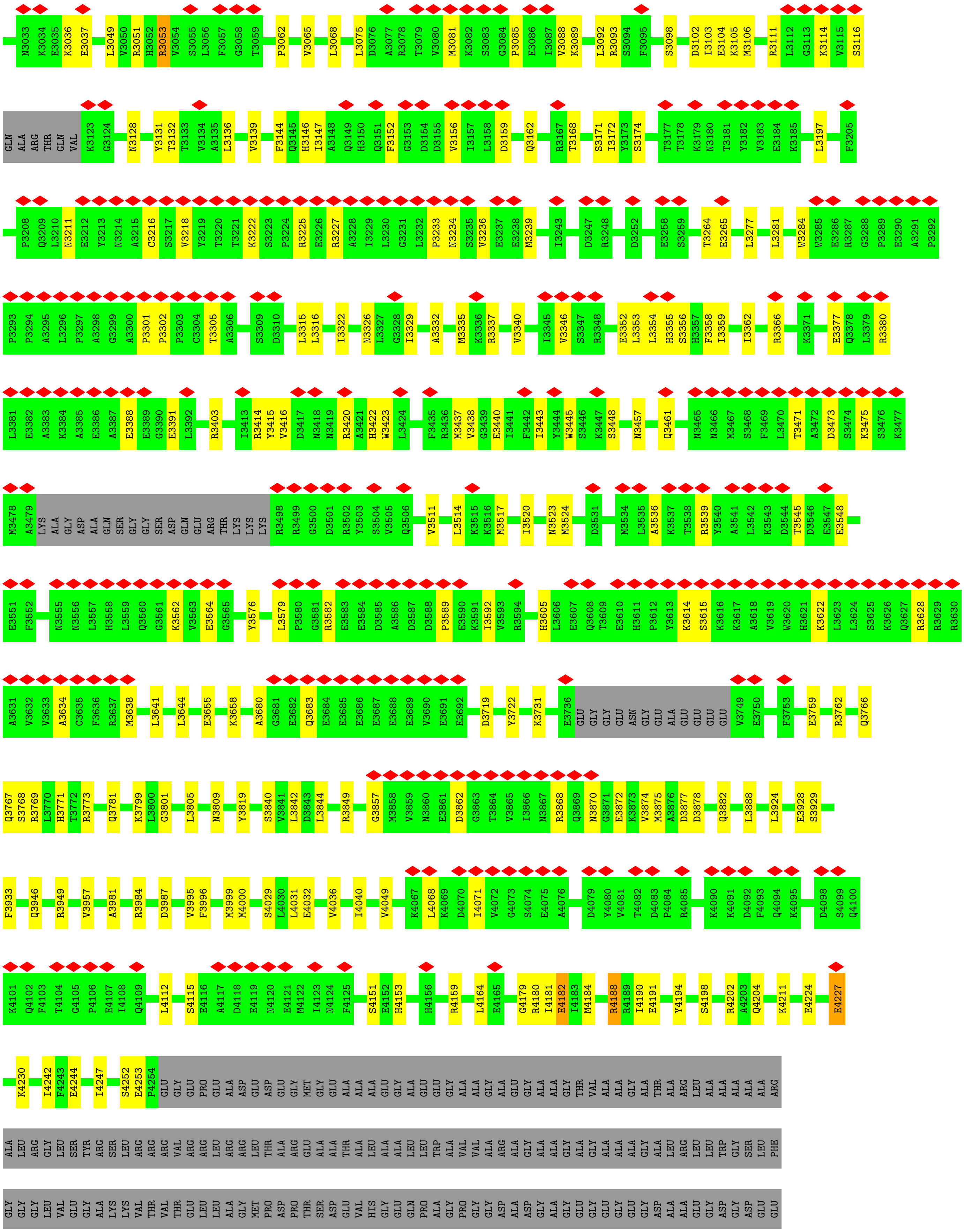
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K4230 I4242 F4243 E4244 I4247 S4252 E4253 P4254 GLU GLY GLU PRO GLU ALA ASP GLU ASP GLU GLY MET GLY GLU ALA ALA ALA GLU GLY ALA GLU GLU GLY ALA ALA GLY ALA GLU GLY ALA ALA GLY THR VAL ALA ALA GLY ALA THR ALA ARG LEU ALA ALA ALA ALA ALA ARG
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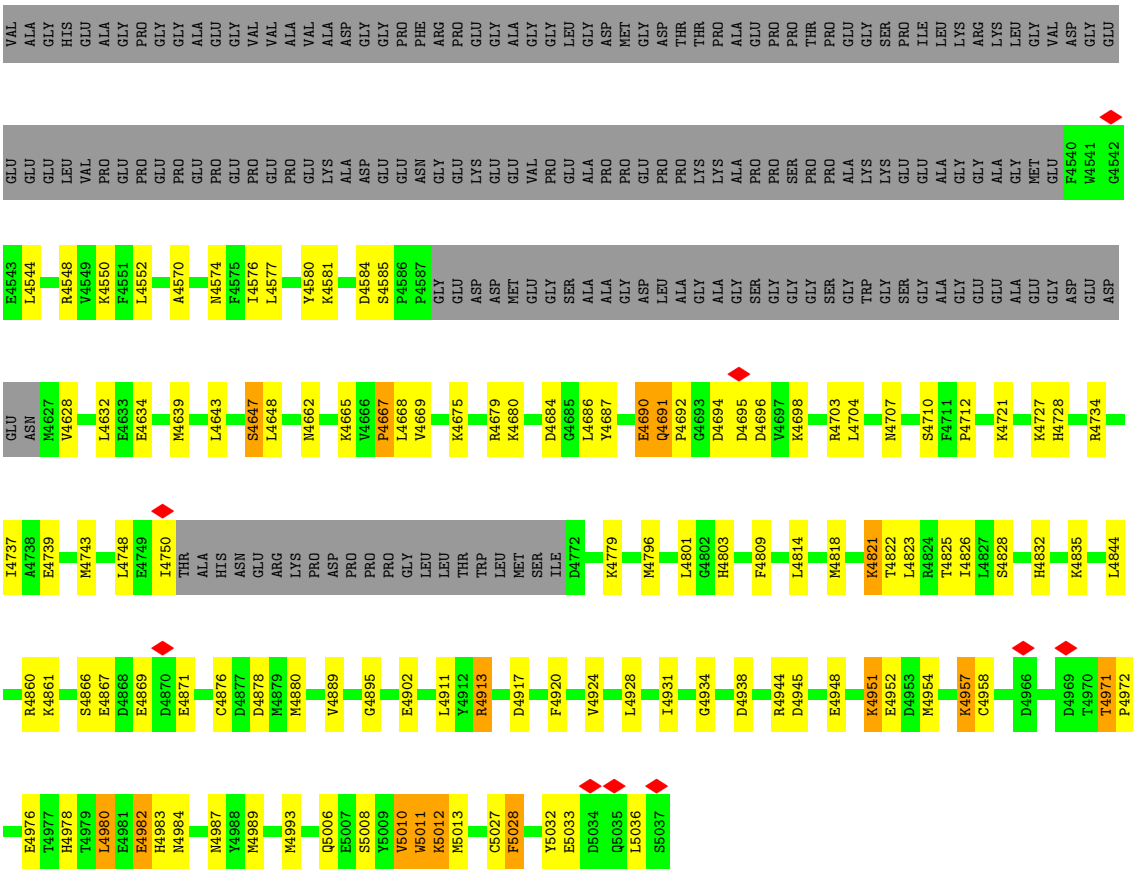
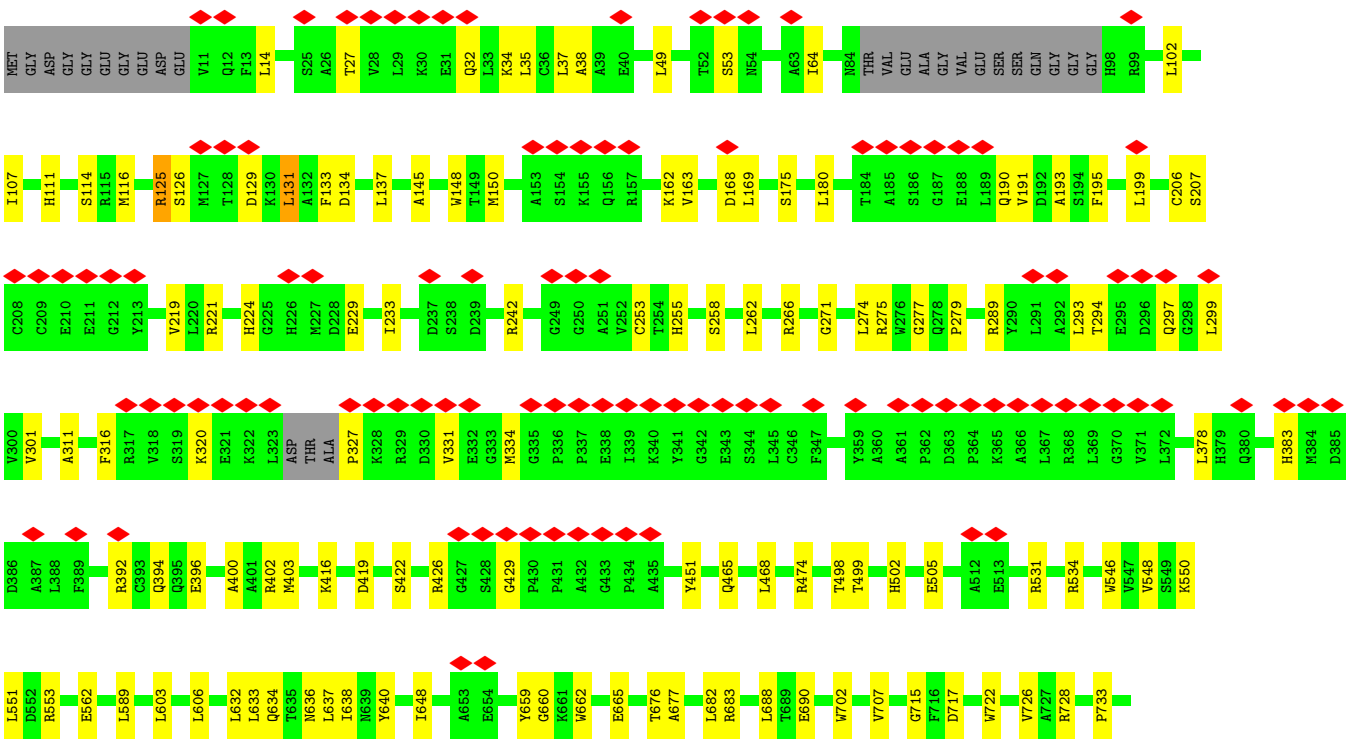
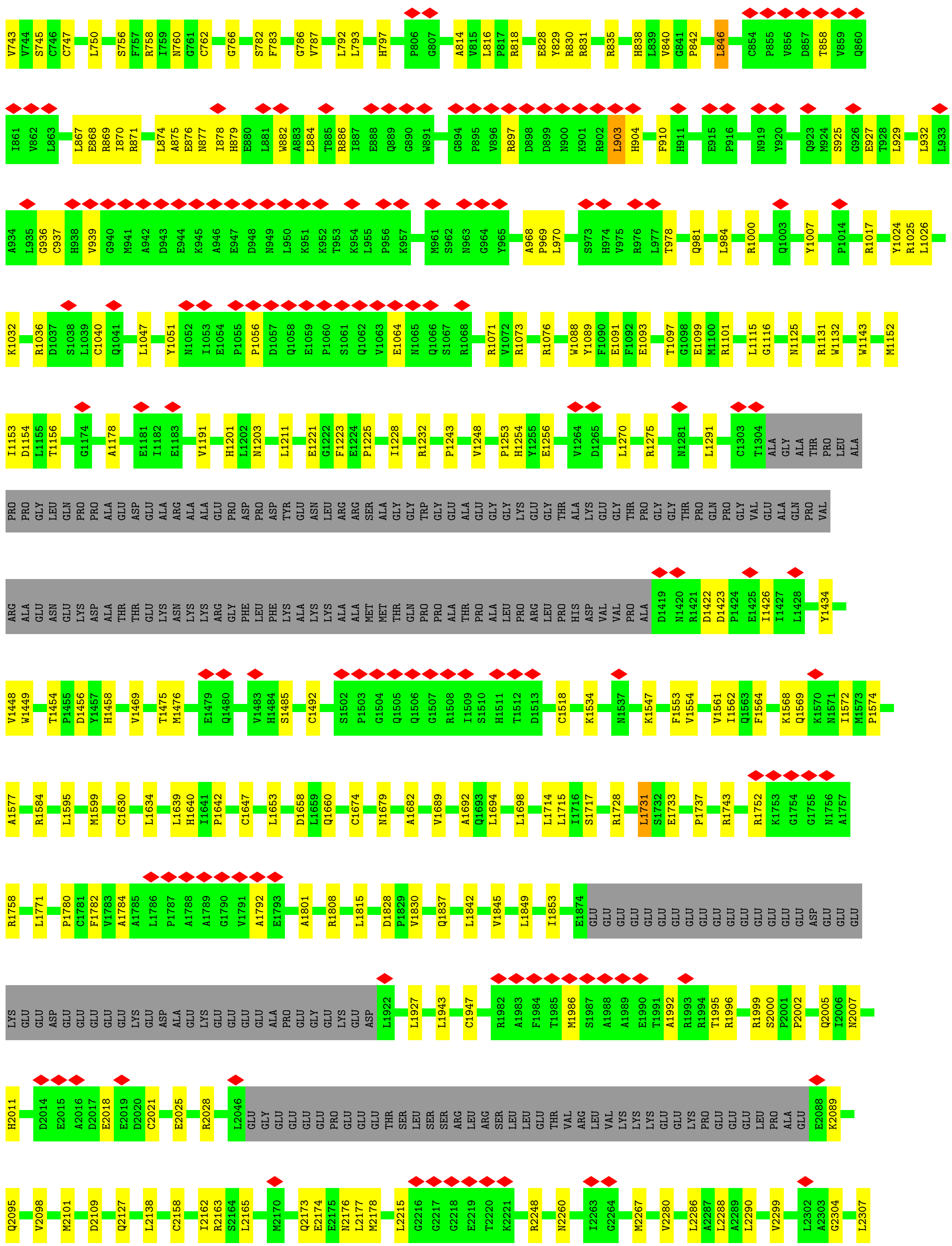
GLY GLY GLY LEU VAL GLU GLY ALA LYS LYS VAL THR VAL THR GLU LEU LEU ALA GLY MET PRO ASP PRO THR SER ASP GLU VAL HIS GLY GLU GLN PRO ALA GLY PRO GLY GLY ASP ALA ASP GLY ALA GLY GLU GLY GLU GLY GLU GLY ASP ALA ALA GLU GLY ASP GLY ASP GLU GLU



• Molecule 1: Ryanodine receptor 1

Chain C:

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PRO PRO GLY LEU GLN PRO PRO ALA GLU ASP GLU ALA ARG ALA ALA GLU PRO ASP PRO ASP TYR GLU ASN LEU ARG ARG SER ALA GLY GLY TRP GLY GLU ALA GLU GLY GLY LYS GLU GLY THR ALA LYS GLU GLY THR PRO GLY GLY THR PRO GLN PRO GLY VAL GLU ALA GLN PRO VAL
ARG ALA GLU ASN GLU LYS ASP ALA THR THR GLU LYS ASN LYS LYS ARG GLY PHE LEU PHE LYS ALA LYS LYS ALA ALA MET MET THR GLN PRO PRO ALA THR PRO ALA LEU PRO ARG LEU PRO HIS ASP VAL VAL PRO ALA D1419 N1420 R1421 D1422 D1423 P1424 E1425 I1426 I1427 L1428 Y1434
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LYS GLU GLU ASP GLU GLU GLU GLU GLU LYS GLU ASP ALA GLU LYS GLU GLU GLU GLU ALA PRO GLU GLY GLU LYS GLU ASP L1922 L1927 L1943 C1947 R1982 A1983 F1984 T1985 M1986 S1987 A1988 A1989 E1990 T1991 A1992 R1993 R1994 T1995 R1996 R1999 S2000 P2001 P2002 Q2005 I2006 N2007
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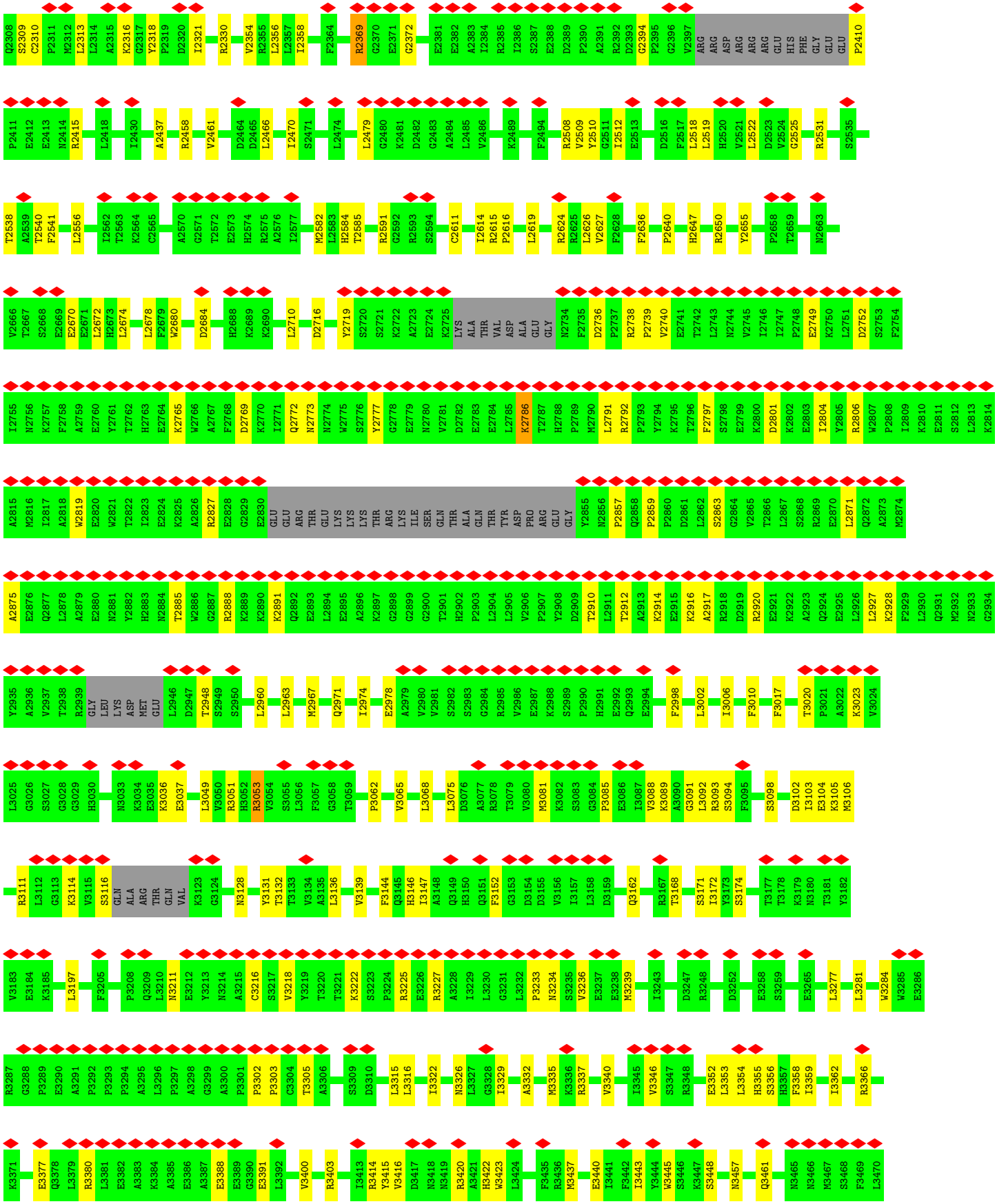
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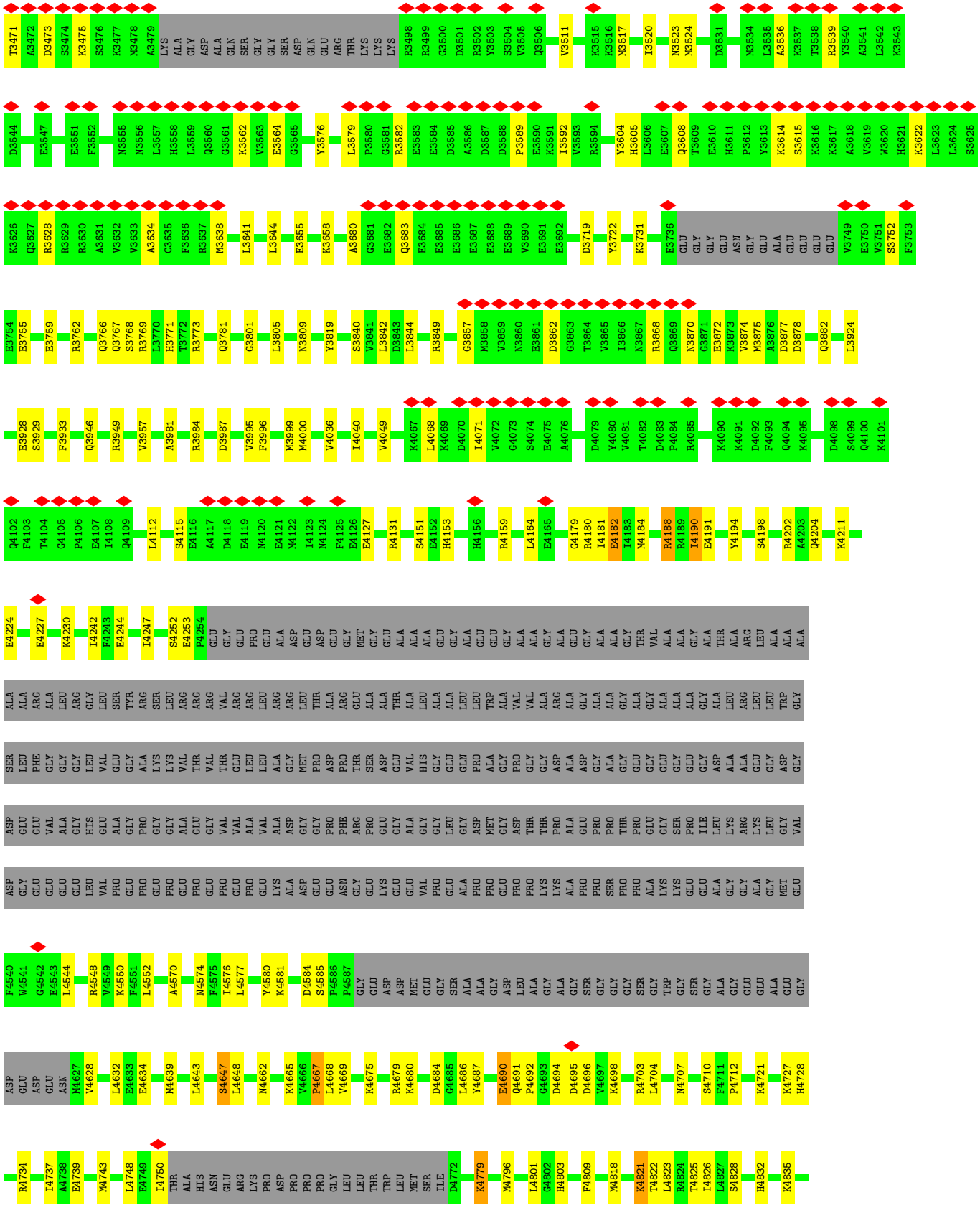
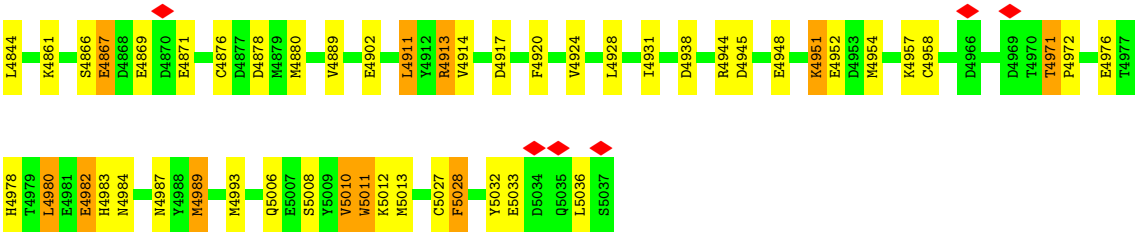
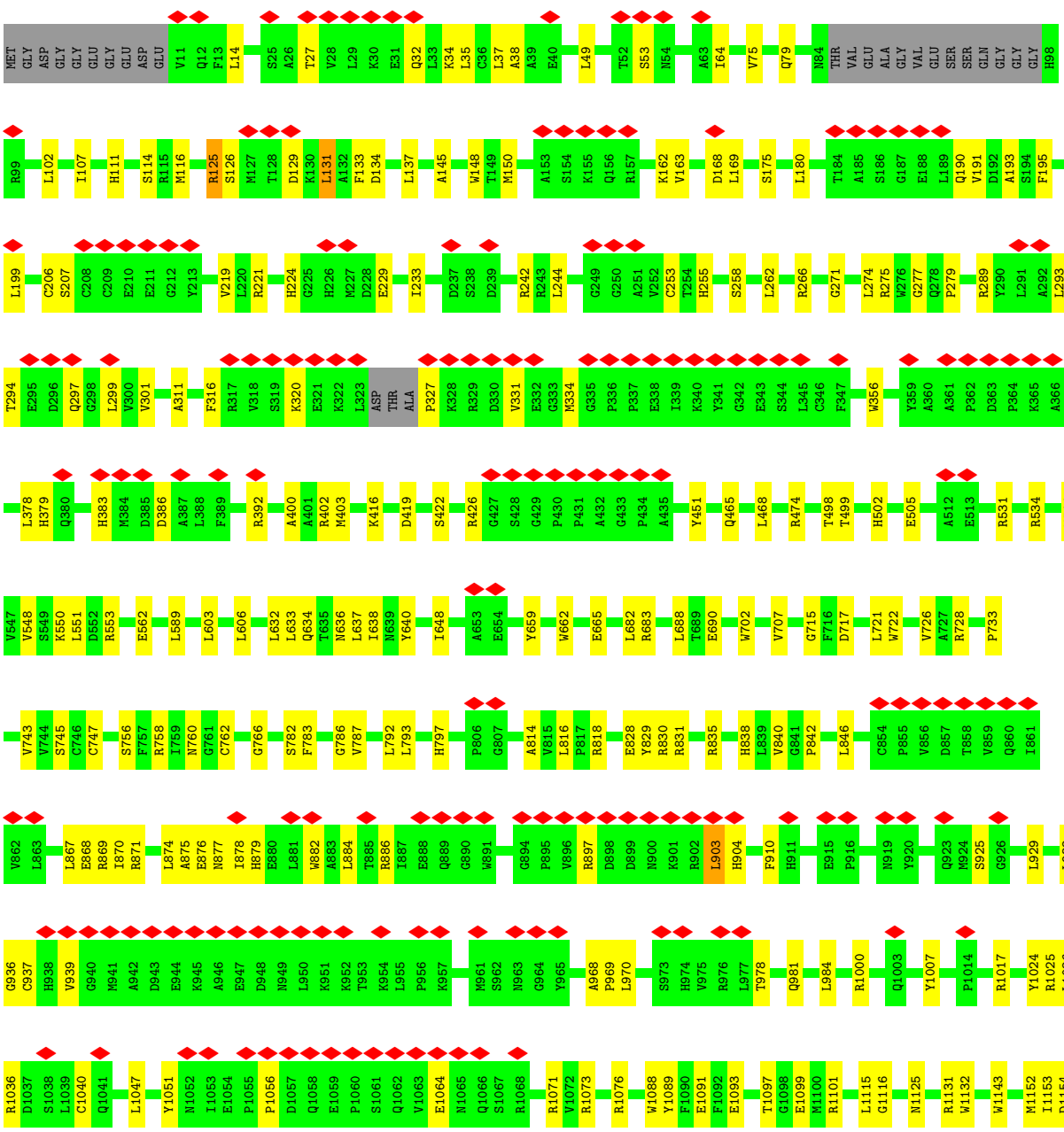
R3111 L3112 G3113 K3114 V3115 S3116 GLN ALA ARG THR GLN VAL K3123 G3124 N3128 Y3131 T3132 T3133 V3134 A3135 L3136 V3139 F3144 Q3145 H3146 I3147 A3148 Q3149 H3150 Q3151 F3152 G3153 D3154 D3155 V3156 I3157 L3158 D3159 Q3162 R3167 T3168 S3171 I3172 Y3173 S3174 T3177 T3178 K3179 N3180 T3181 Y3182
V3183 E3184 K3185 L3197 F3205 P3208 Q3209 L3210 N3211 E3212 Y3213 N3214 A3215 C3216 S3217 V3218 Y3219 T3220 T3221 K3222 S3223 P3224 R3225 E3226 R3227 A3228 I3229 L3230 G3231 L3232 P3233 N3234 S3235 V3236 E3237 E3238 M3239 I3243 D3247 R3248 D3252 E3258 S3259 E3265 L3277 L3281 W3284 W3285 E3286
R3287 G3288 P3289 E3290 A3291 P3292 P3293 P3294 A3295 L3296 P3297 A3298 G3299 A3300 P3301 P3302 P3303 C3304 T3305 A3306 S3309 D3310 L3315 L3316 I3322 N3326 L3327 G3328 I3329 A3332 M3335 K3336 R3337 V3340 I3345 V3346 S3347 R3348 E3352 L3353 L3354 H3355 S3356 H3357 F3358 I3359 I3362 R3366
K3371 E3377 Q3378 L3379 R3380 L3381 E3382 A3383 K3384 A3385 E3386 A3387 E3388 E3389 G3390 E3391 L3392 V3400 R3403 I3413 R3414 Y3415 V3416 D3417 N3418 N3419 R3420 A3421 H3422 W3423 L3424 F3435 R3436 M3437 E3440 I3441 F3442 I3443 Y3444 W3445 S3446 K3447 S3448 N3457 Q3461 N3465 N3466 M3467 S3468 F3469 L3470

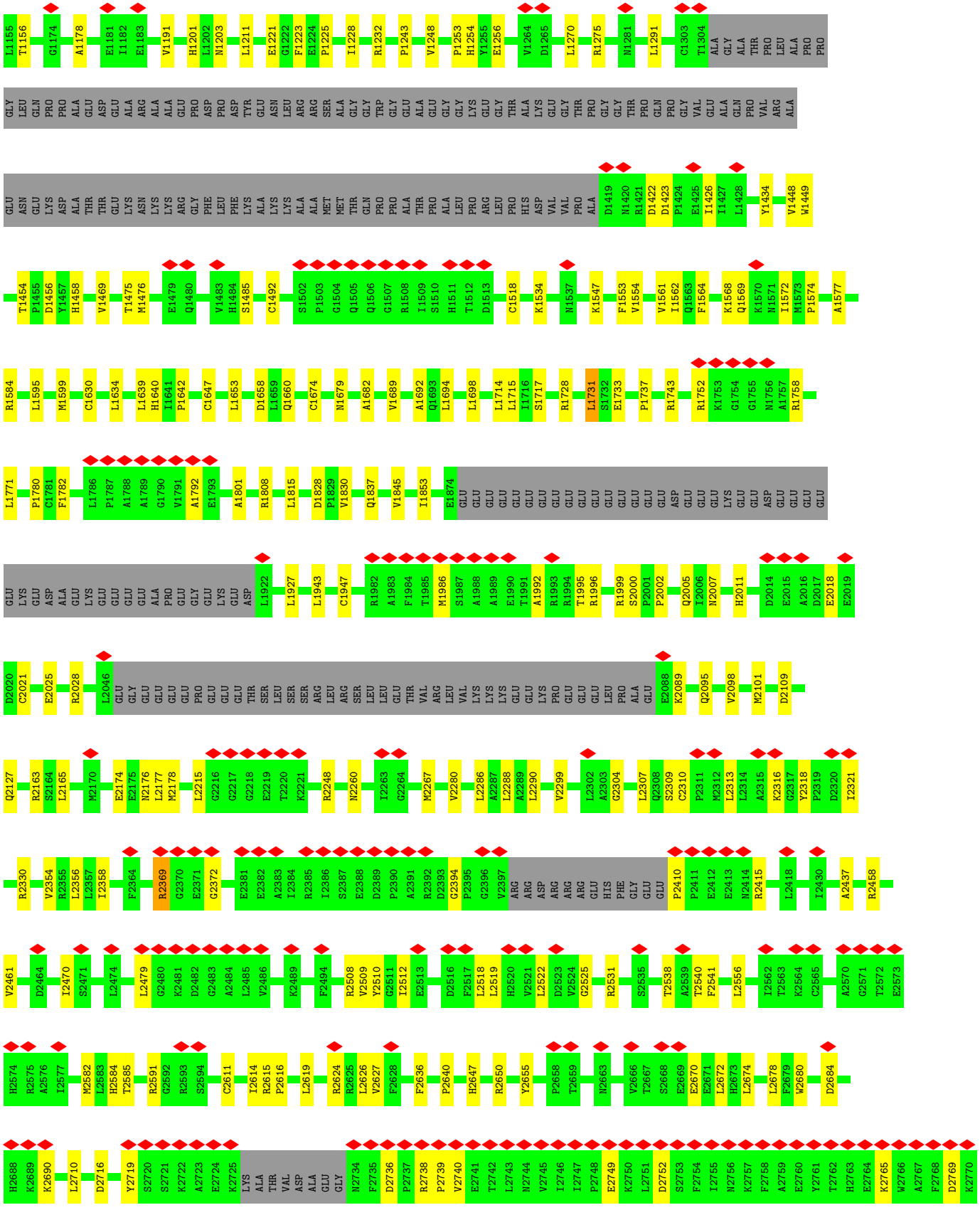


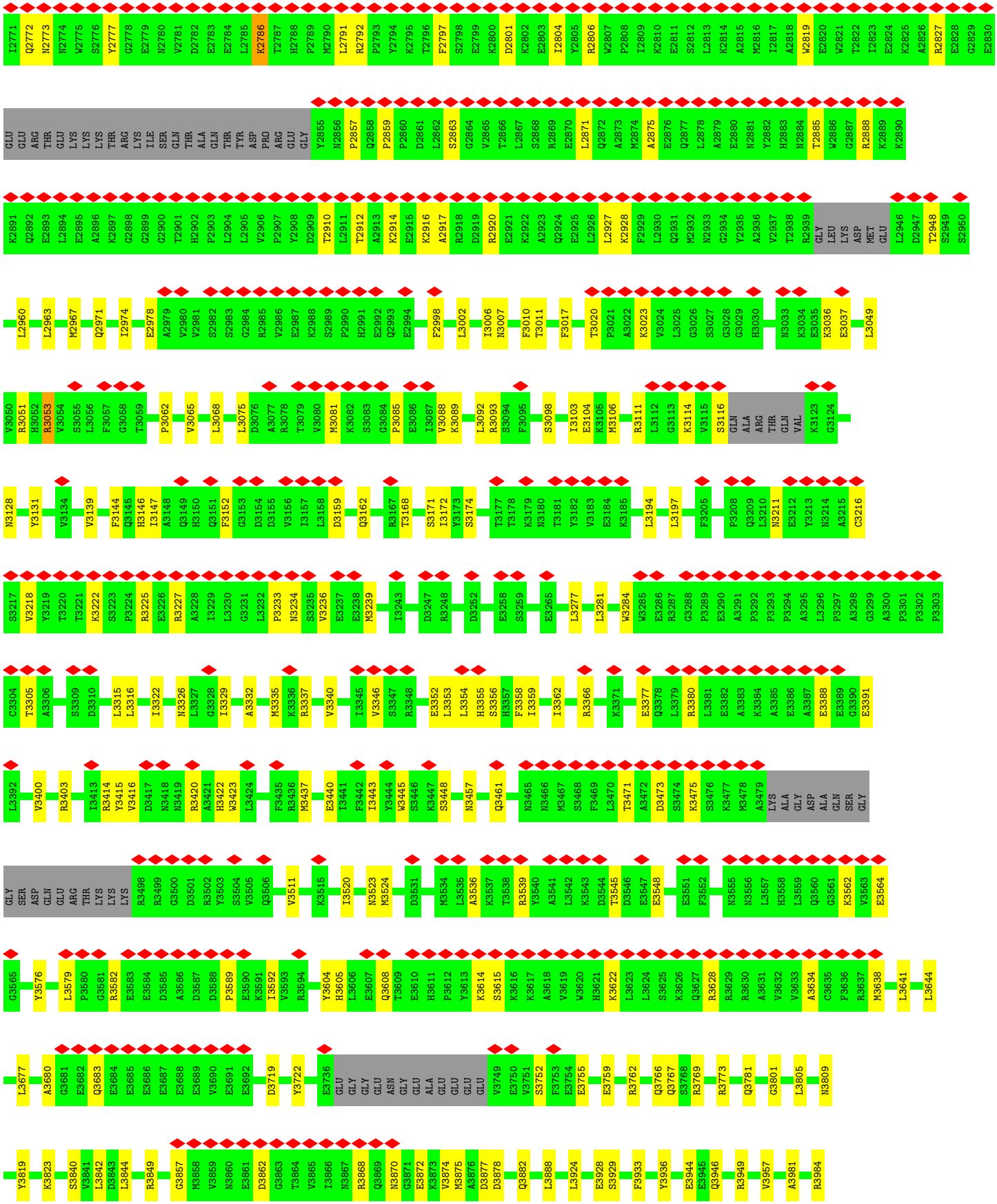


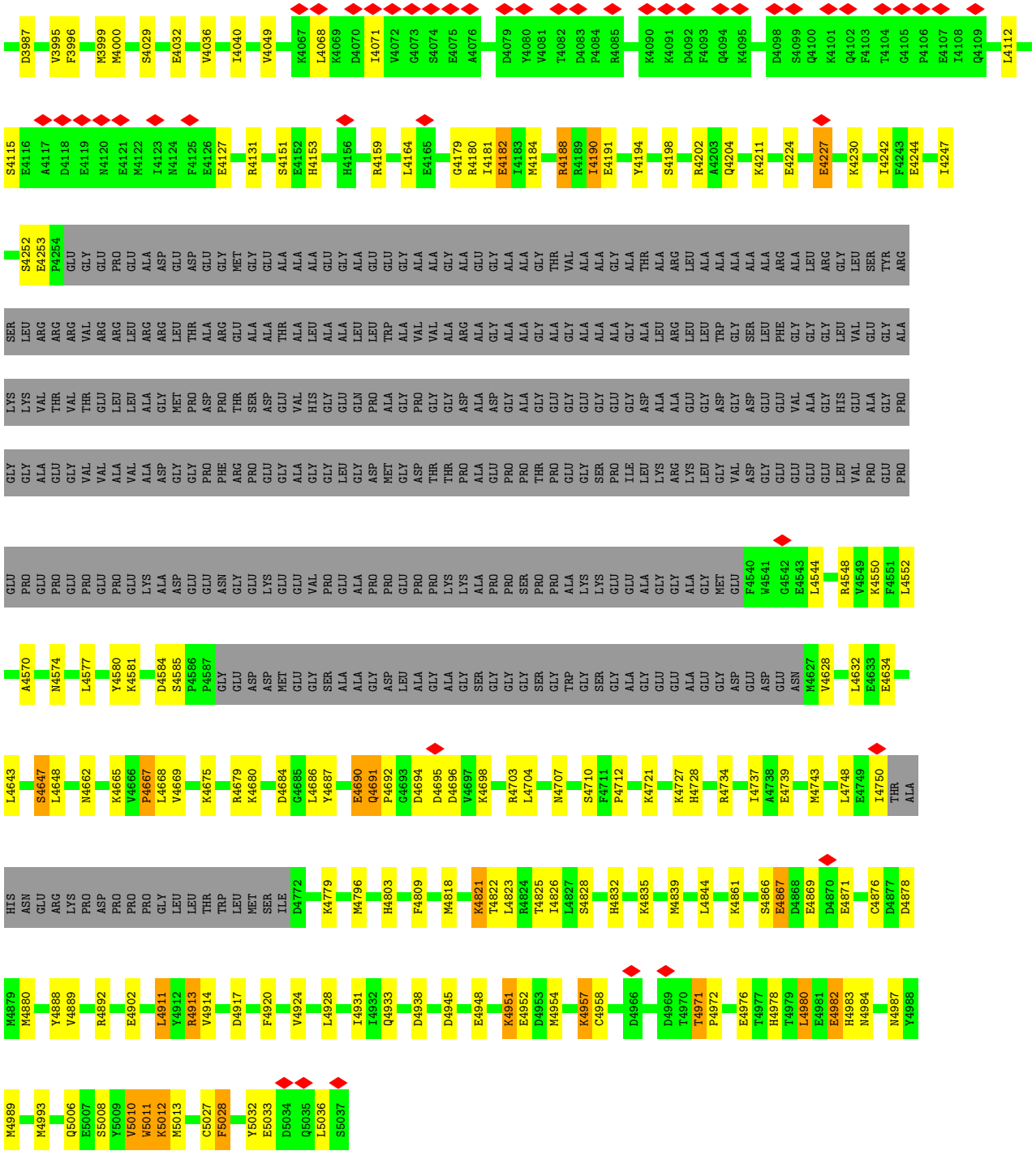
• Molecule 1: Ryanodine receptor 1

Chain D:



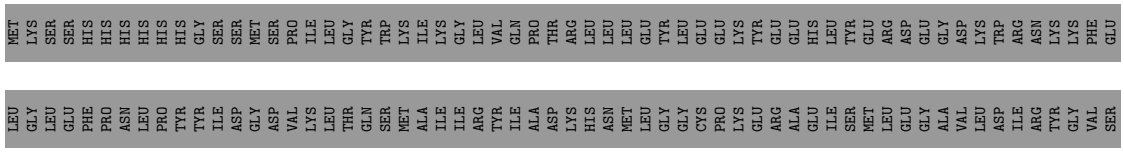


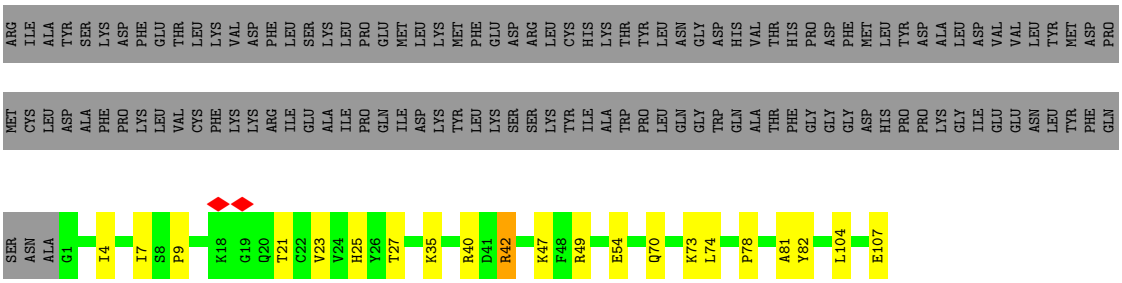

I2771 Q2772 N2773 N2774 W2775 S2776 Y2777 G2778 E2779 N2780 V2781 D2782 E2783 E2784 L2785 K2786 T2787 H2788 P2789 M2790 L2791 R2792 P2793 Y2794 K2795 T2796 F2797 S2798 E2799 K2800 D2801 K2802 E2803 I2804 Y2805 R2806 W2807 P2808 I2809 K2810 E2811 S2812 L2813 K2814 A2815 M2816 I2817 A2818 W2819 E2820 W2821 T2822 I2823 E2824 K2825 A2826 R2827 E2828 G2829 E2830
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 GLY LEU LYS ASP MET GLU L2946 D2947 T2948 S2949 S2950
L2960 L2963 M2967 Q2971 I2974 E2978 A2979 V2980 V2981 S2982 S2983 G2984 R2985 V2986 E2987 K2988 S2989 P2990 H2991 E2992 Q2993 E2994 F2998 L3002 I3006 N3007 F3010 T3011 F3017 T3020 P3021 A3022 K3023 V3024 L3025 G3026 S3027 G3028 G3029 H3030 N3033 K3034 E3035 K3036 E3037 L3049
V3050 R3051 H3052 R3053 V3054 S3055 L3056 F3057 G3058 T3059 P3062 V3065 L3068 L3075 D3076 A3077 R3078 T3079 V3080 M3081 K3082 S3083 G3084 P3085 E3086 I3087 V3088 K3089 L3092 R3093 S3094 F3095 S3098 I3103 E3104 K3105 M3106 R3111 L3112 G3113 K3114 V3115 S3116 GLN ALA ARG THR GLN VAL K3123 G3124
N3128 Y3131 V3134 V3139 F3144 Q3145 H3146 I3147 A3148 Q3149 H3150 Q3151 F3152 G3153 D3154 D3155 V3156 I3157 L3158 D3159 Q3162 R3167 T3168 S3171 I3172 Y3173 S3174 T3177 T3178 K3179 N3180 T3181 Y3182 V3183 E3184 K3185 L3194 L3197 P3205 P3208 Q3209 L3210 N3211 E3212 Y3213 N3214 A3215 C3216
S3217 V3218 Y3219 T3220 T3221 K3222 S3223 P3224 R3225 E3226 R3227 A3228 I3229 L3230 G3231 L3232 P3233 N3234 S3235 V3236 E3237 E3238 M3239 I3243 D3247 R3248 D3252 E3258 S3259 E3265 L3277 L3281 W3284 W3285 E3286 R3287 G3288 P3289 E3290 A3291 P3292 P3293 P3294 A3295 L3296 P3297 A3298 G3299 A3300 P3301 P3302 P3303
C3304 T3305 A3306 S3309 D3310 L3315 L3316 I3322 N3326 L3327 G3328 I3329 A3332 M3335 K3336 R3337 V3340 I3345 V3346 S3347 R3348 E3352 L3353 L3354 H3355 S3356 H3357 F3358 I3359 I3362 R3366 K3371 E3377 Q3378 L3379 R3380 L3381 E3382 A3383 K3384 A3385 E3386 A3387 E3388 E3389 G3390 E3391
L3392 V3400 R3403 I3413 R3414 Y3415 V3416 D3417 N3418 N3419 R3420 A3421 H3422 W3423 L3424 F3435 R3436 M3437 E3440 I3441 F3442 I3443 Y3444 W3445 S3446 K3447 S3448 N3457 Q3461 N3465 N3466 M3467 S3468 F3469 L3470 T3471 A3472 D3473 S3474 K3475 S3476 K3477 M3478 A3479 LYS ALA GLY ASP ALA GLN SER GLY
GLY SER ASP GLN GLU ARG THR LYS LYS LYS R3498 R3499 G3500 D3501 R3502 Y3503 S3504 V3505 Q3506 V3511 K3515 I3520 N3523 M3524 D3531 M3534 L3535 A3536 K3537 T3538 R3539 Y3540 A3541 L3542 K3543 D3544 T3545 D3546 E3547 E3548 E3551 F3552 N3555 N3556 L3557 H3558 L3559 Q3560 G3561 K3562 V3563 E3564
G3565 Y3576 L3579 P3580 G3581 R3582 E3583 E3584 D3585 A3586 D3587 D3588 P3589 E3590 K3591 I3592 V3593 R3594 Y3604 H3605 L3606 E3607 Q3608 T3609 E3610 H3611 P3612 Y3613 K3614 S3615 K3616 K3617 A3618 V3619 W3620 H3621 K3622 L3623 L3624 S3625 K3626 Q3627 R3628 R3629 R3630 A3631 V3632 V3633 A3634 C3635 F3636 R3637 M3638 L3641 L3644
L3677 A3680 G3681 E3682 Q3683 E3684 E3685 E3686 E3687 E3688 E3689 V3690 E3691 E3692 D3719 Y3722 E3736 GLU GLY GLY GLU ASN GLY GLU ALA GLU GLU GLU GLU V3749 E3750 V3751 S3752 F3753 E3754 E3755 E3759 R3762 Q3766 Q3767 S3768 R3769 R3773 Q3781 G3801 L3805 N3809
Y3819 K3823 S3840 V3841 L3842 D3843 L3844 R3849 G3857 M3858 V3859 N3860 E3861 D3862 G3863 T3864 V3865 I3866 N3867 R3868 Q3869 N3870 G3871 E3872 K3873 V3874 M3875 A3876 D3877 D3878 Q3882 L3888 L3924 E3928 S3929 F3933 Y3936 E3944 E3945 Q3946 R3949 V3957 A3981 R3984



• Molecule 2: Glutathione S-transferase class-mu 26 kDa isozyme,Peptidyl-prolyl cis-trans isomerase FKBP1B

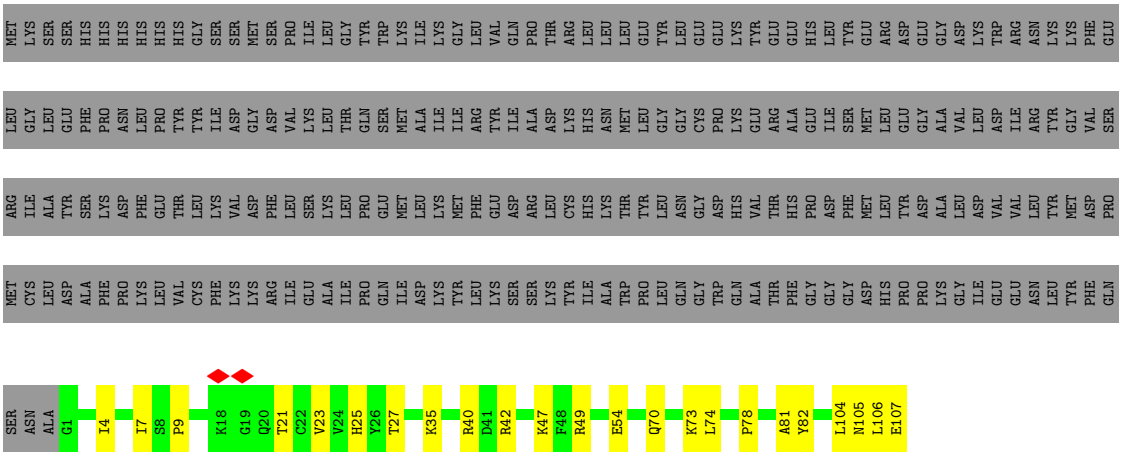
Chain E:





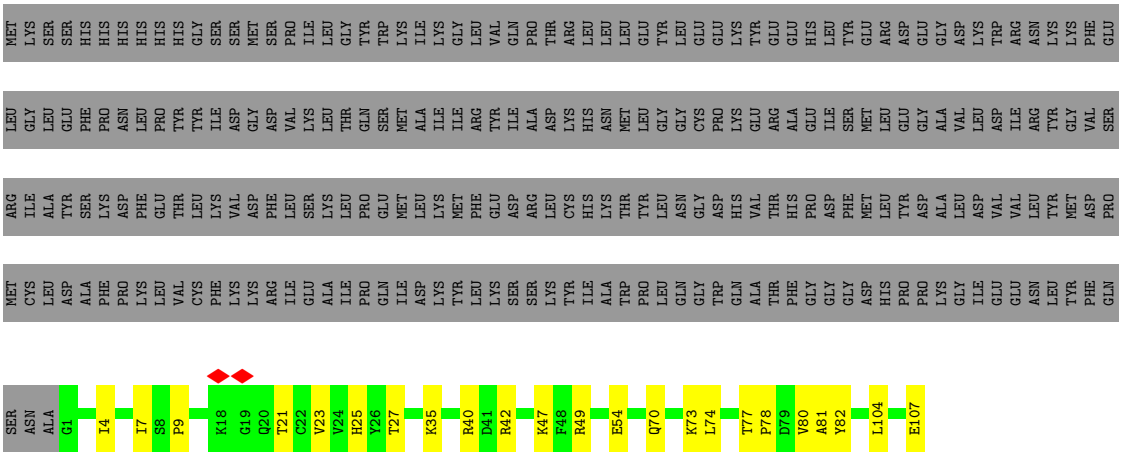
• Molecule 2: Glutathione S-transferase class-mu 26 kDa isozyme,Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F:



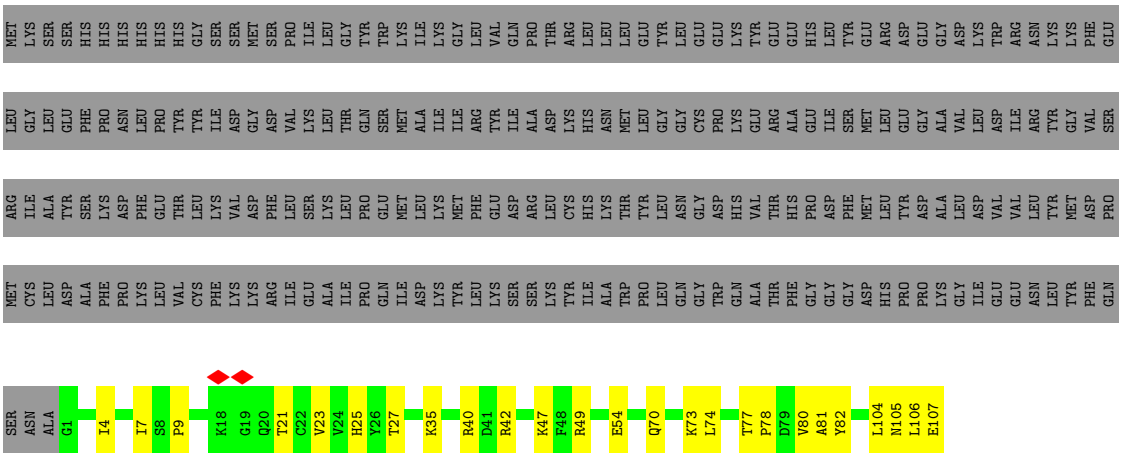
• Molecule 2: Glutathione S-transferase class-mu 26 kDa isozyme,Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain G:



• Molecule 2: Glutathione S-transferase class-mu 26 kDa isozyme,Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H:


MET LYS SER SER HIS HIS HIS HIS HIS HIS GLY SER SER MET SER PRO ILE LEU GLY TYR TRP LYS ILE LYS GLY LEU VAL GLN PRO THR ARG LEU LEU LEU GLU TYR LEU GLU GLU LYS TYR GLU GLU HIS LEU TYR GLU ARG ASP GLU GLY ASP LYS TRP ARG ASN LYS LYS PHE GLU
LEU GLY LEU GLU PHE PRO ASN LEU PRO TYR TYR ILE ASP GLY ASP VAL LYS LEU THR GLN SER MET ALA ILE ILE ARG TYR ILE ALA ASP LYS HIS ASN MET LEU GLY GLY CYS PRO LYS GLU ARG ALA GLU ILE SER MET LEU GLU GLU GLY ALA VAL LEU ASP ILE ARG TYR GLY VAL SER
ARG ILE ALA TYR SER LYS ASP PHE GLU THR LEU LYS VAL ASP PHE LEU SER LYS LEU PRO GLU MET LEU LYS MET PHE GLU ASP ARG LEU CYS HIS LYS THR TYR LEU ASN GLY ASP HIS VAL THR HIS PRO ASP PHE MET LEU TYR ASP ALA LEU VAL VAL LEU TYR MET ASP PRO
MET CYS LEU ASP ALA PHE PRO LYS LEU VAL CYS PHE LYS LYS ARG ILE GLU ALA ILE PRO GLN ILE ASP LYS TYR LEU LYS SER SER LYS TYR ILE ALA TRP PRO LEU GLN GLY TRP GLN ALA THR PHE GLY GLY GLY ASP HIS PRO PRO LYS GLY ILE GLU GLU ASN LEU TYR PHE GLN
SER ASN ALA G1 I4 I7 S8 P9 K18 G19 Q20 T21 C22 V23 V24 H25 Y26 T27 K35 R40 D41 R42 K47 F48 R49 E54 Q70 K73 L74 T77 P78 D79 V80 A81 Y82 L104 N105 L106 E107

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	206618	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.725	Depositor
Minimum map value	-0.299	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.126	Depositor
Map size (Å)	515.2, 515.2, 515.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.288, 1.288, 1.288	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.33	0/35738	0.64	8/48398 (0.0%)
1	B	0.33	0/35738	0.64	8/48398 (0.0%)
1	C	0.33	0/35738	0.64	8/48398 (0.0%)
1	D	0.33	0/35738	0.64	8/48398 (0.0%)
2	E	0.33	0/834	0.65	0/1123
2	F	0.33	0/834	0.65	0/1123
2	G	0.33	0/834	0.65	0/1123
2	H	0.33	0/834	0.64	0/1123
All	All	0.33	0/146288	0.64	32/198084 (0.0%)

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	5028	PHE	CB-CG-CD1	7.53	126.07	120.80
1	C	5028	PHE	CB-CG-CD1	7.43	126.00	120.80
1	B	5028	PHE	CB-CG-CD1	7.42	126.00	120.80
1	D	5028	PHE	CB-CG-CD1	7.42	126.00	120.80
1	A	903	LEU	CA-CB-CG	6.29	129.76	115.30
1	B	903	LEU	CA-CB-CG	6.28	129.75	115.30
1	C	903	LEU	CA-CB-CG	6.28	129.75	115.30
1	D	903	LEU	CA-CB-CG	6.28	129.75	115.30
1	B	1152	MET	CA-CB-CG	5.98	123.47	113.30
1	C	1152	MET	CA-CB-CG	5.98	123.47	113.30
1	D	1152	MET	CA-CB-CG	5.98	123.47	113.30
1	A	1152	MET	CA-CB-CG	5.97	123.45	113.30
1	B	2556	LEU	CA-CB-CG	5.72	128.45	115.30
1	C	2556	LEU	CA-CB-CG	5.72	128.45	115.30
1	D	2556	LEU	CA-CB-CG	5.71	128.43	115.30
1	A	2556	LEU	CA-CB-CG	5.70	128.41	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	3092	LEU	CA-CB-CG	5.58	128.13	115.30
1	B	3092	LEU	CA-CB-CG	5.58	128.12	115.30
1	C	3092	LEU	CA-CB-CG	5.58	128.12	115.30
1	A	5028	PHE	CB-CG-CD2	-5.57	116.91	120.80
1	A	3092	LEU	CA-CB-CG	5.56	128.09	115.30
1	C	5028	PHE	CB-CG-CD2	-5.55	116.91	120.80
1	B	131	LEU	CA-CB-CG	5.48	127.91	115.30
1	B	5028	PHE	CB-CG-CD2	-5.48	116.96	120.80
1	D	131	LEU	CA-CB-CG	5.48	127.91	115.30
1	D	5028	PHE	CB-CG-CD2	-5.48	116.96	120.80
1	A	131	LEU	CA-CB-CG	5.46	127.86	115.30
1	C	131	LEU	CA-CB-CG	5.46	127.86	115.30
1	A	1731	LEU	CA-CB-CG	5.26	127.40	115.30
1	B	1731	LEU	CA-CB-CG	5.25	127.38	115.30
1	C	1731	LEU	CA-CB-CG	5.25	127.38	115.30
1	D	1731	LEU	CA-CB-CG	5.25	127.38	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	34921	0	34546	387	0
1	B	34921	0	34546	399	0
1	C	34921	0	34546	392	0
1	D	34921	0	34546	391	0
2	E	818	0	824	12	0
2	F	818	0	824	12	0
2	G	818	0	824	13	0
2	H	818	0	824	13	0
3	A	22	0	11	2	0
3	B	22	0	11	2	0
3	C	22	0	11	2	0
3	D	22	0	11	2	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
All	All	143048	0	141524	1601	0

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

All (1601) 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)
3:B:5101:CMP:H2	3:B:5101:CMP:C2	0.97	1.49
3:A:5101:CMP:C2	3:A:5101:CMP:H2	0.97	1.49
3:C:5101:CMP:H2	3:C:5101:CMP:C2	0.97	1.48
3:D:5101:CMP:H2	3:D:5101:CMP:C2	0.97	1.47
1:A:3335:MET:SD	1:A:3403:ARG:NH1	2.61	0.74
1:C:3335:MET:SD	1:C:3403:ARG:NH1	2.61	0.74
1:B:3335:MET:SD	1:B:3403:ARG:NH1	2.61	0.73
1:D:3335:MET:SD	1:D:3403:ARG:NH1	2.61	0.73
1:A:4978:HIS:HA	1:A:4982:GLU:HG3	1.71	0.72
1:C:4978:HIS:HA	1:C:4982:GLU:HG3	1.71	0.72
1:B:4978:HIS:HA	1:B:4982:GLU:HG3	1.71	0.72
1:D:4978:HIS:HA	1:D:4982:GLU:HG3	1.71	0.71
1:B:4242:ILE:HG12	1:B:4993:MET:HG2	1.73	0.70
1:A:4242:ILE:HG12	1:A:4993:MET:HG2	1.73	0.70
1:C:3106:MET:SD	1:C:3128:ASN:ND2	2.66	0.69
1:B:3106:MET:SD	1:B:3128:ASN:ND2	2.66	0.69
1:C:4242:ILE:HG12	1:C:4993:MET:HG2	1.73	0.69
1:D:4242:ILE:HG12	1:D:4993:MET:HG2	1.73	0.69
1:D:3106:MET:SD	1:D:3128:ASN:ND2	2.66	0.68
1:B:3634:ALA:O	1:B:3638:MET:HB3	1.94	0.68
1:B:4686:LEU:HA	1:B:4690:GLU:HG3	1.76	0.68
1:A:3634:ALA:O	1:A:3638:MET:HB3	1.94	0.68
1:C:3680:ALA:HB1	1:C:3683:GLN:HE22	1.59	0.68
1:A:3106:MET:SD	1:A:3128:ASN:ND2	2.66	0.67
1:C:4686:LEU:HA	1:C:4690:GLU:HG3	1.76	0.67
1:D:224:HIS:HB3	1:D:229:GLU:HB3	1.77	0.67
1:D:3634:ALA:O	1:D:3638:MET:HB3	1.94	0.67
1:A:4686:LEU:HA	1:A:4690:GLU:HG3	1.76	0.67
1:B:1943:LEU:HD13	1:B:2098:VAL:HG22	1.76	0.67
1:A:224:HIS:HB3	1:A:229:GLU:HB3	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3680:ALA:HB1	1:D:3683:GLN:HE22	1.59	0.67
1:C:3420:ARG:HG3	1:C:3520:ILE:HD11	1.77	0.67
1:C:3634:ALA:O	1:C:3638:MET:HB3	1.94	0.67
1:A:3680:ALA:HB1	1:A:3683:GLN:HE22	1.59	0.67
1:C:224:HIS:HB3	1:C:229:GLU:HB3	1.77	0.67
1:A:2310:CYS:HB3	1:A:2313:LEU:HB2	1.78	0.66
1:B:3420:ARG:HG3	1:B:3520:ILE:HD11	1.77	0.66
1:D:4686:LEU:HA	1:D:4690:GLU:HG3	1.76	0.66
1:B:636:ASN:HD21	2:F:35:LYS:HE3	1.60	0.66
1:C:636:ASN:HD21	2:G:35:LYS:HE3	1.60	0.66
1:A:1943:LEU:HD13	1:A:2098:VAL:HG22	1.76	0.66
1:B:224:HIS:HB3	1:B:229:GLU:HB3	1.77	0.66
1:D:2310:CYS:HB3	1:D:2313:LEU:HB2	1.78	0.66
1:C:1943:LEU:HD13	1:C:2098:VAL:HG22	1.76	0.65
1:D:1943:LEU:HD13	1:D:2098:VAL:HG22	1.76	0.65
1:B:3680:ALA:HB1	1:B:3683:GLN:HE22	1.59	0.65
1:D:636:ASN:HD21	2:H:35:LYS:HE3	1.60	0.65
1:D:3420:ARG:HG3	1:D:3520:ILE:HD11	1.77	0.65
1:A:3332:ALA:HB3	1:A:3403:ARG:HD2	1.79	0.65
1:C:3332:ALA:HB3	1:C:3403:ARG:HD2	1.79	0.65
1:B:2310:CYS:HB3	1:B:2313:LEU:HB2	1.78	0.65
1:B:3332:ALA:HB3	1:B:3403:ARG:HD2	1.79	0.65
2:F:9:PRO:HA	2:F:70:GLN:HG2	1.79	0.65
1:A:3420:ARG:HG3	1:A:3520:ILE:HD11	1.77	0.65
2:E:9:PRO:HA	2:E:70:GLN:HG2	1.79	0.65
1:C:2310:CYS:HB3	1:C:2313:LEU:HB2	1.78	0.64
1:D:3332:ALA:HB3	1:D:3403:ARG:HD2	1.79	0.64
1:B:688:LEU:HD23	1:B:690:GLU:H	1.63	0.64
1:B:2531:ARG:HH12	1:B:2582:MET:HA	1.63	0.64
1:A:2531:ARG:HH12	1:A:2582:MET:HA	1.63	0.64
2:H:9:PRO:HA	2:H:70:GLN:HG2	1.79	0.64
1:C:2531:ARG:HH12	1:C:2582:MET:HA	1.63	0.64
1:C:688:LEU:HD23	1:C:690:GLU:H	1.63	0.63
1:C:1449:TRP:HB2	1:C:1553:PHE:HB2	1.80	0.63
2:G:9:PRO:HA	2:G:70:GLN:HG2	1.79	0.63
1:C:981:GLN:HG2	1:C:1047:LEU:HD11	1.80	0.63
1:A:981:GLN:HG2	1:A:1047:LEU:HD11	1.80	0.63
1:B:1449:TRP:HB2	1:B:1553:PHE:HB2	1.80	0.63
1:B:2007:ASN:O	1:B:2011:HIS:HB2	1.99	0.63
1:C:2007:ASN:O	1:C:2011:HIS:HB2	1.99	0.63
1:A:683:ARG:HG2	1:A:717:ASP:HB3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2007:ASN:O	1:A:2011:HIS:HB2	1.99	0.63
1:D:2007:ASN:O	1:D:2011:HIS:HB2	1.99	0.63
1:D:688:LEU:HD23	1:D:690:GLU:H	1.63	0.63
1:D:683:ARG:HG2	1:D:717:ASP:HB3	1.80	0.63
2:F:25:HIS:HB2	2:F:104:LEU:HD22	1.81	0.63
1:B:219:VAL:O	1:B:392:ARG:NH2	2.32	0.63
1:B:978:THR:OG1	1:B:981:GLN:OE1	2.17	0.63
1:C:219:VAL:O	1:C:392:ARG:NH2	2.32	0.62
1:D:981:GLN:HG2	1:D:1047:LEU:HD11	1.80	0.62
1:D:745:SER:HB2	1:D:758:ARG:HB2	1.81	0.62
1:A:219:VAL:O	1:A:392:ARG:NH2	2.32	0.62
1:A:978:THR:OG1	1:A:981:GLN:OE1	2.17	0.62
1:C:978:THR:OG1	1:C:981:GLN:OE1	2.17	0.62
2:G:25:HIS:HB2	2:G:104:LEU:HD22	1.81	0.62
1:A:688:LEU:HD23	1:A:690:GLU:H	1.62	0.62
1:D:219:VAL:O	1:D:392:ARG:NH2	2.32	0.62
1:D:2531:ARG:HH12	1:D:2582:MET:HA	1.63	0.62
1:A:3103:ILE:HG21	1:A:3168:THR:HG23	1.82	0.62
1:B:981:GLN:HG2	1:B:1047:LEU:HD11	1.80	0.62
1:C:683:ARG:HG2	1:C:717:ASP:HB3	1.80	0.62
1:D:978:THR:OG1	1:D:981:GLN:OE1	2.17	0.62
1:D:3103:ILE:HG21	1:D:3168:THR:HG23	1.82	0.62
1:A:1449:TRP:HB2	1:A:1553:PHE:HB2	1.80	0.62
1:B:683:ARG:HG2	1:B:717:ASP:HB3	1.80	0.62
1:C:835:ARG:NH1	1:C:1093:GLU:OE1	2.33	0.62
1:C:3114:LYS:HD3	1:C:3116:SER:H	1.64	0.62
1:B:3103:ILE:HG21	1:B:3168:THR:HG23	1.82	0.61
1:C:3322:ILE:O	1:C:3326:ASN:ND2	2.33	0.61
1:D:835:ARG:NH1	1:D:1093:GLU:OE1	2.33	0.61
1:D:3114:LYS:HD3	1:D:3116:SER:H	1.64	0.61
1:A:745:SER:HB2	1:A:758:ARG:HB2	1.81	0.61
1:B:745:SER:HB2	1:B:758:ARG:HB2	1.81	0.61
2:E:25:HIS:HB2	2:E:104:LEU:HD22	1.81	0.61
1:A:835:ARG:NH1	1:A:1093:GLU:OE1	2.33	0.61
1:C:745:SER:HB2	1:C:758:ARG:HB2	1.81	0.61
1:A:233:ILE:HD12	1:A:242:ARG:HB3	1.82	0.61
1:A:3020:THR:HG23	1:A:3023:LYS:H	1.65	0.61
1:D:3020:THR:HG23	1:D:3023:LYS:H	1.65	0.61
1:D:1449:TRP:HB2	1:D:1553:PHE:HB2	1.80	0.61
1:A:3322:ILE:O	1:A:3326:ASN:ND2	2.33	0.61
1:B:3020:THR:HG23	1:B:3023:LYS:H	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:233:ILE:HD12	1:D:242:ARG:HB3	1.82	0.61
2:H:25:HIS:HB2	2:H:104:LEU:HD22	1.81	0.61
1:B:233:ILE:HD12	1:B:242:ARG:HB3	1.82	0.61
1:C:897:ARG:HB2	1:C:903:LEU:HD11	1.83	0.61
1:C:3103:ILE:HG21	1:C:3168:THR:HG23	1.82	0.61
1:A:2000:SER:O	1:A:2005:GLN:NE2	2.33	0.61
1:A:3114:LYS:HD3	1:A:3116:SER:H	1.65	0.61
1:B:835:ARG:NH1	1:B:1093:GLU:OE1	2.33	0.61
1:D:1024:TYR:O	1:D:1032:LYS:NZ	2.34	0.61
1:B:3114:LYS:HD3	1:B:3116:SER:H	1.64	0.61
1:D:3868:ARG:HH11	1:D:3870:ASN:HB3	1.66	0.61
1:A:3868:ARG:HH11	1:A:3870:ASN:HB3	1.66	0.61
1:C:1024:TYR:O	1:C:1032:LYS:NZ	2.34	0.60
1:A:1024:TYR:O	1:A:1032:LYS:NZ	2.34	0.60
1:B:2410:PRO:HB3	1:B:2415:ARG:HB3	1.83	0.60
1:B:1024:TYR:O	1:B:1032:LYS:NZ	2.34	0.60
1:C:2000:SER:O	1:C:2005:GLN:NE2	2.33	0.60
1:A:2410:PRO:HB3	1:A:2415:ARG:HB3	1.83	0.60
1:B:897:ARG:HB2	1:B:903:LEU:HD11	1.83	0.60
1:C:3020:THR:HG23	1:C:3023:LYS:H	1.65	0.60
1:D:1569:GLN:HB2	1:D:1572:ILE:HD12	1.84	0.60
1:B:3868:ARG:HH11	1:B:3870:ASN:HB3	1.66	0.60
1:C:233:ILE:HD12	1:C:242:ARG:HB3	1.82	0.60
1:C:2410:PRO:HB3	1:C:2415:ARG:HB3	1.83	0.60
1:C:4049:VAL:HG21	1:C:4159:ARG:HE	1.67	0.60
1:A:1569:GLN:HB2	1:A:1572:ILE:HD12	1.84	0.59
1:C:3868:ARG:HH11	1:C:3870:ASN:HB3	1.66	0.59
1:D:4049:VAL:HG21	1:D:4159:ARG:HE	1.67	0.59
1:C:125:ARG:HH22	1:C:190:GLN:HB3	1.67	0.59
1:B:4049:VAL:HG21	1:B:4159:ARG:HE	1.67	0.59
1:C:633:LEU:HD13	1:C:1639:LEU:HD21	1.84	0.59
1:A:897:ARG:HB2	1:A:903:LEU:HD11	1.83	0.59
1:B:1569:GLN:HB2	1:B:1572:ILE:HD12	1.84	0.59
1:D:35:LEU:HD13	1:D:49:LEU:HD13	1.85	0.59
1:C:34:LYS:H	1:C:53:SER:HB3	1.68	0.59
1:D:34:LYS:H	1:D:53:SER:HB3	1.68	0.59
1:D:3322:ILE:O	1:D:3326:ASN:ND2	2.33	0.59
1:A:1448:VAL:HG22	1:A:1554:VAL:HG23	1.85	0.59
1:D:125:ARG:HH22	1:D:190:GLN:HB3	1.67	0.59
1:D:2410:PRO:HB3	1:D:2415:ARG:HB3	1.83	0.59
1:A:35:LEU:HD13	1:A:49:LEU:HD13	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:633:LEU:HD13	1:A:1639:LEU:HD21	1.84	0.59
1:B:3322:ILE:O	1:B:3326:ASN:ND2	2.33	0.59
1:C:1569:GLN:HB2	1:C:1572:ILE:HD12	1.84	0.59
1:A:125:ARG:HH22	1:A:190:GLN:HB3	1.67	0.59
1:A:293:LEU:HD12	1:A:378:LEU:HD23	1.85	0.59
1:A:4049:VAL:HG21	1:A:4159:ARG:HE	1.67	0.59
1:B:35:LEU:HD13	1:B:49:LEU:HD13	1.85	0.59
1:B:1448:VAL:HG22	1:B:1554:VAL:HG23	1.85	0.59
1:C:1448:VAL:HG22	1:C:1554:VAL:HG23	1.85	0.59
1:D:2000:SER:O	1:D:2005:GLN:NE2	2.33	0.59
1:D:3162:GLN:NE2	1:D:3216:CYS:SG	2.76	0.59
1:A:34:LYS:H	1:A:53:SER:HB3	1.68	0.58
1:B:293:LEU:HD12	1:B:378:LEU:HD23	1.85	0.58
1:B:4920:PHE:O	1:B:4924:VAL:HB	2.03	0.58
1:C:4920:PHE:O	1:C:4924:VAL:HB	2.03	0.58
1:B:125:ARG:HH22	1:B:190:GLN:HB3	1.67	0.58
1:A:3162:GLN:NE2	1:A:3216:CYS:SG	2.76	0.58
1:D:293:LEU:HD12	1:D:378:LEU:HD23	1.85	0.58
1:B:3457:ASN:O	1:B:3461:GLN:NE2	2.37	0.58
1:C:3162:GLN:NE2	1:C:3216:CYS:SG	2.76	0.58
1:D:3457:ASN:O	1:D:3461:GLN:NE2	2.37	0.58
1:A:299:LEU:HD13	1:A:378:LEU:HD22	1.86	0.58
1:C:3017:PHE:O	1:C:3036:LYS:NZ	2.37	0.58
1:C:3457:ASN:O	1:C:3461:GLN:NE2	2.37	0.58
1:D:897:ARG:HB2	1:D:903:LEU:HD11	1.83	0.58
1:D:3377:GLU:HA	1:D:3380:ARG:HG2	1.86	0.58
1:D:4928:LEU:HD23	1:D:4931:ILE:HD12	1.85	0.58
1:A:3872:GLU:HG3	1:A:3874:VAL:H	1.68	0.58
1:C:293:LEU:HD12	1:C:378:LEU:HD23	1.85	0.58
1:D:4920:PHE:O	1:D:4924:VAL:HB	2.03	0.58
1:A:3946:GLN:OE1	1:A:3949:ARG:NH2	2.36	0.58
1:B:34:LYS:H	1:B:53:SER:HB3	1.68	0.58
1:B:633:LEU:HD13	1:B:1639:LEU:HD21	1.84	0.58
1:B:1476:MET:HB2	1:B:1485:SER:HB3	1.86	0.58
1:B:2885:THR:HG22	1:B:2888:ARG:HH12	1.69	0.58
1:C:2885:THR:HG22	1:C:2888:ARG:HH12	1.69	0.58
1:D:633:LEU:HD13	1:D:1639:LEU:HD21	1.84	0.58
1:D:1448:VAL:HG22	1:D:1554:VAL:HG23	1.85	0.58
1:C:35:LEU:HD13	1:C:49:LEU:HD13	1.85	0.58
1:C:3377:GLU:HA	1:C:3380:ARG:HG2	1.86	0.58
1:A:531:ARG:NH2	1:A:562:GLU:OE2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2885:THR:HG22	1:D:2888:ARG:HH12	1.69	0.58
1:A:2885:THR:HG22	1:A:2888:ARG:HH12	1.69	0.57
1:A:4920:PHE:O	1:A:4924:VAL:HB	2.04	0.57
1:B:3017:PHE:O	1:B:3036:LYS:NZ	2.37	0.57
1:B:3162:GLN:NE2	1:B:3216:CYS:SG	2.76	0.57
1:A:3017:PHE:O	1:A:3036:LYS:NZ	2.37	0.57
1:C:3872:GLU:HG3	1:C:3874:VAL:H	1.68	0.57
1:D:3872:GLU:HG3	1:D:3874:VAL:H	1.68	0.57
2:G:27:THR:OG1	2:G:40:ARG:NH1	2.37	0.57
1:B:632:LEU:O	1:B:634:GLN:NE2	2.38	0.57
1:C:632:LEU:O	1:C:634:GLN:NE2	2.38	0.57
1:C:2967:MET:HE3	1:C:3049:LEU:HD13	1.86	0.57
1:D:299:LEU:HD13	1:D:378:LEU:HD22	1.86	0.57
1:D:531:ARG:NH2	1:D:562:GLU:OE2	2.36	0.57
1:D:2978:GLU:OE2	1:D:3053:ARG:NH1	2.37	0.57
1:B:4928:LEU:HD23	1:B:4931:ILE:HD12	1.85	0.57
1:D:1476:MET:HB2	1:D:1485:SER:HB3	1.86	0.57
2:F:27:THR:OG1	2:F:40:ARG:NH1	2.37	0.57
1:A:37:LEU:HD21	1:A:191:VAL:HG21	1.87	0.57
1:B:3872:GLU:HG3	1:B:3874:VAL:H	1.68	0.57
1:C:2978:GLU:OE2	1:C:3053:ARG:NH1	2.37	0.57
2:E:27:THR:OG1	2:E:40:ARG:NH1	2.37	0.57
1:C:1476:MET:HB2	1:C:1485:SER:HB3	1.86	0.57
1:C:4928:LEU:HD23	1:C:4931:ILE:HD12	1.85	0.57
1:D:3562:LYS:HE3	1:D:3564:GLU:HB2	1.87	0.57
1:A:4068:LEU:HA	1:A:4071:ILE:HB	1.87	0.57
1:B:2978:GLU:OE2	1:B:3053:ARG:NH1	2.37	0.57
1:A:3457:ASN:O	1:A:3461:GLN:NE2	2.37	0.57
1:B:37:LEU:HD21	1:B:191:VAL:HG21	1.87	0.57
1:B:299:LEU:HD13	1:B:378:LEU:HD22	1.86	0.57
1:B:2670:GLU:HG2	1:B:2912:THR:HA	1.87	0.57
1:B:3562:LYS:HE3	1:B:3564:GLU:HB2	1.87	0.57
1:D:3017:PHE:O	1:D:3036:LYS:NZ	2.37	0.57
2:H:27:THR:OG1	2:H:40:ARG:NH1	2.37	0.57
1:A:2978:GLU:OE2	1:A:3053:ARG:NH1	2.37	0.56
1:A:4928:LEU:HD23	1:A:4931:ILE:HD12	1.85	0.56
1:C:3081:MET:HG2	1:C:3089:LYS:HE3	1.87	0.56
1:D:632:LEU:O	1:D:634:GLN:NE2	2.38	0.56
1:A:2967:MET:HE3	1:A:3049:LEU:HD13	1.87	0.56
1:B:4068:LEU:HA	1:B:4071:ILE:HB	1.87	0.56
1:A:636:ASN:HD21	2:E:35:LYS:HE3	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1476:MET:HB2	1:A:1485:SER:HB3	1.86	0.56
1:A:2670:GLU:HG2	1:A:2912:THR:HA	1.87	0.56
1:B:1131:ARG:NH1	1:B:1178:ALA:O	2.38	0.56
1:B:3081:MET:HG2	1:B:3089:LYS:HE3	1.87	0.56
1:B:3377:GLU:HA	1:B:3380:ARG:HG2	1.86	0.56
1:C:299:LEU:HD13	1:C:378:LEU:HD22	1.86	0.56
1:C:3562:LYS:HE3	1:C:3564:GLU:HB2	1.87	0.56
1:C:3769:ARG:O	1:C:3773:ARG:NH1	2.38	0.56
1:D:1131:ARG:NH1	1:D:1178:ALA:O	2.38	0.56
1:D:2655:TYR:HB3	1:D:2672:LEU:HD21	1.88	0.56
1:D:3147:ILE:HG23	1:D:3152:PHE:HB2	1.88	0.56
1:D:4068:LEU:HA	1:D:4071:ILE:HB	1.87	0.56
1:A:35:LEU:HB3	1:A:49:LEU:HD22	1.87	0.56
1:A:1131:ARG:NH1	1:A:1178:ALA:O	2.38	0.56
1:A:1291:LEU:HB3	1:A:1595:LEU:HD11	1.88	0.56
1:A:2655:TYR:HB3	1:A:2672:LEU:HD21	1.88	0.56
1:B:882:TRP:O	1:B:886:ARG:NH1	2.39	0.56
1:C:37:LEU:HD21	1:C:191:VAL:HG21	1.87	0.56
1:A:632:LEU:O	1:A:634:GLN:NE2	2.38	0.56
1:A:3377:GLU:HA	1:A:3380:ARG:HG2	1.86	0.56
1:A:3562:LYS:HE3	1:A:3564:GLU:HB2	1.87	0.56
1:D:3769:ARG:O	1:D:3773:ARG:NH1	2.38	0.56
1:A:207:SER:OG	1:A:334:MET:SD	2.64	0.56
1:B:35:LEU:HB3	1:B:49:LEU:HD22	1.87	0.56
1:B:207:SER:OG	1:B:334:MET:SD	2.64	0.56
1:B:2967:MET:HE3	1:B:3049:LEU:HD13	1.86	0.56
1:C:882:TRP:O	1:C:886:ARG:NH1	2.39	0.56
1:B:3524:MET:HA	1:B:3582:ARG:HH12	1.71	0.56
1:C:2670:GLU:HG2	1:C:2912:THR:HA	1.87	0.56
1:D:2765:LYS:NZ	1:D:2859:PRO:O	2.38	0.56
1:A:882:TRP:O	1:A:886:ARG:NH1	2.39	0.56
1:C:1131:ARG:NH1	1:C:1178:ALA:O	2.38	0.56
1:C:1469:VAL:HG13	1:C:1492:CYS:HB3	1.88	0.56
1:C:2021:CYS:O	1:C:2028:ARG:NH2	2.39	0.56
1:D:35:LEU:HB3	1:D:49:LEU:HD22	1.87	0.56
1:A:551:LEU:HB3	1:A:589:LEU:HD11	1.88	0.56
1:A:3081:MET:HG2	1:A:3089:LYS:HE3	1.87	0.56
1:A:3524:MET:HA	1:A:3582:ARG:HH12	1.71	0.56
1:B:2021:CYS:O	1:B:2028:ARG:NH2	2.39	0.56
1:B:3946:GLN:OE1	1:B:3949:ARG:NH2	2.36	0.56
1:C:4068:LEU:HA	1:C:4071:ILE:HB	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1469:VAL:HG13	1:D:1492:CYS:HB3	1.88	0.56
1:D:2670:GLU:HG2	1:D:2912:THR:HA	1.87	0.56
1:B:1469:VAL:HG13	1:B:1492:CYS:HB3	1.88	0.56
1:D:37:LEU:HD21	1:D:191:VAL:HG21	1.87	0.56
1:A:2021:CYS:O	1:A:2028:ARG:NH2	2.39	0.55
1:A:3147:ILE:HG23	1:A:3152:PHE:HB2	1.88	0.55
1:C:1116:GLY:HA3	1:C:1132:TRP:HB3	1.88	0.55
1:C:3147:ILE:HG23	1:C:3152:PHE:HB2	1.88	0.55
1:A:27:THR:OG1	1:A:32:GLN:OE1	2.23	0.55
1:A:867:LEU:HD13	1:A:929:LEU:HB3	1.89	0.55
1:B:531:ARG:NH2	1:B:562:GLU:OE2	2.36	0.55
1:B:1291:LEU:HB3	1:B:1595:LEU:HD11	1.88	0.55
1:B:1454:THR:OG1	1:B:1456:ASP:OD1	2.24	0.55
1:B:3766:GLN:OE1	1:B:3769:ARG:NH2	2.40	0.55
1:C:867:LEU:HD13	1:C:929:LEU:HB3	1.89	0.55
1:C:4976:GLU:O	1:C:4980:LEU:HB2	2.06	0.55
1:D:882:TRP:O	1:D:886:ARG:NH1	2.39	0.55
1:D:2021:CYS:O	1:D:2028:ARG:NH2	2.39	0.55
1:A:1469:VAL:HG13	1:A:1492:CYS:HB3	1.88	0.55
1:B:2777:TYR:HB3	1:B:2791:LEU:HD23	1.89	0.55
1:C:207:SER:OG	1:C:334:MET:SD	2.64	0.55
1:C:1291:LEU:HB3	1:C:1595:LEU:HD11	1.88	0.55
1:C:2655:TYR:HB3	1:C:2672:LEU:HD21	1.88	0.55
1:D:1116:GLY:HA3	1:D:1132:TRP:HB3	1.88	0.55
1:D:3081:MET:HG2	1:D:3089:LYS:HE3	1.87	0.55
1:B:14:LEU:HB2	1:B:163:VAL:HG13	1.88	0.55
1:D:3524:MET:HA	1:D:3582:ARG:HH12	1.71	0.55
1:B:3227:ARG:NH1	1:B:3234:ASN:OD1	2.40	0.55
1:B:4976:GLU:O	1:B:4980:LEU:HB2	2.06	0.55
1:C:35:LEU:HB3	1:C:49:LEU:HD22	1.87	0.55
1:C:3524:MET:O	1:C:3576:TYR:OH	2.24	0.55
1:D:3766:GLN:OE1	1:D:3769:ARG:NH2	2.40	0.55
1:B:27:THR:OG1	1:B:32:GLN:OE1	2.23	0.55
1:B:3147:ILE:HG23	1:B:3152:PHE:HB2	1.88	0.55
1:C:2777:TYR:HB3	1:C:2791:LEU:HD23	1.89	0.55
1:A:2777:TYR:HB3	1:A:2791:LEU:HD23	1.89	0.55
1:B:867:LEU:HD13	1:B:929:LEU:HB3	1.89	0.55
1:C:2765:LYS:NZ	1:C:2859:PRO:O	2.38	0.55
1:D:551:LEU:HB3	1:D:589:LEU:HD11	1.88	0.55
1:D:1291:LEU:HB3	1:D:1595:LEU:HD11	1.88	0.55
1:D:2394:GLY:HA3	1:D:2415:ARG:HH21	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2777:TYR:HB3	1:D:2791:LEU:HD23	1.89	0.55
1:D:4976:GLU:O	1:D:4980:LEU:HB2	2.06	0.55
1:A:14:LEU:HB2	1:A:163:VAL:HG13	1.88	0.55
1:B:2871:LEU:HG	1:B:2927:LEU:HD21	1.89	0.55
1:B:4983:HIS:O	3:B:5101:CMP:N6	2.40	0.55
1:C:4151:SER:HB3	1:C:4164:LEU:HD21	1.88	0.55
1:D:4151:SER:HB3	1:D:4164:LEU:HD21	1.88	0.55
1:A:2394:GLY:HA3	1:A:2415:ARG:HH21	1.72	0.55
1:A:4983:HIS:O	3:A:5101:CMP:N6	2.40	0.55
1:B:2000:SER:O	1:B:2005:GLN:NE2	2.33	0.55
1:C:3766:GLN:OE1	1:C:3769:ARG:NH2	2.40	0.55
2:H:78:PRO:HA	2:H:81:ALA:HB3	1.89	0.55
1:A:828:GLU:O	1:A:1073:ARG:NH1	2.40	0.54
1:A:1116:GLY:HA3	1:A:1132:TRP:HB3	1.88	0.54
1:B:2655:TYR:HB3	1:B:2672:LEU:HD21	1.88	0.54
1:C:3524:MET:HA	1:C:3582:ARG:HH12	1.71	0.54
1:D:207:SER:OG	1:D:334:MET:SD	2.64	0.54
1:D:1089:TYR:HE2	1:D:1211:LEU:HD13	1.72	0.54
1:D:1694:LEU:HB3	1:D:1715:LEU:HD12	1.89	0.54
1:D:3524:MET:O	1:D:3576:TYR:OH	2.24	0.54
1:A:659:TYR:O	1:A:662:TRP:NE1	2.40	0.54
1:A:1089:TYR:HE2	1:A:1211:LEU:HD13	1.72	0.54
1:A:1947:CYS:SG	1:A:2127:GLN:NE2	2.75	0.54
1:A:3766:GLN:OE1	1:A:3769:ARG:NH2	2.40	0.54
1:B:3445:TRP:HZ3	1:B:3511:VAL:HG13	1.73	0.54
1:C:2871:LEU:HG	1:C:2927:LEU:HD21	1.89	0.54
1:D:828:GLU:O	1:D:1073:ARG:NH1	2.40	0.54
1:D:867:LEU:HD13	1:D:929:LEU:HB3	1.89	0.54
1:D:1076:ARG:HB3	1:D:1191:VAL:HG23	1.90	0.54
1:D:4983:HIS:O	3:D:5101:CMP:N6	2.40	0.54
1:A:2288:LEU:O	1:A:3849:ARG:NH1	2.39	0.54
1:A:4913:ARG:NH2	1:D:4888:TYR:OH	2.40	0.54
1:B:1694:LEU:HB3	1:B:1715:LEU:HD12	1.89	0.54
1:C:551:LEU:HB3	1:C:589:LEU:HD11	1.88	0.54
1:C:1694:LEU:HB3	1:C:1715:LEU:HD12	1.89	0.54
1:C:3946:GLN:OE1	1:C:3949:ARG:NH2	2.36	0.54
1:A:4976:GLU:O	1:A:4980:LEU:HB2	2.06	0.54
1:B:2394:GLY:HA3	1:B:2415:ARG:HH21	1.72	0.54
1:C:531:ARG:NH2	1:C:562:GLU:OE2	2.36	0.54
1:D:2967:MET:HE3	1:D:3049:LEU:HD13	1.88	0.54
1:B:551:LEU:HB3	1:B:589:LEU:HD11	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:828:GLU:O	1:B:1073:ARG:NH1	2.40	0.54
1:C:4983:HIS:O	3:C:5101:CMP:N6	2.40	0.54
1:C:1076:ARG:HB3	1:C:1191:VAL:HG23	1.90	0.54
1:C:2519:LEU:HD13	1:C:2522:LEU:HD23	1.90	0.54
1:C:3445:TRP:HZ3	1:C:3511:VAL:HG13	1.72	0.54
1:C:4570:ALA:O	1:C:4574:ASN:ND2	2.41	0.54
1:D:3445:TRP:HZ3	1:D:3511:VAL:HG13	1.73	0.54
1:A:1694:LEU:HB3	1:A:1715:LEU:HD12	1.89	0.54
1:B:1270:LEU:HB2	1:B:1564:PHE:HB2	1.90	0.54
1:C:2394:GLY:HA3	1:C:2415:ARG:HH21	1.72	0.54
1:B:1116:GLY:HA3	1:B:1132:TRP:HB3	1.88	0.54
1:C:14:LEU:HB2	1:C:163:VAL:HG13	1.88	0.54
1:C:1089:TYR:HE2	1:C:1211:LEU:HD13	1.72	0.54
2:G:78:PRO:HA	2:G:81:ALA:HB3	1.89	0.54
1:A:2280:VAL:HG11	1:A:2290:LEU:HD12	1.90	0.54
1:A:3984:ARG:NH2	1:A:3987:ASP:OD2	2.41	0.54
1:A:4151:SER:HB3	1:A:4164:LEU:HD21	1.88	0.54
1:C:828:GLU:O	1:C:1073:ARG:NH1	2.40	0.54
1:C:2765:LYS:HZ3	1:C:2857:PRO:HB2	1.73	0.54
1:D:125:ARG:NH1	1:D:126:SER:OG	2.41	0.54
1:D:2280:VAL:HG11	1:D:2290:LEU:HD12	1.90	0.54
1:D:2871:LEU:HG	1:D:2927:LEU:HD21	1.89	0.54
1:D:3995:VAL:O	1:D:3999:MET:HB2	2.08	0.54
1:D:4570:ALA:O	1:D:4574:ASN:ND2	2.41	0.54
1:A:1076:ARG:HB3	1:A:1191:VAL:HG23	1.90	0.54
1:B:1076:ARG:HB3	1:B:1191:VAL:HG23	1.90	0.54
1:B:1815:LEU:HD22	1:B:1845:VAL:HG21	1.90	0.54
1:B:2801:ASP:HA	1:B:2804:ILE:HG12	1.90	0.54
1:D:27:THR:OG1	1:D:32:GLN:OE1	2.23	0.54
1:A:1815:LEU:HD22	1:A:1845:VAL:HG21	1.90	0.53
1:A:4570:ALA:O	1:A:4574:ASN:ND2	2.41	0.53
1:B:659:TYR:O	1:B:662:TRP:NE1	2.40	0.53
1:B:2458:ARG:NH2	1:B:2509:VAL:O	2.41	0.53
1:C:1784:ALA:O	2:G:82:TYR:OH	2.26	0.53
1:D:14:LEU:HB2	1:D:163:VAL:HG13	1.88	0.53
1:D:2018:GLU:OE1	1:D:2028:ARG:NH1	2.42	0.53
1:A:2765:LYS:NZ	1:A:2859:PRO:O	2.38	0.53
1:B:4151:SER:HB3	1:B:4164:LEU:HD21	1.88	0.53
1:C:659:TYR:O	1:C:662:TRP:NE1	2.40	0.53
1:D:2458:ARG:NH2	1:D:2509:VAL:O	2.41	0.53
1:A:3995:VAL:O	1:A:3999:MET:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3995:VAL:O	1:B:3999:MET:HB2	2.08	0.53
1:C:125:ARG:NH1	1:C:126:SER:OG	2.41	0.53
1:C:1815:LEU:HD22	1:C:1845:VAL:HG21	1.90	0.53
1:C:2458:ARG:NH2	1:C:2509:VAL:O	2.41	0.53
1:D:707:VAL:HG23	1:D:782:SER:HB3	1.91	0.53
1:D:2519:LEU:HD13	1:D:2522:LEU:HD23	1.90	0.53
2:E:78:PRO:HA	2:E:81:ALA:HB3	1.89	0.53
1:B:1089:TYR:HE2	1:B:1211:LEU:HD13	1.72	0.53
1:B:3524:MET:O	1:B:3576:TYR:OH	2.24	0.53
1:B:4570:ALA:O	1:B:4574:ASN:ND2	2.41	0.53
1:C:707:VAL:HG23	1:C:782:SER:HB3	1.91	0.53
1:C:1947:CYS:SG	1:C:2127:GLN:NE2	2.75	0.53
1:C:2801:ASP:HA	1:C:2804:ILE:HG12	1.90	0.53
1:D:1270:LEU:HB2	1:D:1564:PHE:HB2	1.90	0.53
1:D:2288:LEU:O	1:D:3849:ARG:NH1	2.39	0.53
1:A:2871:LEU:HG	1:A:2927:LEU:HD21	1.89	0.53
1:A:4630:TYR:OH	1:B:4860:ARG:NH1	2.38	0.53
1:B:2519:LEU:HD13	1:B:2522:LEU:HD23	1.90	0.53
1:B:3984:ARG:NH2	1:B:3987:ASP:OD2	2.41	0.53
1:C:27:THR:OG1	1:C:32:GLN:OE1	2.23	0.53
1:C:1270:LEU:HB2	1:C:1564:PHE:HB2	1.90	0.53
1:D:1815:LEU:HD22	1:D:1845:VAL:HG21	1.90	0.53
1:A:2458:ARG:NH2	1:A:2509:VAL:O	2.41	0.53
1:B:2280:VAL:HG11	1:B:2290:LEU:HD12	1.90	0.53
1:B:2765:LYS:NZ	1:B:2859:PRO:O	2.38	0.53
1:D:659:TYR:O	1:D:662:TRP:NE1	2.40	0.53
1:D:1243:PRO:O	1:D:1458:HIS:ND1	2.40	0.53
1:D:1454:THR:OG1	1:D:1456:ASP:OD1	2.24	0.53
1:A:2018:GLU:OE1	1:A:2028:ARG:NH1	2.42	0.53
1:C:111:HIS:ND1	1:C:114:SER:OG	2.37	0.53
1:C:3995:VAL:O	1:C:3999:MET:HB2	2.08	0.53
1:D:3984:ARG:NH2	1:D:3987:ASP:OD2	2.41	0.53
1:B:277:GLY:N	1:B:316:PHE:O	2.39	0.53
1:B:3111:ARG:NH2	1:B:3174:SER:OG	2.42	0.53
1:C:2267:MET:O	1:C:2330:ARG:NH1	2.41	0.53
1:C:2288:LEU:O	1:C:3849:ARG:NH1	2.39	0.53
1:C:3227:ARG:NH1	1:C:3234:ASN:OD1	2.40	0.53
1:D:2801:ASP:HA	1:D:2804:ILE:HG12	1.90	0.53
1:D:3111:ARG:NH2	1:D:3174:SER:OG	2.42	0.53
1:A:3445:TRP:HZ3	1:A:3511:VAL:HG13	1.73	0.53
1:A:3769:ARG:O	1:A:3773:ARG:NH1	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:707:VAL:HG23	1:B:782:SER:HB3	1.91	0.53
1:C:3111:ARG:NH2	1:C:3174:SER:OG	2.42	0.53
1:D:3227:ARG:NH1	1:D:3234:ASN:OD1	2.40	0.53
1:A:277:GLY:N	1:A:316:PHE:O	2.39	0.53
1:A:2917:ALA:HA	1:A:2920:ARG:HB3	1.91	0.53
1:C:3984:ARG:NH2	1:C:3987:ASP:OD2	2.41	0.53
1:D:1422:ASP:OD2	1:D:1568:LYS:NZ	2.35	0.53
2:F:78:PRO:HA	2:F:81:ALA:HB3	1.89	0.53
1:A:747:CYS:HB2	1:A:756:SER:HB2	1.91	0.52
1:A:818:ARG:HH12	1:A:1026:LEU:HA	1.74	0.52
1:B:125:ARG:NH1	1:B:126:SER:OG	2.41	0.52
1:B:3767:GLN:OE1	1:B:3809:ASN:ND2	2.41	0.52
1:C:1728:ARG:HA	1:C:1731:LEU:HD23	1.91	0.52
1:C:2018:GLU:OE1	1:C:2028:ARG:NH1	2.42	0.52
1:C:2280:VAL:HG11	1:C:2290:LEU:HD12	1.90	0.52
1:C:2736:ASP:O	1:C:2738:ARG:NH1	2.42	0.52
1:D:2917:ALA:HA	1:D:2920:ARG:HB3	1.91	0.52
1:A:707:VAL:HG23	1:A:782:SER:HB3	1.91	0.52
1:A:2519:LEU:HD13	1:A:2522:LEU:HD23	1.90	0.52
1:A:3227:ARG:NH1	1:A:3234:ASN:OD1	2.40	0.52
1:A:1728:ARG:HA	1:A:1731:LEU:HD23	1.91	0.52
1:A:2736:ASP:O	1:A:2738:ARG:NH1	2.42	0.52
1:A:3524:MET:O	1:A:3576:TYR:OH	2.24	0.52
1:B:747:CYS:HB2	1:B:756:SER:HB2	1.91	0.52
1:D:2736:ASP:O	1:D:2738:ARG:NH1	2.42	0.52
1:A:3051:ARG:O	1:A:3053:ARG:NE	2.33	0.52
1:C:2369[A]:ARG:NH2	1:C:2372:GLY:O	2.39	0.52
1:D:818:ARG:HH12	1:D:1026:LEU:HA	1.74	0.52
1:A:1547:LYS:NZ	1:A:1642:PRO:O	2.43	0.52
1:B:2018:GLU:OE1	1:B:2028:ARG:NH1	2.42	0.52
1:B:3769:ARG:O	1:B:3773:ARG:NH1	2.38	0.52
1:D:277:GLY:N	1:D:316:PHE:O	2.39	0.52
1:D:1782:PHE:O	2:H:82:TYR:OH	2.28	0.52
1:D:2369[A]:ARG:NH2	1:D:2372:GLY:O	2.39	0.52
1:A:1243:PRO:O	1:A:1458:HIS:ND1	2.41	0.52
1:B:1782:PHE:O	2:F:82:TYR:OH	2.28	0.52
1:C:320:LYS:NZ	1:C:383:HIS:O	2.43	0.52
1:D:747:CYS:HB2	1:D:756:SER:HB2	1.91	0.52
1:A:125:ARG:NH1	1:A:126:SER:OG	2.41	0.52
1:D:1547:LYS:NZ	1:D:1642:PRO:O	2.43	0.52
1:A:2801:ASP:HA	1:A:2804:ILE:HG12	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3111:ARG:NH2	1:A:3174:SER:OG	2.42	0.52
1:B:2288:LEU:O	1:B:3849:ARG:NH1	2.39	0.52
1:A:2765:LYS:HZ3	1:A:2857:PRO:HB2	1.74	0.52
1:B:818:ARG:HH12	1:B:1026:LEU:HA	1.74	0.52
1:B:1101:ARG:NH1	1:B:1115:LEU:O	2.43	0.52
1:B:1547:LYS:NZ	1:B:1642:PRO:O	2.43	0.52
1:C:1101:ARG:NH1	1:C:1115:LEU:O	2.43	0.52
1:C:1547:LYS:NZ	1:C:1642:PRO:O	2.43	0.52
1:C:2917:ALA:HA	1:C:2920:ARG:HB3	1.91	0.52
1:C:3414:ARG:HH21	1:C:3473:ASP:HB2	1.75	0.52
1:B:2736:ASP:O	1:B:2738:ARG:NH1	2.42	0.51
1:C:1674:CYS:HG	1:C:1717:SER:HG	1.57	0.51
1:D:1947:CYS:SG	1:D:2127:GLN:NE2	2.75	0.51
1:A:1270:LEU:HB2	1:A:1564:PHE:HB2	1.90	0.51
1:B:3414:ARG:HH21	1:B:3473:ASP:HB2	1.75	0.51
1:D:1101:ARG:NH1	1:D:1115:LEU:O	2.43	0.51
1:C:451:TYR:O	1:C:474:ARG:NH1	2.44	0.51
1:A:168:ASP:HB3	1:A:199:LEU:HD11	1.93	0.51
1:A:4913:ARG:NH2	1:A:4917:ASP:OD2	2.44	0.51
1:B:168:ASP:HB3	1:B:199:LEU:HD11	1.93	0.51
1:B:1728:ARG:HA	1:B:1731:LEU:HD23	1.91	0.51
1:C:2626:LEU:HD22	1:C:2640:PRO:HB3	1.92	0.51
1:D:168:ASP:HB3	1:D:199:LEU:HD11	1.93	0.51
1:D:1728:ARG:HA	1:D:1731:LEU:HD23	1.91	0.51
1:D:2267:MET:O	1:D:2330:ARG:NH1	2.41	0.51
1:D:3414:ARG:HH21	1:D:3473:ASP:HB2	1.75	0.51
1:A:320:LYS:NZ	1:A:383:HIS:O	2.43	0.51
1:A:451:TYR:O	1:A:474:ARG:NH1	2.44	0.51
1:A:1454:THR:OG1	1:A:1456:ASP:OD1	2.24	0.51
1:B:451:TYR:O	1:B:474:ARG:NH1	2.44	0.51
1:C:168:ASP:HB3	1:C:199:LEU:HD11	1.93	0.51
1:C:1243:PRO:O	1:C:1458:HIS:ND1	2.41	0.51
1:D:150:MET:HB2	1:D:169:LEU:HD12	1.93	0.51
2:F:7:ILE:HD11	2:F:73:LYS:HB2	1.93	0.51
1:A:150:MET:HB2	1:A:169:LEU:HD12	1.93	0.51
1:C:747:CYS:HB2	1:C:756:SER:HB2	1.91	0.51
1:D:131:LEU:HD13	1:D:195:PHE:HE2	1.76	0.51
1:D:2626:LEU:HD22	1:D:2640:PRO:HB3	1.92	0.51
1:A:3414:ARG:HH21	1:A:3473:ASP:HB2	1.75	0.51
1:C:818:ARG:HH12	1:C:1026:LEU:HA	1.74	0.51
1:A:1101:ARG:NH1	1:A:1115:LEU:O	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2369[A]:ARG:NH2	1:A:2372:GLY:O	2.39	0.51
1:B:2626:LEU:HD22	1:B:2640:PRO:HB3	1.92	0.51
1:B:3352:GLU:O	1:B:3356:SER:OG	2.29	0.51
1:C:3062:PRO:HA	1:C:3065:VAL:HG12	1.93	0.51
1:D:320:LYS:NZ	1:D:383:HIS:O	2.43	0.51
1:A:939:VAL:HB	1:A:1051:TYR:HB3	1.93	0.51
1:B:2917:ALA:HA	1:B:2920:ARG:HB3	1.91	0.51
1:B:3359:ILE:HD13	1:B:3362:ILE:HD11	1.93	0.51
1:D:3946:GLN:OE1	1:D:3949:ARG:NH2	2.36	0.51
1:A:221:ARG:NH2	1:A:255:HIS:O	2.40	0.51
1:B:150:MET:HB2	1:B:169:LEU:HD12	1.93	0.51
1:B:320:LYS:NZ	1:B:383:HIS:O	2.43	0.51
1:D:3051:ARG:O	1:D:3053:ARG:NE	2.33	0.51
1:A:1927:LEU:HD13	1:A:2101:MET:HG3	1.93	0.50
1:B:939:VAL:HB	1:B:1051:TYR:HB3	1.93	0.50
1:B:1243:PRO:O	1:B:1458:HIS:ND1	2.41	0.50
1:B:3089:LYS:HE2	1:B:3093:ARG:HH21	1.76	0.50
1:B:4913:ARG:NH2	1:B:4917:ASP:OD2	2.44	0.50
1:D:939:VAL:HB	1:D:1051:TYR:HB3	1.94	0.50
1:A:2626:LEU:HD22	1:A:2640:PRO:HB3	1.92	0.50
1:A:3359:ILE:HD13	1:A:3362:ILE:HD11	1.93	0.50
1:D:2765:LYS:HZ1	1:D:2857:PRO:HB2	1.75	0.50
1:D:3062:PRO:HA	1:D:3065:VAL:HG12	1.93	0.50
2:G:7:ILE:HD11	2:G:73:LYS:HB2	1.93	0.50
1:A:131:LEU:HD13	1:A:195:PHE:HE2	1.76	0.50
1:B:3068:LEU:HD23	1:B:3139:VAL:HG21	1.93	0.50
1:B:932:LEU:HB3	1:B:937:CYS:HB3	1.94	0.50
1:C:1454:THR:OG1	1:C:1456:ASP:OD1	2.24	0.50
1:D:1099:GLU:OE2	1:D:1125:ASN:ND2	2.36	0.50
1:D:1927:LEU:HD13	1:D:2101:MET:HG3	1.93	0.50
1:D:3068:LEU:HD23	1:D:3139:VAL:HG21	1.93	0.50
1:A:932:LEU:HB3	1:A:937:CYS:HB3	1.94	0.50
1:A:3352:GLU:O	1:A:3356:SER:OG	2.29	0.50
1:B:3051:ARG:HA	1:B:3131:TYR:CZ	2.47	0.50
1:C:932:LEU:HB3	1:C:937:CYS:HB3	1.94	0.50
1:C:939:VAL:HB	1:C:1051:TYR:HB3	1.93	0.50
1:D:451:TYR:O	1:D:474:ARG:NH1	2.44	0.50
1:D:3352:GLU:O	1:D:3356:SER:OG	2.29	0.50
1:A:3068:LEU:HD23	1:A:3139:VAL:HG21	1.93	0.50
1:A:3767:GLN:OE1	1:A:3809:ASN:ND2	2.41	0.50
1:C:131:LEU:HD13	1:C:195:PHE:HE2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:ARG:NH2	1:C:255:HIS:O	2.40	0.50
1:C:2614:ILE:O	1:C:2650:ARG:NH2	2.45	0.50
1:C:2749:GLU:HG3	1:C:2752:ASP:HB2	1.94	0.50
1:C:3068:LEU:HD23	1:C:3139:VAL:HG21	1.93	0.50
2:E:7:ILE:HD11	2:E:73:LYS:HB2	1.93	0.50
1:C:1099:GLU:OE2	1:C:1125:ASN:ND2	2.36	0.50
1:C:3359:ILE:HD13	1:C:3362:ILE:HD11	1.93	0.50
1:D:932:LEU:HB3	1:D:937:CYS:HB3	1.94	0.50
1:C:3767:GLN:OE1	1:C:3809:ASN:ND2	2.41	0.50
1:D:3051:ARG:HA	1:D:3131:TYR:CZ	2.47	0.50
1:A:3051:ARG:HA	1:A:3131:TYR:CZ	2.47	0.50
1:C:3051:ARG:HA	1:C:3131:TYR:CZ	2.47	0.50
1:C:3089:LYS:HE2	1:C:3093:ARG:HH21	1.76	0.50
1:D:1674:CYS:HG	1:D:1717:SER:HG	1.59	0.50
1:A:870:ILE:HG13	1:A:874:LEU:HD23	1.94	0.49
1:A:1099:GLU:OE2	1:A:1125:ASN:ND2	2.36	0.49
1:B:1099:GLU:OE2	1:B:1125:ASN:ND2	2.36	0.49
1:B:2267:MET:O	1:B:2330:ARG:NH1	2.41	0.49
1:C:150:MET:HB2	1:C:169:LEU:HD12	1.93	0.49
1:A:3062:PRO:HA	1:A:3065:VAL:HG12	1.93	0.49
1:A:4917:ASP:HB2	1:D:4888:TYR:HE1	1.78	0.49
1:B:3840:SER:OG	1:B:3877:ASP:OD1	2.29	0.49
1:D:786:GLY:N	1:D:1630:CYS:O	2.46	0.49
1:D:1064:GLU:O	1:D:1071:ARG:NH2	2.46	0.49
1:D:3359:ILE:HD13	1:D:3362:ILE:HD11	1.93	0.49
1:A:116:MET:HB2	1:A:137:LEU:HD13	1.94	0.49
1:A:3089:LYS:HE2	1:A:3093:ARG:HH21	1.76	0.49
1:D:2614:ILE:O	1:D:2650:ARG:NH2	2.45	0.49
2:H:7:ILE:HD11	2:H:73:LYS:HB2	1.93	0.49
1:A:2736:ASP:OD1	1:A:2736:ASP:N	2.46	0.49
1:B:426:ARG:N	1:B:505:GLU:O	2.45	0.49
1:B:870:ILE:HG13	1:B:874:LEU:HD23	1.94	0.49
1:B:1927:LEU:HD13	1:B:2101:MET:HG3	1.93	0.49
1:B:3523:ASN:O	1:B:3582:ARG:NH2	2.45	0.49
1:C:870:ILE:HG13	1:C:874:LEU:HD23	1.94	0.49
1:D:2749:GLU:HG3	1:D:2752:ASP:HB2	1.94	0.49
1:B:131:LEU:HD13	1:B:195:PHE:HE2	1.76	0.49
1:B:134:ASP:OD1	1:B:134:ASP:N	2.46	0.49
1:C:1927:LEU:HD13	1:C:2101:MET:HG3	1.93	0.49
1:D:111:HIS:ND1	1:D:114:SER:OG	2.37	0.49
1:A:2267:MET:O	1:A:2330:ARG:NH1	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1064:GLU:O	1:B:1071:ARG:NH2	2.46	0.49
1:B:3062:PRO:HA	1:B:3065:VAL:HG12	1.93	0.49
1:C:116:MET:HB2	1:C:137:LEU:HD13	1.94	0.49
1:C:277:GLY:N	1:C:316:PHE:O	2.39	0.49
1:A:111:HIS:ND1	1:A:114:SER:OG	2.37	0.49
1:A:1064:GLU:O	1:A:1071:ARG:NH2	2.46	0.49
1:A:2309:SER:OG	1:A:2321:ILE:O	2.30	0.49
1:B:818:ARG:NH2	1:B:1025:ARG:O	2.46	0.49
1:C:3523:ASN:O	1:C:3582:ARG:NH2	2.45	0.49
1:D:2437:ALA:O	1:D:2508:ARG:NH2	2.46	0.49
1:C:2002:PRO:HB3	1:C:3641:LEU:HD13	1.95	0.49
1:C:2437:ALA:O	1:C:2508:ARG:NH2	2.46	0.49
1:D:1561:VAL:HG12	1:D:1562:ILE:HG23	1.95	0.49
1:A:1653:LEU:HD23	1:A:1660:GLN:HA	1.95	0.49
1:A:3523:ASN:O	1:A:3582:ARG:NH2	2.45	0.49
1:A:4247:ILE:HD11	1:A:4667:PRO:HB2	1.95	0.49
1:B:2749:GLU:HG3	1:B:2752:ASP:HB2	1.94	0.49
1:A:1422:ASP:OD2	1:A:1568:LYS:NZ	2.36	0.49
1:B:266:ARG:NH2	1:B:331:VAL:O	2.39	0.49
1:B:2369[A]:ARG:NH2	1:B:2372:GLY:O	2.39	0.49
1:C:1064:GLU:O	1:C:1071:ARG:NH2	2.46	0.49
1:C:1422:ASP:OD2	1:C:1568:LYS:NZ	2.36	0.49
1:C:1561:VAL:HG12	1:C:1562:ILE:HG23	1.95	0.49
1:C:2309:SER:OG	1:C:2321:ILE:O	2.30	0.49
1:C:3380:ARG:HH22	1:C:3448:SER:HA	1.78	0.49
1:D:3089:LYS:HE2	1:D:3093:ARG:HH21	1.76	0.49
1:D:4913:ARG:NH2	1:D:4917:ASP:OD2	2.44	0.49
1:A:1561:VAL:HG12	1:A:1562:ILE:HG23	1.95	0.48
1:A:2002:PRO:HB3	1:A:3641:LEU:HD13	1.95	0.48
1:B:116:MET:HB2	1:B:137:LEU:HD13	1.94	0.48
1:C:38:ALA:HB1	1:C:64:ILE:HG13	1.95	0.48
1:D:221:ARG:NH2	1:D:255:HIS:O	2.40	0.48
1:D:289:ARG:HB3	1:D:301:VAL:HB	1.95	0.48
1:D:2736:ASP:OD1	1:D:2736:ASP:N	2.46	0.48
1:A:2437:ALA:O	1:A:2508:ARG:NH2	2.46	0.48
1:C:818:ARG:NH2	1:C:1025:ARG:O	2.46	0.48
1:C:875:ALA:O	1:C:879:HIS:ND1	2.47	0.48
1:D:38:ALA:HB1	1:D:64:ILE:HG13	1.95	0.48
1:D:870:ILE:HG13	1:D:874:LEU:HD23	1.94	0.48
1:D:2309:SER:OG	1:D:2321:ILE:O	2.30	0.48
1:D:3767:GLN:OE1	1:D:3809:ASN:ND2	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:875:ALA:O	1:B:879:HIS:ND1	2.46	0.48
1:C:289:ARG:HB3	1:C:301:VAL:HB	1.95	0.48
1:D:3380:ARG:HH22	1:D:3448:SER:HA	1.78	0.48
1:D:3523:ASN:O	1:D:3582:ARG:NH2	2.45	0.48
2:H:4:ILE:HG22	2:H:74:LEU:HG	1.96	0.48
1:A:38:ALA:HB1	1:A:64:ILE:HG13	1.95	0.48
1:A:637:LEU:HD12	1:A:1692:ALA:HB1	1.96	0.48
1:B:2437:ALA:O	1:B:2508:ARG:NH2	2.46	0.48
1:B:4247:ILE:HD11	1:B:4667:PRO:HB2	1.95	0.48
1:C:786:GLY:N	1:C:1630:CYS:O	2.46	0.48
1:C:1733:GLU:OE2	1:C:2163:ARG:NH2	2.46	0.48
1:A:2971:GLN:HA	1:A:2974:ILE:HG12	1.95	0.48
1:B:637:LEU:HD12	1:B:1692:ALA:HB1	1.96	0.48
1:B:1698:LEU:HD21	1:B:1715:LEU:HD13	1.95	0.48
1:D:1808:ARG:NH1	1:D:1853:ILE:O	2.43	0.48
2:E:4:ILE:HG22	2:E:74:LEU:HG	1.96	0.48
1:A:1698:LEU:HD21	1:A:1715:LEU:HD13	1.96	0.48
1:A:2749:GLU:HG3	1:A:2752:ASP:HB2	1.94	0.48
1:B:1561:VAL:HG12	1:B:1562:ILE:HG23	1.95	0.48
1:B:2627:VAL:HG22	1:B:2678:LEU:HG	1.96	0.48
1:B:2971:GLN:HA	1:B:2974:ILE:HG12	1.95	0.48
1:C:2627:VAL:HG22	1:C:2678:LEU:HG	1.96	0.48
1:C:4247:ILE:HD11	1:C:4667:PRO:HB2	1.95	0.48
1:D:134:ASP:OD1	1:D:134:ASP:N	2.46	0.48
1:D:875:ALA:O	1:D:879:HIS:ND1	2.47	0.48
1:D:2002:PRO:HB3	1:D:3641:LEU:HD13	1.95	0.48
1:D:2971:GLN:HA	1:D:2974:ILE:HG12	1.95	0.48
2:F:4:ILE:HG22	2:F:74:LEU:HG	1.96	0.48
2:G:4:ILE:HG22	2:G:74:LEU:HG	1.96	0.48
1:A:875:ALA:O	1:A:879:HIS:ND1	2.46	0.48
1:B:289:ARG:HB3	1:B:301:VAL:HB	1.95	0.48
1:B:1947:CYS:SG	1:B:2127:GLN:NE2	2.75	0.48
1:B:3380:ARG:HH22	1:B:3448:SER:HA	1.78	0.48
1:D:2627:VAL:HG22	1:D:2678:LEU:HG	1.96	0.48
1:A:3380:ARG:HH22	1:A:3448:SER:HA	1.78	0.48
1:B:221:ARG:NH2	1:B:255:HIS:O	2.40	0.48
1:C:1653:LEU:HD23	1:C:1660:GLN:HA	1.95	0.48
1:C:2971:GLN:HA	1:C:2974:ILE:HG12	1.95	0.48
1:C:3352:GLU:O	1:C:3356:SER:OG	2.29	0.48
1:C:3443:ILE:HG12	1:C:3605:HIS:HD2	1.79	0.48
1:D:818:ARG:NH2	1:D:1025:ARG:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1653:LEU:HD23	1:D:1660:GLN:HA	1.95	0.48
1:A:289:ARG:HB3	1:A:301:VAL:HB	1.95	0.48
1:A:1733:GLU:OE2	1:A:2163:ARG:NH2	2.46	0.48
1:A:2614:ILE:O	1:A:2650:ARG:NH2	2.45	0.48
1:B:38:ALA:HB1	1:B:64:ILE:HG13	1.95	0.48
1:B:1674:CYS:HG	1:B:1717:SER:HG	1.58	0.48
1:C:1658:ASP:OD1	1:C:1658:ASP:N	2.47	0.48
1:D:1733:GLU:OE2	1:D:2163:ARG:NH2	2.46	0.48
1:D:1996:ARG:HA	1:D:1999:ARG:HG2	1.96	0.48
1:D:3037:GLU:HG2	1:D:3085:PRO:HD2	1.96	0.48
1:A:648:ILE:HG23	1:A:814:ALA:HB3	1.96	0.48
1:B:1808:ARG:NH1	1:B:1853:ILE:O	2.43	0.48
1:D:116:MET:HB2	1:D:137:LEU:HD13	1.94	0.48
1:D:3443:ILE:HG12	1:D:3605:HIS:HD2	1.79	0.48
1:D:5011:TRP:HD1	1:D:5011:TRP:HA	1.66	0.48
1:A:818:ARG:NH2	1:A:1025:ARG:O	2.46	0.47
1:A:2627:VAL:HG22	1:A:2678:LEU:HG	1.96	0.47
1:B:3233:PRO:HG2	1:B:3239:MET:HA	1.96	0.47
1:C:637:LEU:HD12	1:C:1692:ALA:HB1	1.96	0.47
1:C:3037:GLU:HG2	1:C:3085:PRO:HD2	1.96	0.47
1:C:3840:SER:OG	1:C:3877:ASP:OD1	2.29	0.47
1:D:648:ILE:HG23	1:D:814:ALA:HB3	1.96	0.47
1:D:4247:ILE:HD11	1:D:4667:PRO:HB2	1.95	0.47
1:B:648:ILE:HG23	1:B:814:ALA:HB3	1.96	0.47
1:B:3051:ARG:O	1:B:3053:ARG:NE	2.33	0.47
1:D:4190:ILE:H	1:D:4190:ILE:HG12	1.49	0.47
1:A:816:LEU:HD23	1:A:818:ARG:H	1.79	0.47
1:A:3037:GLU:HG2	1:A:3085:PRO:HD2	1.96	0.47
1:A:3277:LEU:HD23	1:A:3315:LEU:HD13	1.96	0.47
1:B:1232:ARG:NH2	1:B:1828:ASP:O	2.41	0.47
1:B:3277:LEU:HD23	1:B:3315:LEU:HD13	1.96	0.47
1:B:1733:GLU:OE2	1:B:2163:ARG:NH2	2.46	0.47
1:B:2512:ILE:HG21	1:B:2518:LEU:HD13	1.96	0.47
1:B:3159:ASP:OD1	1:B:3159:ASP:N	2.45	0.47
1:C:1698:LEU:HD21	1:C:1715:LEU:HD13	1.95	0.47
1:A:4892:ARG:NH1	1:B:4895:GLY:O	2.45	0.47
1:C:2248:ARG:HG2	1:C:2286:LEU:HD21	1.97	0.47
1:C:2512:ILE:HG21	1:C:2518:LEU:HD13	1.96	0.47
1:A:2792:ARG:HB2	1:A:2797:PHE:HD1	1.80	0.47
1:C:4913:ARG:NH2	1:C:4917:ASP:OD2	2.44	0.47
1:D:133:PHE:O	1:D:193:ALA:N	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2248:ARG:HG2	1:D:2286:LEU:HD21	1.97	0.47
1:A:1996:ARG:HA	1:A:1999:ARG:HG2	1.96	0.47
1:A:4112:LEU:O	1:A:4115:SER:OG	2.32	0.47
1:B:133:PHE:O	1:B:193:ALA:N	2.40	0.47
1:B:1653:LEU:HD23	1:B:1660:GLN:HA	1.95	0.47
1:B:1996:ARG:HA	1:B:1999:ARG:HG2	1.96	0.47
1:B:2002:PRO:HB3	1:B:3641:LEU:HD13	1.95	0.47
1:B:2248:ARG:HG2	1:B:2286:LEU:HD21	1.97	0.47
1:B:2309:SER:OG	1:B:2321:ILE:O	2.30	0.47
1:B:2614:ILE:O	1:B:2650:ARG:NH2	2.45	0.47
1:B:3443:ILE:HG12	1:B:3605:HIS:HD2	1.79	0.47
1:C:134:ASP:N	1:C:134:ASP:OD1	2.46	0.47
1:C:426:ARG:N	1:C:505:GLU:O	2.45	0.47
1:C:682:LEU:HD13	1:C:787:VAL:HG11	1.97	0.47
1:C:816:LEU:HD23	1:C:818:ARG:H	1.80	0.47
1:C:1996:ARG:HA	1:C:1999:ARG:HG2	1.96	0.47
1:C:3233:PRO:HG2	1:C:3239:MET:HA	1.96	0.47
1:C:3277:LEU:HD23	1:C:3315:LEU:HD13	1.96	0.47
1:C:4948:GLU:HA	1:C:4951:LYS:HE3	1.97	0.47
1:D:816:LEU:HD23	1:D:818:ARG:H	1.80	0.47
1:D:2719:TYR:HB3	1:D:2948:THR:HG21	1.97	0.47
1:A:1577:ALA:HB1	1:A:1584:ARG:HD3	1.97	0.47
1:A:2512:ILE:HG21	1:A:2518:LEU:HD13	1.96	0.47
1:C:648:ILE:HG23	1:C:814:ALA:HB3	1.96	0.47
1:C:1577:ALA:HB1	1:C:1584:ARG:HD3	1.97	0.47
1:D:682:LEU:HD13	1:D:787:VAL:HG11	1.97	0.47
2:H:21:THR:N	2:H:107:GLU:OE2	2.48	0.47
1:A:1674:CYS:SG	1:A:1717:SER:OG	2.73	0.47
1:A:2248:ARG:HG2	1:A:2286:LEU:HD21	1.97	0.47
1:B:3037:GLU:HG2	1:B:3085:PRO:HD2	1.96	0.47
1:C:2095:GLN:HG3	1:C:2127:GLN:HB3	1.97	0.47
1:D:637:LEU:HD12	1:D:1692:ALA:HB1	1.96	0.47
1:D:2531:ARG:NH1	1:D:2585:THR:OG1	2.48	0.47
1:A:868:GLU:HA	1:A:871:ARG:HB2	1.97	0.47
1:A:2531:ARG:NH1	1:A:2585:THR:OG1	2.48	0.47
1:B:111:HIS:ND1	1:B:114:SER:OG	2.37	0.47
1:C:499:THR:HG23	1:C:502:HIS:H	1.80	0.47
1:C:715:GLY:O	1:C:722:TRP:N	2.48	0.47
1:C:1782:PHE:O	2:G:82:TYR:OH	2.28	0.47
1:C:4867:GLU:H	1:C:4867:GLU:HG2	1.50	0.47
1:D:1577:ALA:HB1	1:D:1584:ARG:HD3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2512:ILE:HG21	1:D:2518:LEU:HD13	1.96	0.47
1:D:3233:PRO:HG2	1:D:3239:MET:HA	1.96	0.47
1:D:4948:GLU:HA	1:D:4951:LYS:HE3	1.97	0.47
2:E:23:VAL:HG22	2:E:47:LYS:HG2	1.97	0.47
1:A:1640:HIS:HA	1:A:1647:CYS:HA	1.97	0.46
1:A:2095:GLN:HG3	1:A:2127:GLN:HB3	1.97	0.46
1:A:3443:ILE:HG12	1:A:3605:HIS:HD2	1.79	0.46
1:B:1658:ASP:OD1	1:B:1658:ASP:N	2.47	0.46
1:B:2531:ARG:NH1	1:B:2585:THR:OG1	2.48	0.46
1:B:2792:ARG:HB2	1:B:2797:PHE:HD1	1.80	0.46
1:D:499:THR:HG23	1:D:502:HIS:H	1.80	0.46
1:D:868:GLU:HA	1:D:871:ARG:HB2	1.98	0.46
1:A:786:GLY:N	1:A:1630:CYS:O	2.46	0.46
1:A:1784:ALA:O	2:E:82:TYR:OH	2.25	0.46
1:A:4948:GLU:HA	1:A:4951:LYS:HE3	1.97	0.46
1:B:786:GLY:N	1:B:1630:CYS:O	2.46	0.46
1:B:1577:ALA:HB1	1:B:1584:ARG:HD3	1.97	0.46
1:B:2719:TYR:HB3	1:B:2948:THR:HG21	1.97	0.46
1:B:3075:LEU:O	1:B:3146:HIS:NE2	2.46	0.46
1:B:3781:GLN:NE2	1:B:3819:TYR:OH	2.41	0.46
1:C:1780:PRO:HD3	1:C:1801:ALA:H	1.81	0.46
1:C:2739:PRO:HB3	1:C:2888:ARG:HH11	1.81	0.46
1:C:4643:LEU:O	1:C:4647:SER:HB3	2.15	0.46
1:D:1698:LEU:HD21	1:D:1715:LEU:HD13	1.96	0.46
1:D:2739:PRO:HB3	1:D:2888:ARG:HH11	1.81	0.46
2:F:21:THR:N	2:F:107:GLU:OE2	2.48	0.46
2:H:23:VAL:HG22	2:H:47:LYS:HG2	1.97	0.46
1:A:262:LEU:HD13	1:A:274:LEU:HD11	1.97	0.46
1:A:4643:LEU:O	1:A:4647:SER:HB3	2.15	0.46
1:B:499:THR:HG23	1:B:502:HIS:H	1.81	0.46
1:B:3103:ILE:HD11	1:B:3172:ILE:HB	1.98	0.46
1:A:2479:LEU:HB2	1:A:2541:PHE:HZ	1.81	0.46
1:A:2591:ARG:HG2	1:A:2636:PHE:HB3	1.98	0.46
1:B:1640:HIS:HA	1:B:1647:CYS:HA	1.97	0.46
1:C:829:TYR:HB3	1:C:1073:ARG:HH11	1.81	0.46
1:C:2461:VAL:O	1:C:2510:TYR:OH	2.30	0.46
1:C:2719:TYR:HB3	1:C:2948:THR:HG21	1.97	0.46
2:G:23:VAL:HG22	2:G:47:LYS:HG2	1.97	0.46
1:A:2470:ILE:HG22	1:A:2525:GLY:HA3	1.97	0.46
1:A:3233:PRO:HG2	1:A:3239:MET:HA	1.96	0.46
1:B:2739:PRO:HB3	1:B:2888:ARG:HH11	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4643:LEU:O	1:B:4647:SER:HB3	2.15	0.46
1:C:2792:ARG:HB2	1:C:2797:PHE:HD1	1.80	0.46
1:D:1423:ASP:HB2	1:D:1426:ILE:HG22	1.98	0.46
1:D:2479:LEU:HB2	1:D:2541:PHE:HZ	1.81	0.46
1:D:2591:ARG:HG2	1:D:2636:PHE:HB3	1.98	0.46
1:D:3103:ILE:HD11	1:D:3172:ILE:HB	1.98	0.46
1:D:3862:ASP:OD1	1:D:3862:ASP:N	2.45	0.46
2:E:21:THR:N	2:E:107:GLU:OE2	2.48	0.46
2:F:23:VAL:HG22	2:F:47:LYS:HG2	1.97	0.46
1:A:4188:ARG:HA	1:A:4188:ARG:HD2	1.58	0.46
1:B:715:GLY:O	1:B:722:TRP:N	2.48	0.46
1:B:3981:ALA:HB2	1:B:4040:ILE:HG12	1.97	0.46
1:B:4675:LYS:HG3	1:B:4679:ARG:HE	1.81	0.46
1:C:1291:LEU:HD13	1:C:1595:LEU:HD21	1.98	0.46
1:C:2025:GLU:OE2	1:C:2028:ARG:NH1	2.49	0.46
1:C:2531:ARG:NH1	1:C:2585:THR:OG1	2.48	0.46
1:C:3075:LEU:O	1:C:3146:HIS:NE2	2.46	0.46
1:D:1640:HIS:HA	1:D:1647:CYS:HA	1.97	0.46
1:A:134:ASP:OD1	1:A:134:ASP:N	2.46	0.46
1:A:4179:GLY:O	1:A:4194:TYR:HA	2.16	0.46
1:B:148:TRP:CZ3	1:B:180:LEU:HB2	2.51	0.46
1:B:682:LEU:HD13	1:B:787:VAL:HG11	1.97	0.46
1:B:884:LEU:HB2	1:B:969:PRO:HD3	1.98	0.46
1:B:1780:PRO:HD3	1:B:1801:ALA:H	1.81	0.46
1:B:2461:VAL:O	1:B:2510:TYR:OH	2.30	0.46
1:B:2470:ILE:HG22	1:B:2525:GLY:HA3	1.97	0.46
1:C:426:ARG:NH1	1:C:429:GLY:O	2.41	0.46
1:C:1640:HIS:HA	1:C:1647:CYS:HA	1.97	0.46
1:C:2470:ILE:HG22	1:C:2525:GLY:HA3	1.97	0.46
1:C:2538:THR:HG23	1:C:2540:THR:H	1.81	0.46
1:C:3218:VAL:O	1:C:3222:LYS:HB2	2.16	0.46
1:D:416:LYS:HB3	1:D:416:LYS:HE2	1.76	0.46
1:D:715:GLY:O	1:D:722:TRP:N	2.48	0.46
1:D:2470:ILE:HG22	1:D:2525:GLY:HA3	1.97	0.46
1:D:2792:ARG:HB2	1:D:2797:PHE:HD1	1.80	0.46
1:D:3579:LEU:HB2	1:D:3582:ARG:HG2	1.98	0.46
1:D:4643:LEU:O	1:D:4647:SER:HB3	2.15	0.46
1:A:4930:ALA:HB2	1:D:4933:GLN:HG2	1.97	0.46
1:B:816:LEU:HD23	1:B:818:ARG:H	1.80	0.46
1:B:2025:GLU:OE2	1:B:2028:ARG:NH1	2.49	0.46
1:B:2670:GLU:HG3	1:B:2674:LEU:HD13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4179:GLY:O	1:B:4194:TYR:HA	2.16	0.46
1:C:868:GLU:HA	1:C:871:ARG:HB2	1.98	0.46
1:C:3579:LEU:HB2	1:C:3582:ARG:HG2	1.98	0.46
1:D:2025:GLU:OE2	1:D:2028:ARG:NH1	2.49	0.46
1:D:2538:THR:HG23	1:D:2540:THR:H	1.81	0.46
1:A:2025:GLU:OE2	1:A:2028:ARG:NH1	2.49	0.46
1:A:2719:TYR:HB3	1:A:2948:THR:HG21	1.97	0.46
1:A:3579:LEU:HB2	1:A:3582:ARG:HG2	1.98	0.46
1:B:3536:ALA:HA	1:B:3539:ARG:HG2	1.98	0.46
1:C:262:LEU:HD13	1:C:274:LEU:HD11	1.97	0.46
1:C:3233:PRO:HD2	1:C:3239:MET:HG2	1.98	0.46
1:C:4675:LYS:HG3	1:C:4679:ARG:HE	1.81	0.46
1:D:266:ARG:NH2	1:D:331:VAL:O	2.39	0.46
1:D:3218:VAL:O	1:D:3222:LYS:HB2	2.16	0.46
1:A:426:ARG:N	1:A:505:GLU:O	2.45	0.46
1:A:1291:LEU:HD13	1:A:1595:LEU:HD21	1.98	0.46
1:A:3218:VAL:O	1:A:3222:LYS:HB2	2.16	0.46
1:A:4675:LYS:HG3	1:A:4679:ARG:HE	1.81	0.46
1:B:868:GLU:HA	1:B:871:ARG:HB2	1.98	0.46
1:B:2479:LEU:HB2	1:B:2541:PHE:HZ	1.81	0.46
1:C:548:VAL:HA	1:C:551:LEU:HG	1.98	0.46
1:C:1232:ARG:NH2	1:C:1828:ASP:O	2.41	0.46
1:C:3981:ALA:HB2	1:C:4040:ILE:HG12	1.97	0.46
1:C:4188:ARG:HD2	1:C:4188:ARG:HA	1.58	0.46
1:D:548:VAL:HA	1:D:551:LEU:HG	1.98	0.46
1:D:829:TYR:HB3	1:D:1073:ARG:HH11	1.81	0.46
1:A:1780:PRO:HD3	1:A:1801:ALA:H	1.81	0.45
1:A:3536:ALA:HA	1:A:3539:ARG:HG2	1.98	0.45
1:A:3981:ALA:HB2	1:A:4040:ILE:HG12	1.97	0.45
1:B:4948:GLU:HA	1:B:4951:LYS:HE3	1.97	0.45
1:C:253:CYS:O	1:C:258:SER:OG	2.34	0.45
1:C:2479:LEU:HB2	1:C:2541:PHE:HZ	1.81	0.45
1:C:3731:LYS:HA	1:C:3731:LYS:HD3	1.76	0.45
1:D:426:ARG:N	1:D:505:GLU:O	2.45	0.45
1:D:4179:GLY:O	1:D:4194:TYR:HA	2.16	0.45
1:D:4648:LEU:HD12	1:D:4803:HIS:HE1	1.81	0.45
1:D:4971:THR:HG22	1:D:4972:PRO:HD2	1.98	0.45
1:A:2680:TRP:O	1:A:2684:ASP:HB2	2.17	0.45
1:A:4971:THR:HG22	1:A:4972:PRO:HD2	1.98	0.45
1:B:2591:ARG:HG2	1:B:2636:PHE:HB3	1.98	0.45
1:C:107:ILE:N	1:C:148:TRP:O	2.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2095:GLN:HG3	1:D:2127:GLN:HB3	1.97	0.45
1:D:3277:LEU:HD23	1:D:3315:LEU:HD13	1.96	0.45
1:D:4675:LYS:HG3	1:D:4679:ARG:HE	1.81	0.45
1:A:499:THR:HG23	1:A:502:HIS:H	1.80	0.45
1:A:682:LEU:HD13	1:A:787:VAL:HG11	1.97	0.45
1:A:4648:LEU:HD12	1:A:4803:HIS:HE1	1.81	0.45
1:B:1422:ASP:OD2	1:B:1568:LYS:NZ	2.35	0.45
1:B:2095:GLN:HG3	1:B:2127:GLN:HB3	1.97	0.45
1:B:3233:PRO:HD2	1:B:3239:MET:HG2	1.98	0.45
1:B:3579:LEU:HB2	1:B:3582:ARG:HG2	1.98	0.45
1:B:5011:TRP:HD1	1:B:5011:TRP:HA	1.66	0.45
1:C:2670:GLU:HG3	1:C:2674:LEU:HD13	1.98	0.45
1:D:2670:GLU:HG3	1:D:2674:LEU:HD13	1.98	0.45
1:D:3981:ALA:HB2	1:D:4040:ILE:HG12	1.97	0.45
1:A:148:TRP:CZ3	1:A:180:LEU:HB2	2.51	0.45
1:A:884:LEU:HB2	1:A:969:PRO:HD3	1.98	0.45
1:A:2769:ASP:HA	1:A:2772:GLN:HB2	1.98	0.45
1:B:546:TRP:CE2	1:B:550:LYS:HE2	2.52	0.45
1:B:829:TYR:HB3	1:B:1073:ARG:HH11	1.81	0.45
1:B:1423:ASP:HB2	1:B:1426:ILE:HG22	1.97	0.45
1:B:2680:TRP:O	1:B:2684:ASP:HB2	2.17	0.45
1:B:4648:LEU:HD12	1:B:4803:HIS:HE1	1.81	0.45
1:C:266:ARG:NH2	1:C:331:VAL:O	2.39	0.45
1:C:1434:TYR:HA	1:C:1518:CYS:O	2.17	0.45
1:C:3051:ARG:O	1:C:3053:ARG:NE	2.33	0.45
1:C:3719:ASP:HB2	1:C:3722:TYR:HB3	1.98	0.45
1:C:4179:GLY:O	1:C:4194:TYR:HA	2.16	0.45
1:D:148:TRP:CZ3	1:D:180:LEU:HB2	2.51	0.45
1:D:1992:ALA:HA	1:D:1995:THR:HG22	1.98	0.45
1:D:4984:ASN:HB3	1:D:4987:ASN:HB2	1.99	0.45
1:A:831:ARG:HG3	1:A:840:VAL:HG21	1.99	0.45
1:A:2670:GLU:HG3	1:A:2674:LEU:HD13	1.98	0.45
1:B:2538:THR:HG23	1:B:2540:THR:H	1.81	0.45
1:C:831:ARG:HG3	1:C:840:VAL:HG21	1.99	0.45
1:C:1000:ARG:HA	1:C:1000:ARG:HD3	1.80	0.45
1:C:2591:ARG:HG2	1:C:2636:PHE:HB3	1.98	0.45
1:C:3536:ALA:HA	1:C:3539:ARG:HG2	1.98	0.45
1:D:1434:TYR:HA	1:D:1518:CYS:O	2.17	0.45
1:D:2916:LYS:HD3	1:D:2920:ARG:HH21	1.82	0.45
1:D:4036:VAL:HG12	1:D:4153:HIS:HA	1.99	0.45
1:A:2916:LYS:HD3	1:A:2920:ARG:HH21	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3233:PRO:HD2	1:A:3239:MET:HG2	1.98	0.45
1:A:4190:ILE:H	1:A:4190:ILE:HG12	1.49	0.45
1:B:4112:LEU:O	1:B:4115:SER:OG	2.32	0.45
1:B:4984:ASN:HB3	1:B:4987:ASN:HB2	1.99	0.45
1:C:884:LEU:HB2	1:C:969:PRO:HD3	1.98	0.45
1:C:1423:ASP:HB2	1:C:1426:ILE:HG22	1.98	0.45
1:C:1992:ALA:HA	1:C:1995:THR:HG22	1.98	0.45
1:D:546:TRP:CE2	1:D:550:LYS:HE2	2.52	0.45
1:D:831:ARG:HG3	1:D:840:VAL:HG21	1.99	0.45
1:D:1291:LEU:HD13	1:D:1595:LEU:HD21	1.98	0.45
2:G:21:THR:N	2:G:107:GLU:OE2	2.48	0.45
1:A:133:PHE:O	1:A:193:ALA:N	2.40	0.45
1:A:3352:GLU:HA	1:A:3355:HIS:HE1	1.82	0.45
1:A:4957:LYS:HB2	1:A:4957:LYS:HE2	1.64	0.45
1:B:1291:LEU:HD13	1:B:1595:LEU:HD21	1.98	0.45
1:B:4828:SER:O	1:B:4832:HIS:HB2	2.17	0.45
1:C:148:TRP:CZ3	1:C:180:LEU:HB2	2.51	0.45
1:C:546:TRP:CE2	1:C:550:LYS:HE2	2.52	0.45
1:C:3103:ILE:HD11	1:C:3172:ILE:HB	1.98	0.45
1:D:145:ALA:HA	1:D:175:SER:HB3	1.99	0.45
1:D:1036:ARG:O	1:D:1040:CYS:HB2	2.17	0.45
1:D:3536:ALA:HA	1:D:3539:ARG:HG2	1.98	0.45
1:D:3759:GLU:OE1	1:D:3762:ARG:NH2	2.50	0.45
1:A:253:CYS:O	1:A:258:SER:OG	2.34	0.45
1:A:266:ARG:NH2	1:A:331:VAL:O	2.39	0.45
1:A:2739:PRO:HB3	1:A:2888:ARG:HH11	1.81	0.45
1:A:3103:ILE:HD11	1:A:3172:ILE:HB	1.98	0.45
1:A:4984:ASN:HB3	1:A:4987:ASN:HB2	1.99	0.45
1:B:726:VAL:HB	1:B:728:ARG:HH21	1.82	0.45
1:B:4971:THR:HG22	1:B:4972:PRO:HD2	1.98	0.45
1:C:133:PHE:O	1:C:193:ALA:N	2.40	0.45
1:C:1036:ARG:O	1:C:1040:CYS:HB2	2.17	0.45
1:C:4036:VAL:HG12	1:C:4153:HIS:HA	1.99	0.45
1:C:4648:LEU:HD12	1:C:4803:HIS:HE1	1.81	0.45
1:C:4971:THR:HG22	1:C:4972:PRO:HD2	1.98	0.45
1:D:253:CYS:O	1:D:258:SER:OG	2.34	0.45
1:D:2769:ASP:HA	1:D:2772:GLN:HB2	1.99	0.45
1:A:548:VAL:HA	1:A:551:LEU:HG	1.98	0.45
1:A:1423:ASP:HB2	1:A:1426:ILE:HG22	1.98	0.45
1:A:1434:TYR:HA	1:A:1518:CYS:O	2.17	0.45
1:A:1780:PRO:O	2:E:42:ARG:NH1	2.28	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1992:ALA:HA	1:A:1995:THR:HG22	1.98	0.45
1:A:3759:GLU:OE1	1:A:3762:ARG:NH2	2.50	0.45
1:A:4036:VAL:HG12	1:A:4153:HIS:HA	1.99	0.45
1:A:4867:GLU:H	1:A:4867:GLU:HG2	1.50	0.45
1:B:831:ARG:HG3	1:B:840:VAL:HG21	1.99	0.45
1:B:1992:ALA:HA	1:B:1995:THR:HG22	1.98	0.45
1:B:2736:ASP:OD1	1:B:2736:ASP:N	2.46	0.45
1:B:2916:LYS:HD3	1:B:2920:ARG:HH21	1.82	0.45
1:B:3218:VAL:O	1:B:3222:LYS:HB2	2.16	0.45
1:C:2680:TRP:O	1:C:2684:ASP:HB2	2.17	0.45
1:D:1780:PRO:HD3	1:D:1801:ALA:H	1.81	0.45
1:D:2165:LEU:HD21	1:D:2177:LEU:HD23	1.99	0.45
1:D:3352:GLU:HA	1:D:3355:HIS:HE1	1.82	0.45
1:A:294:THR:HG23	1:A:297:GLN:H	1.82	0.45
1:A:546:TRP:CE2	1:A:550:LYS:HE2	2.52	0.45
1:A:715:GLY:O	1:A:722:TRP:N	2.48	0.45
1:A:829:TYR:HB3	1:A:1073:ARG:HH11	1.81	0.45
1:A:5011:TRP:HD1	1:A:5011:TRP:HA	1.66	0.45
1:B:262:LEU:HD13	1:B:274:LEU:HD11	1.98	0.45
1:B:1036:ARG:O	1:B:1040:CYS:HB2	2.17	0.45
1:B:3051:ARG:CZ	1:B:3098:SER:HB3	2.47	0.45
1:B:4188:ARG:HA	1:B:4188:ARG:HD2	1.58	0.45
1:C:498:THR:HA	1:C:553:ARG:HH22	1.82	0.45
1:C:3352:GLU:HA	1:C:3355:HIS:HE1	1.82	0.45
1:C:4823:LEU:HD23	1:C:4823:LEU:HA	1.84	0.45
1:D:294:THR:HG23	1:D:297:GLN:H	1.82	0.45
1:D:2974:ILE:HD12	1:D:3053:ARG:HH12	1.82	0.45
1:D:4687:TYR:HE2	1:D:4703:ARG:HG2	1.82	0.45
1:A:640:TYR:HD2	1:A:1634:LEU:HB3	1.83	0.44
1:A:1007:TYR:O	1:A:1017:ARG:NH2	2.50	0.44
1:A:3326:ASN:HB3	1:A:3329:ILE:HD13	1.99	0.44
1:B:548:VAL:HA	1:B:551:LEU:HG	1.98	0.44
1:C:726:VAL:HB	1:C:728:ARG:HH21	1.82	0.44
1:C:1568:LYS:HE2	1:C:1574:PRO:HD3	1.99	0.44
1:C:4984:ASN:HB3	1:C:4987:ASN:HB2	1.99	0.44
1:D:3719:ASP:HB2	1:D:3722:TYR:HB3	1.98	0.44
1:D:4828:SER:O	1:D:4832:HIS:HB2	2.17	0.44
1:A:129:ASP:OD1	1:A:129:ASP:N	2.50	0.44
1:A:145:ALA:HA	1:A:175:SER:HB3	1.99	0.44
1:A:2165:LEU:HD21	1:A:2177:LEU:HD23	1.99	0.44
1:A:3051:ARG:CZ	1:A:3098:SER:HB3	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3329:ILE:HD11	1:A:3332:ALA:HB2	1.99	0.44
1:B:3719:ASP:HB2	1:B:3722:TYR:HB3	1.98	0.44
1:C:4828:SER:O	1:C:4832:HIS:HB2	2.17	0.44
1:D:262:LEU:HD13	1:D:274:LEU:HD11	1.98	0.44
1:A:76:ARG:HH12	1:D:3936:TYR:HB2	1.82	0.44
1:A:726:VAL:HB	1:A:728:ARG:HH21	1.82	0.44
1:A:2974:ILE:HD12	1:A:3053:ARG:HH12	1.82	0.44
1:B:145:ALA:HA	1:B:175:SER:HB3	1.99	0.44
1:B:1256:GLU:HB3	1:B:1275:ARG:HD2	2.00	0.44
1:B:3759:GLU:OE1	1:B:3762:ARG:NH2	2.50	0.44
1:C:294:THR:HG23	1:C:297:GLN:H	1.82	0.44
1:C:2916:LYS:HD3	1:C:2920:ARG:HH21	1.82	0.44
1:C:3281:LEU:HD12	1:C:3315:LEU:HD22	1.99	0.44
1:D:726:VAL:HB	1:D:728:ARG:HH21	1.82	0.44
1:D:3233:PRO:HD2	1:D:3239:MET:HG2	1.98	0.44
1:A:877:ASN:HA	1:A:970:LEU:H	1.83	0.44
1:A:1036:ARG:O	1:A:1040:CYS:HB2	2.17	0.44
1:A:2538:THR:HG23	1:A:2540:THR:H	1.81	0.44
1:B:3329:ILE:HD11	1:B:3332:ALA:HB2	1.99	0.44
1:B:4036:VAL:HG12	1:B:4153:HIS:HA	1.99	0.44
1:C:665:GLU:HB2	1:C:792:LEU:HB2	2.00	0.44
1:C:858:THR:OG1	1:C:927:GLU:OE2	2.33	0.44
1:C:936:GLY:HA3	1:C:1056:PRO:HB3	1.99	0.44
1:C:1007:TYR:O	1:C:1017:ARG:NH2	2.50	0.44
1:C:2998:PHE:HA	1:C:3002:LEU:HD13	2.00	0.44
1:C:3051:ARG:CZ	1:C:3098:SER:HB3	2.47	0.44
1:D:102:LEU:HA	1:D:162:LYS:HA	2.00	0.44
1:D:665:GLU:HB2	1:D:792:LEU:HB2	2.00	0.44
1:D:2680:TRP:O	1:D:2684:ASP:HB2	2.17	0.44
1:D:2875:ALA:HB2	1:D:2927:LEU:HD22	2.00	0.44
1:D:3281:LEU:HD12	1:D:3315:LEU:HD22	1.99	0.44
1:A:603:LEU:HA	1:A:606:LEU:HD12	2.00	0.44
1:A:884:LEU:HD13	1:A:968:ALA:H	1.83	0.44
1:A:2875:ALA:HB2	1:A:2927:LEU:HD22	2.00	0.44
1:B:102:LEU:HA	1:B:162:LYS:HA	2.00	0.44
1:B:2769:ASP:HA	1:B:2772:GLN:HB2	1.99	0.44
1:B:2875:ALA:HB2	1:B:2927:LEU:HD22	2.00	0.44
1:B:3284:TRP:HB3	1:B:3305:THR:HG21	2.00	0.44
1:B:3352:GLU:HA	1:B:3355:HIS:HE1	1.82	0.44
1:C:640:TYR:HD2	1:C:1634:LEU:HB3	1.82	0.44
1:C:884:LEU:HD13	1:C:968:ALA:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2875:ALA:HB2	1:C:2927:LEU:HD22	2.00	0.44
1:C:3759:GLU:OE1	1:C:3762:ARG:NH2	2.50	0.44
1:D:884:LEU:HB2	1:D:969:PRO:HD3	1.98	0.44
1:D:2461:VAL:O	1:D:2510:TYR:OH	2.30	0.44
1:D:4867:GLU:H	1:D:4867:GLU:HG2	1.50	0.44
1:A:102:LEU:HA	1:A:162:LYS:HA	2.00	0.44
1:B:640:TYR:HD2	1:B:1634:LEU:HB3	1.82	0.44
1:B:1434:TYR:HA	1:B:1518:CYS:O	2.17	0.44
1:B:5012:LYS:HE3	1:B:5012:LYS:HB3	1.69	0.44
1:C:1842:LEU:HD23	1:C:1842:LEU:HA	1.87	0.44
1:C:3388:GLU:HA	1:C:3391:GLU:HB3	1.99	0.44
1:C:4576:ILE:HG23	1:C:4639:MET:HE3	2.00	0.44
1:D:3051:ARG:CZ	1:D:3098:SER:HB3	2.47	0.44
1:D:3996:PHE:O	1:D:4000:MET:HG2	2.18	0.44
1:A:1256:GLU:HB3	1:A:1275:ARG:HD2	2.00	0.44
1:A:3006:ILE:HD12	1:A:3010:PHE:HE2	1.83	0.44
1:A:3284:TRP:HB3	1:A:3305:THR:HG21	2.00	0.44
1:A:3996:PHE:O	1:A:4000:MET:HG2	2.18	0.44
1:A:4828:SER:O	1:A:4832:HIS:HB2	2.17	0.44
1:B:426:ARG:NH1	1:B:429:GLY:O	2.41	0.44
1:B:498:THR:HA	1:B:553:ARG:HH22	1.82	0.44
1:B:877:ASN:HA	1:B:970:LEU:H	1.83	0.44
1:B:2215:LEU:HD23	1:B:2260:ASN:HB3	2.00	0.44
1:B:3316:LEU:HD11	1:B:3353:LEU:HD11	2.00	0.44
1:B:3366:ARG:NH1	1:B:3440:GLU:OE1	2.47	0.44
1:B:4687:TYR:HE2	1:B:4703:ARG:HG2	1.82	0.44
1:C:129:ASP:OD1	1:C:129:ASP:N	2.50	0.44
1:C:869:ARG:HE	1:C:869:ARG:HB3	1.64	0.44
1:C:1808:ARG:HD3	1:C:1853:ILE:HG22	2.00	0.44
1:C:2215:LEU:HD23	1:C:2260:ASN:HB3	2.00	0.44
1:C:4112:LEU:O	1:C:4115:SER:OG	2.32	0.44
1:D:498:THR:HA	1:D:553:ARG:HH22	1.82	0.44
1:D:603:LEU:HA	1:D:606:LEU:HD12	2.00	0.44
1:A:3719:ASP:HB2	1:A:3722:TYR:HB3	1.98	0.44
1:B:603:LEU:HA	1:B:606:LEU:HD12	2.00	0.44
1:B:884:LEU:HD13	1:B:968:ALA:H	1.83	0.44
1:B:1007:TYR:O	1:B:1017:ARG:NH2	2.50	0.44
1:B:1849:LEU:HD23	1:B:1849:LEU:HA	1.87	0.44
1:B:2165:LEU:HD21	1:B:2177:LEU:HD23	1.99	0.44
1:B:3326:ASN:HB3	1:B:3329:ILE:HD13	1.99	0.44
1:C:3316:LEU:HD11	1:C:3353:LEU:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4687:TYR:HE2	1:C:4703:ARG:HG2	1.82	0.44
1:D:3006:ILE:HD12	1:D:3010:PHE:HE2	1.83	0.44
1:A:244:LEU:HD23	1:A:244:LEU:HA	1.90	0.44
1:A:793:LEU:HB2	1:A:797:HIS:HB2	2.00	0.44
1:B:2998:PHE:HA	1:B:3002:LEU:HD13	2.00	0.44
1:C:877:ASN:HA	1:C:970:LEU:H	1.83	0.44
1:D:129:ASP:N	1:D:129:ASP:OD1	2.50	0.44
1:D:1007:TYR:O	1:D:1017:ARG:NH2	2.49	0.44
1:A:936:GLY:HA3	1:A:1056:PRO:HB3	1.99	0.43
1:A:1808:ARG:NH1	1:A:1853:ILE:O	2.43	0.43
1:A:4687:TYR:HE2	1:A:4703:ARG:HG2	1.82	0.43
1:B:3006:ILE:HD12	1:B:3010:PHE:HE2	1.83	0.43
1:C:2740:VAL:HG21	1:C:2819:TRP:HE1	1.83	0.43
1:D:936:GLY:HA3	1:D:1056:PRO:HB3	1.99	0.43
1:D:2215:LEU:HD23	1:D:2260:ASN:HB3	2.00	0.43
1:D:4244:GLU:HG2	1:D:4668:LEU:HD13	2.01	0.43
1:A:2215:LEU:HD23	1:A:2260:ASN:HB3	2.00	0.43
1:B:766:GLY:HA2	1:B:1475:THR:O	2.18	0.43
1:B:936:GLY:HA3	1:B:1056:PRO:HB3	1.99	0.43
1:B:1568:LYS:HE2	1:B:1574:PRO:HD3	1.99	0.43
1:C:145:ALA:HA	1:C:175:SER:HB3	1.99	0.43
1:C:766:GLY:HA2	1:C:1475:THR:O	2.18	0.43
1:C:1256:GLU:HB3	1:C:1275:ARG:HD2	2.00	0.43
1:C:3366:ARG:NH1	1:C:3440:GLU:OE1	2.47	0.43
1:C:3842:LEU:HB2	1:C:3929:SER:HB2	2.01	0.43
1:C:5011:TRP:HD1	1:C:5011:TRP:HA	1.66	0.43
1:D:3388:GLU:HA	1:D:3391:GLU:HB3	1.99	0.43
1:A:498:THR:HA	1:A:553:ARG:HH22	1.82	0.43
1:B:1221:GLU:HG3	1:B:1223:PHE:HD1	1.83	0.43
1:B:1808:ARG:HD3	1:B:1853:ILE:HG22	2.00	0.43
1:B:4957:LYS:HB2	1:B:4957:LYS:HE2	1.64	0.43
1:C:2165:LEU:HD21	1:C:2177:LEU:HD23	1.99	0.43
1:C:4190:ILE:H	1:C:4190:ILE:HG12	1.49	0.43
1:D:640:TYR:HD2	1:D:1634:LEU:HB3	1.82	0.43
1:D:766:GLY:HA2	1:D:1475:THR:O	2.18	0.43
1:D:1256:GLU:HB3	1:D:1275:ARG:HD2	2.00	0.43
1:D:1568:LYS:HE2	1:D:1574:PRO:HD3	1.99	0.43
1:D:3840:SER:OG	1:D:3877:ASP:OD1	2.29	0.43
1:A:465:GLN:HA	1:A:468:LEU:HB2	2.00	0.43
1:B:4576:ILE:HG23	1:B:4639:MET:HE3	2.00	0.43
1:D:1808:ARG:HD3	1:D:1853:ILE:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2716:ASP:N	1:D:2716:ASP:OD1	2.50	0.43
1:D:3316:LEU:HD11	1:D:3353:LEU:HD11	2.00	0.43
1:A:4576:ILE:HG23	1:A:4639:MET:HE3	2.00	0.43
1:B:294:THR:HG23	1:B:297:GLN:H	1.82	0.43
1:C:102:LEU:HA	1:C:162:LYS:HA	2.00	0.43
1:C:603:LEU:HA	1:C:606:LEU:HD12	2.00	0.43
1:C:2974:ILE:HD12	1:C:3053:ARG:HH12	1.82	0.43
1:C:3006:ILE:HD12	1:C:3010:PHE:HE2	1.83	0.43
1:C:4944:ARG:NE	1:D:4938:ASP:OD1	2.51	0.43
1:D:3844:LEU:HD21	1:D:3933:PHE:HA	2.01	0.43
1:A:766:GLY:HA2	1:A:1475:THR:O	2.18	0.43
1:A:1221:GLU:HG3	1:A:1223:PHE:HD1	1.83	0.43
1:A:1737:PRO:HD3	1:A:1771:LEU:HG	2.00	0.43
1:A:3281:LEU:HD12	1:A:3315:LEU:HD22	1.99	0.43
1:A:3366:ARG:NH1	1:A:3440:GLU:OE1	2.47	0.43
1:B:721:LEU:HD23	1:B:721:LEU:HA	1.90	0.43
1:B:2740:VAL:HG21	1:B:2819:TRP:HE1	1.83	0.43
1:B:2974:ILE:HD12	1:B:3053:ARG:HH12	1.82	0.43
1:B:3388:GLU:HA	1:B:3391:GLU:HB3	1.99	0.43
1:C:1221:GLU:HG3	1:C:1223:PHE:HD1	1.83	0.43
1:C:4244:GLU:HG2	1:C:4668:LEU:HD13	2.01	0.43
1:D:2740:VAL:HG21	1:D:2819:TRP:HE1	1.83	0.43
1:D:3326:ASN:HB3	1:D:3329:ILE:HD13	1.99	0.43
1:D:4112:LEU:O	1:D:4115:SER:OG	2.32	0.43
1:A:400:ALA:HA	1:A:403:MET:HG2	2.01	0.43
1:A:665:GLU:HB2	1:A:792:LEU:HB2	2.00	0.43
1:A:3388:GLU:HA	1:A:3391:GLU:HB3	1.99	0.43
1:B:400:ALA:HA	1:B:403:MET:HG2	2.01	0.43
1:B:4244:GLU:HG2	1:B:4668:LEU:HD13	2.01	0.43
1:C:793:LEU:HB2	1:C:797:HIS:HB2	2.00	0.43
1:C:1225:PRO:HG2	1:C:1228:ILE:HD13	2.01	0.43
1:C:1849:LEU:HD23	1:C:1849:LEU:HA	1.87	0.43
1:C:2769:ASP:HA	1:C:2772:GLN:HB2	1.99	0.43
1:C:3329:ILE:HD11	1:C:3332:ALA:HB2	1.99	0.43
1:C:3996:PHE:O	1:C:4000:MET:HG2	2.18	0.43
1:D:877:ASN:HA	1:D:970:LEU:H	1.83	0.43
1:D:1225:PRO:HG2	1:D:1228:ILE:HD13	2.01	0.43
1:D:1737:PRO:HD3	1:D:1771:LEU:HG	2.01	0.43
1:D:3329:ILE:HD11	1:D:3332:ALA:HB2	1.99	0.43
1:D:3471:THR:O	1:D:3475:LYS:HG3	2.19	0.43
1:A:1225:PRO:HG2	1:A:1228:ILE:HD13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1658:ASP:OD1	1:A:1658:ASP:N	2.47	0.43
1:A:3842:LEU:HB2	1:A:3929:SER:HB2	2.01	0.43
1:B:2354:VAL:O	1:B:2358:ILE:HG12	2.19	0.43
1:B:2765:LYS:HZ3	1:B:2857:PRO:HB2	1.83	0.43
1:B:3211:ASN:HB3	1:B:3236:VAL:HG21	2.01	0.43
1:B:3731:LYS:HA	1:B:3731:LYS:HD3	1.76	0.43
1:B:3842:LEU:HB2	1:B:3929:SER:HB2	2.01	0.43
1:B:3996:PHE:O	1:B:4000:MET:HG2	2.18	0.43
1:C:3037:GLU:HG3	1:C:3088:VAL:HG21	2.01	0.43
1:C:3211:ASN:HB3	1:C:3236:VAL:HG21	2.01	0.43
1:C:3844:LEU:HD21	1:C:3933:PHE:HA	2.01	0.43
1:A:279:PRO:HD3	1:A:327:PRO:HB3	2.01	0.43
1:A:3346:VAL:HG22	1:A:3415:TYR:HB2	2.01	0.43
1:A:3471:THR:O	1:A:3475:LYS:HG3	2.19	0.43
1:B:1225:PRO:HG2	1:B:1228:ILE:HD13	2.01	0.43
1:B:1792:ALA:O	1:B:2176:ASN:ND2	2.52	0.43
1:B:3281:LEU:HD12	1:B:3315:LEU:HD22	1.99	0.43
1:C:876:GLU:HG2	1:C:910:PHE:CE2	2.54	0.43
1:C:2354:VAL:O	1:C:2358:ILE:HG12	2.19	0.43
1:C:3284:TRP:HB3	1:C:3305:THR:HG21	2.00	0.43
1:D:1830:VAL:HB	1:D:1837:GLN:HG3	2.01	0.43
1:D:3366:ARG:NH1	1:D:3440:GLU:OE1	2.47	0.43
1:A:886:ARG:HE	1:A:904:HIS:HB2	1.84	0.43
1:A:1568:LYS:HE2	1:A:1574:PRO:HD3	1.99	0.43
1:A:1792:ALA:O	1:A:2176:ASN:ND2	2.52	0.43
1:A:2354:VAL:O	1:A:2358:ILE:HG12	2.19	0.43
1:A:2740:VAL:HG21	1:A:2819:TRP:HE1	1.83	0.43
1:B:665:GLU:HB2	1:B:792:LEU:HB2	2.00	0.43
1:B:783:PHE:HB2	1:B:787:VAL:HG21	2.01	0.43
1:B:793:LEU:HB2	1:B:797:HIS:HB2	2.00	0.43
1:C:886:ARG:HE	1:C:904:HIS:HB2	1.84	0.43
1:C:3326:ASN:HB3	1:C:3329:ILE:HD13	1.99	0.43
1:C:3801:GLY:O	1:C:3805:LEU:HB2	2.19	0.43
1:D:721:LEU:HD23	1:D:721:LEU:HA	1.90	0.43
1:D:793:LEU:HB2	1:D:797:HIS:HB2	2.00	0.43
1:D:876:GLU:HG2	1:D:910:PHE:CE2	2.54	0.43
1:D:886:ARG:HE	1:D:904:HIS:HB2	1.84	0.43
1:D:3346:VAL:HG22	1:D:3415:TYR:HB2	2.01	0.43
1:A:2998:PHE:HA	1:A:3002:LEU:HD13	2.00	0.42
1:B:1000:ARG:HA	1:B:1000:ARG:HD3	1.80	0.42
1:B:3844:LEU:HD21	1:B:3933:PHE:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:400:ALA:HA	1:C:403:MET:HG2	2.01	0.42
1:C:783:PHE:HB2	1:C:787:VAL:HG21	2.01	0.42
1:C:1248:VAL:HG12	1:C:1599:MET:HG3	2.01	0.42
1:C:2466:LEU:HD23	1:C:2466:LEU:HA	1.88	0.42
1:C:2716:ASP:OD1	1:C:2716:ASP:N	2.50	0.42
1:C:3781:GLN:NE2	1:C:3819:TYR:OH	2.41	0.42
1:D:884:LEU:HD13	1:D:968:ALA:H	1.83	0.42
1:D:2354:VAL:O	1:D:2358:ILE:HG12	2.19	0.42
1:D:3211:ASN:HB3	1:D:3236:VAL:HG21	2.01	0.42
2:G:49:ARG:N	2:G:54:GLU:OE2	2.52	0.42
1:A:876:GLU:HG2	1:A:910:PHE:CE2	2.54	0.42
1:A:3211:ASN:HB3	1:A:3236:VAL:HG21	2.01	0.42
1:A:3316:LEU:HD11	1:A:3353:LEU:HD11	2.00	0.42
1:A:3875:MET:HB3	1:A:3878:ASP:HB3	2.02	0.42
1:B:416:LYS:HB3	1:B:416:LYS:HE2	1.76	0.42
1:B:876:GLU:HG2	1:B:910:PHE:CE2	2.54	0.42
1:B:886:ARG:HE	1:B:904:HIS:HB2	1.84	0.42
1:B:1689:VAL:HG21	1:B:1714:LEU:HD21	2.01	0.42
1:B:3799:LYS:HE3	1:B:3799:LYS:HB2	1.94	0.42
1:B:3862:ASP:OD1	1:B:3862:ASP:N	2.45	0.42
1:C:465:GLN:HA	1:C:468:LEU:HB2	2.00	0.42
1:C:3471:THR:O	1:C:3475:LYS:HG3	2.19	0.42
1:D:2165:LEU:HD22	1:D:2174:GLU:HG2	2.01	0.42
1:A:3075:LEU:O	1:A:3146:HIS:NE2	2.46	0.42
1:A:3801:GLY:O	1:A:3805:LEU:HB2	2.19	0.42
1:B:253:CYS:O	1:B:258:SER:OG	2.34	0.42
1:B:3471:THR:O	1:B:3475:LYS:HG3	2.19	0.42
1:D:244:LEU:HD23	1:D:244:LEU:HA	1.90	0.42
1:D:1792:ALA:O	1:D:2176:ASN:ND2	2.52	0.42
1:D:2611:CYS:HA	1:D:2614:ILE:HG22	2.02	0.42
1:D:3284:TRP:HB3	1:D:3305:THR:HG21	2.00	0.42
2:H:49:ARG:N	2:H:54:GLU:OE2	2.52	0.42
1:A:1808:ARG:HD3	1:A:1853:ILE:HG22	2.00	0.42
1:A:2927:LEU:HD12	1:A:2927:LEU:HA	1.87	0.42
1:A:4244:GLU:HG2	1:A:4668:LEU:HD13	2.01	0.42
1:B:129:ASP:N	1:B:129:ASP:OD1	2.50	0.42
1:B:3362:ILE:HG13	1:B:3437:MET:HG2	2.01	0.42
1:B:3801:GLY:O	1:B:3805:LEU:HB2	2.19	0.42
1:C:1634:LEU:HD23	1:C:1634:LEU:HA	1.91	0.42
1:C:3628:ARG:NH2	1:C:3857:GLY:O	2.53	0.42
1:C:3875:MET:HB3	1:C:3878:ASP:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:279:PRO:HD3	1:D:327:PRO:HB3	2.01	0.42
1:D:400:ALA:HA	1:D:403:MET:HG2	2.01	0.42
1:D:1221:GLU:HG3	1:D:1223:PHE:HD1	1.83	0.42
1:D:1253:PRO:HG2	1:D:1254:HIS:CD2	2.54	0.42
1:D:3801:GLY:O	1:D:3805:LEU:HB2	2.19	0.42
1:A:743:VAL:HB	1:A:760:ASN:HA	2.02	0.42
1:A:3628:ARG:NH2	1:A:3857:GLY:O	2.53	0.42
1:B:2611:CYS:HA	1:B:2614:ILE:HG22	2.02	0.42
1:B:3037:GLU:HG3	1:B:3088:VAL:HG21	2.01	0.42
1:B:3875:MET:HB3	1:B:3878:ASP:HB3	2.02	0.42
1:C:206:CYS:HB2	1:C:271:GLY:HA3	2.01	0.42
1:C:1253:PRO:HG2	1:C:1254:HIS:CD2	2.54	0.42
1:C:1689:VAL:HG21	1:C:1714:LEU:HD21	2.01	0.42
1:C:2138:LEU:HD23	1:C:2138:LEU:HA	1.90	0.42
1:C:2616:PRO:HA	1:C:2619:LEU:HD12	2.02	0.42
1:D:1248:VAL:HG12	1:D:1599:MET:HG3	2.01	0.42
1:D:2616:PRO:HA	1:D:2619:LEU:HD12	2.02	0.42
1:A:1248:VAL:HG12	1:A:1599:MET:HG3	2.01	0.42
1:A:4182:GLU:HA	1:A:4191:GLU:O	2.20	0.42
1:A:5012:LYS:HB3	1:A:5012:LYS:HE3	1.69	0.42
1:B:743:VAL:HB	1:B:760:ASN:HA	2.02	0.42
1:B:1248:VAL:HG12	1:B:1599:MET:HG3	2.01	0.42
1:B:1830:VAL:HB	1:B:1837:GLN:HG3	2.01	0.42
1:B:2624:ARG:HG3	1:B:2910:THR:HB	2.02	0.42
1:B:2716:ASP:OD1	1:B:2716:ASP:N	2.50	0.42
1:B:3641:LEU:HA	1:B:3644:LEU:HD23	2.01	0.42
1:C:1792:ALA:O	1:C:2176:ASN:ND2	2.52	0.42
1:C:2611:CYS:HA	1:C:2614:ILE:HG22	2.02	0.42
1:D:107:ILE:N	1:D:148:TRP:O	2.40	0.42
1:D:206:CYS:HB2	1:D:271:GLY:HA3	2.01	0.42
1:D:206:CYS:SG	1:D:207:SER:N	2.93	0.42
1:D:1689:VAL:HG21	1:D:1714:LEU:HD21	2.02	0.42
1:D:3037:GLU:HG3	1:D:3088:VAL:HG21	2.01	0.42
1:D:3159:ASP:OD1	1:D:3159:ASP:N	2.45	0.42
1:D:3875:MET:HB3	1:D:3878:ASP:HB3	2.02	0.42
1:D:4188:ARG:HD2	1:D:4188:ARG:HA	1.58	0.42
1:A:1689:VAL:HG21	1:A:1714:LEU:HD21	2.01	0.42
1:A:2960:LEU:HD23	1:A:2963:LEU:HD12	2.01	0.42
1:A:5006:GLN:O	1:A:5010:VAL:HG12	2.20	0.42
1:B:1253:PRO:HG2	1:B:1254:HIS:CD2	2.54	0.42
1:B:2165:LEU:HD22	1:B:2174:GLU:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4944:ARG:NE	1:C:4938:ASP:OD1	2.51	0.42
1:C:1737:PRO:HD3	1:C:1771:LEU:HG	2.01	0.42
1:C:1830:VAL:HB	1:C:1837:GLN:HG3	2.01	0.42
1:C:2165:LEU:HD22	1:C:2174:GLU:HG2	2.01	0.42
1:C:2316:LYS:HD3	1:C:2318:TYR:HE1	1.84	0.42
1:C:2624:ARG:HG3	1:C:2910:THR:HB	2.02	0.42
1:C:3641:LEU:HA	1:C:3644:LEU:HD23	2.01	0.42
1:D:1674:CYS:SG	1:D:1717:SER:OG	2.73	0.42
1:D:5012:LYS:HB3	1:D:5012:LYS:HE3	1.69	0.42
2:F:49:ARG:N	2:F:54:GLU:OE2	2.52	0.42
1:A:1253:PRO:HG2	1:A:1254:HIS:CD2	2.54	0.42
1:A:2611:CYS:HA	1:A:2614:ILE:HG22	2.02	0.42
1:A:3641:LEU:HA	1:A:3644:LEU:HD23	2.01	0.42
1:A:3844:LEU:HD21	1:A:3933:PHE:HA	2.01	0.42
1:A:4227:GLU:H	1:A:4227:GLU:HG3	1.55	0.42
1:B:206:CYS:SG	1:B:207:SER:N	2.93	0.42
1:C:3353:LEU:HD23	1:C:3358:PHE:HE2	1.85	0.42
1:C:4801:LEU:HD23	1:C:4801:LEU:HA	1.88	0.42
1:D:2998:PHE:HA	1:D:3002:LEU:HD13	2.00	0.42
1:D:5006:GLN:O	1:D:5010:VAL:HG12	2.20	0.42
1:A:2316:LYS:HD3	1:A:2318:TYR:HE1	1.85	0.42
1:B:2960:LEU:HD23	1:B:2963:LEU:HD12	2.01	0.42
1:B:3346:VAL:HG22	1:B:3415:TYR:HB2	2.01	0.42
1:B:4821:LYS:O	1:B:4825:THR:HG23	2.20	0.42
1:C:279:PRO:HD3	1:C:327:PRO:HB3	2.01	0.42
1:C:419:ASP:HA	1:C:422:SER:HB3	2.02	0.42
1:C:743:VAL:HB	1:C:760:ASN:HA	2.02	0.42
1:C:846:LEU:HD22	1:C:846:LEU:HA	1.89	0.42
1:C:1154:ASP:OD1	1:C:1156:THR:OG1	2.38	0.42
1:C:1808:ARG:NH1	1:C:1853:ILE:O	2.43	0.42
1:C:2672:LEU:HD23	1:C:2672:LEU:HA	1.83	0.42
1:C:2960:LEU:HD23	1:C:2963:LEU:HD12	2.01	0.42
1:C:3337:ARG:HA	1:C:3340:VAL:HG22	2.02	0.42
1:C:3346:VAL:HG22	1:C:3415:TYR:HB2	2.01	0.42
1:C:4727:LYS:HG2	1:C:4728:HIS:CD2	2.55	0.42
1:D:878:ILE:HD11	1:D:925:SER:HB2	2.02	0.42
1:D:3353:LEU:HD23	1:D:3358:PHE:HE2	1.85	0.42
1:D:3628:ARG:NH2	1:D:3857:GLY:O	2.53	0.42
1:D:3781:GLN:NE2	1:D:3819:TYR:OH	2.41	0.42
1:D:3842:LEU:HB2	1:D:3929:SER:HB2	2.01	0.42
1:D:4821:LYS:O	1:D:4825:THR:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4727:LYS:HG2	1:A:4728:HIS:CD2	2.55	0.42
1:B:465:GLN:HA	1:B:468:LEU:HB2	2.00	0.42
1:B:869:ARG:CZ	1:B:870:ILE:HB	2.50	0.42
1:B:1737:PRO:HD3	1:B:1771:LEU:HG	2.01	0.42
1:B:2891:LYS:HA	1:B:2891:LYS:HD3	1.97	0.42
1:B:3628:ARG:NH2	1:B:3857:GLY:O	2.53	0.42
1:B:4227:GLU:H	1:B:4227:GLU:HG3	1.55	0.42
1:C:3362:ILE:HG13	1:C:3437:MET:HG2	2.01	0.42
1:C:5006:GLN:O	1:C:5010:VAL:HG12	2.20	0.42
1:D:743:VAL:HB	1:D:760:ASN:HA	2.02	0.42
1:D:1088:TRP:HB2	1:D:1153:ILE:HG22	2.02	0.42
1:D:1658:ASP:OD1	1:D:1658:ASP:N	2.47	0.42
1:D:2863:SER:HA	1:D:2928:LYS:HG3	2.02	0.42
1:D:3007:ASN:O	1:D:3011:THR:OG1	2.33	0.42
1:D:4227:GLU:H	1:D:4227:GLU:HG3	1.55	0.42
1:A:783:PHE:HB2	1:A:787:VAL:HG21	2.01	0.41
1:A:878:ILE:HD11	1:A:925:SER:HB2	2.02	0.41
1:A:1097:THR:HA	1:A:1143:TRP:HE1	1.85	0.41
1:A:2624:ARG:HG3	1:A:2910:THR:HB	2.02	0.41
1:A:3144:PHE:CZ	1:A:3197:LEU:HD13	2.55	0.41
1:B:206:CYS:HB2	1:B:271:GLY:HA3	2.01	0.41
1:B:279:PRO:HD3	1:B:327:PRO:HB3	2.01	0.41
1:B:293:LEU:HB3	1:B:311:ALA:HB1	2.02	0.41
1:B:838:HIS:CE1	1:B:1201:HIS:HB2	2.55	0.41
1:B:863:LEU:HA	1:B:864:PRO:HD3	1.85	0.41
1:B:4727:LYS:HG2	1:B:4728:HIS:CD2	2.55	0.41
1:C:4821:LYS:O	1:C:4825:THR:HG23	2.20	0.41
1:D:465:GLN:HA	1:D:468:LEU:HB2	2.00	0.41
1:D:638:ILE:HD11	1:D:702:TRP:HE3	1.85	0.41
1:D:2299:VAL:HG11	1:D:2356:LEU:HB3	2.03	0.41
1:D:2765:LYS:HA	1:D:2765:LYS:HD3	1.89	0.41
1:D:3641:LEU:HA	1:D:3644:LEU:HD23	2.01	0.41
1:D:3823:LYS:HA	1:D:3823:LYS:HD3	1.90	0.41
1:D:3924:LEU:O	1:D:3928:GLU:HG2	2.20	0.41
1:D:4182:GLU:HA	1:D:4191:GLU:O	2.20	0.41
1:A:356:TRP:O	1:A:379:HIS:N	2.53	0.41
1:A:3781:GLN:NE2	1:A:3819:TYR:OH	2.41	0.41
1:A:4031:LEU:HD23	1:A:4031:LEU:HA	1.88	0.41
1:B:1097:THR:HA	1:B:1143:TRP:HE1	1.85	0.41
1:B:2616:PRO:HB3	1:B:2647:HIS:HE1	1.85	0.41
1:B:3144:PHE:CZ	1:B:3197:LEU:HD13	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1088:TRP:HB2	1:C:1153:ILE:HG22	2.02	0.41
1:C:1097:THR:HA	1:C:1143:TRP:HE1	1.85	0.41
1:C:2891:LYS:HA	1:C:2891:LYS:HD3	1.97	0.41
1:D:2672:LEU:HD22	1:D:2710:LEU:HD23	2.02	0.41
2:E:49:ARG:N	2:E:54:GLU:OE2	2.52	0.41
1:A:75:VAL:O	1:A:79:GLN:HG2	2.21	0.41
1:A:846:LEU:HD22	1:A:846:LEU:HA	1.89	0.41
1:A:1830:VAL:HB	1:A:1837:GLN:HG3	2.01	0.41
1:A:2299:VAL:HG11	1:A:2356:LEU:HB3	2.03	0.41
1:A:3037:GLU:HG3	1:A:3088:VAL:HG21	2.01	0.41
1:A:3353:LEU:HD23	1:A:3358:PHE:HE2	1.85	0.41
1:A:3924:LEU:O	1:A:3928:GLU:HG2	2.20	0.41
1:B:75:VAL:O	1:B:79:GLN:HG2	2.21	0.41
1:C:2616:PRO:HB3	1:C:2647:HIS:HE1	1.85	0.41
1:D:75:VAL:O	1:D:79:GLN:HG2	2.21	0.41
1:D:2624:ARG:HG3	1:D:2910:THR:HB	2.02	0.41
1:D:4029:SER:HA	1:D:4032:GLU:HG3	2.02	0.41
1:A:426:ARG:NH1	1:A:429:GLY:O	2.41	0.41
1:A:2165:LEU:HD22	1:A:2174:GLU:HG2	2.01	0.41
1:A:2863:SER:HA	1:A:2928:LYS:HG3	2.02	0.41
1:A:3362:ILE:HG13	1:A:3437:MET:HG2	2.02	0.41
1:B:1842:LEU:HD23	1:B:1842:LEU:HA	1.87	0.41
1:B:2616:PRO:HA	1:B:2619:LEU:HD12	2.02	0.41
1:B:3416:VAL:O	1:B:3420:ARG:N	2.53	0.41
1:B:3924:LEU:O	1:B:3928:GLU:HG2	2.20	0.41
1:B:4182:GLU:HA	1:B:4191:GLU:O	2.20	0.41
1:C:869:ARG:CZ	1:C:870:ILE:HB	2.50	0.41
1:C:878:ILE:HD11	1:C:925:SER:HB2	2.02	0.41
1:C:2773:ASN:OD1	1:C:2786:LYS:NZ	2.48	0.41
1:C:4779:LYS:HB3	1:C:4779:LYS:HE3	1.87	0.41
1:C:4911:LEU:HA	1:C:4914:VAL:HG22	2.03	0.41
1:D:3416:VAL:O	1:D:3420:ARG:N	2.53	0.41
1:D:3944:GLU:OE1	1:D:3946:GLN:N	2.50	0.41
1:A:206:CYS:HB2	1:A:271:GLY:HA3	2.01	0.41
1:A:419:ASP:HA	1:A:422:SER:HB3	2.02	0.41
1:A:638:ILE:HD11	1:A:702:TRP:HE3	1.85	0.41
1:A:1088:TRP:HB2	1:A:1153:ILE:HG22	2.02	0.41
1:A:3823:LYS:HA	1:A:3823:LYS:HD3	1.90	0.41
1:B:1154:ASP:OD1	1:B:1156:THR:OG1	2.38	0.41
1:B:1634:LEU:HD23	1:B:1634:LEU:HA	1.91	0.41
1:B:2672:LEU:HD23	1:B:2672:LEU:HA	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4031:LEU:HD23	1:B:4031:LEU:HA	1.88	0.41
1:C:3091:GLY:O	1:C:3094:SER:OG	2.36	0.41
1:D:783:PHE:HB2	1:D:787:VAL:HG21	2.01	0.41
1:D:1154:ASP:OD1	1:D:1156:THR:OG1	2.38	0.41
1:A:2616:PRO:HA	1:A:2619:LEU:HD12	2.01	0.41
1:A:4821:LYS:O	1:A:4825:THR:HG23	2.20	0.41
1:A:4917:ASP:OD2	1:D:4888:TYR:OH	2.29	0.41
1:A:4937:ILE:HG12	1:B:4934:GLY:HA2	2.02	0.41
1:B:2299:VAL:HG11	1:B:2356:LEU:HB3	2.02	0.41
1:B:3353:LEU:HD23	1:B:3358:PHE:HE2	1.85	0.41
1:C:638:ILE:HD11	1:C:702:TRP:HE3	1.85	0.41
1:D:293:LEU:HB3	1:D:311:ALA:HB1	2.02	0.41
1:D:869:ARG:CZ	1:D:870:ILE:HB	2.50	0.41
1:D:3888:LEU:HD23	1:D:3888:LEU:HA	1.89	0.41
1:D:4727:LYS:HG2	1:D:4728:HIS:CD2	2.55	0.41
1:D:4911:LEU:HA	1:D:4914:VAL:HG22	2.03	0.41
1:A:1154:ASP:OD1	1:A:1156:THR:OG1	2.38	0.41
1:A:2716:ASP:N	1:A:2716:ASP:OD1	2.50	0.41
1:A:3354:LEU:HD22	1:A:3423:TRP:HE1	1.86	0.41
1:A:3655:GLU:HA	1:A:3658:LYS:HG2	2.03	0.41
1:B:4801:LEU:HD23	1:B:4801:LEU:HA	1.88	0.41
1:C:394:GLN:HE22	1:C:396:GLU:HB2	1.86	0.41
1:C:733:PRO:HG2	1:C:762:CYS:HB3	2.03	0.41
1:C:838:HIS:CE1	1:C:1201:HIS:HB2	2.56	0.41
1:C:2304:GLY:HA2	1:C:2307:LEU:HG	2.02	0.41
1:D:733:PRO:HG2	1:D:762:CYS:HB3	2.03	0.41
1:D:1097:THR:HA	1:D:1143:TRP:HE1	1.85	0.41
1:D:2304:GLY:HA2	1:D:2307:LEU:HG	2.02	0.41
1:D:2616:PRO:HB3	1:D:2647:HIS:HE1	1.85	0.41
2:H:105:ASN:OD1	2:H:106:LEU:N	2.54	0.41
1:A:293:LEU:HB3	1:A:311:ALA:HB1	2.02	0.41
1:A:1634:LEU:HD23	1:A:1634:LEU:HA	1.91	0.41
1:A:2672:LEU:HD22	1:A:2710:LEU:HD23	2.02	0.41
1:A:3132:THR:HG23	1:A:3136:LEU:HD22	2.03	0.41
1:B:1042:ALA:O	1:B:1045:THR:OG1	2.36	0.41
1:B:2316:LYS:HD3	1:B:2318:TYR:HE1	1.84	0.41
1:B:3337:ARG:HA	1:B:3340:VAL:HG22	2.02	0.41
1:B:4814:LEU:HD23	1:B:4814:LEU:HA	1.91	0.41
1:C:206:CYS:SG	1:C:207:SER:N	2.93	0.41
1:C:1792:ALA:HA	1:C:2173:GLN:HA	2.03	0.41
1:C:2299:VAL:HG11	1:C:2356:LEU:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2672:LEU:HD22	1:C:2710:LEU:HD23	2.02	0.41
1:C:4989:MET:HE2	1:C:4989:MET:HB2	1.92	0.41
1:D:2960:LEU:HD23	1:D:2963:LEU:HD12	2.01	0.41
1:D:3589:PRO:HA	1:D:3592:ILE:HG22	2.03	0.41
1:D:3677:LEU:HD23	1:D:3677:LEU:HA	1.91	0.41
1:D:4823:LEU:HA	1:D:4823:LEU:HD23	1.84	0.41
1:D:4957:LYS:HE2	1:D:4957:LYS:HB2	1.64	0.41
1:A:206:CYS:SG	1:A:207:SER:N	2.93	0.41
1:A:383:HIS:N	1:A:386:ASP:OD2	2.54	0.41
1:A:2616:PRO:HB3	1:A:2647:HIS:HE1	1.85	0.41
1:A:3337:ARG:HA	1:A:3340:VAL:HG22	2.02	0.41
1:A:3589:PRO:HA	1:A:3592:ILE:HG22	2.03	0.41
1:A:3882:GLN:HG3	1:A:3957:VAL:HG22	2.03	0.41
1:A:4895:GLY:O	1:D:4892:ARG:NH1	2.46	0.41
1:A:4911:LEU:HA	1:A:4914:VAL:HG22	2.03	0.41
1:A:4944:ARG:NE	1:B:4938:ASP:OD1	2.51	0.41
1:B:356:TRP:O	1:B:379:HIS:N	2.54	0.41
1:B:638:ILE:HD11	1:B:702:TRP:HE3	1.85	0.41
1:B:878:ILE:HD11	1:B:925:SER:HB2	2.02	0.41
1:B:880:GLU:HB3	1:B:883:ALA:HB3	2.03	0.41
1:B:1091:GLU:HB2	1:B:1203:ASN:HB3	2.03	0.41
1:B:1792:ALA:HA	1:B:2173:GLN:HA	2.03	0.41
1:B:2158:CYS:O	1:B:2162:ILE:HG12	2.21	0.41
1:B:2304:GLY:HA2	1:B:2307:LEU:HG	2.02	0.41
1:B:3102:ASP:HA	1:B:3105:LYS:HE2	2.03	0.41
1:B:3104:GLU:HG2	1:B:3171:SER:HB3	2.03	0.41
1:B:5006:GLN:O	1:B:5010:VAL:HG12	2.20	0.41
1:C:293:LEU:HB3	1:C:311:ALA:HB1	2.02	0.41
1:C:1679:ASN:HA	1:C:1682:ALA:HB3	2.03	0.41
1:C:2109:ASP:OD1	1:C:2109:ASP:N	2.54	0.41
1:C:2863:SER:HA	1:C:2928:LYS:HG3	2.02	0.41
1:C:3102:ASP:HA	1:C:3105:LYS:HE2	2.03	0.41
1:C:3104:GLU:HG2	1:C:3171:SER:HB3	2.03	0.41
1:C:3400:VAL:HG23	1:C:3403:ARG:HE	1.86	0.41
1:C:3655:GLU:HA	1:C:3658:LYS:HG2	2.03	0.41
1:C:4182:GLU:HA	1:C:4191:GLU:O	2.20	0.41
1:D:356:TRP:O	1:D:379:HIS:N	2.54	0.41
1:D:383:HIS:N	1:D:386:ASP:OD2	2.54	0.41
1:D:2109:ASP:N	1:D:2109:ASP:OD1	2.54	0.41
1:D:3144:PHE:CZ	1:D:3197:LEU:HD13	2.55	0.41
1:D:3337:ARG:HA	1:D:3340:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3752:SER:OG	1:D:3755:GLU:OE1	2.39	0.41
1:D:4839:MET:HE3	1:D:4839:MET:HB3	1.98	0.41
2:F:105:ASN:OD1	2:F:106:LEU:N	2.54	0.41
1:B:1088:TRP:HB2	1:B:1153:ILE:HG22	2.02	0.41
1:B:2109:ASP:OD1	1:B:2109:ASP:N	2.54	0.41
1:B:3888:LEU:HD23	1:B:3888:LEU:HA	1.90	0.41
1:B:4686:LEU:O	1:B:4691:GLN:N	2.50	0.41
1:C:416:LYS:HB3	1:C:416:LYS:HE2	1.76	0.41
1:C:2158:CYS:O	1:C:2162:ILE:HG12	2.21	0.41
1:C:3144:PHE:CZ	1:C:3197:LEU:HD13	2.56	0.41
1:C:4675:LYS:HD2	1:C:4679:ARG:HH21	1.86	0.41
1:D:2690:LYS:HA	1:D:2690:LYS:HD2	1.90	0.41
2:G:77:THR:HG22	2:G:80:VAL:HG22	2.03	0.41
1:A:733:PRO:HG2	1:A:762:CYS:HB3	2.03	0.40
1:A:838:HIS:CE1	1:A:1201:HIS:HB2	2.55	0.40
1:A:4029:SER:HA	1:A:4032:GLU:HG3	2.02	0.40
1:A:4675:LYS:HD2	1:A:4679:ARG:HH21	1.86	0.40
1:A:4723:LYS:HB3	1:A:4723:LYS:HE2	1.98	0.40
1:B:383:HIS:N	1:B:386:ASP:OD2	2.54	0.40
1:B:2711:PRO:HA	1:B:2712:PRO:HD3	1.94	0.40
1:B:3589:PRO:HA	1:B:3592:ILE:HG22	2.03	0.40
1:B:4029:SER:HA	1:B:4032:GLU:HG3	2.02	0.40
1:D:419:ASP:HA	1:D:422:SER:HB3	2.02	0.40
1:D:838:HIS:CE1	1:D:1201:HIS:HB2	2.55	0.40
1:D:3362:ILE:HG13	1:D:3437:MET:HG2	2.02	0.40
1:A:1128:ARG:HB2	1:A:1130:GLN:HE22	1.87	0.40
1:A:2461:VAL:O	1:A:2510:TYR:OH	2.30	0.40
1:A:3172:ILE:HG21	1:A:3194:LEU:HD13	2.03	0.40
1:A:3545:THR:HG23	1:A:3548:GLU:H	1.87	0.40
1:B:733:PRO:HG2	1:B:762:CYS:HB3	2.03	0.40
1:B:3545:THR:HG23	1:B:3548:GLU:H	1.87	0.40
1:B:3768:SER:HA	1:B:3771:HIS:CD2	2.57	0.40
1:B:3882:GLN:HG3	1:B:3957:VAL:HG22	2.03	0.40
1:C:660:GLY:O	1:C:750:LEU:N	2.53	0.40
1:C:3354:LEU:HD22	1:C:3423:TRP:HE1	1.86	0.40
1:C:3416:VAL:HG11	1:C:3517:MET:HE1	2.03	0.40
1:C:3604:TYR:O	1:C:3608:GLN:HG2	2.22	0.40
1:C:3862:ASP:OD1	1:C:3862:ASP:N	2.45	0.40
1:D:1679:ASN:HA	1:D:1682:ALA:HB3	2.03	0.40
1:D:2773:ASN:OD1	1:D:2786:LYS:NZ	2.48	0.40
1:D:3075:LEU:O	1:D:3146:HIS:NE2	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3545:THR:HG23	1:D:3548:GLU:H	1.86	0.40
1:D:3604:TYR:O	1:D:3608:GLN:HG2	2.22	0.40
1:D:3882:GLN:HG3	1:D:3957:VAL:HG22	2.03	0.40
1:D:4686:LEU:O	1:D:4691:GLN:N	2.50	0.40
1:A:869:ARG:CZ	1:A:870:ILE:HB	2.50	0.40
1:A:2304:GLY:HA2	1:A:2307:LEU:HG	2.02	0.40
1:A:3438:VAL:HG21	1:A:3517:MET:HG3	2.03	0.40
1:A:3768:SER:HA	1:A:3771:HIS:CD2	2.56	0.40
1:B:676:THR:HG22	1:B:677:ALA:H	1.87	0.40
1:B:846:LEU:HD22	1:B:846:LEU:HA	1.89	0.40
1:B:1128:ARG:HB2	1:B:1130:GLN:HE22	1.87	0.40
1:B:3132:THR:HG23	1:B:3136:LEU:HD22	2.03	0.40
1:B:3264:THR:OG1	1:B:3265:GLU:OE1	2.39	0.40
1:B:3354:LEU:HD22	1:B:3423:TRP:HE1	1.86	0.40
1:B:3438:VAL:HG21	1:B:3517:MET:HG3	2.04	0.40
1:C:3132:THR:HG23	1:C:3136:LEU:HD22	2.03	0.40
1:C:3768:SER:HA	1:C:3771:HIS:CD2	2.57	0.40
1:C:3924:LEU:O	1:C:3928:GLU:HG2	2.20	0.40
1:C:4127:GLU:O	1:C:4131:ARG:HB2	2.22	0.40
1:D:2316:LYS:HD3	1:D:2318:TYR:HE1	1.85	0.40
1:D:3104:GLU:HG2	1:D:3171:SER:HB3	2.03	0.40
1:D:3354:LEU:HD22	1:D:3423:TRP:HE1	1.86	0.40
2:H:77:THR:HG22	2:H:80:VAL:HG22	2.03	0.40
1:A:183:SER:O	1:A:183:SER:OG	2.38	0.40
1:A:880:GLU:HB3	1:A:883:ALA:HB3	2.03	0.40
1:A:1792:ALA:HA	1:A:2173:GLN:HA	2.03	0.40
1:A:2711:PRO:HA	1:A:2712:PRO:HD3	1.94	0.40
1:A:3104:GLU:HG2	1:A:3171:SER:HB3	2.03	0.40
1:A:3400:VAL:HG23	1:A:3403:ARG:HE	1.86	0.40
1:B:2672:LEU:HD22	1:B:2710:LEU:HD23	2.02	0.40
1:B:3152:PHE:HB3	1:B:3156:VAL:HG23	2.03	0.40
1:B:3301:PRO:HA	1:B:3302:PRO:HD3	1.92	0.40
1:B:3511:VAL:HG12	1:B:3514:LEU:HD12	2.04	0.40
1:B:3655:GLU:HA	1:B:3658:LYS:HG2	2.03	0.40
1:B:4823:LEU:HA	1:B:4823:LEU:HD23	1.84	0.40
1:C:932:LEU:HD22	1:C:984:LEU:HD21	2.04	0.40
1:C:1091:GLU:HB2	1:C:1203:ASN:HB3	2.03	0.40
1:C:3589:PRO:HA	1:C:3592:ILE:HG22	2.03	0.40
1:C:3752:SER:OG	1:C:3755:GLU:OE1	2.39	0.40
1:D:932:LEU:HD22	1:D:984:LEU:HD21	2.04	0.40
1:D:3172:ILE:HG21	1:D:3194:LEU:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3400:VAL:HG23	1:D:3403:ARG:HE	1.86	0.40
1:D:4127:GLU:O	1:D:4131:ARG:HB2	2.22	0.40
1:A:3752:SER:OG	1:A:3755:GLU:OE1	2.39	0.40
1:A:4821:LYS:H	1:A:4821:LYS:HG2	1.75	0.40
1:B:394:GLN:HE22	1:B:396:GLU:HB2	1.86	0.40
1:B:2863:SER:HA	1:B:2928:LYS:HG3	2.02	0.40
1:B:4675:LYS:HD2	1:B:4679:ARG:HH21	1.86	0.40
1:C:676:THR:HG22	1:C:677:ALA:H	1.87	0.40
1:C:3302:PRO:HA	1:C:3303:PRO:HD3	1.98	0.40
1:C:3882:GLN:HG3	1:C:3957:VAL:HG22	2.03	0.40
1:D:1000:ARG:HA	1:D:1000:ARG:HD3	1.80	0.40
1:D:1091:GLU:HB2	1:D:1203:ASN:HB3	2.03	0.40
1:D:1232:ARG:NH2	1:D:1828:ASP:O	2.41	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	4355/5037 (86%)	4218 (97%)	133 (3%)	4 (0%)	51	83
1	B	4355/5037 (86%)	4219 (97%)	132 (3%)	4 (0%)	51	83
1	C	4355/5037 (86%)	4219 (97%)	132 (3%)	4 (0%)	51	83
1	D	4355/5037 (86%)	4219 (97%)	132 (3%)	4 (0%)	51	83
2	E	105/350 (30%)	103 (98%)	2 (2%)	0	100	100
2	F	105/350 (30%)	103 (98%)	2 (2%)	0	100	100
2	G	105/350 (30%)	103 (98%)	2 (2%)	0	100	100
2	H	105/350 (30%)	103 (98%)	2 (2%)	0	100	100
All	All	17840/21548 (83%)	17287 (97%)	537 (3%)	16 (0%)	54	83

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3615	SER
1	B	3615	SER
1	C	3615	SER
1	D	3615	SER
1	A	4691	GLN
1	B	4691	GLN
1	C	4691	GLN
1	D	4691	GLN
1	A	4712	PRO
1	B	4712	PRO
1	C	4712	PRO
1	D	4712	PRO
1	A	842	PRO
1	B	842	PRO
1	C	842	PRO
1	D	842	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	3807/4276 (89%)	3687 (97%)	120 (3%)	39	69
1	B	3807/4276 (89%)	3687 (97%)	120 (3%)	39	69
1	C	3807/4276 (89%)	3687 (97%)	120 (3%)	39	69
1	D	3807/4276 (89%)	3687 (97%)	120 (3%)	39	69
2	E	88/304 (29%)	87 (99%)	1 (1%)	73	87
2	F	88/304 (29%)	87 (99%)	1 (1%)	73	87
2	G	88/304 (29%)	87 (99%)	1 (1%)	73	87
2	H	88/304 (29%)	87 (99%)	1 (1%)	73	87
All	All	15580/18320 (85%)	15096 (97%)	484 (3%)	44	70

All (484) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	125	ARG
1	A	275	ARG
1	A	402	ARG
1	A	534	ARG
1	A	830	ARG
1	A	846	LEU
1	A	1534	LYS
1	A	1743[A]	ARG
1	A	1743[B]	ARG
1	A	1752	ARG
1	A	1758	ARG
1	A	1986	MET
1	A	2089	LYS
1	A	2178	MET
1	A	2369[A]	ARG
1	A	2369[B]	ARG
1	A	2584[A]	HIS
1	A	2584[B]	HIS
1	A	2615	ARG
1	A	2786	LYS
1	A	2806	ARG
1	A	2827	ARG
1	A	2914	LYS
1	A	3053	ARG
1	A	3225	ARG
1	A	3422[A]	HIS
1	A	3422[B]	HIS
1	A	3614	LYS
1	A	3622	LYS
1	A	4180	ARG
1	A	4181	ILE
1	A	4182	GLU
1	A	4184	MET
1	A	4188	ARG
1	A	4190	ILE
1	A	4198	SER
1	A	4202	ARG
1	A	4204	GLN
1	A	4211	LYS
1	A	4224	GLU
1	A	4227	GLU
1	A	4230	LYS
1	A	4252	SER

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Mol	Chain	Res	Type
1	A	4253	GLU
1	A	4544	LEU
1	A	4548	ARG
1	A	4550	LYS
1	A	4552	LEU
1	A	4577	LEU
1	A	4580	TYR
1	A	4581	LYS
1	A	4584	ASP
1	A	4585	SER
1	A	4628	VAL
1	A	4632	LEU
1	A	4634	GLU
1	A	4647	SER
1	A	4662	ASN
1	A	4665	LYS
1	A	4667	PRO
1	A	4669	VAL
1	A	4680	LYS
1	A	4684	ASP
1	A	4690	GLU
1	A	4692	PRO
1	A	4694	ASP
1	A	4695	ASP
1	A	4696	ASP
1	A	4698	LYS
1	A	4704	LEU
1	A	4707	ASN
1	A	4710	SER
1	A	4721	LYS
1	A	4734	ARG
1	A	4737	ILE
1	A	4739	GLU
1	A	4743	MET
1	A	4748	LEU
1	A	4750	ILE
1	A	4779	LYS
1	A	4796	MET
1	A	4809	PHE
1	A	4818	MET
1	A	4821	LYS
1	A	4822	THR

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Mol	Chain	Res	Type
1	A	4826	ILE
1	A	4835	LYS
1	A	4844	LEU
1	A	4861	LYS
1	A	4866	SER
1	A	4867	GLU
1	A	4869	GLU
1	A	4871	GLU
1	A	4876	CYS
1	A	4878	ASP
1	A	4880	MET
1	A	4889	VAL
1	A	4902	GLU
1	A	4911	LEU
1	A	4913	ARG
1	A	4945	ASP
1	A	4951	LYS
1	A	4952	GLU
1	A	4954	MET
1	A	4957	LYS
1	A	4958	CYS
1	A	4971	THR
1	A	4980	LEU
1	A	4982	GLU
1	A	4989	MET
1	A	5008	SER
1	A	5010	VAL
1	A	5011	TRP
1	A	5012	LYS
1	A	5013	MET
1	A	5027	CYS
1	A	5028	PHE
1	A	5032	TYR
1	A	5033	GLU
1	A	5036	LEU
1	B	125	ARG
1	B	275	ARG
1	B	402	ARG
1	B	534	ARG
1	B	830	ARG
1	B	846	LEU
1	B	1534	LYS

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Mol	Chain	Res	Type
1	B	1743[A]	ARG
1	B	1743[B]	ARG
1	B	1752	ARG
1	B	1758	ARG
1	B	1986	MET
1	B	2089	LYS
1	B	2178	MET
1	B	2369[A]	ARG
1	B	2369[B]	ARG
1	B	2584[A]	HIS
1	B	2584[B]	HIS
1	B	2615	ARG
1	B	2786	LYS
1	B	2806	ARG
1	B	2827	ARG
1	B	2914	LYS
1	B	3053	ARG
1	B	3225	ARG
1	B	3422[A]	HIS
1	B	3422[B]	HIS
1	B	3614	LYS
1	B	3622	LYS
1	B	4180	ARG
1	B	4181	ILE
1	B	4182	GLU
1	B	4184	MET
1	B	4188	ARG
1	B	4190	ILE
1	B	4198	SER
1	B	4202	ARG
1	B	4204	GLN
1	B	4211	LYS
1	B	4224	GLU
1	B	4227	GLU
1	B	4230	LYS
1	B	4252	SER
1	B	4253	GLU
1	B	4544	LEU
1	B	4548	ARG
1	B	4550	LYS
1	B	4552	LEU
1	B	4577	LEU

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Mol	Chain	Res	Type
1	B	4580	TYR
1	B	4581	LYS
1	B	4584	ASP
1	B	4585	SER
1	B	4628	VAL
1	B	4632	LEU
1	B	4634	GLU
1	B	4647	SER
1	B	4662	ASN
1	B	4665	LYS
1	B	4667	PRO
1	B	4669	VAL
1	B	4680	LYS
1	B	4684	ASP
1	B	4690	GLU
1	B	4692	PRO
1	B	4694	ASP
1	B	4695	ASP
1	B	4696	ASP
1	B	4698	LYS
1	B	4704	LEU
1	B	4707	ASN
1	B	4710	SER
1	B	4721	LYS
1	B	4734	ARG
1	B	4737	ILE
1	B	4739	GLU
1	B	4743	MET
1	B	4748	LEU
1	B	4750	ILE
1	B	4779	LYS
1	B	4796	MET
1	B	4809	PHE
1	B	4818	MET
1	B	4821	LYS
1	B	4822	THR
1	B	4826	ILE
1	B	4835	LYS
1	B	4844	LEU
1	B	4861	LYS
1	B	4866	SER
1	B	4867	GLU

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Mol	Chain	Res	Type
1	B	4869	GLU
1	B	4871	GLU
1	B	4876	CYS
1	B	4878	ASP
1	B	4880	MET
1	B	4889	VAL
1	B	4902	GLU
1	B	4911	LEU
1	B	4913	ARG
1	B	4945	ASP
1	B	4951	LYS
1	B	4952	GLU
1	B	4954	MET
1	B	4957	LYS
1	B	4958	CYS
1	B	4971	THR
1	B	4980	LEU
1	B	4982	GLU
1	B	4989	MET
1	B	5008	SER
1	B	5010	VAL
1	B	5011	TRP
1	B	5012	LYS
1	B	5013	MET
1	B	5027	CYS
1	B	5028	PHE
1	B	5032	TYR
1	B	5033	GLU
1	B	5036	LEU
1	C	125	ARG
1	C	275	ARG
1	C	402	ARG
1	C	534	ARG
1	C	830	ARG
1	C	846	LEU
1	C	1534	LYS
1	C	1743[A]	ARG
1	C	1743[B]	ARG
1	C	1752	ARG
1	C	1758	ARG
1	C	1986	MET
1	C	2089	LYS

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Mol	Chain	Res	Type
1	C	2178	MET
1	C	2369[A]	ARG
1	C	2369[B]	ARG
1	C	2584[A]	HIS
1	C	2584[B]	HIS
1	C	2615	ARG
1	C	2786	LYS
1	C	2806	ARG
1	C	2827	ARG
1	C	2914	LYS
1	C	3053	ARG
1	C	3225	ARG
1	C	3422[A]	HIS
1	C	3422[B]	HIS
1	C	3614	LYS
1	C	3622	LYS
1	C	4180	ARG
1	C	4181	ILE
1	C	4182	GLU
1	C	4184	MET
1	C	4188	ARG
1	C	4190	ILE
1	C	4198	SER
1	C	4202	ARG
1	C	4204	GLN
1	C	4211	LYS
1	C	4224	GLU
1	C	4227	GLU
1	C	4230	LYS
1	C	4252	SER
1	C	4253	GLU
1	C	4544	LEU
1	C	4548	ARG
1	C	4550	LYS
1	C	4552	LEU
1	C	4577	LEU
1	C	4580	TYR
1	C	4581	LYS
1	C	4584	ASP
1	C	4585	SER
1	C	4628	VAL
1	C	4632	LEU

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Mol	Chain	Res	Type
1	C	4634	GLU
1	C	4647	SER
1	C	4662	ASN
1	C	4665	LYS
1	C	4667	PRO
1	C	4669	VAL
1	C	4680	LYS
1	C	4684	ASP
1	C	4690	GLU
1	C	4692	PRO
1	C	4694	ASP
1	C	4695	ASP
1	C	4696	ASP
1	C	4698	LYS
1	C	4704	LEU
1	C	4707	ASN
1	C	4710	SER
1	C	4721	LYS
1	C	4734	ARG
1	C	4737	ILE
1	C	4739	GLU
1	C	4743	MET
1	C	4748	LEU
1	C	4750	ILE
1	C	4779	LYS
1	C	4796	MET
1	C	4809	PHE
1	C	4818	MET
1	C	4821	LYS
1	C	4822	THR
1	C	4826	ILE
1	C	4835	LYS
1	C	4844	LEU
1	C	4861	LYS
1	C	4866	SER
1	C	4867	GLU
1	C	4869	GLU
1	C	4871	GLU
1	C	4876	CYS
1	C	4878	ASP
1	C	4880	MET
1	C	4889	VAL

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Mol	Chain	Res	Type
1	C	4902	GLU
1	C	4911	LEU
1	C	4913	ARG
1	C	4945	ASP
1	C	4951	LYS
1	C	4952	GLU
1	C	4954	MET
1	C	4957	LYS
1	C	4958	CYS
1	C	4971	THR
1	C	4980	LEU
1	C	4982	GLU
1	C	4989	MET
1	C	5008	SER
1	C	5010	VAL
1	C	5011	TRP
1	C	5012	LYS
1	C	5013	MET
1	C	5027	CYS
1	C	5028	PHE
1	C	5032	TYR
1	C	5033	GLU
1	C	5036	LEU
1	D	125	ARG
1	D	275	ARG
1	D	402	ARG
1	D	534	ARG
1	D	830	ARG
1	D	846	LEU
1	D	1534	LYS
1	D	1743[A]	ARG
1	D	1743[B]	ARG
1	D	1752	ARG
1	D	1758	ARG
1	D	1986	MET
1	D	2089	LYS
1	D	2178	MET
1	D	2369[A]	ARG
1	D	2369[B]	ARG
1	D	2584[A]	HIS
1	D	2584[B]	HIS
1	D	2615	ARG

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Mol	Chain	Res	Type
1	D	2786	LYS
1	D	2806	ARG
1	D	2827	ARG
1	D	2914	LYS
1	D	3053	ARG
1	D	3225	ARG
1	D	3422[A]	HIS
1	D	3422[B]	HIS
1	D	3614	LYS
1	D	3622	LYS
1	D	4180	ARG
1	D	4181	ILE
1	D	4182	GLU
1	D	4184	MET
1	D	4188	ARG
1	D	4190	ILE
1	D	4198	SER
1	D	4202	ARG
1	D	4204	GLN
1	D	4211	LYS
1	D	4224	GLU
1	D	4227	GLU
1	D	4230	LYS
1	D	4252	SER
1	D	4253	GLU
1	D	4544	LEU
1	D	4548	ARG
1	D	4550	LYS
1	D	4552	LEU
1	D	4577	LEU
1	D	4580	TYR
1	D	4581	LYS
1	D	4584	ASP
1	D	4585	SER
1	D	4628	VAL
1	D	4632	LEU
1	D	4634	GLU
1	D	4647	SER
1	D	4662	ASN
1	D	4665	LYS
1	D	4667	PRO
1	D	4669	VAL

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Mol	Chain	Res	Type
1	D	4680	LYS
1	D	4684	ASP
1	D	4690	GLU
1	D	4692	PRO
1	D	4694	ASP
1	D	4695	ASP
1	D	4696	ASP
1	D	4698	LYS
1	D	4704	LEU
1	D	4707	ASN
1	D	4710	SER
1	D	4721	LYS
1	D	4734	ARG
1	D	4737	ILE
1	D	4739	GLU
1	D	4743	MET
1	D	4748	LEU
1	D	4750	ILE
1	D	4779	LYS
1	D	4796	MET
1	D	4809	PHE
1	D	4818	MET
1	D	4821	LYS
1	D	4822	THR
1	D	4826	ILE
1	D	4835	LYS
1	D	4844	LEU
1	D	4861	LYS
1	D	4866	SER
1	D	4867	GLU
1	D	4869	GLU
1	D	4871	GLU
1	D	4876	CYS
1	D	4878	ASP
1	D	4880	MET
1	D	4889	VAL
1	D	4902	GLU
1	D	4911	LEU
1	D	4913	ARG
1	D	4945	ASP
1	D	4951	LYS
1	D	4952	GLU

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Mol	Chain	Res	Type
1	D	4954	MET
1	D	4957	LYS
1	D	4958	CYS
1	D	4971	THR
1	D	4980	LEU
1	D	4982	GLU
1	D	4989	MET
1	D	5008	SER
1	D	5010	VAL
1	D	5011	TRP
1	D	5012	LYS
1	D	5013	MET
1	D	5027	CYS
1	D	5028	PHE
1	D	5032	TYR
1	D	5033	GLU
1	D	5036	LEU
2	E	42	ARG
2	F	42	ARG
2	G	42	ARG
2	H	42	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	636	ASN
1	A	877	ASN
1	A	1660	GLN
1	A	2284	ASN
1	A	2962	GLN
1	A	3162	GLN
1	A	3461	GLN
1	A	3605	HIS
1	A	4043	GLN
1	A	4246	GLN
1	A	4707	ASN
1	A	4728	HIS
1	A	4973	HIS
1	A	4984	ASN
1	A	5003	HIS
1	A	5035	GLN
1	B	636	ASN

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Mol	Chain	Res	Type
1	B	877	ASN
1	B	1660	GLN
1	B	2284	ASN
1	B	2962	GLN
1	B	3162	GLN
1	B	3461	GLN
1	B	3605	HIS
1	B	4043	GLN
1	B	4246	GLN
1	B	4707	ASN
1	B	4728	HIS
1	B	4973	HIS
1	B	4984	ASN
1	B	5003	HIS
1	B	5035	GLN
1	C	636	ASN
1	C	877	ASN
1	C	1660	GLN
1	C	2284	ASN
1	C	2962	GLN
1	C	3162	GLN
1	C	3461	GLN
1	C	3605	HIS
1	C	4043	GLN
1	C	4246	GLN
1	C	4707	ASN
1	C	4728	HIS
1	C	4973	HIS
1	C	4984	ASN
1	C	5003	HIS
1	C	5035	GLN
1	D	636	ASN
1	D	877	ASN
1	D	2284	ASN
1	D	2772	GLN
1	D	2962	GLN
1	D	3162	GLN
1	D	3461	GLN
1	D	4043	GLN
1	D	4246	GLN
1	D	4707	ASN
1	D	4728	HIS

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Mol	Chain	Res	Type
1	D	4984	ASN
1	D	5003	HIS
1	D	5035	GLN
2	E	87	HIS
2	F	87	HIS
2	G	87	HIS
2	H	87	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	CMP	C	5101	-	22,25,25	1.36	4 (18%)	24,39,39	1.48	5 (20%)
3	CMP	D	5101	-	22,25,25	1.36	4 (18%)	24,39,39	1.48	5 (20%)
3	CMP	A	5101	-	22,25,25	1.36	4 (18%)	24,39,39	1.48	5 (20%)
3	CMP	B	5101	-	22,25,25	1.36	4 (18%)	24,39,39	1.48	5 (20%)

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	CMP	C	5101	-	-	0/0/31/31	0/4/4/4
3	CMP	D	5101	-	-	0/0/31/31	0/4/4/4
3	CMP	A	5101	-	-	0/0/31/31	0/4/4/4
3	CMP	B	5101	-	-	0/0/31/31	0/4/4/4

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	5101	CMP	P-O3'	3.21	1.63	1.57
3	D	5101	CMP	P-O3'	3.21	1.63	1.57
3	C	5101	CMP	P-O3'	3.21	1.63	1.57
3	A	5101	CMP	P-O3'	3.21	1.63	1.57
3	D	5101	CMP	O5'-C5'	-2.57	1.42	1.46
3	B	5101	CMP	O5'-C5'	-2.56	1.42	1.46
3	C	5101	CMP	O5'-C5'	-2.56	1.42	1.46
3	A	5101	CMP	O5'-C5'	-2.56	1.42	1.46
3	A	5101	CMP	C5-C4	2.31	1.47	1.40
3	B	5101	CMP	C5-C4	2.31	1.47	1.40
3	D	5101	CMP	C5-C4	2.30	1.47	1.40
3	C	5101	CMP	C5-C4	2.30	1.47	1.40
3	B	5101	CMP	P-O5'	2.08	1.60	1.57
3	D	5101	CMP	P-O5'	2.08	1.60	1.57
3	C	5101	CMP	P-O5'	2.08	1.60	1.57
3	A	5101	CMP	P-O5'	2.08	1.60	1.57

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	5101	CMP	N3-C2-N1	-3.35	123.44	128.68
3	A	5101	CMP	N3-C2-N1	-3.35	123.44	128.68
3	D	5101	CMP	N3-C2-N1	-3.35	123.44	128.68
3	B	5101	CMP	N3-C2-N1	-3.35	123.45	128.68
3	B	5101	CMP	O2P-P-O1P	3.23	118.86	108.73
3	C	5101	CMP	O2P-P-O1P	3.23	118.85	108.73
3	D	5101	CMP	O2P-P-O1P	3.23	118.85	108.73
3	A	5101	CMP	O2P-P-O1P	3.23	118.85	108.73
3	B	5101	CMP	O5'-P-O3'	-3.01	101.53	105.68
3	D	5101	CMP	O5'-P-O3'	-3.01	101.53	105.68
3	A	5101	CMP	O5'-P-O3'	-3.01	101.53	105.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	5101	CMP	O5'-P-O3'	-3.01	101.53	105.68
3	B	5101	CMP	C4-C5-N7	-2.34	106.96	109.40
3	A	5101	CMP	C4-C5-N7	-2.34	106.96	109.40
3	C	5101	CMP	C4-C5-N7	-2.34	106.96	109.40
3	D	5101	CMP	C4-C5-N7	-2.34	106.96	109.40
3	A	5101	CMP	O3'-C3'-C2'	2.05	117.61	115.61
3	B	5101	CMP	O3'-C3'-C2'	2.05	117.61	115.61
3	D	5101	CMP	O3'-C3'-C2'	2.05	117.61	115.61
3	C	5101	CMP	O3'-C3'-C2'	2.04	117.61	115.61

There are no chirality outliers.

There are no torsion outliers.

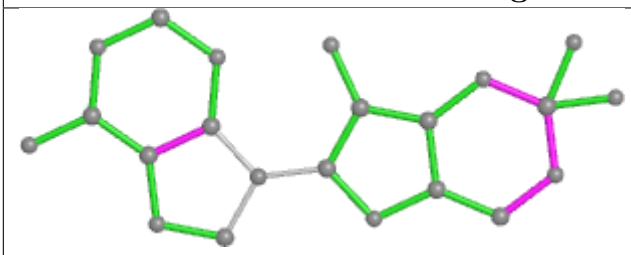
There are no ring outliers.

4 monomers are involved in 8 short contacts:

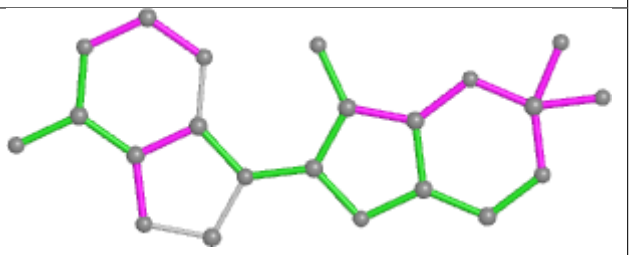
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	5101	CMP	2	0
3	D	5101	CMP	2	0
3	A	5101	CMP	2	0
3	B	5101	CMP	2	0

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

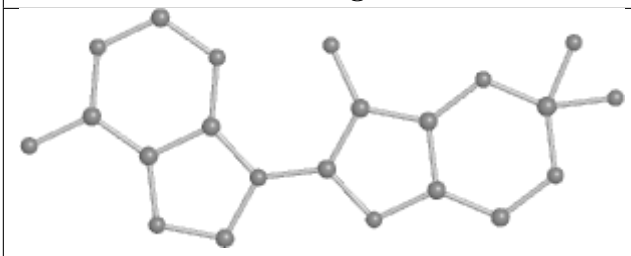
Ligand CMP C 5101



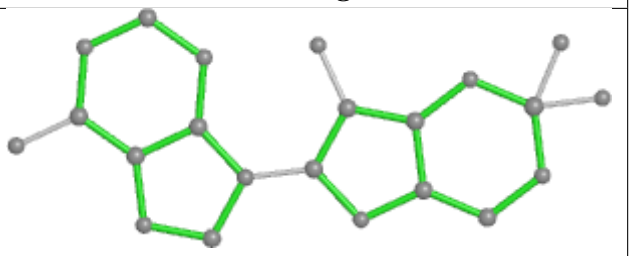
Bond lengths



Bond angles

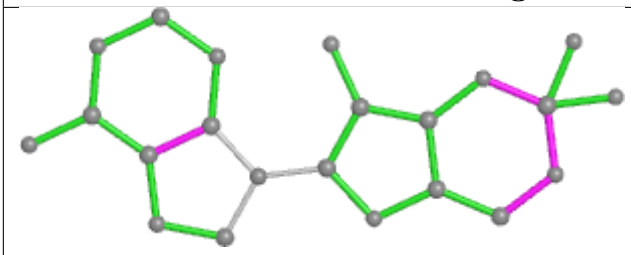


Torsions

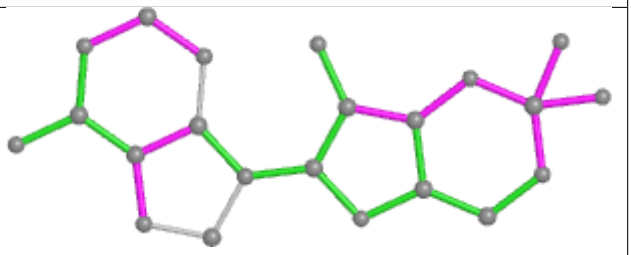


Rings

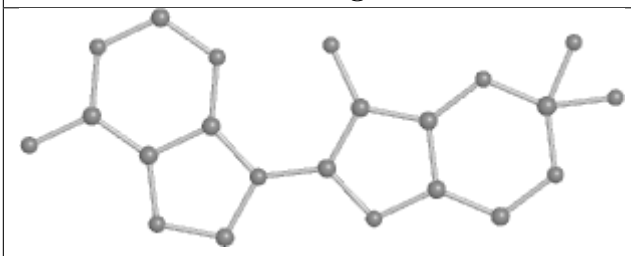
Ligand CMP D 5101



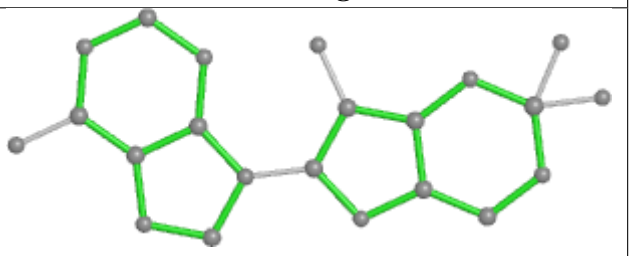
Bond lengths



Bond angles

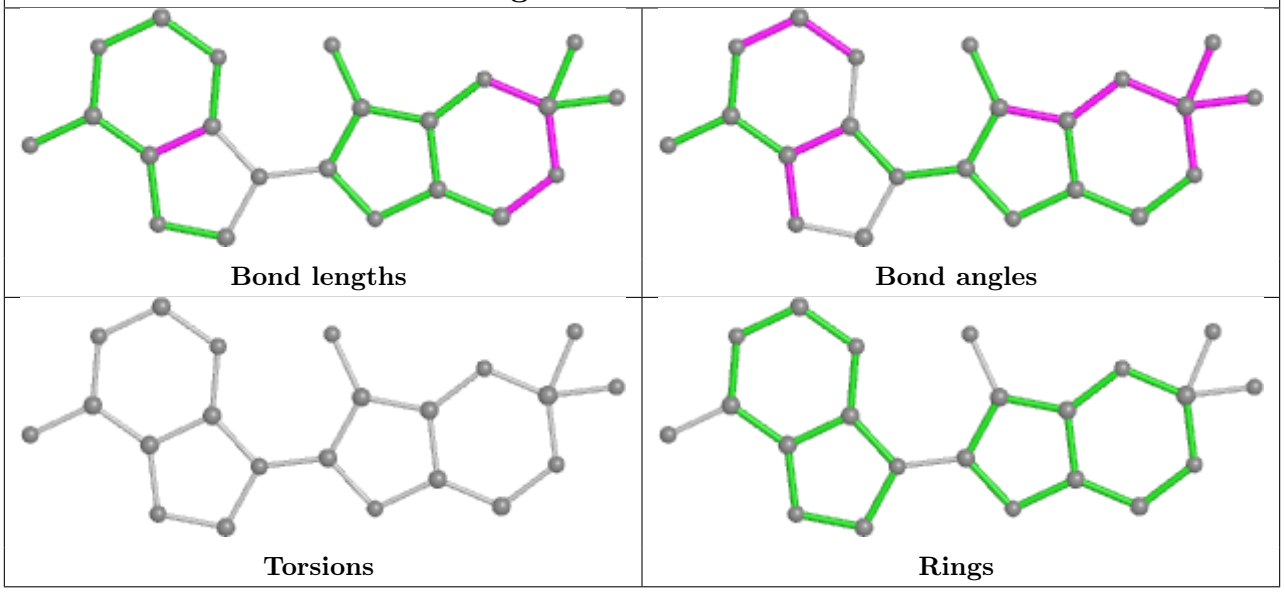


Torsions

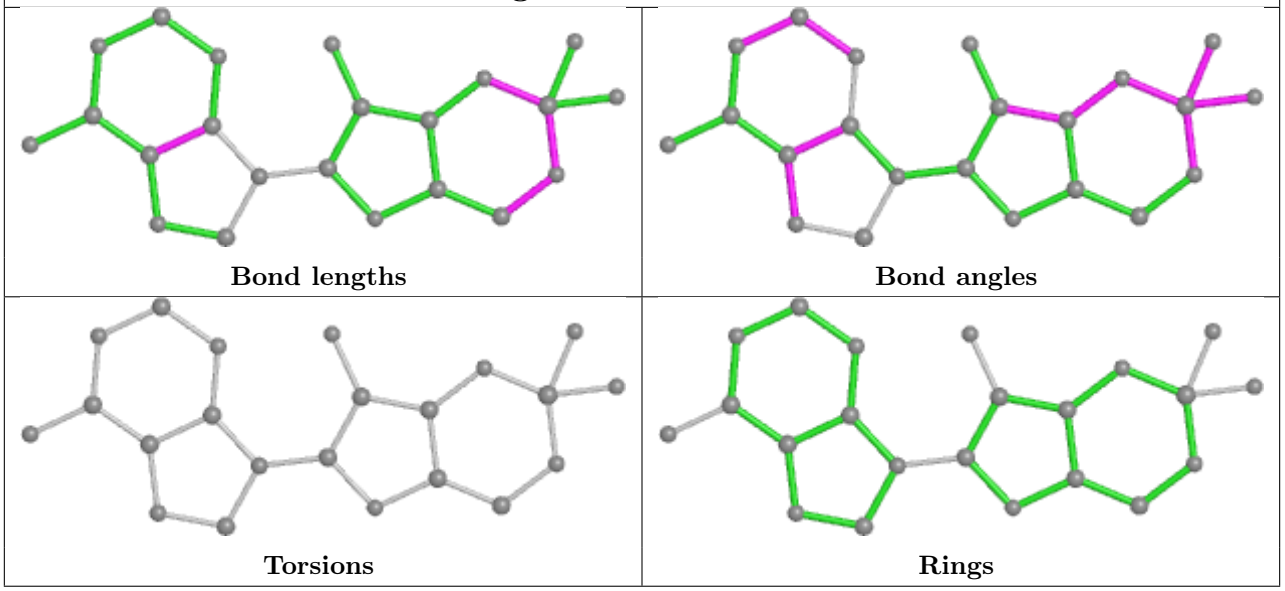


Rings

Ligand CMP A 5101



Ligand CMP B 5101



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

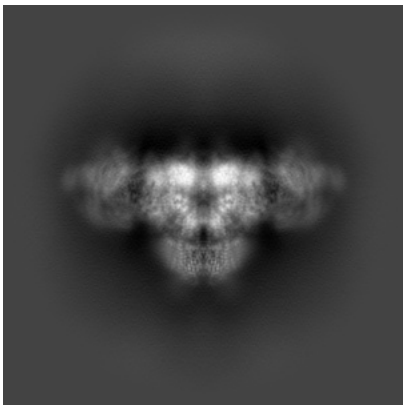
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-40428. These allow visual inspection of the internal detail of the map and identification of artifacts.

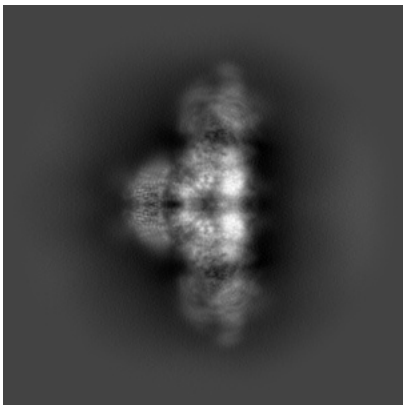
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

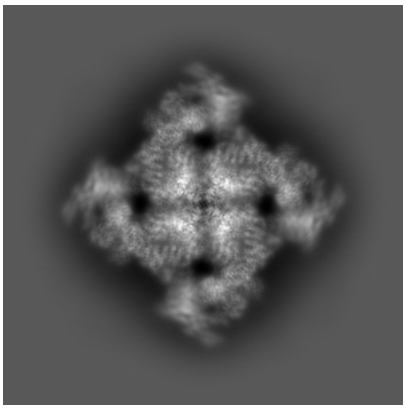
6.1.1 Primary map



X

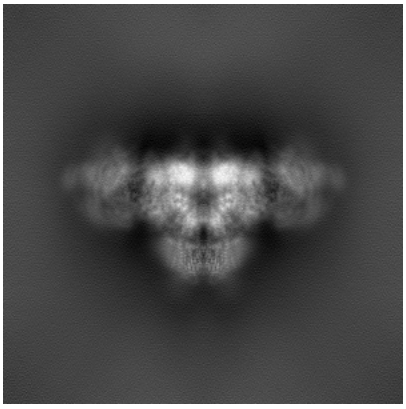


Y

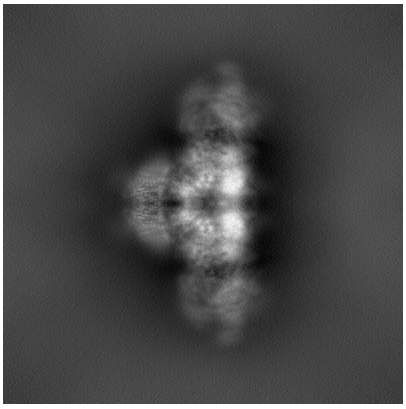


Z

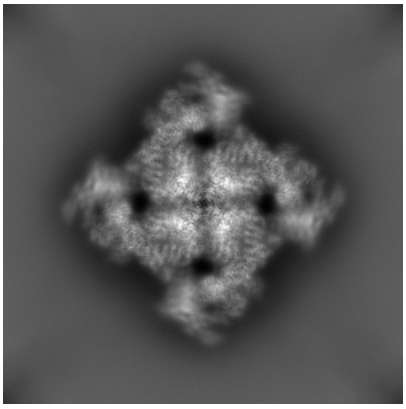
6.1.2 Raw map



X



Y

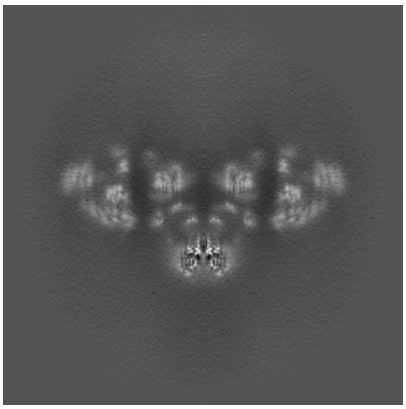


Z

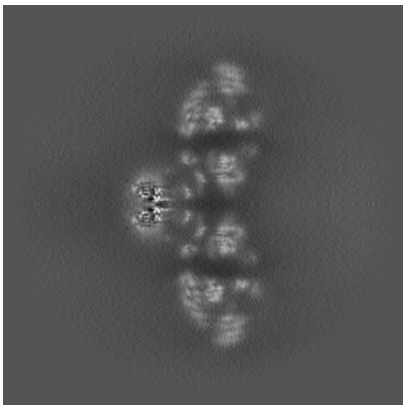
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

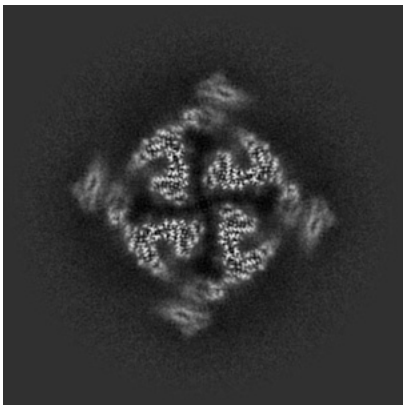
6.2.1 Primary map



X Index: 200

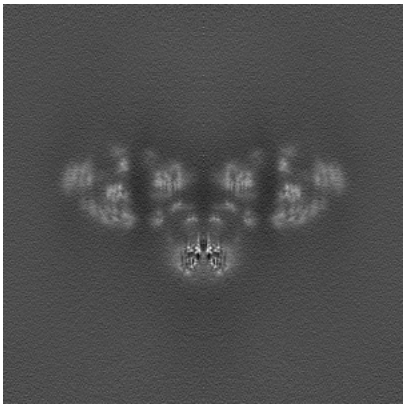


Y Index: 200

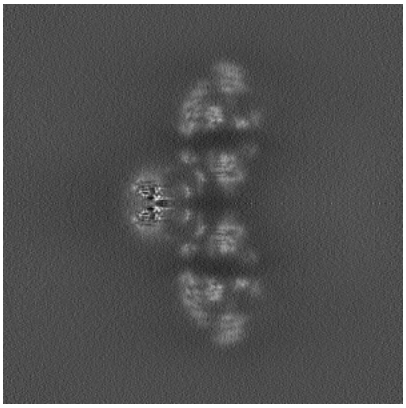


Z Index: 200

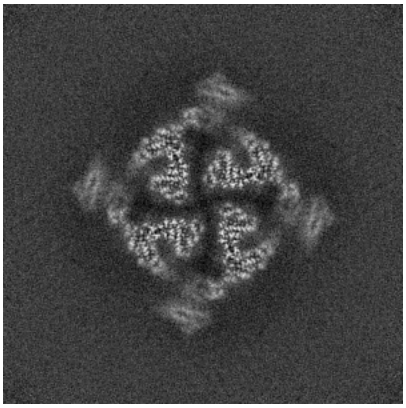
6.2.2 Raw map



X Index: 200



Y Index: 200

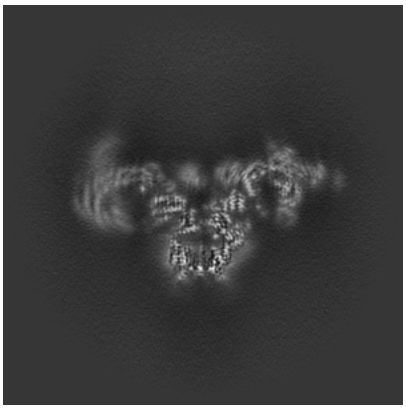


Z Index: 200

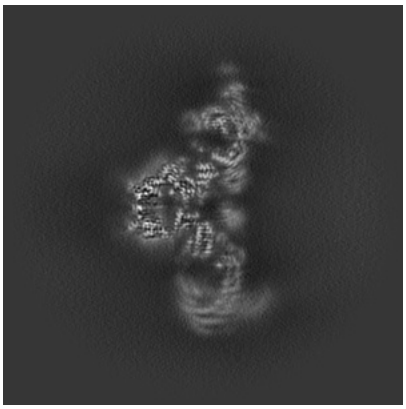
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

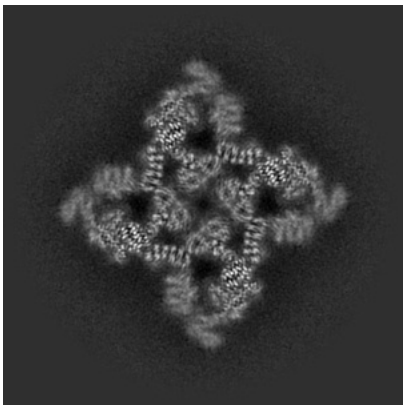
6.3.1 Primary map



X Index: 182

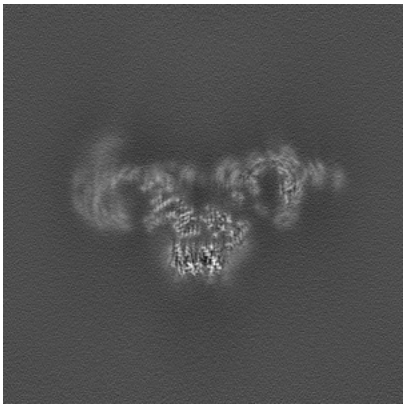


Y Index: 218

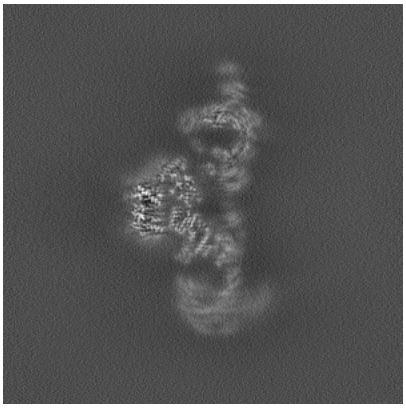


Z Index: 224

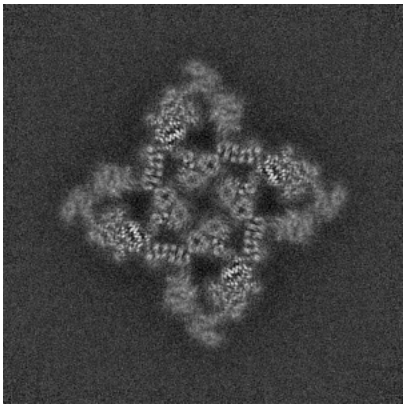
6.3.2 Raw map



X Index: 186



Y Index: 214

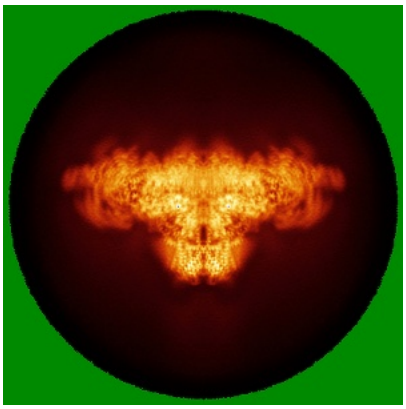


Z Index: 223

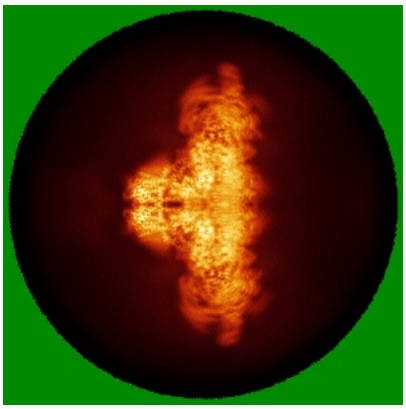
The images above show the largest variance slices of the map in three orthogonal directions.

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

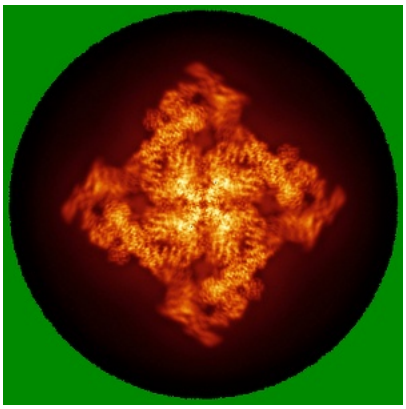
6.4.1 Primary map



X

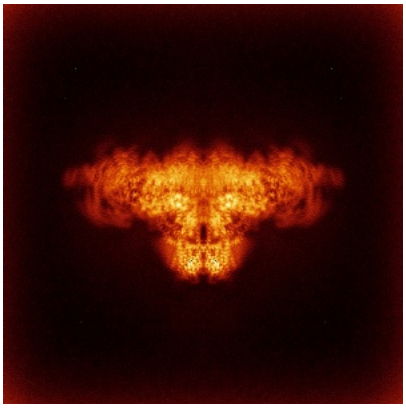


Y

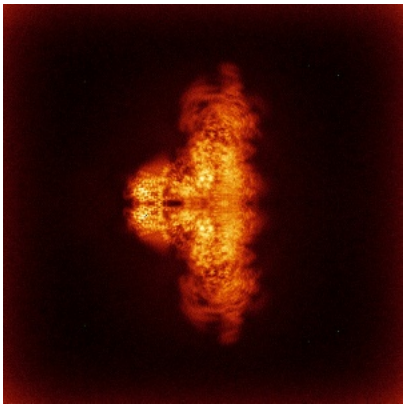


Z

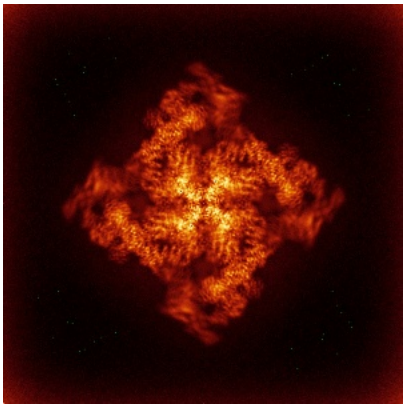
6.4.2 Raw map



X



Y

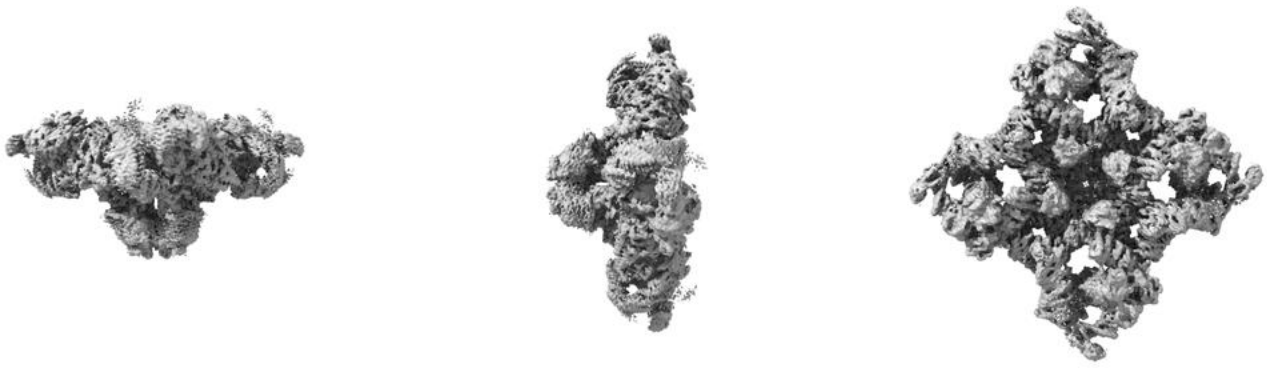


Z

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

6.5 Orthogonal surface views (i)

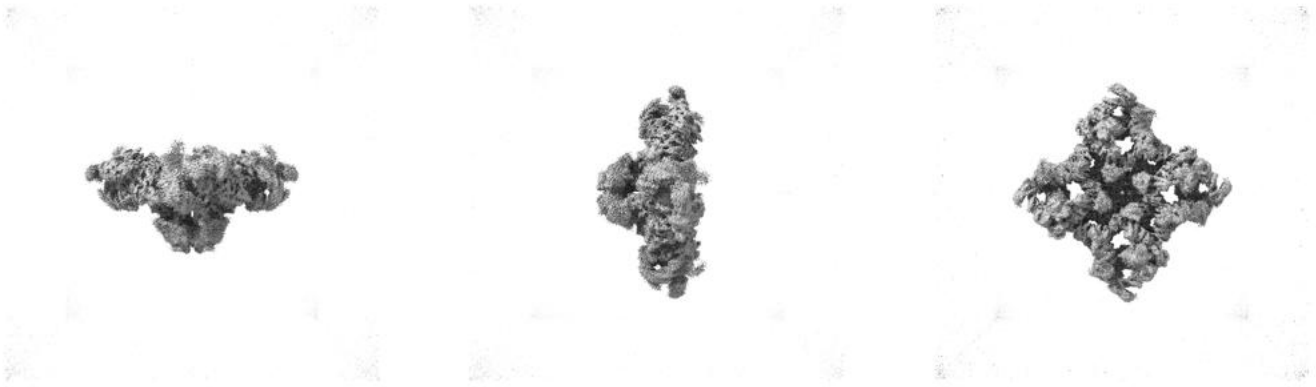
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.126. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

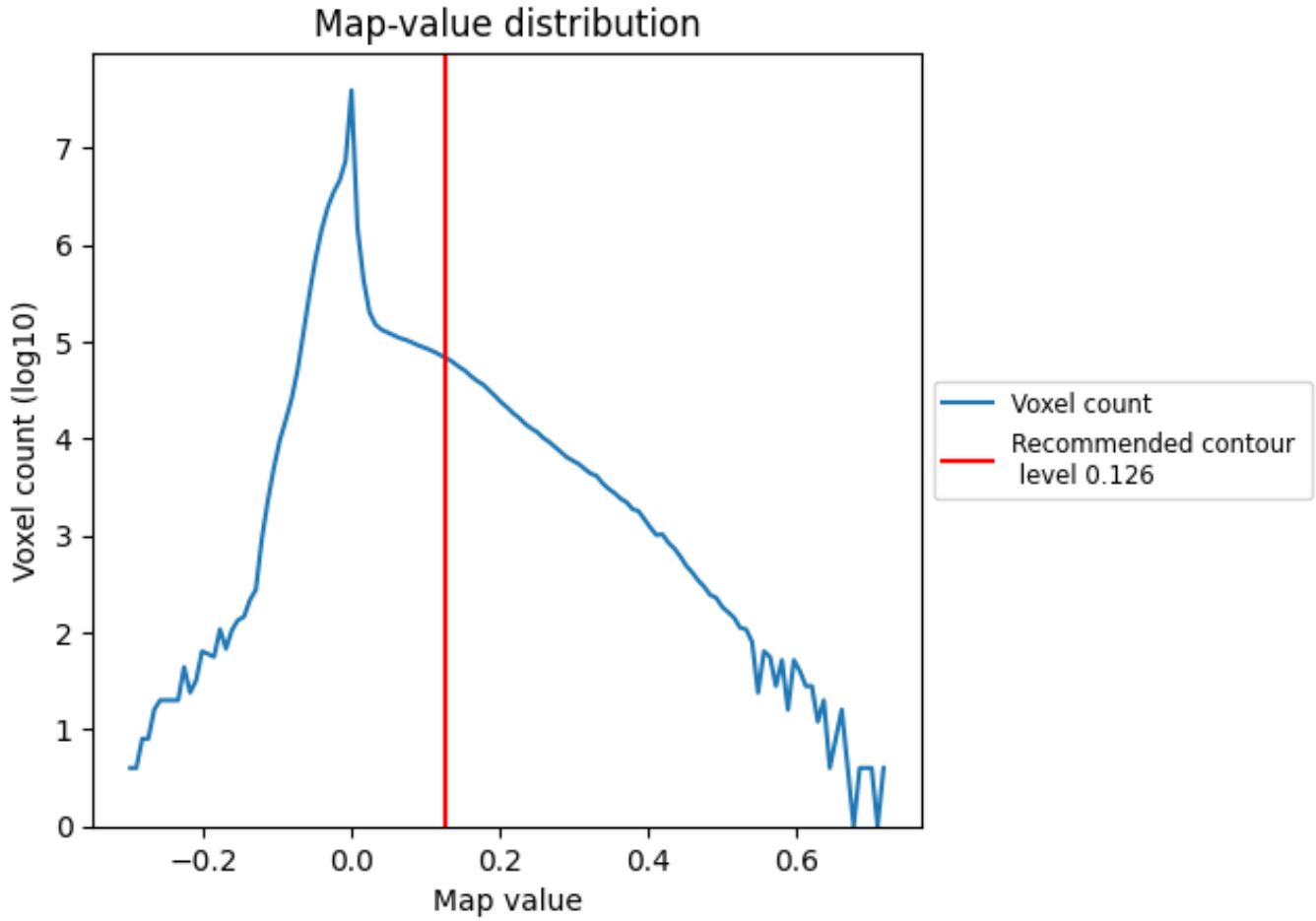
6.6 Mask visualisation (i)

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

7 Map analysis

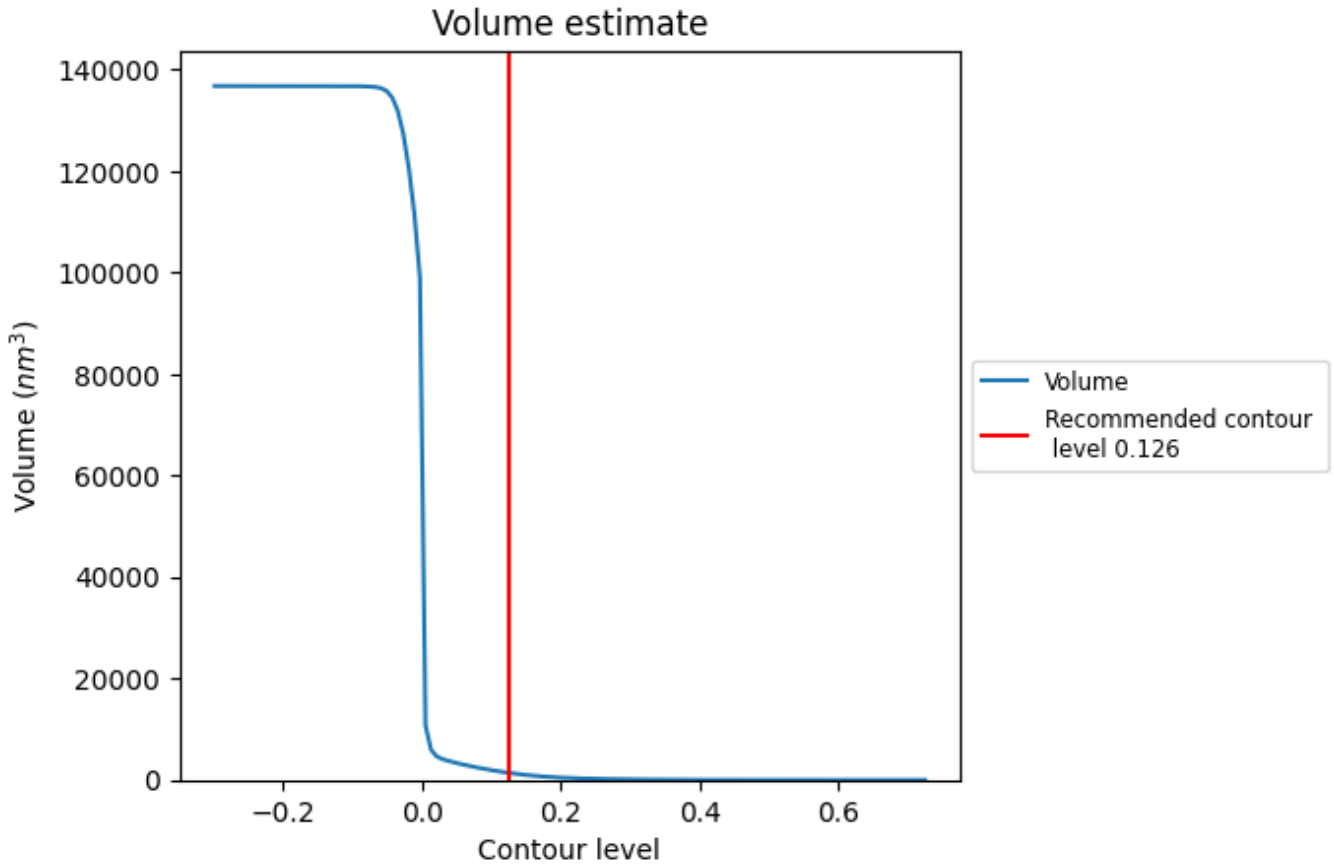
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

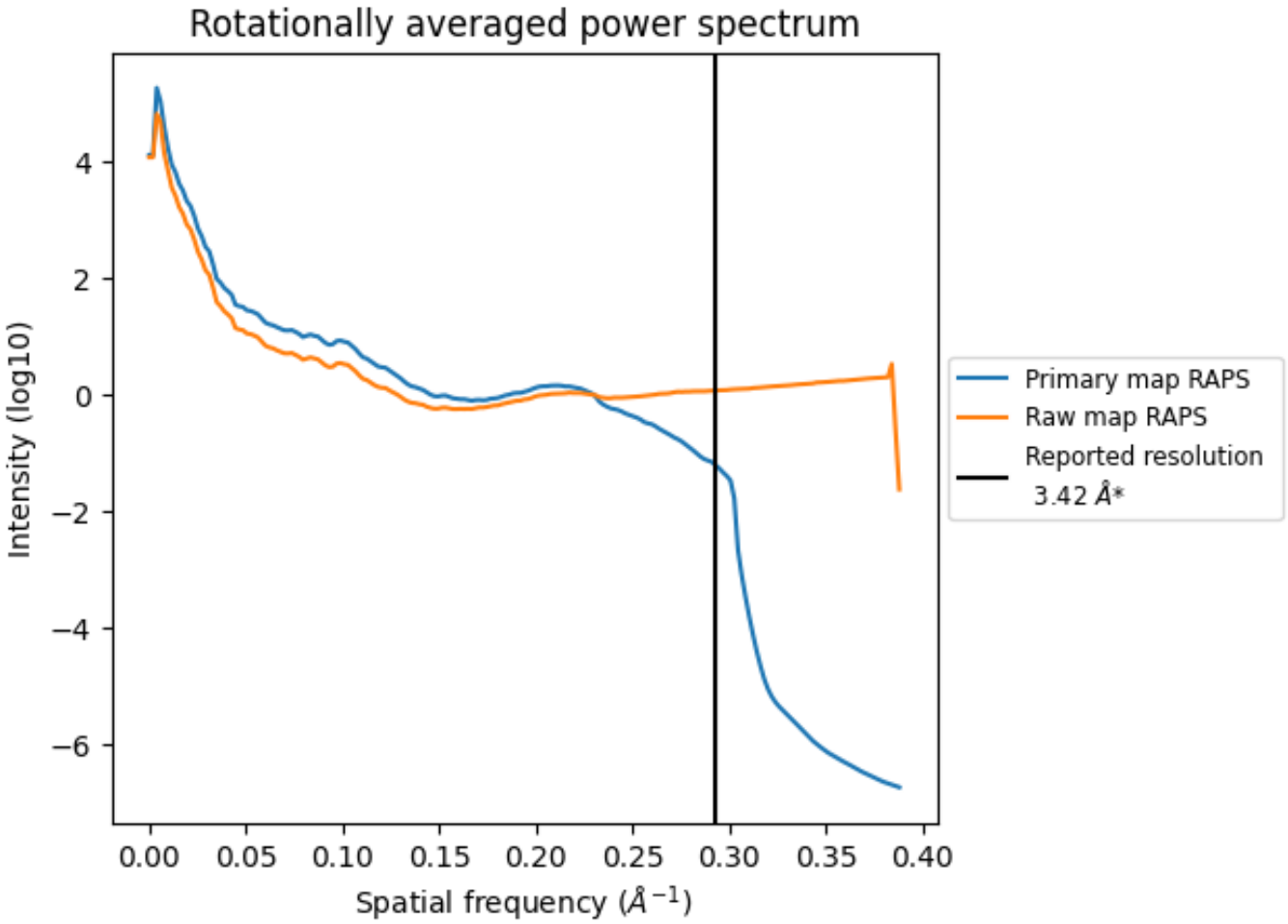
7.2 Volume estimate



The volume at the recommended contour level is 1379 nm^3; this corresponds to an approximate mass of 1246 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)

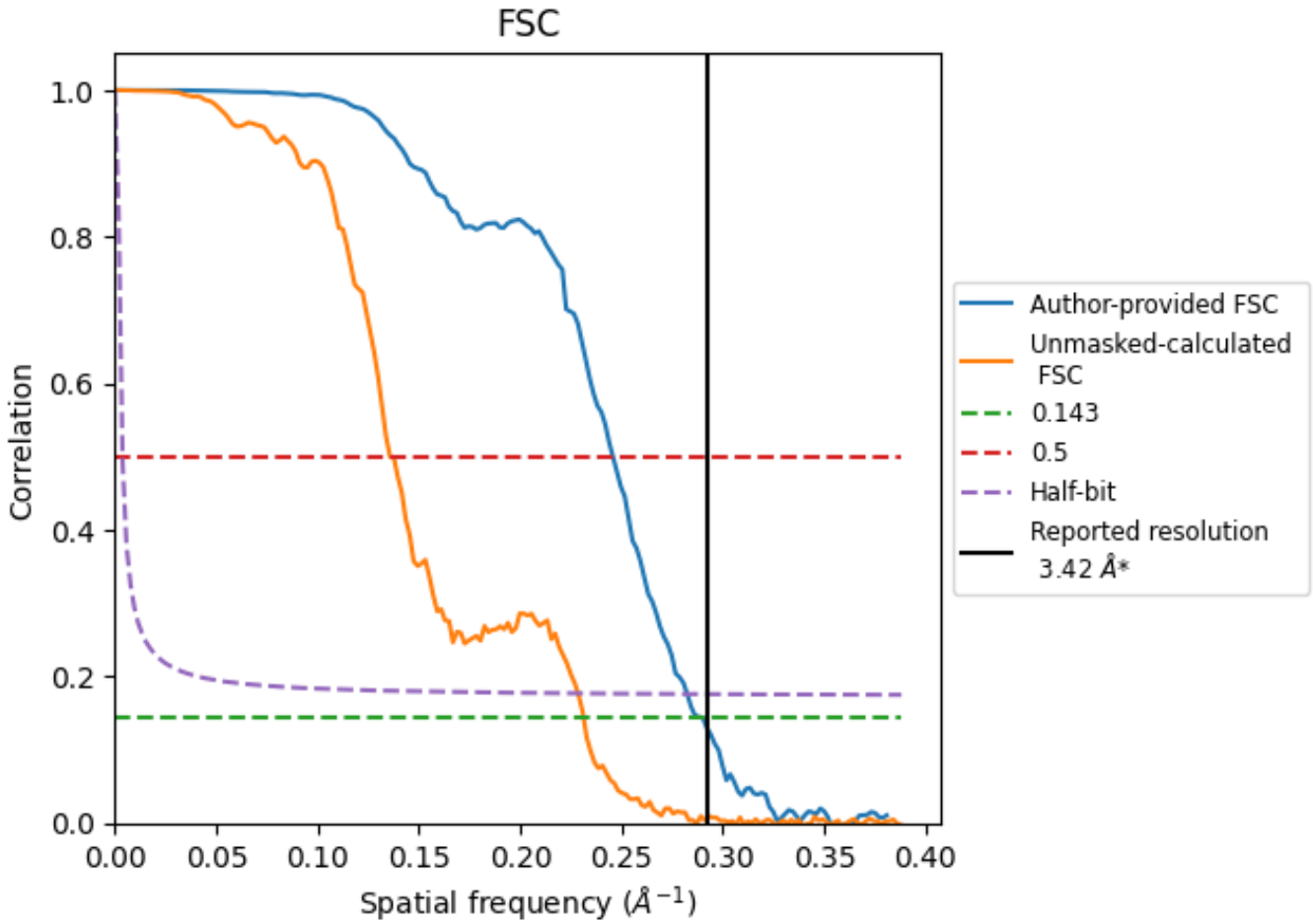


*Reported resolution corresponds to spatial frequency of 0.292 Å^{-1}

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 0.292 Å^{-1}

8.2 Resolution estimates (i)

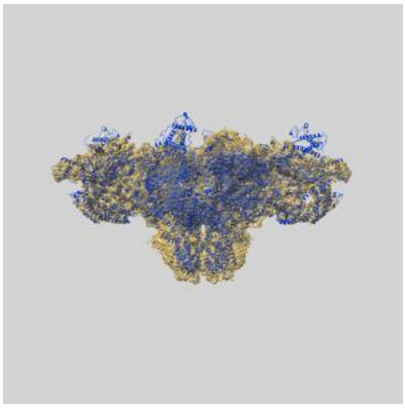
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.42	-	-
Author-provided FSC curve	3.45	4.07	3.54
Unmasked-calculated*	4.32	7.36	4.37

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.32 differs from the reported value 3.42 by more than 10 %

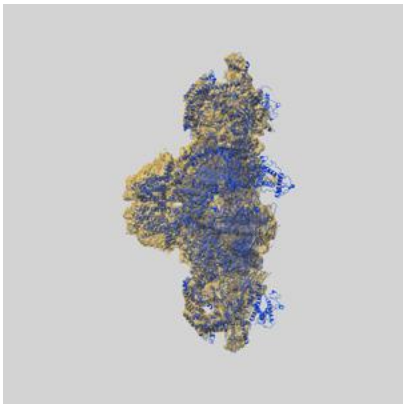
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-40428 and PDB model 8SET. Per-residue inclusion information can be found in section 3 on page 8.

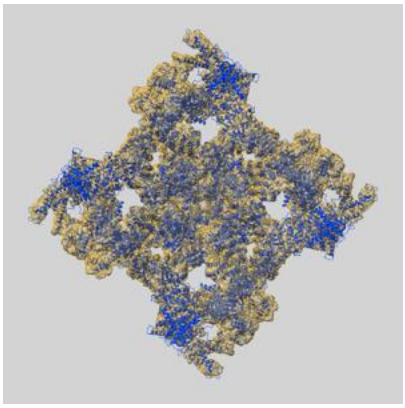
9.1 Map-model overlay



X



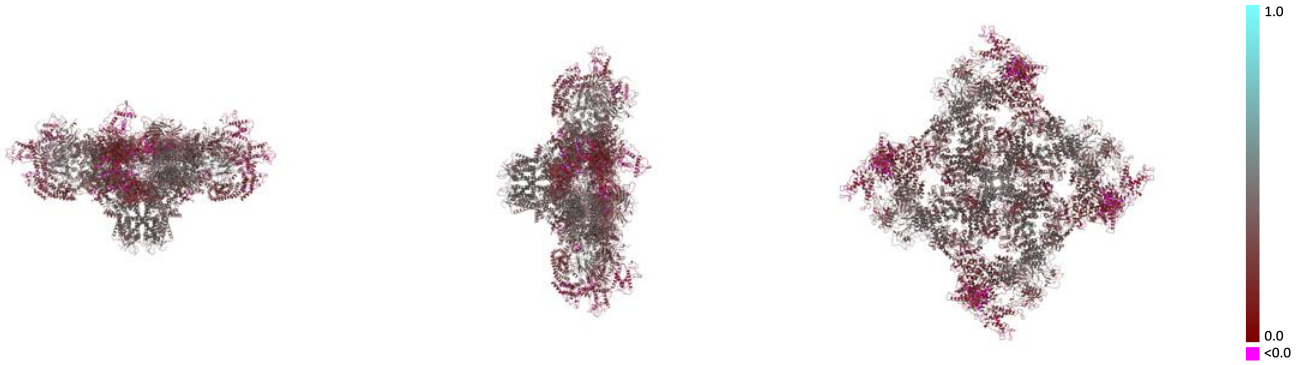
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.126 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.

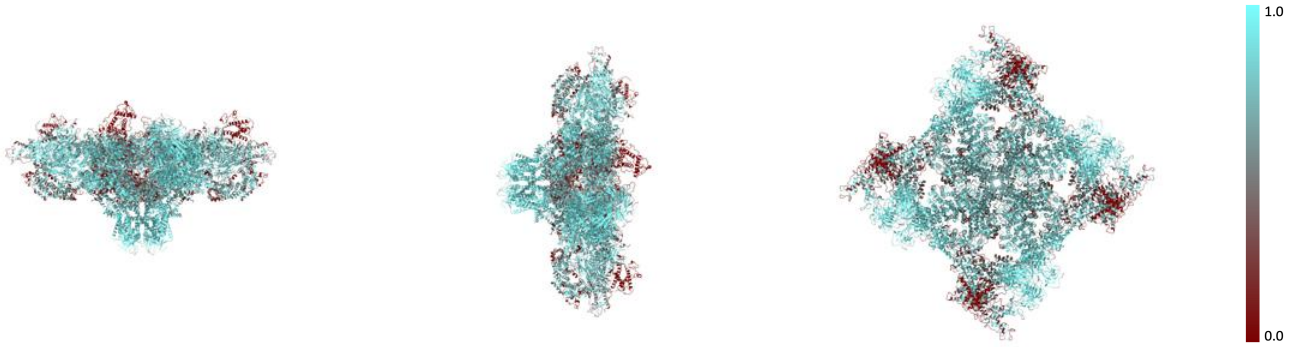
9.2 Q-score mapped to coordinate model (i)



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.

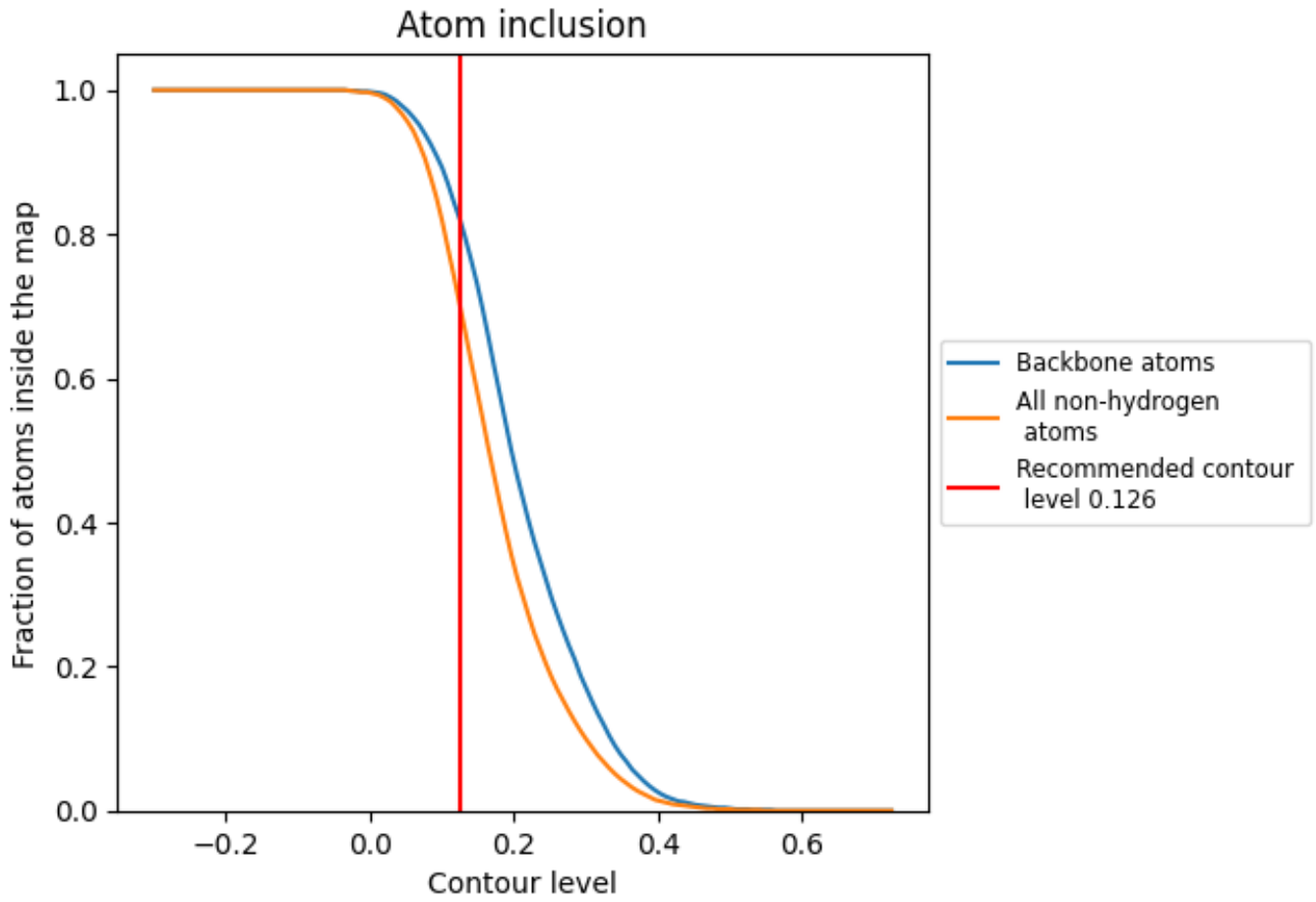
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.126).

9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 70% 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 (0.126) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6990	0.3090
A	0.6960	0.3070
B	0.6960	0.3070
C	0.6960	0.3070
D	0.6960	0.3070
E	0.8410	0.3850
F	0.8410	0.3870
G	0.8410	0.3850
H	0.8410	0.3860