Full wwPDB EM Validation Report

Jul 10, 2023 – 03:00 PM EDT

PDB ID	:	8SEQ
EMDB ID	:	EMD-40425
Title	:	Cryo-EM Structure of RyR1 + AMP
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	:	3.40 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:

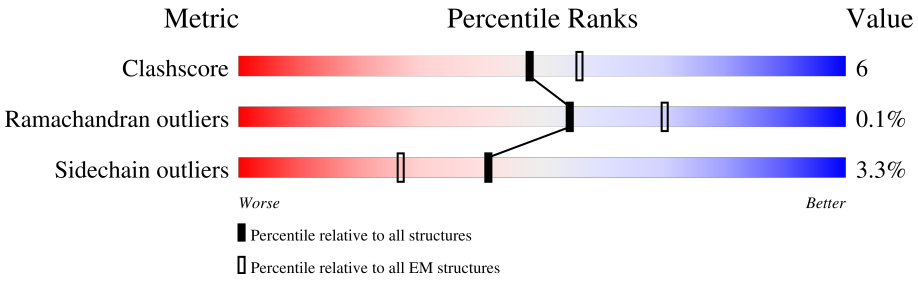
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.40 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	18% 70% 16% • 13%
1	B	5037	18% 70% 16% • 13%
1	C	5037	18% 70% 17% • 13%
1	D	5037	18% 70% 16% • 13%
2	E	350	26% • 69%
2	F	350	26% • 69%
2	G	350	26% • 69%
2	H	350	26% • 69%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 142952 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	4376	Total	C	N	O	S	9	0
			34896	22197	6022	6441	236		
1	B	4376	Total	C	N	O	S	9	0
			34896	22197	6022	6441	236		
1	C	4376	Total	C	N	O	S	9	0
			34896	22197	6022	6441	236		
1	D	4376	Total	C	N	O	S	9	0
			34896	22197	6022	6441	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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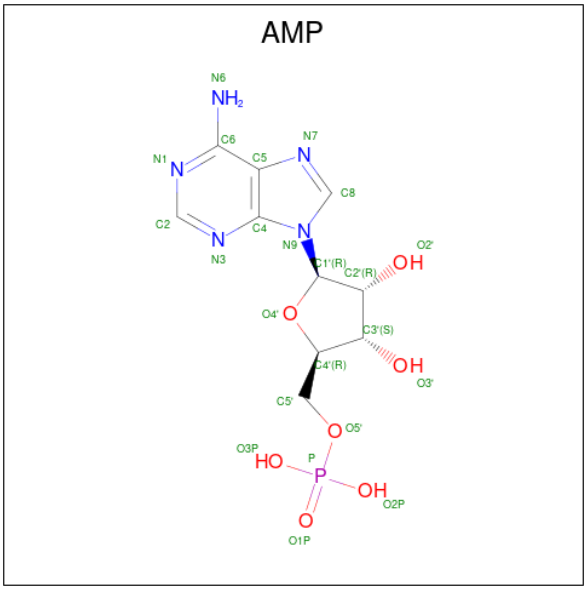
Chain	Residue	Modelled	Actual	Comment	Reference
H	-7	ASN	-	linker	UNP P08515
H	-6	LEU	-	linker	UNP P08515
H	-5	TYR	-	linker	UNP P08515
H	-4	PHE	-	linker	UNP P08515
H	-3	GLN	-	linker	UNP P08515
H	-2	SER	-	linker	UNP P08515
H	-1	ASN	-	linker	UNP P08515
H	0	ALA	-	linker	UNP P08515

- Molecule 3 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			23	10	5	7	1	
3	B	1	Total	C	N	O	P	0
			23	10	5	7	1	
3	C	1	Total	C	N	O	P	0
			23	10	5	7	1	
3	D	1	Total	C	N	O	P	0
			23	10	5	7	1	

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

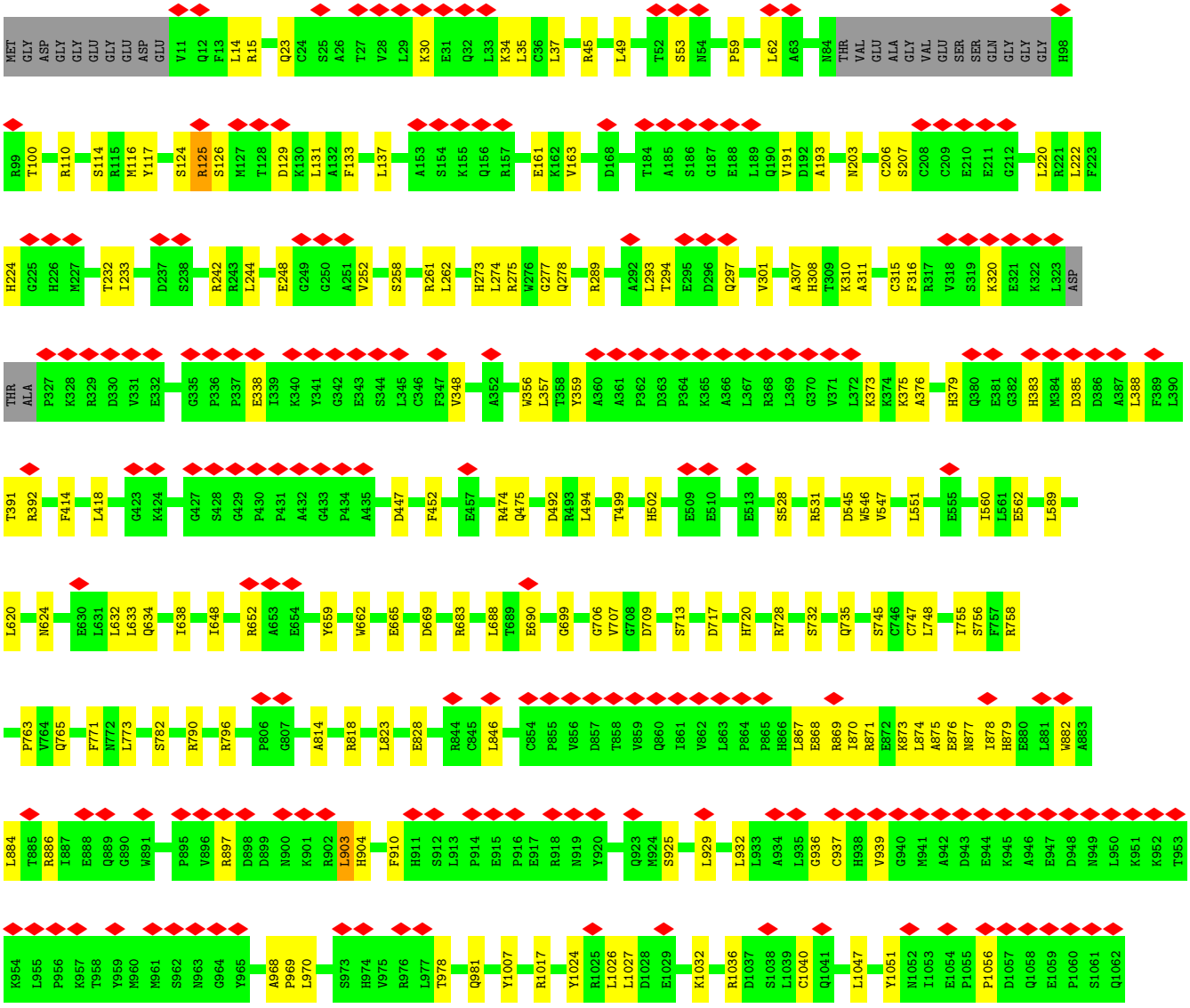
Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total Zn 1 1	0
4	B	1	Total Zn 1 1	0
4	C	1	Total Zn 1 1	0
4	D	1	Total Zn 1 1	0

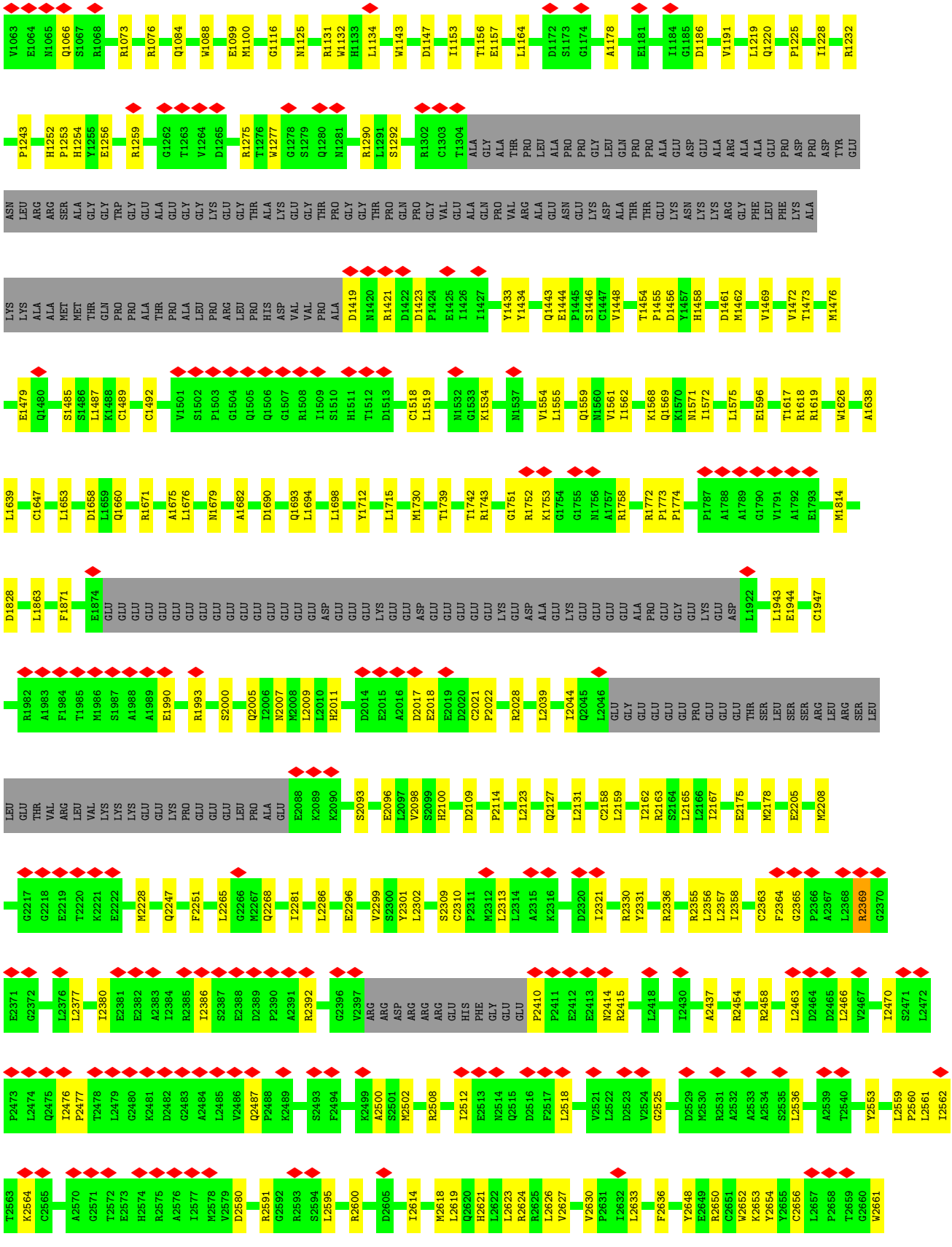
3 Residue-property plots (i)

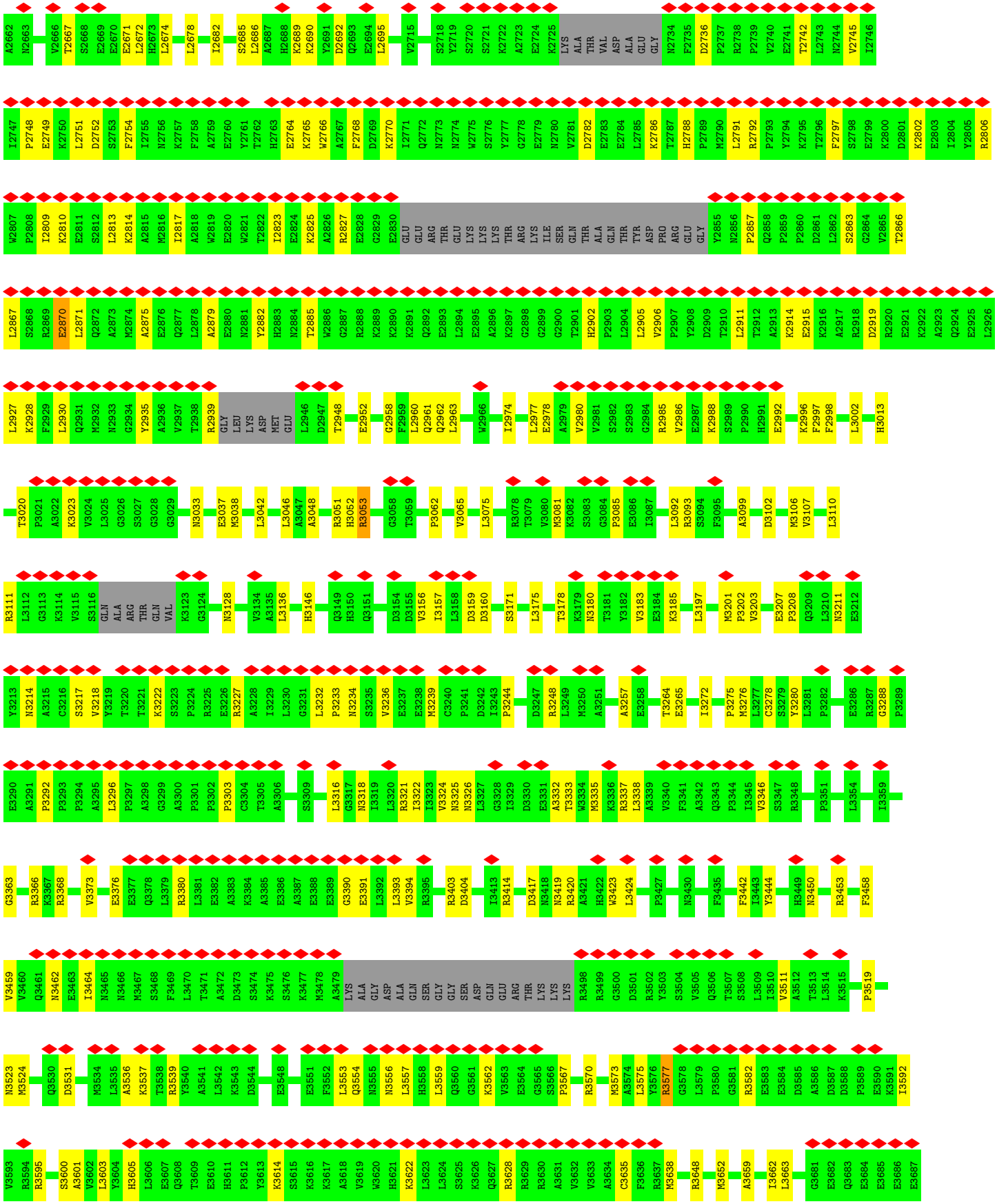
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

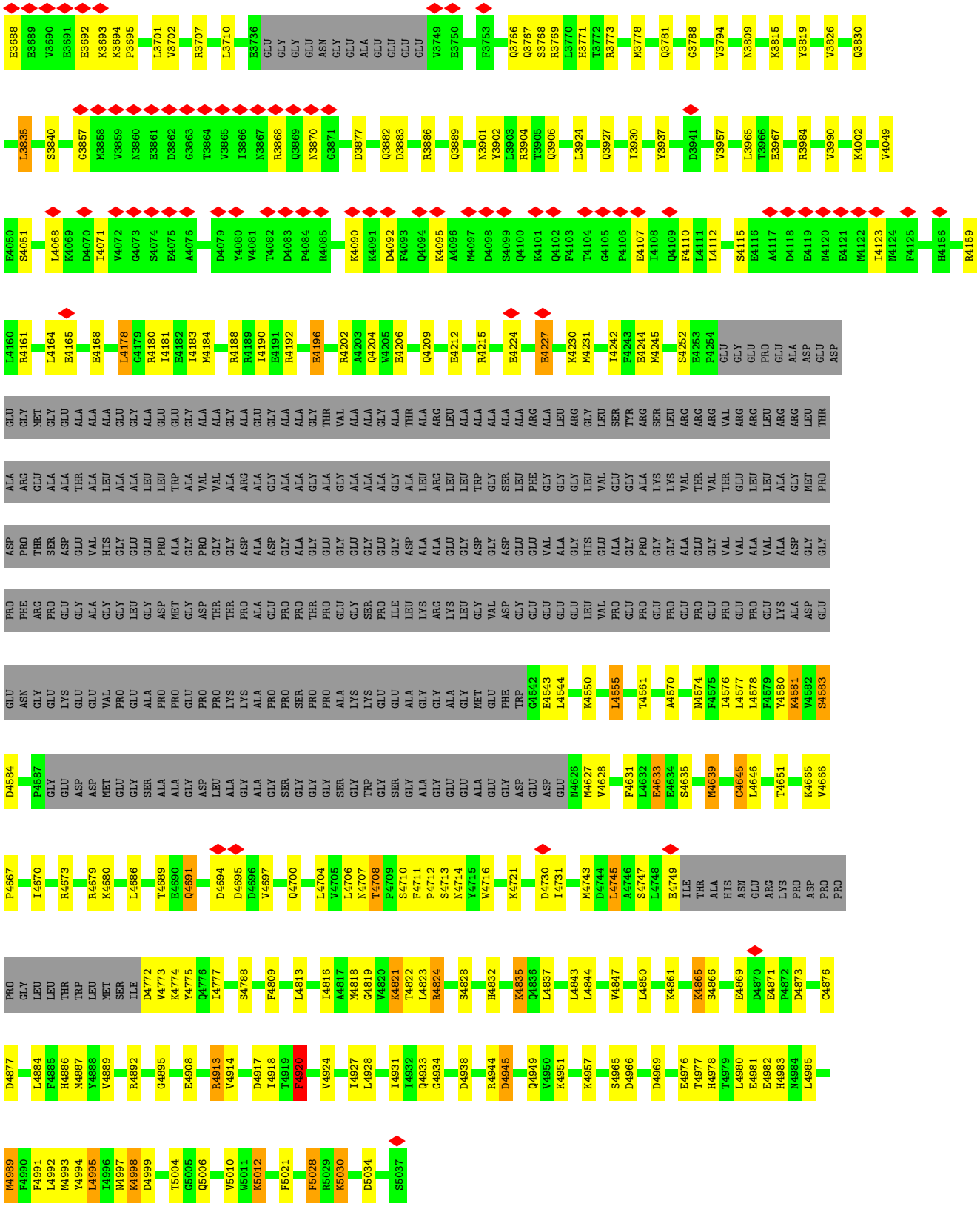
- Molecule 1: Ryanodine receptor 1

Chain A:



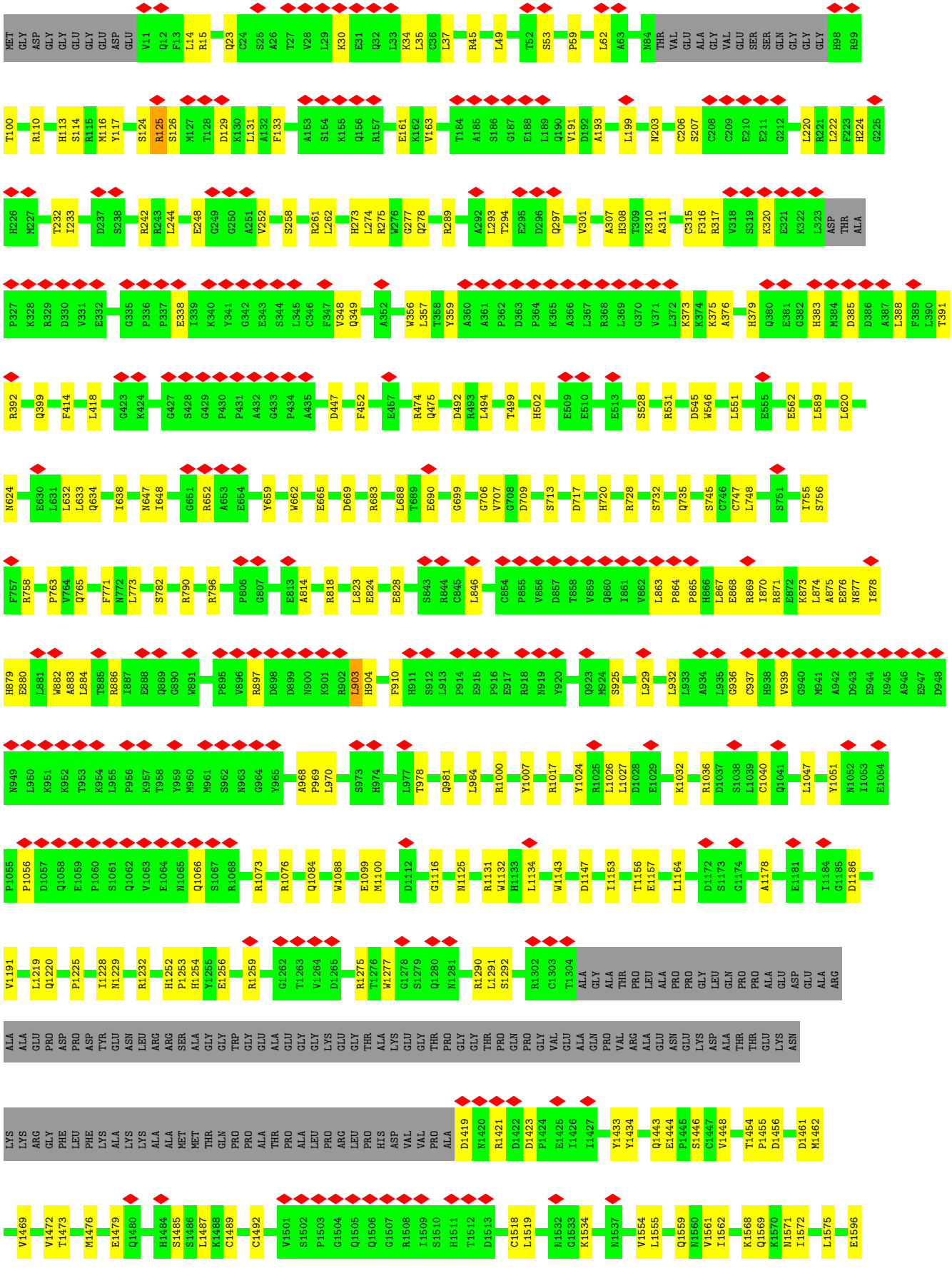

V1063 E1064 N1065 Q1066 S1067 R1068 R1073 R1076 Q1084 W1088 E1099 M1100 G1116 N1125 R1131 W1132 H1133 L1134 W1143 D1147 I1153 T1156 E1157 L1164 D1172 S1173 G1174 A1178 E1181 I1184 G1185 D1186 V1191 L1219 Q1220 P1225 I1228 R1232
P1243 H1252 P1253 H1254 Y1255 E1256 R1259 G1262 T1263 V1264 D1265 R1275 T1276 W1277 G1278 S1279 Q1280 N1281 R1290 L1291 S1292 R1302 C1303 T1304 ALA GLY ALA THR PRO LEU ALA ALA PRO PRO GLY LEU GLN PRO PRO ALA GLU ASP GLU ALA ARG ALA ALA GLU PRO ASP PRO ASP TYR GLU
ASN LEU ARG ARG SER ALA GLY GLY TRP GLY GLU ALA GLU GLY GLY LYS GLU GLY THR ALA LYS GLU GLY THR PRO GLY GLY THR PRO GLN PRO GLY VAL GLU ALA GLN PRO VAL ARG ALA GLU ASN GLU LYS ASP ALA THR THR GLU LYS ASN LYS LYS ARG GLY PHE LEU PHE LYS ALA
LYS LYS ALA ALA MET MET THR GLN PRO PRO ALA THR PRO ALA LEU PRO ARG LEU PRO HIS ASP VAL VAL PRO ALA D1419 N1420 R1421 D1422 D1423 P1424 E1425 I1426 I1427 Y1433 Y1434 Q1443 E1444 P1445 S1446 C1447 V1448 T1454 P1455 D1456 Y1457 H1458 D1461 M1462 V1469 V1472 T1473 M1476
E1479 Q1480 S1485 S1486 L1487 K1488 C1489 C1492 Y1501 S1502 P1503 G1504 Q1505 Q1506 G1507 R1508 I1509 S1510 H1511 T1512 D1513 C1518 L1519 N1532 G1533 K1534 N1537 V1554 L1555 Q1559 N1560 V1561 I1562 K1568 Q1569 K1570 N1571 I1572 L1575 E1596 T1617 R1618 R1619 W1626 A1638
L1639 C1647 L1653 D1658 L1659 Q1660 R1671 A1675 L1676 N1679 A1682 D1690 Q1693 L1694 L1698 Y1712 L1715 M1730 T1739 T1742 R1743 G1751 R1752 K1753 G1754 G1755 N1756 A1757 R1758 R1772 P1773 P1774 P1787 A1788 A1789 G1790 V1791 A1792 E1793 M1814
D1828 L1863 F1871 E1874 GLU GLU GLU


A2662 N2663 V2666 T2667 S2668 E2669 E2670 E2671 L2672 H2673 L2674 L2678 I2682 S2685 L2686 A2687 H2688 K2689 K2690 Y2691 D2692 Q2693 E2694 L2695 V2715 S2718 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 F2758 A2759 E2760 Y2761 T2762 H2763 E2764 K2765 W2766 A2767 F2768 D2769 K2770 I2771 Q2772 N2773 N2774 W2775 S2776 Y2777 G2778 E2779 N2780 V2781 D2782 E2783 E2784 L2785 K2786 T2787 H2788 P2789 M2790 L2791 R2792 P2793 Y2794 K2795 T2796 F2797 S2798 E2799 K2800 D2801 K2802 E2803 I2804 Y2805 R2806
W2807 P2808 I2809 K2810 E2811 S2812 L2813 K2814 A2815 M2816 I2817 A2818 W2819 E2820 W2821 T2822 I2823 E2824 K2825 A2826 R2827 E2828 G2829 E2830 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 E2952 G2958 F2959 L2960 Q2961 Q2962 L2963 W2966 I2974 L2977 E2978 A2979 V2980 V2981 S2982 S2983 G2984 R2985 V2986 E2987 K2988 S2989 P2990 H2991 E2992 K2996 F2997 F2998 L3002 H3013
T3020 P3021 A3022 K3023 V3024 L3025 G3026 S3027 G3028 G3029 N3033 E3037 M3038 L3042 L3046 A3047 A3048 R3051 H3052 R3053 G3058 T3059 P3062 V3065 L3075 R3078 T3079 V3080 M3081 K3082 S3083 G3084 P3085 E3086 I3087 L3092 R3093 S3094 F3095 A3099 D3102 M3106 V3107 L3110
R3111 L3112 G3113 K3114 V3115 S3116 GLN ALA ARG THR GLN VAL K3123 G3124 M3128 V3134 A3135 L3136 H3146 Q3149 H3150 Q3151 D3154 D3155 V3156 I3157 L3158 D3159 D3160 S3171 L3175 T3178 K3179 N3180 T3181 Y3182 V3183 E3184 K3185 L3197 M3201 P3202 V3203 E3207 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 C3240 P3241 D3242 I3243 P3244 D3247 R3248 L3249 M3250 A3251 A3257 E3258 T3264 E3265 I3272 P3275 M3276 L3277 C3278 S3279 Y3280 L3281 P3282 E3286 R3287 G3288 P3289
E3290 A3291 P3292 P3293 P3294 A3295 L3296 P3297 A3298 G3299 A3300 P3301 P3302 P3303 C3304 T3305 A3306 S3309 L3316 G3317 N3318 I3319 L3320 R3321 I3322 I3323 V3324 N3325 N3326 L3327 G3328 I3329 D3330 E3331 A3332 T3333 W3334 M3335 K3336 R3337 L3338 A3339 V3340 F3341 A3342 Q3343 P3344 I3345 V3346 S3347 R3348 P3351 L3354 I3359
G3363 R3366 K3367 R3368 V3373 E3376 E3377 Q3378 L3379 R3380 L3381 E3382 A3383 K3384 A3385 E3386 A3387 E3388 E3389 G3390 E3391 L3392 L3393 V3394 R3395 R3403 D3404 I3413 R3414 D3417 N3418 N3419 R3420 A3421 H3422 W3423 L3424 P3427 N3430 F3435 F3442 I3443 Y3444 H3449 N3450 R3453 F3458
V3459 V3460 Q3461 N3462 E3463 I3464 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 T3507 S3508 L3509 I3510 V3511 A3512 T3513 L3514 K3515 P3519
N3523 M3524 Q3530 D3531 M3534 L3535 A3536 K3537 T3538 R3539 Y3540 A3541 L3542 K3543 D3544 E3548 E3551 F3552 L3553 Q3554 N3555 N3556 L3557 H3558 L3559 Q3560 G3561 K3562 V3563 E3564 G3565 S3566 P3567 R3570 M3573 A3574 L3575 Y3576 R3577 G3578 L3579 P3580 G3581 R3582 E3583 E3584 D3585 A3586 D3587 D3588 P3589 E3590 K3591 I3592
V3593 R3594 R3595 S3600 A3601 V3602 L3603 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 R3648 M3652 A3659 I3662 L3663 G3681 E3682 Q3683 E3684 E3685 E3686 E3687



• Molecule 1: Ryanodine receptor 1

Chain B:


MET GLY ASP GLY GLY GLU GLY GLU ASP GLU V11 Q12 F13 L14 R15 Q23 C24 S25 A26 T27 V28 L29 K30 E31 Q32 L33 K34 L35 C36 L37 R45 L49 T52 S53 P59 L62 A63 N84 THR VAL GLU ALA GLY VAL GLU SER SER GLN GLY GLY GLY H98 R99
T100 R110 H113 S114 R115 M116 Y117 S124 R125 S126 M127 T128 D129 K130 L131 A132 F133 A153 S154 K155 Q156 R157 E161 K162 V163 T184 A185 S186 G187 E188 L189 Q190 V191 D192 A193 L199 N203 C206 S207 C208 C209 E210 E211 G212 L220 R221 L222 F223 H224 G225
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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 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
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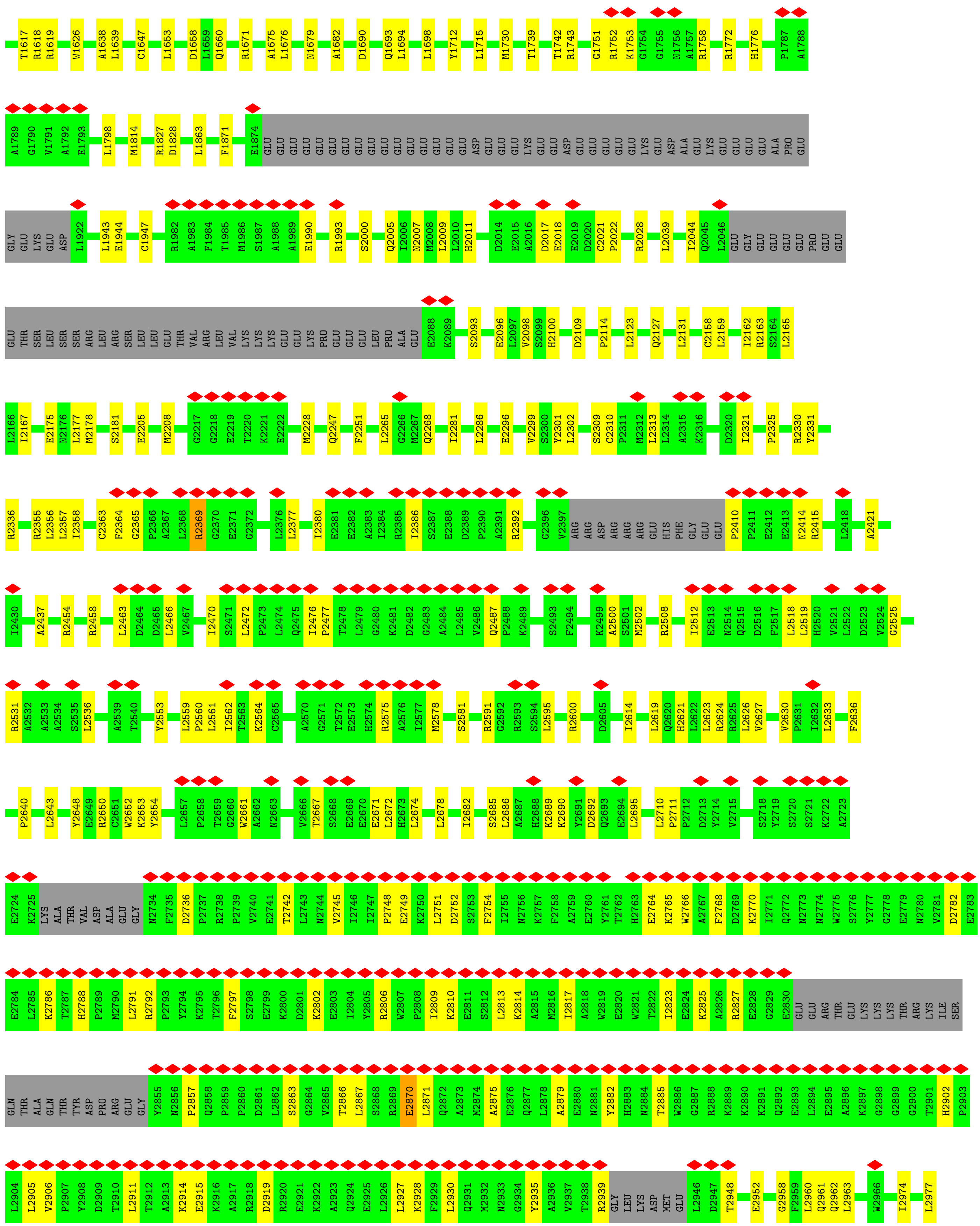
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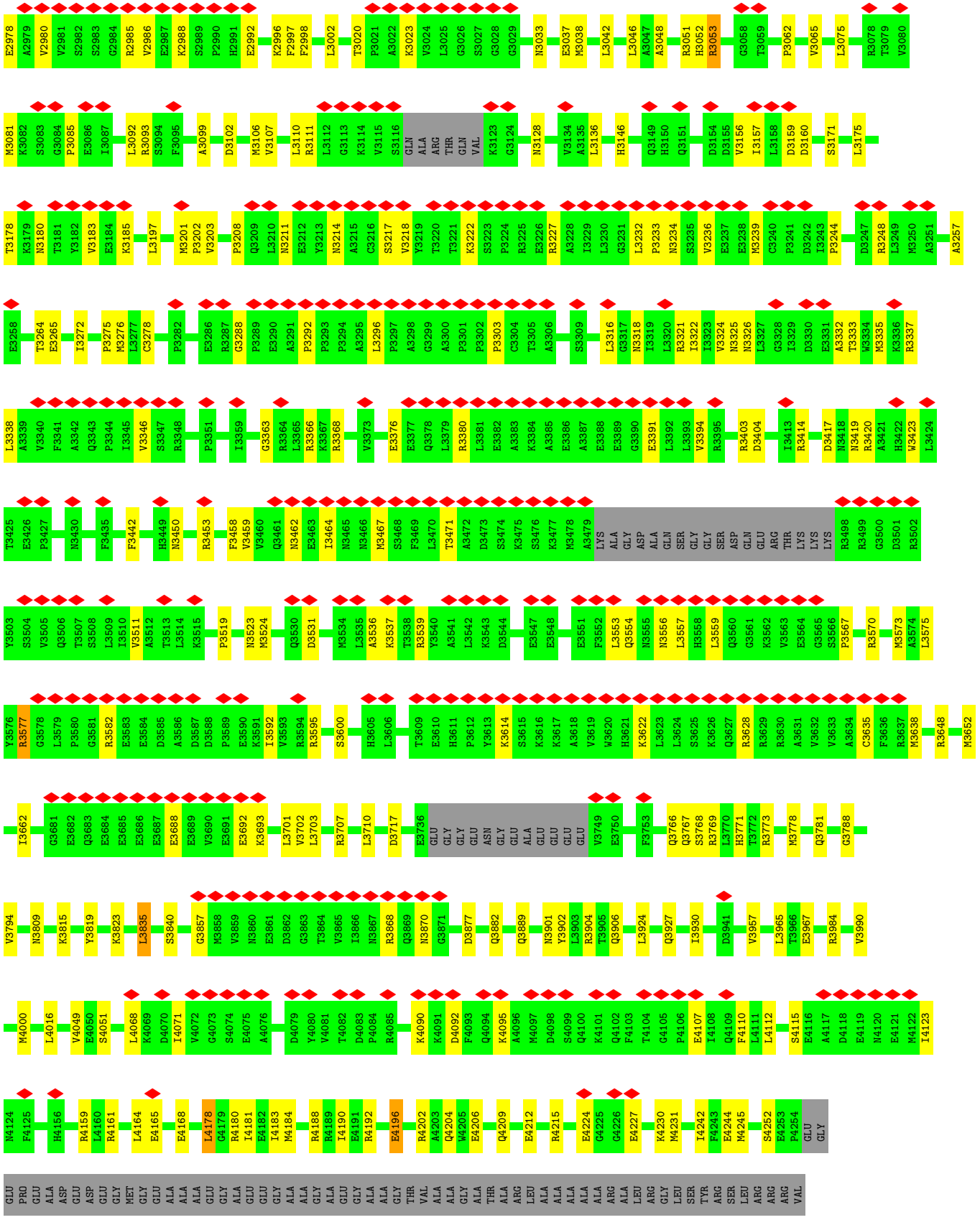
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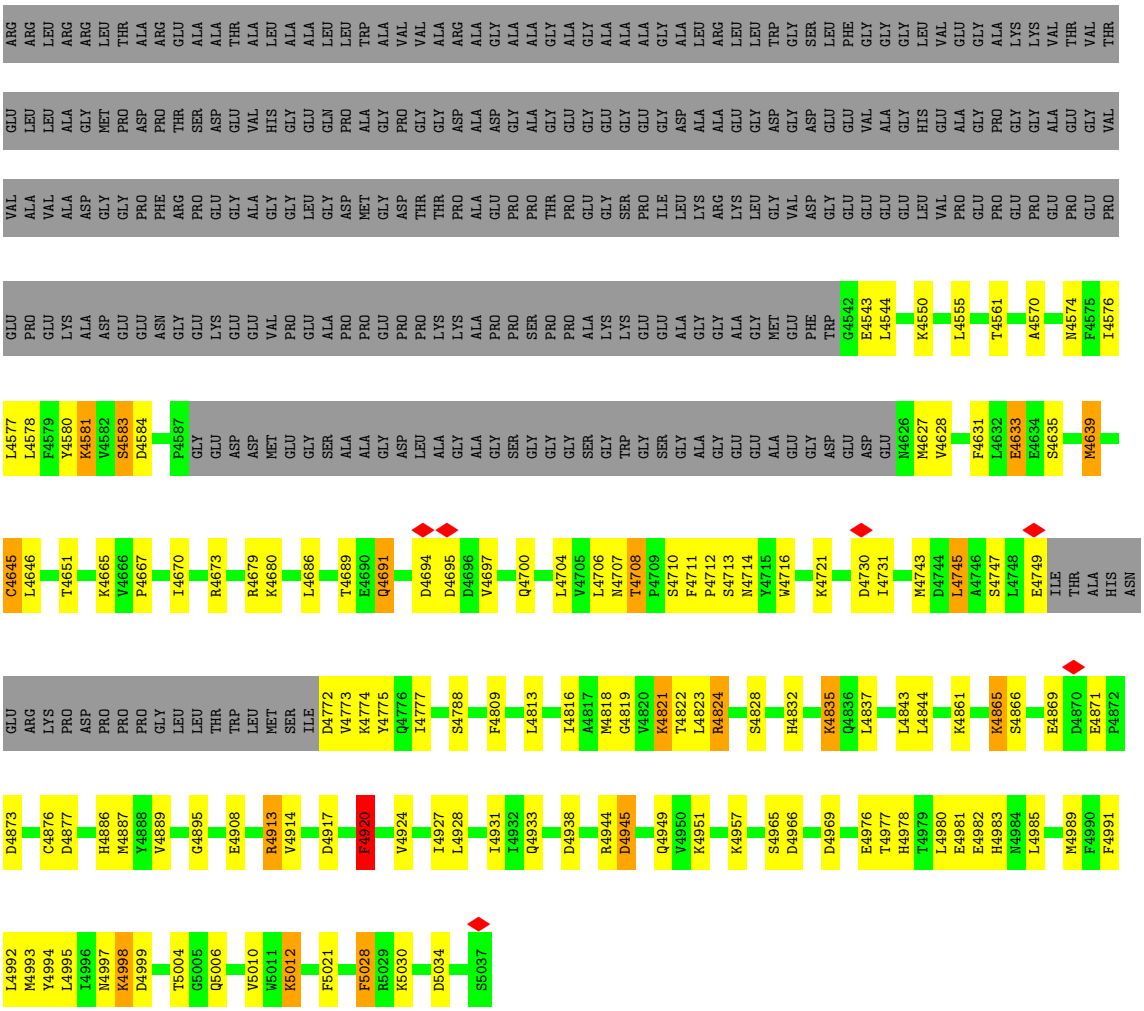
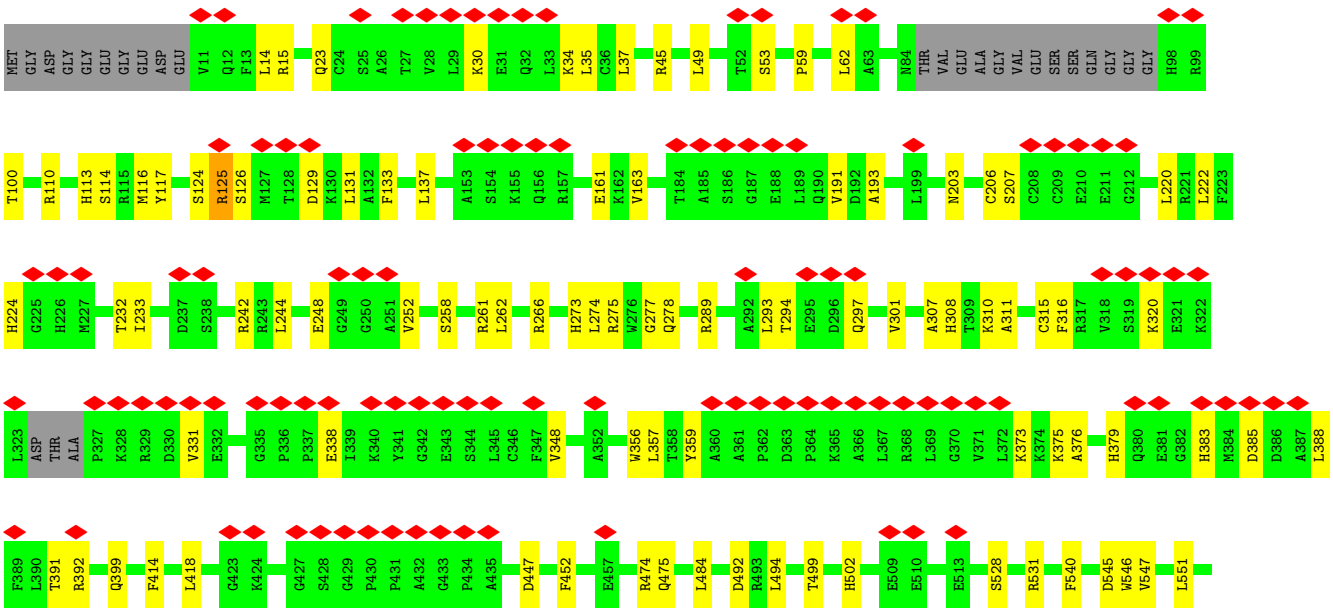
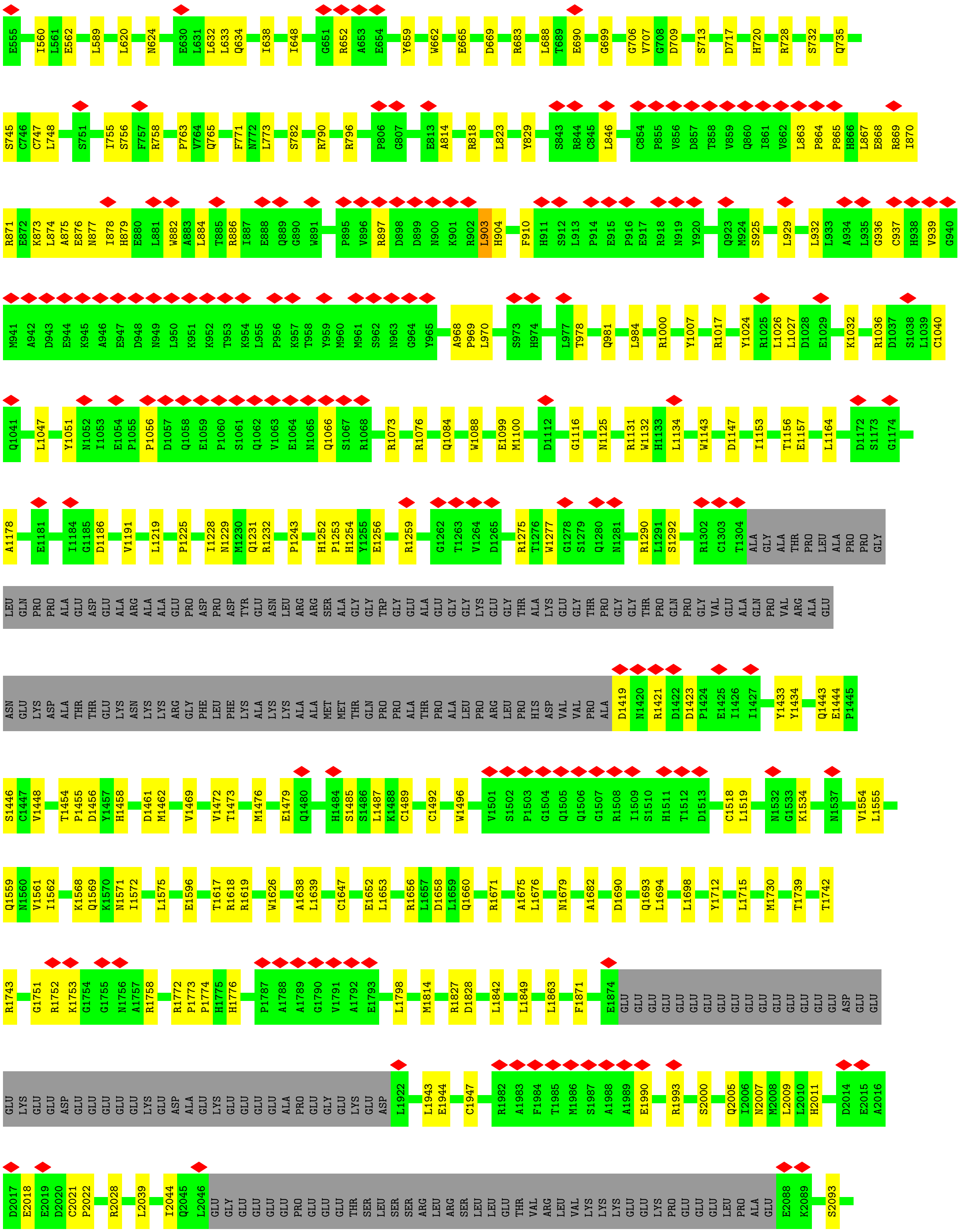


• Molecule 1: Ryanodine receptor 1

Chain C:

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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
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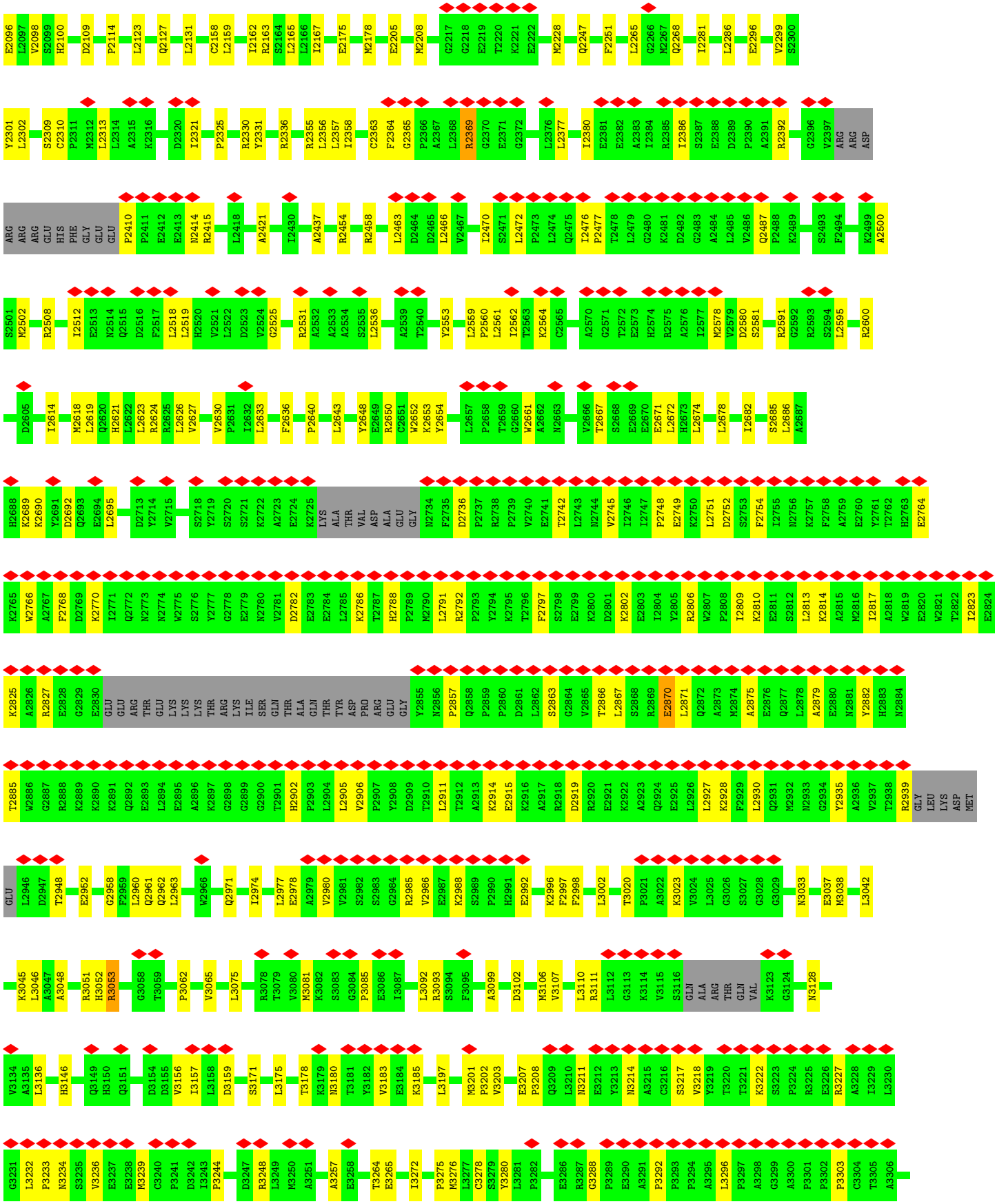
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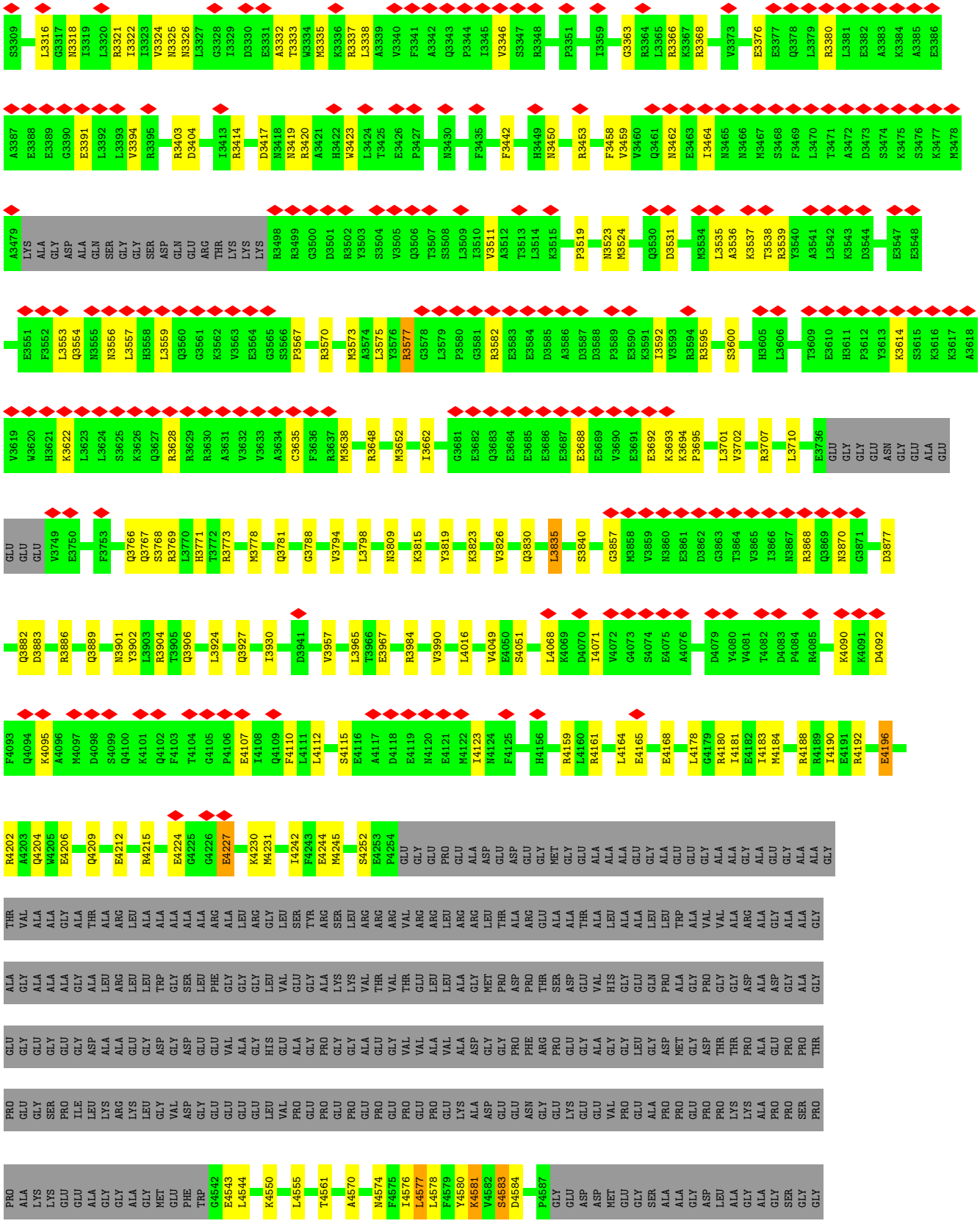
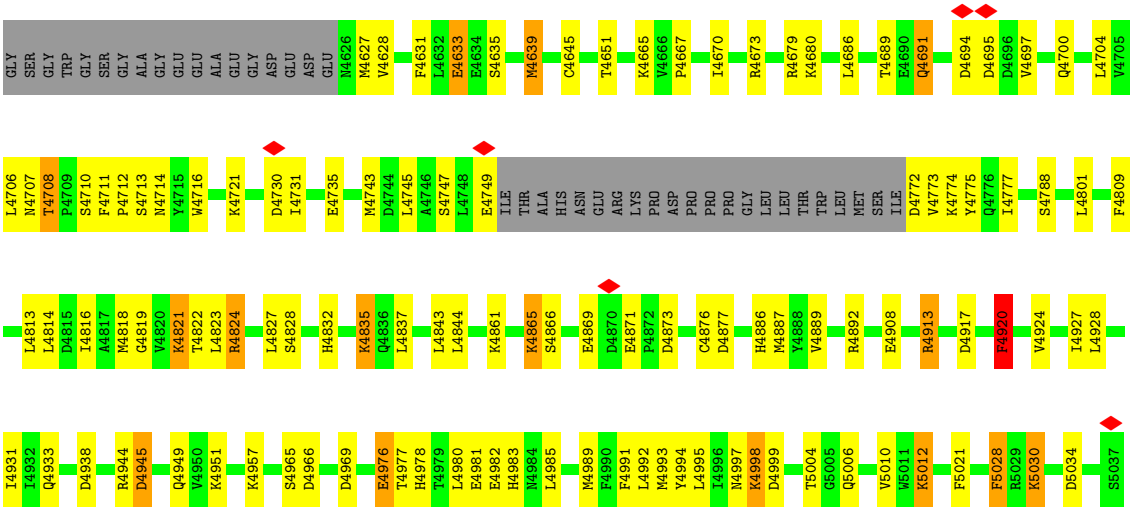
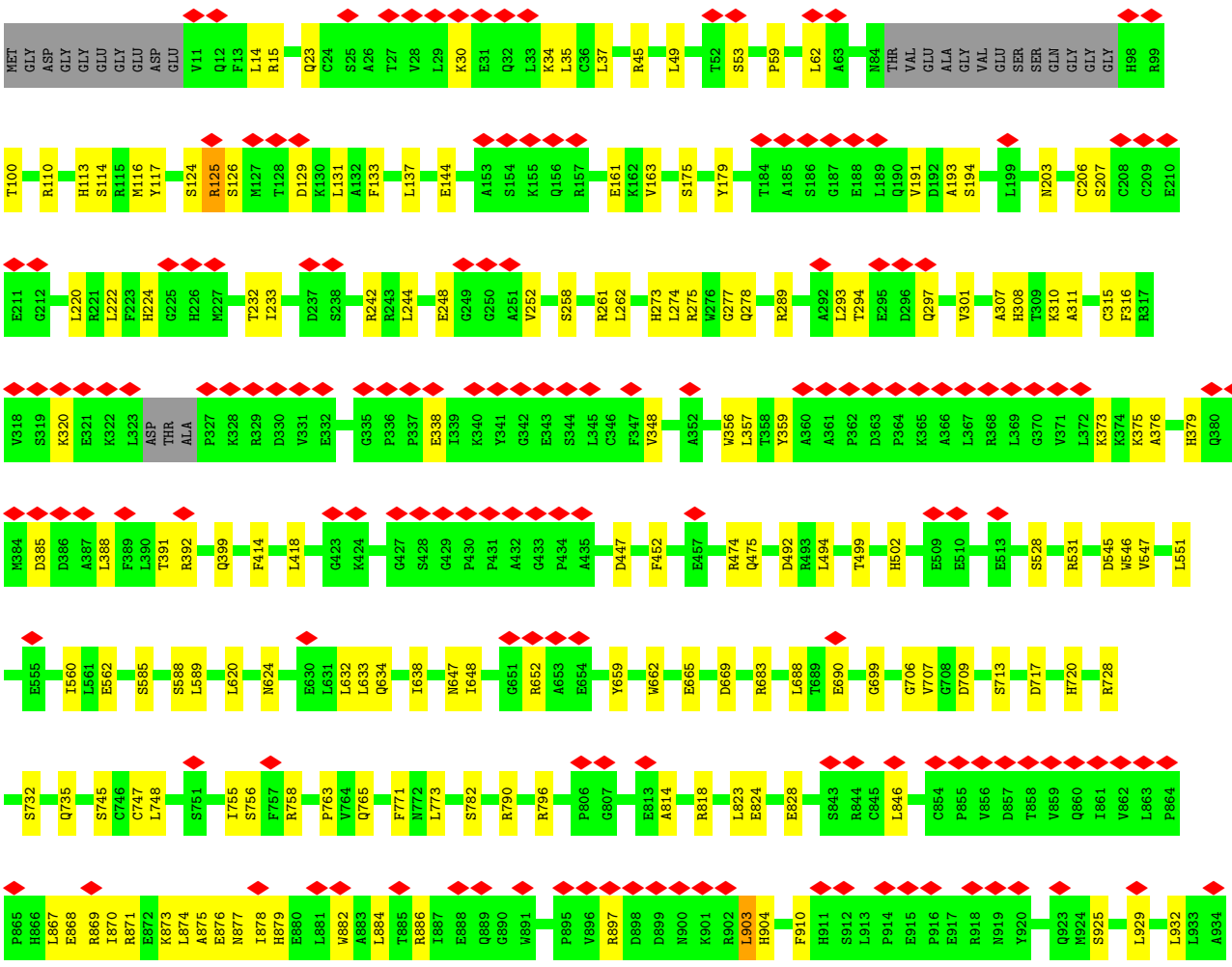
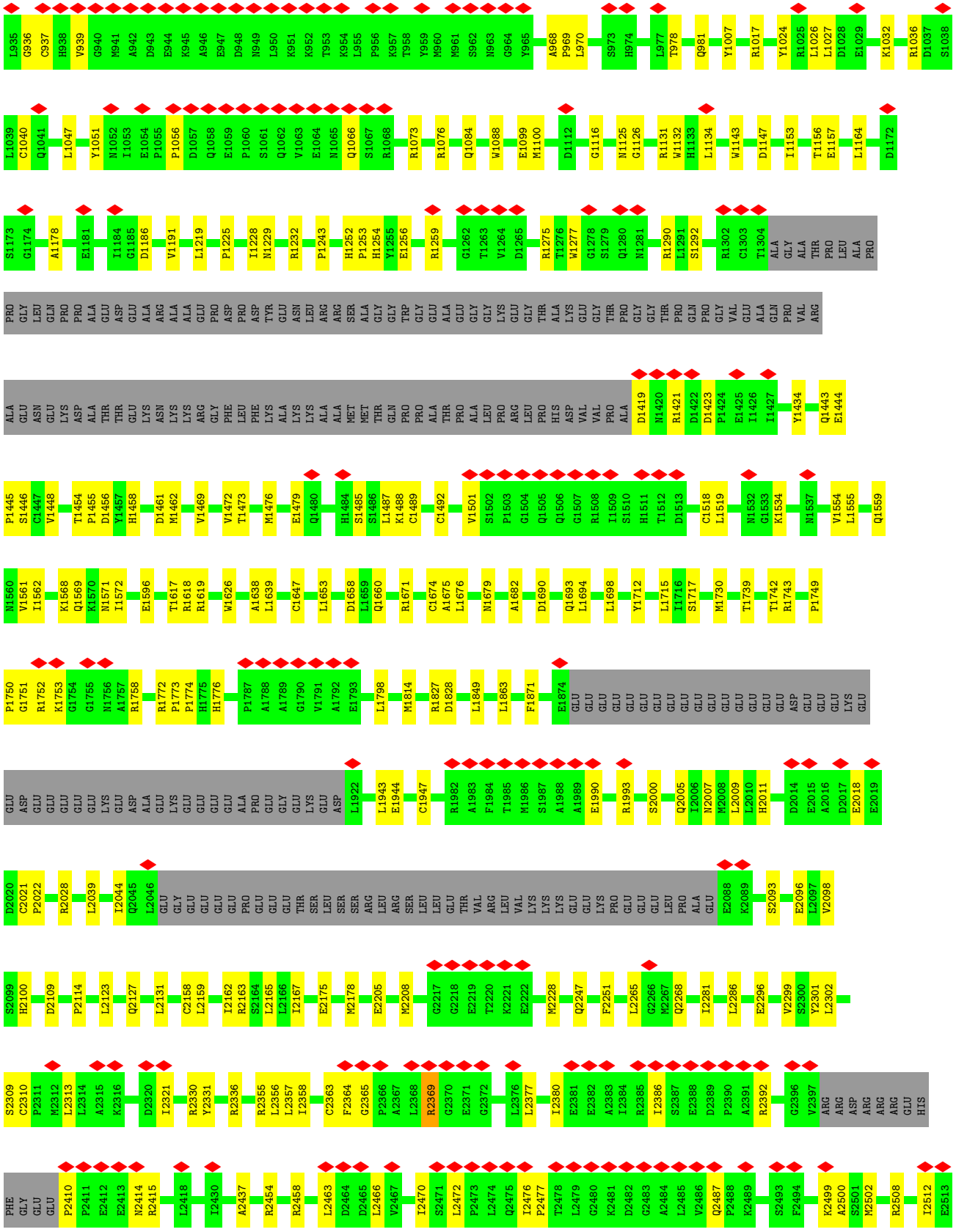




• Molecule 1: Ryanodine receptor 1

Chain D:

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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 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 Y1434 Q1443 E1444
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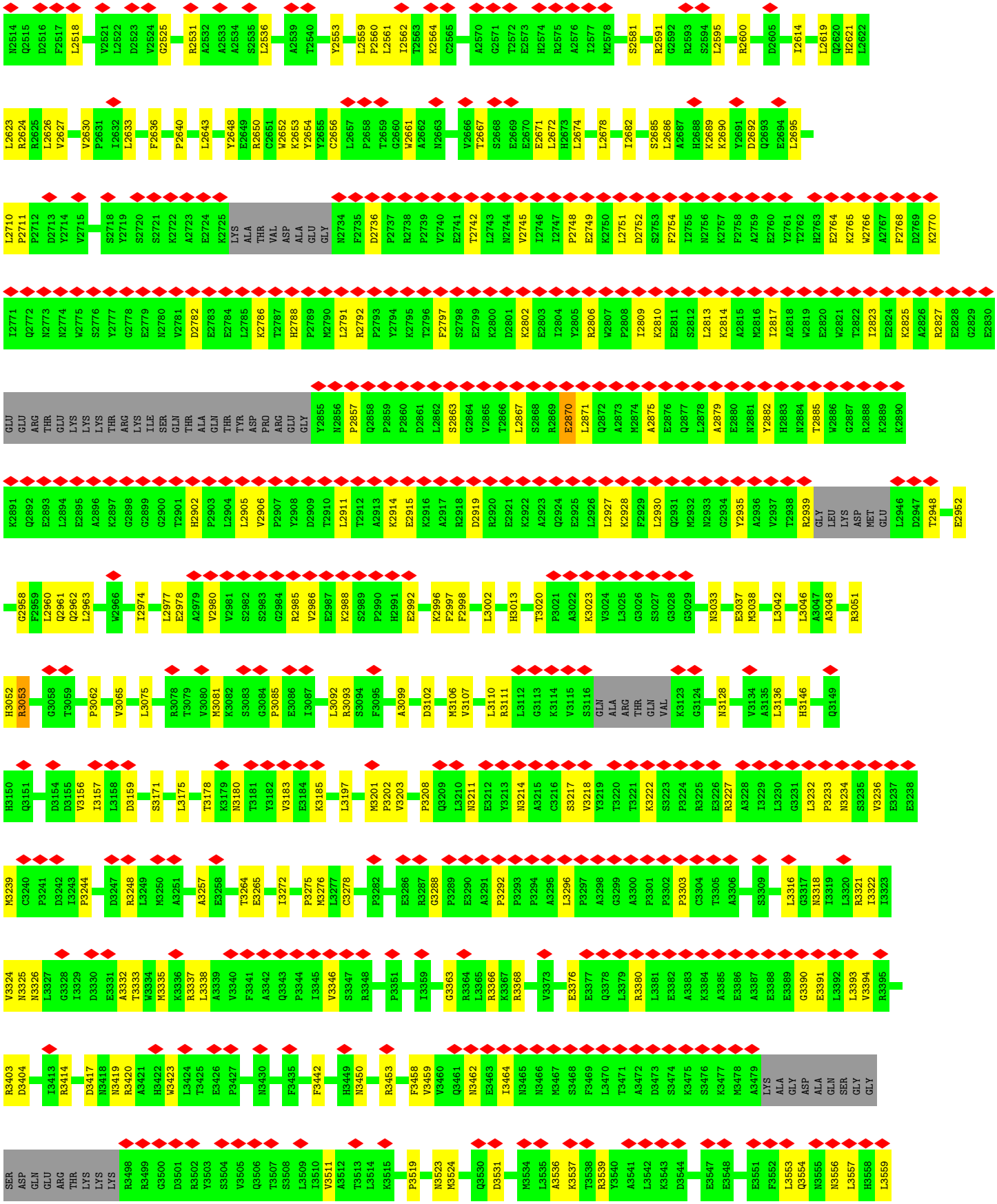
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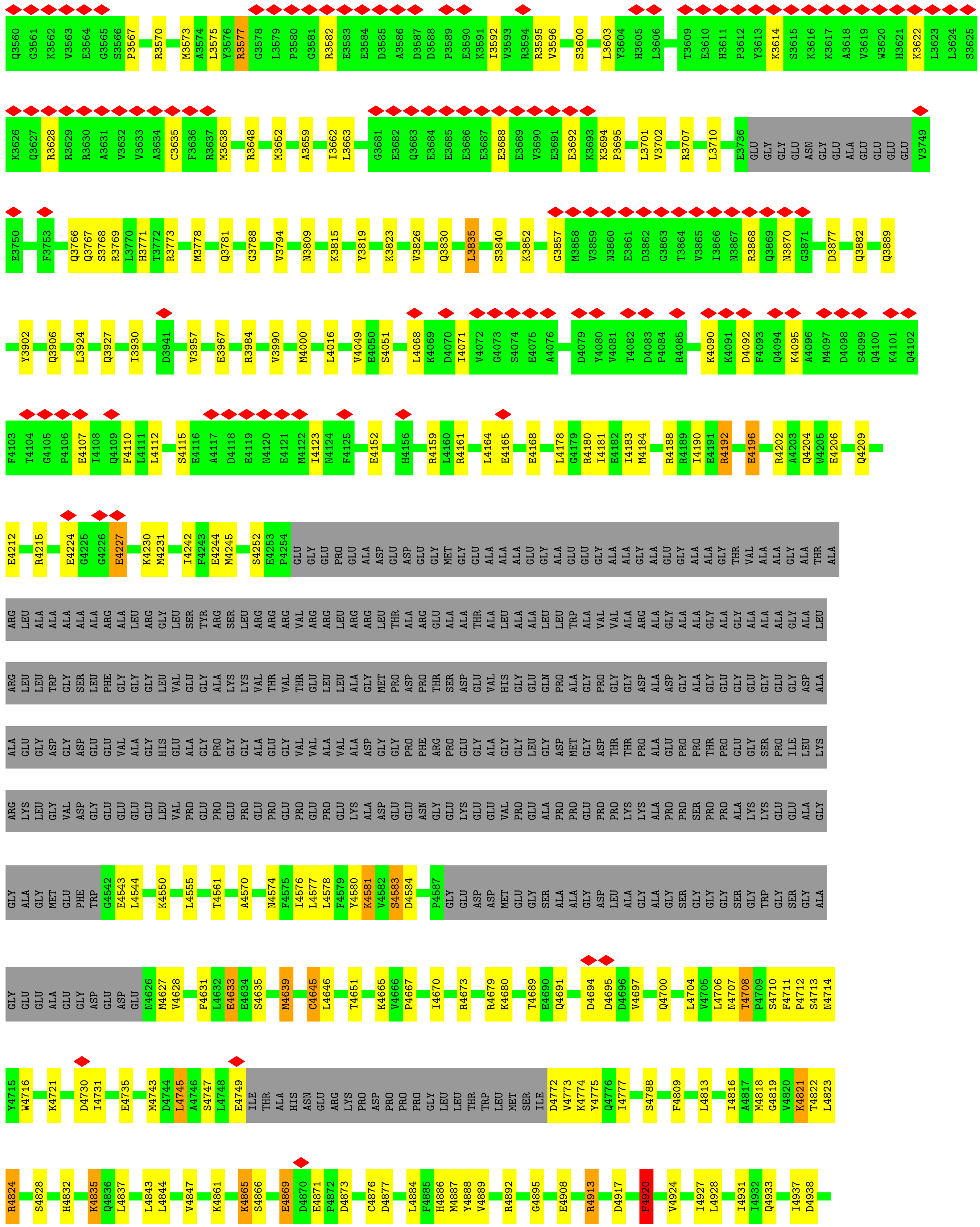
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ARG LEU LEU TRP GLY SER LEU PHE GLY GLY GLY LEU VAL GLU GLY ALA LYS LYS VAL THR VAL THR GLU LEU LEU ALA GLY MET PRO ASP PRO THR SER ASP GLU VAL HIS GLY GLU GLN PRO ALA GLY PRO GLY GLY ASP ALA ASP GLY ALA GLY GLU GLY GLU GLY GLU GLY ASP ALA
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ARG LYS LEU GLY VAL ASP GLY GLU GLU GLU GLU LEU VAL PRO GLU PRO GLU PRO GLU PRO GLU PRO GLU PRO GLU LYS ALA ASP GLU GLU ASN GLY GLU LYS GLU GLU VAL PRO GLU ALA PRO PRO GLU PRO PRO LYS LYS ALA PRO PRO SER PRO PRO ALA LYS LYS GLU GLU ALA GLY
GLY ALA GLY MET GLU PHE TRP G4542 E4543 L4544 K4550 L4555 T4561 A4570 N4574 F4575 I4576 L4577 L4578 F4579 Y4580 K4581 V4582 S4583 D4584 P4587 GLY GLU ASP ASP MET GLU GLY GLY SER ALA ALA GLY ASP LEU ALA GLY ALA GLY SER GLY GLY GLY SER GLY TRP GLY SER GLY ALA
GLY GLU GLU ALA GLU GLY ASP GLY ASP GLU N4626 M4627 V4628 F4631 L4632 E4633 E4634 S4635 M4639 C4645 L4646 T4651 K4665 V4666 P4667 I4670 R4673 R4679 K4680 T4689 E4690 Q4691 D4694 D4695 D4696 V4697 Q4700 L4704 V4705 L4706 N4707 T4708 P4709 S4710 F4711 P4712 S4713 N4714
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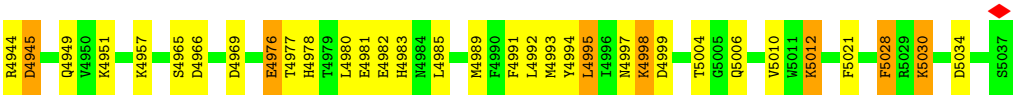
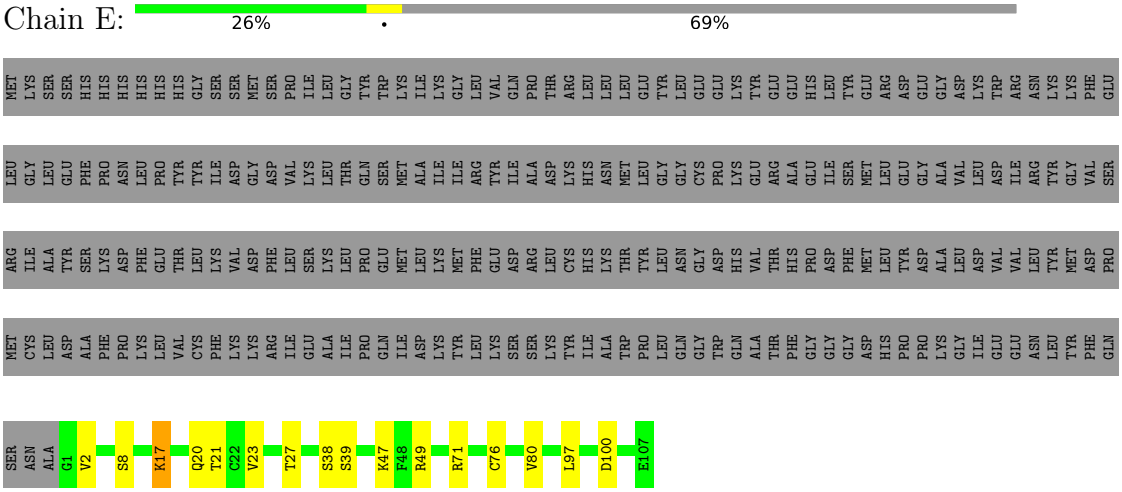


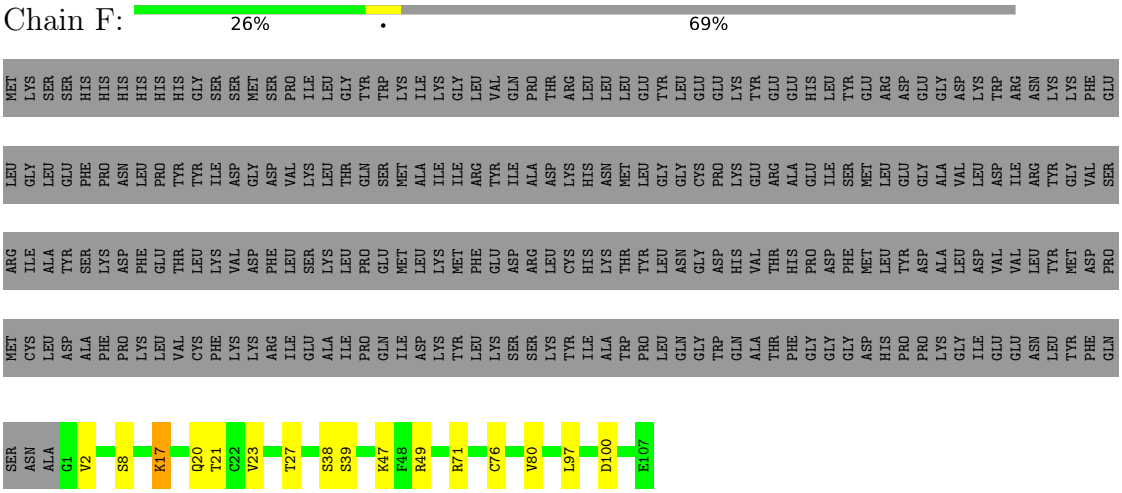
• Molecule 2: Glutathione S-transferase class-mu 26 kDa isozyme,Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain E:



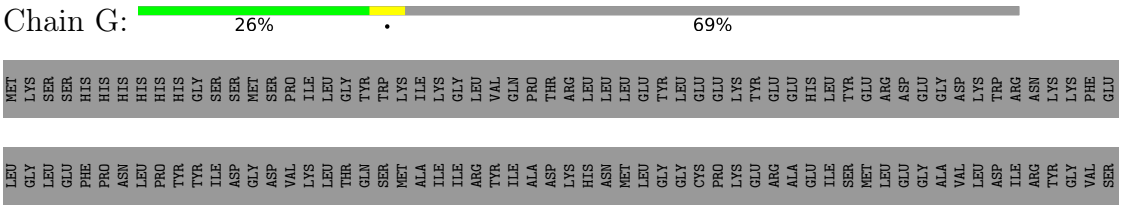
• Molecule 2: Glutathione S-transferase class-mu 26 kDa isozyme,Peptidyl-prolyl cis-trans isomerase FKBP1B

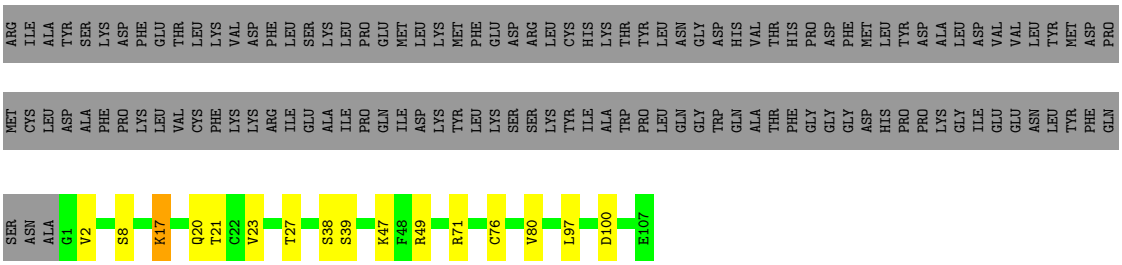
Chain F:



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

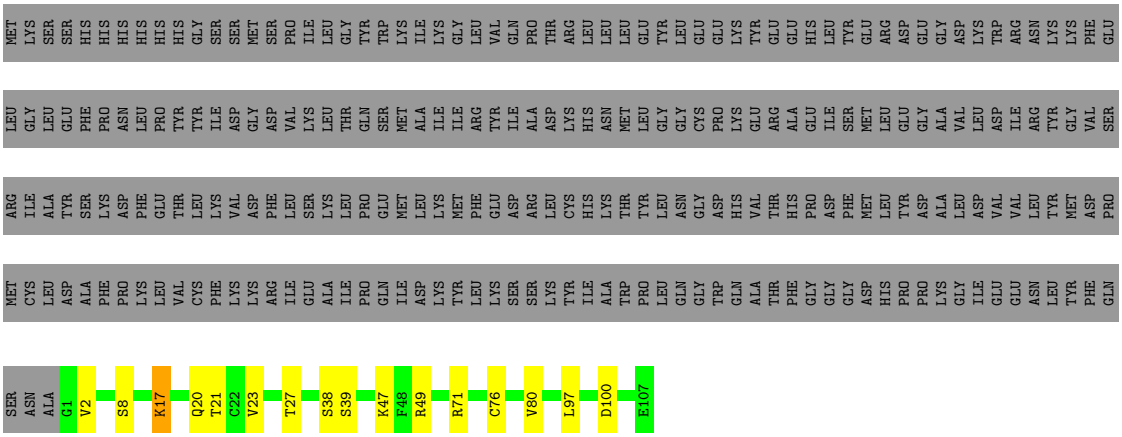
Chain G:





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

Chain H:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	133836	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	0.741	Depositor
Minimum map value	-0.326	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.132	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 (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.34	0/35710	0.66	21/48359 (0.0%)
1	B	0.34	0/35710	0.66	21/48359 (0.0%)
1	C	0.34	0/35710	0.66	20/48359 (0.0%)
1	D	0.34	0/35710	0.66	20/48359 (0.0%)
2	E	0.31	0/834	0.64	0/1123
2	F	0.31	0/834	0.64	0/1123
2	G	0.31	0/834	0.64	0/1123
2	H	0.31	0/834	0.64	0/1123
All	All	0.34	0/146176	0.66	82/197928 (0.0%)

There are no bond length outliers.

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	4945	ASP	CB-CG-OD1	10.69	127.92	118.30
1	C	4945	ASP	CB-CG-OD1	10.66	127.90	118.30
1	A	4945	ASP	CB-CG-OD1	10.58	127.82	118.30
1	D	4945	ASP	CB-CG-OD1	10.58	127.82	118.30
1	B	3417	ASP	CB-CG-OD1	8.19	125.67	118.30
1	A	3417	ASP	CB-CG-OD1	8.12	125.60	118.30
1	C	3417	ASP	CB-CG-OD1	8.12	125.60	118.30
1	D	3417	ASP	CB-CG-OD1	8.12	125.60	118.30
1	B	3835	LEU	CB-CG-CD2	-7.02	99.06	111.00
1	C	3835	LEU	CB-CG-CD2	-7.02	99.06	111.00
1	A	3835	LEU	CB-CG-CD2	-7.02	99.07	111.00
1	D	3835	LEU	CB-CG-CD2	-7.02	99.07	111.00
1	D	4920	PHE	CB-CG-CD1	6.94	125.66	120.80
1	C	4920	PHE	CB-CG-CD1	6.93	125.65	120.80
1	A	4920	PHE	CB-CG-CD1	6.93	125.65	120.80
1	C	5028	PHE	CB-CG-CD1	6.88	125.62	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	4920	PHE	CB-CG-CD1	6.88	125.61	120.80
1	D	5028	PHE	CB-CG-CD1	6.87	125.61	120.80
1	A	5028	PHE	CB-CG-CD1	6.86	125.60	120.80
1	B	5028	PHE	CB-CG-CD1	6.81	125.57	120.80
1	B	4196	GLU	CA-CB-CG	6.61	127.95	113.40
1	C	4196	GLU	CA-CB-CG	6.61	127.95	113.40
1	D	4196	GLU	CA-CB-CG	6.61	127.95	113.40
1	A	4196	GLU	CA-CB-CG	6.60	127.92	113.40
1	A	903	LEU	CA-CB-CG	6.41	130.04	115.30
1	B	903	LEU	CA-CB-CG	6.40	130.02	115.30
1	C	903	LEU	CA-CB-CG	6.40	130.02	115.30
1	D	903	LEU	CA-CB-CG	6.40	130.02	115.30
1	A	3835	LEU	CA-CB-CG	6.28	129.74	115.30
1	B	3835	LEU	CA-CB-CG	6.27	129.72	115.30
1	D	3835	LEU	CA-CB-CG	6.26	129.71	115.30
1	C	3835	LEU	CA-CB-CG	6.25	129.69	115.30
1	B	3085	PRO	CA-N-CD	-5.91	103.23	111.50
1	C	3085	PRO	CA-N-CD	-5.91	103.23	111.50
1	D	3085	PRO	CA-N-CD	-5.91	103.23	111.50
1	A	3085	PRO	CA-N-CD	-5.89	103.26	111.50
1	B	3197	LEU	CA-CB-CG	5.88	128.83	115.30
1	C	3197	LEU	CA-CB-CG	5.87	128.80	115.30
1	D	3197	LEU	CA-CB-CG	5.86	128.78	115.30
1	A	3197	LEU	CA-CB-CG	5.85	128.76	115.30
1	D	131	LEU	CA-CB-CG	5.84	128.73	115.30
1	B	131	LEU	CA-CB-CG	5.84	128.72	115.30
1	C	131	LEU	CA-CB-CG	5.81	128.67	115.30
1	A	131	LEU	CA-CB-CG	5.81	128.66	115.30
1	A	3296	LEU	CA-CB-CG	5.54	128.05	115.30
1	C	3296	LEU	CA-CB-CG	5.54	128.04	115.30
1	D	3296	LEU	CA-CB-CG	5.54	128.04	115.30
1	B	3296	LEU	CA-CB-CG	5.51	127.98	115.30
1	D	3701	LEU	CA-CB-CG	5.48	127.90	115.30
1	A	3701	LEU	CA-CB-CG	5.47	127.88	115.30
1	B	3701	LEU	CA-CB-CG	5.47	127.88	115.30
1	C	3701	LEU	CA-CB-CG	5.47	127.88	115.30
1	A	2751	LEU	CA-CB-CG	5.34	127.58	115.30
1	C	2751	LEU	CA-CB-CG	5.34	127.58	115.30
1	D	2751	LEU	CA-CB-CG	5.33	127.55	115.30
1	B	2751	LEU	CA-CB-CG	5.32	127.54	115.30
1	C	5028	PHE	CB-CG-CD2	-5.29	117.10	120.80
1	D	5028	PHE	CB-CG-CD2	-5.28	117.11	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	4196	GLU	CB-CA-C	-5.26	99.88	110.40
1	B	4196	GLU	CB-CA-C	-5.26	99.88	110.40
1	C	4196	GLU	CB-CA-C	-5.26	99.88	110.40
1	D	4196	GLU	CB-CA-C	-5.25	99.91	110.40
1	A	3531	ASP	CB-CG-OD1	5.24	123.01	118.30
1	A	5028	PHE	CB-CG-CD2	-5.24	117.14	120.80
1	D	4920	PHE	CB-CG-CD2	-5.22	117.15	120.80
1	B	3531	ASP	CB-CG-OD1	5.21	122.99	118.30
1	C	3531	ASP	CB-CG-OD1	5.21	122.99	118.30
1	D	3531	ASP	CB-CG-OD1	5.21	122.98	118.30
1	B	5028	PHE	CB-CG-CD2	-5.19	117.17	120.80
1	A	3085	PRO	N-CD-CG	-5.15	95.48	103.20
1	A	4920	PHE	CB-CG-CD2	-5.14	117.20	120.80
1	A	3835	LEU	CB-CG-CD1	5.14	119.74	111.00
1	D	3835	LEU	CB-CG-CD1	5.14	119.74	111.00
1	B	3085	PRO	N-CD-CG	-5.13	95.50	103.20
1	C	3085	PRO	N-CD-CG	-5.13	95.50	103.20
1	C	4920	PHE	CB-CG-CD2	-5.13	117.21	120.80
1	D	3085	PRO	N-CD-CG	-5.13	95.51	103.20
1	C	3835	LEU	CB-CG-CD1	5.11	119.69	111.00
1	B	3835	LEU	CB-CG-CD1	5.11	119.69	111.00
1	B	4920	PHE	CB-CG-CD2	-5.10	117.23	120.80
1	A	4178	LEU	CA-CB-CG	5.00	126.81	115.30
1	B	4178	LEU	CA-CB-CG	5.00	126.81	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	34896	0	34522	451	0
1	B	34896	0	34522	440	0
1	C	34896	0	34522	448	0
1	D	34896	0	34522	451	0
2	E	818	0	824	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	818	0	824	8	0
2	G	818	0	824	8	0
2	H	818	0	824	8	0
3	A	23	0	12	1	0
3	B	23	0	12	1	0
3	C	23	0	12	1	0
3	D	23	0	12	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
All	All	142952	0	141432	1789	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 (1789) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4242:ILE:HG12	1:B:4993:MET:HG2	1.71	0.73
1:A:4242:ILE:HG12	1:A:4993:MET:HG2	1.71	0.72
1:D:4242:ILE:HG12	1:D:4993:MET:HG2	1.71	0.72
1:C:4242:ILE:HG12	1:C:4993:MET:HG2	1.71	0.71
1:D:233:ILE:HD12	1:D:242:ARG:HB3	1.73	0.71
1:C:1476:MET:HB3	1:C:1485:SER:HB3	1.73	0.71
1:A:233:ILE:HD12	1:A:242:ARG:HB3	1.73	0.71
1:B:1476:MET:HB3	1:B:1485:SER:HB3	1.73	0.70
1:C:233:ILE:HD12	1:C:242:ARG:HB3	1.73	0.70
1:C:3042:LEU:O	1:C:3046:LEU:HB2	1.91	0.70
1:A:1476:MET:HB3	1:A:1485:SER:HB3	1.73	0.70
1:B:3042:LEU:O	1:B:3046:LEU:HB2	1.91	0.70
1:D:3042:LEU:O	1:D:3046:LEU:HB2	1.91	0.69
1:B:233:ILE:HD12	1:B:242:ARG:HB3	1.73	0.69
1:D:1476:MET:HB3	1:D:1485:SER:HB3	1.73	0.69
1:A:3042:LEU:O	1:A:3046:LEU:HB2	1.91	0.69
1:B:745:SER:HB2	1:B:758:ARG:HB2	1.74	0.68
1:C:745:SER:HB2	1:C:758:ARG:HB2	1.74	0.68
1:D:745:SER:HB2	1:D:758:ARG:HB2	1.74	0.68
1:C:688:LEU:HD23	1:C:690:GLU:H	1.59	0.67
1:A:745:SER:HB2	1:A:758:ARG:HB2	1.74	0.67
1:D:688:LEU:HD23	1:D:690:GLU:H	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3346:VAL:HG11	1:D:3414:ARG:HB3	1.77	0.67
1:A:4978:HIS:HA	1:A:4982:GLU:HG3	1.77	0.66
1:A:3257:ALA:HB1	1:A:3321:ARG:HD2	1.76	0.66
1:C:3257:ALA:HB1	1:C:3321:ARG:HD2	1.76	0.66
1:A:688:LEU:HD23	1:A:690:GLU:H	1.59	0.66
1:A:3346:VAL:HG11	1:A:3414:ARG:HB3	1.77	0.66
1:B:688:LEU:HD23	1:B:690:GLU:H	1.59	0.66
1:B:3257:ALA:HB1	1:B:3321:ARG:HD2	1.76	0.66
1:D:3257:ALA:HB1	1:D:3321:ARG:HD2	1.76	0.66
1:B:4581:LYS:NZ	1:C:4877:ASP:O	2.28	0.66
1:C:4978:HIS:HA	1:C:4982:GLU:HG3	1.77	0.66
1:C:3346:VAL:HG11	1:C:3414:ARG:HB3	1.77	0.65
1:C:4581:LYS:NZ	1:D:4877:ASP:O	2.28	0.65
1:D:1116:GLY:HA3	1:D:1132:TRP:HB3	1.78	0.65
1:C:1116:GLY:HA3	1:C:1132:TRP:HB3	1.78	0.65
1:B:3346:VAL:HG11	1:B:3414:ARG:HB3	1.77	0.65
1:C:2007:ASN:O	1:C:2011:HIS:HB2	1.97	0.65
1:D:4978:HIS:HA	1:D:4982:GLU:HG3	1.77	0.65
1:A:4821:LYS:HG3	1:A:4824:ARG:HH21	1.62	0.65
1:B:1116:GLY:HA3	1:B:1132:TRP:HB3	1.78	0.65
1:B:4821:LYS:HG3	1:B:4824:ARG:HH21	1.62	0.65
1:B:4924:VAL:HA	1:B:4928:LEU:HD12	1.79	0.65
1:A:2961:GLN:NE2	1:A:3038:MET:SD	2.70	0.65
1:B:2007:ASN:O	1:B:2011:HIS:HB2	1.97	0.65
1:B:4978:HIS:HA	1:B:4982:GLU:HG3	1.77	0.64
1:A:4924:VAL:HA	1:A:4928:LEU:HD12	1.79	0.64
1:D:4821:LYS:HG3	1:D:4824:ARG:HH21	1.62	0.64
1:A:1116:GLY:HA3	1:A:1132:TRP:HB3	1.78	0.64
1:A:2007:ASN:O	1:A:2011:HIS:HB2	1.97	0.64
1:B:3332:ALA:HB3	1:B:3403:ARG:HD2	1.80	0.64
1:D:2007:ASN:O	1:D:2011:HIS:HB2	1.97	0.64
1:D:2961:GLN:NE2	1:D:3038:MET:SD	2.70	0.64
1:C:3332:ALA:HB3	1:C:3403:ARG:HD2	1.80	0.64
1:C:4924:VAL:HA	1:C:4928:LEU:HD12	1.79	0.64
1:A:3332:ALA:HB3	1:A:3403:ARG:HD2	1.80	0.64
1:A:1569:GLN:HB2	1:A:1572:ILE:HD12	1.80	0.64
1:B:2797:PHE:HE2	1:B:2802:LYS:HD3	1.63	0.64
1:D:4924:VAL:HA	1:D:4928:LEU:HD12	1.79	0.64
1:B:2958:GLY:O	1:B:2962:GLN:NE2	2.31	0.63
1:C:2797:PHE:HE2	1:C:2802:LYS:HD3	1.63	0.63
1:D:3332:ALA:HB3	1:D:3403:ARG:HD2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2958:GLY:O	1:D:2962:GLN:NE2	2.31	0.63
1:D:1569:GLN:HB2	1:D:1572:ILE:HD12	1.80	0.63
1:A:2958:GLY:O	1:A:2962:GLN:NE2	2.31	0.63
1:C:2958:GLY:O	1:C:2962:GLN:NE2	2.31	0.63
1:C:4821:LYS:HG3	1:C:4824:ARG:HH21	1.62	0.63
1:B:2961:GLN:NE2	1:B:3038:MET:SD	2.70	0.63
1:A:2797:PHE:HE2	1:A:2802:LYS:HD3	1.63	0.63
1:D:2797:PHE:HE2	1:D:2802:LYS:HD3	1.63	0.63
1:B:3075:LEU:O	1:B:3146:HIS:NE2	2.32	0.63
1:D:3075:LEU:O	1:D:3146:HIS:NE2	2.32	0.63
1:A:981:GLN:HG2	1:A:1047:LEU:HD11	1.81	0.62
1:B:659:TYR:O	1:B:662:TRP:NE1	2.33	0.62
1:B:1990:GLU:HB2	1:B:1993:ARG:HE	1.65	0.62
1:C:1024:TYR:O	1:C:1032:LYS:NZ	2.33	0.62
1:A:1990:GLU:HB2	1:A:1993:ARG:HE	1.64	0.62
1:A:3075:LEU:O	1:A:3146:HIS:NE2	2.32	0.62
1:C:1569:GLN:HB2	1:C:1572:ILE:HD12	1.80	0.62
1:C:659:TYR:O	1:C:662:TRP:NE1	2.32	0.62
1:D:659:TYR:O	1:D:662:TRP:NE1	2.32	0.62
1:A:659:TYR:O	1:A:662:TRP:NE1	2.32	0.62
1:A:3051:ARG:O	1:A:3053:ARG:NE	2.31	0.62
1:B:2978:GLU:OE2	1:B:3053:ARG:NH1	2.31	0.62
1:B:1569:GLN:HB2	1:B:1572:ILE:HD12	1.80	0.62
1:C:244:LEU:HD13	1:C:375:LYS:HD2	1.82	0.62
1:A:1024:TYR:O	1:A:1032:LYS:NZ	2.33	0.61
1:B:244:LEU:HD13	1:B:375:LYS:HD2	1.82	0.61
1:B:1024:TYR:O	1:B:1032:LYS:NZ	2.33	0.61
1:B:3051:ARG:O	1:B:3053:ARG:NE	2.31	0.61
1:C:1990:GLU:HB2	1:C:1993:ARG:HE	1.64	0.61
1:D:2978:GLU:OE2	1:D:3053:ARG:NH1	2.31	0.61
1:B:2630:VAL:HG12	1:B:2682:ILE:HD11	1.83	0.61
1:C:981:GLN:HG2	1:C:1047:LEU:HD11	1.81	0.61
1:D:981:GLN:HG2	1:D:1047:LEU:HD11	1.81	0.61
1:A:244:LEU:HD13	1:A:375:LYS:HD2	1.82	0.61
1:A:897:ARG:HB2	1:A:903:LEU:HD11	1.83	0.61
1:B:981:GLN:HG2	1:B:1047:LEU:HD11	1.81	0.61
1:C:3051:ARG:O	1:C:3053:ARG:NE	2.31	0.61
1:A:978:THR:OG1	1:A:981:GLN:OE1	2.19	0.61
1:A:3081:MET:HG3	1:A:3156:VAL:HA	1.83	0.61
1:D:1990:GLU:HB2	1:D:1993:ARG:HE	1.65	0.61
1:C:2630:VAL:HG12	1:C:2682:ILE:HD11	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3368:ARG:NH2	1:A:3404:ASP:OD2	2.34	0.61
1:B:3236:VAL:HA	1:B:3239:MET:HG3	1.83	0.61
1:D:244:LEU:HD13	1:D:375:LYS:HD2	1.82	0.61
1:D:1024:TYR:O	1:D:1032:LYS:NZ	2.33	0.61
1:A:3236:VAL:HA	1:A:3239:MET:HG3	1.83	0.61
1:D:897:ARG:HB2	1:D:903:LEU:HD11	1.83	0.61
1:D:3236:VAL:HA	1:D:3239:MET:HG3	1.83	0.60
1:D:3368:ARG:NH2	1:D:3404:ASP:OD2	2.34	0.60
1:A:2630:VAL:HG12	1:A:2682:ILE:HD11	1.83	0.60
1:B:897:ARG:HB2	1:B:903:LEU:HD11	1.83	0.60
1:C:897:ARG:HB2	1:C:903:LEU:HD11	1.83	0.60
1:D:3051:ARG:O	1:D:3053:ARG:NE	2.31	0.60
1:D:3081:MET:HG3	1:D:3156:VAL:HA	1.83	0.60
2:G:17:LYS:HG3	2:G:20:GLN:HE22	1.66	0.60
1:C:652:ARG:HB3	1:C:773:LEU:HD21	1.83	0.60
1:C:2961:GLN:NE2	1:C:3038:MET:SD	2.70	0.60
1:C:2978:GLU:OE2	1:C:3053:ARG:NH1	2.31	0.60
1:A:652:ARG:HB3	1:A:773:LEU:HD21	1.83	0.60
1:C:707:VAL:HG13	1:C:713:SER:HB2	1.83	0.60
1:A:2685:SER:O	1:A:2689:LYS:HB2	2.02	0.60
1:D:2630:VAL:HG12	1:D:2682:ILE:HD11	1.83	0.60
1:B:707:VAL:HG13	1:B:713:SER:HB2	1.83	0.60
1:B:2685:SER:O	1:B:2689:LYS:HB2	2.02	0.60
1:B:3081:MET:HG3	1:B:3156:VAL:HA	1.83	0.60
1:C:978:THR:OG1	1:C:981:GLN:OE1	2.19	0.60
1:C:3236:VAL:HA	1:C:3239:MET:HG3	1.83	0.60
1:B:978:THR:OG1	1:B:981:GLN:OE1	2.19	0.60
1:B:2992:GLU:OE2	1:B:2996:LYS:NZ	2.34	0.60
1:C:3075:LEU:O	1:C:3146:HIS:NE2	2.32	0.60
1:C:3368:ARG:NH2	1:C:3404:ASP:OD2	2.34	0.60
1:D:978:THR:OG1	1:D:981:GLN:OE1	2.19	0.60
1:A:707:VAL:HG13	1:A:713:SER:HB2	1.83	0.59
1:B:652:ARG:HB3	1:B:773:LEU:HD21	1.83	0.59
1:B:3368:ARG:NH2	1:B:3404:ASP:OD2	2.34	0.59
2:E:17:LYS:HG3	2:E:20:GLN:HE22	1.66	0.59
2:H:17:LYS:HG3	2:H:20:GLN:HE22	1.66	0.59
1:B:2619:LEU:HB3	1:B:2623:LEU:HD13	1.85	0.59
1:C:2992:GLU:OE2	1:C:2996:LYS:NZ	2.34	0.59
1:D:707:VAL:HG13	1:D:713:SER:HB2	1.84	0.59
2:F:17:LYS:HG3	2:F:20:GLN:HE22	1.66	0.59
1:A:475:GLN:NE2	1:A:528:SER:O	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1232:ARG:NH2	1:A:1828:ASP:O	2.35	0.59
1:A:2992:GLU:OE2	1:A:2996:LYS:NZ	2.34	0.59
1:C:2619:LEU:HB3	1:C:2623:LEU:HD13	1.85	0.59
1:D:652:ARG:HB3	1:D:773:LEU:HD21	1.83	0.59
1:D:1232:ARG:NH2	1:D:1828:ASP:O	2.35	0.59
1:D:2992:GLU:OE2	1:D:2996:LYS:NZ	2.34	0.59
1:A:551:LEU:HB3	1:A:589:LEU:HD11	1.85	0.59
1:C:1232:ARG:NH2	1:C:1828:ASP:O	2.35	0.59
1:C:3081:MET:HG3	1:C:3156:VAL:HA	1.83	0.59
1:D:551:LEU:HB3	1:D:589:LEU:HD11	1.85	0.59
1:D:2685:SER:O	1:D:2689:LYS:HB2	2.02	0.59
1:B:475:GLN:NE2	1:B:528:SER:O	2.36	0.58
1:C:551:LEU:HB3	1:C:589:LEU:HD11	1.85	0.58
1:D:2871:LEU:HG	1:D:2927:LEU:HD21	1.85	0.58
1:B:551:LEU:HB3	1:B:589:LEU:HD11	1.85	0.58
1:B:1252:HIS:O	1:B:1275:ARG:NH2	2.37	0.58
1:D:475:GLN:NE2	1:D:528:SER:O	2.36	0.58
1:D:1943:LEU:HD13	1:D:2098:VAL:HG22	1.86	0.58
1:B:1232:ARG:NH2	1:B:1828:ASP:O	2.35	0.58
1:C:475:GLN:NE2	1:C:528:SER:O	2.36	0.58
1:C:4994:TYR:OH	1:C:4998:LYS:NZ	2.35	0.58
1:A:882:TRP:O	1:A:886:ARG:NH1	2.37	0.58
1:A:2871:LEU:HG	1:A:2927:LEU:HD21	1.85	0.58
1:C:1252:HIS:O	1:C:1275:ARG:NH2	2.36	0.58
1:D:1252:HIS:O	1:D:1275:ARG:NH2	2.37	0.58
1:C:763:PRO:O	1:C:765:GLN:NE2	2.37	0.58
1:D:2619:LEU:HB3	1:D:2623:LEU:HD13	1.85	0.58
1:A:161:GLU:HB3	1:D:3984:ARG:HH22	1.68	0.58
1:A:1252:HIS:O	1:A:1275:ARG:NH2	2.36	0.58
1:A:4581:LYS:NZ	1:B:4877:ASP:O	2.35	0.58
1:C:1943:LEU:HD13	1:C:2098:VAL:HG22	1.86	0.58
1:C:2685:SER:O	1:C:2689:LYS:HB2	2.02	0.58
1:B:882:TRP:O	1:B:886:ARG:NH1	2.37	0.58
1:D:289:ARG:HB3	1:D:301:VAL:HB	1.85	0.58
1:B:62:LEU:HD23	1:B:261:ARG:HH12	1.69	0.58
1:B:3990:VAL:HG13	1:B:4051:SER:HB3	1.86	0.58
1:C:289:ARG:HB3	1:C:301:VAL:HB	1.86	0.58
1:C:882:TRP:O	1:C:886:ARG:NH1	2.37	0.58
1:C:2823:ILE:HD11	1:C:2935:TYR:HB3	1.86	0.58
1:C:3990:VAL:HG13	1:C:4051:SER:HB3	1.86	0.58
1:D:882:TRP:O	1:D:886:ARG:NH1	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2619:LEU:HB3	1:A:2623:LEU:HD13	1.85	0.57
1:D:638:ILE:HD12	1:D:1638:ALA:HB3	1.86	0.57
1:C:2463:LEU:HA	1:C:2466:LEU:HD12	1.86	0.57
1:C:2871:LEU:HG	1:C:2927:LEU:HD21	1.85	0.57
1:C:3524:MET:HA	1:C:3582:ARG:HH22	1.70	0.57
1:C:3702:VAL:HG13	1:C:3778:MET:HG2	1.86	0.57
1:D:763:PRO:O	1:D:765:GLN:NE2	2.37	0.57
1:D:3702:VAL:HG13	1:D:3778:MET:HG2	1.86	0.57
1:A:763:PRO:O	1:A:765:GLN:NE2	2.37	0.57
1:A:62:LEU:HD23	1:A:261:ARG:HH12	1.69	0.57
1:B:289:ARG:HB3	1:B:301:VAL:HB	1.86	0.57
1:B:1943:LEU:HD13	1:B:2098:VAL:HG22	1.86	0.57
1:B:2309:SER:OG	1:B:2321:ILE:O	2.22	0.57
1:D:3524:MET:HA	1:D:3582:ARG:HH22	1.70	0.57
1:A:638:ILE:HD12	1:A:1638:ALA:HB3	1.86	0.57
1:A:2309:SER:OG	1:A:2321:ILE:O	2.22	0.57
1:B:3524:MET:HA	1:B:3582:ARG:HH22	1.70	0.57
1:A:1561:VAL:HG12	1:A:1562:ILE:HG13	1.87	0.57
1:A:3635:CYS:HA	1:A:3638:MET:HG3	1.86	0.57
1:C:2595:LEU:O	1:C:2600:ARG:NH1	2.38	0.57
1:C:3052:HIS:NE2	1:C:3128:ASN:OD1	2.35	0.57
1:D:2309:SER:OG	1:D:2321:ILE:O	2.22	0.57
1:B:2871:LEU:HG	1:B:2927:LEU:HD21	1.85	0.57
1:D:2823:ILE:HD11	1:D:2935:TYR:HB3	1.86	0.57
1:D:3990:VAL:HG13	1:D:4051:SER:HB3	1.86	0.57
1:A:1943:LEU:HD13	1:A:2098:VAL:HG22	1.86	0.57
1:A:2463:LEU:HA	1:A:2466:LEU:HD12	1.86	0.57
1:B:348:VAL:HB	1:B:357:LEU:HD22	1.87	0.57
1:C:62:LEU:HD23	1:C:261:ARG:HH12	1.69	0.57
1:C:2021:CYS:O	1:C:2028:ARG:NH2	2.38	0.57
1:D:2653:LYS:HB2	1:D:2661:TRP:HE3	1.70	0.57
1:D:3766:GLN:OE1	1:D:3769:ARG:NH2	2.38	0.57
1:B:747:CYS:HB2	1:B:756:SER:HB2	1.87	0.57
1:B:763:PRO:O	1:B:765:GLN:NE2	2.37	0.57
1:B:1653:LEU:O	1:B:1660:GLN:NE2	2.38	0.57
1:B:2595:LEU:O	1:B:2600:ARG:NH1	2.38	0.57
1:B:3635:CYS:HA	1:B:3638:MET:HG3	1.86	0.57
1:B:4994:TYR:OH	1:B:4998:LYS:NZ	2.35	0.57
1:C:728:ARG:NH2	1:C:1489:CYS:SG	2.78	0.57
1:A:1653:LEU:O	1:A:1660:GLN:NE2	2.38	0.57
1:A:2595:LEU:O	1:A:2600:ARG:NH1	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2792:ARG:HB2	1:A:2797:PHE:HD1	1.70	0.57
1:A:3769:ARG:O	1:A:3773:ARG:NH1	2.38	0.57
1:A:3990:VAL:HG13	1:A:4051:SER:HB3	1.86	0.57
1:D:62:LEU:HD23	1:D:261:ARG:HH12	1.69	0.57
1:D:1561:VAL:HG12	1:D:1562:ILE:HG13	1.87	0.57
1:D:2018:GLU:OE1	1:D:2028:ARG:NH1	2.38	0.57
1:D:2792:ARG:HB2	1:D:2797:PHE:HD1	1.70	0.57
1:A:289:ARG:HB3	1:A:301:VAL:HB	1.86	0.56
1:C:3766:GLN:OE1	1:C:3769:ARG:NH2	2.38	0.56
1:D:133:PHE:O	1:D:193:ALA:N	2.38	0.56
1:D:728:ARG:NH2	1:D:1489:CYS:SG	2.78	0.56
1:A:2823:ILE:HD11	1:A:2935:TYR:HB3	1.86	0.56
1:B:638:ILE:HD12	1:B:1638:ALA:HB3	1.86	0.56
1:B:2000:SER:O	1:B:2005:GLN:NE2	2.33	0.56
1:C:1561:VAL:HG12	1:C:1562:ILE:HG13	1.87	0.56
1:D:2021:CYS:O	1:D:2028:ARG:NH2	2.38	0.56
1:A:348:VAL:HB	1:A:357:LEU:HD22	1.87	0.56
1:A:3766:GLN:OE1	1:A:3769:ARG:NH2	2.38	0.56
1:B:2653:LYS:HB2	1:B:2661:TRP:HE3	1.70	0.56
1:B:3766:GLN:OE1	1:B:3769:ARG:NH2	2.38	0.56
1:C:638:ILE:HD12	1:C:1638:ALA:HB3	1.86	0.56
1:C:3214:ASN:HB3	1:C:3217:SER:HB2	1.86	0.56
1:D:747:CYS:HB2	1:D:756:SER:HB2	1.87	0.56
1:A:728:ARG:NH2	1:A:1489:CYS:SG	2.78	0.56
1:A:2018:GLU:OE1	1:A:2028:ARG:NH1	2.38	0.56
1:B:2463:LEU:HA	1:B:2466:LEU:HD12	1.86	0.56
1:D:2463:LEU:HA	1:D:2466:LEU:HD12	1.86	0.56
1:D:2595:LEU:O	1:D:2600:ARG:NH1	2.38	0.56
1:A:2977:LEU:HA	1:A:2980:VAL:HG22	1.88	0.56
1:B:1454:THR:OG1	1:B:1456:ASP:OD1	2.23	0.56
1:B:1561:VAL:HG12	1:B:1562:ILE:HG13	1.87	0.56
1:B:2792:ARG:HB2	1:B:2797:PHE:HD1	1.70	0.56
1:B:3769:ARG:O	1:B:3773:ARG:NH1	2.38	0.56
1:C:2792:ARG:HB2	1:C:2797:PHE:HD1	1.70	0.56
1:D:3635:CYS:HA	1:D:3638:MET:HG3	1.86	0.56
1:D:4570:ALA:O	1:D:4574:ASN:ND2	2.39	0.56
1:A:3702:VAL:HG13	1:A:3778:MET:HG2	1.86	0.56
1:B:2021:CYS:O	1:B:2028:ARG:NH2	2.38	0.56
1:B:3702:VAL:HG13	1:B:3778:MET:HG2	1.86	0.56
1:D:348:VAL:HB	1:D:357:LEU:HD22	1.87	0.56
1:D:1694:LEU:HB3	1:D:1715:LEU:HD12	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2977:LEU:HA	1:D:2980:VAL:HG22	1.87	0.56
1:A:34:LYS:HB3	1:A:53:SER:HB3	1.87	0.56
1:A:133:PHE:O	1:A:193:ALA:N	2.38	0.56
1:A:683:ARG:NH1	1:A:707:VAL:O	2.34	0.56
1:A:2021:CYS:O	1:A:2028:ARG:NH2	2.38	0.56
1:B:3052:HIS:NE2	1:B:3128:ASN:OD1	2.35	0.56
1:D:3769:ARG:O	1:D:3773:ARG:NH1	2.38	0.56
1:A:4938:ASP:OD1	1:D:4944:ARG:NH2	2.36	0.56
1:B:728:ARG:NH2	1:B:1489:CYS:SG	2.78	0.56
1:B:2823:ILE:HD11	1:B:2935:TYR:HB3	1.86	0.56
1:B:3214:ASN:HB3	1:B:3217:SER:HB2	1.86	0.56
1:B:4570:ALA:O	1:B:4574:ASN:ND2	2.39	0.56
1:A:2653:LYS:HB2	1:A:2661:TRP:HE3	1.70	0.56
1:B:3048:ALA:O	1:B:3053:ARG:NH2	2.39	0.56
1:C:1694:LEU:HB3	1:C:1715:LEU:HD12	1.88	0.56
1:C:2018:GLU:OE1	1:C:2028:ARG:NH1	2.38	0.56
1:D:1653:LEU:O	1:D:1660:GLN:NE2	2.38	0.56
1:D:4994:TYR:OH	1:D:4998:LYS:NZ	2.35	0.56
1:C:2512:ILE:HG21	1:C:2518:LEU:HD13	1.88	0.56
1:D:3048:ALA:O	1:D:3053:ARG:NH2	2.39	0.56
1:A:747:CYS:HB2	1:A:756:SER:HB2	1.87	0.55
1:A:2000:SER:O	1:A:2005:GLN:NE2	2.32	0.55
1:A:3524:MET:HA	1:A:3582:ARG:HH22	1.70	0.55
1:B:1694:LEU:HB3	1:B:1715:LEU:HD12	1.88	0.55
1:B:2018:GLU:OE1	1:B:2028:ARG:NH1	2.38	0.55
1:B:2977:LEU:HA	1:B:2980:VAL:HG22	1.87	0.55
1:C:683:ARG:NH1	1:C:707:VAL:O	2.34	0.55
1:C:3459:VAL:HG13	1:C:3464:ILE:HB	1.89	0.55
1:A:707:VAL:HG23	1:A:782:SER:HB3	1.88	0.55
1:A:3459:VAL:HG13	1:A:3464:ILE:HB	1.89	0.55
1:B:707:VAL:HG23	1:B:782:SER:HB3	1.88	0.55
1:C:348:VAL:HB	1:C:357:LEU:HD22	1.87	0.55
1:C:2927:LEU:HD12	1:C:2930:LEU:HD12	1.88	0.55
1:C:4570:ALA:O	1:C:4574:ASN:ND2	2.39	0.55
1:D:3214:ASN:HB3	1:D:3217:SER:HB2	1.87	0.55
1:D:4583:SER:HB2	1:D:4631:PHE:HE1	1.72	0.55
1:A:277:GLY:HA2	1:A:315:CYS:HB3	1.89	0.55
1:A:1454:THR:OG1	1:A:1456:ASP:OD1	2.23	0.55
1:B:34:LYS:HB3	1:B:53:SER:HB3	1.87	0.55
1:C:2653:LYS:HB2	1:C:2661:TRP:HE3	1.70	0.55
1:D:277:GLY:HA2	1:D:315:CYS:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2114:PRO:HB3	1:D:3707:ARG:HH12	1.72	0.55
1:D:3099:ALA:HA	1:D:3136:LEU:HD21	1.89	0.55
1:A:1694:LEU:HB3	1:A:1715:LEU:HD12	1.88	0.55
1:A:2512:ILE:HG21	1:A:2518:LEU:HD13	1.88	0.55
1:A:4583:SER:HB2	1:A:4631:PHE:HE1	1.72	0.55
1:C:3635:CYS:HA	1:C:3638:MET:HG3	1.86	0.55
1:A:3214:ASN:HB3	1:A:3217:SER:HB2	1.87	0.55
1:B:133:PHE:O	1:B:193:ALA:N	2.38	0.55
1:B:2512:ILE:HG21	1:B:2518:LEU:HD13	1.88	0.55
1:B:3459:VAL:HG13	1:B:3464:ILE:HB	1.89	0.55
1:C:633:LEU:HD13	1:C:1639:LEU:HD21	1.89	0.55
1:C:3769:ARG:O	1:C:3773:ARG:NH1	2.38	0.55
1:A:3048:ALA:O	1:A:3053:ARG:NH2	2.39	0.55
1:A:4570:ALA:O	1:A:4574:ASN:ND2	2.39	0.55
1:B:2265:LEU:O	1:B:2330:ARG:NH1	2.39	0.55
1:C:1653:LEU:O	1:C:1660:GLN:NE2	2.38	0.55
1:C:3048:ALA:O	1:C:3053:ARG:NH2	2.39	0.55
1:C:3419:ASN:OD1	1:C:3423:TRP:NE1	2.40	0.55
1:D:3459:VAL:HG13	1:D:3464:ILE:HB	1.89	0.55
1:D:23:GLN:NE2	1:D:203:ASN:OD1	2.40	0.55
1:A:1730:MET:O	1:A:1772:ARG:NH1	2.40	0.55
1:C:747:CYS:HB2	1:C:756:SER:HB2	1.87	0.55
1:C:2265:LEU:O	1:C:2330:ARG:NH1	2.39	0.55
1:C:2977:LEU:HA	1:C:2980:VAL:HG22	1.87	0.55
1:C:4583:SER:HB2	1:C:4631:PHE:HE1	1.72	0.55
1:D:1730:MET:O	1:D:1772:ARG:NH1	2.40	0.55
1:D:2000:SER:O	1:D:2005:GLN:NE2	2.33	0.55
1:A:2114:PRO:HB3	1:A:3707:ARG:HH12	1.72	0.55
1:B:633:LEU:HD13	1:B:1639:LEU:HD21	1.89	0.55
1:B:3419:ASN:OD1	1:B:3423:TRP:NE1	2.40	0.55
1:C:23:GLN:NE2	1:C:203:ASN:OD1	2.40	0.55
1:C:796:ARG:O	1:C:1619:ARG:NH2	2.40	0.55
1:B:796:ARG:O	1:B:1619:ARG:NH2	2.40	0.54
1:A:796:ARG:O	1:A:1619:ARG:NH2	2.40	0.54
1:A:2978:GLU:OE2	1:A:3053:ARG:NH1	2.31	0.54
1:A:3419:ASN:OD1	1:A:3423:TRP:NE1	2.40	0.54
1:B:1730:MET:O	1:B:1772:ARG:NH1	2.40	0.54
1:B:2114:PRO:HB3	1:B:3707:ARG:HH12	1.72	0.54
1:B:3840:SER:OG	1:B:3877:ASP:OD1	2.24	0.54
1:B:4583:SER:HB2	1:B:4631:PHE:HE1	1.72	0.54
1:C:2114:PRO:HB3	1:C:3707:ARG:HH12	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:34:LYS:HB3	1:D:53:SER:HB3	1.87	0.54
1:A:2265:LEU:O	1:A:2330:ARG:NH1	2.40	0.54
1:B:23:GLN:NE2	1:B:203:ASN:OD1	2.40	0.54
1:C:3099:ALA:HA	1:C:3136:LEU:HD21	1.89	0.54
1:A:23:GLN:NE2	1:A:203:ASN:OD1	2.40	0.54
1:A:2927:LEU:HD12	1:A:2930:LEU:HD12	1.88	0.54
1:D:2265:LEU:O	1:D:2330:ARG:NH1	2.39	0.54
1:C:707:VAL:HG23	1:C:782:SER:HB3	1.88	0.54
1:D:707:VAL:HG23	1:D:782:SER:HB3	1.88	0.54
1:D:4886:HIS:HD2	1:D:4920:PHE:HE2	1.56	0.54
1:A:1944:GLU:HB3	1:A:2123:LEU:HD21	1.90	0.54
1:A:2131:LEU:HD12	1:A:3662:ILE:HG23	1.90	0.54
1:C:34:LYS:HB3	1:C:53:SER:HB3	1.87	0.54
1:A:867:LEU:HD13	1:A:929:LEU:HB3	1.90	0.54
1:B:3099:ALA:HA	1:B:3136:LEU:HD21	1.89	0.54
1:B:4886:HIS:HD2	1:B:4920:PHE:HE2	1.56	0.54
1:C:1730:MET:O	1:C:1772:ARG:NH1	2.40	0.54
1:C:1944:GLU:HB3	1:C:2123:LEU:HD21	1.90	0.54
1:C:2309:SER:OG	1:C:2321:ILE:O	2.22	0.54
1:D:669:ASP:OD1	1:D:790:ARG:NH1	2.40	0.54
1:A:2247:GLN:NE2	1:A:2281:ILE:O	2.41	0.54
1:A:3099:ALA:HA	1:A:3136:LEU:HD21	1.88	0.54
1:A:4886:HIS:HD2	1:A:4920:PHE:HE2	1.56	0.54
1:B:632:LEU:O	1:B:634:GLN:NE2	2.40	0.54
1:B:669:ASP:OD1	1:B:790:ARG:NH1	2.40	0.54
1:B:1944:GLU:HB3	1:B:2123:LEU:HD21	1.90	0.54
1:B:2247:GLN:NE2	1:B:2281:ILE:O	2.41	0.54
1:C:669:ASP:OD1	1:C:790:ARG:NH1	2.40	0.54
1:C:867:LEU:HD13	1:C:929:LEU:HB3	1.90	0.54
1:C:4112:LEU:O	1:C:4115:SER:OG	2.25	0.54
1:D:633:LEU:HD13	1:D:1639:LEU:HD21	1.89	0.54
1:D:2512:ILE:HG21	1:D:2518:LEU:HD13	1.88	0.54
1:D:3380:ARG:NH2	1:D:3450:ASN:OD1	2.41	0.54
1:A:4112:LEU:O	1:A:4115:SER:OG	2.25	0.54
1:B:2927:LEU:HD12	1:B:2930:LEU:HD12	1.89	0.54
1:C:277:GLY:HA2	1:C:315:CYS:HB3	1.89	0.54
1:C:1277:TRP:O	1:C:1559:GLN:NE2	2.41	0.54
1:C:3380:ARG:NH2	1:C:3450:ASN:OD1	2.40	0.54
1:D:632:LEU:O	1:D:634:GLN:NE2	2.40	0.54
1:D:1277:TRP:O	1:D:1559:GLN:NE2	2.41	0.54
1:B:3380:ARG:NH2	1:B:3450:ASN:OD1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:632:LEU:O	1:A:634:GLN:NE2	2.40	0.53
1:A:669:ASP:OD1	1:A:790:ARG:NH1	2.40	0.53
1:B:277:GLY:HA2	1:B:315:CYS:HB3	1.89	0.53
1:B:867:LEU:HD13	1:B:929:LEU:HB3	1.90	0.53
1:B:2131:LEU:HD12	1:B:3662:ILE:HG23	1.90	0.53
1:D:1454:THR:OG1	1:D:1456:ASP:OD1	2.23	0.53
1:D:4112:LEU:O	1:D:4115:SER:OG	2.25	0.53
1:A:633:LEU:HD13	1:A:1639:LEU:HD21	1.89	0.53
1:A:4994:TYR:OH	1:A:4998:LYS:NZ	2.35	0.53
1:B:3322:ILE:O	1:B:3326:ASN:ND2	2.41	0.53
1:D:796:ARG:O	1:D:1619:ARG:NH2	2.40	0.53
1:D:1944:GLU:HB3	1:D:2123:LEU:HD21	1.90	0.53
1:D:2927:LEU:HD12	1:D:2930:LEU:HD12	1.88	0.53
1:D:3322:ILE:O	1:D:3326:ASN:ND2	2.41	0.53
1:D:3419:ASN:OD1	1:D:3423:TRP:NE1	2.40	0.53
1:C:3882:GLN:HG3	1:C:3957:VAL:HG22	1.91	0.53
1:D:867:LEU:HD13	1:D:929:LEU:HB3	1.90	0.53
1:A:1277:TRP:O	1:A:1559:GLN:NE2	2.41	0.53
1:A:3380:ARG:NH2	1:A:3450:ASN:OD1	2.41	0.53
1:B:1277:TRP:O	1:B:1559:GLN:NE2	2.41	0.53
1:C:2000:SER:O	1:C:2005:GLN:NE2	2.33	0.53
1:D:3107:VAL:HG11	1:D:3171:SER:HB2	1.91	0.53
1:A:3322:ILE:O	1:A:3326:ASN:ND2	2.41	0.53
1:A:3924:LEU:HD21	1:A:3984:ARG:HH21	1.73	0.53
1:C:632:LEU:O	1:C:634:GLN:NE2	2.40	0.53
1:D:3524:MET:O	1:D:3595:ARG:NH1	2.42	0.53
1:D:3882:GLN:HG3	1:D:3957:VAL:HG22	1.91	0.53
1:A:2960:LEU:HD23	1:A:2963:LEU:HD12	1.91	0.53
1:A:3882:GLN:HG3	1:A:3957:VAL:HG22	1.91	0.53
1:B:2960:LEU:HD23	1:B:2963:LEU:HD12	1.91	0.53
1:D:125:ARG:NH1	1:D:126:SER:OG	2.42	0.53
1:D:1066:GLN:NE2	1:D:1461:ASP:OD1	2.39	0.53
1:B:3767:GLN:OE1	1:B:3809:ASN:ND2	2.38	0.53
1:C:4886:HIS:HD2	1:C:4920:PHE:HE2	1.56	0.53
1:D:3208:PRO:HA	1:D:3211:ASN:HB2	1.91	0.53
1:B:3020:THR:HG23	1:B:3023:LYS:H	1.74	0.53
1:B:3524:MET:O	1:B:3595:ARG:NH1	2.42	0.53
1:C:3524:MET:O	1:C:3595:ARG:NH1	2.42	0.53
1:D:683:ARG:NH1	1:D:707:VAL:O	2.34	0.53
1:D:1099:GLU:OE2	1:D:1125:ASN:ND2	2.40	0.53
1:D:2131:LEU:HD12	1:D:3662:ILE:HG23	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3984:ARG:HH22	1:B:161:GLU:HB3	1.74	0.53
1:B:3984:ARG:HH22	1:C:161:GLU:HB3	1.74	0.53
1:C:3573:MET:HB3	1:C:3577:ARG:HH21	1.73	0.53
1:D:3573:MET:HB3	1:D:3577:ARG:HH21	1.73	0.53
1:A:818:ARG:NH2	1:A:1027:LEU:O	2.42	0.53
1:A:4161:ARG:HA	1:A:4164:LEU:HD13	1.91	0.53
1:C:133:PHE:O	1:C:193:ALA:N	2.38	0.53
1:C:3020:THR:HG23	1:C:3023:LYS:H	1.74	0.53
1:B:3573:MET:HB3	1:B:3577:ARG:HH21	1.73	0.52
1:C:1066:GLN:NE2	1:C:1461:ASP:OD1	2.39	0.52
1:C:3984:ARG:HH22	1:D:161:GLU:HB3	1.74	0.52
1:D:1674:CYS:HG	1:D:1717:SER:HG	1.56	0.52
1:B:224:HIS:NE2	1:B:385:ASP:O	2.42	0.52
1:C:3107:VAL:HG11	1:C:3171:SER:HB2	1.91	0.52
1:C:3924:LEU:HD21	1:C:3984:ARG:HH21	1.74	0.52
1:A:1739:THR:OG1	1:A:1742:THR:OG1	2.25	0.52
1:B:818:ARG:NH2	1:B:1027:LEU:O	2.42	0.52
1:B:3208:PRO:HA	1:B:3211:ASN:HB2	1.91	0.52
1:B:4866:SER:HB3	1:B:4873:ASP:HB2	1.92	0.52
1:C:222:LEU:HD23	1:C:388:LEU:HD13	1.92	0.52
1:C:224:HIS:NE2	1:C:385:ASP:O	2.42	0.52
1:C:1443:GLN:NE2	1:C:1555:LEU:O	2.40	0.52
1:C:2131:LEU:HD12	1:C:3662:ILE:HG23	1.90	0.52
1:D:222:LEU:HD23	1:D:388:LEU:HD13	1.92	0.52
1:A:1443:GLN:NE2	1:A:1555:LEU:O	2.41	0.52
1:A:2268[A]:GLN:OE1	1:A:2414:ASN:ND2	2.43	0.52
1:A:2268[B]:GLN:OE1	1:A:2414:ASN:ND2	2.43	0.52
1:A:3524:MET:O	1:A:3595:ARG:NH1	2.42	0.52
1:A:3573:MET:HB3	1:A:3577:ARG:HH21	1.73	0.52
1:A:4107:GLU:HA	1:A:4110:PHE:HB3	1.92	0.52
1:B:3107:VAL:HG11	1:B:3171:SER:HB2	1.91	0.52
1:C:818:ARG:NH2	1:C:1027:LEU:O	2.42	0.52
1:D:2268[A]:GLN:OE1	1:D:2414:ASN:ND2	2.43	0.52
1:D:3052:HIS:NE2	1:D:3128:ASN:OD1	2.35	0.52
1:D:3924:LEU:HD21	1:D:3984:ARG:HH21	1.74	0.52
1:D:4161:ARG:HA	1:D:4164:LEU:HD13	1.91	0.52
1:B:125:ARG:NH1	1:B:126:SER:OG	2.42	0.52
1:B:3882:GLN:HG3	1:B:3957:VAL:HG22	1.90	0.52
1:C:125:ARG:NH1	1:C:126:SER:OG	2.42	0.52
1:C:4866:SER:HB3	1:C:4873:ASP:HB2	1.92	0.52
1:D:3767:GLN:OE1	1:D:3809:ASN:ND2	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3208:PRO:HA	1:A:3211:ASN:HB2	1.91	0.52
1:A:3556:ASN:HA	1:A:3559:LEU:HD23	1.92	0.52
1:B:222:LEU:HD23	1:B:388:LEU:HD13	1.92	0.52
1:C:2247:GLN:NE2	1:C:2281:ILE:O	2.41	0.52
1:A:125:ARG:NH1	1:A:126:SER:OG	2.42	0.52
1:B:2365:GLY:O	1:B:2369[B]:ARG:NE	2.39	0.52
1:B:3924:LEU:HD21	1:B:3984:ARG:HH21	1.73	0.52
1:D:818:ARG:NH2	1:D:1027:LEU:O	2.42	0.52
1:D:4107:GLU:HA	1:D:4110:PHE:HB3	1.92	0.52
1:A:3318:ASN:OD1	1:A:3321:ARG:NH1	2.43	0.52
1:A:4866:SER:HB3	1:A:4873:ASP:HB2	1.92	0.52
1:A:4877:ASP:O	1:D:4581:LYS:NZ	2.42	0.52
1:B:3318:ASN:OD1	1:B:3321:ARG:NH1	2.43	0.52
1:C:2879:ALA:HB1	1:C:2919:ASP:HB3	1.92	0.52
1:C:3318:ASN:OD1	1:C:3321:ARG:NH1	2.43	0.52
1:D:3020:THR:HG23	1:D:3023:LYS:H	1.74	0.52
1:D:3556:ASN:HA	1:D:3559:LEU:HD23	1.92	0.52
1:D:4866:SER:HB3	1:D:4873:ASP:HB2	1.92	0.52
1:A:2879:ALA:HB1	1:A:2919:ASP:HB3	1.92	0.52
1:B:1443:GLN:NE2	1:B:1555:LEU:O	2.41	0.52
1:D:2247:GLN:NE2	1:D:2281:ILE:O	2.41	0.52
1:D:2960:LEU:HD23	1:D:2963:LEU:HD12	1.91	0.52
1:A:3020:THR:HG23	1:A:3023:LYS:H	1.74	0.52
1:B:2268[A]:GLN:OE1	1:B:2414:ASN:ND2	2.43	0.52
1:B:2879:ALA:HB1	1:B:2919:ASP:HB3	1.92	0.52
1:C:2268[A]:GLN:OE1	1:C:2414:ASN:ND2	2.43	0.52
1:D:2268[B]:GLN:OE1	1:D:2414:ASN:ND2	2.43	0.52
1:A:4914:VAL:HG11	1:D:4884:LEU:HD11	1.92	0.51
1:B:2268[B]:GLN:OE1	1:B:2414:ASN:ND2	2.43	0.51
1:B:4068:LEU:HA	1:B:4071:ILE:HB	1.92	0.51
1:B:4161:ARG:HA	1:B:4164:LEU:HD13	1.91	0.51
1:B:4823:LEU:HD22	1:C:4843:LEU:HD22	1.91	0.51
1:C:3322:ILE:O	1:C:3326:ASN:ND2	2.41	0.51
1:C:4708:THR:HG21	1:C:4775:TYR:HB2	1.93	0.51
1:D:224:HIS:NE2	1:D:385:ASP:O	2.42	0.51
1:D:1443:GLN:NE2	1:D:1555:LEU:O	2.40	0.51
1:A:4068:LEU:HA	1:A:4071:ILE:HB	1.92	0.51
1:B:1084:GLN:NE2	1:B:1186:ASP:O	2.43	0.51
1:C:2749:GLU:HG3	1:C:2752:ASP:HB2	1.93	0.51
1:D:3458:PHE:O	1:D:3462:ASN:ND2	2.36	0.51
1:D:3596:VAL:O	1:D:3600:SER:OG	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:HIS:NE2	1:A:385:ASP:O	2.42	0.51
1:B:45:ARG:NH2	1:B:447:ASP:OD1	2.42	0.51
1:D:2437:ALA:O	1:D:2508:ARG:NH2	2.44	0.51
1:D:2749:GLU:HG3	1:D:2752:ASP:HB2	1.93	0.51
1:D:4708:THR:HG21	1:D:4775:TYR:HB2	1.93	0.51
1:A:222:LEU:HD23	1:A:388:LEU:HD13	1.92	0.51
1:A:796:ARG:HG3	1:A:1619:ARG:HH22	1.74	0.51
1:A:1099:GLU:OE2	1:A:1125:ASN:ND2	2.40	0.51
1:C:2960:LEU:HD23	1:C:2963:LEU:HD12	1.91	0.51
1:D:3318:ASN:OD1	1:D:3321:ARG:NH1	2.43	0.51
1:B:356:TRP:O	1:B:379:HIS:N	2.43	0.51
1:B:2749:GLU:HG3	1:B:2752:ASP:HB2	1.93	0.51
1:C:3556:ASN:HA	1:C:3559:LEU:HD23	1.92	0.51
1:B:3781:GLN:NE2	1:B:3819:TYR:OH	2.40	0.51
1:C:4161:ARG:HA	1:C:4164:LEU:HD13	1.91	0.51
1:C:4823:LEU:HD22	1:D:4843:LEU:HD22	1.91	0.51
1:D:1947:CYS:SG	1:D:2127:GLN:NE2	2.79	0.51
1:D:2365:GLY:O	1:D:2369[B]:ARG:NE	2.39	0.51
1:D:2879:ALA:HB1	1:D:2919:ASP:HB3	1.92	0.51
1:A:818:ARG:HH12	1:A:1026:LEU:HA	1.76	0.51
1:A:3052:HIS:NE2	1:A:3128:ASN:OD1	2.35	0.51
1:B:1947:CYS:SG	1:B:2127:GLN:NE2	2.79	0.51
1:B:2437:ALA:O	1:B:2508:ARG:NH2	2.44	0.51
1:C:356:TRP:O	1:C:379:HIS:N	2.43	0.51
1:C:2268[B]:GLN:OE1	1:C:2414:ASN:ND2	2.43	0.51
1:D:45:ARG:NH2	1:D:447:ASP:OD1	2.42	0.51
1:D:4068:LEU:HA	1:D:4071:ILE:HB	1.93	0.51
1:B:818:ARG:HH12	1:B:1026:LEU:HA	1.76	0.51
1:B:1225:PRO:HG2	1:B:1228:ILE:HD13	1.93	0.51
1:B:1618:ARG:NH2	1:B:1619:ARG:O	2.44	0.51
1:B:3107:VAL:O	1:B:3111:ARG:HB2	2.11	0.51
1:B:4107:GLU:HA	1:B:4110:PHE:HB3	1.92	0.51
1:C:320:LYS:NZ	1:C:383:HIS:O	2.44	0.51
1:C:4107:GLU:HA	1:C:4110:PHE:HB3	1.92	0.51
1:A:2437:ALA:O	1:A:2508:ARG:NH2	2.44	0.51
1:A:2749:GLU:HG3	1:A:2752:ASP:HB2	1.93	0.51
1:B:796:ARG:HG3	1:B:1619:ARG:HH22	1.74	0.51
1:B:2806:ARG:HD2	1:B:2810:LYS:HZ3	1.75	0.51
1:B:3556:ASN:HA	1:B:3559:LEU:HD23	1.92	0.51
1:A:356:TRP:O	1:A:379:HIS:N	2.43	0.51
1:A:1225:PRO:HG2	1:A:1228:ILE:HD13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4708:THR:HG21	1:B:4775:TYR:HB2	1.93	0.51
1:C:796:ARG:HG3	1:C:1619:ARG:HH22	1.74	0.51
1:C:1084:GLN:NE2	1:C:1186:ASP:O	2.43	0.51
1:C:3771:HIS:O	1:C:3815:LYS:NZ	2.44	0.51
1:A:45:ARG:NH2	1:A:447:ASP:OD1	2.42	0.50
1:A:320:LYS:NZ	1:A:383:HIS:O	2.44	0.50
1:A:3107:VAL:HG11	1:A:3171:SER:HB2	1.91	0.50
1:C:1454:THR:OG1	1:C:1456:ASP:OD1	2.23	0.50
1:C:1739:THR:OG1	1:C:1742:THR:OG1	2.25	0.50
1:C:3458:PHE:O	1:C:3462:ASN:ND2	2.36	0.50
1:D:1739:THR:OG1	1:D:1742:THR:OG1	2.25	0.50
1:A:2788:HIS:HB3	1:A:2791:LEU:HD23	1.93	0.50
1:B:273:HIS:CE1	1:B:338:GLU:H	2.30	0.50
1:C:1618:ARG:NH2	1:C:1619:ARG:O	2.44	0.50
1:C:3208:PRO:HA	1:C:3211:ASN:HB2	1.91	0.50
1:A:545:ASP:N	1:A:545:ASP:OD1	2.44	0.50
1:A:2754:PHE:HE2	1:A:2813:LEU:HD11	1.76	0.50
1:B:1676:LEU:HD22	1:B:2167:ILE:HD12	1.93	0.50
1:B:2745:VAL:HG13	1:B:2814:LYS:HD2	1.94	0.50
1:C:273:HIS:CE1	1:C:338:GLU:H	2.29	0.50
1:C:1225:PRO:HG2	1:C:1228:ILE:HD13	1.93	0.50
1:D:273:HIS:CE1	1:D:338:GLU:H	2.29	0.50
1:A:706:GLY:N	1:A:709:ASP:OD2	2.39	0.50
1:A:1066:GLN:NE2	1:A:1461:ASP:OD1	2.39	0.50
1:B:2754:PHE:HE2	1:B:2813:LEU:HD11	1.76	0.50
1:B:2788:HIS:HB3	1:B:2791:LEU:HD23	1.93	0.50
1:C:1751:GLY:HA3	1:C:1758:ARG:HE	1.77	0.50
1:C:2745:VAL:HG13	1:C:2814:LYS:HD2	1.94	0.50
1:C:3107:VAL:O	1:C:3111:ARG:HB2	2.11	0.50
1:C:4068:LEU:HA	1:C:4071:ILE:HB	1.93	0.50
1:D:3107:VAL:O	1:D:3111:ARG:HB2	2.11	0.50
1:D:3771:HIS:O	1:D:3815:LYS:NZ	2.44	0.50
1:A:273:HIS:CE1	1:A:338:GLU:H	2.29	0.50
1:A:1084:GLN:NE2	1:A:1186:ASP:O	2.43	0.50
1:A:1679:ASN:HA	1:A:1682:ALA:HB3	1.93	0.50
1:A:1947:CYS:SG	1:A:2127:GLN:NE2	2.79	0.50
1:A:2299:VAL:HG11	1:A:2356:LEU:HB3	1.93	0.50
1:C:3781:GLN:NE2	1:C:3819:TYR:OH	2.40	0.50
1:C:3868:ARG:HH11	1:C:3870:ASN:HB3	1.76	0.50
1:D:3840:SER:OG	1:D:3877:ASP:OD1	2.24	0.50
1:A:932:LEU:HB3	1:A:937:CYS:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1618:ARG:NH2	1:A:1619:ARG:O	2.44	0.50
1:A:3840:SER:OG	1:A:3877:ASP:OD1	2.24	0.50
1:A:3868:ARG:HH11	1:A:3870:ASN:HB3	1.76	0.50
1:A:4204:GLN:HG2	1:A:4245:MET:HG2	1.94	0.50
1:B:2764:GLU:HG3	1:B:2857:PRO:HB3	1.94	0.50
1:C:2437:ALA:O	1:C:2508:ARG:NH2	2.44	0.50
1:D:2745:VAL:HG13	1:D:2814:LYS:HD2	1.94	0.50
1:A:3107:VAL:O	1:A:3111:ARG:HB2	2.11	0.50
1:A:3458:PHE:O	1:A:3462:ASN:ND2	2.36	0.50
1:A:3767:GLN:OE1	1:A:3809:ASN:ND2	2.38	0.50
1:A:4708:THR:HG21	1:A:4775:TYR:HB2	1.93	0.50
1:A:4892:ARG:NH1	1:B:4895:GLY:O	2.37	0.50
1:B:932:LEU:HB3	1:B:937:CYS:HB3	1.94	0.50
1:B:2310:CYS:HB3	1:B:2313:LEU:HB2	1.94	0.50
1:C:648:ILE:HG23	1:C:814:ALA:HB3	1.94	0.50
1:C:2299:VAL:HG11	1:C:2356:LEU:HB3	1.93	0.50
1:C:2764:GLU:HG3	1:C:2857:PRO:HB3	1.94	0.50
1:D:545:ASP:N	1:D:545:ASP:OD1	2.44	0.50
1:B:1739:THR:OG1	1:B:1742:THR:OG1	2.25	0.50
1:B:4204:GLN:HG2	1:B:4245:MET:HG2	1.94	0.50
1:D:796:ARG:HG3	1:D:1619:ARG:HH22	1.74	0.50
1:A:1676:LEU:HD22	1:A:2167:ILE:HD12	1.93	0.50
1:A:4917:ASP:HB2	1:D:4888:TYR:HE1	1.76	0.50
1:B:1679:ASN:HA	1:B:1682:ALA:HB3	1.93	0.50
1:B:2882:TYR:O	1:B:2885:THR:OG1	2.28	0.50
1:C:2882:TYR:O	1:C:2885:THR:OG1	2.28	0.50
1:C:3227:ARG:NH1	1:C:3234:ASN:OD1	2.37	0.50
1:C:3767:GLN:OE1	1:C:3809:ASN:ND2	2.38	0.50
1:D:356:TRP:O	1:D:379:HIS:N	2.43	0.50
1:D:2764:GLU:HG3	1:D:2857:PRO:HB3	1.94	0.50
1:A:2764:GLU:HG3	1:A:2857:PRO:HB3	1.94	0.49
1:C:758:ARG:HA	1:C:763:PRO:HA	1.94	0.49
1:C:4204:GLN:HG2	1:C:4245:MET:HG2	1.94	0.49
1:D:758:ARG:HA	1:D:763:PRO:HA	1.94	0.49
1:D:1618:ARG:NH2	1:D:1619:ARG:O	2.44	0.49
1:D:1676:LEU:HD22	1:D:2167:ILE:HD12	1.93	0.49
1:D:3244:PRO:HA	1:D:3248:ARG:HH21	1.76	0.49
1:D:3868:ARG:HH11	1:D:3870:ASN:HB3	1.76	0.49
1:B:320:LYS:NZ	1:B:383:HIS:O	2.44	0.49
1:B:3244:PRO:HA	1:B:3248:ARG:HH21	1.76	0.49
1:C:45:ARG:NH2	1:C:447:ASP:OD1	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2310:CYS:HB3	1:C:2313:LEU:HB2	1.94	0.49
1:D:932:LEU:HB3	1:D:937:CYS:HB3	1.94	0.49
1:D:1225:PRO:HG2	1:D:1228:ILE:HD13	1.93	0.49
1:D:1423:ASP:N	1:D:1571:ASN:OD1	2.45	0.49
1:D:2648:TYR:O	1:D:2652:TRP:HB3	2.12	0.49
1:D:3781:GLN:NE2	1:D:3819:TYR:OH	2.40	0.49
2:E:21:THR:HA	2:E:49:ARG:HA	1.94	0.49
1:B:545:ASP:N	1:B:545:ASP:OD1	2.44	0.49
1:B:4112:LEU:O	1:B:4115:SER:OG	2.25	0.49
1:C:818:ARG:HH12	1:C:1026:LEU:HA	1.76	0.49
1:C:932:LEU:HB3	1:C:937:CYS:HB3	1.94	0.49
1:D:2788:HIS:HB3	1:D:2791:LEU:HD23	1.93	0.49
1:A:2648:TYR:O	1:A:2652:TRP:HB3	2.12	0.49
1:A:3244:PRO:HA	1:A:3248:ARG:HH21	1.76	0.49
1:B:683:ARG:NH1	1:B:707:VAL:O	2.34	0.49
1:B:1131:ARG:NH1	1:B:1178:ALA:O	2.46	0.49
1:B:2299:VAL:HG11	1:B:2356:LEU:HB3	1.93	0.49
1:C:1676:LEU:HD22	1:C:2167:ILE:HD12	1.93	0.49
1:C:2648:TYR:O	1:C:2652:TRP:HB3	2.13	0.49
1:C:3244:PRO:HA	1:C:3248:ARG:HH21	1.76	0.49
1:D:648:ILE:HG23	1:D:814:ALA:HB3	1.94	0.49
1:D:818:ARG:HH12	1:D:1026:LEU:HA	1.76	0.49
1:D:4204:GLN:HG2	1:D:4245:MET:HG2	1.94	0.49
1:A:2768:PHE:HD1	1:A:2857:PRO:HG2	1.78	0.49
1:A:4090:LYS:HG2	1:A:4123:ILE:HD11	1.95	0.49
1:A:4828:SER:O	1:A:4832:HIS:HB2	2.12	0.49
1:B:1066:GLN:NE2	1:B:1461:ASP:OD1	2.39	0.49
1:B:3391:GLU:HA	1:B:3394:VAL:HG22	1.95	0.49
1:B:3868:ARG:HH11	1:B:3870:ASN:HB3	1.76	0.49
1:B:4828:SER:O	1:B:4832:HIS:HB2	2.13	0.49
1:D:320:LYS:NZ	1:D:383:HIS:O	2.44	0.49
1:D:1256:GLU:HB3	1:D:1275:ARG:HE	1.77	0.49
1:D:2754:PHE:HE2	1:D:2813:LEU:HD11	1.76	0.49
1:A:2745:VAL:HG13	1:A:2814:LYS:HD2	1.94	0.49
1:A:3202:PRO:O	1:A:3214:ASN:ND2	2.45	0.49
1:B:1256:GLU:HB3	1:B:1275:ARG:HE	1.77	0.49
1:B:1751:GLY:HA3	1:B:1758:ARG:HE	1.77	0.49
1:B:4090:LYS:HG2	1:B:4123:ILE:HD11	1.95	0.49
1:C:262:LEU:HD13	1:C:274:LEU:HD11	1.94	0.49
1:C:1099:GLU:OE2	1:C:1125:ASN:ND2	2.40	0.49
1:C:1679:ASN:HA	1:C:1682:ALA:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2299:VAL:HG11	1:D:2356:LEU:HB3	1.93	0.49
1:D:2470:ILE:O	1:D:2499:LYS:NZ	2.39	0.49
1:D:2742:THR:O	1:D:2814:LYS:NZ	2.46	0.49
1:D:4999:ASP:OD1	1:D:4999:ASP:N	2.46	0.49
1:A:939:VAL:HB	1:A:1051:TYR:HB3	1.95	0.49
1:A:1131:ARG:NH1	1:A:1178:ALA:O	2.46	0.49
1:A:3180:ASN:HB2	1:A:3183:VAL:HG23	1.95	0.49
1:A:3391:GLU:HA	1:A:3394:VAL:HG22	1.95	0.49
1:A:4928:LEU:HD23	1:A:4931:ILE:HD12	1.95	0.49
1:B:3180:ASN:HB2	1:B:3183:VAL:HG23	1.95	0.49
1:C:936:GLY:HA3	1:C:1056:PRO:HB3	1.95	0.49
1:C:2998:PHE:HA	1:C:3002:LEU:HD13	1.95	0.49
1:C:3575:LEU:HD23	1:D:1219:LEU:HD22	1.95	0.49
1:C:4828:SER:O	1:C:4832:HIS:HB2	2.13	0.49
1:D:1679:ASN:HA	1:D:1682:ALA:HB3	1.93	0.49
1:D:1751:GLY:HA3	1:D:1758:ARG:HE	1.77	0.49
2:F:21:THR:HA	2:F:49:ARG:HA	1.94	0.49
2:H:21:THR:HA	2:H:49:ARG:HA	1.94	0.49
1:A:1423:ASP:N	1:A:1571:ASN:OD1	2.45	0.49
1:A:3051:ARG:NH2	1:A:3102:ASP:OD1	2.46	0.49
1:B:3771:HIS:O	1:B:3815:LYS:NZ	2.44	0.49
1:C:2788:HIS:HB3	1:C:2791:LEU:HD23	1.93	0.49
1:C:3051:ARG:NH2	1:C:3102:ASP:OD1	2.46	0.49
1:C:3523:ASN:O	1:C:3582:ARG:NH2	2.46	0.49
1:D:717:ASP:OD1	1:D:720:HIS:N	2.41	0.49
1:D:3227:ARG:NH1	1:D:3234:ASN:OD1	2.37	0.49
2:G:21:THR:HA	2:G:49:ARG:HA	1.94	0.49
1:A:870:ILE:HG13	1:A:874:LEU:HD23	1.95	0.49
1:A:2093:SER:OG	1:A:2096:GLU:OE1	2.31	0.49
1:B:2768:PHE:HD1	1:B:2857:PRO:HG2	1.78	0.49
1:C:2093:SER:OG	1:C:2096:GLU:OE1	2.31	0.49
1:D:939:VAL:HB	1:D:1051:TYR:HB3	1.95	0.49
1:D:2310:CYS:HB3	1:D:2313:LEU:HB2	1.94	0.49
1:A:262:LEU:HD13	1:A:274:LEU:HD11	1.95	0.49
1:B:5012:LYS:HD3	1:B:5012:LYS:HA	1.64	0.49
1:C:870:ILE:HG13	1:C:874:LEU:HD23	1.95	0.49
1:D:1131:ARG:NH1	1:D:1178:ALA:O	2.46	0.49
1:D:3391:GLU:HA	1:D:3394:VAL:HG22	1.95	0.49
1:A:648:ILE:HG23	1:A:814:ALA:HB3	1.94	0.48
1:A:758:ARG:HA	1:A:763:PRO:HA	1.94	0.48
1:A:2365:GLY:O	1:A:2369[B]:ARG:NE	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3902:TYR:O	1:A:3906:GLN:NE2	2.45	0.48
1:B:717:ASP:OD1	1:B:720:HIS:N	2.41	0.48
1:B:870:ILE:HG13	1:B:874:LEU:HD23	1.95	0.48
1:C:4944:ARG:NH2	1:D:4938:ASP:OD1	2.43	0.48
1:D:2093:SER:OG	1:D:2096:GLU:OE1	2.31	0.48
1:D:2386:ILE:HG23	1:D:2392:ARG:HG3	1.95	0.48
1:B:939:VAL:HB	1:B:1051:TYR:HB3	1.95	0.48
1:C:2754:PHE:HE2	1:C:2813:LEU:HD11	1.76	0.48
1:C:3391:GLU:HA	1:C:3394:VAL:HG22	1.95	0.48
1:C:3442:PHE:HE1	1:C:3511:VAL:HG12	1.78	0.48
1:D:4821:LYS:HE2	1:D:4821:LYS:HB2	1.54	0.48
1:D:4828:SER:O	1:D:4832:HIS:HB2	2.12	0.48
1:A:1256:GLU:HB3	1:A:1275:ARG:HE	1.77	0.48
1:A:4227:GLU:H	1:A:4227:GLU:HG3	1.43	0.48
1:B:758:ARG:HA	1:B:763:PRO:HA	1.94	0.48
1:B:2093:SER:OG	1:B:2096:GLU:OE1	2.31	0.48
1:B:2736:ASP:OD1	1:B:2736:ASP:N	2.47	0.48
1:C:1256:GLU:HB3	1:C:1275:ARG:HE	1.77	0.48
1:C:1423:ASP:N	1:C:1571:ASN:OD1	2.45	0.48
1:C:2512:ILE:HD13	1:C:2561:LEU:HD11	1.95	0.48
1:A:1751:GLY:HA3	1:A:1758:ARG:HE	1.77	0.48
1:A:3781:GLN:NE2	1:A:3819:TYR:OH	2.40	0.48
1:B:648:ILE:HG23	1:B:814:ALA:HB3	1.94	0.48
1:C:1131:ARG:NH1	1:C:1178:ALA:O	2.46	0.48
1:C:2742:THR:O	1:C:2814:LYS:NZ	2.46	0.48
1:D:3180:ASN:HB2	1:D:3183:VAL:HG23	1.95	0.48
1:D:4928:LEU:HD23	1:D:4931:ILE:HD12	1.95	0.48
1:A:936:GLY:HA3	1:A:1056:PRO:HB3	1.95	0.48
1:B:1099:GLU:OE2	1:B:1125:ASN:ND2	2.40	0.48
1:B:2512:ILE:HD13	1:B:2561:LEU:HD11	1.95	0.48
1:B:4928:LEU:HD23	1:B:4931:ILE:HD12	1.95	0.48
1:B:4999:ASP:OD1	1:B:4999:ASP:N	2.46	0.48
1:D:3442:PHE:HE1	1:D:3511:VAL:HG12	1.78	0.48
1:D:4090:LYS:HG2	1:D:4123:ILE:HD11	1.95	0.48
1:A:356:TRP:N	1:A:379:HIS:O	2.38	0.48
1:A:359:TYR:HA	1:A:376:ALA:HA	1.96	0.48
1:A:3442:PHE:HE1	1:A:3511:VAL:HG12	1.78	0.48
1:A:3523:ASN:O	1:A:3582:ARG:NH2	2.46	0.48
1:A:3788:GLY:HA2	1:A:3835:LEU:HD12	1.96	0.48
1:B:2648:TYR:O	1:B:2652:TRP:HB3	2.13	0.48
1:C:886:ARG:HE	1:C:904:HIS:HB2	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2377:LEU:HA	1:C:2380:ILE:HG22	1.96	0.48
1:C:3794:VAL:HG11	1:C:3835:LEU:HD21	1.96	0.48
1:D:870:ILE:HG13	1:D:874:LEU:HD23	1.95	0.48
1:D:886:ARG:HE	1:D:904:HIS:HB2	1.79	0.48
1:D:936:GLY:HA3	1:D:1056:PRO:HB3	1.95	0.48
1:D:2768:PHE:HD1	1:D:2857:PRO:HG2	1.78	0.48
1:A:1253:PRO:O	1:A:1275:ARG:NH1	2.46	0.48
1:A:4165:GLU:HA	1:A:4168:GLU:HG2	1.95	0.48
1:B:359:TYR:HA	1:B:376:ALA:HA	1.96	0.48
1:B:936:GLY:HA3	1:B:1056:PRO:HB3	1.95	0.48
1:B:1698:LEU:HD21	1:B:1715:LEU:HD13	1.95	0.48
1:B:2165:LEU:HD12	1:B:2178:MET:HB3	1.95	0.48
1:B:3051:ARG:NH2	1:B:3102:ASP:OD1	2.46	0.48
1:B:3363:GLY:HA2	1:B:3366:ARG:HG2	1.96	0.48
1:B:4835:LYS:HB3	1:B:4835:LYS:HE2	1.56	0.48
1:C:3180:ASN:HB2	1:C:3183:VAL:HG23	1.95	0.48
1:C:4165:GLU:HA	1:C:4168:GLU:HG2	1.95	0.48
1:C:4928:LEU:HD23	1:C:4931:ILE:HD12	1.95	0.48
1:D:2165:LEU:HD12	1:D:2178:MET:HB3	1.95	0.48
1:B:3575:LEU:HD23	1:C:1219:LEU:HD22	1.95	0.48
1:B:3794:VAL:HG11	1:B:3835:LEU:HD21	1.96	0.48
1:C:875:ALA:O	1:C:879:HIS:ND1	2.47	0.48
1:C:2165:LEU:HD12	1:C:2178:MET:HB3	1.95	0.48
1:C:4090:LYS:HG2	1:C:4123:ILE:HD11	1.95	0.48
1:D:748:LEU:HD13	1:D:755:ILE:HG12	1.96	0.48
1:A:886:ARG:HE	1:A:904:HIS:HB2	1.79	0.48
1:A:2998:PHE:HA	1:A:3002:LEU:HD13	1.95	0.48
1:B:706:GLY:N	1:B:709:ASP:OD2	2.39	0.48
1:B:875:ALA:O	1:B:879:HIS:ND1	2.47	0.48
1:B:1253:PRO:O	1:B:1275:ARG:NH1	2.46	0.48
1:C:939:VAL:HB	1:C:1051:TYR:HB3	1.95	0.48
1:C:1253:PRO:O	1:C:1275:ARG:NH1	2.46	0.48
1:C:2768:PHE:HD1	1:C:2857:PRO:HG2	1.78	0.48
1:D:262:LEU:HD13	1:D:274:LEU:HD11	1.94	0.48
1:D:1448:VAL:HG22	1:D:1554:VAL:HG23	1.96	0.48
1:D:2512:ILE:HD13	1:D:2561:LEU:HD11	1.95	0.48
1:A:110:ARG:NH2	1:A:117:TYR:OH	2.47	0.48
1:A:1448:VAL:HG22	1:A:1554:VAL:HG23	1.96	0.48
1:A:2310:CYS:HB3	1:A:2313:LEU:HB2	1.94	0.48
1:A:2386:ILE:HG23	1:A:2392:ARG:HG3	1.95	0.48
1:A:2863:SER:HA	1:A:2928:LYS:HG3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:LEU:HD13	1:B:274:LEU:HD11	1.94	0.48
1:B:2742:THR:O	1:B:2814:LYS:NZ	2.46	0.48
1:B:3537:LYS:NZ	1:B:3600:SER:O	2.44	0.48
1:C:110:ARG:NH2	1:C:117:TYR:OH	2.47	0.48
1:C:248:GLU:HG2	1:C:252:VAL:HG21	1.96	0.48
1:C:359:TYR:HA	1:C:376:ALA:HA	1.96	0.48
1:C:1100:MET:HB2	1:C:1143:TRP:HZ2	1.79	0.48
1:C:2736:ASP:OD1	1:C:2736:ASP:N	2.47	0.48
1:A:877:ASN:HA	1:A:970:LEU:H	1.79	0.47
1:B:886:ARG:HE	1:B:904:HIS:HB2	1.79	0.47
1:C:748:LEU:HD13	1:C:755:ILE:HG12	1.96	0.47
1:C:2365:GLY:O	1:C:2369[B]:ARG:NE	2.39	0.47
1:C:2870[A]:GLU:OE1	1:C:2939:ARG:NH2	2.47	0.47
1:C:3902:TYR:O	1:C:3906:GLN:NE2	2.45	0.47
1:D:875:ALA:O	1:D:879:HIS:ND1	2.47	0.47
1:D:1100:MET:HB2	1:D:1143:TRP:HZ2	1.79	0.47
1:D:2863:SER:HA	1:D:2928:LYS:HG3	1.96	0.47
1:D:2998:PHE:HA	1:D:3002:LEU:HD13	1.95	0.47
1:D:3523:ASN:O	1:D:3582:ARG:NH2	2.46	0.47
1:A:1292:SER:OG	1:A:1596:GLU:N	2.44	0.47
1:A:2165:LEU:HD12	1:A:2178:MET:HB3	1.95	0.47
1:A:3159:ASP:OD1	1:A:3159:ASP:N	2.46	0.47
1:A:3227:ARG:NH1	1:A:3234:ASN:OD1	2.37	0.47
1:A:3363:GLY:HA2	1:A:3366:ARG:HG2	1.96	0.47
1:B:2377:LEU:HA	1:B:2380:ILE:HG22	1.96	0.47
1:B:2998:PHE:HA	1:B:3002:LEU:HD13	1.95	0.47
1:C:877:ASN:HA	1:C:970:LEU:H	1.79	0.47
1:D:110:ARG:NH2	1:D:117:TYR:OH	2.47	0.47
1:D:359:TYR:HA	1:D:376:ALA:HA	1.96	0.47
1:D:1253:PRO:O	1:D:1275:ARG:NH1	2.46	0.47
1:D:2377:LEU:HA	1:D:2380:ILE:HG22	1.96	0.47
1:D:3233:PRO:HG2	1:D:3239:MET:HA	1.96	0.47
1:D:4835:LYS:HB3	1:D:4835:LYS:HE2	1.56	0.47
1:A:875:ALA:O	1:A:879:HIS:ND1	2.47	0.47
1:A:2736:ASP:OD1	1:A:2736:ASP:N	2.47	0.47
1:B:3442:PHE:HE1	1:B:3511:VAL:HG12	1.78	0.47
1:C:1653:LEU:HD23	1:C:1660:GLN:HA	1.96	0.47
1:C:2477:PRO:HB3	1:C:2487:GLN:HG2	1.97	0.47
1:D:15:ARG:HG3	1:D:100:THR:HA	1.96	0.47
1:D:1712:TYR:OH	1:D:1814:MET:SD	2.72	0.47
1:B:14:LEU:HB2	1:B:163:VAL:HG13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:ARG:HG3	1:B:100:THR:HA	1.96	0.47
1:B:3523:ASN:O	1:B:3582:ARG:NH2	2.46	0.47
1:B:4049:VAL:HG11	1:B:4159:ARG:HH11	1.80	0.47
1:C:545:ASP:OD1	1:C:545:ASP:N	2.44	0.47
1:C:3840:SER:OG	1:C:3877:ASP:OD1	2.24	0.47
1:D:2736:ASP:N	1:D:2736:ASP:OD1	2.47	0.47
1:D:4165:GLU:HA	1:D:4168:GLU:HG2	1.95	0.47
1:A:868:GLU:HA	1:A:871:ARG:HB2	1.97	0.47
1:A:2748:PRO:HG2	1:A:2817:ILE:HD13	1.97	0.47
1:B:3233:PRO:HG2	1:B:3239:MET:HA	1.96	0.47
1:C:356:TRP:N	1:C:379:HIS:O	2.38	0.47
1:D:868:GLU:HA	1:D:871:ARG:HB2	1.97	0.47
1:D:1469:VAL:HG13	1:D:1492:CYS:HB3	1.96	0.47
1:D:2875:ALA:HB2	1:D:2927:LEU:HD22	1.97	0.47
1:A:1698:LEU:HD21	1:A:1715:LEU:HD13	1.95	0.47
1:C:15:ARG:HG3	1:C:100:THR:HA	1.96	0.47
1:D:37:LEU:HD21	1:D:191:VAL:HG21	1.97	0.47
1:D:2870[A]:GLU:OE1	1:D:2939:ARG:NH2	2.47	0.47
1:D:3567:PRO:HA	1:D:3570:ARG:HD3	1.96	0.47
1:D:3902:TYR:O	1:D:3906:GLN:NE2	2.45	0.47
1:A:15:ARG:HG3	1:A:100:THR:HA	1.96	0.47
1:A:1469:VAL:HG13	1:A:1492:CYS:HB3	1.96	0.47
1:A:1653:LEU:HD23	1:A:1660:GLN:HA	1.96	0.47
1:A:2870[A]:GLU:OE1	1:A:2939:ARG:NH2	2.47	0.47
1:A:3233:PRO:HG2	1:A:3239:MET:HA	1.96	0.47
1:A:3537:LYS:NZ	1:A:3600:SER:O	2.44	0.47
1:A:4895:GLY:O	1:D:4892:ARG:NH1	2.45	0.47
1:A:4999:ASP:N	1:A:4999:ASP:OD1	2.46	0.47
1:B:35:LEU:HD13	1:B:49:LEU:HD13	1.97	0.47
1:B:877:ASN:HA	1:B:970:LEU:H	1.79	0.47
1:B:1100:MET:HB2	1:B:1143:TRP:HZ2	1.79	0.47
1:B:1469:VAL:HG13	1:B:1492:CYS:HB3	1.96	0.47
1:B:2386:ILE:HG23	1:B:2392:ARG:HG3	1.95	0.47
1:B:2748:PRO:HG2	1:B:2817:ILE:HD13	1.97	0.47
1:B:2867:LEU:HD12	1:B:2928:LYS:HZ3	1.79	0.47
1:B:3567:PRO:HA	1:B:3570:ARG:HD3	1.96	0.47
1:B:4944:ARG:NH2	1:C:4938:ASP:OD1	2.43	0.47
1:C:37:LEU:HD21	1:C:191:VAL:HG21	1.97	0.47
1:C:1698:LEU:HD21	1:C:1715:LEU:HD13	1.95	0.47
1:C:2875:ALA:HB2	1:C:2927:LEU:HD22	1.97	0.47
1:C:3363:GLY:HA2	1:C:3366:ARG:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4227:GLU:H	1:C:4227:GLU:HG3	1.43	0.47
1:D:35:LEU:HD13	1:D:49:LEU:HD13	1.97	0.47
1:D:877:ASN:HA	1:D:970:LEU:H	1.79	0.47
1:D:1698:LEU:HD21	1:D:1715:LEU:HD13	1.95	0.47
1:D:1753:LYS:HB3	1:D:1758:ARG:HD2	1.96	0.47
1:D:2477:PRO:HB3	1:D:2487:GLN:HG2	1.97	0.47
1:D:2692:ASP:HB3	1:D:2695:LEU:HB3	1.96	0.47
1:D:2748:PRO:HG2	1:D:2817:ILE:HD13	1.97	0.47
1:D:2882:TYR:O	1:D:2885:THR:OG1	2.28	0.47
1:A:37:LEU:HD21	1:A:191:VAL:HG21	1.97	0.47
1:A:1100:MET:HB2	1:A:1143:TRP:HZ2	1.79	0.47
1:A:2512:ILE:HD13	1:A:2561:LEU:HD11	1.95	0.47
1:A:2692:ASP:HB3	1:A:2695:LEU:HB3	1.96	0.47
1:A:2742:THR:O	1:A:2814:LYS:NZ	2.46	0.47
1:B:356:TRP:N	1:B:379:HIS:O	2.38	0.47
1:B:1292:SER:OG	1:B:1596:GLU:N	2.44	0.47
1:B:1653:LEU:HD23	1:B:1660:GLN:HA	1.96	0.47
1:B:1712:TYR:OH	1:B:1814:MET:SD	2.72	0.47
1:C:35:LEU:HD13	1:C:49:LEU:HD13	1.97	0.47
1:C:1469:VAL:HG13	1:C:1492:CYS:HB3	1.96	0.47
1:C:2863:SER:HA	1:C:2928:LYS:HG3	1.96	0.47
1:D:1292:SER:OG	1:D:1596:GLU:N	2.44	0.47
1:D:2614:ILE:O	1:D:2650:ARG:NH2	2.43	0.47
1:D:2806:ARG:HD2	1:D:2810:LYS:HZ3	1.79	0.47
1:A:248:GLU:HG2	1:A:252:VAL:HG21	1.96	0.47
1:B:248:GLU:HG2	1:B:252:VAL:HG21	1.96	0.47
1:B:2870[A]:GLU:OE1	1:B:2939:ARG:NH2	2.47	0.47
1:B:3788:GLY:HA2	1:B:3835:LEU:HD12	1.96	0.47
1:C:3316:LEU:HD11	1:C:3346:VAL:HA	1.97	0.47
1:C:4694:ASP:HA	1:C:4700:GLN:HE21	1.80	0.47
1:D:706:GLY:N	1:D:709:ASP:OD2	2.39	0.47
1:D:3051:ARG:NH2	1:D:3102:ASP:OD1	2.46	0.47
2:F:23:VAL:HG22	2:F:47:LYS:HG2	1.97	0.47
1:A:14:LEU:HB2	1:A:163:VAL:HG13	1.97	0.47
1:B:748:LEU:HD13	1:B:755:ILE:HG12	1.96	0.47
1:B:1753:LYS:HB3	1:B:1758:ARG:HD2	1.96	0.47
1:C:3567:PRO:HA	1:C:3570:ARG:HD3	1.96	0.47
1:C:4999:ASP:N	1:C:4999:ASP:OD1	2.46	0.47
1:D:3333:THR:O	1:D:3337:ARG:NH1	2.48	0.47
1:D:3788:GLY:HA2	1:D:3835:LEU:HD12	1.96	0.47
1:D:4694:ASP:HA	1:D:4700:GLN:HE21	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:27:THR:HB	2:F:100:ASP:HB3	1.97	0.47
2:G:27:THR:HB	2:G:100:ASP:HB3	1.97	0.47
1:A:2377:LEU:HA	1:A:2380:ILE:HG22	1.96	0.46
1:A:3536:ALA:HA	1:A:3539:ARG:HG2	1.97	0.46
1:A:3567:PRO:HA	1:A:3570:ARG:HD3	1.97	0.46
1:A:3794:VAL:HG11	1:A:3835:LEU:HD21	1.96	0.46
1:B:2863:SER:HA	1:B:2928:LYS:HG3	1.96	0.46
1:B:3333:THR:O	1:B:3337:ARG:NH1	2.48	0.46
1:C:1292:SER:OG	1:C:1596:GLU:N	2.44	0.46
1:D:248:GLU:HG2	1:D:252:VAL:HG21	1.96	0.46
1:D:1653:LEU:HD23	1:D:1660:GLN:HA	1.96	0.46
1:D:3794:VAL:HG11	1:D:3835:LEU:HD21	1.96	0.46
2:E:23:VAL:HG22	2:E:47:LYS:HG2	1.97	0.46
2:F:8:SER:HB2	2:F:71:ARG:HB2	1.97	0.46
2:G:23:VAL:HG22	2:G:47:LYS:HG2	1.97	0.46
1:A:1712:TYR:OH	1:A:1814:MET:SD	2.72	0.46
1:A:1753:LYS:HB3	1:A:1758:ARG:HD2	1.97	0.46
1:B:37:LEU:HD21	1:B:191:VAL:HG21	1.97	0.46
1:C:14:LEU:HB2	1:C:163:VAL:HG13	1.97	0.46
1:C:3788:GLY:HA2	1:C:3835:LEU:HD12	1.96	0.46
1:D:294:THR:HG23	1:D:297:GLN:H	1.81	0.46
1:D:3202:PRO:O	1:D:3214:ASN:ND2	2.45	0.46
2:E:8:SER:HB2	2:E:71:ARG:HB2	1.97	0.46
2:H:23:VAL:HG22	2:H:47:LYS:HG2	1.97	0.46
1:A:717:ASP:OD1	1:A:720:HIS:N	2.41	0.46
1:A:4835:LYS:HB3	1:A:4835:LYS:HE2	1.56	0.46
1:B:110:ARG:NH2	1:B:117:TYR:OH	2.47	0.46
1:B:2109:ASP:OD1	1:B:2109:ASP:N	2.49	0.46
1:C:1947:CYS:SG	1:C:2127:GLN:NE2	2.79	0.46
1:C:2386:ILE:HG23	1:C:2392:ARG:HG3	1.95	0.46
1:C:2623:LEU:HD12	1:C:2626:LEU:HD12	1.97	0.46
1:A:294:THR:HG23	1:A:297:GLN:H	1.81	0.46
1:A:2466:LEU:HB3	1:A:2502:MET:HE1	1.97	0.46
1:A:3316:LEU:HD11	1:A:3346:VAL:HA	1.97	0.46
1:A:3333:THR:O	1:A:3337:ARG:NH1	2.48	0.46
1:B:3316:LEU:HD11	1:B:3346:VAL:HA	1.97	0.46
1:C:1753:LYS:HB3	1:C:1758:ARG:HD2	1.96	0.46
1:C:2109:ASP:N	1:C:2109:ASP:OD1	2.49	0.46
1:C:4049:VAL:HG11	1:C:4159:ARG:HH11	1.80	0.46
1:D:492:ASP:OD1	1:D:546:TRP:NE1	2.42	0.46
1:A:748:LEU:HD13	1:A:755:ILE:HG12	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2882:TYR:O	1:A:2885:THR:OG1	2.28	0.46
1:B:277:GLY:N	1:B:316:PHE:O	2.48	0.46
1:B:884:LEU:HB2	1:B:969:PRO:HD3	1.98	0.46
1:B:3902:TYR:O	1:B:3906:GLN:NE2	2.45	0.46
1:C:868:GLU:HA	1:C:871:ARG:HB2	1.97	0.46
1:C:1448:VAL:HG22	1:C:1554:VAL:HG23	1.96	0.46
1:C:2748:PRO:HG2	1:C:2817:ILE:HD13	1.97	0.46
1:C:3233:PRO:HG2	1:C:3239:MET:HA	1.96	0.46
1:C:3537:LYS:NZ	1:C:3600:SER:O	2.44	0.46
1:D:1243:PRO:O	1:D:1458:HIS:ND1	2.34	0.46
1:D:3363:GLY:HA2	1:D:3366:ARG:HG2	1.96	0.46
1:A:161:GLU:OE1	1:D:3984:ARG:NH1	2.49	0.46
1:A:4049:VAL:HG11	1:A:4159:ARG:HH11	1.80	0.46
1:A:4694:ASP:HA	1:A:4700:GLN:HE21	1.80	0.46
1:B:232:THR:HG22	1:B:258:SER:HB3	1.98	0.46
1:B:1448:VAL:HG22	1:B:1554:VAL:HG23	1.96	0.46
1:B:2477:PRO:HB3	1:B:2487:GLN:HG2	1.97	0.46
1:B:2623:LEU:HD12	1:B:2626:LEU:HD12	1.97	0.46
1:B:4165:GLU:HA	1:B:4168:GLU:HG2	1.95	0.46
1:B:4865:LYS:HA	1:B:4865:LYS:HD2	1.49	0.46
1:C:5012:LYS:HD3	1:C:5012:LYS:HA	1.64	0.46
1:D:14:LEU:HB2	1:D:163:VAL:HG13	1.97	0.46
1:D:2623:LEU:HD12	1:D:2626:LEU:HD12	1.97	0.46
2:H:8:SER:HB2	2:H:71:ARG:HB2	1.97	0.46
1:B:275:ARG:NH1	1:B:278:GLN:OE1	2.49	0.46
1:B:492:ASP:OD1	1:B:546:TRP:NE1	2.42	0.46
1:B:868:GLU:HA	1:B:871:ARG:HB2	1.97	0.46
1:B:2410:PRO:HB3	1:B:2415:ARG:HB3	1.97	0.46
1:B:2692:ASP:HB3	1:B:2695:LEU:HB3	1.96	0.46
1:D:3275:PRO:HA	1:D:3278:CYS:HB2	1.98	0.46
1:D:4049:VAL:HG11	1:D:4159:ARG:HH11	1.80	0.46
1:A:2109:ASP:N	1:A:2109:ASP:OD1	2.49	0.46
1:A:2627:VAL:HG22	1:A:2678:LEU:HG	1.98	0.46
1:A:3771:HIS:O	1:A:3815:LYS:NZ	2.44	0.46
1:B:620:LEU:O	1:B:624:ASN:ND2	2.49	0.46
1:B:2742:THR:HB	1:B:2814:LYS:HG2	1.98	0.46
1:B:2875:ALA:HB2	1:B:2927:LEU:HD22	1.97	0.46
1:B:3536:ALA:HA	1:B:3539:ARG:HG2	1.97	0.46
1:B:4694:ASP:HA	1:B:4700:GLN:HE21	1.80	0.46
1:C:294:THR:HG23	1:C:297:GLN:H	1.81	0.46
1:C:3175:LEU:O	1:C:3178:THR:OG1	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3202:PRO:O	1:C:3214:ASN:ND2	2.45	0.46
1:C:3536:ALA:HA	1:C:3539:ARG:HG2	1.97	0.46
1:D:277:GLY:N	1:D:316:PHE:O	2.48	0.46
1:D:1084:GLN:NE2	1:D:1186:ASP:O	2.43	0.46
2:H:27:THR:HB	2:H:100:ASP:HB3	1.97	0.46
1:A:35:LEU:HD13	1:A:49:LEU:HD13	1.97	0.46
1:A:1473:THR:HA	1:A:1487:LEU:O	2.16	0.46
1:A:2470:ILE:HG22	1:A:2525:GLY:HA3	1.98	0.46
1:A:2477:PRO:HB3	1:A:2487:GLN:HG2	1.97	0.46
1:B:1423:ASP:N	1:B:1571:ASN:OD1	2.45	0.46
1:C:732:SER:HB2	1:C:735:GLN:HB3	1.98	0.46
1:C:2410:PRO:HB3	1:C:2415:ARG:HB3	1.97	0.46
1:C:2500:ALA:HB2	1:C:2553:TYR:HD1	1.81	0.46
1:C:3275:PRO:HA	1:C:3278:CYS:HB2	1.98	0.46
1:D:732:SER:HB2	1:D:735:GLN:HB3	1.98	0.46
1:D:2410:PRO:HB3	1:D:2415:ARG:HB3	1.97	0.46
1:D:3316:LEU:HD11	1:D:3346:VAL:HA	1.97	0.46
1:D:4631:PHE:HE2	1:D:4633:GLU:HG2	1.81	0.46
1:A:531:ARG:NH2	1:A:562:GLU:OE2	2.37	0.46
1:A:620:LEU:O	1:A:624:ASN:ND2	2.49	0.46
1:A:4989:MET:HE3	1:A:4989:MET:HB3	1.82	0.46
1:B:3159:ASP:OD1	1:B:3159:ASP:N	2.46	0.46
1:B:3275:PRO:HA	1:B:3278:CYS:HB2	1.98	0.46
1:C:2692:ASP:HB3	1:C:2695:LEU:HB3	1.96	0.46
1:C:3333:THR:O	1:C:3337:ARG:NH1	2.48	0.46
1:D:2109:ASP:OD1	1:D:2109:ASP:N	2.49	0.46
2:G:8:SER:HB2	2:G:71:ARG:HB2	1.97	0.46
1:A:3275:PRO:HA	1:A:3278:CYS:HB2	1.98	0.45
1:C:277:GLY:N	1:C:316:PHE:O	2.48	0.45
1:D:275:ARG:NH1	1:D:278:GLN:OE1	2.49	0.45
1:D:665:GLU:HG2	1:D:745:SER:HA	1.98	0.45
1:A:232:THR:HG22	1:A:258:SER:HB3	1.98	0.45
1:A:277:GLY:N	1:A:316:PHE:O	2.48	0.45
1:C:275:ARG:NH1	1:C:278:GLN:OE1	2.49	0.45
1:D:1473:THR:HA	1:D:1487:LEU:O	2.16	0.45
1:D:2500:ALA:HB2	1:D:2553:TYR:HD1	1.81	0.45
1:D:3536:ALA:HA	1:D:3539:ARG:HG2	1.97	0.45
1:A:2500:ALA:HB2	1:A:2553:TYR:HD1	1.81	0.45
1:B:2559:LEU:HA	1:B:2562:ILE:HD12	1.99	0.45
1:A:884:LEU:HB2	1:A:969:PRO:HD3	1.98	0.45
1:A:2623:LEU:HD12	1:A:2626:LEU:HD12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1473:THR:HA	1:B:1487:LEU:O	2.16	0.45
1:C:620:LEU:O	1:C:624:ASN:ND2	2.49	0.45
1:C:4631:PHE:HE2	1:C:4633:GLU:HG2	1.81	0.45
1:D:2627:VAL:HG22	1:D:2678:LEU:HG	1.98	0.45
1:A:665:GLU:HG2	1:A:745:SER:HA	1.98	0.45
1:A:2875:ALA:HB2	1:A:2927:LEU:HD22	1.97	0.45
1:A:3175:LEU:O	1:A:3178:THR:OG1	2.33	0.45
1:A:4576:ILE:HG23	1:A:4639:MET:HG2	1.99	0.45
1:B:4631:PHE:HE2	1:B:4633:GLU:HG2	1.81	0.45
1:B:4821:LYS:HE2	1:B:4821:LYS:HB2	1.54	0.45
1:C:2466:LEU:HB3	1:C:2502:MET:HE1	1.99	0.45
1:C:2559:LEU:HA	1:C:2562:ILE:HD12	1.99	0.45
1:D:620:LEU:O	1:D:624:ASN:ND2	2.49	0.45
1:D:5030:LYS:HE2	1:D:5030:LYS:HB2	1.76	0.45
1:A:232:THR:HG21	1:A:252:VAL:HG12	1.99	0.45
1:A:699:GLY:N	1:A:1647:CYS:O	2.50	0.45
1:A:2742:THR:HB	1:A:2814:LYS:HG2	1.98	0.45
1:A:4049:VAL:HG21	1:A:4159:ARG:HG2	1.99	0.45
1:C:699:GLY:N	1:C:1647:CYS:O	2.50	0.45
1:C:876:GLU:HG2	1:C:910:PHE:CE2	2.52	0.45
1:C:2667:THR:HG21	1:C:2672:LEU:HD21	1.99	0.45
1:C:4581:LYS:HE3	1:C:4581:LYS:HB3	1.82	0.45
1:D:771:PHE:HB3	1:D:1472:VAL:HG23	1.99	0.45
1:D:884:LEU:HB2	1:D:969:PRO:HD3	1.98	0.45
1:D:1671:ARG:O	1:D:1675:ALA:HB2	2.17	0.45
1:D:2742:THR:HB	1:D:2814:LYS:HG2	1.98	0.45
1:A:275:ARG:NH1	1:A:278:GLN:OE1	2.49	0.45
1:B:732:SER:HB2	1:B:735:GLN:HB3	1.98	0.45
1:B:2500:ALA:HB2	1:B:2553:TYR:HD1	1.81	0.45
1:C:884:LEU:HB2	1:C:969:PRO:HD3	1.98	0.45
1:C:1519:LEU:HD21	1:C:1572:ILE:HD13	1.99	0.45
1:D:232:THR:HG21	1:D:252:VAL:HG12	1.99	0.45
1:D:2466:LEU:HB3	1:D:2502:MET:HE1	1.98	0.45
2:E:27:THR:HB	2:E:100:ASP:HB3	1.97	0.45
1:A:1116:GLY:O	1:A:1134:LEU:N	2.50	0.45
1:A:2986:VAL:HG22	1:A:2988:LYS:H	1.82	0.45
1:A:3519:PRO:HB3	1:B:1220:GLN:HB2	1.99	0.45
1:A:4184:MET:N	1:A:5021:PHE:O	2.50	0.45
1:B:294:THR:HG23	1:B:297:GLN:H	1.81	0.45
1:B:665:GLU:HG2	1:B:745:SER:HA	1.98	0.45
1:B:2039:LEU:HB3	1:B:2044:ILE:HB	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:LYS:HA	1:C:30:LYS:HD2	1.79	0.45
1:C:206:CYS:SG	1:C:207:SER:N	2.90	0.45
1:C:1000:ARG:HD3	1:C:1000:ARG:HA	1.82	0.45
1:C:1473:THR:HA	1:C:1487:LEU:O	2.16	0.45
1:D:585:SER:O	1:D:588:SER:OG	2.28	0.45
2:G:38:SER:OG	2:G:39:SER:N	2.50	0.45
1:A:2410:PRO:HB3	1:A:2415:ARG:HB3	1.97	0.45
1:B:2470:ILE:HG22	1:B:2525:GLY:HA3	1.98	0.45
1:B:2614:ILE:O	1:B:2650:ARG:NH2	2.43	0.45
1:B:2667:THR:HG21	1:B:2672:LEU:HD21	1.99	0.45
1:B:4576:ILE:HG23	1:B:4639:MET:HG2	1.99	0.45
1:C:2470:ILE:HG22	1:C:2525:GLY:HA3	1.98	0.45
1:C:2742:THR:HB	1:C:2814:LYS:HG2	1.98	0.45
1:C:2806:ARG:HD2	1:C:2810:LYS:HZ3	1.82	0.45
1:D:232:THR:HG22	1:D:258:SER:HB3	1.98	0.45
1:D:876:GLU:HG2	1:D:910:PHE:CE2	2.52	0.45
1:D:1658:ASP:N	1:D:1658:ASP:OD1	2.50	0.45
1:D:1690:ASP:HB2	1:D:1693:GLN:HG3	1.99	0.45
1:A:1671:ARG:O	1:A:1675:ALA:HB2	2.17	0.45
1:A:3693:LYS:HD2	1:A:3693:LYS:HA	1.78	0.45
1:A:4202:ARG:O	1:A:4206:GLU:HG2	2.17	0.45
1:A:4631:PHE:HE2	1:A:4633:GLU:HG2	1.81	0.45
1:B:1671:ARG:O	1:B:1675:ALA:HB2	2.17	0.45
1:C:1419:ASP:OD1	1:C:1421:ARG:NH1	2.50	0.45
1:D:4202:ARG:O	1:D:4206:GLU:HG2	2.17	0.45
1:D:4745:LEU:H	1:D:4745:LEU:HG	1.55	0.45
2:H:38:SER:OG	2:H:39:SER:N	2.50	0.45
1:A:732:SER:HB2	1:A:735:GLN:HB3	1.98	0.44
1:B:876:GLU:HG2	1:B:910:PHE:CE2	2.52	0.44
1:B:1658:ASP:OD1	1:B:1658:ASP:N	2.50	0.44
1:C:771:PHE:HB3	1:C:1472:VAL:HG23	1.99	0.44
1:C:1690:ASP:HB2	1:C:1693:GLN:HG3	1.99	0.44
1:C:2627:VAL:HG22	1:C:2678:LEU:HG	1.98	0.44
1:C:4049:VAL:HG21	1:C:4159:ARG:HG2	1.99	0.44
1:D:356:TRP:N	1:D:379:HIS:O	2.38	0.44
1:D:2296:GLU:HA	1:D:2299:VAL:HG12	1.99	0.44
1:D:3420:ARG:HH22	1:D:3519:PRO:HG2	1.82	0.44
1:A:206:CYS:SG	1:A:207:SER:N	2.90	0.44
1:A:876:GLU:HG2	1:A:910:PHE:CE2	2.52	0.44
1:A:1156:THR:OG1	1:A:1157:GLU:OE1	2.36	0.44
1:A:4821:LYS:HE2	1:A:4821:LYS:HB2	1.54	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:CYS:SG	1:B:207:SER:N	2.90	0.44
1:B:531:ARG:NH2	1:B:562:GLU:OE2	2.37	0.44
1:B:1116:GLY:O	1:B:1134:LEU:N	2.50	0.44
1:B:1147:ASP:HB3	1:B:1164:LEU:HD11	2.00	0.44
1:B:3202:PRO:O	1:B:3214:ASN:ND2	2.45	0.44
1:C:232:THR:HG22	1:C:258:SER:HB3	1.98	0.44
1:C:823:LEU:HD12	1:C:823:LEU:HA	1.89	0.44
1:D:206:CYS:SG	1:D:207:SER:N	2.90	0.44
1:D:1116:GLY:O	1:D:1134:LEU:N	2.50	0.44
1:D:2470:ILE:HG22	1:D:2525:GLY:HA3	1.98	0.44
1:D:2559:LEU:HA	1:D:2562:ILE:HD12	1.99	0.44
1:D:2770:LYS:HD2	1:D:2788:HIS:H	1.82	0.44
1:A:2559:LEU:HA	1:A:2562:ILE:HD12	1.99	0.44
1:A:4938:ASP:CG	1:D:4944:ARG:HH21	2.20	0.44
1:B:2466:LEU:HB3	1:B:2502:MET:HE1	2.00	0.44
1:C:499:THR:HG23	1:C:502:HIS:H	1.83	0.44
1:C:1147:ASP:HB3	1:C:1164:LEU:HD11	2.00	0.44
1:A:499:THR:HG23	1:A:502:HIS:H	1.83	0.44
1:A:1658:ASP:N	1:A:1658:ASP:OD1	2.50	0.44
1:A:2039:LEU:HB3	1:A:2044:ILE:HB	1.99	0.44
1:B:499:THR:HG23	1:B:502:HIS:H	1.83	0.44
1:B:2986:VAL:HG22	1:B:2988:LYS:H	1.82	0.44
1:C:4913:ARG:NH2	1:C:4917:ASP:OD2	2.51	0.44
1:D:30:LYS:HA	1:D:30:LYS:HD2	1.79	0.44
1:D:3159:ASP:OD1	1:D:3159:ASP:N	2.46	0.44
1:A:1147:ASP:HB3	1:A:1164:LEU:HD11	2.00	0.44
1:A:1220:GLN:HB2	1:D:3519:PRO:HB3	1.99	0.44
1:A:1243:PRO:O	1:A:1458:HIS:ND1	2.33	0.44
1:A:2355:ARG:HA	1:A:2358:ILE:HG12	1.99	0.44
1:A:2654:TYR:HA	1:A:2661:TRP:H	1.83	0.44
1:A:2770:LYS:HD2	1:A:2788:HIS:H	1.83	0.44
1:A:4865:LYS:HA	1:A:4865:LYS:HD2	1.49	0.44
1:B:863:LEU:HA	1:B:864:PRO:HD3	1.85	0.44
1:C:717:ASP:OD1	1:C:720:HIS:N	2.41	0.44
1:C:4865:LYS:HD2	1:C:4865:LYS:HA	1.49	0.44
1:D:4576:ILE:HG23	1:D:4639:MET:HG2	1.99	0.44
1:A:161:GLU:HB3	1:D:3984:ARG:NH2	2.32	0.44
1:A:1690:ASP:HB2	1:A:1693:GLN:HG3	1.99	0.44
1:A:5012:LYS:HD3	1:A:5012:LYS:HA	1.64	0.44
1:B:2355:ARG:HA	1:B:2358:ILE:HG12	1.99	0.44
1:B:4202:ARG:O	1:B:4206:GLU:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:232:THR:HG21	1:C:252:VAL:HG12	1.99	0.44
1:C:665:GLU:HG2	1:C:745:SER:HA	1.98	0.44
1:C:2355:ARG:HA	1:C:2358:ILE:HG12	1.99	0.44
1:C:2614:ILE:O	1:C:2650:ARG:NH2	2.43	0.44
1:C:2770:LYS:HD2	1:C:2788:HIS:H	1.83	0.44
1:D:1519:LEU:HD21	1:D:1572:ILE:HD13	1.99	0.44
1:D:2251:PHE:HB2	1:D:2286:LEU:HD13	2.00	0.44
1:D:2560:PRO:O	1:D:2564:LYS:HD2	2.18	0.44
1:D:2654:TYR:HA	1:D:2661:TRP:H	1.83	0.44
1:D:2667:THR:HG21	1:D:2672:LEU:HD21	1.99	0.44
1:D:2986:VAL:HG22	1:D:2988:LYS:H	1.82	0.44
2:E:38:SER:OG	2:E:39:SER:N	2.50	0.44
1:A:308:HIS:HD2	1:A:310:LYS:HB3	1.83	0.44
1:A:771:PHE:HB3	1:A:1472:VAL:HG23	1.99	0.44
1:A:2671:GLU:HA	1:A:2674:LEU:HB2	2.00	0.44
1:A:3420:ARG:HH22	1:A:3519:PRO:HG2	1.82	0.44
1:A:4983:HIS:O	3:A:5101:AMP:N6	2.51	0.44
1:B:771:PHE:HB3	1:B:1472:VAL:HG23	1.99	0.44
1:B:1519:LEU:HD21	1:B:1572:ILE:HD13	1.99	0.44
1:B:2560:PRO:O	1:B:2564:LYS:HD2	2.18	0.44
1:B:2806:ARG:HA	1:B:2809:ILE:HD13	2.00	0.44
1:B:3321:ARG:HA	1:B:3324:VAL:HG12	2.00	0.44
1:C:414:PHE:O	1:C:418:LEU:HB2	2.18	0.44
1:C:2039:LEU:HB3	1:C:2044:ILE:HB	1.99	0.44
1:C:2251:PHE:HB2	1:C:2286:LEU:HD13	2.00	0.44
1:D:1147:ASP:HB3	1:D:1164:LEU:HD11	2.00	0.44
1:D:3092:LEU:HD12	1:D:3093:ARG:HG3	2.00	0.44
1:A:414:PHE:O	1:A:418:LEU:HB2	2.18	0.44
1:A:2806:ARG:HA	1:A:2809:ILE:HD13	2.00	0.44
1:B:1156:THR:OG1	1:B:1157:GLU:OE1	2.35	0.44
1:B:2770:LYS:HD2	1:B:2788:HIS:H	1.83	0.44
1:C:308:HIS:HD2	1:C:310:LYS:HB3	1.83	0.44
1:C:1671:ARG:O	1:C:1675:ALA:HB2	2.17	0.44
1:C:1712:TYR:OH	1:C:1814:MET:SD	2.72	0.44
1:D:2633:LEU:HG	1:D:2695:LEU:HD21	2.00	0.44
1:D:4913:ARG:NH2	1:D:4917:ASP:OD2	2.51	0.44
2:F:38:SER:OG	2:F:39:SER:N	2.50	0.44
1:A:452:PHE:HE1	1:A:474:ARG:HB3	1.83	0.44
1:A:492:ASP:OD1	1:A:546:TRP:NE1	2.42	0.44
1:A:2621:HIS:HB3	1:A:2624:ARG:HH21	1.83	0.44
1:A:3321:ARG:HA	1:A:3324:VAL:HG12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:699:GLY:N	1:B:1647:CYS:O	2.50	0.44
1:B:3218:VAL:O	1:B:3222:LYS:HB2	2.18	0.44
1:C:1156:THR:OG1	1:C:1157:GLU:OE1	2.36	0.44
1:C:1652:GLU:OE1	1:C:1656:ARG:NH2	2.46	0.44
1:C:2296:GLU:HA	1:C:2299:VAL:HG12	1.99	0.44
1:C:4202:ARG:O	1:C:4206:GLU:HG2	2.17	0.44
1:D:3218:VAL:O	1:D:3222:LYS:HB2	2.18	0.44
1:D:3694:LYS:HA	1:D:3695:PRO:HD3	1.90	0.44
1:D:4049:VAL:HG21	1:D:4159:ARG:HG2	1.99	0.44
1:A:683:ARG:HG2	1:A:717:ASP:HB3	2.00	0.43
1:B:3264:THR:OG1	1:B:3265:GLU:OE1	2.36	0.43
1:C:2472:LEU:HD23	1:C:2472:LEU:HA	1.87	0.43
1:C:2560:PRO:O	1:C:2564:LYS:HD2	2.18	0.43
1:C:2633:LEU:HG	1:C:2695:LEU:HD21	2.00	0.43
1:C:2825:LYS:NZ	1:C:2935:TYR:OH	2.45	0.43
1:C:3420:ARG:HH22	1:C:3519:PRO:HG2	1.82	0.43
1:C:4576:ILE:HG23	1:C:4639:MET:HG2	1.99	0.43
1:C:4983:HIS:O	3:C:5101:AMP:N6	2.51	0.43
1:D:1419:ASP:OD1	1:D:1421:ARG:NH1	2.50	0.43
1:D:4184:MET:N	1:D:5021:PHE:O	2.50	0.43
2:E:76:CYS:HB3	2:E:97:LEU:HB2	2.00	0.43
2:H:76:CYS:HB3	2:H:97:LEU:HB2	2.00	0.43
1:A:2357:LEU:HB3	1:A:2364:PHE:HE1	1.83	0.43
1:A:2667:THR:HG21	1:A:2672:LEU:HD21	1.99	0.43
1:A:4823:LEU:HD23	1:A:4823:LEU:HA	1.79	0.43
1:A:4965:SER:O	1:A:4969:ASP:HB2	2.18	0.43
1:B:232:THR:HG21	1:B:252:VAL:HG12	1.99	0.43
1:B:452:PHE:HE1	1:B:474:ARG:HB3	1.83	0.43
1:B:683:ARG:HG2	1:B:717:ASP:HB3	2.00	0.43
1:B:1036:ARG:O	1:B:1040:CYS:HB2	2.18	0.43
1:B:2686:LEU:HB3	1:B:2997:PHE:HE1	1.83	0.43
1:B:3592:ILE:HG22	1:B:3595:ARG:HH21	1.83	0.43
1:B:4049:VAL:HG21	1:B:4159:ARG:HG2	1.99	0.43
1:B:4823:LEU:HA	1:B:4823:LEU:HD23	1.79	0.43
1:C:2357:LEU:HB3	1:C:2364:PHE:HE1	1.83	0.43
1:C:3798:LEU:HD23	1:C:3798:LEU:HA	1.89	0.43
1:D:2621:HIS:HB3	1:D:2624:ARG:HH21	1.83	0.43
1:D:2806:ARG:HA	1:D:2809:ILE:HD13	2.00	0.43
1:A:2175:GLU:HG3	1:A:2228:MET:HB2	2.00	0.43
1:A:2633:LEU:HG	1:A:2695:LEU:HD21	2.00	0.43
1:A:2766:TRP:HE1	1:A:2788:HIS:HB2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3092:LEU:HD12	1:A:3093:ARG:HG3	1.99	0.43
1:A:4823:LEU:HD22	1:B:4843:LEU:HD22	1.99	0.43
1:B:1690:ASP:HB2	1:B:1693:GLN:HG3	1.99	0.43
1:B:2782:ASP:N	1:B:2782:ASP:OD1	2.52	0.43
1:B:4184:MET:N	1:B:5021:PHE:O	2.50	0.43
1:B:4913:ARG:NH2	1:B:4917:ASP:OD2	2.51	0.43
1:C:1116:GLY:O	1:C:1134:LEU:N	2.50	0.43
1:C:1658:ASP:N	1:C:1658:ASP:OD1	2.50	0.43
1:C:2591:ARG:HG2	1:C:2636:PHE:HB3	2.01	0.43
1:C:2986:VAL:HG22	1:C:2988:LYS:H	1.82	0.43
1:C:4965:SER:O	1:C:4969:ASP:HB2	2.18	0.43
1:D:452:PHE:HE1	1:D:474:ARG:HB3	1.83	0.43
1:D:1036:ARG:O	1:D:1040:CYS:HB2	2.18	0.43
1:D:3227:ARG:HA	1:D:3232:LEU:HD12	2.01	0.43
1:D:3264:THR:OG1	1:D:3265:GLU:OE1	2.36	0.43
1:D:4227:GLU:H	1:D:4227:GLU:HG3	1.43	0.43
1:D:4823:LEU:HD23	1:D:4823:LEU:HA	1.79	0.43
2:E:2:VAL:HG23	2:E:80:VAL:HG21	2.01	0.43
1:A:2782:ASP:N	1:A:2782:ASP:OD1	2.52	0.43
1:A:4934:GLY:HA2	1:D:4937:ILE:HG12	2.00	0.43
1:B:124:SER:HB2	1:B:133:PHE:HA	2.01	0.43
1:B:414:PHE:O	1:B:418:LEU:HB2	2.18	0.43
1:B:2159:LEU:HG	1:B:2163:ARG:HE	1.84	0.43
1:B:2627:VAL:HG22	1:B:2678:LEU:HG	1.98	0.43
1:B:2654:TYR:HA	1:B:2661:TRP:H	1.83	0.43
1:B:3092:LEU:HD12	1:B:3093:ARG:HG3	2.00	0.43
1:C:1036:ARG:O	1:C:1040:CYS:HB2	2.18	0.43
1:C:2930:LEU:O	1:C:2935:TYR:N	2.49	0.43
1:C:3694:LYS:HA	1:C:3695:PRO:HD3	1.90	0.43
1:D:414:PHE:O	1:D:418:LEU:HB2	2.18	0.43
1:A:2560:PRO:O	1:A:2564:LYS:HD2	2.18	0.43
1:A:2686:LEU:HB3	1:A:2997:PHE:HE1	1.83	0.43
1:B:308:HIS:HD2	1:B:310:LYS:HB3	1.83	0.43
1:B:2591:ARG:HG2	1:B:2636:PHE:HB3	2.01	0.43
1:B:3458:PHE:O	1:B:3462:ASN:ND2	2.36	0.43
1:B:4965:SER:O	1:B:4969:ASP:HB2	2.18	0.43
1:B:4983:HIS:O	3:B:5101:AMP:N6	2.51	0.43
1:C:2621:HIS:HB3	1:C:2624:ARG:HH21	1.83	0.43
1:C:2806:ARG:HA	1:C:2809:ILE:HD13	2.00	0.43
1:C:3092:LEU:HD12	1:C:3093:ARG:HG3	2.00	0.43
1:C:3227:ARG:HA	1:C:3232:LEU:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3535:LEU:O	1:C:3538:THR:OG1	2.32	0.43
1:D:2039:LEU:HB3	1:D:2044:ILE:HB	1.99	0.43
1:D:3157:ILE:HB	1:D:3202:PRO:HG3	2.01	0.43
1:D:4965:SER:O	1:D:4969:ASP:HB2	2.18	0.43
1:A:1519:LEU:HD21	1:A:1572:ILE:HD13	1.99	0.43
1:A:2158:CYS:O	1:A:2162:ILE:HG12	2.19	0.43
1:A:2251:PHE:HB2	1:A:2286:LEU:HD13	2.00	0.43
1:A:4670:ILE:HB	1:A:4714:ASN:HD22	1.84	0.43
1:B:2621:HIS:HB3	1:B:2624:ARG:HH21	1.83	0.43
1:B:2633:LEU:HG	1:B:2695:LEU:HD21	2.00	0.43
1:C:492:ASP:OD1	1:C:546:TRP:NE1	2.42	0.43
1:C:2654:TYR:HA	1:C:2661:TRP:H	1.83	0.43
1:C:3592:ILE:HG22	1:C:3595:ARG:HH21	1.83	0.43
1:C:3693:LYS:HD2	1:C:3693:LYS:HA	1.78	0.43
1:D:308:HIS:HD2	1:D:310:LYS:HB3	1.83	0.43
1:D:499:THR:HG23	1:D:502:HIS:H	1.83	0.43
1:D:3592:ILE:HG22	1:D:3595:ARG:HH21	1.83	0.43
1:D:4983:HIS:O	3:D:5101:AMP:N6	2.51	0.43
1:A:1036:ARG:O	1:A:1040:CYS:HB2	2.18	0.43
1:A:2296:GLU:HA	1:A:2299:VAL:HG12	1.99	0.43
1:A:4913:ARG:NH2	1:A:4917:ASP:OD2	2.51	0.43
1:A:5030:LYS:HB2	1:A:5030:LYS:HE2	1.76	0.43
1:B:823:LEU:HD23	1:B:1617:THR:HB	2.01	0.43
1:B:1419:ASP:OD1	1:B:1421:ARG:NH1	2.50	0.43
1:B:2205:GLU:O	1:B:2208:MET:N	2.52	0.43
1:C:2009:LEU:HD23	1:C:2022:PRO:HD2	2.01	0.43
1:C:2686:LEU:HB3	1:C:2997:PHE:HE1	1.83	0.43
1:C:3218:VAL:O	1:C:3222:LYS:HB2	2.18	0.43
1:C:3321:ARG:HA	1:C:3324:VAL:HG12	2.00	0.43
1:C:4670:ILE:HB	1:C:4714:ASN:HD22	1.84	0.43
1:D:2671:GLU:HA	1:D:2674:LEU:HB2	2.00	0.43
1:D:4670:ILE:HB	1:D:4714:ASN:HD22	1.84	0.43
1:A:1007:TYR:O	1:A:1017:ARG:NH2	2.51	0.43
1:A:3227:ARG:HA	1:A:3232:LEU:HD12	2.01	0.43
1:A:4884:LEU:HD11	1:B:4914:VAL:HG11	2.01	0.43
1:B:2296:GLU:HA	1:B:2299:VAL:HG12	1.99	0.43
1:B:2476:ILE:HG23	1:B:2536:LEU:HD21	2.01	0.43
1:B:2575:ARG:HA	1:B:2575:ARG:HD2	1.79	0.43
1:B:2766:TRP:HE1	1:B:2788:HIS:HB2	1.84	0.43
1:B:2911:LEU:HD13	1:B:2915:GLU:HG3	2.00	0.43
1:B:3420:ARG:HH22	1:B:3519:PRO:HG2	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:823:LEU:HD23	1:C:1617:THR:HB	2.01	0.43
1:D:1156:THR:OG1	1:D:1157:GLU:OE1	2.36	0.43
1:D:2205:GLU:O	1:D:2208:MET:N	2.52	0.43
1:D:2357:LEU:HB3	1:D:2364:PHE:HE1	1.83	0.43
1:D:2782:ASP:OD1	1:D:2782:ASP:N	2.52	0.43
1:A:2301:TYR:HB3	1:A:2331:TYR:CE2	2.54	0.43
1:A:3575:LEU:HD23	1:B:1219:LEU:HD22	2.00	0.43
1:A:4745:LEU:H	1:A:4745:LEU:HG	1.55	0.43
1:B:113:HIS:NE2	1:B:399:GLN:O	2.51	0.43
1:B:2177:LEU:O	1:B:2181:SER:OG	2.36	0.43
1:C:1444:GLU:HG2	1:C:1446:SER:H	1.84	0.43
1:C:2766:TRP:HE1	1:C:2788:HIS:HB2	1.84	0.43
1:C:3264:THR:OG1	1:C:3265:GLU:OE1	2.36	0.43
1:C:4892:ARG:NH1	1:D:4895:GLY:O	2.48	0.43
1:D:113:HIS:NE2	1:D:399:GLN:O	2.51	0.43
1:D:683:ARG:HG2	1:D:717:ASP:HB3	2.00	0.43
1:D:2765:LYS:HA	1:D:2765:LYS:HD3	1.87	0.43
2:G:76:CYS:HB3	2:G:97:LEU:HB2	2.00	0.43
2:H:2:VAL:HG23	2:H:80:VAL:HG21	2.01	0.43
1:A:293:LEU:H	1:A:311:ALA:HB1	1.84	0.43
1:A:2591:ARG:HG2	1:A:2636:PHE:HB3	2.01	0.43
1:A:4977:THR:O	1:A:4981:GLU:HB2	2.19	0.43
1:B:765:GLN:NE2	1:B:1479:GLU:OE1	2.52	0.43
1:B:1000:ARG:HA	1:B:1000:ARG:HD3	1.82	0.43
1:B:1444:GLU:HG2	1:B:1446:SER:H	1.84	0.43
1:B:2009:LEU:HD23	1:B:2022:PRO:HD2	2.01	0.43
1:B:2301:TYR:HB3	1:B:2331:TYR:CE2	2.54	0.43
1:B:4686:LEU:O	1:B:4691:GLN:N	2.49	0.43
1:C:706:GLY:N	1:C:709:ASP:OD2	2.39	0.43
1:C:1007:TYR:O	1:C:1017:ARG:NH2	2.51	0.43
1:C:2911:LEU:HD13	1:C:2915:GLU:HG3	2.00	0.43
1:C:3901:ASN:OD1	1:C:3904:ARG:NH1	2.34	0.43
1:D:765:GLN:NE2	1:D:1479:GLU:OE1	2.52	0.43
1:D:3537:LYS:HZ1	1:D:3603:LEU:HB2	1.84	0.43
1:D:4991:PHE:HE2	1:D:5010:VAL:HG11	1.84	0.43
1:A:2948:THR:HG23	1:A:2952:GLU:HB2	2.01	0.42
1:A:3218:VAL:O	1:A:3222:LYS:HB2	2.18	0.42
1:A:3424:LEU:HD23	1:A:3424:LEU:HA	1.88	0.42
1:B:2251:PHE:HB2	1:B:2286:LEU:HD13	2.00	0.42
1:B:3106:MET:HG3	1:B:3110:LEU:HD13	2.01	0.42
1:B:3889:GLN:HG3	1:B:3967:GLU:HG3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:452:PHE:HE1	1:C:474:ARG:HB3	1.83	0.42
1:C:1231[B]:GLN:H	1:C:1231[B]:GLN:HG3	1.61	0.42
1:C:2671:GLU:HA	1:C:2674:LEU:HB2	2.00	0.42
1:C:3218:VAL:HG22	1:C:3227:ARG:HD3	2.00	0.42
1:D:3218:VAL:HG22	1:D:3227:ARG:HD3	2.00	0.42
1:D:3927:GLN:HA	1:D:3930:ILE:HG22	2.01	0.42
1:D:4977:THR:O	1:D:4981:GLU:HB2	2.19	0.42
1:A:1219:LEU:HD22	1:D:3575:LEU:HD23	2.01	0.42
1:A:1444:GLU:HG2	1:A:1446:SER:H	1.84	0.42
1:A:2205:GLU:O	1:A:2208:MET:N	2.52	0.42
1:A:3106:MET:HG3	1:A:3110:LEU:HD13	2.01	0.42
1:B:1076:ARG:HB3	1:B:1191:VAL:HG23	2.01	0.42
1:B:1291:LEU:HD23	1:B:1291:LEU:HA	1.91	0.42
1:B:2671:GLU:HA	1:B:2674:LEU:HB2	2.00	0.42
1:B:2974:ILE:HD12	1:B:3053:ARG:HH12	1.84	0.42
1:B:4581:LYS:HE3	1:B:4581:LYS:HB3	1.82	0.42
1:B:4977:THR:O	1:B:4981:GLU:HB2	2.20	0.42
1:C:1066:GLN:HG3	1:C:1462:MET:HG2	2.01	0.42
1:C:2205:GLU:O	1:C:2208:MET:N	2.52	0.42
1:C:2301:TYR:HB3	1:C:2331:TYR:CE2	2.54	0.42
1:C:2476:ILE:HG23	1:C:2536:LEU:HD21	2.01	0.42
1:C:2519:LEU:HD12	1:C:2578:MET:HE1	2.01	0.42
1:C:4821:LYS:HB2	1:C:4821:LYS:HE2	1.54	0.42
1:C:4977:THR:O	1:C:4981:GLU:HB2	2.20	0.42
1:D:114:SER:HB2	1:D:116:MET:HG3	2.02	0.42
1:D:2355:ARG:HA	1:D:2358:ILE:HG12	1.99	0.42
1:D:3768:SER:HA	1:D:3771:HIS:CD2	2.54	0.42
1:A:823:LEU:HD22	1:A:1626:TRP:HB3	2.01	0.42
1:A:823:LEU:HD23	1:A:1617:THR:HB	2.01	0.42
1:A:1419:ASP:OD1	1:A:1421:ARG:NH1	2.50	0.42
1:A:2302:LEU:HD23	1:A:2363:CYS:HB3	2.02	0.42
1:A:2974:ILE:HD12	1:A:3053:ARG:HH12	1.84	0.42
1:A:3207:GLU:OE1	1:A:3280:TYR:OH	2.33	0.42
1:A:3335:MET:HE3	1:A:3338:LEU:HD23	2.00	0.42
1:A:3554:GLN:HA	1:A:3557:LEU:HG	2.02	0.42
1:A:3768:SER:HA	1:A:3771:HIS:CD2	2.54	0.42
1:B:1007:TYR:O	1:B:1017:ARG:NH2	2.51	0.42
1:B:2519:LEU:HD12	1:B:2578:MET:HE1	2.01	0.42
1:B:3157:ILE:HB	1:B:3202:PRO:HG3	2.00	0.42
1:B:3218:VAL:HG22	1:B:3227:ARG:HD3	2.01	0.42
1:B:3335:MET:HE3	1:B:3338:LEU:HD23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4016:LEU:HD12	1:B:4016:LEU:HA	1.84	0.42
1:C:114:SER:HB2	1:C:116:MET:HG3	2.02	0.42
1:C:683:ARG:HG2	1:C:717:ASP:HB3	2.00	0.42
1:C:2159:LEU:HG	1:C:2163:ARG:HE	1.84	0.42
1:C:2175:GLU:HG3	1:C:2228:MET:HB2	2.00	0.42
1:C:3159:ASP:OD1	1:C:3159:ASP:N	2.46	0.42
1:C:3768:SER:HA	1:C:3771:HIS:CD2	2.54	0.42
1:C:4092:ASP:HA	1:C:4095:LYS:HG2	2.02	0.42
1:D:823:LEU:HD23	1:D:1617:THR:HB	2.01	0.42
1:D:1444:GLU:HG2	1:D:1446:SER:H	1.84	0.42
1:D:2009:LEU:HD23	1:D:2022:PRO:HD2	2.01	0.42
1:D:2302:LEU:HD23	1:D:2363:CYS:HB3	2.02	0.42
1:D:2591:ARG:HG2	1:D:2636:PHE:HB3	2.00	0.42
1:D:2948:THR:HG23	1:D:2952:GLU:HB2	2.01	0.42
1:D:3321:ARG:HA	1:D:3324:VAL:HG12	2.00	0.42
2:F:2:VAL:HG23	2:F:80:VAL:HG21	2.01	0.42
1:A:2624:ARG:HD2	1:A:2906:VAL:HG11	2.02	0.42
1:A:2867:LEU:HD12	1:A:2928:LYS:HZ3	1.84	0.42
1:A:3592:ILE:HG22	1:A:3595:ARG:HH21	1.83	0.42
1:B:293:LEU:H	1:B:311:ALA:HB1	1.84	0.42
1:B:869:ARG:CZ	1:B:870:ILE:HB	2.50	0.42
1:B:884:LEU:HD13	1:B:968:ALA:H	1.84	0.42
1:C:765:GLN:NE2	1:C:1479:GLU:OE1	2.52	0.42
1:C:884:LEU:HD13	1:C:968:ALA:H	1.84	0.42
1:C:2974:ILE:HD12	1:C:3053:ARG:HH12	1.84	0.42
1:C:3889:GLN:HG3	1:C:3967:GLU:HG3	2.01	0.42
1:C:4814:LEU:HD23	1:C:4814:LEU:HA	1.89	0.42
1:C:4991:PHE:HE2	1:C:5010:VAL:HG11	1.84	0.42
1:D:2159:LEU:HG	1:D:2163:ARG:HE	1.84	0.42
1:D:2175:GLU:HG3	1:D:2228:MET:HB2	2.00	0.42
2:F:76:CYS:HB3	2:F:97:LEU:HB2	2.00	0.42
1:A:1076:ARG:HB3	1:A:1191:VAL:HG23	2.01	0.42
1:A:3264:THR:OG1	1:A:3265:GLU:OE1	2.36	0.42
1:B:30:LYS:HA	1:B:30:LYS:HD2	1.80	0.42
1:B:1066:GLN:HG3	1:B:1462:MET:HG2	2.01	0.42
1:B:2158:CYS:O	1:B:2162:ILE:HG12	2.19	0.42
1:B:2302:LEU:HD23	1:B:2363:CYS:HB3	2.02	0.42
1:B:3227:ARG:HA	1:B:3232:LEU:HD12	2.01	0.42
1:C:2302:LEU:HD23	1:C:2363:CYS:HB3	2.02	0.42
1:C:4184:MET:N	1:C:5021:PHE:O	2.50	0.42
1:C:5030:LYS:HE2	1:C:5030:LYS:HB2	1.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:828:GLU:O	1:D:1073:ARG:NH1	2.53	0.42
1:D:878:ILE:HD11	1:D:925:SER:HB2	2.02	0.42
1:A:30:LYS:HD2	1:A:30:LYS:HA	1.79	0.42
1:A:878:ILE:HD11	1:A:925:SER:HB2	2.02	0.42
1:A:884:LEU:HD13	1:A:968:ALA:H	1.84	0.42
1:A:3927:GLN:HA	1:A:3930:ILE:HG22	2.01	0.42
1:A:4991:PHE:HE2	1:A:5010:VAL:HG11	1.84	0.42
1:B:199:LEU:HD12	1:B:199:LEU:HA	1.90	0.42
1:C:863:LEU:HA	1:C:864:PRO:HD3	1.85	0.42
1:C:3157:ILE:HB	1:C:3202:PRO:HG3	2.00	0.42
1:C:3288:GLY:HA2	1:C:3303:PRO:HB3	2.01	0.42
1:D:1007:TYR:O	1:D:1017:ARG:NH2	2.51	0.42
1:D:2686:LEU:HB3	1:D:2997:PHE:HE1	1.83	0.42
1:A:1066:GLN:HG3	1:A:1462:MET:HG2	2.01	0.42
1:A:2009:LEU:HD23	1:A:2022:PRO:HD2	2.01	0.42
1:A:2911:LEU:HD13	1:A:2915:GLU:HG3	2.00	0.42
1:A:2930:LEU:O	1:A:2935:TYR:N	2.49	0.42
1:A:3218:VAL:HG22	1:A:3227:ARG:HD3	2.00	0.42
1:A:3288:GLY:HA2	1:A:3303:PRO:HB3	2.01	0.42
1:A:3582:ARG:HD3	1:A:3582:ARG:HA	1.88	0.42
1:B:114:SER:HB2	1:B:116:MET:HG3	2.02	0.42
1:B:2039:LEU:HD22	1:B:2044:ILE:HG13	2.02	0.42
1:B:2175:GLU:HG3	1:B:2228:MET:HB2	2.00	0.42
1:B:2472:LEU:HA	1:B:2472:LEU:HD23	1.87	0.42
1:C:2867:LEU:HD12	1:C:2928:LYS:HZ3	1.85	0.42
1:C:3207:GLU:OE1	1:C:3280:TYR:OH	2.33	0.42
1:C:3927:GLN:HA	1:C:3930:ILE:HG22	2.01	0.42
1:C:4827:LEU:HD23	1:C:4827:LEU:HA	1.89	0.42
1:C:4976:GLU:H	1:C:4976:GLU:HG2	1.59	0.42
1:D:124:SER:HB2	1:D:133:PHE:HA	2.01	0.42
1:D:1434:TYR:HA	1:D:1518:CYS:O	2.20	0.42
1:D:2158:CYS:O	1:D:2162:ILE:HG12	2.19	0.42
1:D:2301:TYR:HB3	1:D:2331:TYR:CE2	2.54	0.42
1:D:2624:ARG:HD2	1:D:2906:VAL:HG11	2.02	0.42
1:D:2867:LEU:HD12	1:D:2928:LYS:HZ3	1.85	0.42
1:D:3175:LEU:O	1:D:3178:THR:OG1	2.33	0.42
1:D:3335:MET:HE3	1:D:3338:LEU:HD23	2.02	0.42
1:D:4092:ASP:HA	1:D:4095:LYS:HG2	2.02	0.42
2:G:2:VAL:HG23	2:G:80:VAL:HG21	2.01	0.42
1:A:765:GLN:NE2	1:A:1479:GLU:OE1	2.52	0.42
1:A:2039:LEU:HD22	1:A:2044:ILE:HG13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2159:LEU:HG	1:A:2163:ARG:HE	1.84	0.42
1:A:2580:ASP:HB2	1:A:2618:MET:HE1	2.02	0.42
1:A:3157:ILE:HB	1:A:3202:PRO:HG3	2.00	0.42
1:A:3889:GLN:HG3	1:A:3967:GLU:HG3	2.01	0.42
1:B:2357:LEU:HB3	1:B:2364:PHE:HE1	1.83	0.42
1:B:2825:LYS:NZ	1:B:2935:TYR:OH	2.45	0.42
1:B:2902:HIS:HB3	1:B:2905:LEU:HG	2.02	0.42
1:B:3554:GLN:HA	1:B:3557:LEU:HG	2.01	0.42
1:B:3710:LEU:HD21	1:B:3781:GLN:HG2	2.02	0.42
1:B:4092:ASP:HA	1:B:4095:LYS:HG2	2.02	0.42
1:C:124:SER:HB2	1:C:133:PHE:HA	2.01	0.42
1:C:293:LEU:H	1:C:311:ALA:HB1	1.84	0.42
1:D:699:GLY:N	1:D:1647:CYS:O	2.50	0.42
1:D:2766:TRP:HE1	1:D:2788:HIS:HB2	1.84	0.42
1:A:1773:PRO:HA	1:A:1774:PRO:HD3	1.94	0.42
1:C:1253:PRO:HG2	1:C:1254:HIS:CD2	2.55	0.42
1:C:3648:ARG:O	1:C:3652:MET:HG2	2.20	0.42
1:D:59:PRO:HD3	1:D:307:ALA:HB3	2.02	0.42
1:D:823:LEU:HD22	1:D:1626:TRP:HB3	2.01	0.42
1:D:1066:GLN:HG3	1:D:1462:MET:HG2	2.01	0.42
1:D:1253:PRO:HG2	1:D:1254:HIS:CD2	2.55	0.42
1:D:1773:PRO:HA	1:D:1774:PRO:HD3	1.94	0.42
1:D:2911:LEU:HD13	1:D:2915:GLU:HG3	2.00	0.42
1:D:4865:LYS:HA	1:D:4865:LYS:HD2	1.49	0.42
1:A:3575:LEU:HD12	1:A:3575:LEU:HA	1.93	0.42
1:A:4645:CYS:SG	1:A:4646:LEU:N	2.93	0.42
1:B:418:LEU:HD11	1:B:494:LEU:HD22	2.02	0.42
1:B:2948:THR:HG23	1:B:2952:GLU:HB2	2.01	0.42
1:B:3376:GLU:O	1:B:3380:ARG:HG2	2.20	0.42
1:B:3539:ARG:NH1	1:B:3553:LEU:HG	2.35	0.42
1:B:3648:ARG:O	1:B:3652:MET:HG2	2.20	0.42
1:B:4645:CYS:SG	1:B:4646:LEU:N	2.93	0.42
1:B:4670:ILE:HB	1:B:4714:ASN:HD22	1.84	0.42
1:B:4991:PHE:HE2	1:B:5010:VAL:HG11	1.84	0.42
1:C:869:ARG:CZ	1:C:870:ILE:HB	2.50	0.42
1:C:878:ILE:HD11	1:C:925:SER:HB2	2.02	0.42
1:C:1773:PRO:HA	1:C:1774:PRO:HD3	1.94	0.42
1:C:2782:ASP:OD1	1:C:2782:ASP:N	2.52	0.42
1:C:3965:LEU:HD23	1:C:3965:LEU:HA	1.94	0.42
1:D:3106:MET:HG3	1:D:3110:LEU:HD13	2.01	0.42
1:A:114:SER:HB2	1:A:116:MET:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1253:PRO:HG2	1:A:1254:HIS:CD2	2.55	0.41
1:B:1290:ARG:HH12	1:B:1455:PRO:HA	1.85	0.41
1:B:1434:TYR:HA	1:B:1518:CYS:O	2.20	0.41
1:B:3033:ASN:O	1:B:3037:GLU:HG2	2.21	0.41
1:B:3823:LYS:HA	1:B:3823:LYS:HD3	1.83	0.41
1:C:1434:TYR:HA	1:C:1518:CYS:O	2.20	0.41
1:C:3106:MET:HG3	1:C:3110:LEU:HD13	2.01	0.41
1:C:3335:MET:HE3	1:C:3338:LEU:HD23	2.02	0.41
1:D:293:LEU:H	1:D:311:ALA:HB1	1.84	0.41
1:D:869:ARG:CZ	1:D:870:ILE:HB	2.50	0.41
1:D:3889:GLN:HG3	1:D:3967:GLU:HG3	2.02	0.41
1:A:828:GLU:O	1:A:1073:ARG:NH1	2.53	0.41
1:A:1568:LYS:O	1:A:1569:GLN:NE2	2.53	0.41
1:A:2614:ILE:O	1:A:2650:ARG:NH2	2.43	0.41
1:B:878:ILE:HD11	1:B:925:SER:HB2	2.02	0.41
1:B:2624:ARG:HD2	1:B:2906:VAL:HG11	2.02	0.41
1:B:3227:ARG:NH1	1:B:3234:ASN:OD1	2.37	0.41
1:B:3768:SER:HA	1:B:3771:HIS:CD2	2.54	0.41
1:C:418:LEU:HD11	1:C:494:LEU:HD22	2.02	0.41
1:C:2624:ARG:HD2	1:C:2906:VAL:HG11	2.02	0.41
1:C:2948:THR:HG23	1:C:2952:GLU:HB2	2.01	0.41
1:C:3033:ASN:O	1:C:3037:GLU:HG2	2.21	0.41
1:C:4835:LYS:HE2	1:C:4835:LYS:HB3	1.56	0.41
1:D:1568:LYS:O	1:D:1569:GLN:NE2	2.53	0.41
1:D:1749:PRO:HA	1:D:1750:PRO:HD3	1.95	0.41
1:A:124:SER:HB2	1:A:133:PHE:HA	2.01	0.41
1:A:2454:ARG:CZ	1:A:2458:ARG:HH21	2.34	0.41
1:A:4686:LEU:O	1:A:4691:GLN:N	2.49	0.41
1:A:4995:LEU:HD23	1:A:4995:LEU:HA	1.93	0.41
1:B:2682:ILE:HD13	1:B:2682:ILE:HA	1.93	0.41
1:B:3160:ASP:OD1	1:B:3160:ASP:N	2.53	0.41
1:B:3288:GLY:HA2	1:B:3303:PRO:HB3	2.01	0.41
1:B:3467:MET:O	1:B:3471:THR:OG1	2.37	0.41
1:C:1849:LEU:HD23	1:C:1849:LEU:HA	1.87	0.41
1:C:2454:ARG:CZ	1:C:2458:ARG:HH21	2.34	0.41
1:C:3823:LYS:HD3	1:C:3823:LYS:HA	1.83	0.41
1:D:1076:ARG:HB3	1:D:1191:VAL:HG23	2.01	0.41
1:D:3288:GLY:HA2	1:D:3303:PRO:HB3	2.01	0.41
1:D:3554:GLN:HA	1:D:3557:LEU:HG	2.02	0.41
1:B:823:LEU:HD22	1:B:1626:TRP:HB3	2.01	0.41
1:B:2454:ARG:CZ	1:B:2458:ARG:HH21	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3628:ARG:NH2	1:B:3857:GLY:O	2.54	0.41
1:B:3693:LYS:HA	1:B:3693:LYS:HD2	1.78	0.41
1:C:59:PRO:HD3	1:C:307:ALA:HB3	2.02	0.41
1:C:129:ASP:N	1:C:129:ASP:OD1	2.54	0.41
1:C:823:LEU:HD22	1:C:1626:TRP:HB3	2.01	0.41
1:C:1076:ARG:HB3	1:C:1191:VAL:HG23	2.01	0.41
1:C:1290:ARG:HH12	1:C:1455:PRO:HA	1.85	0.41
1:C:2902:HIS:HB3	1:C:2905:LEU:HG	2.02	0.41
1:C:3272:ILE:O	1:C:3276:MET:HG2	2.20	0.41
1:D:531:ARG:NH2	1:D:562:GLU:OE2	2.37	0.41
1:D:2476:ILE:HG23	1:D:2536:LEU:HD21	2.01	0.41
1:D:2974:ILE:HD12	1:D:3053:ARG:HH12	1.84	0.41
1:D:4995:LEU:HD23	1:D:4995:LEU:HA	1.94	0.41
1:A:59:PRO:HD3	1:A:307:ALA:HB3	2.02	0.41
1:A:1863:LEU:HB3	1:A:1871:PHE:HD2	1.86	0.41
1:A:4944:ARG:NH2	1:B:4938:ASP:O	2.54	0.41
1:B:220:LEU:HB2	1:B:391:THR:O	2.20	0.41
1:B:3175:LEU:O	1:B:3178:THR:OG1	2.33	0.41
1:C:137:LEU:HD23	1:C:137:LEU:HA	1.87	0.41
1:C:531:ARG:NH2	1:C:562:GLU:OE2	2.37	0.41
1:C:3376:GLU:O	1:C:3380:ARG:HG2	2.20	0.41
1:D:3272:ILE:O	1:D:3276:MET:HG2	2.20	0.41
1:D:3376:GLU:O	1:D:3380:ARG:HG2	2.20	0.41
1:D:3823:LYS:HD3	1:D:3823:LYS:HA	1.83	0.41
1:D:4843:LEU:O	1:D:4847:VAL:HG13	2.21	0.41
1:A:418:LEU:HD11	1:A:494:LEU:HD22	2.02	0.41
1:A:823:LEU:HD12	1:A:823:LEU:HA	1.89	0.41
1:A:3033:ASN:O	1:A:3037:GLU:HG2	2.20	0.41
1:A:3539:ARG:NH1	1:A:3553:LEU:HG	2.35	0.41
1:A:4092:ASP:HA	1:A:4095:LYS:HG2	2.02	0.41
1:A:4843:LEU:O	1:A:4847:VAL:HG13	2.21	0.41
1:B:828:GLU:O	1:B:1073:ARG:NH1	2.53	0.41
1:B:1229:ASN:HB2	1:B:1827:ARG:HG3	2.03	0.41
1:B:3927:GLN:HA	1:B:3930:ILE:HG22	2.01	0.41
1:C:1863:LEU:HB3	1:C:1871:PHE:HD2	1.86	0.41
1:D:137:LEU:HA	1:D:137:LEU:HD23	1.88	0.41
1:D:418:LEU:HD11	1:D:494:LEU:HD22	2.02	0.41
1:D:873:LYS:HG2	1:D:970:LEU:HD13	2.02	0.41
1:D:884:LEU:HD13	1:D:968:ALA:H	1.84	0.41
1:D:1088:TRP:HB2	1:D:1153:ILE:HG22	2.01	0.41
1:D:2825:LYS:NZ	1:D:2935:TYR:OH	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:LEU:HB2	1:A:391:THR:O	2.20	0.41
1:A:2806:ARG:HD2	1:A:2810:LYS:HZ3	1.86	0.41
1:A:3062:PRO:HA	1:A:3065:VAL:HG22	2.03	0.41
1:A:3373:VAL:HG11	1:A:3444:TYR:HB3	2.03	0.41
1:B:129:ASP:N	1:B:129:ASP:OD1	2.54	0.41
1:B:932:LEU:HD22	1:B:984:LEU:HD21	2.03	0.41
1:C:49:LEU:HD23	1:C:49:LEU:HA	1.93	0.41
1:C:1243:PRO:O	1:C:1458:HIS:ND1	2.33	0.41
1:C:2158:CYS:O	1:C:2162:ILE:HG12	2.19	0.41
1:C:2866:THR:OG1	1:C:2867:LEU:N	2.54	0.41
1:C:3883:ASP:HA	1:C:3886:ARG:HB3	2.03	0.41
1:D:2454:ARG:CZ	1:D:2458:ARG:HH21	2.34	0.41
1:D:3648:ARG:O	1:D:3652:MET:HG2	2.20	0.41
1:A:869:ARG:CZ	1:A:870:ILE:HB	2.50	0.41
1:A:1259:ARG:HH12	1:A:1596:GLU:HA	1.85	0.41
1:A:1434:TYR:HA	1:A:1518:CYS:O	2.20	0.41
1:A:2866:THR:OG1	1:A:2867:LEU:N	2.54	0.41
1:A:3659:ALA:HA	1:A:3663:LEU:HD12	2.03	0.41
1:A:3694:LYS:HA	1:A:3695:PRO:HD3	1.90	0.41
1:A:3937:TYR:O	1:A:4002:LYS:NZ	2.44	0.41
1:B:2930:LEU:O	1:B:2935:TYR:N	2.49	0.41
1:C:113:HIS:NE2	1:C:399:GLN:O	2.51	0.41
1:C:2039:LEU:HD22	1:C:2044:ILE:HG13	2.02	0.41
1:C:3582:ARG:HD3	1:C:3582:ARG:HA	1.87	0.41
1:D:129:ASP:OD1	1:D:129:ASP:N	2.54	0.41
1:D:2039:LEU:HD22	1:D:2044:ILE:HG13	2.02	0.41
1:D:2656:CYS:SG	1:D:3013:HIS:NE2	2.93	0.41
1:D:3033:ASN:O	1:D:3037:GLU:HG2	2.21	0.41
1:D:3659:ALA:HA	1:D:3663:LEU:HD12	2.03	0.41
1:A:137:LEU:HD23	1:A:137:LEU:HA	1.87	0.41
1:A:873:LYS:HG2	1:A:970:LEU:HD13	2.02	0.41
1:A:1088:TRP:HB2	1:A:1153:ILE:HG22	2.01	0.41
1:A:2017:ASP:OD1	1:A:2017:ASP:N	2.54	0.41
1:A:2476:ILE:HG23	1:A:2536:LEU:HD21	2.01	0.41
1:A:2765:LYS:HA	1:A:2765:LYS:HD3	1.87	0.41
1:A:3272:ILE:O	1:A:3276:MET:HG2	2.20	0.41
1:A:3376:GLU:O	1:A:3380:ARG:HG2	2.20	0.41
1:A:3628:ARG:NH2	1:A:3857:GLY:O	2.54	0.41
1:A:3710:LEU:HD21	1:A:3781:GLN:HG2	2.02	0.41
1:A:3883:ASP:HA	1:A:3886:ARG:HB3	2.03	0.41
1:A:3965:LEU:HD23	1:A:3965:LEU:HA	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4850:LEU:HD23	1:A:4850:LEU:HA	1.93	0.41
1:B:1253:PRO:HG2	1:B:1254:HIS:CD2	2.55	0.41
1:B:1568:LYS:O	1:B:1569:GLN:NE2	2.53	0.41
1:B:3062:PRO:HA	1:B:3065:VAL:HG22	2.03	0.41
1:B:3703:LEU:HD23	1:B:3703:LEU:HA	1.93	0.41
1:B:3901:ASN:OD1	1:B:3904:ARG:NH1	2.34	0.41
1:C:547:VAL:HB	1:C:560:ILE:HD11	2.03	0.41
1:C:829:TYR:HB3	1:C:1073:ARG:HH11	1.86	0.41
1:C:1088:TRP:HB2	1:C:1153:ILE:HG22	2.02	0.41
1:C:1433:TYR:HB3	1:C:1575:LEU:HD23	2.03	0.41
1:C:1446:SER:O	1:C:1496:TRP:NE1	2.43	0.41
1:C:1842:LEU:HD23	1:C:1842:LEU:HA	1.95	0.41
1:C:2580:ASP:HB2	1:C:2618:MET:HE1	2.03	0.41
1:C:2971:GLN:HG2	1:C:3045:LYS:NZ	2.36	0.41
1:C:3539:ARG:NH1	1:C:3553:LEU:HG	2.35	0.41
1:C:3554:GLN:HA	1:C:3557:LEU:HG	2.02	0.41
1:D:49:LEU:HD23	1:D:49:LEU:HA	1.93	0.41
1:D:2472:LEU:HD23	1:D:2472:LEU:HA	1.87	0.41
1:D:2902:HIS:HB3	1:D:2905:LEU:HG	2.02	0.41
1:D:4645:CYS:SG	1:D:4646:LEU:N	2.93	0.41
1:A:2902:HIS:HB3	1:A:2905:LEU:HG	2.02	0.41
1:A:3562:LYS:HE2	1:A:3562:LYS:HB2	1.92	0.41
1:B:865:PRO:HA	1:B:868:GLU:HG2	2.03	0.41
1:B:1433:TYR:HB3	1:B:1575:LEU:HD23	2.03	0.41
1:B:2531:ARG:HH22	1:B:2581:SER:HB2	1.85	0.41
1:B:2640:PRO:HA	1:B:2643:LEU:HB3	2.03	0.41
1:B:4813:LEU:O	1:B:4816:ILE:HG12	2.20	0.41
1:C:865:PRO:HA	1:C:868:GLU:HG2	2.03	0.41
1:C:1229:ASN:HB2	1:C:1827:ARG:HG3	2.03	0.41
1:C:1259:ARG:HH12	1:C:1596:GLU:HA	1.85	0.41
1:C:3826:VAL:HG12	1:C:3830:GLN:HG3	2.03	0.41
1:C:4813:LEU:O	1:C:4816:ILE:HG12	2.20	0.41
1:D:547:VAL:HB	1:D:560:ILE:HD11	2.03	0.41
1:D:1126:GLY:HA3	1:D:1143:TRP:CZ3	2.56	0.41
1:D:2710:LEU:HA	1:D:2711:PRO:HD3	1.98	0.41
1:D:3201:MET:HG2	1:D:3203:VAL:H	1.86	0.41
1:D:3628:ARG:NH2	1:D:3857:GLY:O	2.54	0.41
1:D:3852:LYS:HE3	1:D:3852:LYS:HB3	1.94	0.41
1:A:1433:TYR:HB3	1:A:1575:LEU:HD23	2.03	0.40
1:A:2656:CYS:SG	1:A:3013:HIS:NE2	2.93	0.40
1:A:3201:MET:HG2	1:A:3203:VAL:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3537:LYS:HZ1	1:A:3603:LEU:HB2	1.86	0.40
1:A:3648:ARG:O	1:A:3652:MET:HG2	2.20	0.40
1:A:3826:VAL:HG12	1:A:3830:GLN:HG3	2.03	0.40
1:A:4581:LYS:HE3	1:A:4581:LYS:HB3	1.82	0.40
1:A:4918:ILE:HD11	1:D:4888:TYR:HA	2.03	0.40
1:B:1863:LEU:HB3	1:B:1871:PHE:HD2	1.86	0.40
1:B:2159:LEU:HD21	1:B:2163:ARG:HH21	1.86	0.40
1:B:2710:LEU:HA	1:B:2711:PRO:HD3	1.98	0.40
1:B:3965:LEU:HD23	1:B:3965:LEU:HA	1.94	0.40
1:C:220:LEU:HB2	1:C:391:THR:O	2.20	0.40
1:C:2531:ARG:HH22	1:C:2581:SER:HB2	1.85	0.40
1:C:3062:PRO:HA	1:C:3065:VAL:HG22	2.03	0.40
1:C:3628:ARG:NH2	1:C:3857:GLY:O	2.54	0.40
1:C:4577:LEU:HD12	1:C:4577:LEU:HA	1.94	0.40
1:D:220:LEU:HB2	1:D:391:THR:O	2.20	0.40
1:D:1259:ARG:HH12	1:D:1596:GLU:HA	1.85	0.40
1:D:1488:LYS:HB2	1:D:1488:LYS:HE3	1.86	0.40
1:D:2531:ARG:HH22	1:D:2581:SER:HB2	1.85	0.40
1:D:3710:LEU:HD21	1:D:3781:GLN:HG2	2.02	0.40
1:A:1290:ARG:HH12	1:A:1455:PRO:HA	1.85	0.40
1:A:3390:GLY:HA2	1:A:3393:LEU:HD13	2.04	0.40
1:A:3601:ALA:O	1:A:3605:HIS:ND1	2.40	0.40
1:A:4555:LEU:HD12	1:A:4555:LEU:HA	1.94	0.40
1:A:4666:VAL:O	1:A:4670:ILE:HG12	2.21	0.40
1:A:4813:LEU:O	1:A:4816:ILE:HG12	2.20	0.40
1:B:1088:TRP:HB2	1:B:1153:ILE:HG22	2.02	0.40
1:B:1259:ARG:HH12	1:B:1596:GLU:HA	1.85	0.40
1:B:2866:THR:OG1	1:B:2867:LEU:N	2.54	0.40
1:B:3201:MET:HG2	1:B:3203:VAL:H	1.86	0.40
1:B:3272:ILE:O	1:B:3276:MET:HG2	2.20	0.40
1:B:4745:LEU:H	1:B:4745:LEU:HG	1.55	0.40
1:C:1568:LYS:O	1:C:1569:GLN:NE2	2.53	0.40
1:C:1776:HIS:HB3	1:C:1798:LEU:HD13	2.04	0.40
1:C:3573:MET:HB3	1:C:3577:ARG:NH2	2.36	0.40
1:C:4686:LEU:O	1:C:4691:GLN:N	2.49	0.40
1:D:2159:LEU:HD21	1:D:2163:ARG:HH21	1.86	0.40
1:D:2640:PRO:HA	1:D:2643:LEU:HB3	2.03	0.40
1:D:4152:GLU:OE1	1:D:4192:ARG:NH1	2.51	0.40
1:D:4976:GLU:H	1:D:4976:GLU:HG2	1.59	0.40
1:A:3160:ASP:OD1	1:A:3160:ASP:N	2.53	0.40
1:A:4843:LEU:HD22	1:D:4823:LEU:HD22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:PRO:HD3	1:B:307:ALA:HB3	2.02	0.40
1:B:873:LYS:HG2	1:B:970:LEU:HD13	2.02	0.40
1:B:2765:LYS:HA	1:B:2765:LYS:HD3	1.87	0.40
1:B:4000:MET:HG2	1:B:4016:LEU:HD23	2.04	0.40
1:C:2640:PRO:HA	1:C:2643:LEU:HB3	2.04	0.40
1:C:3201:MET:HG2	1:C:3203:VAL:H	1.86	0.40
1:C:4016:LEU:HD12	1:C:4016:LEU:HA	1.84	0.40
1:D:179:TYR:N	1:D:194:SER:O	2.54	0.40
1:D:1776:HIS:HB3	1:D:1798:LEU:HD13	2.04	0.40
1:D:1849:LEU:HD23	1:D:1849:LEU:HA	1.87	0.40
1:D:3573:MET:HB3	1:D:3577:ARG:NH2	2.36	0.40
1:D:3826:VAL:HG12	1:D:3830:GLN:HG3	2.04	0.40
1:D:4993:MET:HE2	1:D:4993:MET:HB3	2.00	0.40
1:A:129:ASP:OD1	1:A:129:ASP:N	2.54	0.40
1:A:2825:LYS:NZ	1:A:2935:TYR:OH	2.45	0.40
1:A:3901:ASN:OD1	1:A:3904:ARG:NH1	2.34	0.40
1:B:647:ASN:ND2	1:B:824:GLU:OE2	2.54	0.40
1:B:1776:HIS:HB3	1:B:1798:LEU:HD13	2.04	0.40
1:B:2325:PRO:HB2	1:B:2421:ALA:HB1	2.04	0.40
1:C:484:LEU:HD21	1:C:540:PHE:HE1	1.87	0.40
1:C:873:LYS:HG2	1:C:970:LEU:HD13	2.02	0.40
1:C:932:LEU:HD22	1:C:984:LEU:HD21	2.03	0.40
1:D:144:GLU:HG3	1:D:175:SER:HB3	2.04	0.40
1:D:647:ASN:ND2	1:D:824:GLU:OE2	2.54	0.40
1:D:1229:ASN:HB2	1:D:1827:ARG:HG3	2.03	0.40
1:D:1863:LEU:HB3	1:D:1871:PHE:HD2	1.86	0.40
1:D:3390:GLY:HA2	1:D:3393:LEU:HD13	2.04	0.40
1:D:3539:ARG:NH1	1:D:3553:LEU:HG	2.35	0.40
1:D:4000:MET:HG2	1:D:4016:LEU:HD23	2.04	0.40
1:D:4813:LEU:O	1:D:4816:ILE:HG12	2.20	0.40
1:D:4869:GLU:H	1:D:4869:GLU:HG2	1.74	0.40
1:D:5012:LYS:HD3	1:D:5012:LYS:HA	1.64	0.40
1:A:547:VAL:HB	1:A:560:ILE:HD11	2.03	0.40
1:A:2159:LEU:HD21	1:A:2163:ARG:HH21	1.86	0.40
1:B:317:ARG:HH12	1:B:349:GLN:N	2.20	0.40
1:B:880:GLU:HB3	1:B:883:ALA:HB3	2.03	0.40
1:B:2017:ASP:OD1	1:B:2017:ASP:N	2.54	0.40
1:B:3717:ASP:N	1:B:3717:ASP:OD1	2.54	0.40
1:C:266:ARG:NH2	1:C:331:VAL:O	2.51	0.40
1:C:2325:PRO:HB2	1:C:2421:ALA:HB1	2.04	0.40
1:C:3710:LEU:HD21	1:C:3781:GLN:HG2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4801:LEU:HD23	1:C:4801:LEU:HA	1.87	0.40
1:D:1290:ARG:HH12	1:D:1455:PRO:HA	1.85	0.40
1:D:1445:PRO:HG2	1:D:1501:VAL:HG11	2.04	0.40
1:D:3062:PRO:HA	1:D:3065:VAL:HG22	2.03	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	4353/5037 (86%)	4199 (96%)	149 (3%)	5 (0%)	51 82
1	B	4353/5037 (86%)	4199 (96%)	149 (3%)	5 (0%)	51 82
1	C	4353/5037 (86%)	4200 (96%)	148 (3%)	5 (0%)	51 82
1	D	4353/5037 (86%)	4199 (96%)	149 (3%)	5 (0%)	51 82
2	E	105/350 (30%)	102 (97%)	3 (3%)	0	100 100
2	F	105/350 (30%)	102 (97%)	3 (3%)	0	100 100
2	G	105/350 (30%)	102 (97%)	3 (3%)	0	100 100
2	H	105/350 (30%)	102 (97%)	3 (3%)	0	100 100
All	All	17832/21548 (83%)	17205 (96%)	607 (3%)	20 (0%)	54 82

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3692	GLU
1	A	4691	GLN
1	B	3692	GLU
1	B	4691	GLN
1	C	3692	GLU
1	C	4691	GLN

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Mol	Chain	Res	Type
1	D	3692	GLU
1	D	4691	GLN
1	A	4712	PRO
1	B	4712	PRO
1	C	4712	PRO
1	D	4712	PRO
1	A	4819	GLY
1	B	4819	GLY
1	C	4819	GLY
1	D	4819	GLY
1	A	3292	PRO
1	B	3292	PRO
1	C	3292	PRO
1	D	3292	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	3805/4276 (89%)	3675 (97%)	130 (3%)	37	65
1	B	3805/4276 (89%)	3675 (97%)	130 (3%)	37	65
1	C	3805/4276 (89%)	3674 (97%)	131 (3%)	37	65
1	D	3805/4276 (89%)	3674 (97%)	131 (3%)	37	65
2	E	88/304 (29%)	87 (99%)	1 (1%)	73	86
2	F	88/304 (29%)	87 (99%)	1 (1%)	73	86
2	G	88/304 (29%)	87 (99%)	1 (1%)	73	86
2	H	88/304 (29%)	87 (99%)	1 (1%)	73	86
All	All	15572/18320 (85%)	15046 (97%)	526 (3%)	41	65

All (526) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	125	ARG

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Mol	Chain	Res	Type
1	A	373	LYS
1	A	392	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	2100[A]	HIS
1	A	2100[B]	HIS
1	A	2336	ARG
1	A	2369[A]	ARG
1	A	2369[B]	ARG
1	A	2690	LYS
1	A	2786	LYS
1	A	2827	ARG
1	A	2870[A]	GLU
1	A	2870[B]	GLU
1	A	2914	LYS
1	A	2985	ARG
1	A	3053	ARG
1	A	3185	LYS
1	A	3325	ASN
1	A	3453	ARG
1	A	3577	ARG
1	A	3614	LYS
1	A	3622	LYS
1	A	3688	GLU
1	A	4178	LEU
1	A	4180	ARG
1	A	4181	ILE
1	A	4183	ILE
1	A	4188	ARG
1	A	4190	ILE
1	A	4192	ARG
1	A	4196	GLU
1	A	4209	GLN
1	A	4212	GLU
1	A	4215	ARG
1	A	4224	GLU
1	A	4227	GLU
1	A	4230	LYS
1	A	4231	MET

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Mol	Chain	Res	Type
1	A	4244	GLU
1	A	4252	SER
1	A	4543	GLU
1	A	4544	LEU
1	A	4550	LYS
1	A	4555	LEU
1	A	4561	THR
1	A	4577	LEU
1	A	4578	LEU
1	A	4580	TYR
1	A	4581	LYS
1	A	4583	SER
1	A	4584	ASP
1	A	4627	MET
1	A	4628	VAL
1	A	4633	GLU
1	A	4635	SER
1	A	4639	MET
1	A	4645	CYS
1	A	4651	THR
1	A	4665	LYS
1	A	4667	PRO
1	A	4673	ARG
1	A	4679	ARG
1	A	4680	LYS
1	A	4689	THR
1	A	4695	ASP
1	A	4697	VAL
1	A	4704	LEU
1	A	4706	LEU
1	A	4707	ASN
1	A	4708	THR
1	A	4710	SER
1	A	4711	PHE
1	A	4713	SER
1	A	4716	TRP
1	A	4721	LYS
1	A	4730	ASP
1	A	4731	ILE
1	A	4743	MET
1	A	4745	LEU
1	A	4747	SER

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Mol	Chain	Res	Type
1	A	4749	GLU
1	A	4772	ASP
1	A	4773	VAL
1	A	4774	LYS
1	A	4777	ILE
1	A	4788	SER
1	A	4809	PHE
1	A	4818	MET
1	A	4821	LYS
1	A	4822	THR
1	A	4824	ARG
1	A	4835	LYS
1	A	4837	LEU
1	A	4844	LEU
1	A	4861	LYS
1	A	4865	LYS
1	A	4869	GLU
1	A	4871	GLU
1	A	4876	CYS
1	A	4887	MET
1	A	4889	VAL
1	A	4908	GLU
1	A	4913	ARG
1	A	4920	PHE
1	A	4927	ILE
1	A	4933	GLN
1	A	4945	ASP
1	A	4949	GLN
1	A	4951	LYS
1	A	4957	LYS
1	A	4966	ASP
1	A	4976	GLU
1	A	4980	LEU
1	A	4985	LEU
1	A	4989	MET
1	A	4992	LEU
1	A	4995	LEU
1	A	4997	ASN
1	A	4998	LYS
1	A	5004	THR
1	A	5006	GLN
1	A	5012	LYS

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Mol	Chain	Res	Type
1	A	5028	PHE
1	A	5030	LYS
1	A	5034	ASP
1	B	125	ARG
1	B	373	LYS
1	B	392	ARG
1	B	846	LEU
1	B	1534	LYS
1	B	1743[A]	ARG
1	B	1743[B]	ARG
1	B	1752	ARG
1	B	2100[A]	HIS
1	B	2100[B]	HIS
1	B	2336	ARG
1	B	2369[A]	ARG
1	B	2369[B]	ARG
1	B	2690	LYS
1	B	2786	LYS
1	B	2827	ARG
1	B	2870[A]	GLU
1	B	2870[B]	GLU
1	B	2914	LYS
1	B	2985	ARG
1	B	3053	ARG
1	B	3185	LYS
1	B	3325	ASN
1	B	3453	ARG
1	B	3577	ARG
1	B	3614	LYS
1	B	3622	LYS
1	B	3688	GLU
1	B	4178	LEU
1	B	4180	ARG
1	B	4181	ILE
1	B	4183	ILE
1	B	4188	ARG
1	B	4190	ILE
1	B	4192	ARG
1	B	4196	GLU
1	B	4209	GLN
1	B	4212	GLU
1	B	4215	ARG

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Mol	Chain	Res	Type
1	B	4224	GLU
1	B	4227	GLU
1	B	4230	LYS
1	B	4231	MET
1	B	4244	GLU
1	B	4252	SER
1	B	4543	GLU
1	B	4544	LEU
1	B	4550	LYS
1	B	4555	LEU
1	B	4561	THR
1	B	4577	LEU
1	B	4578	LEU
1	B	4580	TYR
1	B	4581	LYS
1	B	4583	SER
1	B	4584	ASP
1	B	4627	MET
1	B	4628	VAL
1	B	4633	GLU
1	B	4635	SER
1	B	4639	MET
1	B	4645	CYS
1	B	4651	THR
1	B	4665	LYS
1	B	4667	PRO
1	B	4673	ARG
1	B	4679	ARG
1	B	4680	LYS
1	B	4689	THR
1	B	4695	ASP
1	B	4697	VAL
1	B	4704	LEU
1	B	4706	LEU
1	B	4707	ASN
1	B	4708	THR
1	B	4710	SER
1	B	4711	PHE
1	B	4713	SER
1	B	4716	TRP
1	B	4721	LYS
1	B	4730	ASP

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Mol	Chain	Res	Type
1	B	4731	ILE
1	B	4743	MET
1	B	4745	LEU
1	B	4747	SER
1	B	4749	GLU
1	B	4772	ASP
1	B	4773	VAL
1	B	4774	LYS
1	B	4777	ILE
1	B	4788	SER
1	B	4809	PHE
1	B	4818	MET
1	B	4821	LYS
1	B	4822	THR
1	B	4824	ARG
1	B	4835	LYS
1	B	4837	LEU
1	B	4844	LEU
1	B	4861	LYS
1	B	4865	LYS
1	B	4869	GLU
1	B	4871	GLU
1	B	4876	CYS
1	B	4887	MET
1	B	4889	VAL
1	B	4908	GLU
1	B	4913	ARG
1	B	4920	PHE
1	B	4927	ILE
1	B	4933	GLN
1	B	4945	ASP
1	B	4949	GLN
1	B	4951	LYS
1	B	4957	LYS
1	B	4966	ASP
1	B	4976	GLU
1	B	4980	LEU
1	B	4985	LEU
1	B	4989	MET
1	B	4992	LEU
1	B	4995	LEU
1	B	4997	ASN

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Mol	Chain	Res	Type
1	B	4998	LYS
1	B	5004	THR
1	B	5006	GLN
1	B	5012	LYS
1	B	5028	PHE
1	B	5030	LYS
1	B	5034	ASP
1	C	125	ARG
1	C	373	LYS
1	C	392	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	2100[A]	HIS
1	C	2100[B]	HIS
1	C	2336	ARG
1	C	2369[A]	ARG
1	C	2369[B]	ARG
1	C	2690	LYS
1	C	2786	LYS
1	C	2827	ARG
1	C	2870[A]	GLU
1	C	2870[B]	GLU
1	C	2914	LYS
1	C	2985	ARG
1	C	3053	ARG
1	C	3185	LYS
1	C	3325	ASN
1	C	3453	ARG
1	C	3577	ARG
1	C	3614	LYS
1	C	3622	LYS
1	C	3688	GLU
1	C	4178	LEU
1	C	4180	ARG
1	C	4181	ILE
1	C	4183	ILE
1	C	4188	ARG
1	C	4190	ILE
1	C	4192	ARG

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Mol	Chain	Res	Type
1	C	4196	GLU
1	C	4209	GLN
1	C	4212	GLU
1	C	4215	ARG
1	C	4224	GLU
1	C	4227	GLU
1	C	4230	LYS
1	C	4231	MET
1	C	4244	GLU
1	C	4252	SER
1	C	4543	GLU
1	C	4544	LEU
1	C	4550	LYS
1	C	4555	LEU
1	C	4561	THR
1	C	4577	LEU
1	C	4578	LEU
1	C	4580	TYR
1	C	4581	LYS
1	C	4583	SER
1	C	4584	ASP
1	C	4627	MET
1	C	4628	VAL
1	C	4633	GLU
1	C	4635	SER
1	C	4639	MET
1	C	4645	CYS
1	C	4651	THR
1	C	4665	LYS
1	C	4667	PRO
1	C	4673	ARG
1	C	4679	ARG
1	C	4680	LYS
1	C	4689	THR
1	C	4695	ASP
1	C	4697	VAL
1	C	4704	LEU
1	C	4706	LEU
1	C	4707	ASN
1	C	4708	THR
1	C	4710	SER
1	C	4711	PHE

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Mol	Chain	Res	Type
1	C	4713	SER
1	C	4716	TRP
1	C	4721	LYS
1	C	4730	ASP
1	C	4731	ILE
1	C	4735	GLU
1	C	4743	MET
1	C	4745	LEU
1	C	4747	SER
1	C	4749	GLU
1	C	4772	ASP
1	C	4773	VAL
1	C	4774	LYS
1	C	4777	ILE
1	C	4788	SER
1	C	4809	PHE
1	C	4818	MET
1	C	4821	LYS
1	C	4822	THR
1	C	4824	ARG
1	C	4835	LYS
1	C	4837	LEU
1	C	4844	LEU
1	C	4861	LYS
1	C	4865	LYS
1	C	4869	GLU
1	C	4871	GLU
1	C	4876	CYS
1	C	4887	MET
1	C	4889	VAL
1	C	4908	GLU
1	C	4913	ARG
1	C	4920	PHE
1	C	4927	ILE
1	C	4933	GLN
1	C	4945	ASP
1	C	4949	GLN
1	C	4951	LYS
1	C	4957	LYS
1	C	4966	ASP
1	C	4976	GLU
1	C	4980	LEU

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Mol	Chain	Res	Type
1	C	4985	LEU
1	C	4989	MET
1	C	4992	LEU
1	C	4995	LEU
1	C	4997	ASN
1	C	4998	LYS
1	C	5004	THR
1	C	5006	GLN
1	C	5012	LYS
1	C	5028	PHE
1	C	5030	LYS
1	C	5034	ASP
1	D	125	ARG
1	D	373	LYS
1	D	392	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	2100[A]	HIS
1	D	2100[B]	HIS
1	D	2336	ARG
1	D	2369[A]	ARG
1	D	2369[B]	ARG
1	D	2690	LYS
1	D	2786	LYS
1	D	2827	ARG
1	D	2870[A]	GLU
1	D	2870[B]	GLU
1	D	2914	LYS
1	D	2985	ARG
1	D	3053	ARG
1	D	3185	LYS
1	D	3325	ASN
1	D	3453	ARG
1	D	3577	ARG
1	D	3614	LYS
1	D	3622	LYS
1	D	3688	GLU
1	D	4178	LEU
1	D	4180	ARG

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Mol	Chain	Res	Type
1	D	4181	ILE
1	D	4183	ILE
1	D	4188	ARG
1	D	4190	ILE
1	D	4192	ARG
1	D	4196	GLU
1	D	4209	GLN
1	D	4212	GLU
1	D	4215	ARG
1	D	4224	GLU
1	D	4227	GLU
1	D	4230	LYS
1	D	4231	MET
1	D	4244	GLU
1	D	4252	SER
1	D	4543	GLU
1	D	4544	LEU
1	D	4550	LYS
1	D	4555	LEU
1	D	4561	THR
1	D	4577	LEU
1	D	4578	LEU
1	D	4580	TYR
1	D	4581	LYS
1	D	4583	SER
1	D	4584	ASP
1	D	4627	MET
1	D	4628	VAL
1	D	4633	GLU
1	D	4635	SER
1	D	4639	MET
1	D	4645	CYS
1	D	4651	THR
1	D	4665	LYS
1	D	4667	PRO
1	D	4673	ARG
1	D	4679	ARG
1	D	4680	LYS
1	D	4689	THR
1	D	4695	ASP
1	D	4697	VAL
1	D	4704	LEU

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Mol	Chain	Res	Type
1	D	4706	LEU
1	D	4707	ASN
1	D	4708	THR
1	D	4710	SER
1	D	4711	PHE
1	D	4713	SER
1	D	4716	TRP
1	D	4721	LYS
1	D	4730	ASP
1	D	4731	ILE
1	D	4735	GLU
1	D	4743	MET
1	D	4745	LEU
1	D	4747	SER
1	D	4749	GLU
1	D	4772	ASP
1	D	4773	VAL
1	D	4774	LYS
1	D	4777	ILE
1	D	4788	SER
1	D	4809	PHE
1	D	4818	MET
1	D	4821	LYS
1	D	4822	THR
1	D	4824	ARG
1	D	4835	LYS
1	D	4837	LEU
1	D	4844	LEU
1	D	4861	LYS
1	D	4865	LYS
1	D	4869	GLU
1	D	4871	GLU
1	D	4876	CYS
1	D	4887	MET
1	D	4889	VAL
1	D	4908	GLU
1	D	4913	ARG
1	D	4920	PHE
1	D	4927	ILE
1	D	4933	GLN
1	D	4945	ASP
1	D	4949	GLN

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Mol	Chain	Res	Type
1	D	4951	LYS
1	D	4957	LYS
1	D	4966	ASP
1	D	4976	GLU
1	D	4980	LEU
1	D	4985	LEU
1	D	4989	MET
1	D	4992	LEU
1	D	4995	LEU
1	D	4997	ASN
1	D	4998	LYS
1	D	5004	THR
1	D	5006	GLN
1	D	5012	LYS
1	D	5028	PHE
1	D	5030	LYS
1	D	5034	ASP
2	E	17	LYS
2	F	17	LYS
2	G	17	LYS
2	H	17	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	475	GLN
1	A	479	GLN
1	A	533	ASN
1	A	877	ASN
1	A	2127	GLN
1	A	2498	HIS
1	A	2877	GLN
1	A	2962	GLN
1	A	4133	GLN
1	A	4700	GLN
1	A	4707	ASN
1	A	4728	HIS
1	A	4886	HIS
1	B	475	GLN
1	B	479	GLN
1	B	533	ASN
1	B	877	ASN

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Mol	Chain	Res	Type
1	B	2127	GLN
1	B	2498	HIS
1	B	2877	GLN
1	B	2962	GLN
1	B	4133	GLN
1	B	4700	GLN
1	B	4707	ASN
1	B	4728	HIS
1	B	4886	HIS
1	C	475	GLN
1	C	479	GLN
1	C	533	ASN
1	C	877	ASN
1	C	2498	HIS
1	C	2877	GLN
1	C	2962	GLN
1	C	4133	GLN
1	C	4700	GLN
1	C	4728	HIS
1	C	4886	HIS
1	D	475	GLN
1	D	479	GLN
1	D	533	ASN
1	D	877	ASN
1	D	2127	GLN
1	D	2498	HIS
1	D	2877	GLN
1	D	2962	GLN
1	D	4133	GLN
1	D	4700	GLN
1	D	4728	HIS
1	D	4886	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	AMP	B	5101	-	22,25,25	0.83	1 (4%)	25,38,38	1.23	2 (8%)
3	AMP	C	5101	-	22,25,25	0.83	1 (4%)	25,38,38	1.23	2 (8%)
3	AMP	D	5101	-	22,25,25	0.83	1 (4%)	25,38,38	1.23	2 (8%)
3	AMP	A	5101	-	22,25,25	0.83	1 (4%)	25,38,38	1.23	2 (8%)

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	AMP	B	5101	-	-	2/6/26/26	0/3/3/3
3	AMP	C	5101	-	-	2/6/26/26	0/3/3/3
3	AMP	D	5101	-	-	2/6/26/26	0/3/3/3
3	AMP	A	5101	-	-	2/6/26/26	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	5101	AMP	C5-C4	2.18	1.46	1.40
3	D	5101	AMP	C5-C4	2.18	1.46	1.40
3	C	5101	AMP	C5-C4	2.17	1.46	1.40
3	B	5101	AMP	C5-C4	2.17	1.46	1.40

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	5101	AMP	N3-C2-N1	-3.31	123.50	128.68
3	D	5101	AMP	N3-C2-N1	-3.31	123.50	128.68
3	C	5101	AMP	N3-C2-N1	-3.31	123.50	128.68
3	A	5101	AMP	N3-C2-N1	-3.31	123.51	128.68
3	A	5101	AMP	C4-C5-N7	-2.29	107.01	109.40
3	D	5101	AMP	C4-C5-N7	-2.29	107.02	109.40
3	B	5101	AMP	C4-C5-N7	-2.28	107.02	109.40
3	C	5101	AMP	C4-C5-N7	-2.28	107.02	109.40

There are no chirality outliers.

All (8) torsion outliers are listed below:

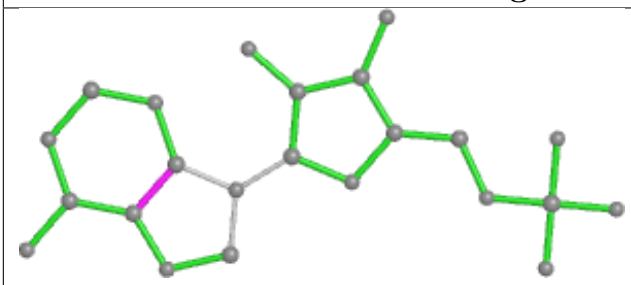
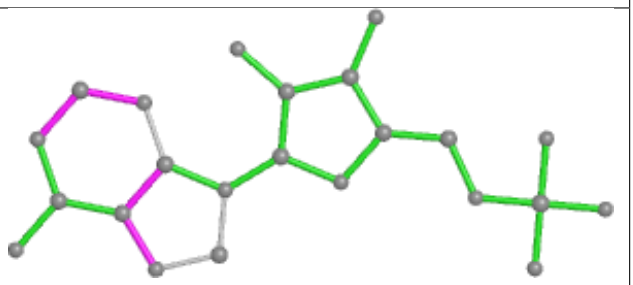
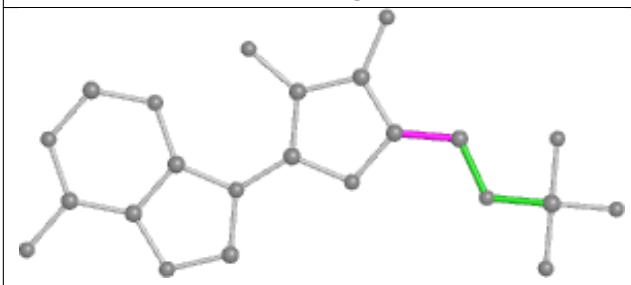
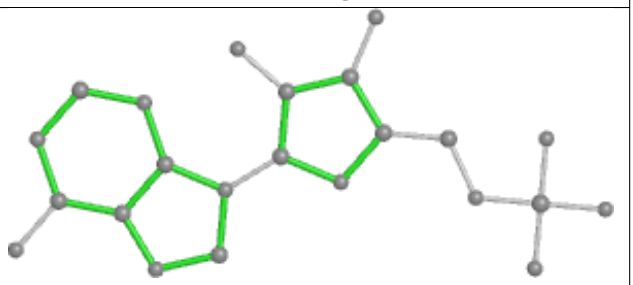
Mol	Chain	Res	Type	Atoms
3	A	5101	AMP	O4'-C4'-C5'-O5'
3	B	5101	AMP	O4'-C4'-C5'-O5'
3	C	5101	AMP	O4'-C4'-C5'-O5'
3	D	5101	AMP	O4'-C4'-C5'-O5'
3	A	5101	AMP	C3'-C4'-C5'-O5'
3	B	5101	AMP	C3'-C4'-C5'-O5'
3	C	5101	AMP	C3'-C4'-C5'-O5'
3	D	5101	AMP	C3'-C4'-C5'-O5'

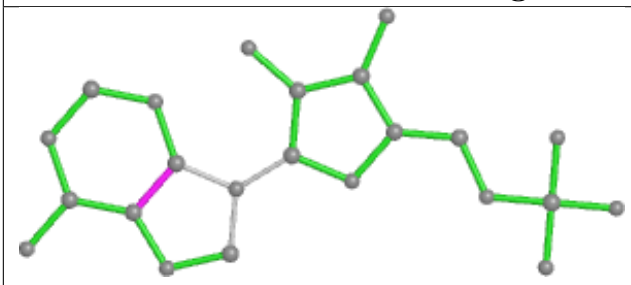
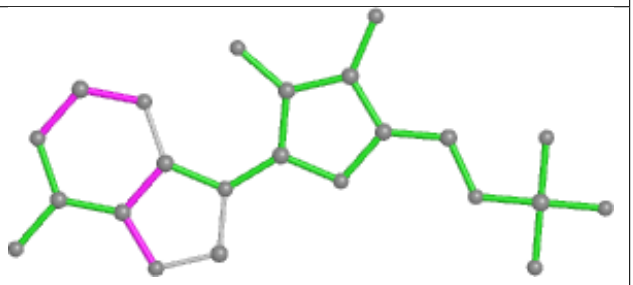
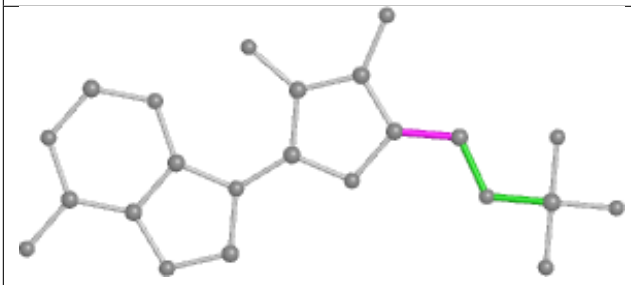
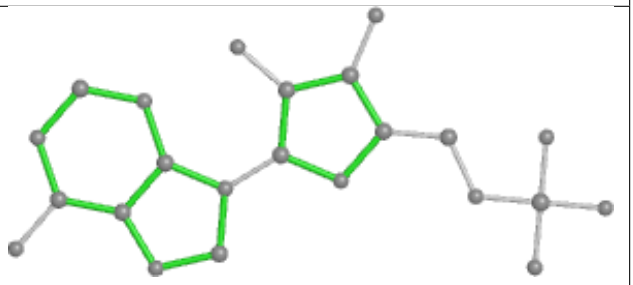
There are no ring outliers.

4 monomers are involved in 4 short contacts:

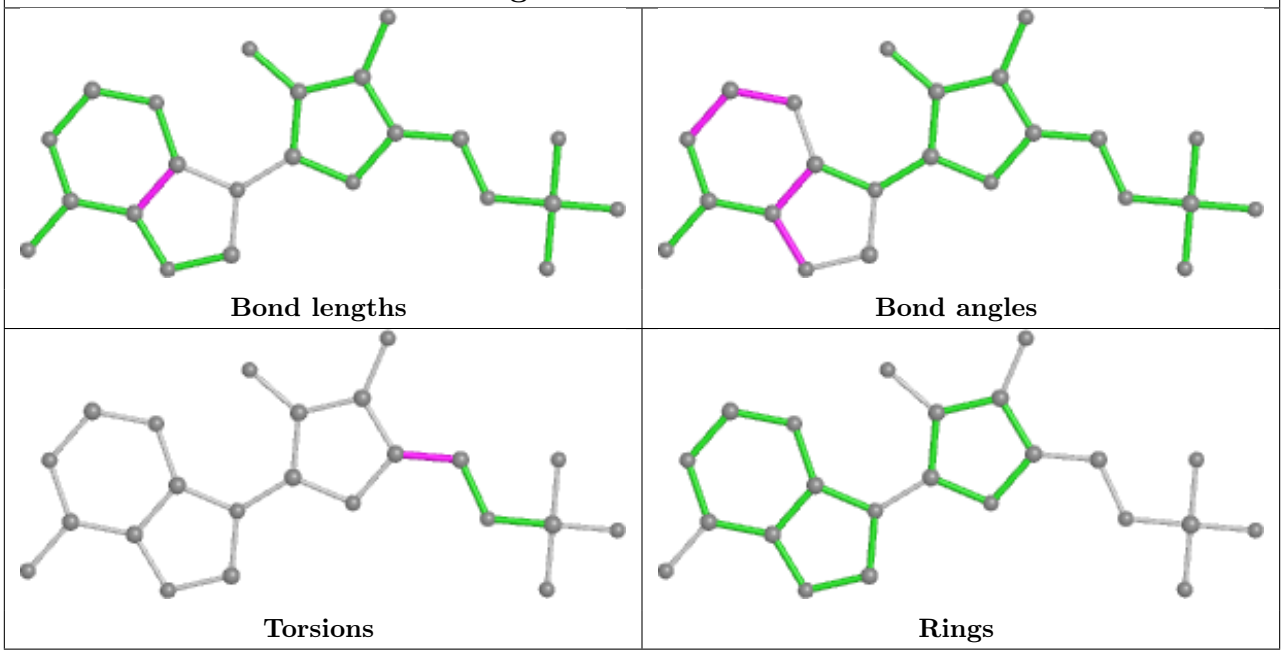
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	5101	AMP	1	0
3	C	5101	AMP	1	0
3	D	5101	AMP	1	0
3	A	5101	AMP	1	0

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

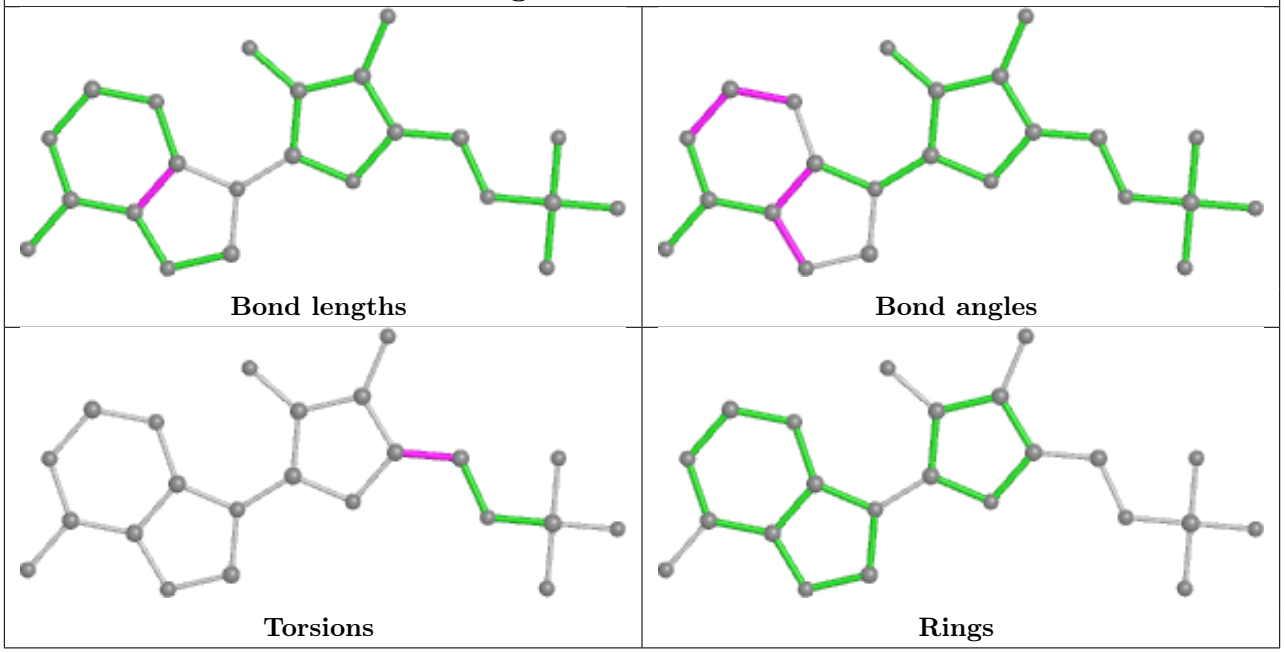
Ligand AMP B 5101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand AMP C 5101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand AMP D 5101



Ligand AMP A 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.

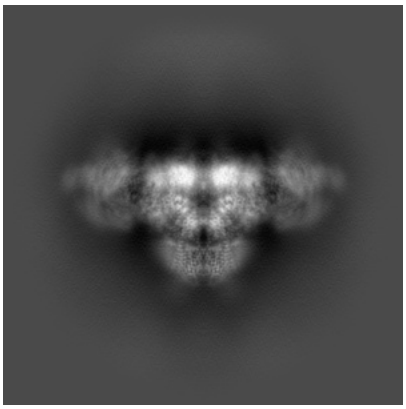
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-40425. These allow visual inspection of the internal detail of the map and identification of artifacts.

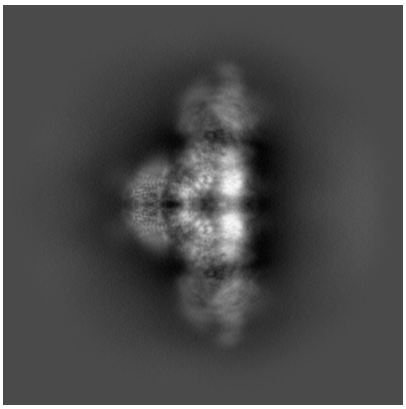
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

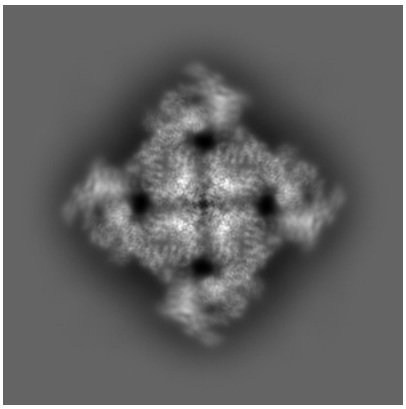
6.1.1 Primary map



X

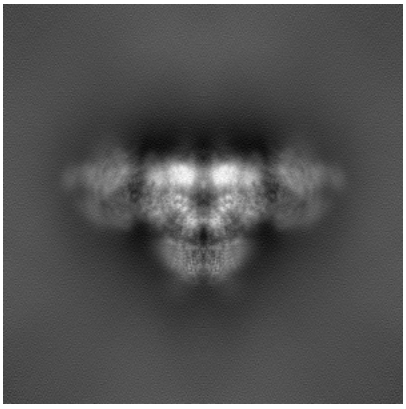


Y

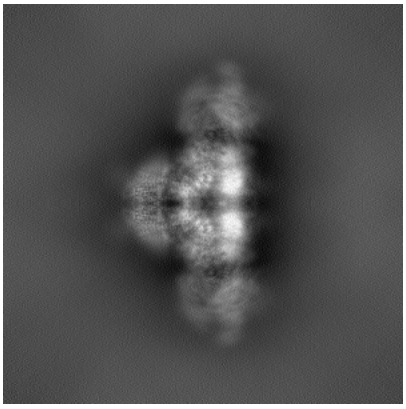


Z

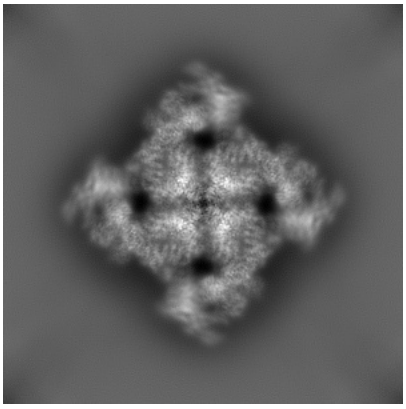
6.1.2 Raw map



X



Y

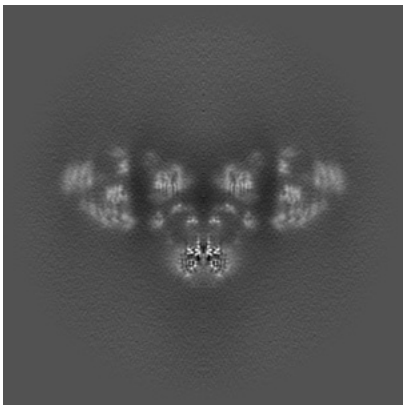


Z

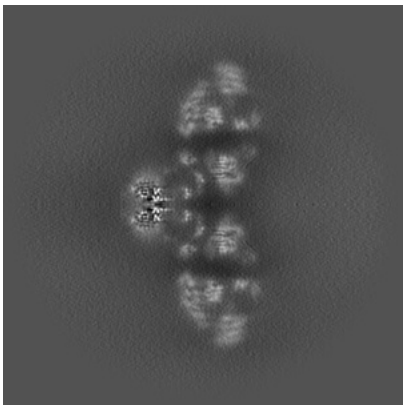
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

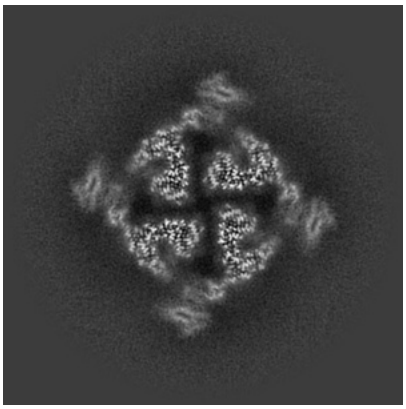
6.2.1 Primary map



X Index: 200

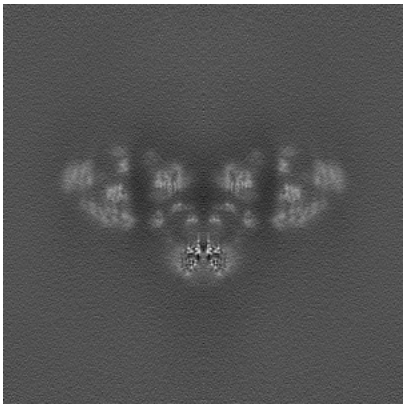


Y Index: 200

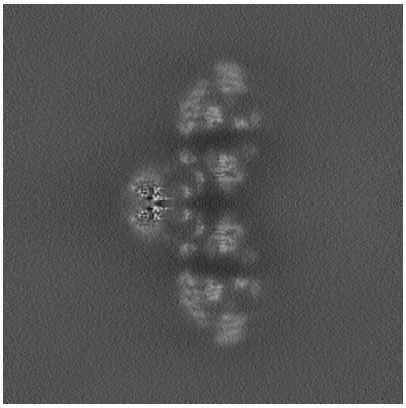


Z Index: 200

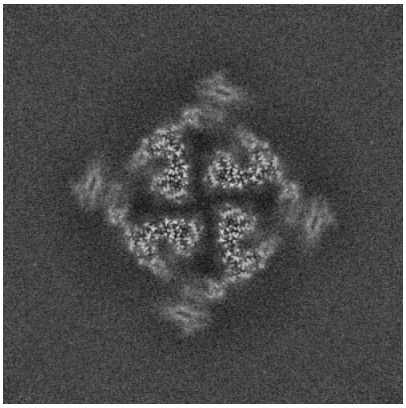
6.2.2 Raw map



X Index: 200



Y Index: 200

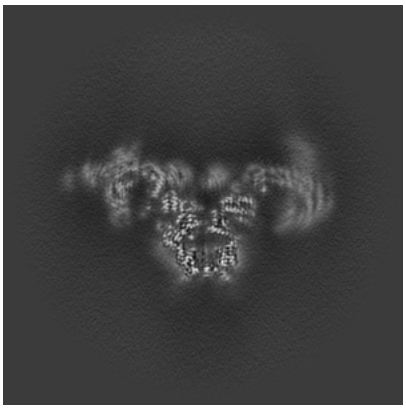


Z Index: 200

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

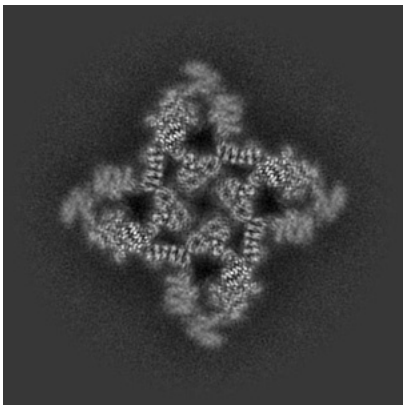
6.3 Largest variance slices (i)

6.3.1 Primary map



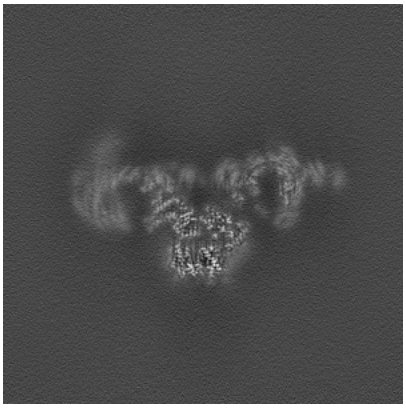
X Index: 218

Y Index: 182



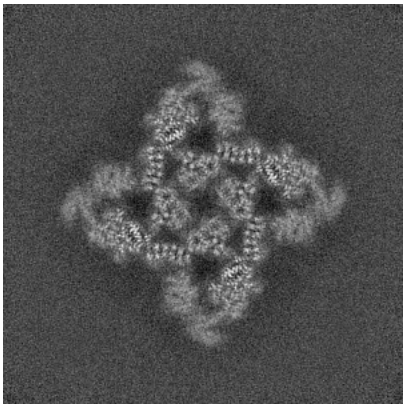
Z Index: 223

6.3.2 Raw map



X Index: 186

Y Index: 186

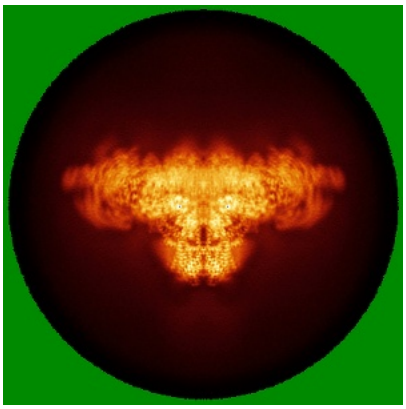


Z Index: 222

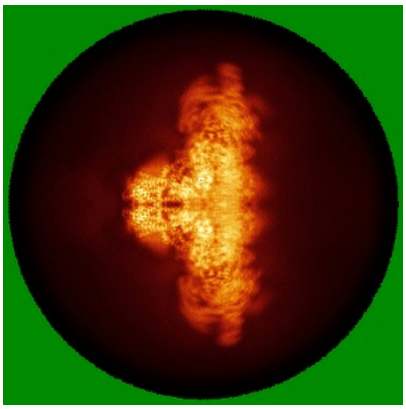
The images above show the largest variance slices of the map in three orthogonal directions.

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

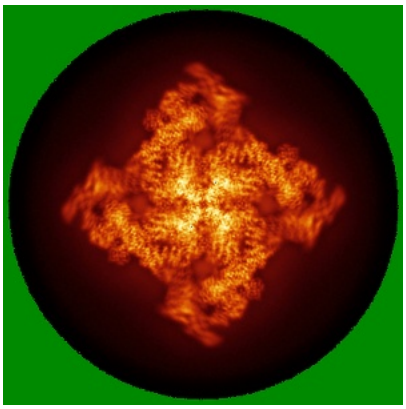
6.4.1 Primary map



X

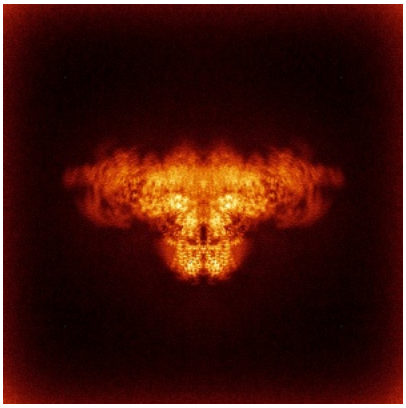


Y

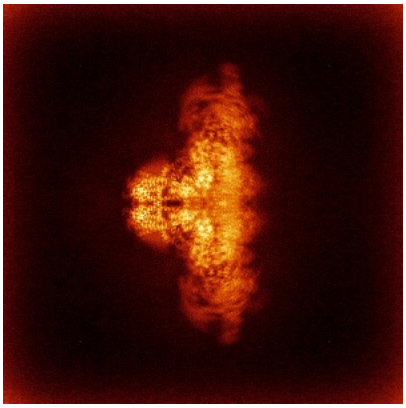


Z

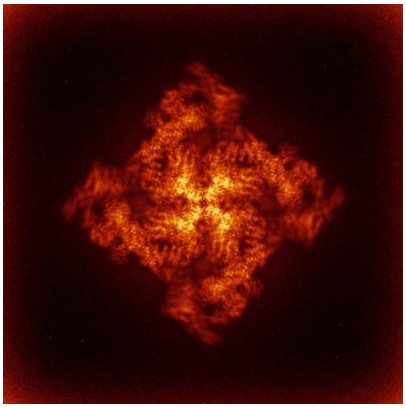
6.4.2 Raw map



X



Y

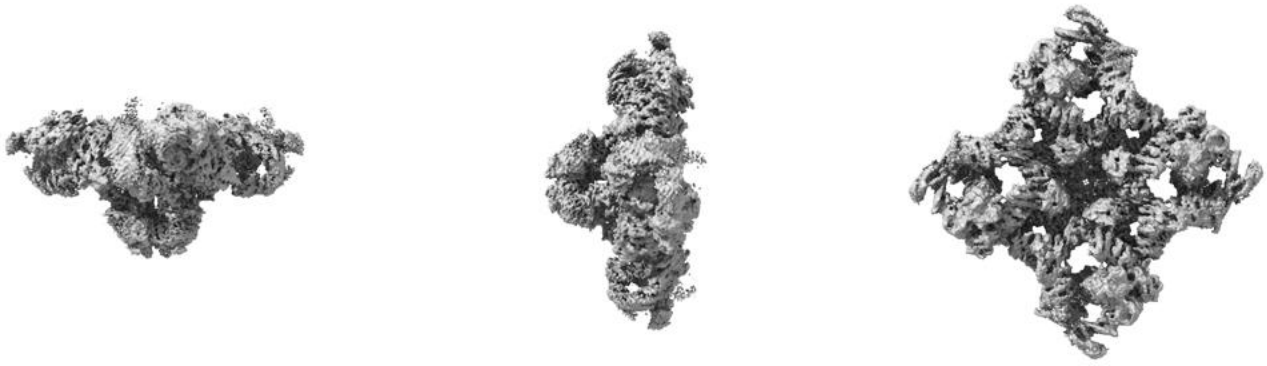


Z

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)

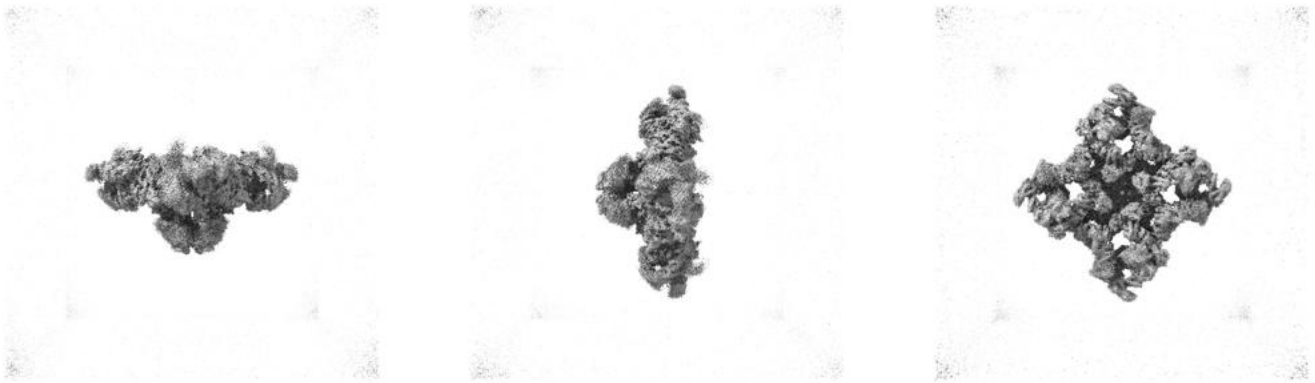
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.132. 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.

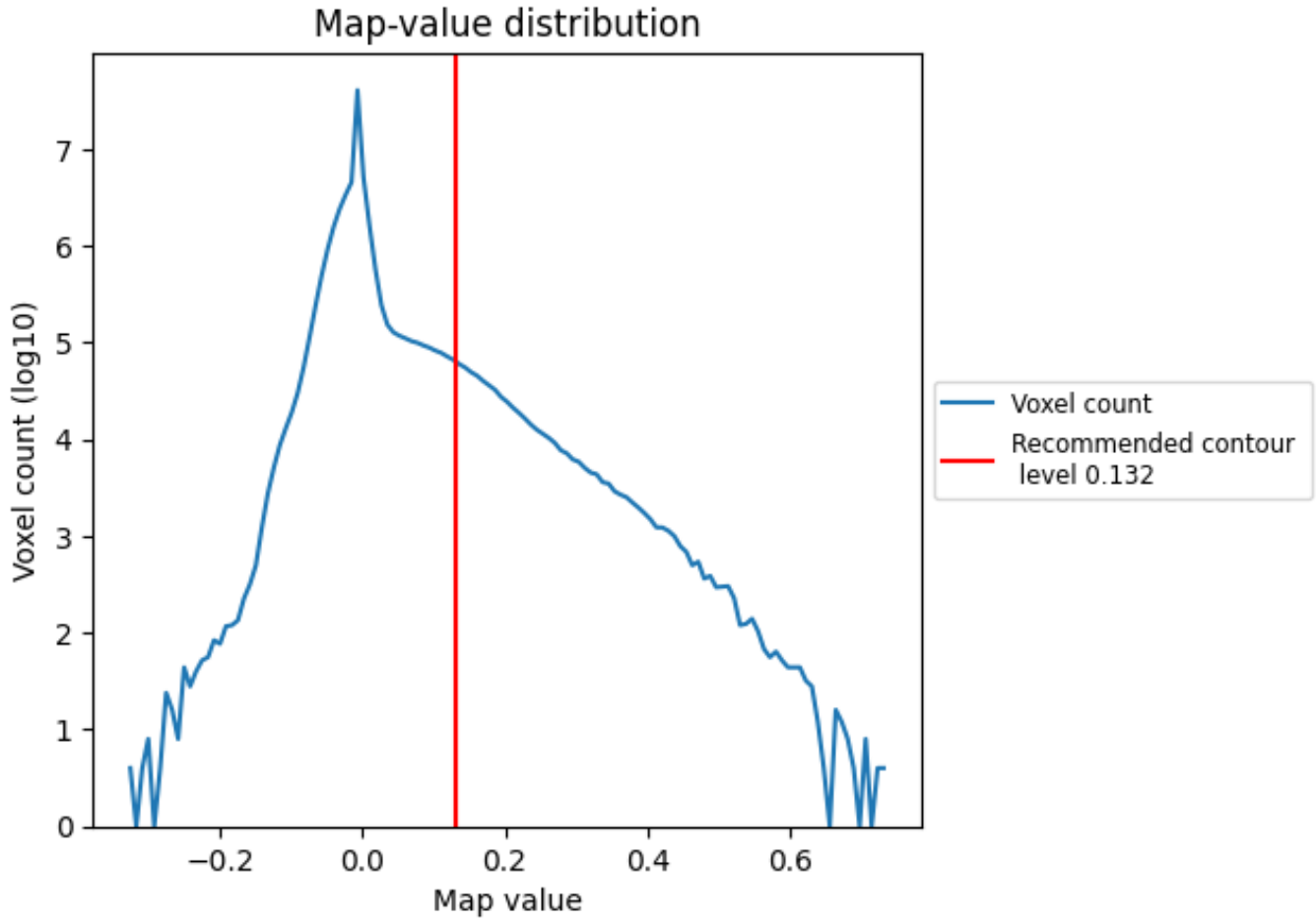
6.6 Mask visualisation (i)

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

7 Map analysis

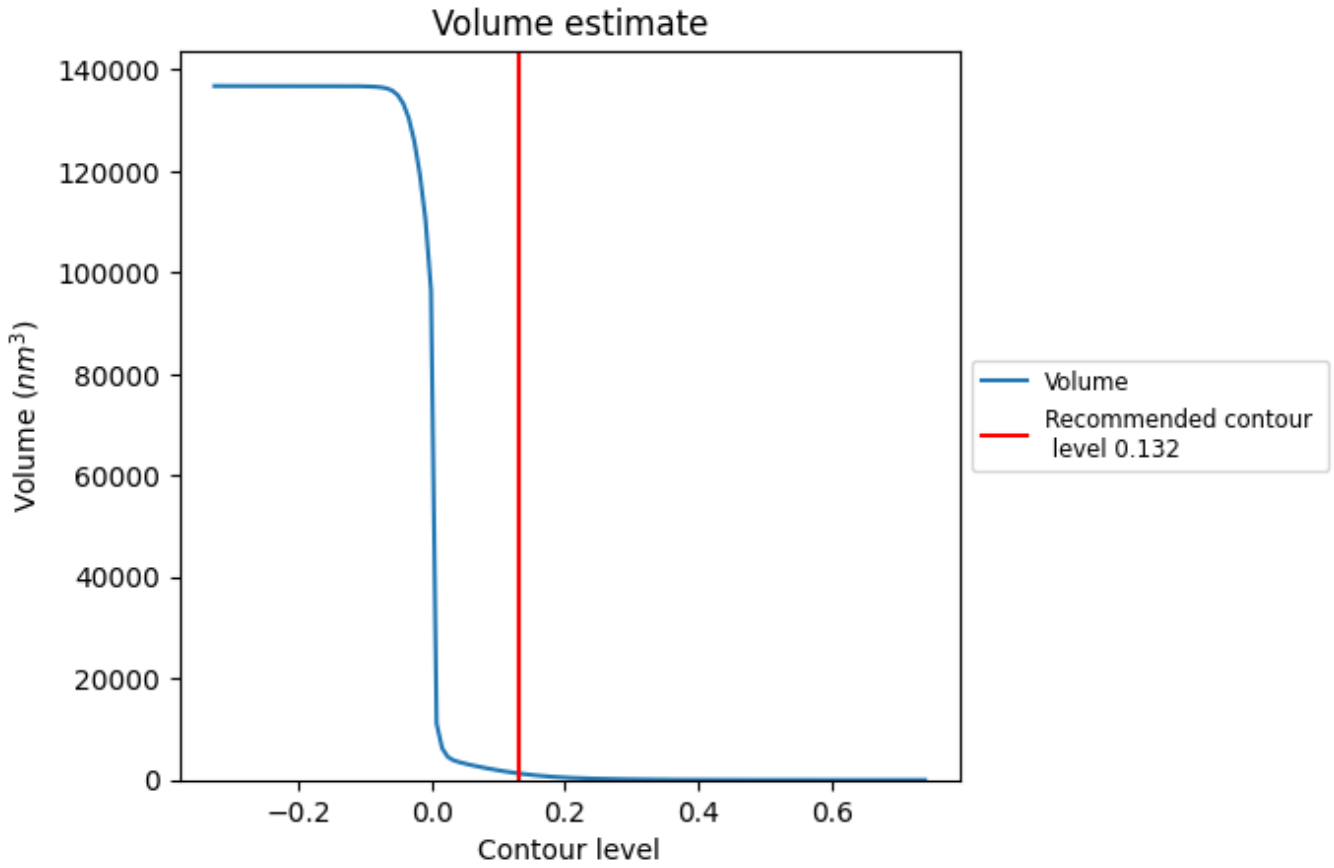
This section contains the results of statistical analysis of the map.

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.

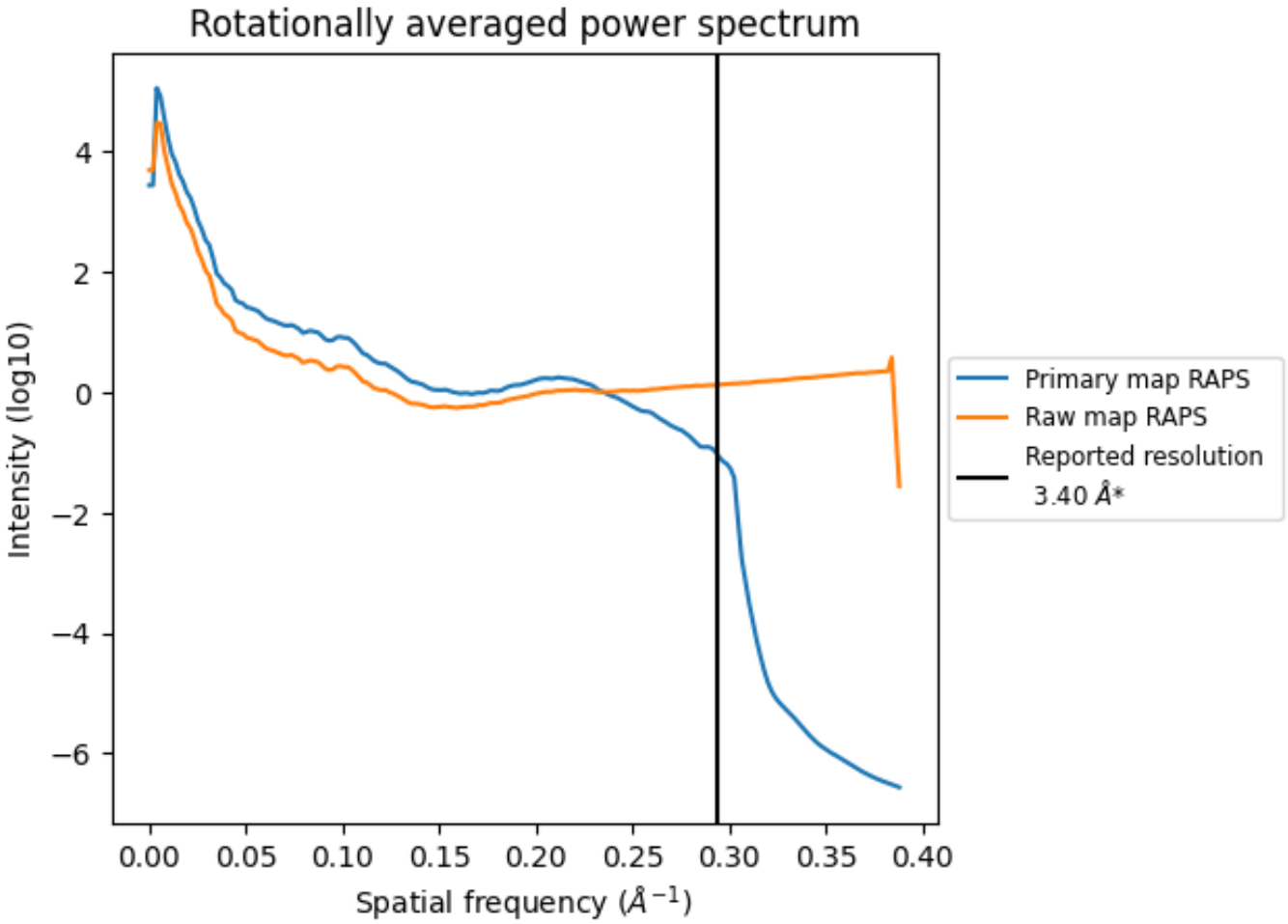
7.2 Volume estimate (i)



The volume at the recommended contour level is 1261 nm^3; this corresponds to an approximate mass of 1139 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)

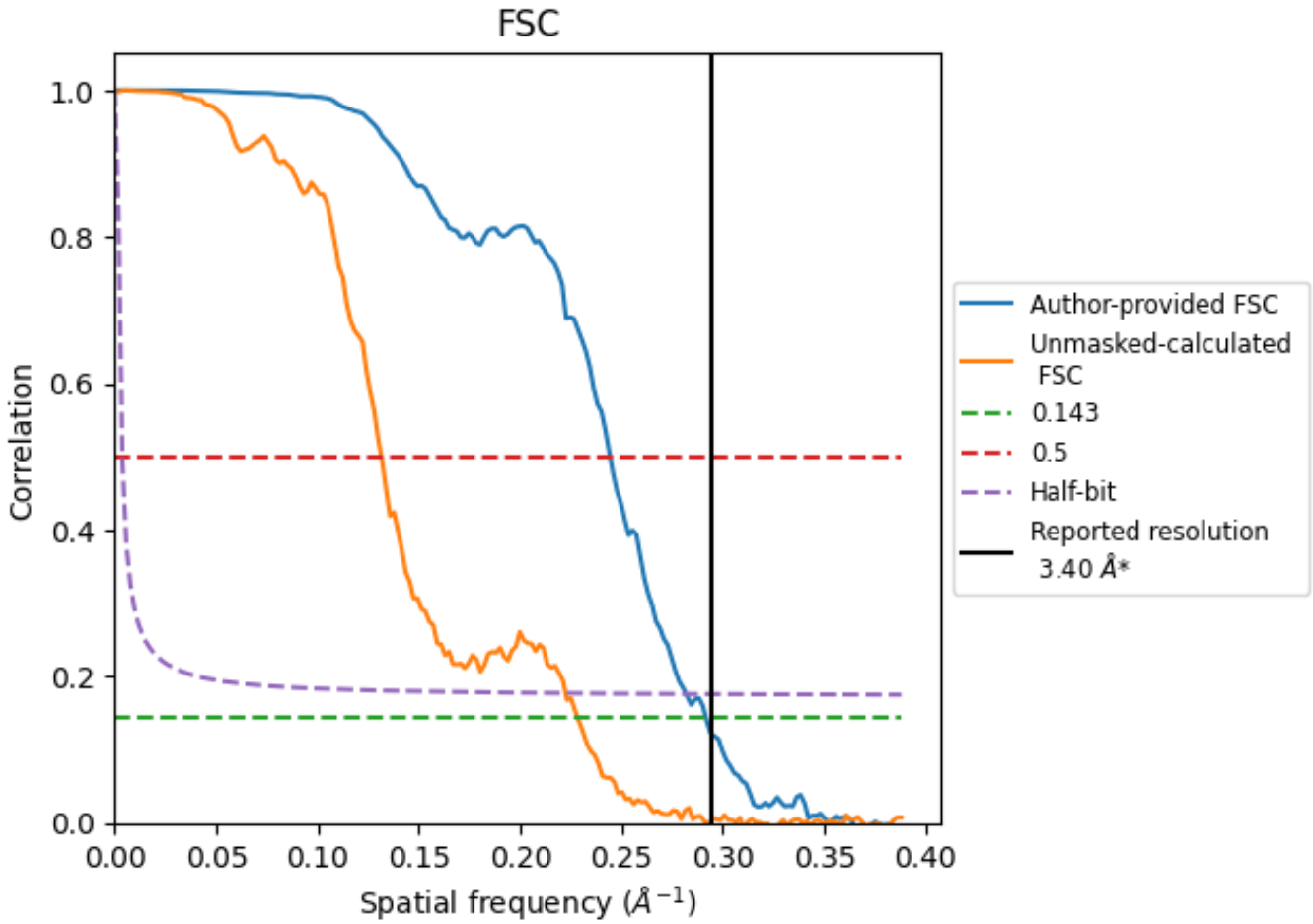


*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

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 0.294 Å^{-1}

8.2 Resolution estimates (i)

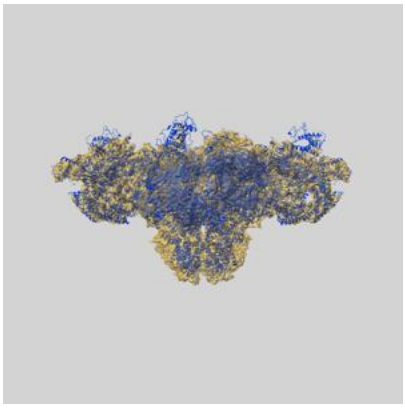
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.43	4.09	3.55
Unmasked-calculated*	4.37	7.60	4.49

*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 4.37 differs from the reported value 3.4 by more than 10 %

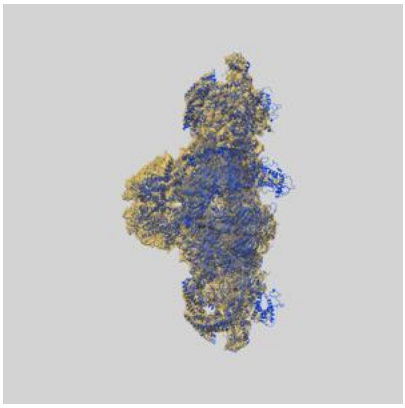
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-40425 and PDB model 8SEQ. Per-residue inclusion information can be found in section 3 on page 8.

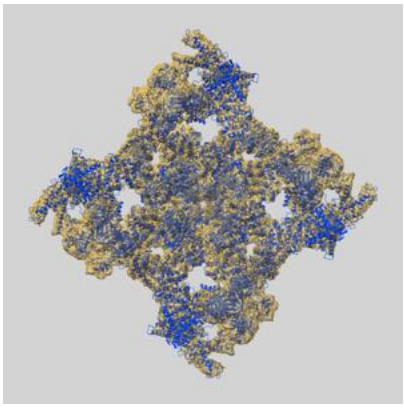
9.1 Map-model overlay



X



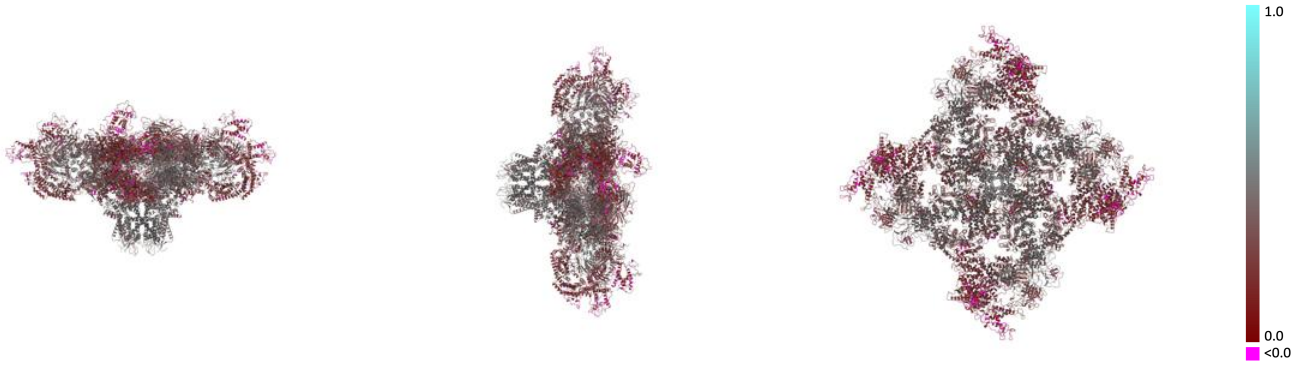
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.132 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.

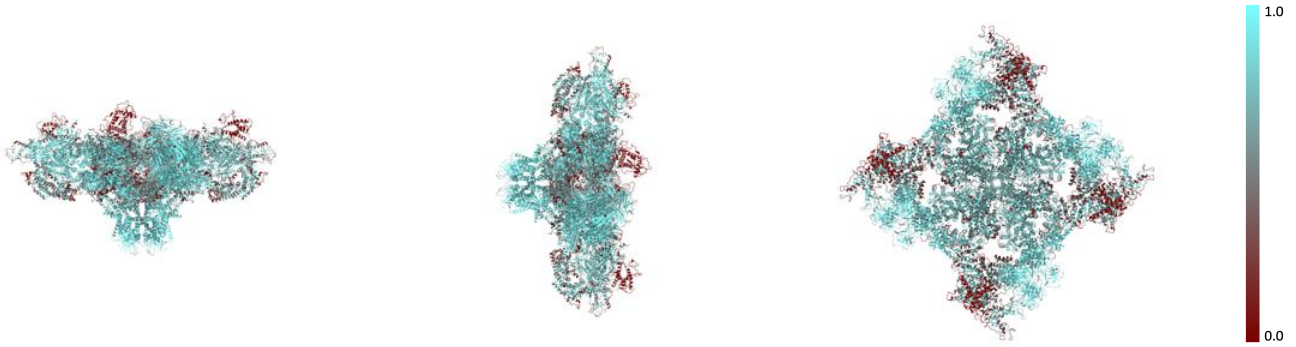
9.2 Q-score mapped to coordinate model



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.

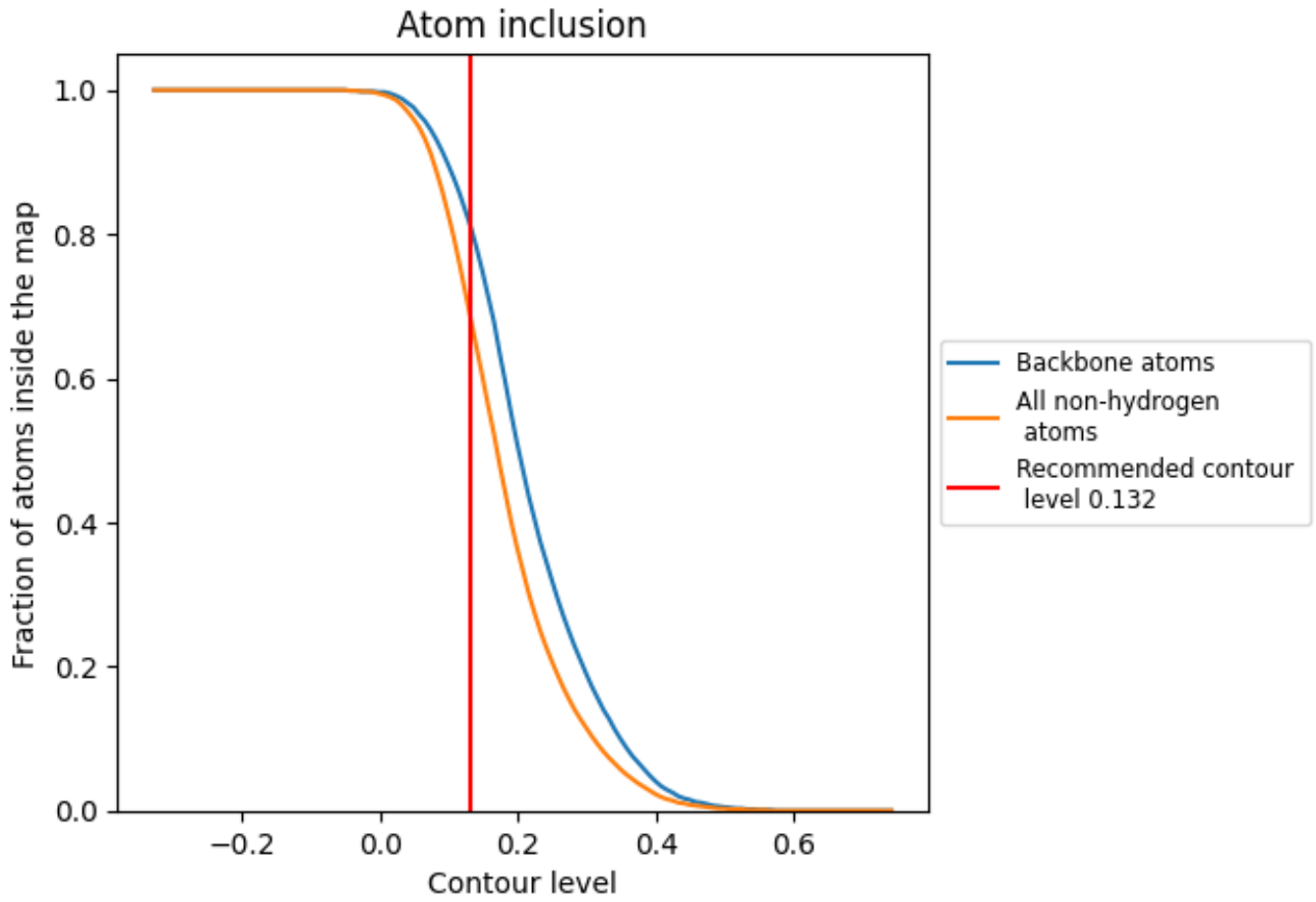
9.3 Atom inclusion mapped to coordinate model



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 (0.132).

9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 68% 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 (0.132) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6820	0.3220
A	0.6780	0.3210
B	0.6790	0.3200
C	0.6790	0.3200
D	0.6790	0.3200
E	0.8500	0.3890
F	0.8500	0.3880
G	0.8500	0.3900
H	0.8500	0.3930