Full wwPDB EM Validation Report ⓘ

Mar 2, 2024 – 11:47 AM EST

PDB ID	:	5T9M
EMDB ID	:	EMD-8372
Title	:	Structure of rabbit RyR1 (Ca2+-only dataset, class 1)
Authors	:	Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.; Frank, J.
Deposited on	:	2016-09-09
Resolution	:	4.00 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:

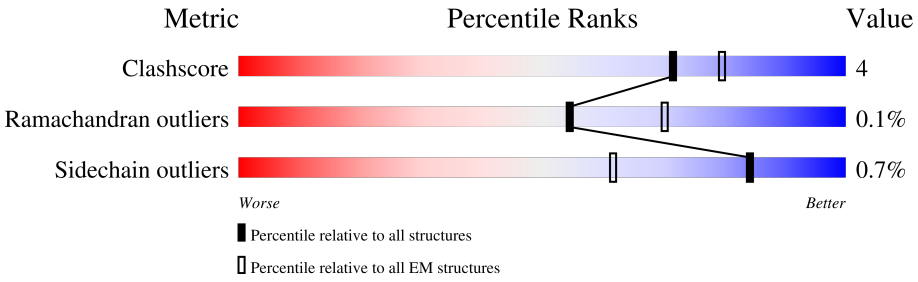
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.00 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	108	13% 88% 11% ·
1	F	108	14% 87% 12% ·
1	H	108	14% 87% 12% ·
1	J	108	13% 88% 11% ·
2	B	4676	19% 81% 8% 11%
2	E	4676	19% 81% 8% 11%
2	G	4676	19% 81% 8% 11%
2	I	4676	19% 81% 8% 11%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 120756 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

- Molecule 2 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		
2	E	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		
2	I	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		
2	G	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

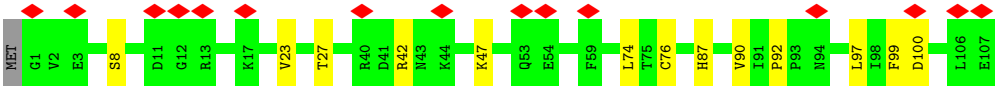
Mol	Chain	Residues	Atoms	AltConf
4	B	1	Total Ca 1 1	0
4	E	1	Total Ca 1 1	0
4	I	1	Total Ca 1 1	0
4	G	1	Total Ca 1 1	0

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.

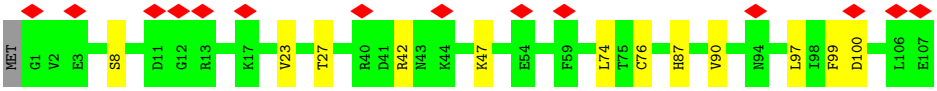
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F:



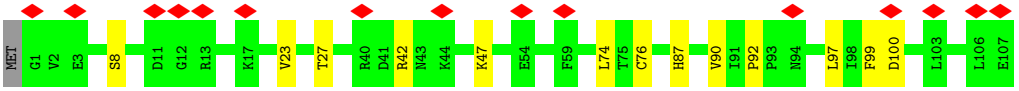
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain A:



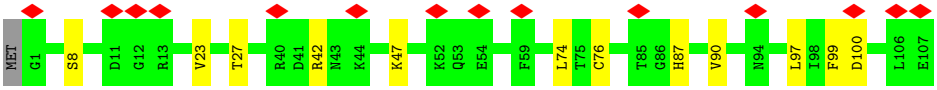
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H:



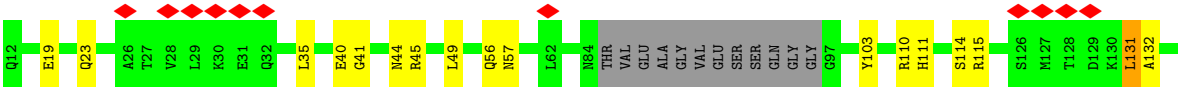
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

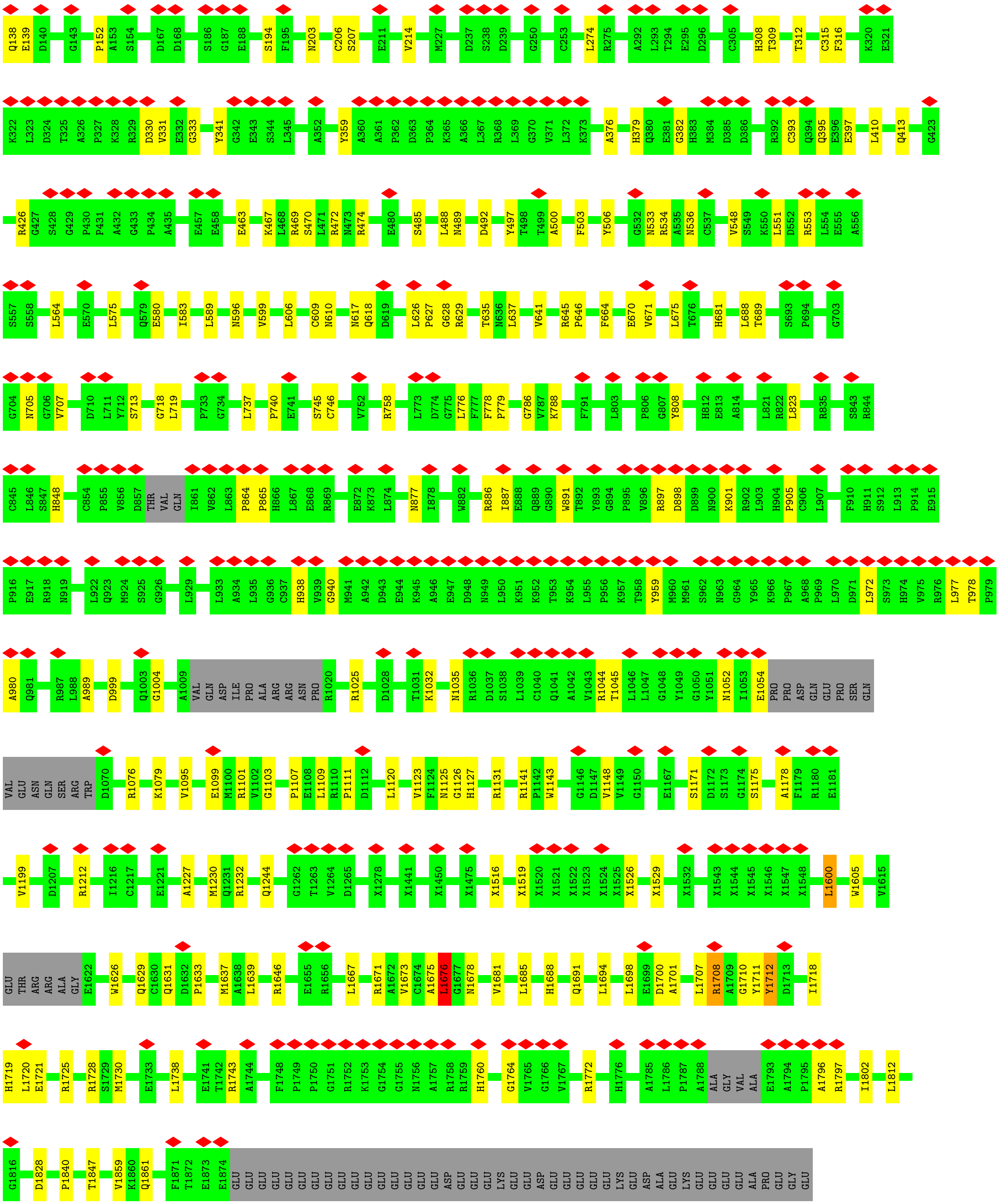
Chain J:



• Molecule 2: Ryanodine receptor 1

Chain B:

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K322 L323 D324 T325 A326 P327 K328 R329 D330 V331 E332 G333 Y341 G342 E343 S344 L345 A352 Y359 A360 A361 P362 D363 P364 K365 A366 L367 R368 L369 G370 V371 L372 K373 A376 H379 Q380 E381 G382 H383 M384 D385 D386 R392 C393 Q394 Q395 E396 E397 L410 Q413 G423
R426 G427 S428 G429 P430 P431 A432 G433 P434 A435 E457 E458 E463 K467 L468 R469 S470 L471 R472 N473 R474 E480 S485 L488 N489 D492 Y497 T498 T499 A500 F503 Y506 G532 N533 R534 A535 N536 C537 V548 S549 K550 L551 D552 R553 L554 E555 A556
S557 S558 L564 E570 L575 Q579 E580 I583 L589 N596 V599 L606 C609 N610 N617 Q618 D619 L626 P627 G628 R629 T635 N636 L637 V641 R645 P646 F664 E670 V671 L675 T676 H681 L688 T689 S693 P694 G703
G704 N705 G706 V707 D710 L711 Y712 S713 G718 L719 P733 G734 L737 P740 E741 S745 C746 V752 R758 L773 D774 G775 L776 F777 F778 P779 G786 V787 K788 F791 L803 P806 G807 Y808 H812 E813 A814 L821 R822 L823 R835 S843 R844
C845 L846 S847 H848 C854 P855 V856 D857 THR VAL GLN I861 V862 L863 P864 P865 H866 L867 E868 R869 E872 K873 L874 N877 I878 W882 R886 I887 E888 Q889 G890 W891 T892 Y893 G894 P895 V896 R897 D898 D899 N900 K901 R902 L903 H904 P905 C906 L907 F910 H911 S912 L913 P914 E915
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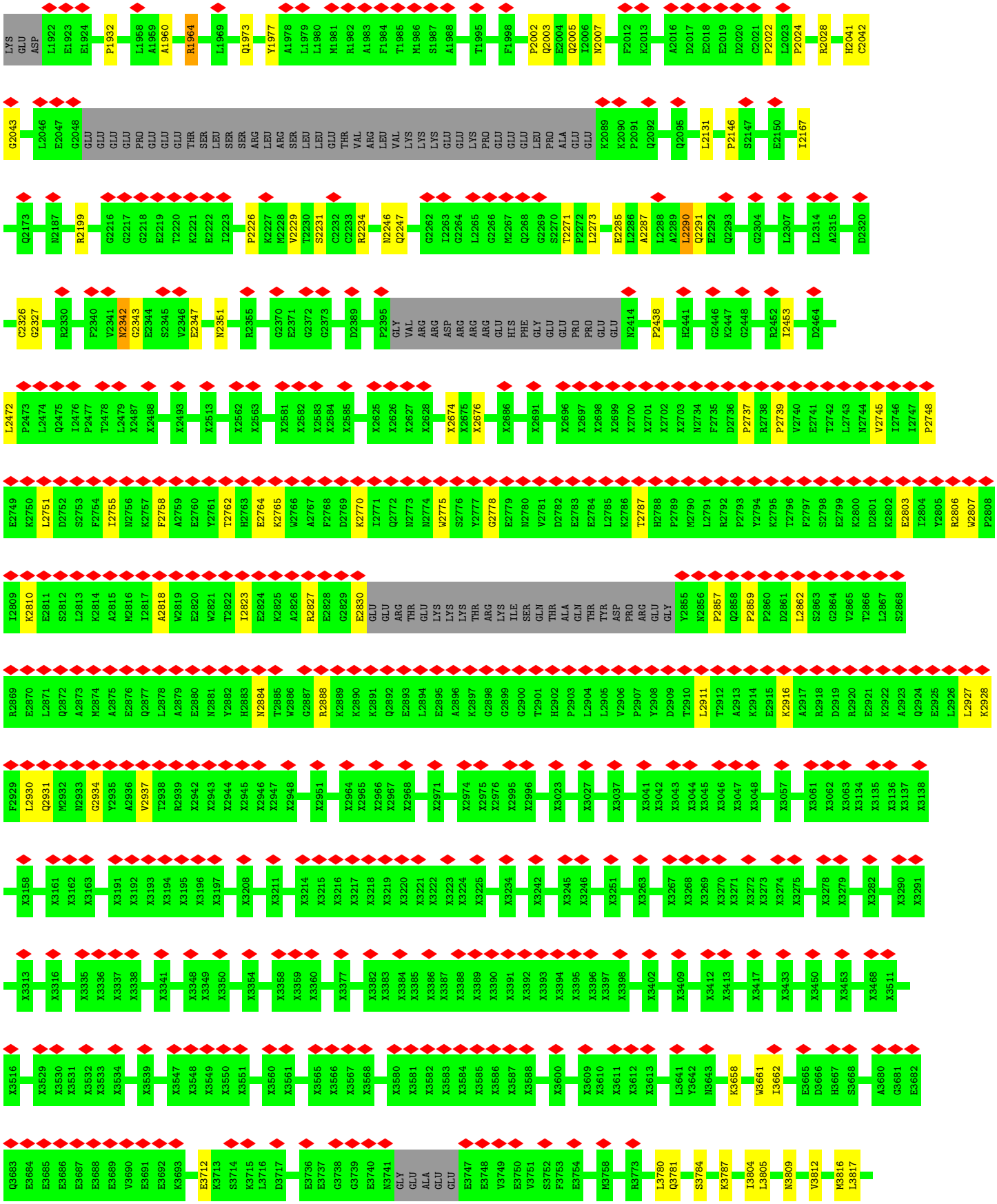
A980 Q981 R987 L988 A989 D999 Q1003 G1004 A1009 VAL GLN ASP ILE PRO ALA ARG ARG ASN PRO R1020 R1025 D1028 T1031 K1032 N1035 R1036 D1037 S1038 L1039 C1040 Q1041 A1042 V1043 R1044 T1045 L1046 L1047 G1048 Y1049 G1050 Y1051 N1052 I1053 E1054 PRO PRO ASP GLN GLU PRO SER GLN
VAL GLU ASN GLN SER ARG TRP D1070 R1076 K1079 V1095 E1099 M1100 R1101 V1102 G1103 P1107 E1108 L1109 R1110 P1111 D1112 L1120 V1123 F1124 N1125 G1126 H1127 R1131 R1141 P1142 W1143 G1146 D1147 V1148 V1149 G1150 E1167 S1171 D1172 S1173 G1174 S1175 A1178 F1179 R1180 E1181
V1199 D1207 R1212 I1216 C1217 E1221 A1227 M1230 Q1231 R1232 Q1244 G1262 T1263 V1264 D1265 X1278 X1441 X1450 X1475 X1516 X1519 X1520 X1521 X1522 X1523 X1524 X1525 X1526 X1529 X1532 X1543 X1544 X1545 X1546 X1547 X1548 L1600 W1605 V1615
GLU THR ARG ARG ALA GLY E1622 W1626 Q1629 C1630 Q1631 D1632 P1633 M1637 A1638 L1639 R1646 E1655 R1656 L1667 R1671 A1672 V1673 C1674 A1675 L1676 G1677 N1678 V1681 L1685 H1688 Q1691 L1694 L1698 E1699 D1700 A1701 L1707 R1708 A1709 G1710 Y1711 Y1712 D1713 I1718
H1719 L1720 E1721 R1725 R1728 S1729 M1730 E1733 L1738 E1741 T1742 R1743 A1744 F1748 P1749 P1750 G1751 R1752 K1753 G1754 G1755 N1756 A1757 R1758 R1759 H1760 G1764 V1765 G1766 V1767 R1772 H1776 A1785 L1786 P1787 A1788 ALA GLY VAL ALA E1793 A1794 P1795 A1796 R1797 I1802 L1812
G1816 D1828 P1840 T1847 V1859 K1860 Q1861 F1871 T1872 E1873 E1874 GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU ASP GLU GLU GLU LYS GLU GLU ASP GLU GLU GLU GLU GLU LYS GLU ASP ALA GLU LYS GLU GLU GLU GLU ALA PRO GLU GLY GLU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G2043 L2046 E2047 G2048 GLU GLU GLU PRO GLU GLU GLU THR SER LEU SER SER ARG LEU ARG SER LEU LEU GLU THR VAL ARG LEU VAL LYS LYS LYS GLU GLU LYS PRO GLU GLU GLU LEU PRO ALA GLU GLU K2089 K2090 P2091 Q2092 Q2095 L2131 P2146 S2147 E2150 I2167
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C2326 G2327 R2330 F2340 V2341 N2342 G2343 E2344 S2345 V2346 E2347 N2351 R2355 G2370 E2371 G2372 G2373 D2389 P2395 GLY VAL ARG ARG ASP ARG ARG ARG GLU HIS PHE GLY GLU GLU PRO PRO GLU GLU N2414 P2438 H2441 G2446 K2447 G2448 R2452 I2453 D2464
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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
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F2929 L2930 Q2931 M2932 N2933 G2934 Y2935 A2936 V2937 T2938 R2939 X2942 X2943 X2944 X2945 X2946 X2947 X2948 X2951 X2964 X2965 X2966 X2967 X2968 X2971 X2974 X2975 X2976 X2995 X2996 X3023 X3027 X3037 X3041 X3042 X3043 X3044 X3045 X3046 X3047 X3048 X3057 X3061 X3062 X3063 X3134 X3135 X3136 X3137 X3138
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X3516 X3529 X3530 X3531 X3532 X3533 X3534 X3539 X3547 X3548 X3549 X3550 X3551 X3560 X3561 X3565 X3566 X3567 X3568 X3580 X3581 X3582 X3583 X3584 X3585 X3586 X3587 X3588 X3600 X3609 X3610 X3611 X3612 X3613 L3641 Y3642 N3643 K3658 W3661 I3662 E3665 D3666 H3667 S3668 A3680 G3681 E3682
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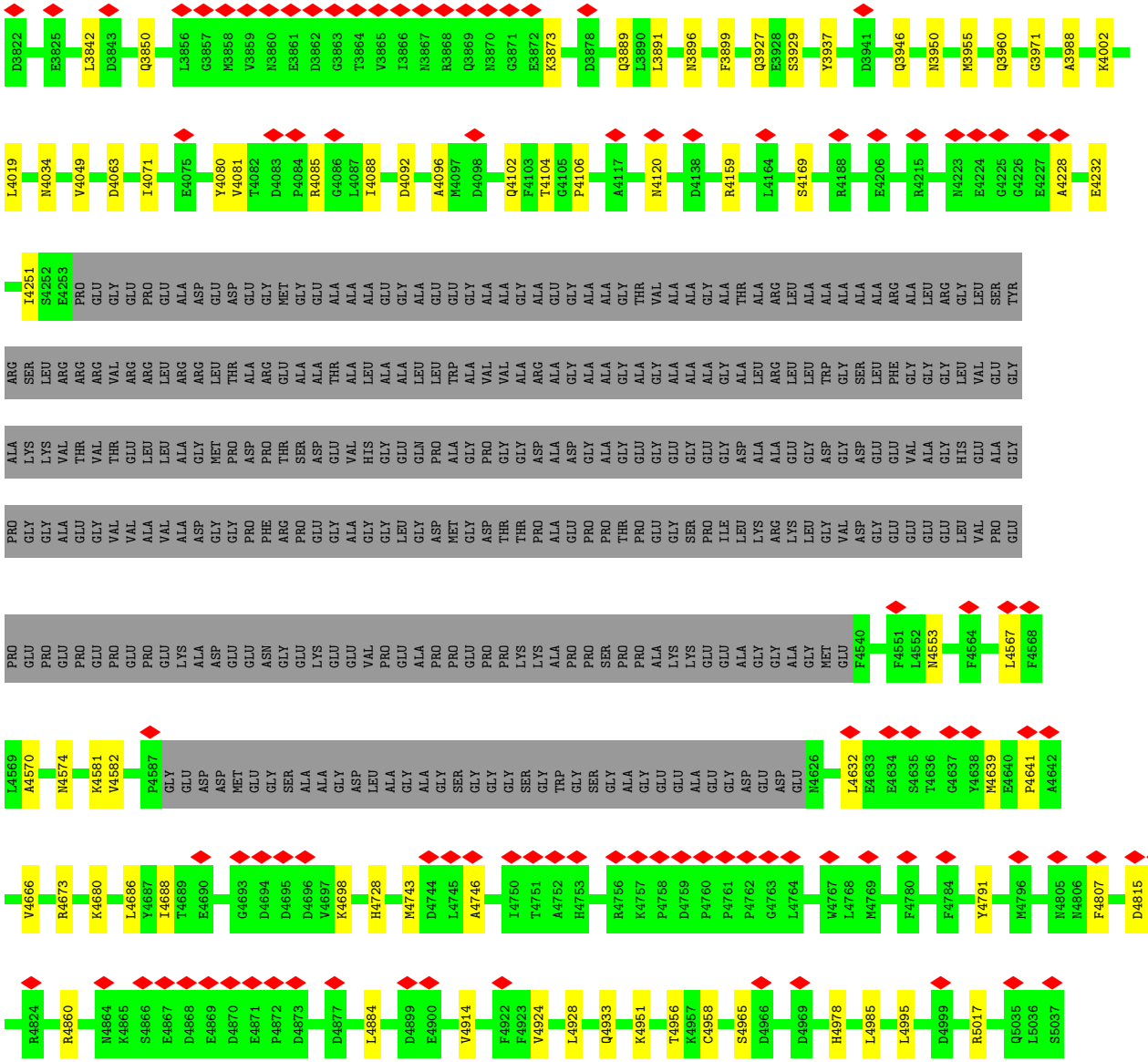
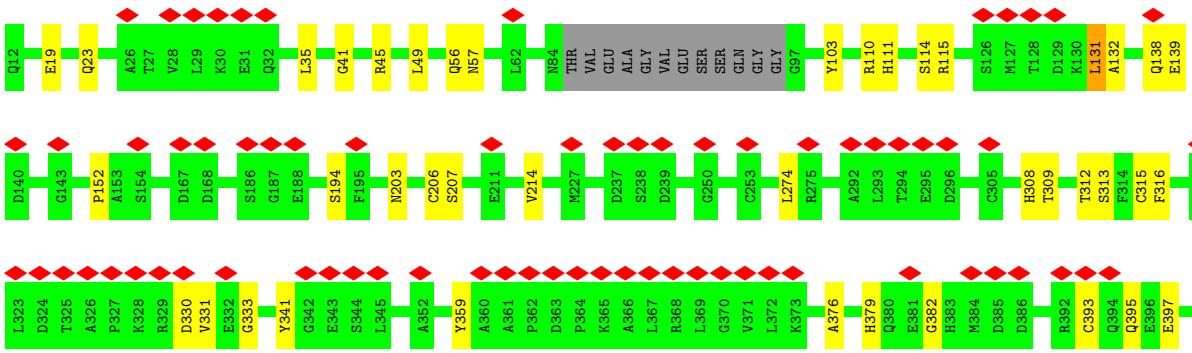
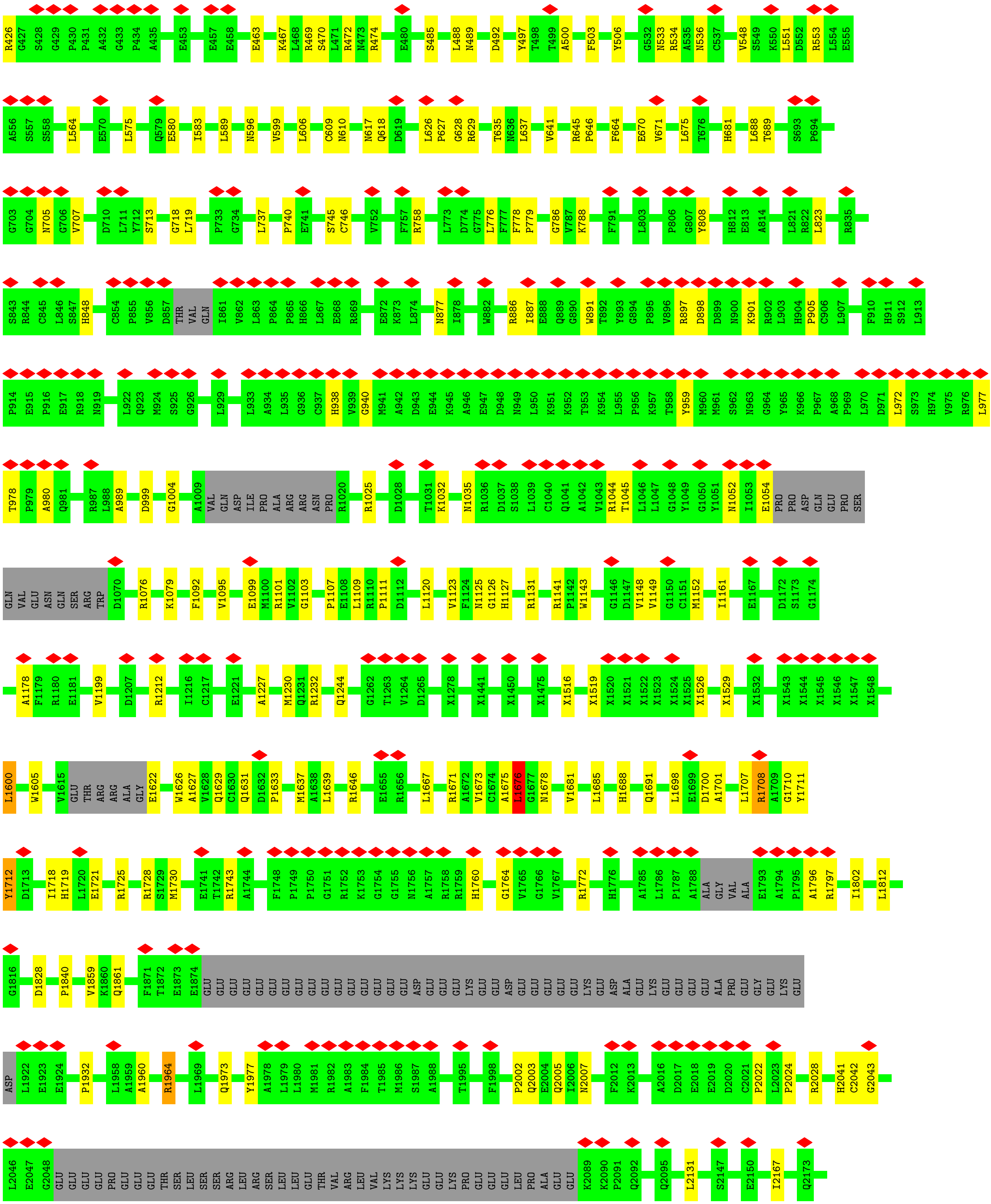


• Molecule 2: Ryanodine receptor 1

Chain E:

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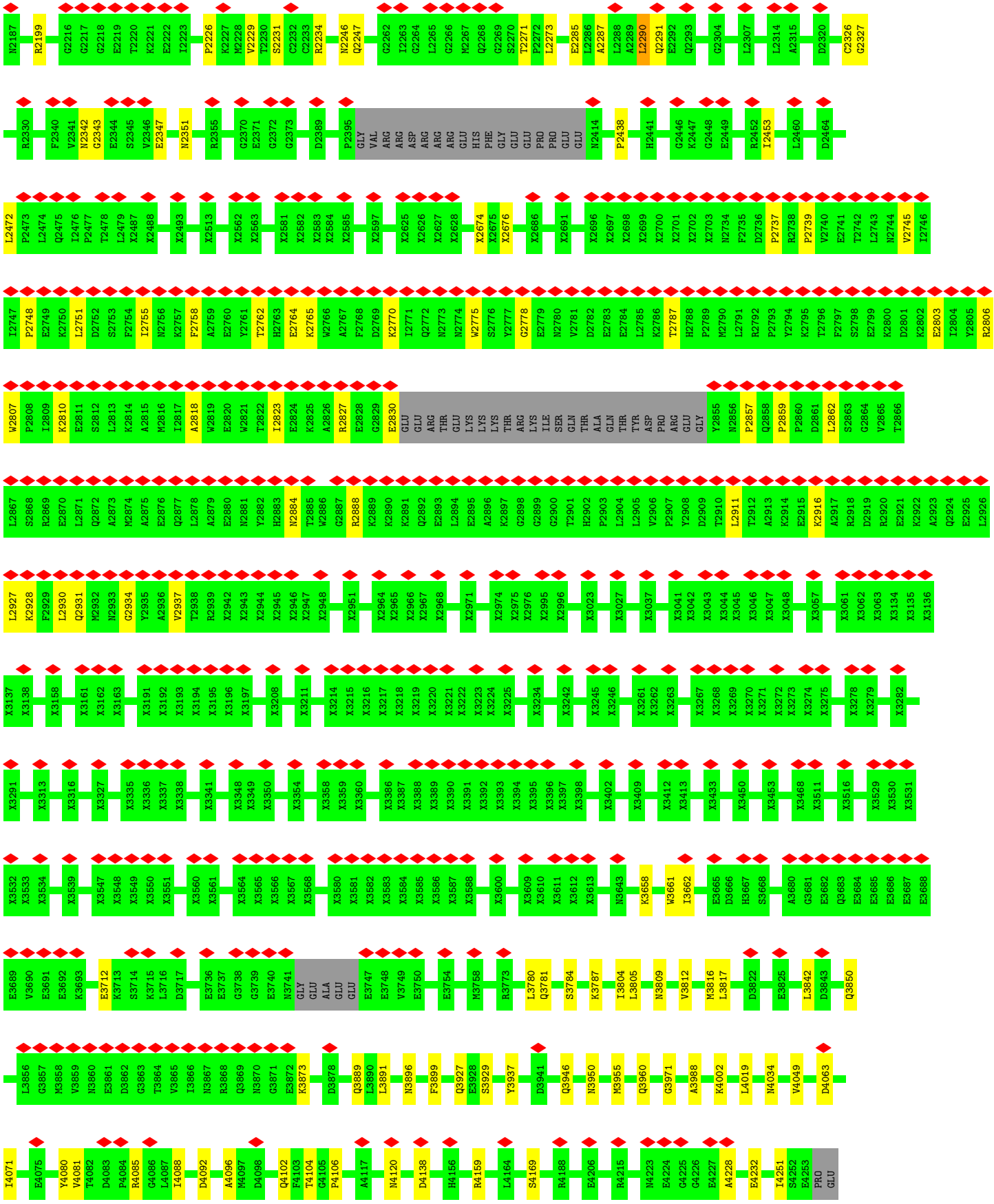
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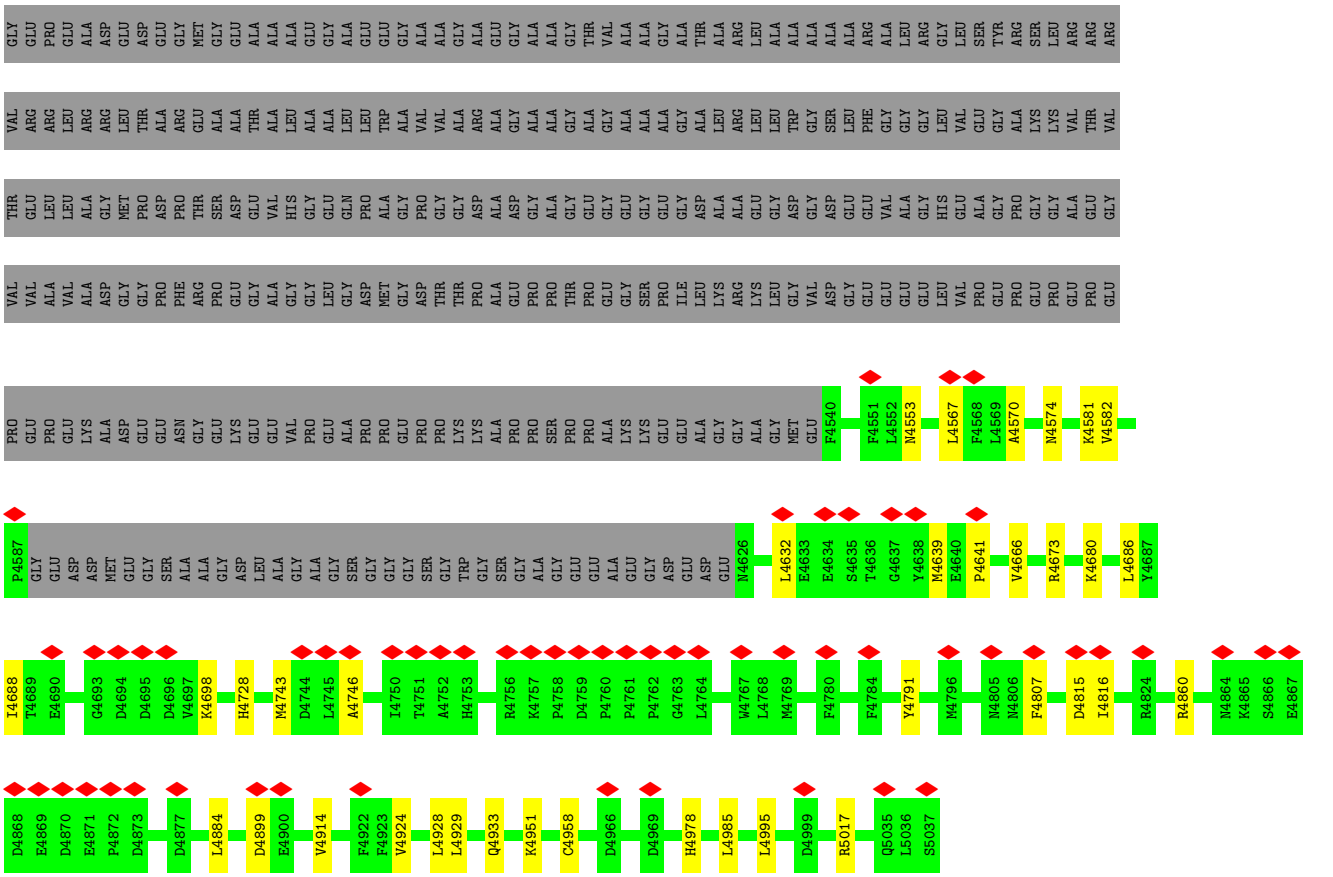
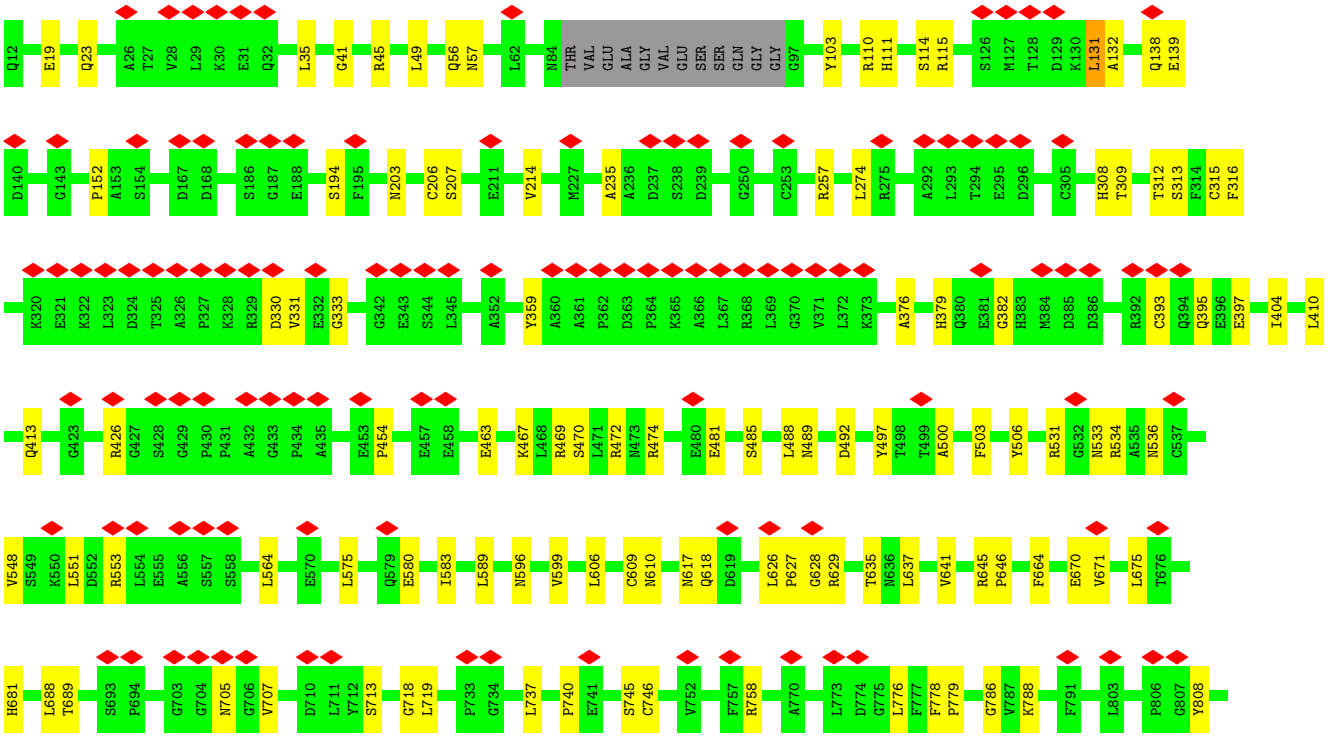
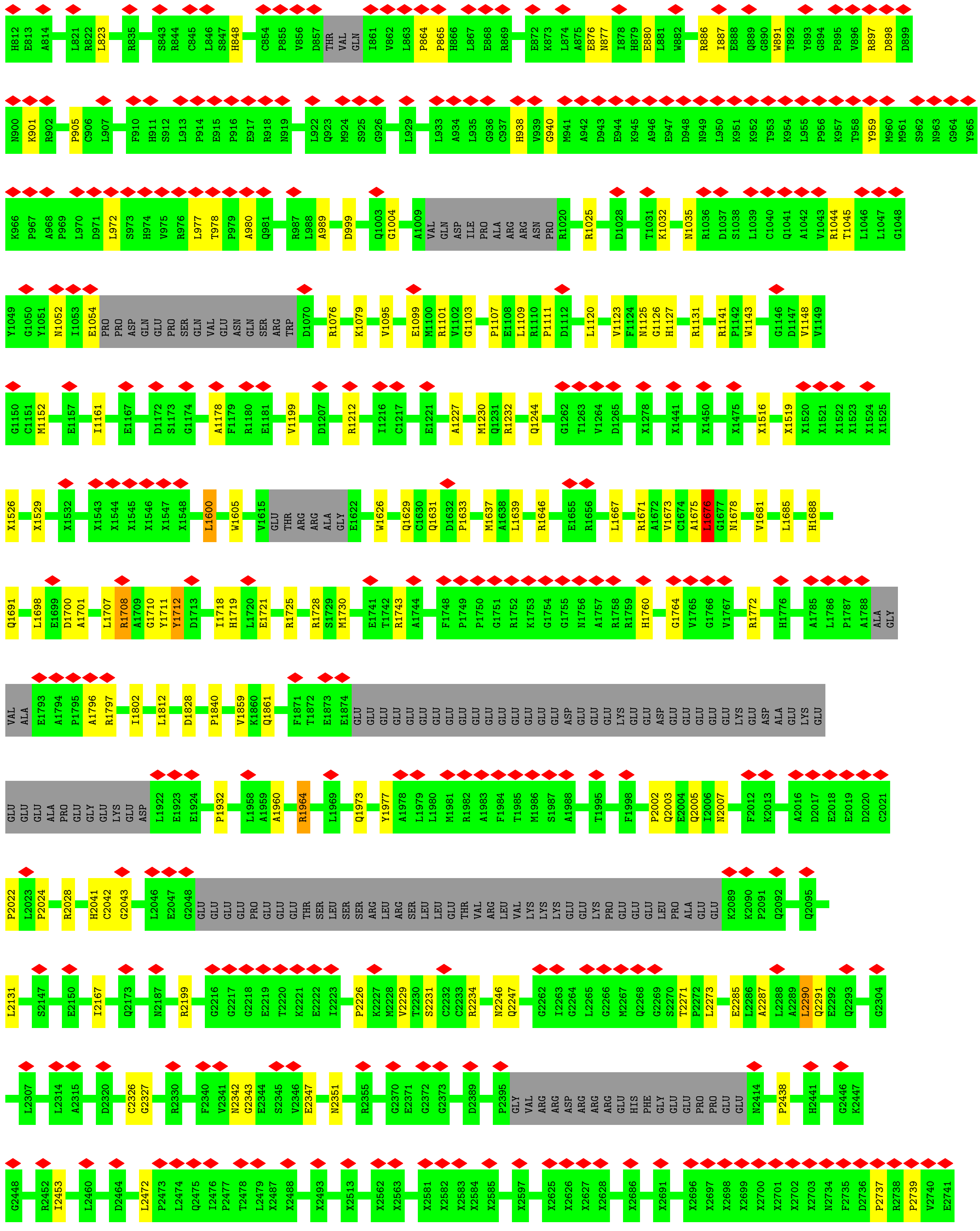


• Molecule 2: Ryanodine receptor 1

Chain I:

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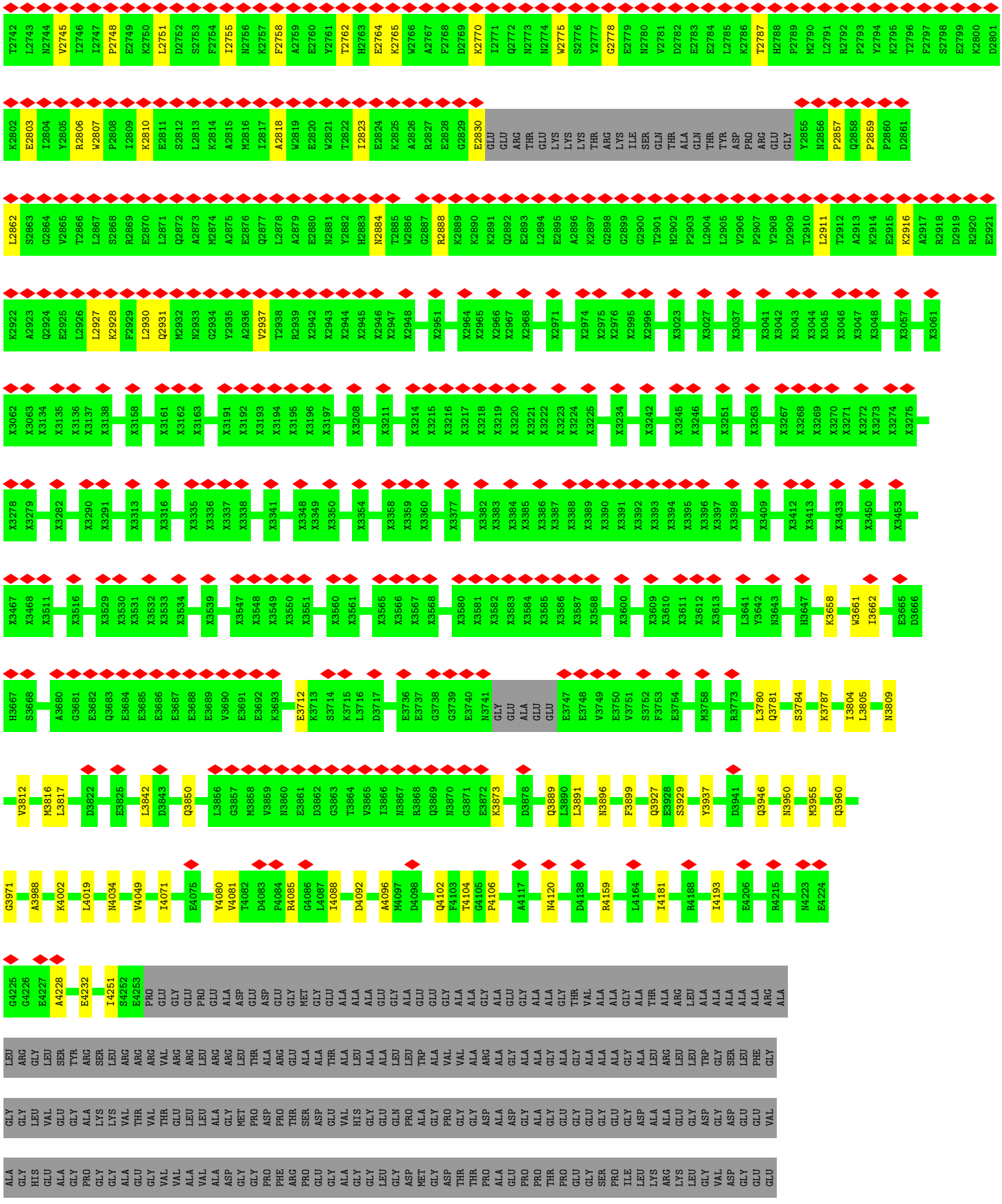
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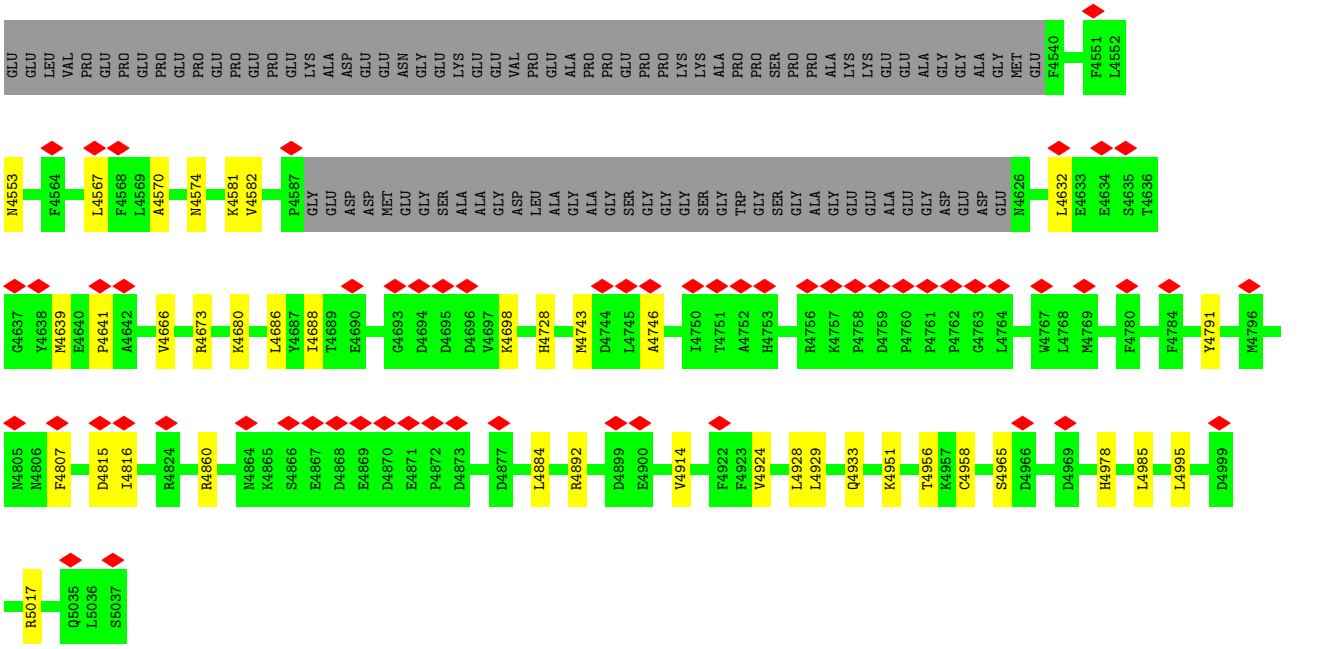
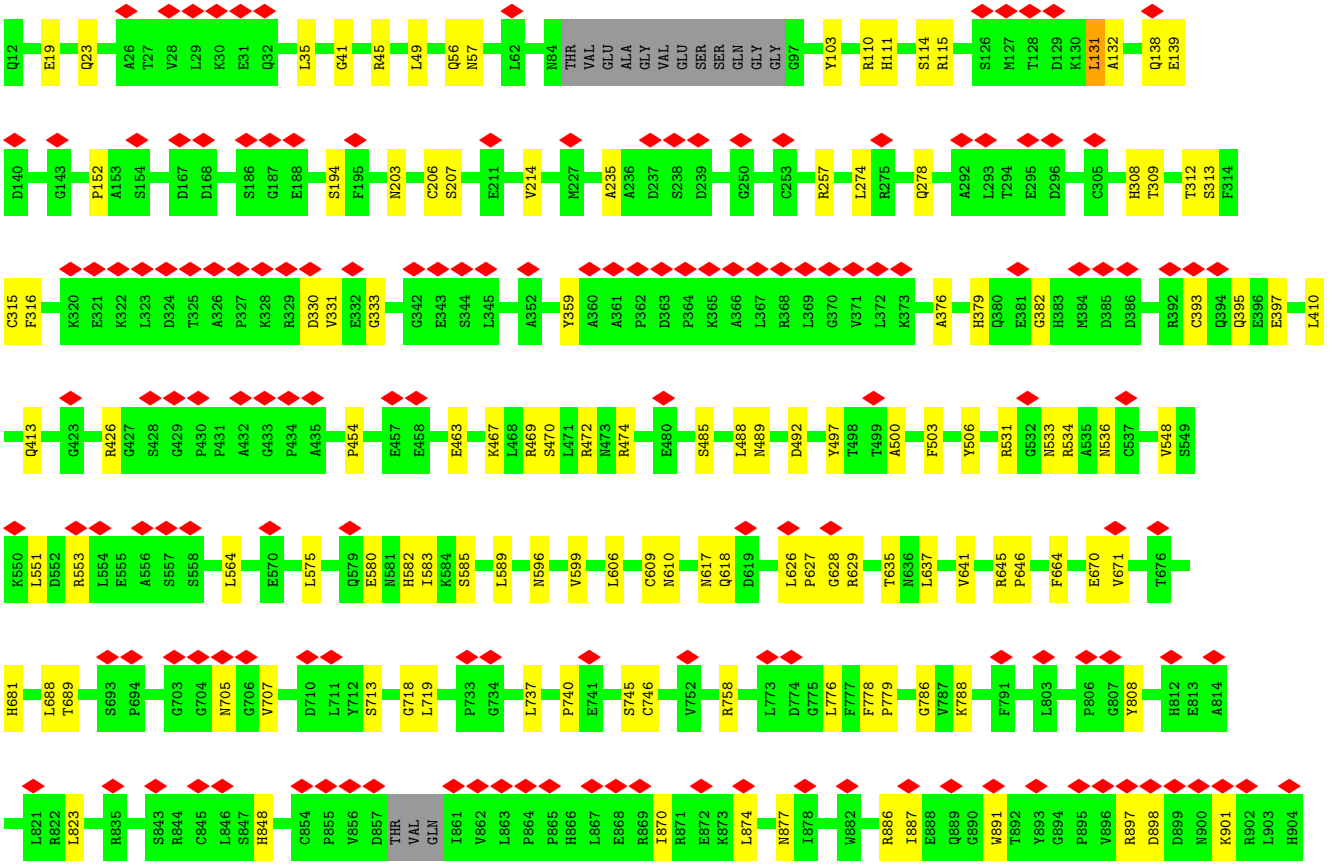
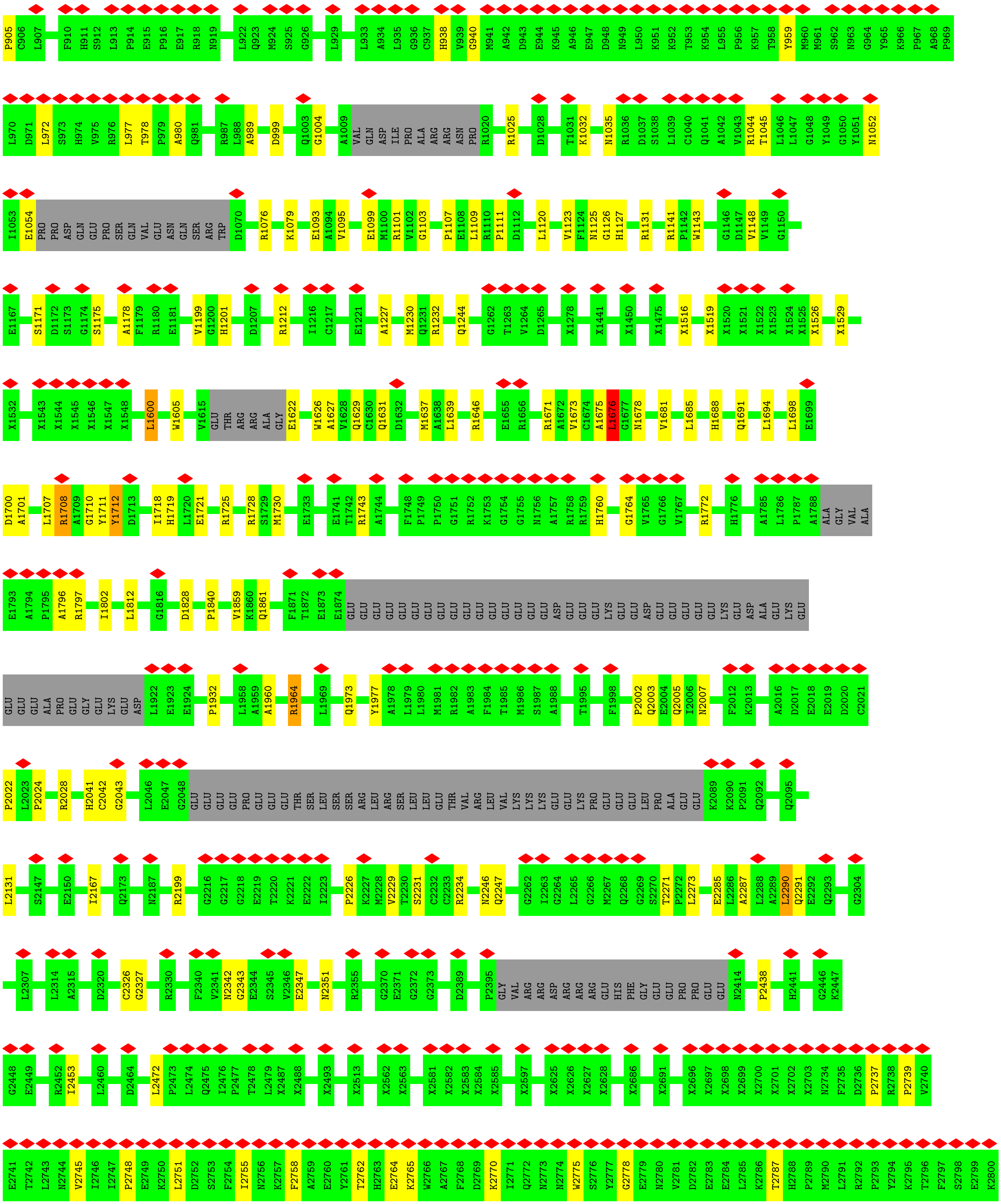


• Molecule 2: Ryanodine receptor 1

Chain G:

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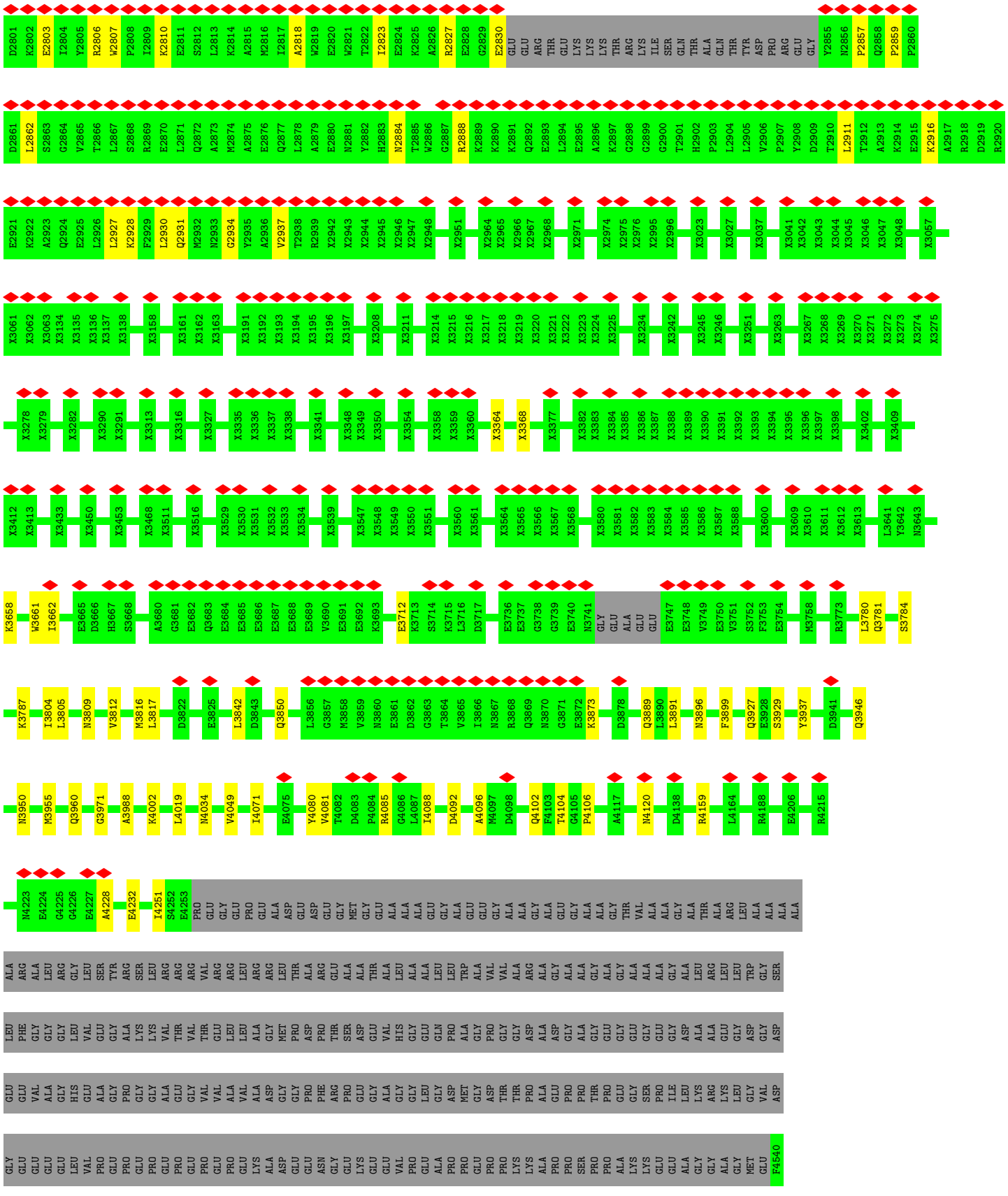
E2741 T2742 L2743 N2744 V2745 I2746 I2747 P2748 E2749 K2750 L2751 D2752 S2753 F2754 I2755 N2756 K2757 F2758 A2759 E2760 Y2761 T2762 H2763 E2764 K2765 W2766 A2767 F2768 D2769 K2770 I2771 Q2772 N2773 N2774 W2775 S2776 Y2777 G2778 E2779 N2780 V2781 D2782 E2783 E2784 L2785 K2786 T2787 H2788 P2789 M2790 L2791 R2792 P2793 Y2794 K2795 T2796 F2797 S2798 E2799 K2800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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 X2942 X2943 X2944 X2945 X2946 X2947 X2948 X2951 X2964 X2965 X2966 X2967 X2968 X2971 X2974 X2975 X2976 X2995 X2996 X3023 X3027 X3037 X3041 X3042 X3043 X3044 X3045 X3046 X3047 X3048 X3057
X3061 X3062 X3063 X3134 X3135 X3136 X3137 X3138 X3158 X3161 X3162 X3163 X3191 X3192 X3193 X3194 X3195 X3196 X3197 X3208 X3211 X3214 X3215 X3216 X3217 X3218 X3219 X3220 X3221 X3222 X3223 X3224 X3225 X3234 X3242 X3245 X3246 X3251 X3263 X3267 X3268 X3269 X3270 X3271 X3272 X3273 X3274 X3275
X3278 X3279 X3282 X3290 X3291 X3313 X3316 X3327 X3335 X3336 X3337 X3338 X3341 X3348 X3349 X3350 X3354 X3358 X3359 X3360 X3364 X3368 X3377 X3382 X3383 X3384 X3385 X3386 X3387 X3388 X3389 X3390 X3391 X3392 X3393 X3394 X3395 X3396 X3397 X3398 X3402 X3409
X3412 X3413 X3433 X3450 X3453 X3468 X3511 X3516 X3529 X3530 X3531 X3532 X3533 X3534 X3539 X3547 X3548 X3549 X3550 X3551 X3560 X3561 X3564 X3565 X3566 X3567 X3568 X3580 X3581 X3582 X3583 X3584 X3585 X3586 X3587 X3588 X3600 X3609 X3610 X3611 X3612 X3613 L3641 Y3642 N3643
K3658 W3661 I3662 E3665 D3666 H3667 S3668 A3680 G3681 E3682 Q3683 E3684 E3685 E3686 E3687 E3688 E3689 V3690 E3691 E3692 K3693 E3712 K3713 S3714 K3715 L3716 D3717 E3736 E3737 G3738 G3739 E3740 N3741 GLY GLU ALA GLU GLU E3747 E3748 V3749 E3750 V3751 S3752 F3753 E3754 M3758 R3773 L3780 Q3781 S3784
K3787 I3804 L3805 N3809 V3812 M3816 L3817 D3822 E3825 L3842 D3843 Q3850 L3856 G3857 M3858 V3859 N3860 E3861 D3862 G3863 T3864 V3865 I3866 N3867 R3868 Q3869 N3870 G3871 E3872 K3873 D3878 Q3889 L3890 L3891 N3896 F3899 Q3927 E3928 S3929 Y3937 D3941 Q3946
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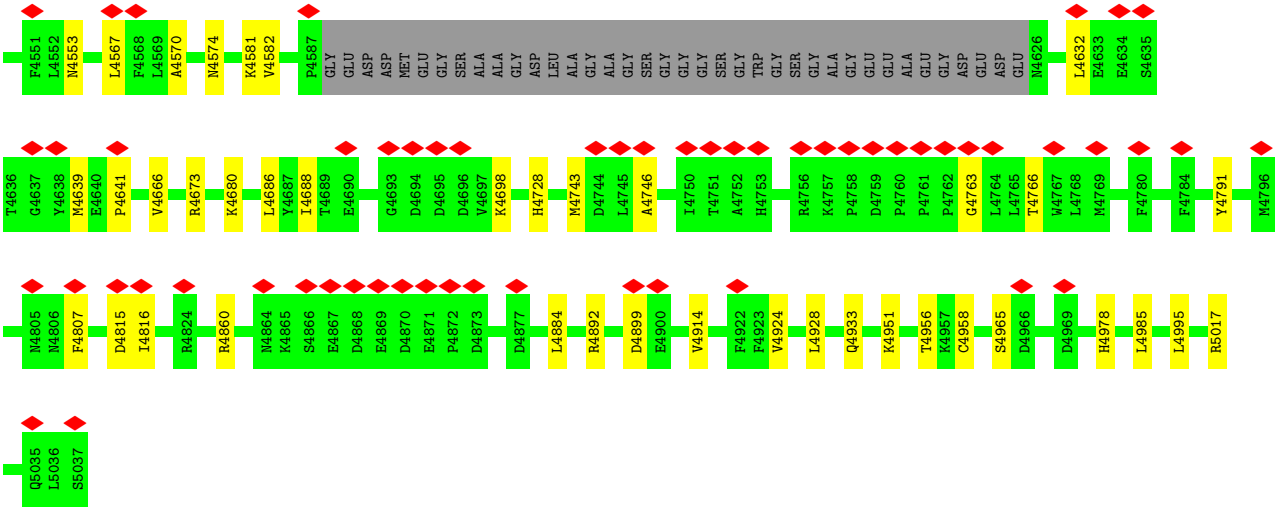
ALA ARG ALA LEU ARG GLY LEU SER TYR ARG SER LEU ARG ARG ARG VAL ARG ARG ARG LEU ALA ARG GLU ALA THR ALA LEU ALA ALA LEU LEU TRP ALA VAL VAL ALA ARG ALA GLY ALA ALA ALA GLY ALA GLY ALA ALA ALA GLY ALA LEU ARG LEU LEU LEU TRP GLY SER
LEU PHE GLY GLY GLY LEU VAL GLU GLY ALA LYS LYS VAL THR VAL THR GLU LEU 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 GLU PRO GLY GLY ASP GLY GLU GLY GLU GLY GLU GLY GLU GLY SER GLU GLY ASP ALA ALA GLU GLY GLY ASP
GLU GLU VAL ALA GLY HIS GLU ALA GLY PRO GLY GLY ALA GLU GLY VAL ALA VAL ALA ASP GLY PRO PHE ARG PRO GLU GLY ALA GLY GLY LEU GLY ASP THR THR PRO ALA GLU PRO PRO GLU GLY SER PRO ILE LEU LYS ARG LYS LEU GLY VAL ASP
GLY GLU GLU GLU LEU VAL PRO GLU PRO GLU PRO GLU PRO GLU PRO GLU PRO GLU LYS ALA ASP GLU GLU ASN GLY GLU LYS GLU GLU VAL PRO GLU ALA PRO PRO PRO LYS LYS ALA PRO PRO SER PRO PRO ALA LYS LYS GLU GLU ALA GLY GLY ALA GLY MET GLU F4540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N4574
K4581 V4582
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L4632 E4633 E4634 S4635
T4636 G4637 Y4638 M4639 E4640 P4641 V4666 R4673 K4680 L4686 Y4687 I4688 T4689 E4690 G4693 D4694 D4695 D4696 V4697 K4698 H4728 M4743 D4744 L4745 A4746 I4750 T4751 A4752 H4753 R4756 K4757 P4758 D4759 P4760 P4761 P4762 G4763 L4764 L4765 T4766 W4767 L4768 M4769 F4780 F4784 Y4791 M4796
N4805 N4806 F4807 D4815 I4816 R4824 R4860 N4864 K4865 S4866 E4867 D4868 E4869 D4870 E4871 P4872 D4873 D4877 L4884 R4892 D4899 E4900 V4914 F4922 F4923 V4924 L4928 Q4933 K4951 T4956 K4957 C4958 S4965 D4966 D4969 H4978 L4985 L4995 R5017
Q5035 L5036 S5037

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55564	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.175	Depositor
Minimum map value	-0.083	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	502.0, 502.0, 502.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.255, 1.255, 1.255	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.31	0/834	0.52	0/1123
1	F	0.31	0/834	0.52	0/1123
1	H	0.31	0/834	0.52	0/1123
1	J	0.31	0/834	0.52	0/1123
2	B	0.30	0/25428	0.55	8/34534 (0.0%)
2	E	0.30	0/25428	0.55	8/34534 (0.0%)
2	G	0.30	0/25428	0.55	8/34534 (0.0%)
2	I	0.30	0/25428	0.55	8/34534 (0.0%)
All	All	0.30	0/105048	0.55	32/142628 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	F	0	1
1	H	0	1
1	J	0	1
2	B	0	14
2	E	0	14
2	G	0	14
2	I	0	14
All	All	0	60

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	131	LEU	CA-CB-CG	8.47	134.78	115.30
2	B	131	LEU	CA-CB-CG	8.46	134.76	115.30
2	E	131	LEU	CA-CB-CG	8.46	134.76	115.30
2	I	131	LEU	CA-CB-CG	8.46	134.75	115.30
2	B	1600	LEU	CA-CB-CG	7.43	132.39	115.30
2	G	1600	LEU	CA-CB-CG	7.41	132.35	115.30
2	I	1600	LEU	CA-CB-CG	7.40	132.33	115.30
2	E	1600	LEU	CA-CB-CG	7.38	132.28	115.30
2	I	1676	LEU	CA-CB-CG	6.69	130.69	115.30
2	B	1676	LEU	CA-CB-CG	6.69	130.69	115.30
2	G	1676	LEU	CA-CB-CG	6.69	130.69	115.30
2	E	1676	LEU	CA-CB-CG	6.69	130.68	115.30
2	E	2290	LEU	CA-CB-CG	6.32	129.83	115.30
2	G	2290	LEU	CA-CB-CG	6.32	129.83	115.30
2	B	2290	LEU	CA-CB-CG	6.31	129.81	115.30
2	I	2290	LEU	CA-CB-CG	6.30	129.79	115.30
2	E	977	LEU	CA-CB-CG	5.43	127.80	115.30
2	I	977	LEU	CA-CB-CG	5.41	127.75	115.30
2	B	977	LEU	CA-CB-CG	5.41	127.75	115.30
2	G	977	LEU	CA-CB-CG	5.40	127.72	115.30
2	B	4985	LEU	CA-CB-CG	5.30	127.50	115.30
2	I	4985	LEU	CA-CB-CG	5.30	127.50	115.30
2	G	4985	LEU	CA-CB-CG	5.29	127.46	115.30
2	E	4985	LEU	CA-CB-CG	5.29	127.46	115.30
2	B	4639	MET	C-N-CA	5.28	134.91	121.70
2	I	4639	MET	C-N-CA	5.28	134.89	121.70
2	E	4639	MET	C-N-CA	5.27	134.87	121.70
2	G	4639	MET	C-N-CA	5.25	134.83	121.70
2	I	688	LEU	CA-CB-CG	5.19	127.23	115.30
2	B	688	LEU	CA-CB-CG	5.18	127.21	115.30
2	G	688	LEU	CA-CB-CG	5.17	127.20	115.30
2	E	688	LEU	CA-CB-CG	5.17	127.18	115.30

There are no chirality outliers.

All (60) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	8	SER	Peptide
2	B	139	GLU	Peptide
2	B	1676	LEU	Peptide
2	B	1712	TYR	Peptide
2	B	1828	ASP	Peptide
2	B	2291	GLN	Peptide

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Mol	Chain	Res	Type	Group
2	B	2342	ASN	Peptide
2	B	2343	GLY	Peptide
2	B	2472	LEU	Peptide
2	B	2807	TRP	Peptide
2	B	312	THR	Peptide
2	B	3971	GLY	Peptide
2	B	4666	VAL	Peptide
2	B	4807	PHE	Peptide
2	B	808	TYR	Peptide
2	E	139	GLU	Peptide
2	E	1676	LEU	Peptide
2	E	1712	TYR	Peptide
2	E	1828	ASP	Peptide
2	E	2291	GLN	Peptide
2	E	2342	ASN	Peptide
2	E	2343	GLY	Peptide
2	E	2472	LEU	Peptide
2	E	2807	TRP	Peptide
2	E	312	THR	Peptide
2	E	3971	GLY	Peptide
2	E	4666	VAL	Peptide
2	E	4807	PHE	Peptide
2	E	808	TYR	Peptide
1	F	8	SER	Peptide
2	G	139	GLU	Peptide
2	G	1676	LEU	Peptide
2	G	1712	TYR	Peptide
2	G	1828	ASP	Peptide
2	G	2291	GLN	Peptide
2	G	2342	ASN	Peptide
2	G	2343	GLY	Peptide
2	G	2472	LEU	Peptide
2	G	2807	TRP	Peptide
2	G	312	THR	Peptide
2	G	3971	GLY	Peptide
2	G	4666	VAL	Peptide
2	G	4807	PHE	Peptide
2	G	808	TYR	Peptide
1	H	8	SER	Peptide
2	I	139	GLU	Peptide
2	I	1676	LEU	Peptide
2	I	1712	TYR	Peptide

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Mol	Chain	Res	Type	Group
2	I	1828	ASP	Peptide
2	I	2291	GLN	Peptide
2	I	2342	ASN	Peptide
2	I	2343	GLY	Peptide
2	I	2472	LEU	Peptide
2	I	2807	TRP	Peptide
2	I	312	THR	Peptide
2	I	3971	GLY	Peptide
2	I	4666	VAL	Peptide
2	I	4807	PHE	Peptide
2	I	808	TYR	Peptide
1	J	8	SER	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	818	0	824	6	0
1	F	818	0	824	7	0
1	H	818	0	824	7	0
1	J	818	0	824	6	0
2	B	29369	0	24721	194	0
2	E	29369	0	24721	194	0
2	G	29369	0	24721	197	0
2	I	29369	0	24721	192	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
All	All	120756	0	102180	783	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 4.

All (783) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4958:CYS:SG	2:E:4978:HIS:CD2	2.72	0.83
2:G:4958:CYS:SG	2:G:4978:HIS:CD2	2.72	0.83
2:I:4958:CYS:SG	2:I:4978:HIS:CD2	2.72	0.82
2:B:4958:CYS:SG	2:B:4978:HIS:CD2	2.72	0.82
1:J:42:ARG:HG2	2:I:1691:GLN:HG2	1.72	0.70
2:E:379:HIS:HD2	2:E:382:GLY:H	1.42	0.68
2:B:379:HIS:HD2	2:B:382:GLY:H	1.42	0.68
2:G:379:HIS:HD2	2:G:382:GLY:H	1.42	0.67
2:I:646:PRO:HD2	2:I:779:PRO:HB2	1.77	0.67
2:I:379:HIS:HD2	2:I:382:GLY:H	1.42	0.66
2:E:646:PRO:HD2	2:E:779:PRO:HB2	1.77	0.66
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.77	0.66
2:I:1721:GLU:OE2	2:I:1725:ARG:NH2	2.29	0.65
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.77	0.65
2:B:1721:GLU:OE2	2:B:1725:ARG:NH2	2.29	0.64
2:G:664:PHE:HB2	2:G:746:CYS:HB2	1.79	0.64
2:B:2755:ILE:HD13	2:B:2810:LYS:HG2	1.80	0.64
2:I:664:PHE:HB2	2:I:746:CYS:HB2	1.79	0.64
2:I:2755:ILE:HD13	2:I:2810:LYS:HG2	1.80	0.64
2:E:2755:ILE:HD13	2:E:2810:LYS:HG2	1.80	0.64
2:E:664:PHE:HB2	2:E:746:CYS:HB2	1.79	0.64
2:G:2755:ILE:HD13	2:G:2810:LYS:HG2	1.80	0.63
2:G:1721:GLU:OE2	2:G:1725:ARG:NH2	2.29	0.63
2:B:664:PHE:HB2	2:B:746:CYS:HB2	1.79	0.62
2:I:641:VAL:HG21	2:I:705:ASN:HA	1.82	0.62
2:B:641:VAL:HG21	2:B:705:ASN:HA	1.81	0.62
2:E:1721:GLU:OE2	2:E:1725:ARG:NH2	2.29	0.62
2:G:641:VAL:HG21	2:G:705:ASN:HA	1.81	0.61
2:E:331:VAL:HG12	2:E:333:GLY:H	1.65	0.61
2:E:641:VAL:HG21	2:E:705:ASN:HA	1.82	0.60
2:B:1519:UNK:HA	2:B:1526:UNK:HA	1.83	0.60
2:G:331:VAL:HG12	2:G:333:GLY:H	1.65	0.60
2:E:1519:UNK:HA	2:E:1526:UNK:HA	1.83	0.60
2:B:331:VAL:HG12	2:B:333:GLY:H	1.65	0.60
2:I:331:VAL:HG12	2:I:333:GLY:H	1.65	0.60
2:G:1519:UNK:HA	2:G:1526:UNK:HA	1.83	0.59
2:E:1079:LYS:NZ	2:E:1107:PRO:O	2.36	0.59
2:G:2739:PRO:HB3	2:G:2884:ASN:HB3	1.85	0.59
2:E:4673:ARG:HH22	2:E:4698:LYS:HB2	1.68	0.59
2:G:1079:LYS:NZ	2:G:1107:PRO:O	2.36	0.59
2:E:4924:VAL:HA	2:E:4928:LEU:HB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2739:PRO:HB3	2:I:2884:ASN:HB3	1.85	0.59
2:B:1079:LYS:NZ	2:B:1107:PRO:O	2.36	0.59
2:B:4924:VAL:HA	2:B:4928:LEU:HB2	1.85	0.59
2:I:1519:UNK:HA	2:I:1526:UNK:HA	1.83	0.59
2:I:4673:ARG:HH22	2:I:4698:LYS:HB2	1.68	0.59
2:B:4673:ARG:HH22	2:B:4698:LYS:HB2	1.68	0.58
2:G:1671:ARG:NH2	2:G:1710:GLY:O	2.36	0.58
2:G:4673:ARG:HH22	2:G:4698:LYS:HB2	1.68	0.58
2:E:2739:PRO:HB3	2:E:2884:ASN:HB3	1.85	0.58
2:B:2739:PRO:HB3	2:B:2884:ASN:HB3	1.85	0.58
2:E:57:ASN:HD22	2:E:308:HIS:HB2	1.68	0.58
2:I:1671:ARG:NH2	2:I:1710:GLY:O	2.36	0.58
2:G:4924:VAL:HA	2:G:4928:LEU:HB2	1.85	0.58
2:E:1671:ARG:NH2	2:E:1710:GLY:O	2.37	0.58
2:I:57:ASN:HD22	2:I:308:HIS:HB2	1.68	0.58
2:I:1079:LYS:NZ	2:I:1107:PRO:O	2.36	0.58
2:G:609:CYS:SG	2:G:610:ASN:N	2.77	0.58
2:B:1671:ARG:NH2	2:B:1710:GLY:O	2.36	0.58
2:I:4924:VAL:HA	2:I:4928:LEU:HB2	1.85	0.58
2:B:609:CYS:SG	2:B:610:ASN:N	2.77	0.58
2:B:4104:THR:HG22	2:B:4106:PRO:HD2	1.87	0.57
2:E:2764:GLU:HG3	2:E:2857:PRO:HB2	1.86	0.57
2:I:3946:GLN:OE1	2:I:3950:ASN:ND2	2.37	0.57
2:E:4104:THR:HG22	2:E:4106:PRO:HD2	1.87	0.57
2:B:3946:GLN:OE1	2:B:3950:ASN:ND2	2.37	0.57
2:B:57:ASN:HD22	2:B:308:HIS:HB2	1.68	0.57
2:B:2764:GLU:HG3	2:B:2857:PRO:HB2	1.86	0.57
2:E:3946:GLN:OE1	2:E:3950:ASN:ND2	2.37	0.57
2:I:609:CYS:SG	2:I:610:ASN:N	2.77	0.57
2:E:609:CYS:SG	2:E:610:ASN:N	2.77	0.57
2:I:4933:GLN:NE2	2:G:4933:GLN:OE1	2.38	0.57
2:G:2287:ALA:HA	2:G:2290:LEU:HD13	1.87	0.57
2:B:2131:LEU:HB3	2:B:3662:ILE:HD13	1.87	0.57
2:I:2131:LEU:HB3	2:I:3662:ILE:HD13	1.87	0.56
2:G:110:ARG:HH21	2:G:115:ARG:HB3	1.70	0.56
2:G:4104:THR:HG22	2:G:4106:PRO:HD2	1.86	0.56
2:I:2287:ALA:HA	2:I:2290:LEU:HD13	1.87	0.56
2:I:2764:GLU:HG3	2:I:2857:PRO:HB2	1.86	0.56
2:G:3946:GLN:OE1	2:G:3950:ASN:ND2	2.37	0.56
2:G:2764:GLU:HG3	2:G:2857:PRO:HB2	1.86	0.56
2:B:4933:GLN:NE2	2:I:4933:GLN:OE1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:718:GLY:HA3	2:I:737:LEU:HA	1.87	0.56
2:G:1730:MET:O	2:G:1772:ARG:NH1	2.39	0.56
2:B:110:ARG:HH21	2:B:115:ARG:HB3	1.70	0.56
2:B:745:SER:HB2	2:B:758:ARG:HB3	1.88	0.56
2:E:4933:GLN:OE1	2:G:4933:GLN:NE2	2.38	0.56
2:I:618:GLN:OE1	2:I:1678:ASN:ND2	2.39	0.56
2:I:4104:THR:HG22	2:I:4106:PRO:HD2	1.87	0.56
2:G:57:ASN:HD22	2:G:308:HIS:HB2	1.68	0.56
2:B:2287:ALA:HA	2:B:2290:LEU:HD13	1.87	0.56
2:E:4049:VAL:HG21	2:E:4159:ARG:HD2	1.88	0.56
2:B:718:GLY:HA3	2:B:737:LEU:HA	1.87	0.56
2:E:110:ARG:HH21	2:E:115:ARG:HB3	1.70	0.56
2:I:745:SER:HB2	2:I:758:ARG:HB3	1.88	0.56
2:G:745:SER:HB2	2:G:758:ARG:HB3	1.88	0.56
2:B:4049:VAL:HG21	2:B:4159:ARG:HD2	1.88	0.56
2:G:2131:LEU:HB3	2:G:3662:ILE:HD13	1.87	0.56
2:G:4049:VAL:HG21	2:G:4159:ARG:HD2	1.88	0.56
2:E:745:SER:HB2	2:E:758:ARG:HB3	1.88	0.55
2:E:2131:LEU:HB3	2:E:3662:ILE:HD13	1.87	0.55
1:F:23:VAL:HG22	1:F:47:LYS:HG2	1.89	0.55
1:A:23:VAL:HG22	1:A:47:LYS:HG2	1.89	0.55
1:J:23:VAL:HG22	1:J:47:LYS:HG2	1.89	0.55
2:I:1743:ARG:O	2:I:1964:ARG:NH2	2.39	0.55
2:E:618:GLN:OE1	2:E:1678:ASN:ND2	2.39	0.55
2:E:718:GLY:HA3	2:E:737:LEU:HA	1.87	0.55
2:I:4049:VAL:HG21	2:I:4159:ARG:HD2	1.88	0.55
2:E:2287:ALA:HA	2:E:2290:LEU:HD13	1.87	0.55
2:I:110:ARG:HH21	2:I:115:ARG:HB3	1.70	0.55
2:B:2803:GLU:OE2	2:B:2806:ARG:NH1	2.40	0.55
2:B:618:GLN:OE1	2:B:1678:ASN:ND2	2.39	0.55
2:E:1730:MET:O	2:E:1772:ARG:NH1	2.39	0.55
2:E:1743:ARG:O	2:E:1964:ARG:NH2	2.39	0.55
1:H:23:VAL:HG22	1:H:47:LYS:HG2	1.89	0.55
2:B:1109:LEU:HA	2:B:1120:LEU:HD21	1.89	0.55
2:E:1109:LEU:HA	2:E:1120:LEU:HD21	1.89	0.55
2:E:2042:CYS:SG	2:E:2043:GLY:N	2.79	0.55
2:G:2803:GLU:OE2	2:G:2806:ARG:NH1	2.40	0.55
2:E:2803:GLU:OE2	2:E:2806:ARG:NH1	2.40	0.55
2:I:426:ARG:HB2	2:I:506:TYR:HA	1.89	0.55
2:G:618:GLN:OE1	2:G:1678:ASN:ND2	2.39	0.55
2:G:718:GLY:HA3	2:G:737:LEU:HA	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3937:TYR:O	2:B:4002:LYS:NZ	2.38	0.55
2:I:670:GLU:HG3	2:I:788:LYS:H	1.72	0.55
2:B:2131:LEU:HD23	2:B:3662:ILE:HB	1.90	0.54
2:I:1730:MET:O	2:I:1772:ARG:NH1	2.39	0.54
2:I:2042:CYS:SG	2:I:2043:GLY:N	2.79	0.54
2:G:1109:LEU:HA	2:G:1120:LEU:HD21	1.89	0.54
2:B:1743:ARG:O	2:B:1964:ARG:NH2	2.39	0.54
2:E:111:HIS:HD2	2:E:114:SER:H	1.55	0.54
2:G:426:ARG:HB2	2:G:506:TYR:HA	1.89	0.54
2:G:575:LEU:HD22	2:G:609:CYS:HB3	1.89	0.54
2:E:670:GLU:HG3	2:E:788:LYS:H	1.72	0.54
2:E:2131:LEU:HD23	2:E:3662:ILE:HB	1.90	0.54
2:I:2803:GLU:OE2	2:I:2806:ARG:NH1	2.40	0.54
2:B:635:THR:HB	2:B:1639:LEU:HD23	1.90	0.54
2:B:1730:MET:O	2:B:1772:ARG:NH1	2.39	0.54
2:I:575:LEU:HD22	2:I:609:CYS:HB3	1.89	0.54
2:G:111:HIS:HD2	2:G:114:SER:H	1.55	0.54
2:B:500:ALA:H	2:B:503:PHE:HB3	1.73	0.54
2:E:426:ARG:HB2	2:E:506:TYR:HA	1.89	0.54
2:I:1109:LEU:HA	2:I:1120:LEU:HD21	1.89	0.54
2:G:635:THR:HB	2:G:1639:LEU:HD23	1.90	0.54
2:E:627:PRO:O	2:E:629:ARG:NH1	2.41	0.54
2:G:23:GLN:OE1	2:G:203:ASN:ND2	2.41	0.54
2:G:500:ALA:H	2:G:503:PHE:HB3	1.73	0.54
2:B:23:GLN:OE1	2:B:203:ASN:ND2	2.41	0.54
2:B:111:HIS:HD2	2:B:114:SER:H	1.55	0.54
2:I:2131:LEU:HD23	2:I:3662:ILE:HB	1.90	0.54
2:G:2131:LEU:HD23	2:G:3662:ILE:HB	1.90	0.54
2:B:2042:CYS:SG	2:B:2043:GLY:N	2.79	0.54
2:E:635:THR:HB	2:E:1639:LEU:HD23	1.90	0.54
2:E:3937:TYR:O	2:E:4002:LYS:NZ	2.38	0.54
2:I:500:ALA:H	2:I:503:PHE:HB3	1.73	0.54
2:G:670:GLU:HG3	2:G:788:LYS:H	1.72	0.54
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.38	0.54
2:B:426:ARG:HB2	2:B:506:TYR:HA	1.89	0.53
2:B:2326:CYS:SG	2:B:2327:GLY:N	2.81	0.53
2:E:469:ARG:HH21	2:E:3712:GLU:HB3	1.73	0.53
2:E:4581:LYS:HD2	2:E:4632:LEU:HD22	1.90	0.53
2:I:4581:LYS:HD2	2:I:4632:LEU:HD22	1.90	0.53
2:E:2326:CYS:SG	2:E:2327:GLY:N	2.81	0.53
2:I:627:PRO:O	2:I:629:ARG:NH1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2042:CYS:SG	2:G:2043:GLY:N	2.79	0.53
2:B:627:PRO:O	2:B:629:ARG:NH1	2.41	0.53
2:E:500:ALA:H	2:E:503:PHE:HB3	1.73	0.53
2:I:2326:CYS:SG	2:I:2327:GLY:N	2.81	0.53
1:A:74:LEU:HB2	1:A:99:PHE:HB2	1.90	0.53
2:B:469:ARG:HH21	2:B:3712:GLU:HB3	1.74	0.53
2:E:23:GLN:OE1	2:E:203:ASN:ND2	2.41	0.53
2:E:575:LEU:HD22	2:E:609:CYS:HB3	1.89	0.53
2:I:635:THR:HB	2:I:1639:LEU:HD23	1.90	0.53
2:G:2326:CYS:SG	2:G:2327:GLY:N	2.81	0.53
2:B:989:ALA:O	2:B:1035:ASN:ND2	2.42	0.53
1:F:74:LEU:HB2	1:F:99:PHE:HB2	1.90	0.53
2:B:670:GLU:HG3	2:B:788:LYS:H	1.72	0.53
2:I:469:ARG:HH21	2:I:3712:GLU:HB3	1.74	0.53
2:G:627:PRO:O	2:G:629:ARG:NH1	2.41	0.53
2:I:23:GLN:OE1	2:I:203:ASN:ND2	2.41	0.53
2:G:1743:ARG:O	2:G:1964:ARG:NH2	2.39	0.53
1:J:74:LEU:HB2	1:J:99:PHE:HB2	1.90	0.53
2:B:575:LEU:HD22	2:B:609:CYS:HB3	1.89	0.53
2:E:989:ALA:O	2:E:1035:ASN:ND2	2.42	0.53
2:I:111:HIS:HD2	2:I:114:SER:H	1.55	0.53
2:I:359:TYR:HA	2:I:376:ALA:HA	1.91	0.53
2:G:469:ARG:HH21	2:G:3712:GLU:HB3	1.74	0.53
2:G:132:ALA:HA	2:G:194:SER:HB2	1.91	0.53
2:B:359:TYR:HA	2:B:376:ALA:HA	1.91	0.52
2:I:3955:MET:HG3	2:I:4019:LEU:HD22	1.92	0.52
1:H:74:LEU:HB2	1:H:99:PHE:HB2	1.90	0.52
2:B:4581:LYS:HD2	2:B:4632:LEU:HD22	1.90	0.52
2:E:103:TYR:HB3	2:E:152:PRO:HD3	1.92	0.52
2:I:132:ALA:HA	2:I:194:SER:HB2	1.91	0.52
2:G:3955:MET:HG3	2:G:4019:LEU:HD22	1.92	0.52
2:B:2758:PHE:O	2:B:2762:THR:N	2.42	0.52
2:G:103:TYR:HB3	2:G:152:PRO:HD3	1.92	0.52
2:B:1764:GLY:HA3	2:B:1859:VAL:HG11	1.91	0.52
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.39	0.52
2:G:972:LEU:O	2:G:1044:ARG:NH2	2.43	0.52
2:I:1764:GLY:HA3	2:I:1859:VAL:HG11	1.91	0.52
2:G:359:TYR:HA	2:G:376:ALA:HA	1.91	0.52
2:G:938:HIS:HB2	2:G:1054:GLU:HB2	1.92	0.52
2:G:4581:LYS:HD2	2:G:4632:LEU:HD22	1.91	0.52
2:B:2347:GLU:O	2:B:2351:ASN:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:551:LEU:HD21	2:E:589:LEU:HD13	1.91	0.52
2:G:1764:GLY:HA3	2:G:1859:VAL:HG11	1.91	0.52
2:I:989:ALA:O	2:I:1035:ASN:ND2	2.42	0.52
2:B:3955:MET:HG3	2:B:4019:LEU:HD22	1.92	0.51
2:B:4791:TYR:OH	2:B:4815:ASP:O	2.28	0.51
2:E:359:TYR:HA	2:E:376:ALA:HA	1.91	0.51
2:B:626:LEU:HG	2:B:628:GLY:H	1.75	0.51
2:E:132:ALA:HA	2:E:194:SER:HB2	1.91	0.51
2:E:972:LEU:O	2:E:1044:ARG:NH2	2.43	0.51
2:I:2347:GLU:O	2:I:2351:ASN:N	2.43	0.51
2:G:989:ALA:O	2:G:1035:ASN:ND2	2.42	0.51
2:B:972:LEU:O	2:B:1044:ARG:NH2	2.43	0.51
2:E:2347:GLU:O	2:E:2351:ASN:N	2.43	0.51
2:I:938:HIS:HB2	2:I:1054:GLU:HB2	1.92	0.51
2:E:626:LEU:HG	2:E:628:GLY:H	1.75	0.51
2:I:551:LEU:HD21	2:I:589:LEU:HD13	1.92	0.51
2:G:626:LEU:HG	2:G:628:GLY:H	1.76	0.51
2:B:45:ARG:HE	2:B:138:GLN:HG3	1.76	0.51
2:E:938:HIS:HB2	2:E:1054:GLU:HB2	1.92	0.51
2:E:1764:GLY:HA3	2:E:1859:VAL:HG11	1.91	0.51
2:E:3955:MET:HG3	2:E:4019:LEU:HD22	1.92	0.51
2:I:972:LEU:O	2:I:1044:ARG:NH2	2.43	0.51
2:G:2347:GLU:O	2:G:2351:ASN:N	2.43	0.51
2:B:103:TYR:HB3	2:B:152:PRO:HD3	1.92	0.51
2:B:132:ALA:HA	2:B:194:SER:HB2	1.91	0.51
2:B:393:CYS:SG	2:B:395:GLN:NE2	2.84	0.51
2:I:4791:TYR:OH	2:I:4815:ASP:O	2.28	0.51
2:G:4791:TYR:OH	2:G:4815:ASP:O	2.28	0.51
2:B:4933:GLN:OE1	2:E:4933:GLN:NE2	2.42	0.51
2:E:45:ARG:HE	2:E:138:GLN:HG3	1.76	0.51
2:I:626:LEU:HG	2:I:628:GLY:H	1.76	0.51
2:I:2758:PHE:O	2:I:2762:THR:N	2.42	0.51
2:G:393:CYS:SG	2:G:395:GLN:NE2	2.84	0.51
2:B:551:LEU:HD21	2:B:589:LEU:HD13	1.92	0.51
2:G:551:LEU:HD21	2:G:589:LEU:HD13	1.91	0.51
2:B:19:GLU:HB2	2:B:206:CYS:HB3	1.93	0.51
2:B:111:HIS:CD2	2:B:114:SER:H	2.29	0.51
2:B:938:HIS:HB2	2:B:1054:GLU:HB2	1.92	0.51
2:B:2927:LEU:HD23	2:B:2930:LEU:HD12	1.92	0.51
2:I:45:ARG:HE	2:I:138:GLN:HG3	1.76	0.51
2:I:103:TYR:HB3	2:I:152:PRO:HD3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:111:HIS:CD2	2:I:114:SER:H	2.29	0.51
2:I:1960:ALA:O	2:I:1964:ARG:NE	2.44	0.51
2:G:45:ARG:HE	2:G:138:GLN:HG3	1.76	0.51
2:E:4791:TYR:OH	2:E:4815:ASP:O	2.28	0.50
2:I:393:CYS:SG	2:I:395:GLN:NE2	2.84	0.50
2:I:395:GLN:NE2	2:I:397:GLU:OE1	2.43	0.50
2:G:606:LEU:O	2:G:617:ASN:ND2	2.45	0.50
2:E:2927:LEU:HD23	2:E:2930:LEU:HD12	1.92	0.50
2:I:395:GLN:HG3	2:I:397:GLU:H	1.77	0.50
2:I:606:LEU:O	2:I:617:ASN:ND2	2.45	0.50
2:G:2758:PHE:O	2:G:2762:THR:N	2.42	0.50
2:G:2911:LEU:HB2	2:G:2916:LYS:HE3	1.93	0.50
1:J:76:CYS:HB2	1:J:97:LEU:HB2	1.94	0.50
2:B:606:LEU:O	2:B:617:ASN:ND2	2.44	0.50
2:E:393:CYS:SG	2:E:395:GLN:NE2	2.84	0.50
2:E:606:LEU:O	2:E:617:ASN:ND2	2.44	0.50
2:E:2911:LEU:HB2	2:E:2916:LYS:HE3	1.93	0.50
2:E:4914:VAL:HG21	2:G:4884:LEU:HD11	1.93	0.50
2:I:19:GLU:HB2	2:I:206:CYS:HB3	1.93	0.50
2:I:776:LEU:HG	2:I:848:HIS:HA	1.94	0.50
2:I:2927:LEU:HD23	2:I:2930:LEU:HD12	1.92	0.50
2:G:111:HIS:CD2	2:G:114:SER:H	2.29	0.50
2:G:1025:ARG:O	2:G:1032:LYS:NZ	2.40	0.50
2:B:395:GLN:HG3	2:B:397:GLU:H	1.77	0.50
2:B:4567:LEU:HD12	2:B:4816:ILE:HD12	1.94	0.50
2:G:2927:LEU:HD23	2:G:2930:LEU:HD12	1.92	0.50
1:H:76:CYS:HB2	1:H:97:LEU:HB2	1.94	0.50
2:B:4884:LEU:HD11	2:I:4914:VAL:HG21	1.92	0.50
2:I:2823:ILE:HG12	2:I:2937:VAL:HG22	1.94	0.50
2:G:776:LEU:HG	2:G:848:HIS:HA	1.94	0.50
2:E:2823:ILE:HG12	2:E:2937:VAL:HG22	1.94	0.50
2:I:4884:LEU:HD11	2:G:4914:VAL:HG21	1.93	0.50
2:G:395:GLN:NE2	2:G:397:GLU:OE1	2.42	0.50
2:B:1691:GLN:HE22	2:B:1802:ILE:HG12	1.77	0.50
2:E:111:HIS:CD2	2:E:114:SER:H	2.29	0.50
2:I:1691:GLN:HE22	2:I:1802:ILE:HG12	1.77	0.50
2:G:4232:GLU:OE2	2:G:5017:ARG:NH1	2.44	0.50
2:E:395:GLN:HG3	2:E:397:GLU:H	1.77	0.50
2:B:3817:LEU:HD13	2:B:3899:PHE:HD1	1.77	0.50
2:E:2003:GLN:O	2:E:2007:ASN:ND2	2.45	0.50
2:I:580:GLU:HG2	2:I:583:ILE:HD11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2003:GLN:O	2:I:2007:ASN:ND2	2.45	0.50
2:I:4570:ALA:O	2:I:4574:ASN:ND2	2.45	0.50
2:I:4743:MET:HB3	2:I:4746:ALA:HB3	1.94	0.50
2:G:395:GLN:HG3	2:G:397:GLU:H	1.77	0.50
2:G:2823:ILE:HG12	2:G:2937:VAL:HG22	1.94	0.50
1:A:76:CYS:HB2	1:A:97:LEU:HB2	1.94	0.49
2:B:35:LEU:HD13	2:B:49:LEU:HD13	1.94	0.49
2:B:4232:GLU:OE2	2:B:5017:ARG:NH1	2.44	0.49
2:E:470:SER:O	2:E:474:ARG:NE	2.38	0.49
2:E:4570:ALA:O	2:E:4574:ASN:ND2	2.45	0.49
2:I:3817:LEU:HD13	2:I:3899:PHE:HD1	1.77	0.49
2:G:1691:GLN:HE22	2:G:1802:ILE:HG12	1.77	0.49
2:G:2003:GLN:O	2:G:2007:ASN:ND2	2.45	0.49
2:G:3817:LEU:HD13	2:G:3899:PHE:HD1	1.77	0.49
2:G:4743:MET:HB3	2:G:4746:ALA:HB3	1.93	0.49
2:B:2748:PRO:HD2	2:B:2751:LEU:HD12	1.94	0.49
2:G:19:GLU:HB2	2:G:206:CYS:HB3	1.93	0.49
2:B:2003:GLN:O	2:B:2007:ASN:ND2	2.45	0.49
2:G:2748:PRO:HD2	2:G:2751:LEU:HD12	1.94	0.49
2:B:776:LEU:HG	2:B:848:HIS:HA	1.93	0.49
2:E:19:GLU:HB2	2:E:206:CYS:HB3	1.94	0.49
2:E:580:GLU:HG2	2:E:583:ILE:HD11	1.94	0.49
2:I:4567:LEU:HD12	2:I:4816:ILE:HD12	1.94	0.49
1:F:76:CYS:HB2	1:F:97:LEU:HB2	1.94	0.49
2:B:2823:ILE:HG12	2:B:2937:VAL:HG22	1.94	0.49
2:G:4570:ALA:O	2:G:4574:ASN:ND2	2.45	0.49
2:E:1691:GLN:HE22	2:E:1802:ILE:HG12	1.77	0.49
2:I:1025:ARG:O	2:I:1032:LYS:NZ	2.40	0.49
2:B:4570:ALA:O	2:B:4574:ASN:ND2	2.45	0.49
2:E:776:LEU:HG	2:E:848:HIS:HA	1.93	0.49
2:B:707:VAL:HG23	2:B:713:SER:HB2	1.95	0.49
2:B:1960:ALA:O	2:B:1964:ARG:NE	2.44	0.49
2:E:2758:PHE:O	2:E:2762:THR:N	2.42	0.49
2:G:580:GLU:HG2	2:G:583:ILE:HD11	1.94	0.49
2:B:463:GLU:OE2	2:B:467:LYS:NZ	2.46	0.49
2:B:4743:MET:HB3	2:B:4746:ALA:HB3	1.94	0.49
2:I:2226:PRO:HA	2:I:2229:VAL:HG12	1.95	0.49
2:E:707:VAL:HG23	2:E:713:SER:HB2	1.95	0.49
2:E:1960:ALA:O	2:E:1964:ARG:NE	2.44	0.49
2:E:35:LEU:HD13	2:E:49:LEU:HD13	1.94	0.48
2:E:671:VAL:HG22	2:E:740:PRO:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:463:GLU:OE2	2:I:467:LYS:NZ	2.46	0.48
2:I:2911:LEU:HB2	2:I:2916:LYS:HE3	1.93	0.48
2:G:463:GLU:OE2	2:G:467:LYS:NZ	2.46	0.48
2:G:671:VAL:HG22	2:G:740:PRO:HG3	1.95	0.48
2:B:2911:LEU:HB2	2:B:2916:LYS:HE3	1.93	0.48
2:G:2226:PRO:HA	2:G:2229:VAL:HG12	1.95	0.48
2:E:877:ASN:HD22	2:E:1045:THR:HG23	1.78	0.48
2:E:2748:PRO:HD2	2:E:2751:LEU:HD12	1.94	0.48
2:I:35:LEU:HD13	2:I:49:LEU:HD13	1.94	0.48
2:G:1960:ALA:O	2:G:1964:ARG:NE	2.44	0.48
2:B:2862:LEU:HB3	2:B:2928:LYS:HB3	1.95	0.48
2:E:1725:ARG:HA	2:E:1728:ARG:HG2	1.96	0.48
2:I:2199:ARG:NH2	2:I:2246:ASN:OD1	2.47	0.48
2:G:2765:LYS:HA	2:G:2859:PRO:HG3	1.96	0.48
2:G:4567:LEU:HD12	2:G:4816:ILE:HD12	1.94	0.48
2:B:315:CYS:SG	2:B:316:PHE:N	2.87	0.48
2:E:497:TYR:HB3	2:E:500:ALA:HB2	1.96	0.48
2:I:707:VAL:HG23	2:I:713:SER:HB2	1.95	0.48
2:I:2748:PRO:HD2	2:I:2751:LEU:HD12	1.94	0.48
2:B:4914:VAL:HG21	2:E:4884:LEU:HD11	1.95	0.48
2:E:4743:MET:HB3	2:E:4746:ALA:HB3	1.94	0.48
2:G:35:LEU:HD13	2:G:49:LEU:HD13	1.94	0.48
2:G:315:CYS:SG	2:G:316:PHE:N	2.87	0.48
2:G:2199:ARG:NH2	2:G:2246:ASN:OD1	2.47	0.48
2:B:1025:ARG:O	2:B:1032:LYS:NZ	2.40	0.48
2:B:2226:PRO:HA	2:B:2229:VAL:HG12	1.95	0.48
2:E:315:CYS:SG	2:E:316:PHE:N	2.87	0.48
2:E:463:GLU:OE2	2:E:467:LYS:NZ	2.46	0.48
2:G:877:ASN:HD22	2:G:1045:THR:HG23	1.78	0.48
2:B:395:GLN:NE2	2:B:397:GLU:OE1	2.43	0.48
2:I:877:ASN:HD22	2:I:1045:THR:HG23	1.78	0.48
2:G:707:VAL:HG23	2:G:713:SER:HB2	1.95	0.48
2:B:1725:ARG:HA	2:B:1728:ARG:HG2	1.96	0.48
2:E:2765:LYS:HA	2:E:2859:PRO:HG3	1.96	0.48
2:E:2778:GLY:HA3	2:E:2787:THR:HB	1.96	0.48
2:E:2862:LEU:HB3	2:E:2928:LYS:HB3	1.95	0.48
2:E:4567:LEU:HD12	2:E:4816:ILE:HD12	1.94	0.48
2:I:315:CYS:SG	2:I:316:PHE:N	2.87	0.48
2:I:2231:SER:HA	2:I:2234:ARG:HG2	1.95	0.48
2:G:497:TYR:HB3	2:G:500:ALA:HB2	1.96	0.48
2:B:580:GLU:HG2	2:B:583:ILE:HD11	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2226:PRO:HA	2:E:2229:VAL:HG12	1.95	0.48
2:E:3817:LEU:HD13	2:E:3899:PHE:HD1	1.77	0.48
2:I:2737:PRO:O	2:I:2888:ARG:NH2	2.47	0.48
2:G:472:ARG:NH2	2:G:3712:GLU:OE2	2.47	0.48
2:G:1718:ILE:HG13	2:G:1719:HIS:CD2	2.49	0.48
2:G:2862:LEU:HB3	2:G:2928:LYS:HB3	1.95	0.48
2:B:671:VAL:HG22	2:B:740:PRO:HG3	1.95	0.47
2:B:877:ASN:HD22	2:B:1045:THR:HG23	1.78	0.47
2:B:2199:ARG:NH2	2:B:2246:ASN:OD1	2.47	0.47
2:E:2737:PRO:O	2:E:2888:ARG:NH2	2.47	0.47
2:I:1675:ALA:HB1	2:I:1676:LEU:HD13	1.96	0.47
1:A:87:HIS:HD2	1:A:90:VAL:HB	1.79	0.47
2:B:1718:ILE:HG13	2:B:1719:HIS:CD2	2.49	0.47
2:B:3889:GLN:OE1	2:B:3960:GLN:NE2	2.48	0.47
2:I:1718:ILE:HG13	2:I:1719:HIS:CD2	2.49	0.47
2:E:395:GLN:NE2	2:E:397:GLU:OE1	2.42	0.47
2:G:470:SER:O	2:G:474:ARG:NE	2.38	0.47
2:G:2737:PRO:O	2:G:2888:ARG:NH2	2.47	0.47
2:G:2778:GLY:HA3	2:G:2787:THR:HB	1.96	0.47
2:B:472:ARG:NH2	2:B:3712:GLU:OE2	2.47	0.47
2:B:1675:ALA:HB1	2:B:1676:LEU:HD13	1.96	0.47
2:B:2231:SER:HA	2:B:2234:ARG:HG2	1.95	0.47
2:I:2002:PRO:HA	2:I:2005:GLN:HB3	1.96	0.47
2:I:3809:ASN:HB3	2:I:3812:VAL:HG22	1.97	0.47
2:G:1725:ARG:HA	2:G:1728:ARG:HG2	1.96	0.47
1:J:27:THR:HB	1:J:100:ASP:HB3	1.97	0.47
2:B:2778:GLY:HA3	2:B:2787:THR:HB	1.96	0.47
2:B:4860:ARG:HD2	2:E:4582:VAL:HG11	1.96	0.47
2:I:497:TYR:HB3	2:I:500:ALA:HB2	1.96	0.47
2:I:2765:LYS:HA	2:I:2859:PRO:HG3	1.96	0.47
2:I:2862:LEU:HB3	2:I:2928:LYS:HB3	1.95	0.47
1:H:27:THR:HB	1:H:100:ASP:HB3	1.96	0.47
2:B:2002:PRO:HA	2:B:2005:GLN:HB3	1.97	0.47
2:B:2737:PRO:O	2:B:2888:ARG:NH2	2.47	0.47
2:B:2765:LYS:HA	2:B:2859:PRO:HG3	1.96	0.47
2:E:2199:ARG:NH2	2:E:2246:ASN:OD1	2.47	0.47
2:I:671:VAL:HG22	2:I:740:PRO:HG3	1.95	0.47
2:I:1103:GLY:HA3	2:I:1123:VAL:HA	1.97	0.47
2:I:1725:ARG:HA	2:I:1728:ARG:HG2	1.96	0.47
2:G:999:ASP:O	2:G:1004:GLY:N	2.48	0.47
2:G:1760:HIS:HE1	2:G:2041:HIS:HA	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2231:SER:HA	2:G:2234:ARG:HG2	1.95	0.47
2:G:3809:ASN:HB3	2:G:3812:VAL:HG22	1.97	0.47
2:G:3889:GLN:OE1	2:G:3960:GLN:NE2	2.48	0.47
1:F:27:THR:HB	1:F:100:ASP:HB3	1.96	0.47
1:F:87:HIS:HD2	1:F:90:VAL:HB	1.79	0.47
1:J:87:HIS:HD2	1:J:90:VAL:HB	1.79	0.47
2:E:472:ARG:NH2	2:E:3712:GLU:OE2	2.47	0.47
2:E:3889:GLN:OE1	2:E:3960:GLN:NE2	2.48	0.47
2:G:56:GLN:O	2:G:309:THR:OG1	2.26	0.47
1:H:87:HIS:HD2	1:H:90:VAL:HB	1.79	0.47
2:B:497:TYR:HB3	2:B:500:ALA:HB2	1.96	0.47
2:B:1103:GLY:HA3	2:B:1123:VAL:HA	1.97	0.47
2:I:472:ARG:NH2	2:I:3712:GLU:OE2	2.47	0.47
2:G:1103:GLY:HA3	2:G:1123:VAL:HA	1.97	0.47
2:I:2778:GLY:HA3	2:I:2787:THR:HB	1.96	0.47
2:G:2271:THR:HG22	2:G:2273:LEU:H	1.80	0.47
2:B:1973:GLN:O	2:B:1977:TYR:N	2.48	0.46
2:B:2271:THR:HG22	2:B:2273:LEU:H	1.80	0.46
2:B:4063:ASP:OD1	2:B:4169:SER:OG	2.26	0.46
2:E:1099:GLU:OE2	2:E:1127:HIS:ND1	2.40	0.46
2:E:1700:ASP:OD2	2:E:1708:ARG:NH2	2.49	0.46
2:E:2231:SER:HA	2:E:2234:ARG:HG2	1.95	0.46
2:I:2271:THR:HG22	2:I:2273:LEU:H	1.80	0.46
2:E:1718:ILE:HG13	2:E:1719:HIS:CD2	2.49	0.46
2:E:1760:HIS:HE1	2:E:2041:HIS:HA	1.79	0.46
2:I:3889:GLN:OE1	2:I:3960:GLN:NE2	2.47	0.46
2:B:470:SER:O	2:B:474:ARG:NE	2.38	0.46
2:B:1244:GLN:OE1	2:B:1646:ARG:NH1	2.49	0.46
2:B:3809:ASN:HB3	2:B:3812:VAL:HG22	1.97	0.46
2:E:2002:PRO:HA	2:E:2005:GLN:HB3	1.96	0.46
2:I:999:ASP:O	2:I:1004:GLY:N	2.48	0.46
2:I:1244:GLN:OE1	2:I:1646:ARG:NH1	2.49	0.46
2:G:4071:ILE:HD11	2:G:4102:GLN:HE21	1.81	0.46
2:B:898:ASP:HB3	2:B:901:LYS:HB2	1.97	0.46
2:E:1973:GLN:O	2:E:1977:TYR:N	2.48	0.46
2:E:3809:ASN:HB3	2:E:3812:VAL:HG22	1.97	0.46
2:E:3850:GLN:HB3	2:E:3873:LYS:HD3	1.98	0.46
2:G:1244:GLN:OE1	2:G:1646:ARG:NH1	2.49	0.46
2:G:1675:ALA:HB1	2:G:1676:LEU:HD13	1.96	0.46
2:G:1700:ASP:OD2	2:G:1708:ARG:NH2	2.49	0.46
2:B:1700:ASP:OD2	2:B:1708:ARG:NH2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1760:HIS:HE1	2:B:2041:HIS:HA	1.79	0.46
2:B:3850:GLN:HB3	2:B:3873:LYS:HD3	1.97	0.46
2:E:1675:ALA:HB1	2:E:1676:LEU:HD13	1.96	0.46
2:I:898:ASP:HB3	2:I:901:LYS:HB2	1.97	0.46
2:I:4071:ILE:HD11	2:I:4102:GLN:HE21	1.81	0.46
2:B:999:ASP:O	2:B:1004:GLY:N	2.48	0.46
2:E:999:ASP:O	2:E:1004:GLY:N	2.48	0.46
2:I:533:ASN:ND2	2:I:536:ASN:OD1	2.42	0.46
2:G:1973:GLN:O	2:G:1977:TYR:N	2.48	0.46
2:G:2022:PRO:O	2:G:2028:ARG:NH2	2.41	0.46
2:G:3850:GLN:HB3	2:G:3873:LYS:HD3	1.97	0.46
2:E:1698:LEU:N	2:E:1712:TYR:OH	2.49	0.46
2:E:4860:ARG:HD2	2:G:4582:VAL:HG11	1.98	0.46
2:I:4232:GLU:OE2	2:I:5017:ARG:NH1	2.44	0.46
2:I:4582:VAL:HG11	2:G:4860:ARG:HD2	1.98	0.46
2:G:645:ARG:HH11	2:G:778:PHE:HE1	1.63	0.46
1:A:27:THR:HB	1:A:100:ASP:HB3	1.96	0.46
2:E:1103:GLY:HA3	2:E:1123:VAL:HA	1.97	0.46
2:I:645:ARG:HH11	2:I:778:PHE:HE1	1.63	0.46
2:I:1698:LEU:N	2:I:1712:TYR:OH	2.49	0.46
2:I:1700:ASP:OD2	2:I:1708:ARG:NH2	2.49	0.46
2:G:2002:PRO:HA	2:G:2005:GLN:HB3	1.97	0.46
2:E:214:VAL:HG12	2:E:274:LEU:HD12	1.98	0.46
2:E:4232:GLU:OE2	2:E:5017:ARG:NH1	2.44	0.46
2:I:1760:HIS:HE1	2:I:2041:HIS:HA	1.79	0.46
2:G:823:LEU:HD23	2:G:1626:TRP:HB3	1.98	0.46
2:B:645:ARG:HH11	2:B:778:PHE:HE1	1.63	0.46
2:B:1698:LEU:N	2:B:1712:TYR:OH	2.49	0.46
2:E:1244:GLN:OE1	2:E:1646:ARG:NH1	2.49	0.46
2:B:214:VAL:HG12	2:B:274:LEU:HD12	1.98	0.45
2:E:2271:THR:HG22	2:E:2273:LEU:H	1.80	0.45
2:I:3891:LEU:HB3	2:I:3899:PHE:HE2	1.81	0.45
2:G:898:ASP:HB3	2:G:901:LYS:HB2	1.97	0.45
2:G:1698:LEU:N	2:G:1712:TYR:OH	2.49	0.45
2:E:788:LYS:HG2	2:E:1629:GLN:HA	1.98	0.45
2:E:1708:ARG:HG2	2:E:1711:TYR:CE2	2.51	0.45
2:I:1708:ARG:HG2	2:I:1711:TYR:CE2	2.51	0.45
2:I:3850:GLN:HB3	2:I:3873:LYS:HD3	1.97	0.45
2:E:3804:ILE:O	2:E:3809:ASN:ND2	2.50	0.45
2:I:823:LEU:HD23	2:I:1626:TRP:HB3	1.98	0.45
2:I:3658:LYS:HA	2:I:3661:TRP:CD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:645:ARG:HH11	2:E:778:PHE:HE1	1.63	0.45
2:I:470:SER:O	2:I:474:ARG:NE	2.38	0.45
2:I:3804:ILE:O	2:I:3809:ASN:ND2	2.50	0.45
2:G:788:LYS:HG2	2:G:1629:GLN:HA	1.98	0.45
2:B:823:LEU:HD23	2:B:1626:TRP:HB3	1.98	0.45
2:E:898:ASP:HB3	2:E:901:LYS:HB2	1.97	0.45
2:E:4071:ILE:HD11	2:E:4102:GLN:HE21	1.81	0.45
2:I:2022:PRO:O	2:I:2028:ARG:NH2	2.41	0.45
2:I:3927:GLN:NE2	2:I:3988:ALA:O	2.47	0.45
2:G:1099:GLU:OE2	2:G:1127:HIS:ND1	2.40	0.45
2:G:3804:ILE:O	2:G:3809:ASN:ND2	2.50	0.45
2:E:1111:PRO:HD3	2:E:1605:TRP:HE1	1.82	0.45
2:I:1973:GLN:O	2:I:1977:TYR:N	2.48	0.45
2:G:3891:LEU:HB3	2:G:3899:PHE:HE2	1.82	0.45
2:B:56:GLN:O	2:B:309:THR:OG1	2.26	0.45
2:B:886:ARG:HB3	2:B:891:TRP:HB2	1.99	0.45
2:B:3891:LEU:HB3	2:B:3899:PHE:HE2	1.81	0.45
2:E:823:LEU:HD23	2:E:1626:TRP:HB3	1.98	0.45
2:I:886:ARG:HB3	2:I:891:TRP:HB2	1.99	0.45
2:B:533:ASN:ND2	2:B:536:ASN:OD1	2.42	0.45
2:B:3658:LYS:HA	2:B:3661:TRP:CD2	2.52	0.45
2:I:596:ASN:HB3	2:I:599:VAL:HG22	1.99	0.45
2:I:4080:TYR:CZ	2:I:4096:ALA:HB3	2.52	0.45
2:G:214:VAL:HG12	2:G:274:LEU:HD12	1.98	0.45
1:F:92:PRO:HD3	2:E:627:PRO:HB2	1.99	0.45
2:B:485:SER:HA	2:B:488:LEU:HB2	1.98	0.45
2:B:1708:ARG:HG2	2:B:1711:TYR:CE2	2.52	0.45
2:B:2342:ASN:OD1	2:B:2342:ASN:N	2.44	0.45
2:B:3804:ILE:O	2:B:3809:ASN:ND2	2.50	0.45
2:B:4080:TYR:CZ	2:B:4096:ALA:HB3	2.52	0.45
2:E:886:ARG:HB3	2:E:891:TRP:HB2	1.99	0.45
2:E:309:THR:O	2:E:313:SER:OG	2.29	0.45
2:I:1099:GLU:OE2	2:I:1127:HIS:ND1	2.40	0.45
2:I:2247:GLN:NE2	2:I:2285:GLU:OE2	2.50	0.45
2:G:886:ARG:HB3	2:G:891:TRP:HB2	1.99	0.45
2:B:4582:VAL:HG11	2:I:4860:ARG:HD2	2.00	0.44
2:E:4080:TYR:CZ	2:E:4096:ALA:HB3	2.52	0.44
2:I:214:VAL:HG12	2:I:274:LEU:HD12	1.98	0.44
2:E:1148:VAL:HG21	2:E:1212:ARG:HG2	2.00	0.44
2:G:1708:ARG:HG2	2:G:1711:TYR:CE2	2.52	0.44
2:G:3658:LYS:HA	2:G:3661:TRP:CD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:ARG:HG2	2:B:1691:GLN:HG2	1.99	0.44
2:B:788:LYS:HG2	2:B:1629:GLN:HA	1.98	0.44
2:I:788:LYS:HG2	2:I:1629:GLN:HA	1.98	0.44
2:G:1111:PRO:HD3	2:G:1605:TRP:HE1	1.82	0.44
2:G:1131:ARG:HH12	2:G:1178:ALA:HB3	1.83	0.44
2:B:596:ASN:HB3	2:B:599:VAL:HG22	1.99	0.44
2:B:1148:VAL:HG21	2:B:1212:ARG:HG2	2.00	0.44
2:B:2247:GLN:NE2	2:B:2285:GLU:OE2	2.50	0.44
2:E:3658:LYS:HA	2:E:3661:TRP:CD2	2.52	0.44
2:I:786:GLY:HA2	2:I:1631:GLN:HA	2.00	0.44
2:I:2745:VAL:HG21	2:I:2818:ALA:HB2	1.99	0.44
2:G:485:SER:HA	2:G:488:LEU:HB2	1.98	0.44
2:G:4080:TYR:CZ	2:G:4096:ALA:HB3	2.52	0.44
2:B:1111:PRO:HD3	2:B:1605:TRP:HE1	1.82	0.44
2:B:4071:ILE:HD11	2:B:4102:GLN:HE21	1.81	0.44
2:E:3891:LEU:HB3	2:E:3899:PHE:HE2	1.81	0.44
2:G:1227:ALA:HB1	2:G:1230:MET:HG3	2.00	0.44
2:G:2247:GLN:NE2	2:G:2285:GLU:OE2	2.50	0.44
2:G:3927:GLN:NE2	2:G:3988:ALA:O	2.47	0.44
2:B:2745:VAL:HG21	2:B:2818:ALA:HB2	1.99	0.44
2:G:596:ASN:HB3	2:G:599:VAL:HG22	1.99	0.44
2:G:689:THR:H	2:G:778:PHE:HE2	1.65	0.44
2:G:1148:VAL:HG21	2:G:1212:ARG:HG2	2.00	0.44
2:G:2745:VAL:HG21	2:G:2818:ALA:HB2	1.99	0.44
2:B:786:GLY:HA2	2:B:1631:GLN:HA	2.00	0.44
2:E:485:SER:HA	2:E:488:LEU:HB2	1.98	0.44
2:E:1025:ARG:O	2:E:1032:LYS:NZ	2.40	0.44
2:E:2247:GLN:NE2	2:E:2285:GLU:OE2	2.50	0.44
2:I:485:SER:HA	2:I:488:LEU:HB2	1.98	0.44
2:E:41:GLY:O	2:E:45:ARG:NH1	2.51	0.44
2:I:1131:ARG:HH12	2:I:1178:ALA:HB3	1.83	0.44
2:B:2884:ASN:O	2:B:2888:ARG:N	2.47	0.43
2:B:3781:GLN:HA	2:B:3784:SER:HB3	2.01	0.43
2:E:56:GLN:O	2:E:309:THR:OG1	2.26	0.43
2:E:1227:ALA:HB1	2:E:1230:MET:HG3	2.00	0.43
2:E:2022:PRO:O	2:E:2028:ARG:NH2	2.41	0.43
2:E:2745:VAL:HG21	2:E:2818:ALA:HB2	1.99	0.43
2:I:41:GLY:O	2:I:45:ARG:NH1	2.51	0.43
2:G:786:GLY:HA2	2:G:1631:GLN:HA	2.00	0.43
2:G:1093:GLU:OE1	2:G:1201:HIS:NE2	2.46	0.43
2:G:1101:ARG:HG2	2:G:1125:ASN:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:786:GLY:HA2	2:E:1631:GLN:HA	2.00	0.43
2:E:887:ILE:HG21	2:E:959:TYR:HA	2.00	0.43
2:E:1101:ARG:HG2	2:E:1125:ASN:HA	2.00	0.43
2:E:3927:GLN:NE2	2:E:3988:ALA:O	2.47	0.43
2:I:1111:PRO:HD3	2:I:1605:TRP:HE1	1.82	0.43
2:G:2830:GLU:OE2	2:G:2931:GLN:NE2	2.52	0.43
2:B:1227:ALA:HB1	2:B:1230:MET:HG3	2.00	0.43
2:I:887:ILE:HG21	2:I:959:TYR:HA	2.00	0.43
2:I:1148:VAL:HG21	2:I:1212:ARG:HG2	2.00	0.43
2:I:1227:ALA:HB1	2:I:1230:MET:HG3	2.00	0.43
2:I:4688:ILE:HG21	2:I:4728:HIS:HB3	1.99	0.43
2:G:41:GLY:O	2:G:45:ARG:NH1	2.51	0.43
2:B:206:CYS:SG	2:B:207:SER:N	2.91	0.43
2:B:2830:GLU:OE2	2:B:2931:GLN:NE2	2.52	0.43
2:E:596:ASN:HB3	2:E:599:VAL:HG22	1.99	0.43
2:E:4688:ILE:HG21	2:E:4728:HIS:HB3	1.99	0.43
2:I:309:THR:O	2:I:313:SER:OG	2.29	0.43
2:I:1812:LEU:HD21	2:I:1861:GLN:HG2	2.00	0.43
2:G:1232:ARG:HH21	2:G:1701:ALA:HB1	1.83	0.43
2:B:41:GLY:O	2:B:45:ARG:NH1	2.51	0.43
2:B:887:ILE:HG21	2:B:959:TYR:HA	2.00	0.43
2:B:1812:LEU:HD21	2:B:1861:GLN:HG2	2.00	0.43
2:E:1131:ARG:HH12	2:E:1178:ALA:HB3	1.83	0.43
2:I:2830:GLU:OE2	2:I:2931:GLN:NE2	2.52	0.43
2:B:4688:ILE:HG21	2:B:4728:HIS:HB3	1.99	0.43
2:G:887:ILE:HG21	2:G:959:TYR:HA	2.00	0.43
2:B:689:THR:H	2:B:778:PHE:HE2	1.65	0.43
2:B:1685:LEU:HA	2:B:1688:HIS:HD2	1.84	0.43
2:E:206:CYS:SG	2:E:207:SER:N	2.91	0.43
2:E:689:THR:H	2:E:778:PHE:HE2	1.65	0.43
2:I:1232:ARG:HH21	2:I:1701:ALA:HB1	1.83	0.43
2:I:4092:ASP:OD1	2:I:4092:ASP:N	2.52	0.43
2:G:4688:ILE:HG21	2:G:4728:HIS:HB3	1.99	0.43
2:B:4081:VAL:HB	2:B:4088:ILE:HD12	2.00	0.43
2:E:1685:LEU:HA	2:E:1688:HIS:HD2	1.84	0.43
2:I:206:CYS:SG	2:I:207:SER:N	2.91	0.43
2:I:2438:PRO:HB3	2:I:2453:ILE:HB	2.00	0.43
2:I:3781:GLN:HA	2:I:3784:SER:HB3	2.01	0.43
2:G:4092:ASP:OD1	2:G:4092:ASP:N	2.52	0.43
2:B:1126:GLY:HA3	2:B:1143:TRP:CE2	2.54	0.43
2:B:1232:ARG:HH21	2:B:1701:ALA:HB1	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:206:CYS:SG	2:G:207:SER:N	2.91	0.43
2:G:548:VAL:HG12	2:G:564:LEU:HD22	2.00	0.43
2:G:1516:UNK:N	2:G:1529:UNK:O	2.52	0.43
2:G:4081:VAL:HB	2:G:4088:ILE:HD12	2.00	0.43
2:B:2024:PRO:O	2:B:2028:ARG:NE	2.45	0.43
2:E:1095:VAL:HB	2:E:1199:VAL:HG23	2.01	0.43
2:E:3781:GLN:HA	2:E:3784:SER:HB3	2.00	0.43
2:E:4899:ASP:OD1	2:G:4892:ARG:NH2	2.52	0.43
2:I:3842:LEU:O	2:I:3929:SER:OG	2.37	0.43
2:G:1685:LEU:HA	2:G:1688:HIS:HD2	1.84	0.43
2:B:1131:ARG:HH12	2:B:1178:ALA:HB3	1.83	0.42
2:B:4092:ASP:OD1	2:B:4092:ASP:N	2.52	0.42
2:E:1126:GLY:HA3	2:E:1143:TRP:CE2	2.54	0.42
2:I:940:GLY:O	2:I:1052:ASN:N	2.52	0.42
2:I:1101:ARG:HG2	2:I:1125:ASN:HA	2.00	0.42
2:G:533:ASN:ND2	2:G:536:ASN:OD1	2.42	0.42
1:F:42:ARG:HG2	2:E:1691:GLN:HG2	2.01	0.42
2:B:2438:PRO:HB3	2:B:2453:ILE:HB	2.00	0.42
2:E:548:VAL:HG12	2:E:564:LEU:HD22	2.00	0.42
2:E:4063:ASP:OD1	2:E:4169:SER:OG	2.26	0.42
2:I:548:VAL:HG12	2:I:564:LEU:HD22	2.00	0.42
2:I:2770:LYS:HB3	2:I:2775:TRP:HB2	2.01	0.42
2:G:940:GLY:O	2:G:1052:ASN:N	2.52	0.42
2:B:940:GLY:O	2:B:1052:ASN:N	2.52	0.42
2:E:1232:ARG:HH21	2:E:1701:ALA:HB1	1.83	0.42
2:E:2770:LYS:HB3	2:E:2775:TRP:HB2	2.01	0.42
2:I:1095:VAL:HB	2:I:1199:VAL:HG23	2.01	0.42
2:G:870:ILE:O	2:G:874:LEU:N	2.42	0.42
2:G:978:THR:HB	2:G:980:ALA:H	1.84	0.42
2:G:1095:VAL:HB	2:G:1199:VAL:HG23	2.01	0.42
2:G:1126:GLY:HA3	2:G:1143:TRP:CE2	2.54	0.42
2:G:1812:LEU:HD21	2:G:1861:GLN:HG2	2.00	0.42
2:G:2770:LYS:HB3	2:G:2775:TRP:HB2	2.01	0.42
2:B:330:ASP:N	2:B:330:ASP:OD1	2.53	0.42
2:B:489:ASN:HA	2:B:492:ASP:HB2	2.02	0.42
2:E:940:GLY:O	2:E:1052:ASN:N	2.52	0.42
2:E:4092:ASP:N	2:E:4092:ASP:OD1	2.52	0.42
2:I:637:LEU:HD23	2:I:1637:MET:HB3	2.01	0.42
2:I:1676:LEU:HD23	2:I:2167:ILE:HG23	2.01	0.42
2:I:1685:LEU:HA	2:I:1688:HIS:HD2	1.84	0.42
2:G:2438:PRO:HB3	2:G:2453:ILE:HB	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:864:PRO:HA	2:B:865:PRO:HD3	1.92	0.42
2:B:978:THR:HB	2:B:980:ALA:H	1.84	0.42
2:B:1099:GLU:OE2	2:B:1127:HIS:ND1	2.40	0.42
2:B:1101:ARG:HG2	2:B:1125:ASN:HA	2.00	0.42
2:B:2022:PRO:HB2	2:B:2024:PRO:HD2	2.01	0.42
2:E:489:ASN:HA	2:E:492:ASP:HB2	2.02	0.42
2:E:1676:LEU:HD23	2:E:2167:ILE:HG23	2.01	0.42
2:I:1126:GLY:HA3	2:I:1143:TRP:CE2	2.54	0.42
2:G:330:ASP:OD1	2:G:330:ASP:N	2.53	0.42
2:G:637:LEU:HD23	2:G:1637:MET:HB3	2.01	0.42
2:G:1694:LEU:O	2:G:1712:TYR:OH	2.29	0.42
1:H:42:ARG:HG2	2:G:1691:GLN:HG2	2.00	0.42
2:B:548:VAL:HG12	2:B:564:LEU:HD22	2.00	0.42
2:E:978:THR:HB	2:E:980:ALA:H	1.84	0.42
2:B:3842:LEU:O	2:B:3929:SER:OG	2.37	0.42
2:E:2022:PRO:HB2	2:E:2024:PRO:HD2	2.01	0.42
2:I:689:THR:H	2:I:778:PHE:HE2	1.65	0.42
2:G:3842:LEU:O	2:G:3929:SER:OG	2.37	0.42
2:B:1707:LEU:HG	2:B:1708:ARG:HG3	2.02	0.42
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	2.01	0.42
2:E:1516:UNK:N	2:E:1529:UNK:O	2.52	0.42
2:E:1707:LEU:HG	2:E:1708:ARG:HG3	2.02	0.42
2:I:4081:VAL:HB	2:I:4088:ILE:HD12	2.00	0.42
2:B:1676:LEU:HD23	2:B:2167:ILE:HG23	2.01	0.42
2:B:1694:LEU:O	2:B:1712:TYR:OH	2.29	0.42
2:E:637:LEU:HD23	2:E:1637:MET:HB3	2.01	0.42
2:E:4251:ILE:HG22	2:E:4553:ASN:HD22	1.85	0.42
2:G:1676:LEU:HD23	2:G:2167:ILE:HG23	2.01	0.42
2:G:2884:ASN:O	2:G:2888:ARG:N	2.47	0.42
2:G:3781:GLN:HA	2:G:3784:SER:HB3	2.01	0.42
2:G:4680:LYS:HD3	2:G:4686:LEU:HD22	2.02	0.42
2:E:2830:GLU:OE2	2:E:2931:GLN:NE2	2.52	0.42
2:G:1171:SER:OG	2:G:1175:SER:N	2.45	0.42
2:G:1673:VAL:HG12	2:G:1681:VAL:HG11	2.02	0.42
2:B:637:LEU:HD23	2:B:1637:MET:HB3	2.01	0.41
2:B:3927:GLN:NE2	2:B:3988:ALA:O	2.47	0.41
2:E:4680:LYS:HD3	2:E:4686:LEU:HD22	2.02	0.41
2:G:3780:LEU:HD11	2:G:3816:MET:HG3	2.01	0.41
2:B:1673:VAL:HG12	2:B:1681:VAL:HG11	2.02	0.41
2:E:1812:LEU:HD21	2:E:1861:GLN:HG2	2.00	0.41
2:E:3780:LEU:HD11	2:E:3816:MET:HG3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:3842:LEU:O	2:E:3929:SER:OG	2.37	0.41
2:E:4929:LEU:HD13	2:E:4929:LEU:HA	1.90	0.41
2:I:876:GLU:O	2:I:880:GLU:N	2.53	0.41
2:I:1673:VAL:HG12	2:I:1681:VAL:HG11	2.02	0.41
2:I:2022:PRO:HB2	2:I:2024:PRO:HD2	2.01	0.41
2:I:4251:ILE:HG22	2:I:4553:ASN:HD22	1.85	0.41
2:G:410:LEU:HD12	2:G:413:GLN:HE21	1.85	0.41
2:G:582:HIS:O	2:G:585:SER:OG	2.29	0.41
2:B:1095:VAL:HB	2:B:1199:VAL:HG23	2.01	0.41
2:E:410:LEU:HD12	2:E:413:GLN:HE21	1.85	0.41
2:E:2438:PRO:HB3	2:E:2453:ILE:HB	2.01	0.41
2:I:454:PRO:HG2	2:I:531:ARG:HH12	1.85	0.41
2:I:1516:UNK:N	2:I:1529:UNK:O	2.53	0.41
2:B:641:VAL:HG11	2:B:681:HIS:HD1	1.86	0.41
2:B:1516:UNK:N	2:B:1529:UNK:O	2.52	0.41
2:B:3780:LEU:HD11	2:B:3816:MET:HG3	2.01	0.41
2:E:1796:ALA:HB1	2:E:1797:ARG:HH21	1.86	0.41
2:I:897:ARG:HB2	2:I:905:PRO:HG3	2.03	0.41
2:G:4251:ILE:HG22	2:G:4553:ASN:HD22	1.85	0.41
2:B:4680:LYS:HD3	2:B:4686:LEU:HD22	2.02	0.41
2:E:1673:VAL:HG12	2:E:1681:VAL:HG11	2.02	0.41
2:B:897:ARG:HB2	2:B:905:PRO:HG3	2.03	0.41
2:B:1796:ALA:HB1	2:B:1797:ARG:HH21	1.86	0.41
2:I:56:GLN:O	2:I:309:THR:OG1	2.26	0.41
2:G:235:ALA:HA	2:G:257:ARG:HD3	2.03	0.41
2:G:489:ASN:HA	2:G:492:ASP:HB2	2.01	0.41
2:G:1707:LEU:HG	2:G:1708:ARG:HG3	2.02	0.41
2:G:2022:PRO:HB2	2:G:2024:PRO:HD2	2.01	0.41
2:B:1738:LEU:HB3	2:B:2146:PRO:HD3	2.03	0.41
2:E:330:ASP:OD1	2:E:330:ASP:N	2.53	0.41
2:E:4081:VAL:HB	2:E:4088:ILE:HD12	2.00	0.41
2:I:235:ALA:HA	2:I:257:ARG:HD3	2.03	0.41
2:I:1707:LEU:HG	2:I:1708:ARG:HG3	2.02	0.41
2:I:3780:LEU:HD11	2:I:3816:MET:HG3	2.01	0.41
2:I:4680:LYS:HD3	2:I:4686:LEU:HD22	2.02	0.41
2:G:454:PRO:HG2	2:G:531:ARG:HH12	1.86	0.41
2:G:897:ARG:HB2	2:G:905:PRO:HG3	2.03	0.41
2:B:2827:ARG:H	2:B:2934:GLY:HA3	1.86	0.41
2:I:641:VAL:HG11	2:I:681:HIS:HD1	1.86	0.41
2:I:864:PRO:HA	2:I:865:PRO:HD3	1.92	0.41
2:I:978:THR:HB	2:I:980:ALA:H	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1796:ALA:HB1	2:I:1797:ARG:HH21	1.86	0.41
2:B:410:LEU:HD12	2:B:413:GLN:HE21	1.85	0.41
2:E:1152:MET:HB2	2:E:1161:ILE:HB	2.03	0.41
2:E:2827:ARG:H	2:E:2934:GLY:HA3	1.86	0.41
2:E:4138:ASP:N	2:E:4138:ASP:OD1	2.54	0.41
2:I:410:LEU:HD12	2:I:413:GLN:HE21	1.85	0.41
2:I:489:ASN:HA	2:I:492:ASP:HB2	2.02	0.41
2:I:1152:MET:HB2	2:I:1161:ILE:HB	2.03	0.41
2:I:4929:LEU:HD13	2:I:4929:LEU:HA	1.90	0.41
2:G:278:GLN:N	2:G:315:CYS:SG	2.83	0.41
2:G:309:THR:O	2:G:313:SER:OG	2.29	0.41
2:E:675:LEU:HD11	2:E:1633:PRO:HB3	2.03	0.41
1:H:92:PRO:HD3	2:G:627:PRO:HB2	2.02	0.40
2:B:1720:LEU:HD12	2:B:1847:THR:HG23	2.03	0.40
2:B:4956:THR:O	2:B:4965:SER:N	2.55	0.40
2:E:533:ASN:ND2	2:E:536:ASN:OD1	2.42	0.40
2:E:897:ARG:HB2	2:E:905:PRO:HG3	2.03	0.40
2:I:4181:ILE:HG22	2:I:4193:ILE:HB	2.03	0.40
2:I:4892:ARG:NH2	2:G:4899:ASP:OD1	2.54	0.40
2:G:4763:GLY:O	2:G:4766:THR:OG1	2.33	0.40
2:E:641:VAL:HG11	2:E:681:HIS:HD1	1.86	0.40
2:I:404:ILE:HG21	2:I:481:GLU:HG3	2.04	0.40
2:I:1667:LEU:HD23	2:I:1671:ARG:HH12	1.87	0.40
2:G:641:VAL:HG11	2:G:681:HIS:HD1	1.86	0.40
2:G:1796:ALA:HB1	2:G:1797:ARG:HH21	1.86	0.40
2:G:4956:THR:O	2:G:4965:SER:N	2.55	0.40
2:B:40:GLU:HB3	2:B:44:ASN:HB3	2.04	0.40
2:B:1171:SER:OG	2:B:1175:SER:N	2.44	0.40
2:B:1667:LEU:HD23	2:B:1671:ARG:HH12	1.87	0.40
2:E:214:VAL:HG22	2:E:341:TYR:CE1	2.57	0.40
2:E:1092:PHE:HB3	2:E:1149:VAL:HB	2.03	0.40
2:E:1622:GLU:N	2:E:1627:ALA:O	2.55	0.40
2:E:1667:LEU:HD23	2:E:1671:ARG:HH12	1.87	0.40
2:E:2674:UNK:O	2:E:2676:UNK:N	2.54	0.40
2:I:330:ASP:OD1	2:I:330:ASP:N	2.53	0.40
2:I:4956:THR:O	2:I:4965:SER:N	2.55	0.40
2:G:1622:GLU:N	2:G:1627:ALA:O	2.55	0.40
2:G:2827:ARG:H	2:G:2934:GLY:HA3	1.86	0.40
2:B:214:VAL:HG22	2:B:341:TYR:CE1	2.57	0.40
2:B:675:LEU:HD11	2:B:1633:PRO:HB3	2.03	0.40
2:B:2674:UNK:O	2:B:2676:UNK:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4251:ILE:HG22	2:B:4553:ASN:HD22	1.85	0.40
2:E:4567:LEU:HA	2:E:4816:ILE:HD12	2.03	0.40
2:I:675:LEU:HD11	2:I:1633:PRO:HB3	2.03	0.40
2:G:3364:UNK:O	2:G:3368:UNK:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	105/108 (97%)	97 (92%)	8 (8%)	0	100	100
1	F	105/108 (97%)	98 (93%)	7 (7%)	0	100	100
1	H	105/108 (97%)	98 (93%)	7 (7%)	0	100	100
1	J	105/108 (97%)	97 (92%)	8 (8%)	0	100	100
2	B	3235/4676 (69%)	2881 (89%)	349 (11%)	5 (0%)	47	79
2	E	3235/4676 (69%)	2883 (89%)	347 (11%)	5 (0%)	47	79
2	G	3235/4676 (69%)	2879 (89%)	351 (11%)	5 (0%)	47	79
2	I	3235/4676 (69%)	2880 (89%)	350 (11%)	5 (0%)	47	79
All	All	13360/19136 (70%)	11913 (89%)	1427 (11%)	20 (0%)	54	84

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1708	ARG
2	E	1708	ARG
2	I	1708	ARG
2	G	1708	ARG
2	B	1932	PRO
2	E	1932	PRO

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Mol	Chain	Res	Type
2	I	1932	PRO
2	G	1932	PRO
2	B	1840	PRO
2	B	4641	PRO
2	E	1840	PRO
2	E	4641	PRO
2	I	1840	PRO
2	I	4641	PRO
2	G	1840	PRO
2	G	4641	PRO
2	B	4228	ALA
2	E	4228	ALA
2	I	4228	ALA
2	G	4228	ALA

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	88/89 (99%)	88 (100%)	0	100	100
1	F	88/89 (99%)	88 (100%)	0	100	100
1	H	88/89 (99%)	88 (100%)	0	100	100
1	J	88/89 (99%)	88 (100%)	0	100	100
2	B	2493/3202 (78%)	2476 (99%)	17 (1%)	84	90
2	E	2493/3202 (78%)	2476 (99%)	17 (1%)	84	90
2	G	2493/3202 (78%)	2476 (99%)	17 (1%)	84	90
2	I	2493/3202 (78%)	2476 (99%)	17 (1%)	84	90
All	All	10324/13164 (78%)	10256 (99%)	68 (1%)	84	90

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

Mol	Chain	Res	Type
2	B	131	LEU

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Mol	Chain	Res	Type
2	B	534	ARG
2	B	553	ARG
2	B	719	LEU
2	B	1076	ARG
2	B	1141	ARG
2	B	1600	LEU
2	B	1676	LEU
2	B	1964	ARG
2	B	3787	LYS
2	B	3805	LEU
2	B	3896	ASN
2	B	4034	ASN
2	B	4085	ARG
2	B	4120	ASN
2	B	4951	LYS
2	B	4995	LEU
2	E	131	LEU
2	E	534	ARG
2	E	553	ARG
2	E	719	LEU
2	E	1076	ARG
2	E	1141	ARG
2	E	1600	LEU
2	E	1676	LEU
2	E	1964	ARG
2	E	3787	LYS
2	E	3805	LEU
2	E	3896	ASN
2	E	4034	ASN
2	E	4085	ARG
2	E	4120	ASN
2	E	4951	LYS
2	E	4995	LEU
2	I	131	LEU
2	I	534	ARG
2	I	553	ARG
2	I	719	LEU
2	I	1076	ARG
2	I	1141	ARG
2	I	1600	LEU
2	I	1676	LEU
2	I	1964	ARG

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Mol	Chain	Res	Type
2	I	3787	LYS
2	I	3805	LEU
2	I	3896	ASN
2	I	4034	ASN
2	I	4085	ARG
2	I	4120	ASN
2	I	4951	LYS
2	I	4995	LEU
2	G	131	LEU
2	G	534	ARG
2	G	553	ARG
2	G	719	LEU
2	G	1076	ARG
2	G	1141	ARG
2	G	1600	LEU
2	G	1676	LEU
2	G	1964	ARG
2	G	3787	LYS
2	G	3805	LEU
2	G	3896	ASN
2	G	4034	ASN
2	G	4085	ARG
2	G	4120	ASN
2	G	4951	LYS
2	G	4995	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (133) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	87	HIS
1	A	87	HIS
1	H	87	HIS
1	J	87	HIS
2	B	23	GLN
2	B	57	ASN
2	B	105	HIS
2	B	111	HIS
2	B	203	ASN
2	B	379	HIS
2	B	383	HIS
2	B	395	GLN
2	B	413	GLN

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Mol	Chain	Res	Type
2	B	479	GLN
2	B	1598	GLN
2	B	1688	HIS
2	B	1691	GLN
2	B	1693	GLN
2	B	1719	HIS
2	B	1760	HIS
2	B	1775	HIS
2	B	2005	GLN
2	B	2127	GLN
2	B	3771	HIS
2	B	3809	ASN
2	B	3896	ASN
2	B	3946	GLN
2	B	3950	ASN
2	B	4034	ASN
2	B	4054	ASN
2	B	4102	GLN
2	B	4120	ASN
2	B	4156	HIS
2	B	4553	ASN
2	B	4806	ASN
2	B	4984	ASN
2	E	23	GLN
2	E	57	ASN
2	E	105	HIS
2	E	111	HIS
2	E	113	HIS
2	E	203	ASN
2	E	379	HIS
2	E	383	HIS
2	E	395	GLN
2	E	413	GLN
2	E	479	GLN
2	E	1598	GLN
2	E	1688	HIS
2	E	1691	GLN
2	E	1693	GLN
2	E	1719	HIS
2	E	1760	HIS
2	E	1775	HIS
2	E	2005	GLN

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Mol	Chain	Res	Type
2	E	2127	GLN
2	E	3771	HIS
2	E	3809	ASN
2	E	3896	ASN
2	E	3946	GLN
2	E	3950	ASN
2	E	4034	ASN
2	E	4054	ASN
2	E	4102	GLN
2	E	4120	ASN
2	E	4156	HIS
2	E	4553	ASN
2	E	4806	ASN
2	E	4984	ASN
2	I	23	GLN
2	I	57	ASN
2	I	105	HIS
2	I	111	HIS
2	I	203	ASN
2	I	379	HIS
2	I	383	HIS
2	I	395	GLN
2	I	413	GLN
2	I	479	GLN
2	I	1598	GLN
2	I	1688	HIS
2	I	1691	GLN
2	I	1693	GLN
2	I	1719	HIS
2	I	1760	HIS
2	I	1775	HIS
2	I	2005	GLN
2	I	2127	GLN
2	I	3771	HIS
2	I	3809	ASN
2	I	3896	ASN
2	I	3946	GLN
2	I	3950	ASN
2	I	4034	ASN
2	I	4054	ASN
2	I	4102	GLN
2	I	4120	ASN

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Mol	Chain	Res	Type
2	I	4156	HIS
2	I	4553	ASN
2	I	4806	ASN
2	I	4984	ASN
2	G	23	GLN
2	G	57	ASN
2	G	105	HIS
2	G	111	HIS
2	G	113	HIS
2	G	203	ASN
2	G	379	HIS
2	G	383	HIS
2	G	395	GLN
2	G	413	GLN
2	G	479	GLN
2	G	1598	GLN
2	G	1688	HIS
2	G	1691	GLN
2	G	1693	GLN
2	G	1719	HIS
2	G	1760	HIS
2	G	1775	HIS
2	G	2005	GLN
2	G	2127	GLN
2	G	3771	HIS
2	G	3809	ASN
2	G	3896	ASN
2	G	3946	GLN
2	G	3950	ASN
2	G	4034	ASN
2	G	4054	ASN
2	G	4102	GLN
2	G	4120	ASN
2	G	4156	HIS
2	G	4553	ASN
2	G	4984	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	I	12
2	B	12
2	G	12
2	E	12

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	3613:UNK	C	3639:THR	N	42.97
1	B	3613:UNK	C	3639:THR	N	42.95
1	G	3613:UNK	C	3639:THR	N	42.95
1	E	3613:UNK	C	3639:THR	N	42.94

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	3163:UNK	C	3170:UNK	N	16.52
1	E	3163:UNK	C	3170:UNK	N	16.52
1	I	3163:UNK	C	3170:UNK	N	16.52
1	G	3163:UNK	C	3170:UNK	N	16.52
1	E	3468:UNK	C	3511:UNK	N	14.99
1	G	3468:UNK	C	3511:UNK	N	14.99
1	B	3468:UNK	C	3511:UNK	N	14.98
1	I	3468:UNK	C	3511:UNK	N	14.98
1	B	3063:UNK	C	3134:UNK	N	14.61
1	E	3063:UNK	C	3134:UNK	N	14.61
1	I	3063:UNK	C	3134:UNK	N	14.61
1	G	3063:UNK	C	3134:UNK	N	14.61
1	B	2703:UNK	C	2734:ASN	N	14.43
1	I	2703:UNK	C	2734:ASN	N	14.43
1	G	2703:UNK	C	2734:ASN	N	14.43
1	E	2703:UNK	C	2734:ASN	N	14.42
1	B	3236:UNK	C	3241:UNK	N	13.59
1	E	3236:UNK	C	3241:UNK	N	13.59
1	I	3236:UNK	C	3241:UNK	N	13.59
1	G	3236:UNK	C	3241:UNK	N	13.59
1	I	1564:UNK	C	1573:MET	N	12.75
1	B	1564:UNK	C	1573:MET	N	12.73
1	G	1564:UNK	C	1573:MET	N	12.73
1	E	1564:UNK	C	1573:MET	N	12.71
1	B	2976:UNK	C	2995:UNK	N	12.12
1	E	2976:UNK	C	2995:UNK	N	12.12
1	I	2976:UNK	C	2995:UNK	N	12.12
1	G	2976:UNK	C	2995:UNK	N	12.12
1	B	3254:UNK	C	3261:UNK	N	8.52
1	E	3254:UNK	C	3261:UNK	N	8.52
1	I	3254:UNK	C	3261:UNK	N	8.52
1	G	3254:UNK	C	3261:UNK	N	8.52
1	B	1297:UNK	C	1430:UNK	N	5.67
1	E	1297:UNK	C	1430:UNK	N	5.67
1	G	1297:UNK	C	1430:UNK	N	5.67
1	I	1297:UNK	C	1430:UNK	N	5.66
1	I	2939:ARG	C	2942:UNK	N	3.56
1	G	2939:ARG	C	2942:UNK	N	3.55
1	B	2939:ARG	C	2942:UNK	N	3.54
1	E	2479:LEU	C	2487:UNK	N	3.53
1	E	2939:ARG	C	2942:UNK	N	3.53
1	B	2479:LEU	C	2487:UNK	N	3.51

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	2479:LEU	C	2487:UNK	N	3.51
1	I	2479:LEU	C	2487:UNK	N	3.49

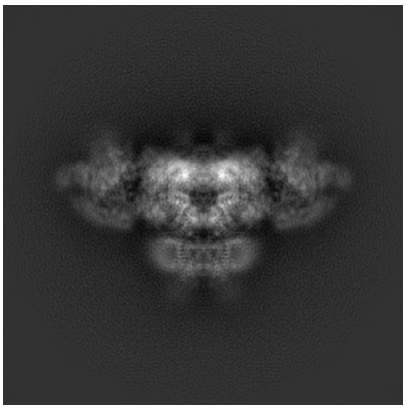
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8372. These allow visual inspection of the internal detail of the map and identification of artifacts.

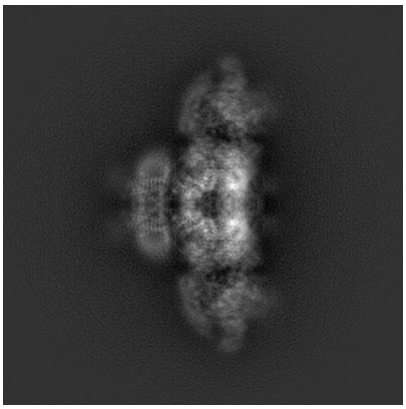
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

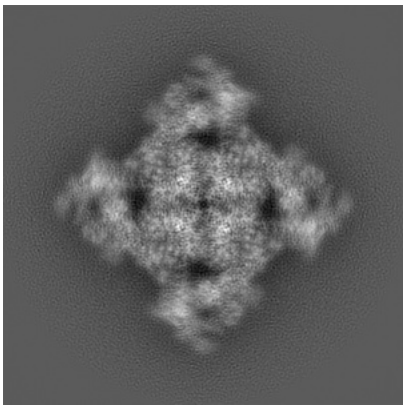
6.1.1 Primary map



X

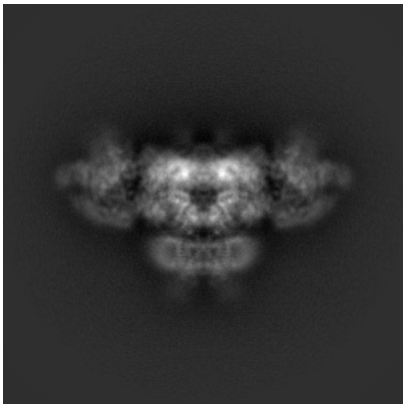


Y

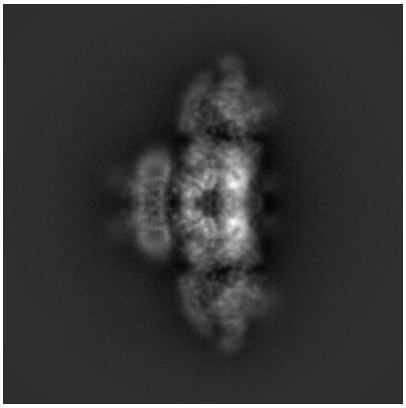


Z

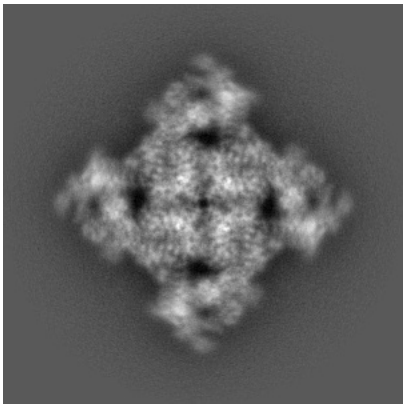
6.1.2 Raw map



X



Y

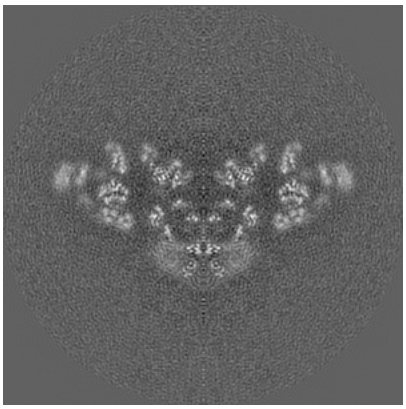


Z

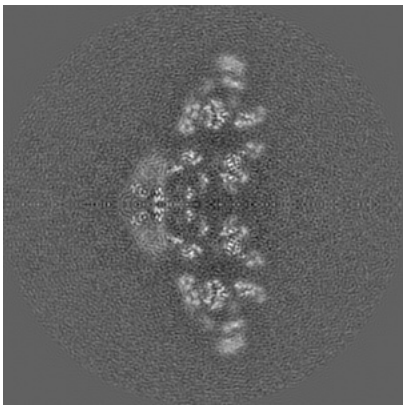
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

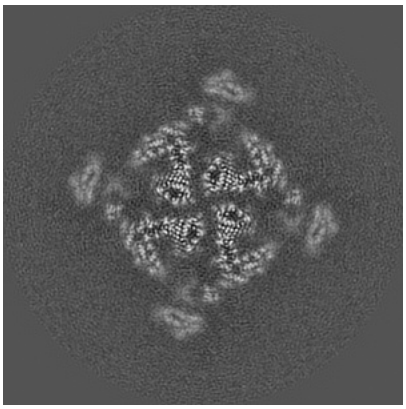
6.2.1 Primary map



X Index: 200

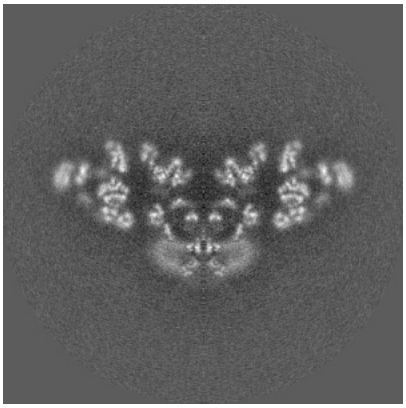


Y Index: 200

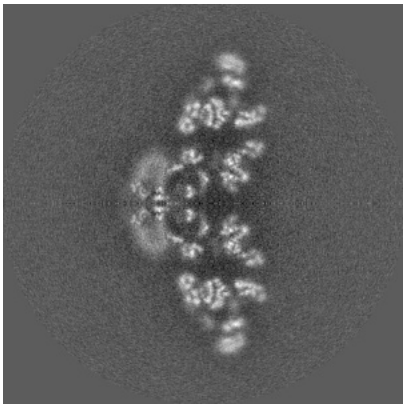


Z Index: 200

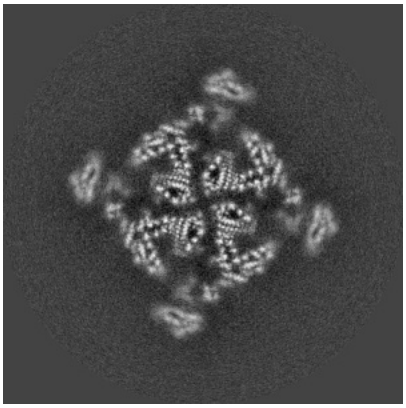
6.2.2 Raw map



X Index: 200



Y Index: 200

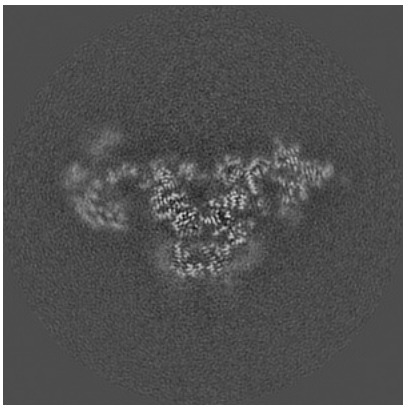


Z Index: 200

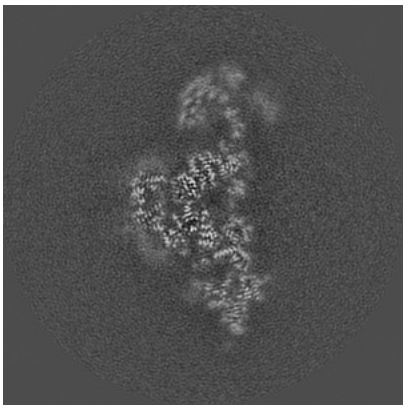
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

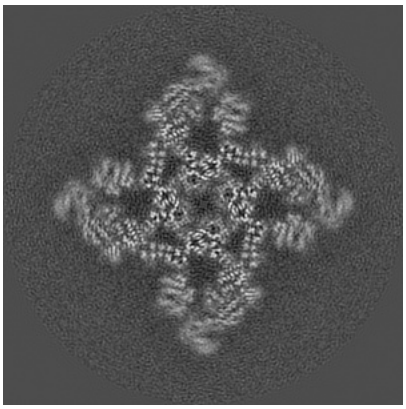
6.3.1 Primary map



X Index: 184

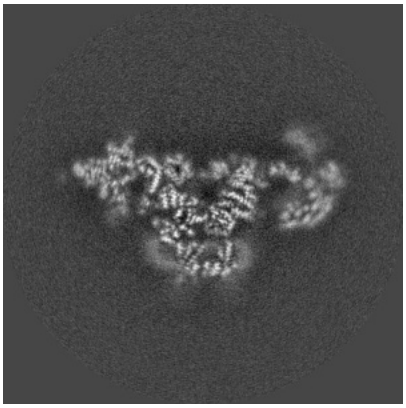


Y Index: 184

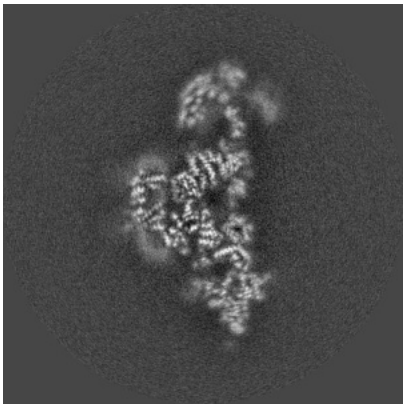


Z Index: 227

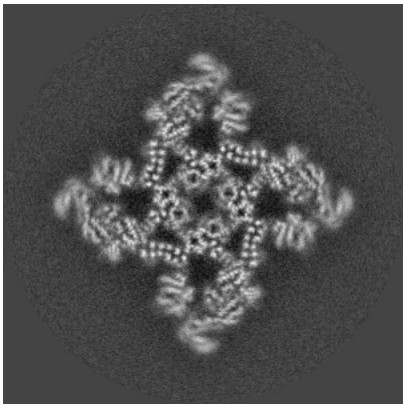
6.3.2 Raw map



X Index: 216



Y Index: 184

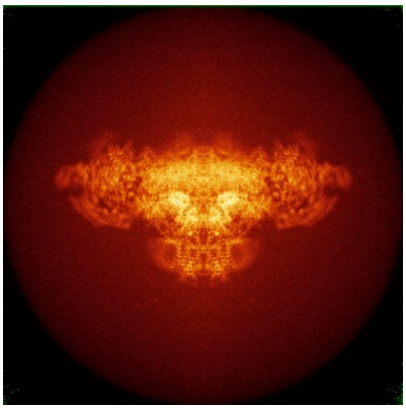


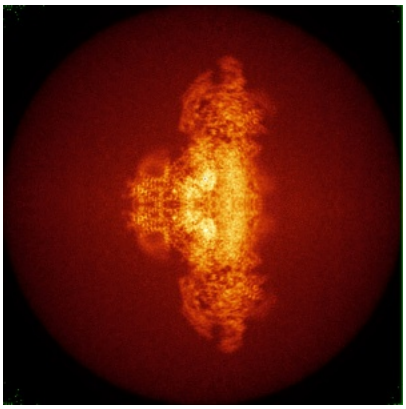
Z Index: 227

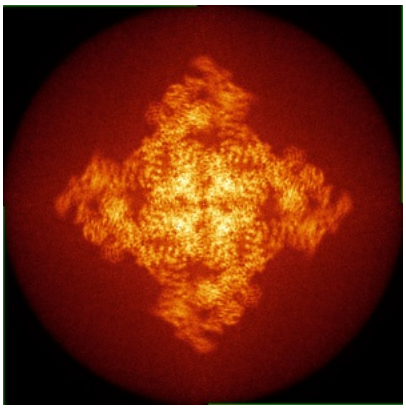
The images above show the largest variance slices of the map in three orthogonal directions.

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

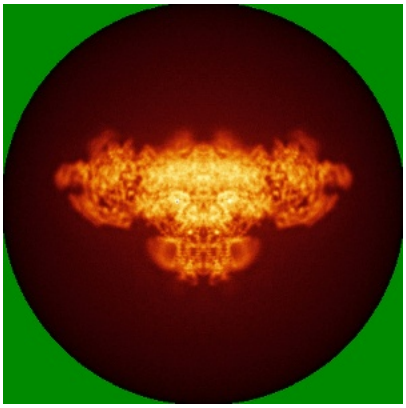
6.4.1 Primary map

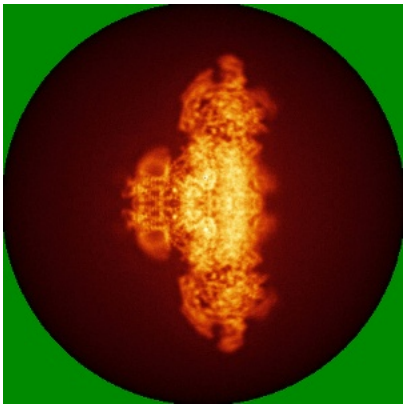

X

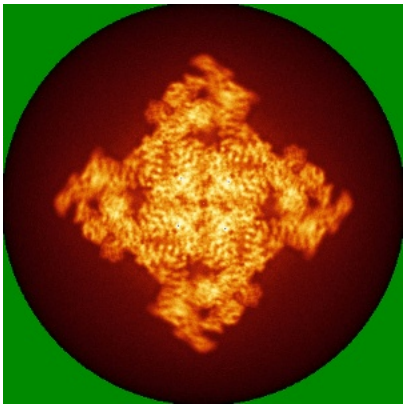

Y


Z

6.4.2 Raw map


X

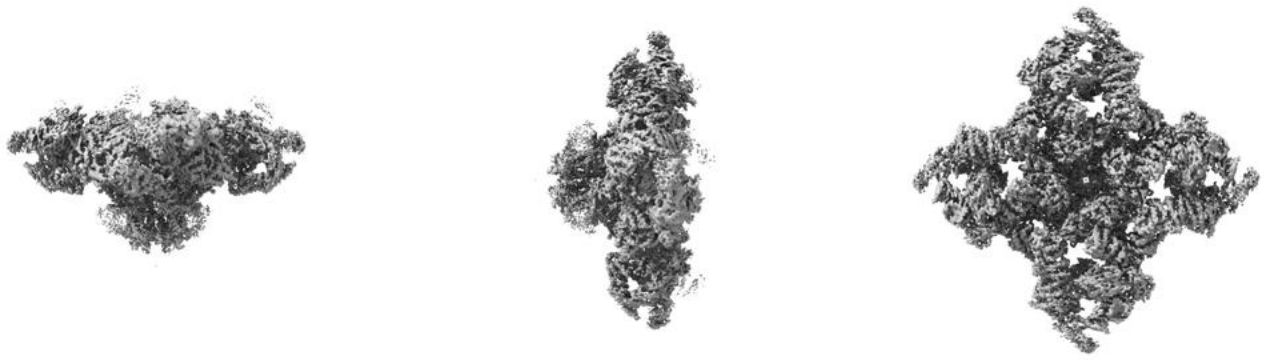

Y


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

6.5.2 Raw map

X Y Z

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

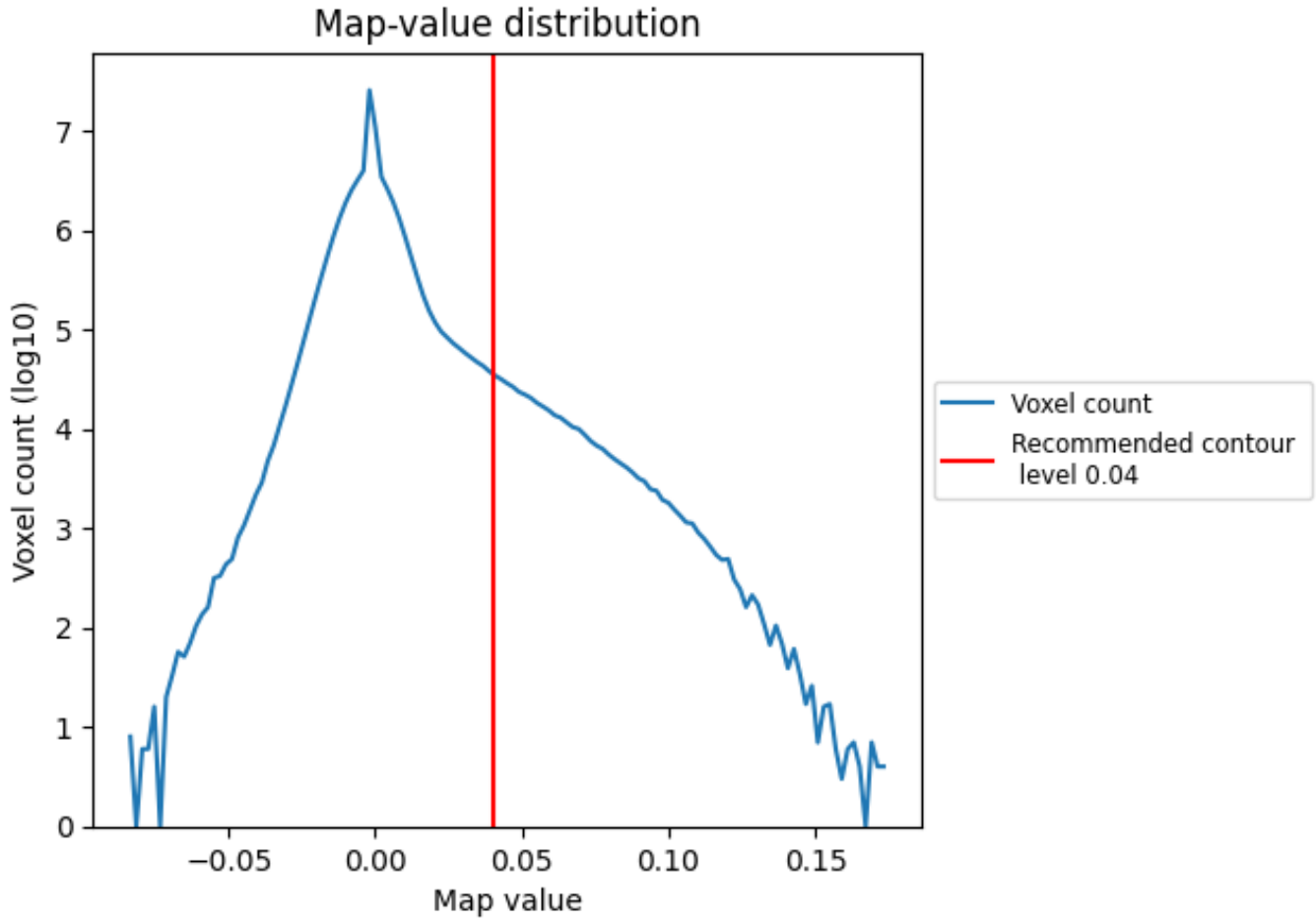
6.6 Mask visualisation (i)

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

7 Map analysis

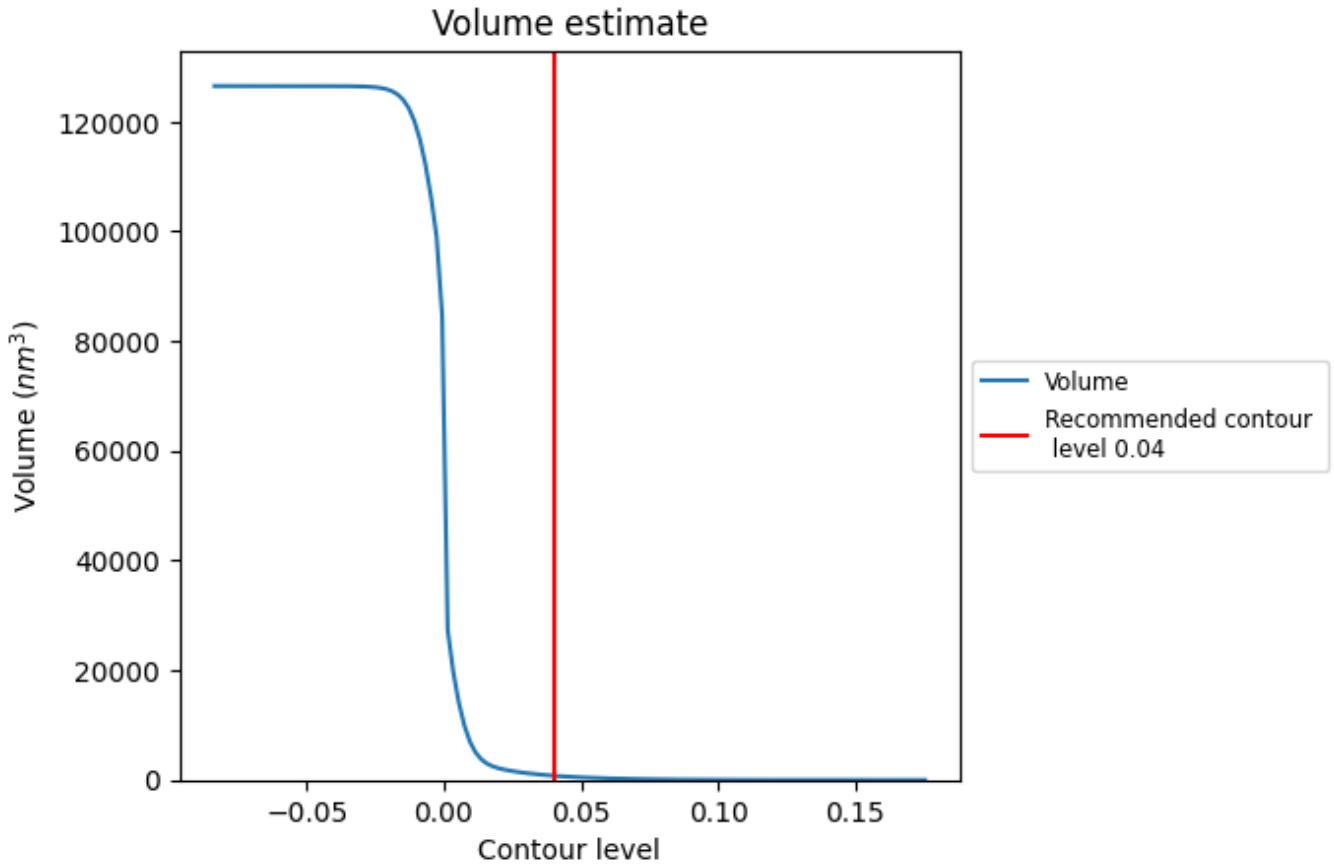
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

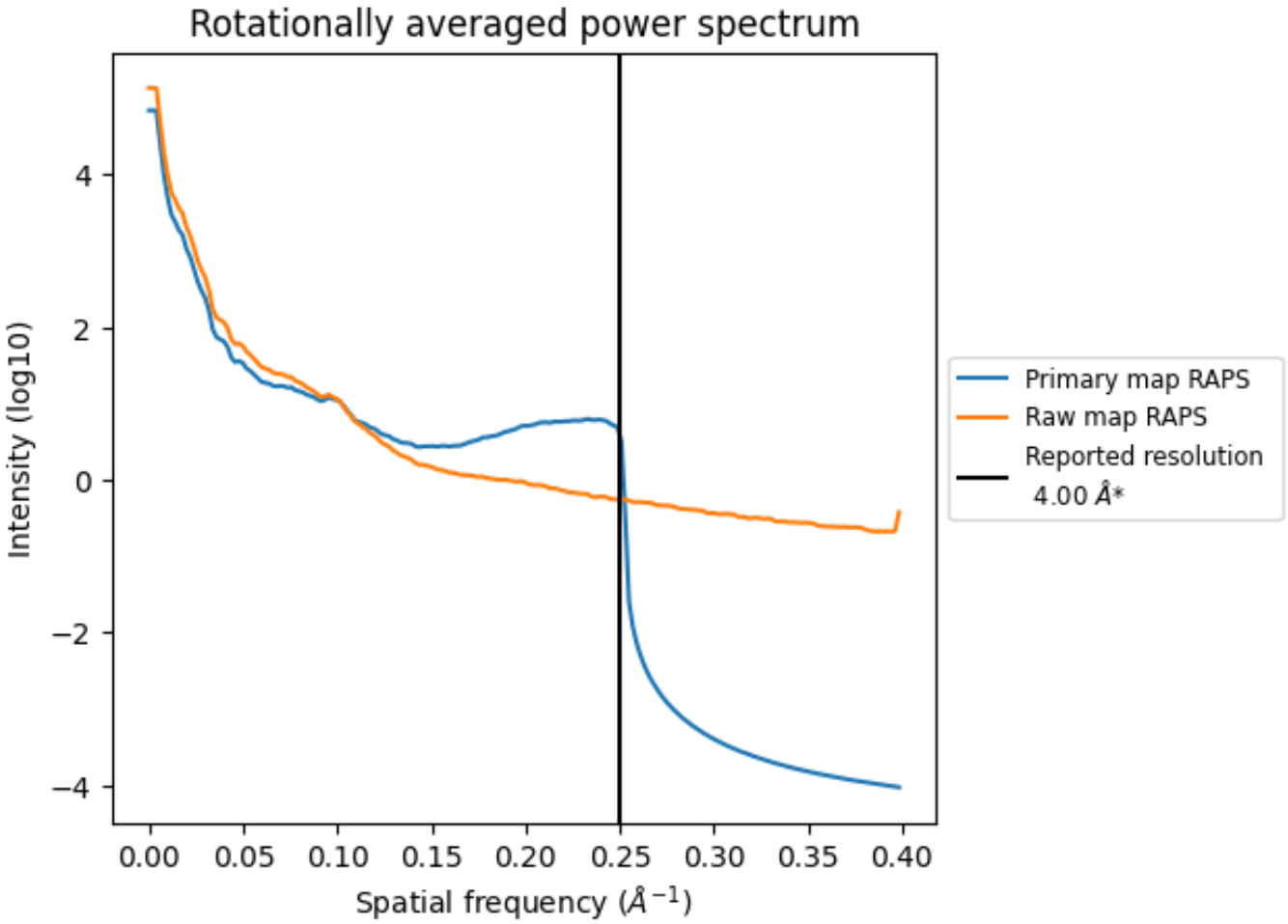
7.2 Volume estimate



The volume at the recommended contour level is 771 nm^3; this corresponds to an approximate mass of 696 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)

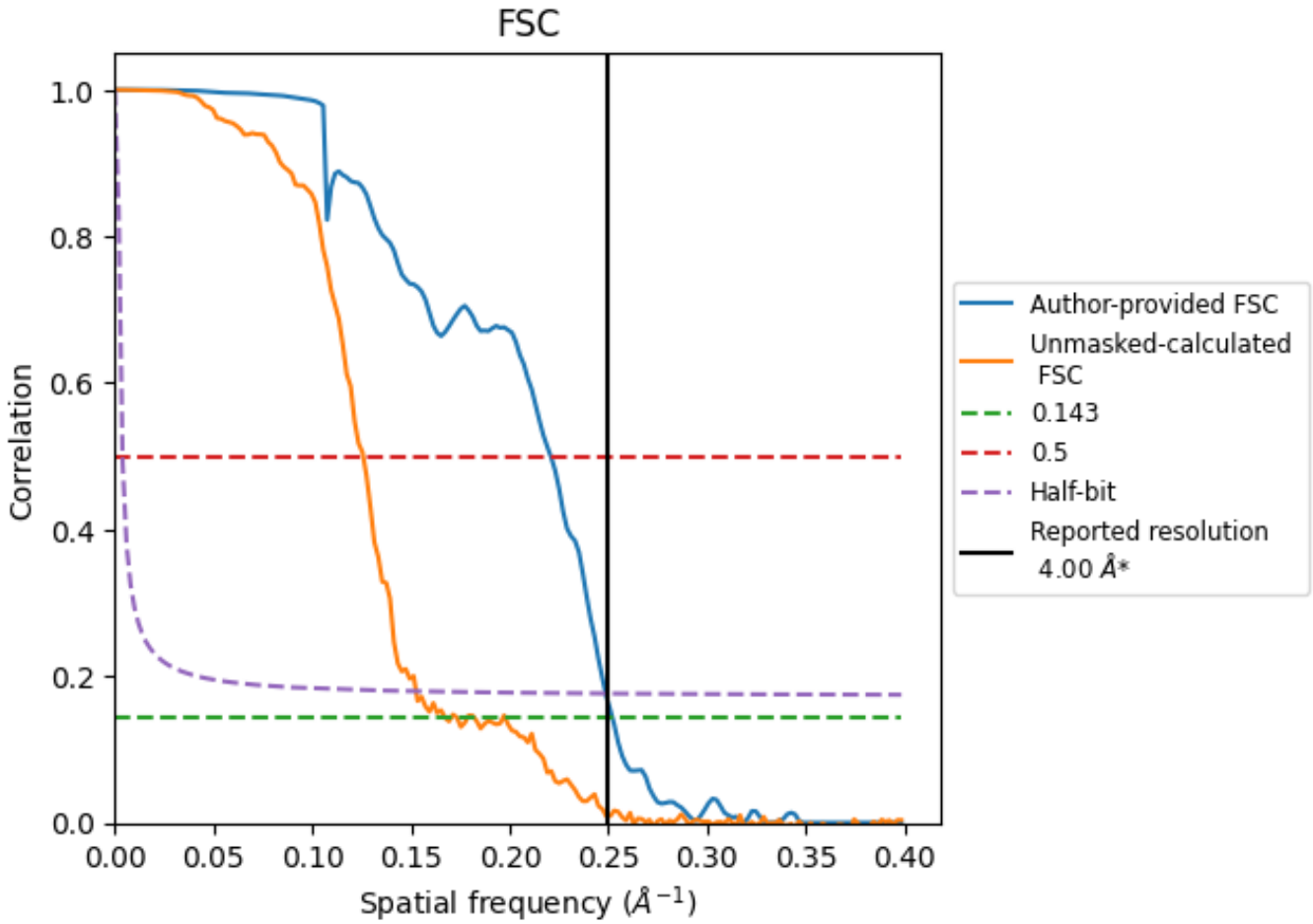


*Reported resolution corresponds to spatial frequency of 0.250 Å^{-1}

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 0.250 Å^{-1}

8.2 Resolution estimates (i)

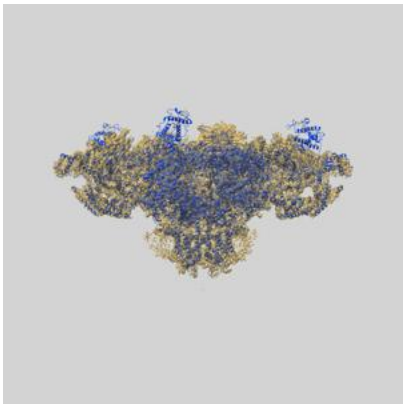
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	3.97	4.53	4.02
Unmasked-calculated*	5.97	7.95	6.55

*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 5.97 differs from the reported value 4.0 by more than 10 %

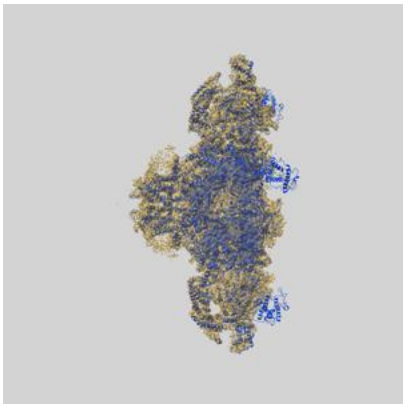
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-8372 and PDB model 5T9M. Per-residue inclusion information can be found in section 3 on page 5.

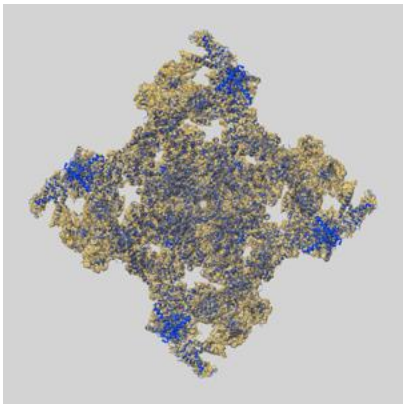
9.1 Map-model overlay



X



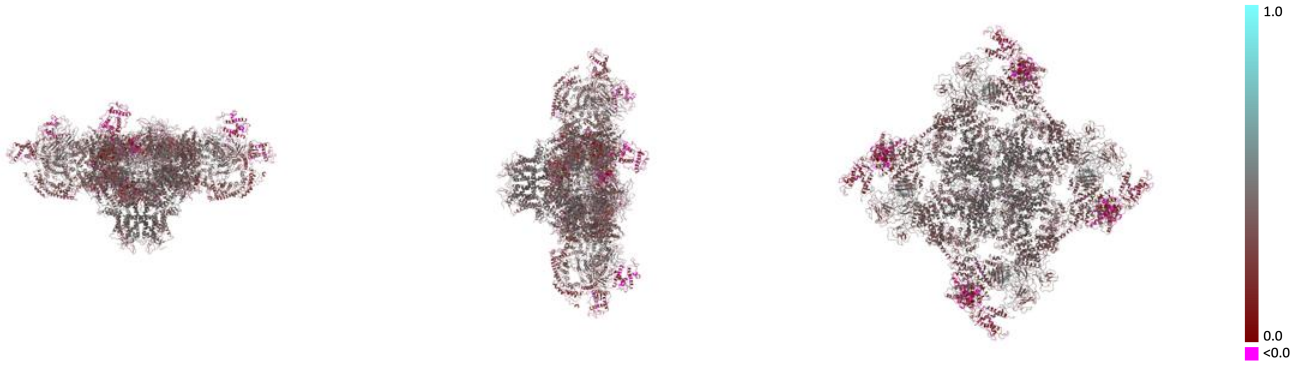
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 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.

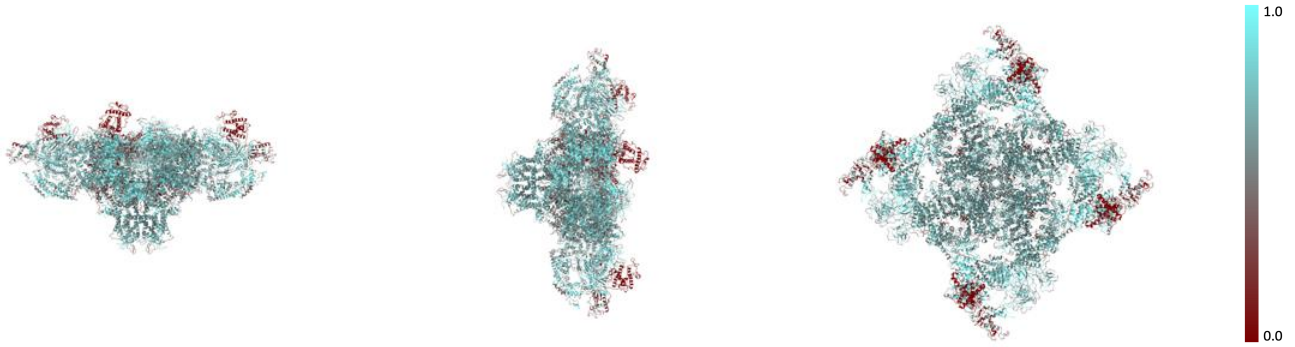
9.2 Q-score mapped to coordinate model



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.

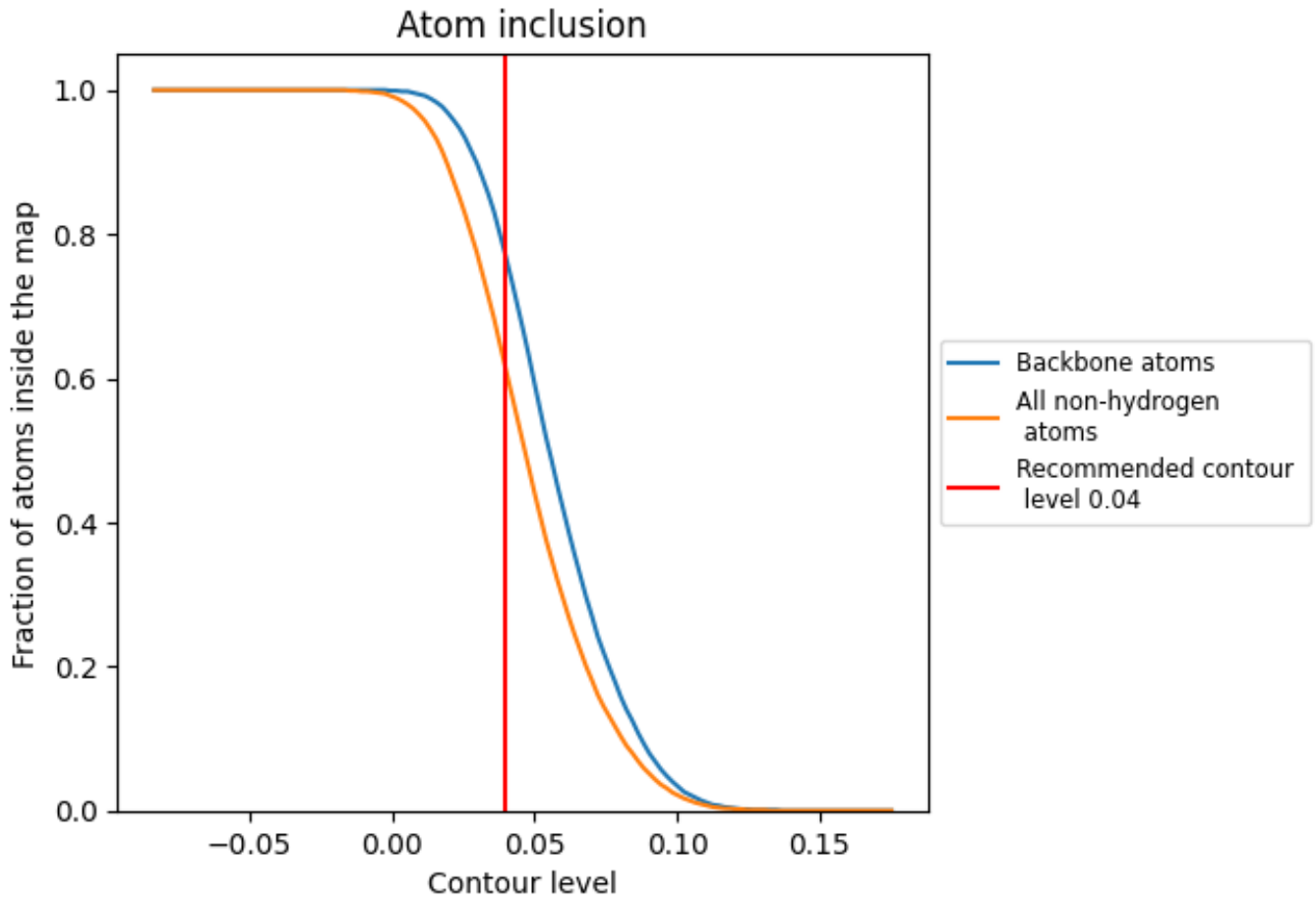
9.3 Atom inclusion mapped to coordinate model



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 (0.04).

9.4 Atom inclusion (i)



At the recommended contour level, 77% of all backbone atoms, 61% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6120	0.3470
A	0.6190	0.3590
B	0.6120	0.3470
E	0.6120	0.3470
F	0.6120	0.3630
G	0.6120	0.3470
H	0.6100	0.3650
I	0.6120	0.3470
J	0.6130	0.3660