Full wwPDB EM Validation Report ⓘ

Nov 11, 2026 – 03:10 PM EST

PDB ID	:	9Z9T / pdb_00009z9t
EMDB ID	:	EMD-73958
Title	:	Open-state rabbit RyR1 with activating ligands (Ca2+/ATP)
Authors	:	Chen, Y.S.; Van Petegem, F.
Deposited on	:	2025-11-18
Resolution	:	2.97 Å(reported)
Based on initial model	:	7TZC

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:

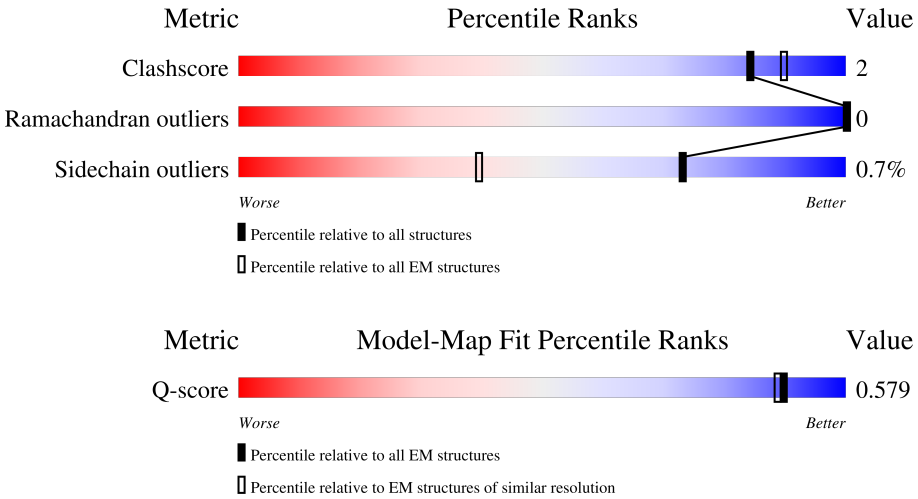
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

1 Overall quality at a glance

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

The reported resolution of this entry is 2.97 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.



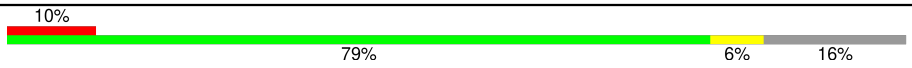
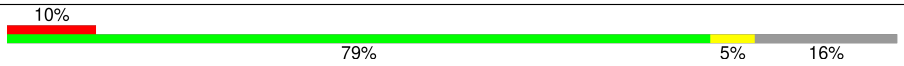
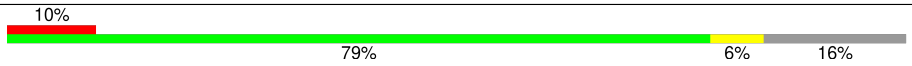
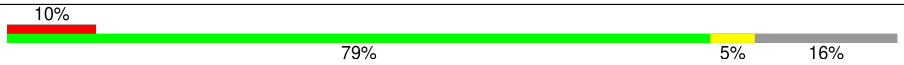
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13205 (2.47 - 3.47)

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	110	90% 7%
1	C	110	90% 8%
1	E	110	90% 8%
1	G	110	90% 8%

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Mol	Chain	Length	Quality of chain
2	B	5037	
2	D	5037	
2	F	5037	
2	H	5037	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 136324 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	A	108	Total	C	N	O	S	0	0
			819	516	144	155	4		
1	C	108	Total	C	N	O	S	0	0
			819	516	144	155	4		
1	E	108	Total	C	N	O	S	0	0
			819	516	144	155	4		
1	G	108	Total	C	N	O	S	0	0
			819	516	144	155	4		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP P68106
A	0	ASN	-	expression tag	UNP P68106
A	1	ALA	-	expression tag	UNP P68106
C	-1	SER	-	expression tag	UNP P68106
C	0	ASN	-	expression tag	UNP P68106
C	1	ALA	-	expression tag	UNP P68106
E	-1	SER	-	expression tag	UNP P68106
E	0	ASN	-	expression tag	UNP P68106
E	1	ALA	-	expression tag	UNP P68106
G	-1	SER	-	expression tag	UNP P68106
G	0	ASN	-	expression tag	UNP P68106
G	1	ALA	-	expression tag	UNP P68106

- Molecule 2 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4246	Total	C	N	O	S	4	0
			33229	21217	5745	6042	225		
2	D	4246	Total	C	N	O	S	4	0
			33229	21217	5745	6042	225		
2	F	4246	Total	C	N	O	S	4	0
			33229	21217	5745	6042	225		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	4246	Total 33229	C 21217	N 5745	O 6042	S 225	4	0

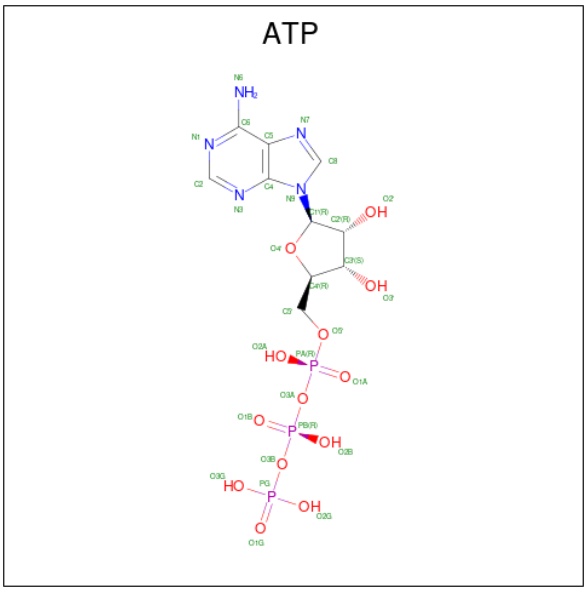
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
3	B	1	Total 1	Zn 1	0
3	D	1	Total 1	Zn 1	0
3	F	1	Total 1	Zn 1	0
3	H	1	Total 1	Zn 1	0

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
4	B	1	Total 1	Ca 1	0
4	D	1	Total 1	Ca 1	0
4	F	1	Total 1	Ca 1	0
4	H	1	Total 1	Ca 1	0

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
5	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	F	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	H	1	Total	C	N	O	P	0
			31	10	5	13	3	

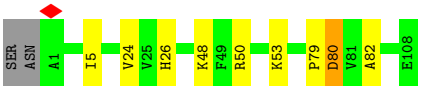
3 Residue-property plots (i)

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 A:

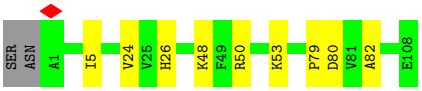




• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain C:

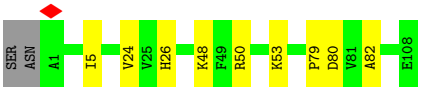




• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain E:

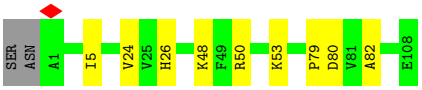




• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain G:

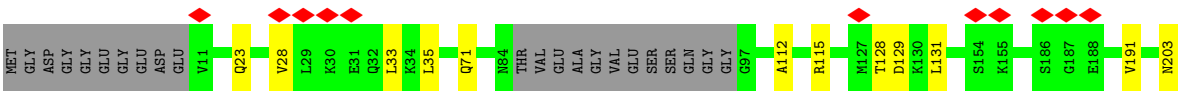


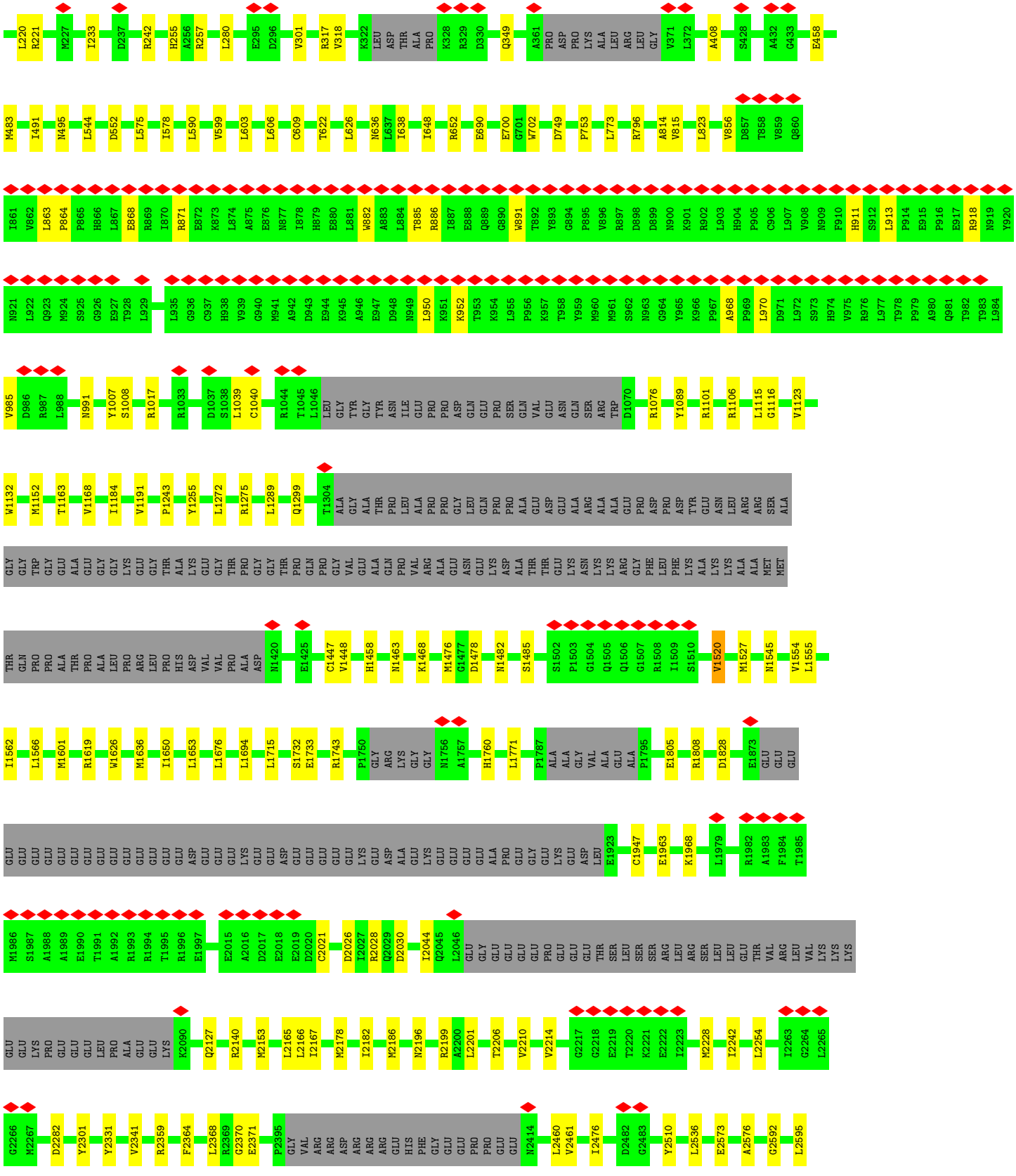


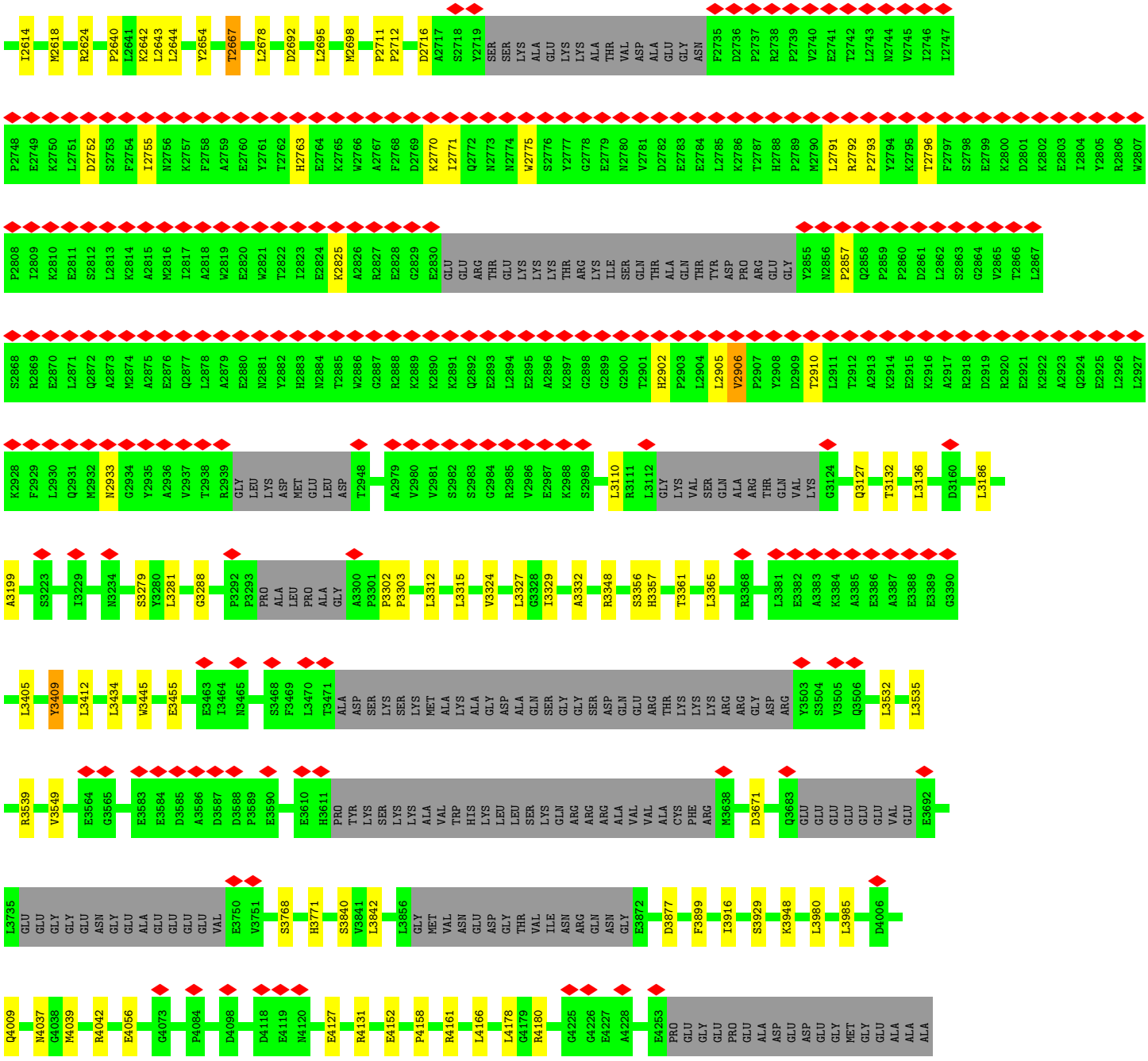
• Molecule 2: Ryanodine receptor 1

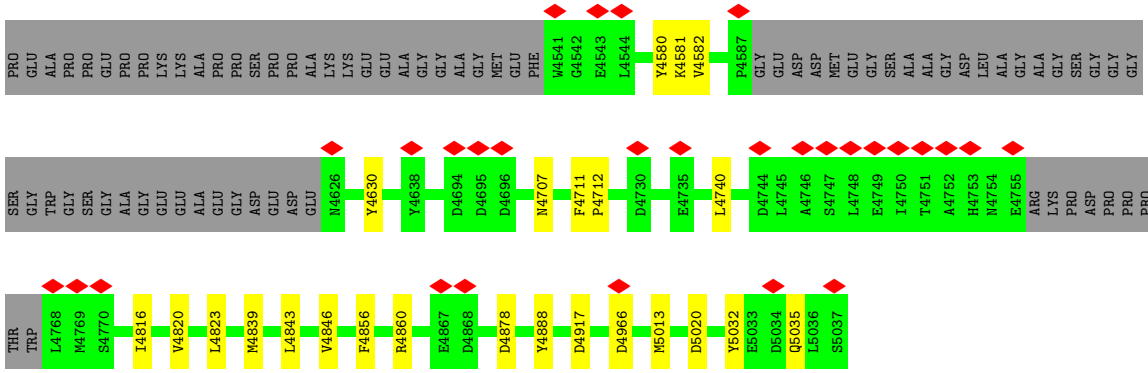
Chain B:






L220 R221 M227 I233 D237 R242 H255 A256 R257 L280 E295 D296 V301 R317 V318 K322 LEU ASP THR ALA PRO K328 R329 D330 Q349 A361 PRO ASP PRO LYS ALA LEU ARG LEU GLY V371 L372 A408 S428 A432 G433 E458
M483 I491 N495 L544 D552 L575 I578 L590 V599 L603 L606 C609 T622 L626 N636 L637 I638 I648 R652 E690 E700 G701 W702 D749 P753 L773 R796 A814 V815 L823 V856 D857 T858 V859 Q860
I861 V862 L863 P864 P865 H866 L867 E868 R869 I870 R871 E872 K873 L874 A875 E876 N877 I878 H879 E880 L881 W882 A883 L884 T885 R886 I887 E888 Q889 G890 W891 T892 Y893 G894 P895 V896 R897 D898 D899 N900 K901 R902 L903 H904 P905 C906 L907 V908 N909 F910 H911 S912 L913 P914 E915 P916 E917 R918 N919 Y920
N921 L922 Q923 M924 S925 G926 E927 T928 L929 L935 G936 C937 H938 V939 G940 M941 A942 D943 E944 K945 A946 E947 D948 N949 L950 K951 K952 T953 K954 L955 P956 K957 T958 Y959 M960 M961 S962 N963 G964 Y965 K966 P967 A968 P969 L970 D971 L972 S973 H974 V975 R976 L977 T978 P979 A980 Q981 T982 T983 L984
V985 D986 R987 L988 N991 Y1007 S1008 R1017 R1033 D1037 S1038 L1039 C1040 R1044 T1045 L1046 LEU GLY TYR GLY TYR ASN ILE GLU PRO PRO ASP GLN GLU PRO SER GLN VAL GLU ASN GLN SER ARG TRP D1070 R1076 Y1089 R1101 R1106 L1115 G1116 V1123
W1132 M1152 T1163 V1168 I1184 V1191 P1243 Y1255 L1272 R1275 L1289 Q1299 T1304 ALA GLY ALA THR PRO LEU ALA PRO PRO GLY LEU GLN PRO PRO ALA GLU ASP GLU ALA ARG ALA ALA GLU PRO ASP PRO ASP TYR GLU ASN LEU ARG ARG SER ALA
GLY GLY TRP GLY GLU ALA GLU GLY GLY LYS GLU GLY THR ALA LYS GLU GLY THR PRO GLY GLY THR PRO GLN PRO GLY VAL GLU ALA 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 ASP N1420 E1425 C1447 V1448 H1458 N1463 K1468 M1476 G1477 D1478 N1482 S1485 S1502 P1503 G1504 Q1505 Q1506 G1507 R1508 I1509 S1510 V1520 M1527 N1545 V1554 L1555
I1562 L1566 M1601 R1619 W1626 M1636 I1650 L1653 L1676 L1694 L1715 S1732 E1733 R1743 P1750 GLY ARG LYS GLY GLY N1756 A1757 H1760 L1771 P1787 ALA ALA GLY VAL ALA GLU ALA P1795 E1805 R1808 D1828 E1873 GLU 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 LYS GLU ASP ALA GLU LYS GLU GLU GLU GLU ALA PRO GLU GLY GLU LYS GLU ASP LEU E1923 C1947 E1963 K1968 L1979 R1982 A1983 F1984 T1985
M1986 S1987 A1988 A1989 E1990 T1991 A1992 R1993 R1994 T1995 R1996 E1997 E2015 A2016 D2017 E2018 E2019 D2020 C2021 D2026 I2027 R2028 Q2029 D2030 I2044 Q2045 L2046 GLU GLY GLU 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 LEU PRO ALA GLU GLU LYS K2090 Q2127 R2140 M2153 L2165 L2166 I2167 M2178 I2182 M2186 N2196 R2199 A2200 L2201 T2206 V2210 V2214 G2217 G2218 E2219 T2220 K2221 E2222 I2223 M2228 I2242 L2254 I2263 G2264 L2265
G2266 M2267 D2282 Y2301 Y2331 V2341 R2359 F2364 L2368 R2369 G2370 E2371 P2395 GLY VAL ARG ARG ASP ARG ARG ARG GLU HIS PHE GLY GLU GLU PRO PRO GLU GLU N2414 L2460 V2461 I2476 D2482 G2483 Y2510 L2536 E2573 A2576 G2592 L2595

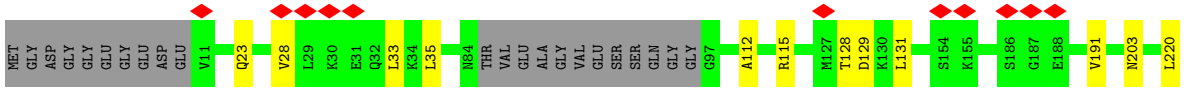

I2614 M2618 R2624 P2640 L2641 K2642 L2643 L2644 Y2654 T2667 L2678 D2692 L2695 M2698 P2711 P2712 D2716 A2717 S2718 Y2719 SER SER LYS ALA GLU LYS LYS ALA THR VAL ASP ALA GLU GLY ASN F2735 D2736 P2737 R2738 P2739 V2740 E2741 T2742 L2743 N2744 V2745 I2746 I2747
P2748 E2749 K2750 L2751 D2752 S2753 F2754 I2755 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 LEU ASP T2948 A2979 V2980 V2981 S2982 S2983 G2984 R2985 V2986 E2987 K2988 S2989 L3110 R3111 L3112 GLY LYS VAL SER GLN ALA ARG THR GLN VAL LYS G3124 Q3127 T3132 L3136 D3160 L3186
A3199 S3223 I3229 N3234 S3279 Y3280 L3281 G3288 P3292 P3293 PRO ALA LEU PRO ALA GLY A3300 P3301 P3302 P3303 L3312 L3315 V3324 L3327 G3328 I3329 A3332 R3348 S3356 H3357 T3361 L3365 R3368 L3381 E3382 A3383 K3384 A3385 E3386 A3387 E3388 E3389 G3390
L3405 Y3409 L3412 L3434 W3445 E3455 E3463 I3464 N3465 S3468 F3469 L3470 T3471 ALA ASP SER LYS SER LYS MET ALA LYS ALA GLY ASP ALA GLN SER GLY GLY SER ASP GLN GLU ARG THR LYS LYS LYS ARG ARG GLY ASP ARG Y3503 S3504 V3505 Q3506 L3532 L3535
B3539 V3549 E3564 G3565 E3583 E3584 D3585 A3586 D3587 D3588 P3589 E3590 E3610 H3611 PRO TYR LYS SER LYS LYS ALA VAL TRP HIS LYS LEU LEU SER LYS GLN ARG ARG ARG ALA VAL VAL ALA CYS PHE ARG M3638 D3671 Q3683 GLU GLU GLU GLU GLU GLU VAL E3692
L3735 GLU GLU GLY GLY GLU ASN GLY GLU ALA GLU GLU GLU GLU VAL E3750 V3751 S3768 H3771 S3840 V3841 L3842 L3856 GLY MET VAL ASN GLU ASP GLY THR VAL ILE ASN ARG GLN ASN GLY E3872 D3877 F3899 I3916 S3929 K3948 L3980 L3985 D4006
Q4009 N4037 G4038 M4039 R4042 E4056 G4073 P4084 D4098 D4118 E4119 N4120 E4127 R4131 E4152 P4158 R4161 L4166 L4178 G4179 R4180 G4225 G4226 E4227 A4228 E4253 PRO GLU GLY GLU PRO GLU ALA ASP GLU ASP GLU GLY MET GLY GLU ALA ALA ALA
GLU GLY ALA GLU GLU GLY ALA ALA GLY ALA ALA GLY ALA GLU GLY ALA ALA GLY THR VAL ALA ALA GLY ALA THR ARG LEU ALA ALA ALA ARG ARG GLY LEU SER TYR ARG SER LEU ARG ARG ARG VAL ARG ARG LEU ARG ARG LEU THR ALA ARG GLU ALA ALA THR ALA LEU
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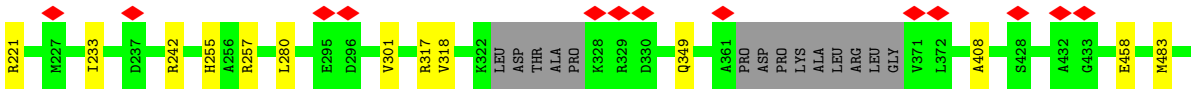


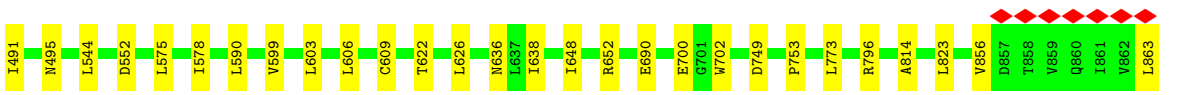
• Molecule 2: Ryanodine receptor 1

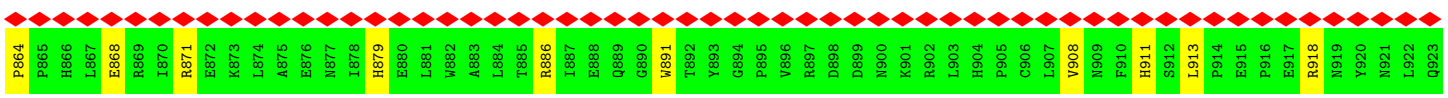
Chain D:

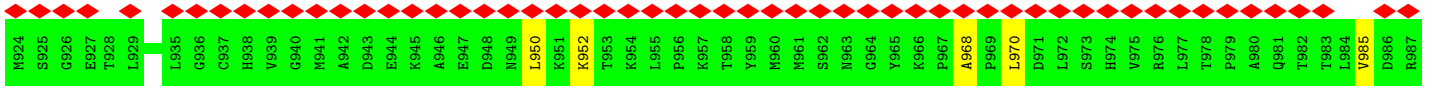


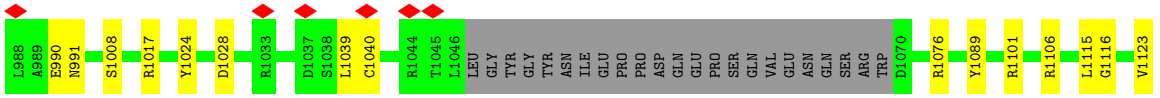


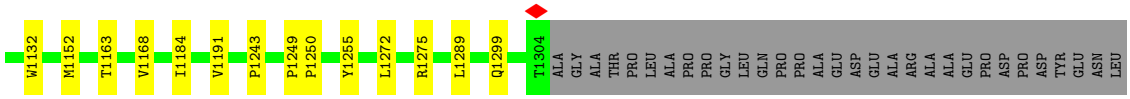


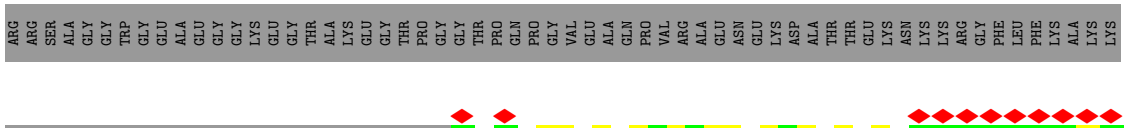


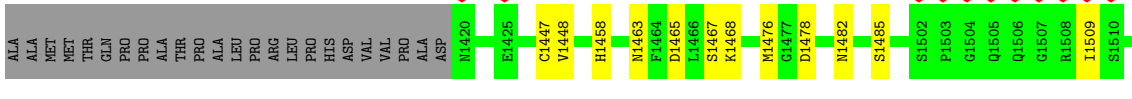


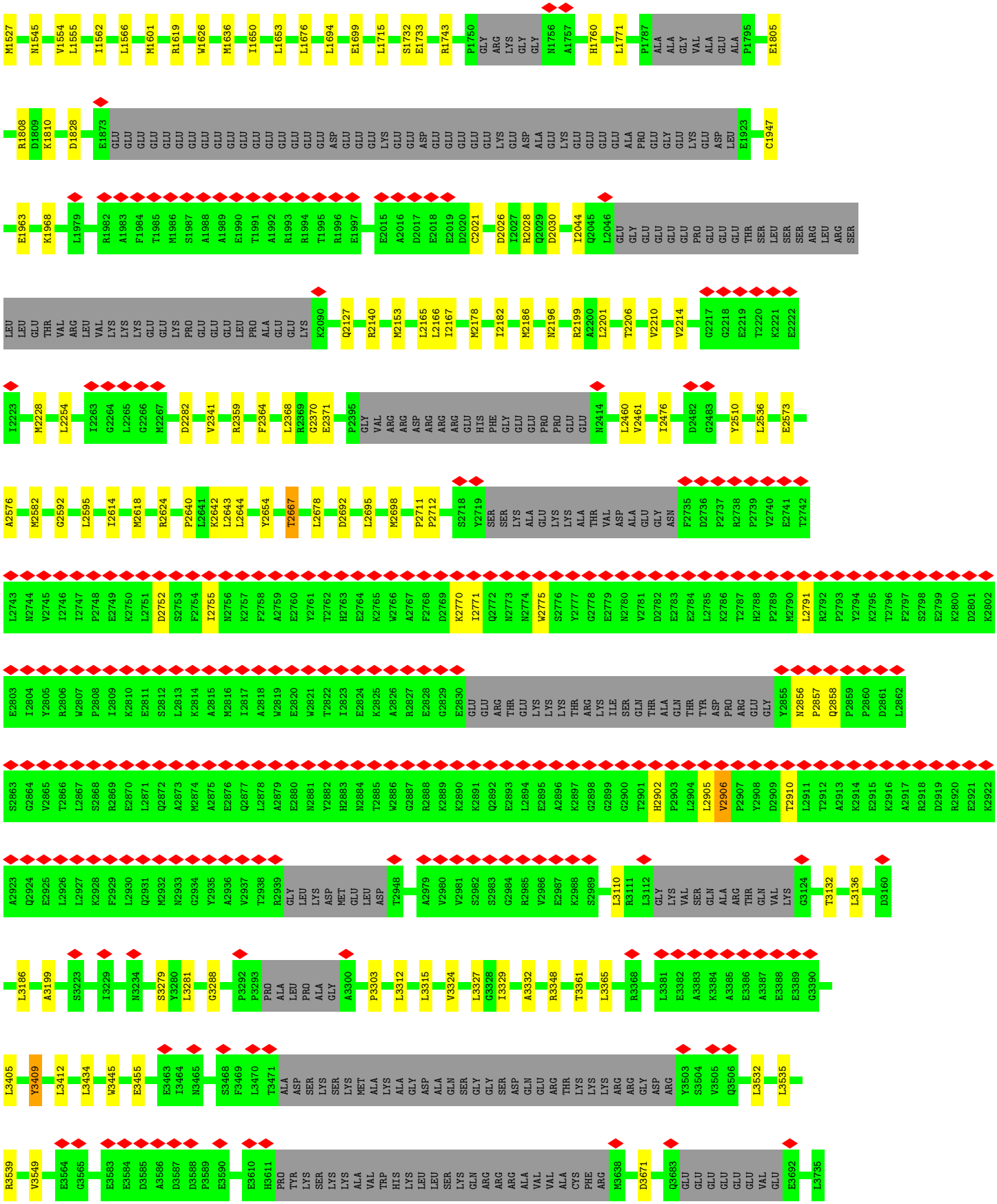


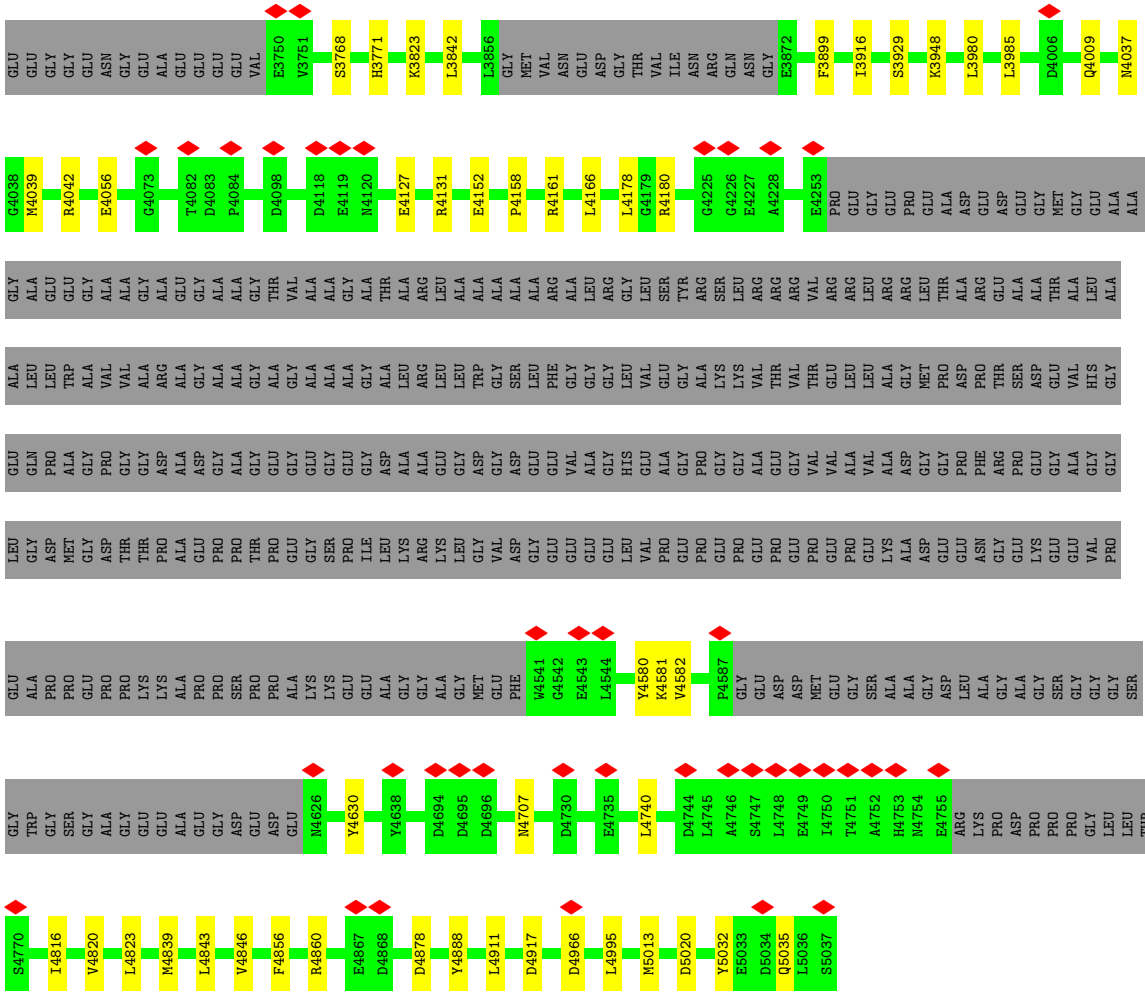








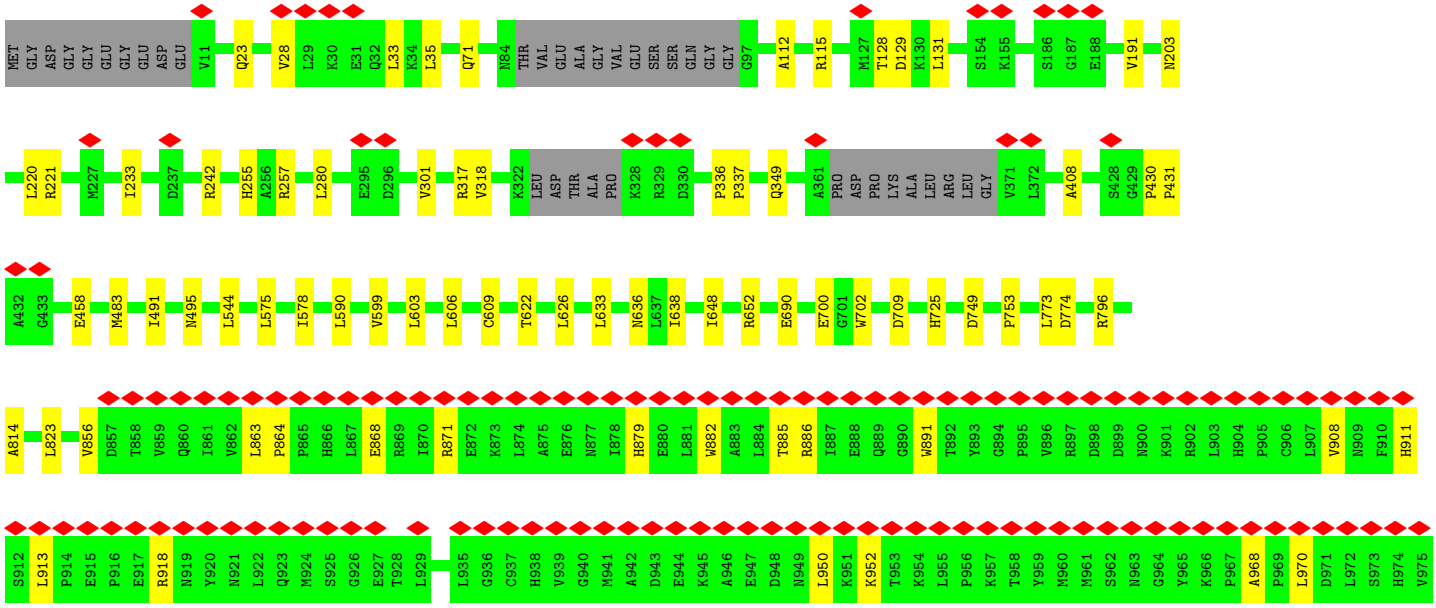

M1527 N1545 V1554 L1555 I1562 L1566 M1601 R1619 W1626 M1636 I1650 L1663 L1676 L1694 E1699 L1715 S1732 E1733 R1743 P1750 GLY ARG LYS GLY N1756 A1757 H1760 L1771 P1787 ALA ALA GLY VAL ALA GLU ALA P1795 E1805
R1808 D1809 K1810 D1828 E1873 GLU GLU GLU

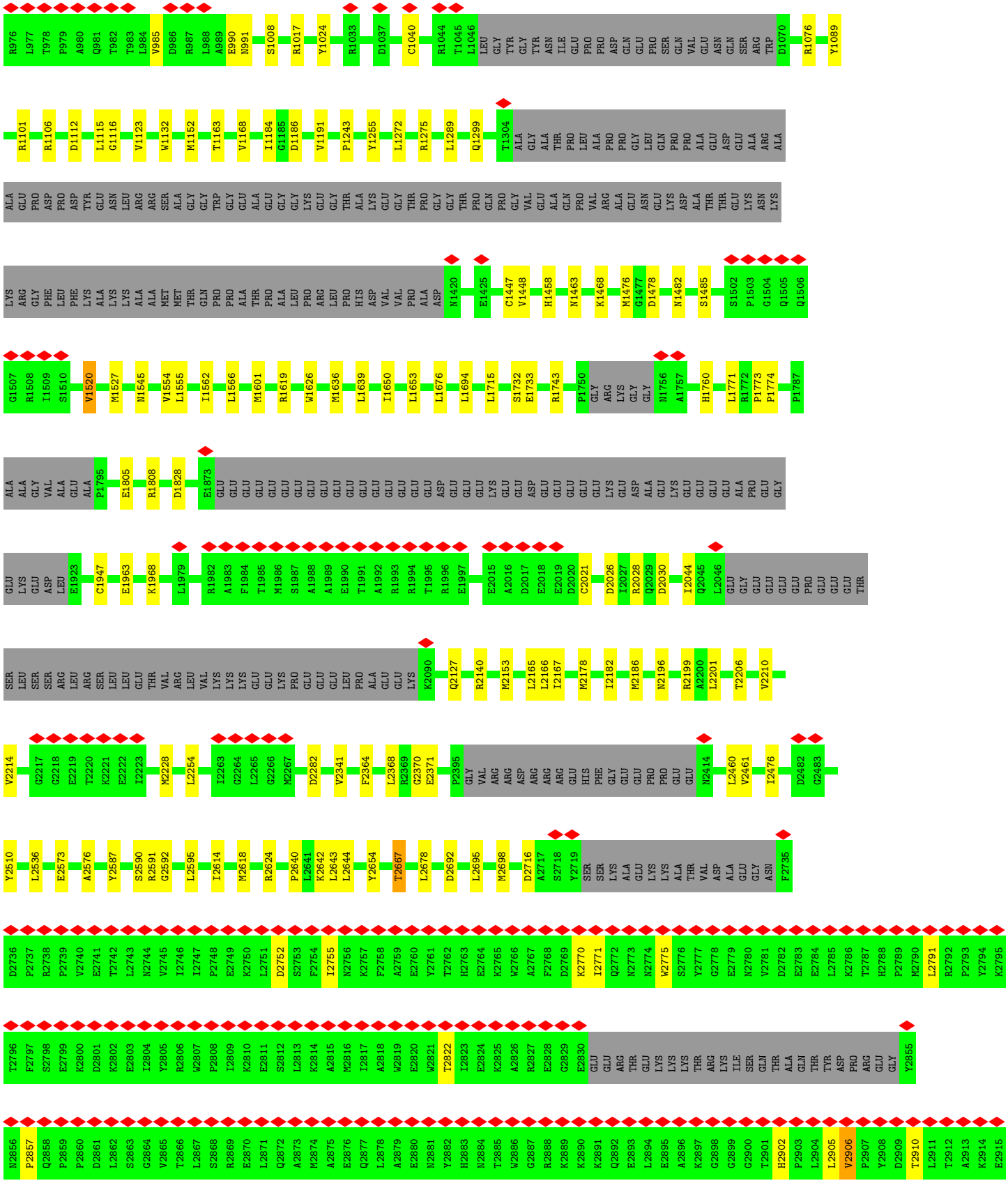


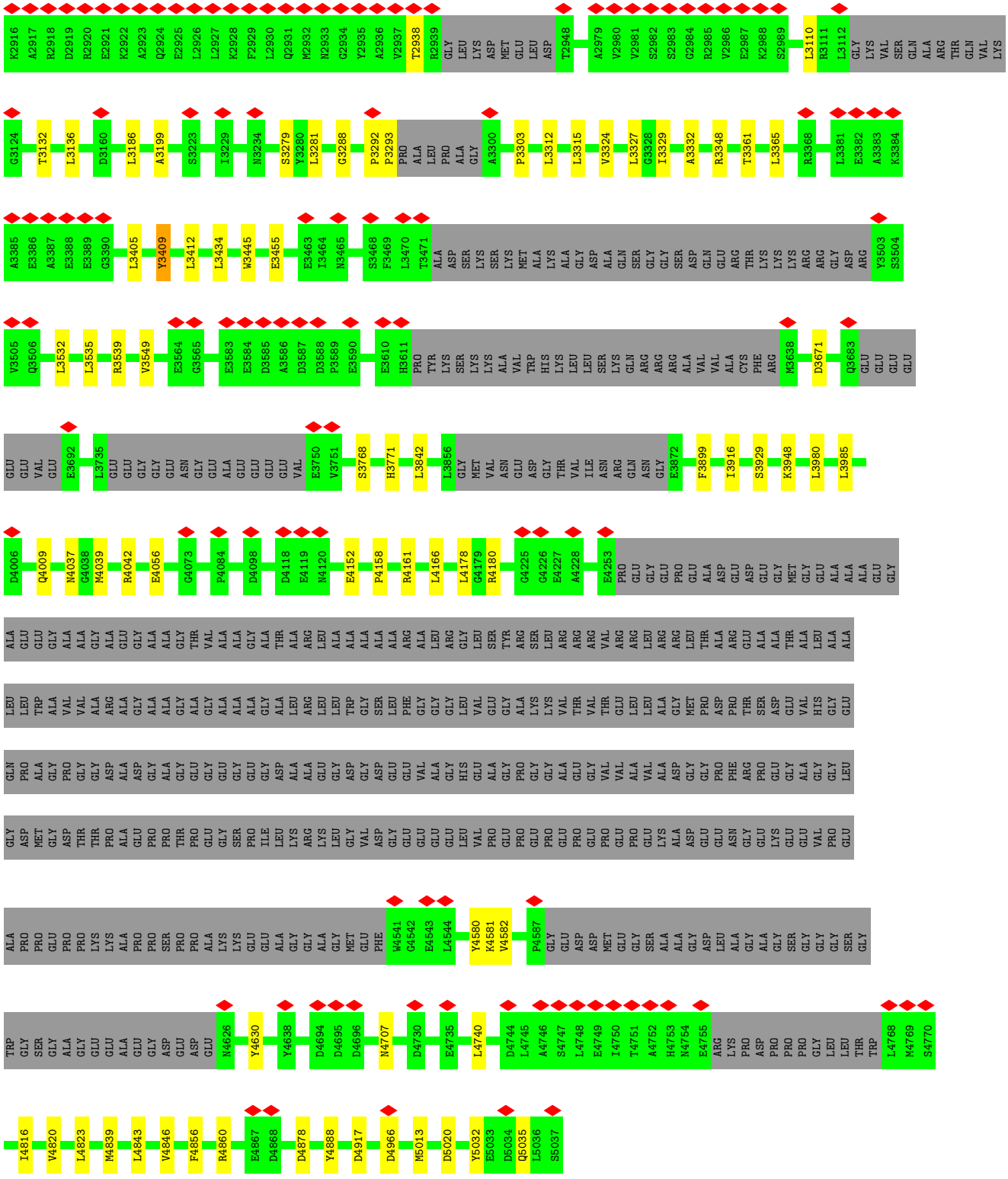
• Molecule 2: Ryanodine receptor 1

Chain F:





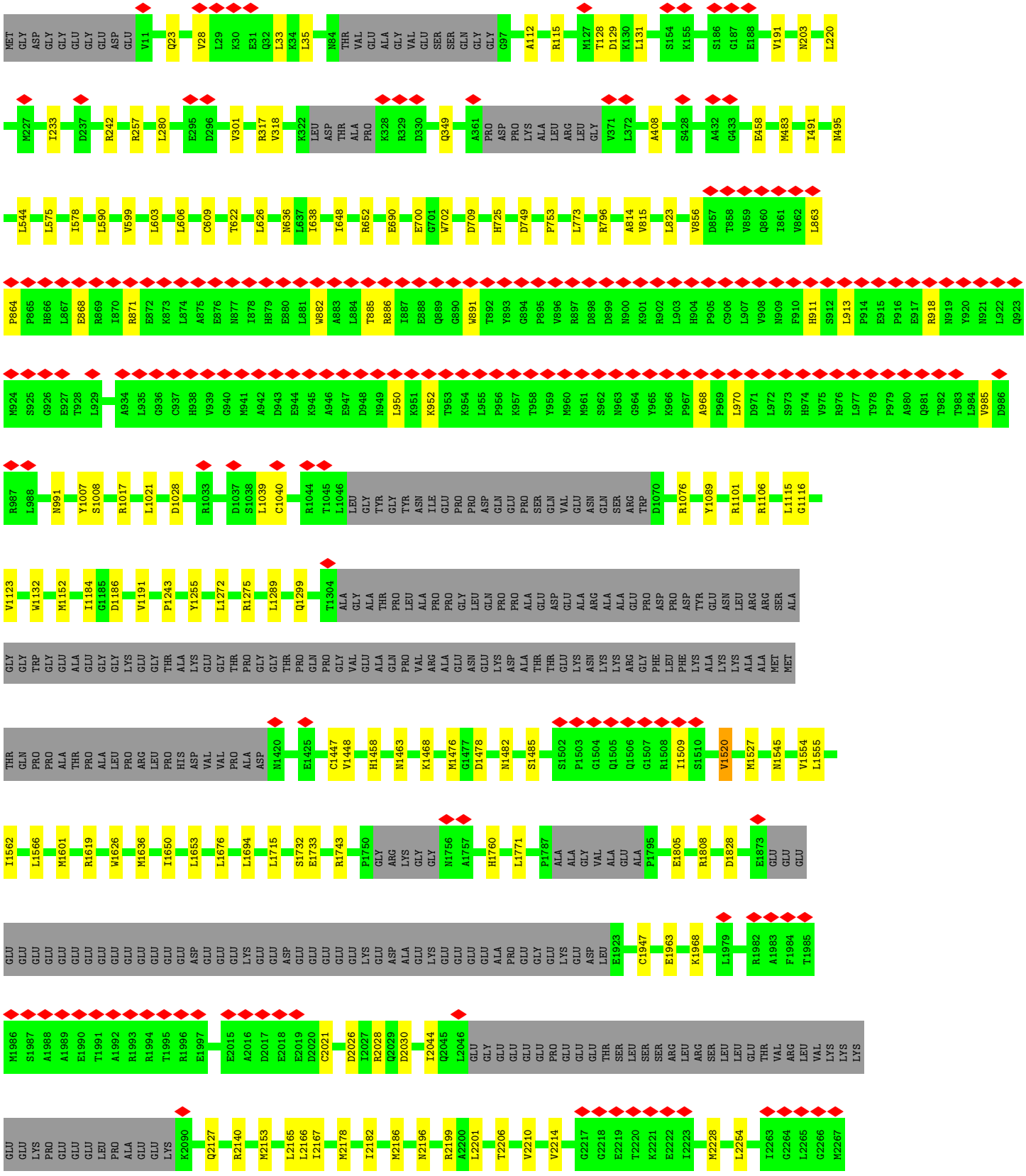

R976 L977 T978 P979 A980 Q981 T982 T983 L984 V985 D986 R987 L988 A989 E990 N991 S1008 R1017 Y1024 R1033 D1037 C1040 R1044 T1045 L1046 LEU GLY TYR GLY TYR ASN ILE GLU PRO PRO ASP GLN GLU PRO SER GLN VAL GLU ASN GLN SER ARG TRP D1070 R1076 Y1089
R1101 R1106 D1112 L1115 G1116 V1123 W1132 M1152 T1163 V1168 I1184 G1185 D1186 V1191 P1243 Y1255 L1272 R1275 L1289 Q1299 T1304 ALA GLY ALA THR PRO LEU ALA PRO PRO GLY LEU GLN PRO PRO ALA GLU ASP GLU ALA ARG ALA
ALA GLU PRO ASP PRO ASP TYR GLU ASN LEU ARG ARG SER ALA GLY GLY TRP GLY GLU ALA GLU GLY GLY LYS GLU GLY THR ALA LYS GLU GLY THR PRO GLY GLY THR PRO GLN PRO GLY VAL GLU ALA 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 ASP N1420 E1425 C1447 V1448 H1458 N1463 K1468 M1476 G1477 D1478 N1482 S1485 S1502 P1503 G1504 Q1505 Q1506
G1507 R1508 I1509 S1510 V1520 M1527 N1545 V1554 L1555 I1562 L1566 M1601 R1619 W1626 M1636 L1639 I1650 L1653 L1676 L1694 L1715 S1732 E1733 R1743 P1750 GLY ARG LYS GLY GLY N1756 A1757 H1760 L1771 R1772 P1773 P1774 P1787
ALA ALA GLY VAL ALA GLU ALA P1795 E1805 R1808 D1828 E1873 GLU GLU GLU

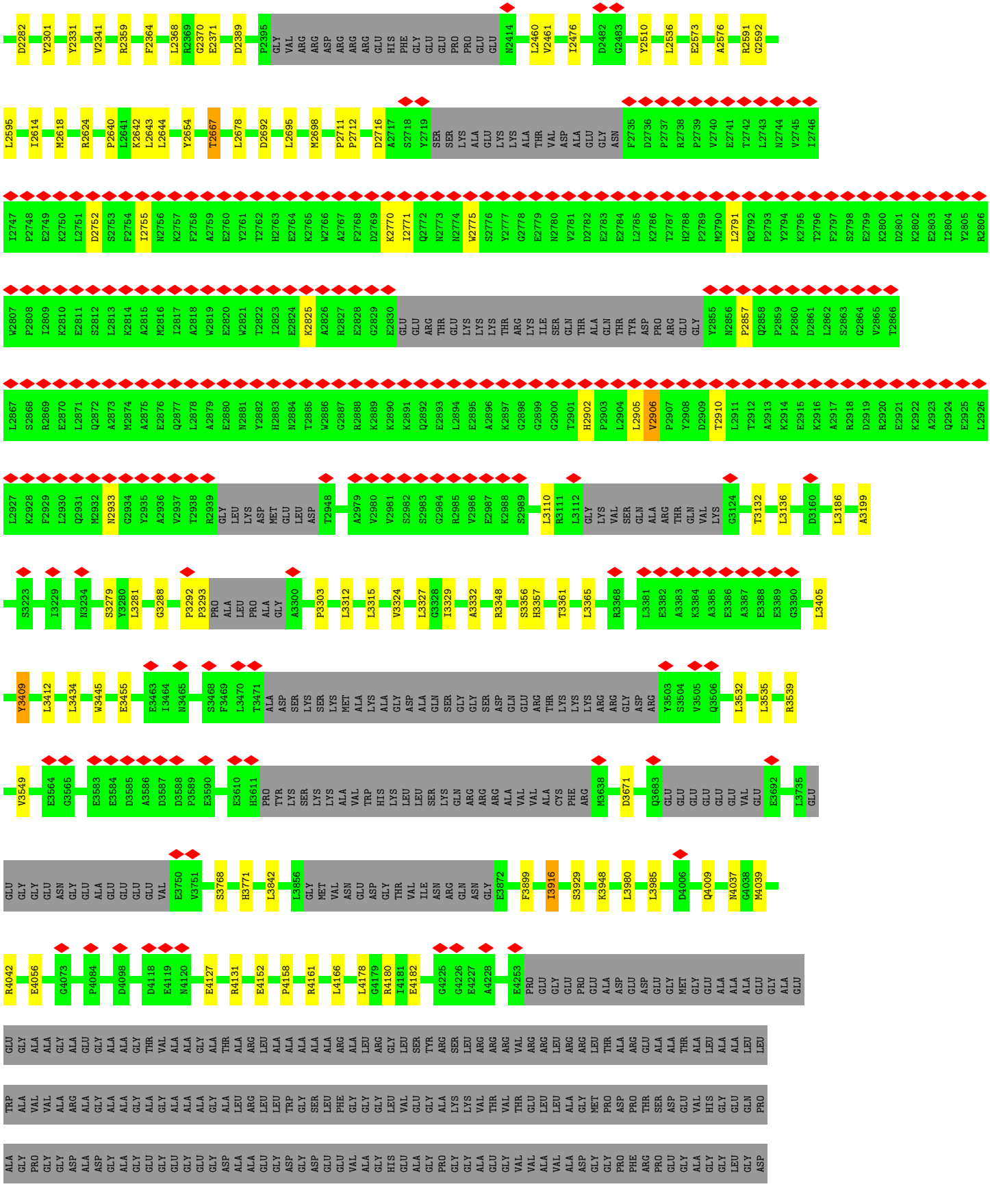


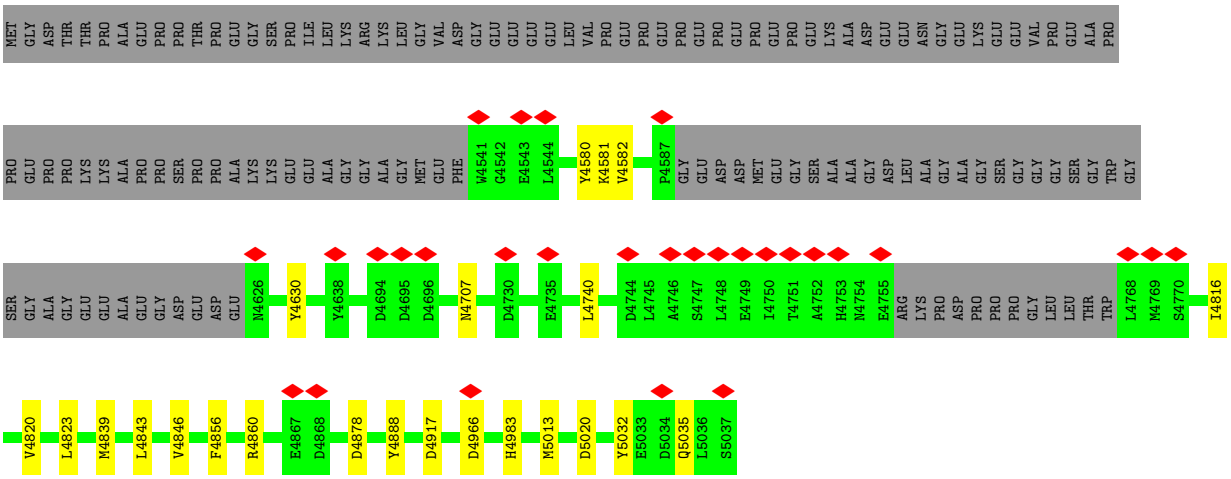
• Molecule 2: Ryanodine receptor 1

Chain H:




MET GLY ASP GLY GLY GLU GLY GLU ASP GLU V11 Q23 V28 L29 K30 E31 Q32 L33 K34 L35 N84 THR VAL GLU ALA GLY VAL GLU SER SER GLN GLY GLY G97 A112 R115 M127 T128 D129 K130 L131 S154 K155 S186 G187 E188 V191 N203 L220
M227 I233 D237 R242 R257 L280 E295 D296 V301 R317 V318 K322 LEU ASP THR ALA PRO K328 R329 D330 Q349 A361 PRO ASP PRO LYS ALA LEU ARG LEU GLY V371 L372 A408 S428 A432 G433 E458 M483 I491 N495
L544 L575 I578 L590 V599 L603 L606 C609 T622 L626 N636 L637 I638 I648 R652 E690 E700 G701 W702 D709 H725 D749 P753 L773 R796 A814 V815 L823 V856 D857 T858 V859 Q860 I861 V862 L863
P864 P865 H866 L867 E868 R869 I870 R871 E872 K873 L874 A875 E876 N877 I878 H879 E880 L881 W882 A883 L884 T885 R886 I887 E888 Q889 G890 W891 T892 Y893 G894 P895 V896 R897 D898 D899 N900 K901 R902 L903 H904 P905 C906 L907 V908 N909 P910 H911 S912 L913 P914 E915 P916 E917 R918 N919 Y920 N921 L922 Q923
M924 S925 G926 E927 T928 L929 A934 L935 G936 C937 H938 V939 G940 M941 A942 D943 E944 K945 A946 E947 D948 N949 L950 K951 K952 T953 K954 L955 P956 K957 T958 Y959 M960 M961 S962 N963 G964 Y965 K966 P967 A968 P969 L970 D971 L972 S973 H974 V975 R976 L977 T978 P979 A980 Q981 T982 T983 L984 V985 D986
R987 L988 N991 Y1007 S1008 R1017 L1021 D1028 R1033 D1037 S1038 L1039 C1040 R1044 T1045 L1046 LEU GLY TYR GLY TYR ASN ILE GLU PRO PRO ASP GLN GLU PRO SER GLN VAL GLU ASN GLN SER ARG TRP D1070 R1076 Y1089 R1101 R1106 L1115 G1116
V1123 W1132 M1152 I1184 G1185 D1186 V1191 P1243 Y1255 L1272 R1275 L1289 Q1299 T1304 ALA GLY ALA THR PRO LEU ALA PRO PRO GLY LEU GLN PRO PRO ALA GLU ASP GLU ALA ARG ALA ALA GLU PRO ASP PRO ASP TYR GLU ASN LEU ARG ARG SER ALA
GLY GLY TRP GLY GLU ALA GLU GLY GLY LYS GLU GLY THR ALA LYS GLU GLY THR PRO GLY GLY THR PRO GLN PRO GLY VAL GLU ALA 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 ASP N1420 E1425 C1447 V1448 H1458 N1463 K1468 M1476 G1477 D1478 N1482 S1485 S1502 P1503 G1504 Q1505 Q1506 G1507 R1508 I1509 S1510 V1520 M1527 N1545 V1554 L1555
I1562 L1566 M1601 R1619 W1626 M1636 I1650 L1653 L1676 L1694 L1715 S1732 E1733 R1743 P1750 GLY ARG LYS GLY GLY N1756 A1757 H1760 L1771 P1787 ALA ALA GLY VAL ALA GLU ALA P1795 E1805 R1808 D1828 E1873 GLU GLU GLU
GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU ASP GLU GLU GLU LYS GLU GLU GLU ASP GLU GLU GLU GLU GLU LYS GLU GLU ASP ALA GLU LYS GLU GLU GLU GLU ALA PRO GLU GLY GLU LYS GLU GLU ASP LEU E1923 C1947 E1963 K1968 L1979 R1982 A1983 F1984 T1985
M1986 S1987 A1988 A1989 E1990 T1991 A1992 R1993 R1994 T1995 R1996 E1997 E2015 A2016 D2017 E2018 E2019 D2020 C2021 D2026 I2027 R2028 Q2029 D2030 I2044 Q2045 L2046 GLU GLY GLU 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 LEU PRO ALA GLU GLU LYS K2090 Q2127 R2140 M2153 L2165 L2166 I2167 M2178 I2182 M2186 N2196 R2199 A2200 L2201 T2206 V2210 V2214 G2217 G2218 E2219 T2220 K2221 E2222 I2223 M2228 L2254 I2263 G2264 L2265 G2266 M2267


D2282 Y2301 Y2331 V2341 R2359 F2364 L2368 R2369 G2370 E2371 D2389 P2395 GLY VAL ARG ARG ASP ARG ARG ARG GLU HIS PHE GLY GLU GLU PRO PRO GLU GLU N2414 L2460 V2461 I2476 D2482 G2483 Y2510 L2536 E2573 A2576 R2591 G2592
L2595 I2614 M2618 R2624 P2640 L2641 K2642 L2643 L2644 Y2654 T2667 L2678 D2692 L2695 M2698 P2711 P2712 D2716 A2717 S2718 Y2719 SER SER LYS ALA GLU LYS LYS ALA THR VAL ASP ALA GLU GLY ASN 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 LEU ASP T2948 A2979 V2980 V2981 S2982 S2983 G2984 R2985 V2986 E2987 K2988 S2989 L3110 R3111 L3112 GLY LYS VAL SER GLN ALA ARG THR GLN VAL LYS G3124 T3132 L3136 D3160 L3186 A3199
S3223 I3229 N3234 S3279 Y3280 L3281 G3288 P3292 P3293 PRO ALA LEU PRO ALA GLY A3300 P3303 L3312 L3315 V3324 L3327 G3328 I3329 A3332 R3348 S3356 H3357 T3381 L3365 R3368 L3381 E3382 A3383 K3384 A3385 E3386 A3387 E3388 E3389 G3390 L3405
Y3409 L3412 L3434 W3445 E3455 E3463 I3464 N3465 S3468 F3469 L3470 T3471 ALA ASP SER LYS SER LYS MET ALA LYS ALA GLY ASP ALA GLN SER GLY GLY SER ASP GLN GLU ARG THR LYS LYS LYS ARG ARG GLY ASP ARG Y3503 S3504 V3505 Q3506 L3532 L3535 R3539
V3549 E3564 G3565 E3583 E3584 D3585 A3586 D3587 D3588 P3589 E3590 E3610 H3611 PRO TYR LYS SER LYS LYS ALA VAL TRP HIS LYS LEU LEU SER LYS GLN ARG ARG ARG ALA VAL VAL ALA CYS PHE ARG M3638 D3671 Q3683 GLU GLU GLU GLU GLU GLU VAL GLU E3692 L3735 GLU
GLU GLY GLY GLU ASN GLY GLU ALA GLU GLU GLU GLU VAL E3750 V3751 S3768 H3771 L3842 L3856 GLY MET VAL ASN GLU ASP GLY THR VAL ILE ASN ARG GLN ASN GLY E3872 F3899 I3916 S3929 K3948 L3980 L3985 D4006 Q4009 N4037 G4038 M4039
R4042 E4056 G4073 P4084 D4098 D4118 E4119 N4120 E4127 R4131 E4152 P4158 R4161 L4166 L4178 G4179 R4180 I4181 E4182 G4225 G4226 E4227 A4228 E4253 PRO GLU GLY GLU PRO GLU ALA ASP GLU ASP GLU GLY MET GLY GLU ALA ALA ALA GLU GLY ALA GLU
GLU GLY ALA ALA GLY ALA GLU GLY ALA ALA GLY GLY THR VAL ALA ALA ALA GLY ALA THR ALA ARG LEU ALA ALA ALA ARG ALA LEU ARG ARG ARG ARG VAL ARG ARG LEU ARG ARG LEU THR ALA ARG GLU ALA ALA THR ALA LEU ALA ALA LEU LEU
TRP ALA VAL VAL ALA ARG ALA ALA ALA GLY GLY ALA ALA GLY GLY ALA ALA GLY GLY ALA LEU ARG LEU LEU TRP GLY SER LEU PHE GLY GLY LEU VAL GLU GLY ALA LYS LYS VAL ALA THR VAL THR GLU LEU LEU ALA ALA LEU ALA GLY PRO PRO THR SER ASP GLU VAL HIS GLY GLU GLN PRO
ALA GLY PRO GLY GLY ASP ALA ASP GLY GLU GLY GLU GLY GLU GLU GLY ASP ALA ALA GLU GLY ASP GLY ASP GLU GLU GLY ALA GLY HIS GLU ALA GLY PRO GLY GLY ALA GLU GLY VAL ALA ALA VAL ALA ASP GLY GLY PRO PRO PHE ARG PRO GLU GLY ALA GLY GLY LEU GLY ASP


MET GLY ASP THR THR PRO ALA GLU PRO PRO THR 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 GLY 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 W4541 G4542 E4543 L4544 Y4580 K4581 V4582 P4587 GLY GLU ASP ASP MET GLU GLY SER ALA ALA GLY ASP LEU ALA GLY ALA GLY SER GLY GLY GLY SER GLY TRP GLY
SER GLY ALA GLY GLU GLU ALA GLU GLY ASP GLU ASP GLU M4626 Y4630 Y4638 D4694 D4695 D4696 M4707 D4730 E4735 L4740 D4744 L4745 A4746 S4747 L4748 E4749 I4750 T4751 A4752 H4753 N4754 E4755 ARG LYS PRO ASP PRO PRO PRO GLY LEU LEU THR TRP L4768 M4769 S4770 I4816
V4820 L4823 M4839 L4843 V4846 F4856 R4860 E4867 D4868 D4878 Y4888 D4917 D4966 H4983 M5013 D5020 Y5032 E5033 D5034 Q5035 L5036 S5037

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	113276	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.712	Depositor
Minimum map value	0.000	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.068	Depositor
Map size (Å)	477.696, 477.696, 477.696	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.933, 0.933, 0.933	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, 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	0.14	0/835	0.35	0/1126
1	C	0.14	0/835	0.35	0/1126
1	E	0.14	0/835	0.35	0/1126
1	G	0.14	0/835	0.35	0/1126
2	B	0.14	0/33991	0.32	0/46110
2	D	0.14	0/33991	0.32	0/46110
2	F	0.14	0/33991	0.32	0/46110
2	H	0.14	0/33991	0.32	0/46110
All	All	0.14	0/139304	0.32	0/188944

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	819	0	818	5	0
1	C	819	0	818	4	0
1	E	819	0	818	4	0
1	G	819	0	818	4	0
2	B	33229	0	32428	165	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	33229	0	32428	164	0
2	F	33229	0	32428	165	0
2	H	33229	0	32428	165	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	F	1	0	0	0	0
3	H	1	0	0	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
4	H	1	0	0	0	0
5	B	31	0	12	0	0
5	D	31	0	12	0	0
5	F	31	0	12	0	0
5	H	31	0	12	0	0
All	All	136324	0	133032	618	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 2.

All (618) 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:D:2371:GLU:N	2:F:128:THR:O	2.25	0.69
2:B:128:THR:O	2:H:2371:GLU:N	2.25	0.69
2:B:2371:GLU:N	2:D:128:THR:O	2.25	0.69
2:F:856:VAL:H	2:F:991:ASN:HD21	1.40	0.68
2:H:856:VAL:H	2:H:991:ASN:HD21	1.40	0.68
2:B:856:VAL:H	2:B:991:ASN:HD21	1.40	0.68
2:D:856:VAL:H	2:D:991:ASN:HD21	1.40	0.68
2:F:2371:GLU:N	2:H:128:THR:O	2.25	0.66
2:D:2214:VAL:HG21	2:D:2228:MET:HG2	1.77	0.65
2:F:2214:VAL:HG21	2:F:2228:MET:HG2	1.77	0.65
2:B:2214:VAL:HG21	2:B:2228:MET:HG2	1.77	0.64
2:H:2214:VAL:HG21	2:H:2228:MET:HG2	1.77	0.64
2:D:868:GLU:O	2:D:871:ARG:HB3	2.00	0.62
2:H:868:GLU:O	2:H:871:ARG:HB3	2.00	0.61
2:B:868:GLU:O	2:B:871:ARG:HB3	2.00	0.61
2:F:868:GLU:O	2:F:871:ARG:HB3	2.00	0.61
2:B:4630:TYR:OH	2:D:4860:ARG:NH1	2.34	0.61
2:B:4860:ARG:NH1	2:H:4630:TYR:OH	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4039:MET:SD	2:B:4042:ARG:NH2	2.74	0.61
2:F:4630:TYR:OH	2:H:4860:ARG:NH1	2.34	0.61
2:B:2614:ILE:HG23	2:B:2618:MET:HE3	1.83	0.61
2:B:4582:VAL:HG23	2:D:4856:PHE:CZ	2.36	0.61
2:D:4582:VAL:HG23	2:F:4856:PHE:CZ	2.36	0.61
2:F:3324:VAL:HG11	2:F:3361:THR:HG22	1.83	0.61
2:H:3324:VAL:HG11	2:H:3361:THR:HG22	1.83	0.61
2:D:2614:ILE:HG23	2:D:2618:MET:HE3	1.83	0.60
2:F:4039:MET:SD	2:F:4042:ARG:NH2	2.74	0.60
2:H:2614:ILE:HG23	2:H:2618:MET:HE3	1.83	0.60
2:B:2624:ARG:NH1	2:B:2910:THR:O	2.35	0.60
2:H:1101:ARG:NH1	2:H:1115:LEU:O	2.35	0.60
2:B:4856:PHE:CZ	2:H:4582:VAL:HG23	2.36	0.60
2:D:4630:TYR:OH	2:F:4860:ARG:NH1	2.34	0.60
2:F:4582:VAL:HG23	2:H:4856:PHE:CZ	2.36	0.60
2:D:3324:VAL:HG11	2:D:3361:THR:HG22	1.83	0.60
2:D:4039:MET:SD	2:D:4042:ARG:NH2	2.74	0.60
2:F:2614:ILE:HG23	2:F:2618:MET:HE3	1.83	0.60
2:H:4039:MET:SD	2:H:4042:ARG:NH2	2.74	0.60
2:B:1101:ARG:NH1	2:B:1115:LEU:O	2.35	0.60
2:B:3324:VAL:HG11	2:B:3361:THR:HG22	1.83	0.60
2:D:1101:ARG:NH1	2:D:1115:LEU:O	2.35	0.60
2:F:2624:ARG:NH1	2:F:2910:THR:O	2.35	0.59
2:F:1101:ARG:NH1	2:F:1115:LEU:O	2.35	0.59
2:D:3539:ARG:HB3	2:D:3549:VAL:HG22	1.85	0.59
2:F:3539:ARG:HB3	2:F:3549:VAL:HG22	1.85	0.58
2:B:3539:ARG:HB3	2:B:3549:VAL:HG22	1.85	0.58
2:H:3539:ARG:HB3	2:H:3549:VAL:HG22	1.85	0.58
2:H:3324:VAL:HA	2:H:3327:LEU:HG	1.86	0.58
2:H:2624:ARG:NH1	2:H:2910:THR:O	2.35	0.57
2:D:2624:ARG:NH1	2:D:2910:THR:O	2.35	0.57
2:D:4888:TYR:OH	2:F:4917:ASP:OD2	2.19	0.57
2:H:1299:GLN:NE2	2:H:1545:ASN:OD1	2.38	0.57
2:B:2654:TYR:O	2:B:2667:THR:OG1	2.23	0.57
2:D:3324:VAL:HA	2:D:3327:LEU:HG	1.86	0.57
2:F:1299:GLN:NE2	2:F:1545:ASN:OD1	2.38	0.57
2:H:2654:TYR:O	2:H:2667:THR:OG1	2.23	0.56
2:F:2770:LYS:HB3	2:F:2775:TRP:HB2	1.86	0.56
2:F:3324:VAL:HA	2:F:3327:LEU:HG	1.86	0.56
2:H:2770:LYS:HB3	2:H:2775:TRP:HB2	1.86	0.56
2:B:3324:VAL:HA	2:B:3327:LEU:HG	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3445:TRP:NE1	2:B:3455:GLU:OE1	2.38	0.56
2:B:4856:PHE:CZ	2:H:4582:VAL:CG2	2.88	0.56
2:B:5013:MET:HE1	2:B:5020:ASP:HB2	1.86	0.56
2:H:5013:MET:HE1	2:H:5020:ASP:HB2	1.86	0.56
2:B:1115:LEU:HD13	2:B:1123:VAL:HG11	1.87	0.56
2:D:5013:MET:HE1	2:D:5020:ASP:HB2	1.86	0.56
2:F:2654:TYR:O	2:F:2667:THR:OG1	2.23	0.56
2:D:1243:PRO:HA	2:D:1601:MET:O	2.06	0.56
2:F:4582:VAL:CG2	2:H:4856:PHE:CZ	2.88	0.56
2:F:4888:TYR:OH	2:H:4917:ASP:OD2	2.19	0.56
2:H:1115:LEU:HD13	2:H:1123:VAL:HG11	1.87	0.56
2:D:2654:TYR:O	2:D:2667:THR:OG1	2.23	0.56
2:D:2770:LYS:HB3	2:D:2775:TRP:HB2	1.86	0.56
2:D:4582:VAL:CG2	2:F:4856:PHE:CZ	2.88	0.56
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	1.86	0.56
2:F:1243:PRO:HA	2:F:1601:MET:O	2.06	0.56
2:H:3445:TRP:NE1	2:H:3455:GLU:OE1	2.38	0.56
2:B:1520:VAL:HG12	2:B:1527:MET:HG2	1.88	0.56
2:B:1243:PRO:HA	2:B:1601:MET:O	2.06	0.56
2:B:1476:MET:HB2	2:B:1485:SER:HB3	1.88	0.56
2:H:1476:MET:HB2	2:H:1485:SER:HB3	1.88	0.56
2:D:1299:GLN:NE2	2:D:1545:ASN:OD1	2.38	0.55
2:D:3445:TRP:NE1	2:D:3455:GLU:OE1	2.38	0.55
2:D:4707:ASN:ND2	2:D:4740:LEU:O	2.39	0.55
2:F:5013:MET:HE1	2:F:5020:ASP:HB2	1.86	0.55
2:B:603:LEU:HA	2:B:606:LEU:HD12	1.89	0.55
2:B:4707:ASN:ND2	2:B:4740:LEU:O	2.39	0.55
2:D:603:LEU:HA	2:D:606:LEU:HD12	1.89	0.55
2:F:3445:TRP:NE1	2:F:3455:GLU:OE1	2.38	0.55
2:B:4582:VAL:CG2	2:D:4856:PHE:CZ	2.88	0.55
2:H:4707:ASN:ND2	2:H:4740:LEU:O	2.39	0.55
2:D:1476:MET:HB2	2:D:1485:SER:HB3	1.88	0.55
2:F:603:LEU:HA	2:F:606:LEU:HD12	1.89	0.55
2:F:1115:LEU:HD13	2:F:1123:VAL:HG11	1.87	0.55
2:F:1520:VAL:HG12	2:F:1527:MET:HG2	1.88	0.55
2:F:3412:LEU:HD11	2:F:3434:LEU:HD21	1.89	0.55
2:F:4707:ASN:ND2	2:F:4740:LEU:O	2.39	0.55
2:H:603:LEU:HA	2:H:606:LEU:HD12	1.89	0.55
2:H:1243:PRO:HA	2:H:1601:MET:O	2.06	0.55
2:D:1115:LEU:HD13	2:D:1123:VAL:HG11	1.87	0.55
2:D:1520:VAL:HG12	2:D:1527:MET:HG2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1743:ARG:NH1	2:B:1963:GLU:OE2	2.40	0.54
2:D:1743:ARG:NH1	2:D:1963:GLU:OE2	2.40	0.54
2:H:1520:VAL:HG12	2:H:1527:MET:HG2	1.88	0.54
2:B:2178:MET:HE2	2:B:2210:VAL:HG11	1.90	0.54
2:H:1743:ARG:NH1	2:H:1963:GLU:OE2	2.40	0.54
2:D:3412:LEU:HD11	2:D:3434:LEU:HD21	1.89	0.54
2:H:2178:MET:HE2	2:H:2210:VAL:HG11	1.90	0.54
2:F:1476:MET:HB2	2:F:1485:SER:HB3	1.88	0.54
2:B:1299:GLN:NE2	2:B:1545:ASN:OD1	2.38	0.54
2:D:2178:MET:HE2	2:D:2210:VAL:HG11	1.90	0.54
2:H:3412:LEU:HD11	2:H:3434:LEU:HD21	1.89	0.54
2:H:4056:GLU:HG2	2:H:4166:LEU:HD13	1.90	0.54
2:B:3412:LEU:HD11	2:B:3434:LEU:HD21	1.89	0.54
2:B:4888:TYR:OH	2:D:4917:ASP:OD2	2.19	0.54
2:D:1008:SER:HB3	2:D:1017:ARG:HB3	1.90	0.54
2:H:1008:SER:HB3	2:H:1017:ARG:HB3	1.90	0.53
2:B:1008:SER:HB3	2:B:1017:ARG:HB3	1.90	0.53
2:F:1008:SER:HB3	2:F:1017:ARG:HB3	1.90	0.53
2:B:4056:GLU:HG2	2:B:4166:LEU:HD13	1.90	0.53
2:F:2178:MET:HE2	2:F:2210:VAL:HG11	1.90	0.53
2:D:3365:LEU:HD13	2:D:3405:LEU:HD23	1.90	0.53
2:D:4056:GLU:HG2	2:D:4166:LEU:HD13	1.90	0.53
2:D:233:ILE:HD12	2:D:242:ARG:HB3	1.90	0.53
2:D:638:ILE:HD11	2:D:1636:MET:HE2	1.91	0.53
2:H:3365:LEU:HD13	2:H:3405:LEU:HD23	1.90	0.53
2:B:3365:LEU:HD13	2:B:3405:LEU:HD23	1.90	0.52
2:F:638:ILE:HD11	2:F:1636:MET:HE2	1.91	0.52
2:H:2770:LYS:HG3	2:H:2791:LEU:HD21	1.92	0.52
2:D:1116:GLY:HA3	2:D:1132:TRP:HB3	1.91	0.52
2:F:1116:GLY:HA3	2:F:1132:TRP:HB3	1.91	0.52
2:H:408:ALA:HB2	2:H:483:MET:HE1	1.91	0.52
2:B:2770:LYS:HG3	2:B:2791:LEU:HD21	1.92	0.52
2:F:4056:GLU:HG2	2:F:4166:LEU:HD13	1.90	0.52
2:B:408:ALA:HB2	2:B:483:MET:HE1	1.91	0.52
2:B:1116:GLY:HA3	2:B:1132:TRP:HB3	1.91	0.52
2:H:1028:ASP:OD1	2:H:1028:ASP:N	2.43	0.52
2:F:233:ILE:HD12	2:F:242:ARG:HB3	1.90	0.52
2:F:3365:LEU:HD13	2:F:3405:LEU:HD23	1.90	0.52
2:H:233:ILE:HD12	2:H:242:ARG:HB3	1.90	0.52
2:B:4917:ASP:OD2	2:H:4888:TYR:OH	2.19	0.52
2:B:638:ILE:HD11	2:B:1636:MET:HE2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:233:ILE:O	2:F:257:ARG:NH1	2.41	0.52
2:F:1743:ARG:NH1	2:F:1963:GLU:OE2	2.40	0.52
2:F:2770:LYS:HG3	2:F:2791:LEU:HD21	1.92	0.52
2:H:1116:GLY:HA3	2:H:1132:TRP:HB3	1.91	0.52
2:F:4152:GLU:OE2	2:F:4180:ARG:NH1	2.44	0.51
2:H:638:ILE:HD11	2:H:1636:MET:HE2	1.91	0.51
2:D:3312:LEU:HD22	2:D:3348:ARG:HG3	1.93	0.51
2:F:408:ALA:HB2	2:F:483:MET:HE1	1.91	0.51
2:F:3312:LEU:HD22	2:F:3348:ARG:HG3	1.93	0.51
2:H:3312:LEU:HD22	2:H:3348:ARG:HG3	1.93	0.51
2:B:233:ILE:HD12	2:B:242:ARG:HB3	1.90	0.51
1:C:79:PRO:HA	1:C:82:ALA:HB3	1.93	0.51
2:D:408:ALA:HB2	2:D:483:MET:HE1	1.91	0.51
2:D:2770:LYS:HG3	2:D:2791:LEU:HD21	1.92	0.51
2:B:1947:CYS:SG	2:B:2127:GLN:NE2	2.83	0.51
2:B:3312:LEU:HD22	2:B:3348:ARG:HG3	1.93	0.51
1:E:79:PRO:HA	1:E:82:ALA:HB3	1.93	0.51
2:H:1968:LYS:NZ	2:H:2030:ASP:OD2	2.43	0.51
2:B:4843:LEU:HD22	2:H:4823:LEU:HD22	1.93	0.51
2:D:233:ILE:O	2:D:257:ARG:NH1	2.41	0.51
2:D:1947:CYS:SG	2:D:2127:GLN:NE2	2.83	0.51
2:H:4152:GLU:OE2	2:H:4180:ARG:NH1	2.44	0.51
2:D:1805:GLU:OE1	2:D:1808:ARG:NH2	2.44	0.51
2:F:1947:CYS:SG	2:F:2127:GLN:NE2	2.83	0.51
2:B:491:ILE:O	2:B:495:ASN:HB2	2.10	0.51
2:D:2642:LYS:HB2	2:D:2698:MET:HE1	1.93	0.51
2:D:4152:GLU:OE2	2:D:4180:ARG:NH1	2.44	0.51
2:F:491:ILE:O	2:F:495:ASN:HB2	2.10	0.51
2:F:2642:LYS:HB2	2:F:2698:MET:HE1	1.93	0.51
2:H:1805:GLU:OE1	2:H:1808:ARG:NH2	2.44	0.51
2:H:1947:CYS:SG	2:H:2127:GLN:NE2	2.83	0.51
2:H:4037:ASN:O	2:H:4042:ARG:NH1	2.44	0.51
2:B:913:LEU:O	2:B:918:ARG:NH2	2.44	0.50
2:D:2902:HIS:HB3	2:D:2905:LEU:HG	1.94	0.50
2:H:233:ILE:O	2:H:257:ARG:NH1	2.41	0.50
2:H:2642:LYS:HB2	2:H:2698:MET:HE1	1.93	0.50
2:D:491:ILE:O	2:D:495:ASN:HB2	2.10	0.50
2:F:2370:GLY:HA3	2:H:129:ASP:OD1	2.12	0.50
2:B:4152:GLU:OE2	2:B:4180:ARG:NH1	2.44	0.50
2:D:1694:LEU:HB3	2:D:1715:LEU:HD12	1.93	0.50
2:F:1968:LYS:NZ	2:F:2030:ASP:OD2	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1968:LYS:NZ	2:D:2030:ASP:OD2	2.43	0.50
2:D:4037:ASN:O	2:D:4042:ARG:NH1	2.44	0.50
2:F:2460:LEU:HD23	2:H:131:LEU:HD22	1.93	0.50
2:F:2902:HIS:HB3	2:F:2905:LEU:HG	1.94	0.50
2:F:4823:LEU:HD22	2:H:4843:LEU:HD22	1.93	0.50
2:B:1968:LYS:NZ	2:B:2030:ASP:OD2	2.43	0.50
2:B:1805:GLU:OE1	2:B:1808:ARG:NH2	2.44	0.50
2:B:2642:LYS:HB2	2:B:2698:MET:HE1	1.93	0.50
2:B:2902:HIS:HB3	2:B:2905:LEU:HG	1.94	0.50
1:G:79:PRO:HA	1:G:82:ALA:HB3	1.93	0.50
2:H:2902:HIS:HB3	2:H:2905:LEU:HG	1.94	0.50
2:D:1448:VAL:HG22	2:D:1554:VAL:HG23	1.93	0.50
2:D:2460:LEU:HD23	2:F:131:LEU:HD22	1.93	0.50
2:D:4823:LEU:HD22	2:F:4843:LEU:HD22	1.93	0.50
2:H:2364:PHE:HB3	2:H:2368:LEU:HB2	1.94	0.50
1:A:79:PRO:HA	1:A:82:ALA:HB3	1.93	0.50
2:B:1694:LEU:HB3	2:B:1715:LEU:HD12	1.93	0.50
2:B:2370:GLY:HA3	2:D:129:ASP:OD1	2.12	0.50
2:H:1448:VAL:HG22	2:H:1554:VAL:HG23	1.93	0.50
2:B:863:LEU:HD12	2:B:864:PRO:HD2	1.94	0.50
2:B:4823:LEU:HD22	2:D:4843:LEU:HD22	1.93	0.50
2:D:2370:GLY:HA3	2:F:129:ASP:OD1	2.12	0.50
2:F:913:LEU:O	2:F:918:ARG:NH2	2.44	0.50
2:F:4037:ASN:O	2:F:4042:ARG:NH1	2.44	0.50
2:H:491:ILE:O	2:H:495:ASN:HB2	2.10	0.50
2:B:233:ILE:O	2:B:257:ARG:NH1	2.41	0.49
2:B:4037:ASN:O	2:B:4042:ARG:NH1	2.44	0.49
2:D:2364:PHE:HB3	2:D:2368:LEU:HB2	1.94	0.49
2:F:1805:GLU:OE1	2:F:1808:ARG:NH2	2.44	0.49
2:H:913:LEU:O	2:H:918:ARG:NH2	2.44	0.49
2:B:1448:VAL:HG22	2:B:1554:VAL:HG23	1.93	0.49
2:D:913:LEU:O	2:D:918:ARG:NH2	2.44	0.49
2:D:1463:ASN:O	2:D:1468:LYS:NZ	2.46	0.49
2:H:863:LEU:HD12	2:H:864:PRO:HD2	1.94	0.49
2:B:129:ASP:OD1	2:H:2370:GLY:HA3	2.12	0.49
2:B:2460:LEU:HD23	2:D:131:LEU:HD22	1.93	0.49
2:F:863:LEU:HD12	2:F:864:PRO:HD2	1.94	0.49
2:H:1463:ASN:O	2:H:1468:LYS:NZ	2.46	0.49
2:F:1694:LEU:HB3	2:F:1715:LEU:HD12	1.93	0.49
2:B:131:LEU:HD22	2:H:2460:LEU:HD23	1.93	0.49
2:B:950:LEU:HD13	2:B:970:LEU:HD13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2364:PHE:HB3	2:B:2368:LEU:HB2	1.94	0.49
2:B:4581:LYS:HG3	2:D:4878:ASP:HB3	1.95	0.49
2:F:1448:VAL:HG22	2:F:1554:VAL:HG23	1.93	0.49
2:F:2716:ASP:OD1	2:F:2716:ASP:N	2.45	0.49
2:H:950:LEU:HD13	2:H:970:LEU:HD13	1.95	0.49
2:H:4966:ASP:OD1	2:H:4966:ASP:N	2.46	0.49
2:F:1463:ASN:O	2:F:1468:LYS:NZ	2.46	0.49
2:H:796:ARG:O	2:H:1619:ARG:NH2	2.45	0.49
2:B:4878:ASP:HB3	2:H:4581:LYS:HG3	1.95	0.49
2:D:1465:ASP:OD1	2:D:1467:SER:OG	2.28	0.49
2:D:2592:GLY:HA3	2:D:2595:LEU:HD12	1.95	0.49
2:F:4581:LYS:HG3	2:H:4878:ASP:HB3	1.95	0.49
2:B:4846:VAL:HG21	2:H:4816:ILE:CD1	2.43	0.49
2:F:823:LEU:HD11	2:F:1626:TRP:HB3	1.95	0.49
2:F:950:LEU:HD13	2:F:970:LEU:HD13	1.95	0.49
2:H:1694:LEU:HB3	2:H:1715:LEU:HD12	1.93	0.49
2:D:950:LEU:HD13	2:D:970:LEU:HD13	1.95	0.48
2:F:2364:PHE:HB3	2:F:2368:LEU:HB2	1.94	0.48
2:D:863:LEU:HD12	2:D:864:PRO:HD2	1.94	0.48
2:F:2592:GLY:HA3	2:F:2595:LEU:HD12	1.95	0.48
2:F:4816:ILE:CD1	2:H:4846:VAL:HG21	2.43	0.48
2:H:911:HIS:O	2:H:918:ARG:NH2	2.47	0.48
2:B:4816:ILE:CD1	2:D:4846:VAL:HG21	2.43	0.48
2:D:4816:ILE:CD1	2:F:4846:VAL:HG21	2.43	0.48
2:D:911:HIS:O	2:D:918:ARG:NH2	2.47	0.48
2:H:3199:ALA:HB2	2:H:3279:SER:HB3	1.95	0.48
1:E:50:ARG:HH21	1:E:53:LYS:HE2	1.79	0.48
2:F:886:ARG:HB3	2:F:891:TRP:HB2	1.96	0.48
1:A:50:ARG:HH21	1:A:53:LYS:HE2	1.79	0.48
2:B:796:ARG:O	2:B:1619:ARG:NH2	2.45	0.48
2:B:911:HIS:O	2:B:918:ARG:NH2	2.47	0.48
2:D:886:ARG:HB3	2:D:891:TRP:HB2	1.96	0.48
2:F:3329:ILE:HD11	2:F:3332:ALA:HB2	1.95	0.48
1:G:50:ARG:HH21	1:G:53:LYS:HE2	1.79	0.48
2:H:3329:ILE:HD11	2:H:3332:ALA:HB2	1.95	0.48
2:D:4581:LYS:HG3	2:F:4878:ASP:HB3	1.95	0.48
2:H:823:LEU:HD11	2:H:1626:TRP:HB3	1.95	0.48
2:B:2592:GLY:HA3	2:B:2595:LEU:HD12	1.95	0.48
2:D:2196:ASN:OD1	2:D:2199:ARG:NH2	2.41	0.48
2:B:823:LEU:HD11	2:B:1626:TRP:HB3	1.95	0.48
2:D:112:ALA:O	2:D:115:ARG:NH1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:112:ALA:O	2:H:115:ARG:NH1	2.47	0.48
2:B:112:ALA:O	2:B:115:ARG:NH1	2.47	0.47
2:D:823:LEU:HD11	2:D:1626:TRP:HB3	1.95	0.47
2:H:2592:GLY:HA3	2:H:2595:LEU:HD12	1.95	0.47
1:C:50:ARG:HH21	1:C:53:LYS:HE2	1.79	0.47
1:G:50:ARG:HE	1:G:53:LYS:HG3	1.79	0.47
2:B:1463:ASN:O	2:B:1468:LYS:NZ	2.46	0.47
2:B:3329:ILE:HD11	2:B:3332:ALA:HB2	1.95	0.47
2:F:1447:CYS:HB3	2:F:1555:LEU:HB3	1.96	0.47
2:B:1447:CYS:HB3	2:B:1555:LEU:HB3	1.96	0.47
1:C:50:ARG:HE	1:C:53:LYS:HG3	1.79	0.47
2:F:112:ALA:O	2:F:115:ARG:NH1	2.47	0.47
2:F:911:HIS:O	2:F:918:ARG:NH2	2.47	0.47
2:F:2640:PRO:O	2:F:2643:LEU:HB3	2.14	0.47
2:H:2716:ASP:OD1	2:H:2716:ASP:N	2.45	0.47
2:B:3199:ALA:HB2	2:B:3279:SER:HB3	1.95	0.47
2:B:4820:VAL:HG21	2:D:4839:MET:SD	2.55	0.47
2:D:3199:ALA:HB2	2:D:3279:SER:HB3	1.95	0.47
2:F:3199:ALA:HB2	2:F:3279:SER:HB3	1.95	0.47
2:F:4820:VAL:HG21	2:H:4839:MET:SD	2.55	0.47
2:H:544:LEU:HD21	2:H:578:ILE:HD13	1.97	0.47
2:H:2021:CYS:HB3	2:H:2028:ARG:HH21	1.80	0.47
2:B:886:ARG:HB3	2:B:891:TRP:HB2	1.96	0.47
2:D:2021:CYS:HB3	2:D:2028:ARG:HH21	1.80	0.47
2:F:796:ARG:O	2:F:1619:ARG:NH2	2.45	0.47
2:B:4839:MET:SD	2:H:4820:VAL:HG21	2.55	0.47
2:D:544:LEU:HD21	2:D:578:ILE:HD13	1.97	0.47
1:E:50:ARG:HE	1:E:53:LYS:HG3	1.79	0.47
2:H:886:ARG:HB3	2:H:891:TRP:HB2	1.96	0.47
2:B:2640:PRO:O	2:B:2643:LEU:HB3	2.14	0.47
2:B:2771:ILE:HD11	2:B:2857:PRO:HD2	1.97	0.47
2:B:4846:VAL:HG21	2:H:4816:ILE:HD11	1.97	0.47
2:D:2228:MET:HE2	2:D:2228:MET:HB2	1.80	0.47
2:D:2640:PRO:O	2:D:2643:LEU:HB3	2.14	0.47
2:B:3842:LEU:HB2	2:B:3929:SER:HB2	1.97	0.46
2:D:4582:VAL:HG23	2:F:4856:PHE:CE1	2.51	0.46
2:D:4820:VAL:HG21	2:F:4839:MET:SD	2.55	0.46
2:F:3842:LEU:HB2	2:F:3929:SER:HB2	1.97	0.46
2:F:4582:VAL:HG23	2:H:4856:PHE:CE1	2.51	0.46
2:H:2771:ILE:HD11	2:H:2857:PRO:HD2	1.97	0.46
2:B:4856:PHE:CE1	2:H:4582:VAL:HG23	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:ARG:HE	1:A:53:LYS:HG3	1.79	0.46
2:D:3281:LEU:HD12	2:D:3315:LEU:HD22	1.97	0.46
2:D:3329:ILE:HD11	2:D:3332:ALA:HB2	1.95	0.46
2:H:2640:PRO:O	2:H:2643:LEU:HB3	2.14	0.46
2:D:622:THR:HG23	2:D:626:LEU:HD12	1.98	0.46
2:D:1447:CYS:HB3	2:D:1555:LEU:HB3	1.96	0.46
2:F:882:TRP:O	2:F:885:THR:OG1	2.32	0.46
2:H:3281:LEU:HD12	2:H:3315:LEU:HD22	1.97	0.46
2:H:3842:LEU:HB2	2:H:3929:SER:HB2	1.97	0.46
2:B:1828:ASP:N	2:B:1828:ASP:OD1	2.49	0.46
2:D:2771:ILE:HD11	2:D:2857:PRO:HD2	1.97	0.46
2:F:636:ASN:HB2	2:F:702:TRP:CZ3	2.51	0.46
2:F:2021:CYS:HB3	2:F:2028:ARG:HH21	1.80	0.46
2:H:2166:LEU:HD11	2:H:2206:THR:HG23	1.97	0.46
2:B:552:ASP:OD1	2:B:552:ASP:N	2.46	0.46
2:B:622:THR:HG23	2:B:626:LEU:HD12	1.98	0.46
2:B:2021:CYS:HB3	2:B:2028:ARG:HH21	1.80	0.46
2:D:636:ASN:HB2	2:D:702:TRP:CZ3	2.51	0.46
2:D:4816:ILE:HD11	2:F:4846:VAL:HG21	1.97	0.46
2:F:2771:ILE:HD11	2:F:2857:PRO:HD2	1.97	0.46
2:H:1089:TYR:HD2	2:H:1152:MET:HG3	1.81	0.46
2:B:544:LEU:HD21	2:B:578:ILE:HD13	1.97	0.46
2:B:2166:LEU:HD11	2:B:2206:THR:HG23	1.97	0.46
2:B:3281:LEU:HD12	2:B:3315:LEU:HD22	1.97	0.46
2:D:1089:TYR:HD2	2:D:1152:MET:HG3	1.81	0.46
2:D:2026:ASP:OD1	2:D:2026:ASP:N	2.49	0.46
2:F:3281:LEU:HD12	2:F:3315:LEU:HD22	1.97	0.46
2:H:636:ASN:HB2	2:H:702:TRP:CZ3	2.51	0.46
2:B:590:LEU:HB2	2:B:599:VAL:HG11	1.97	0.46
2:B:3110:LEU:HD11	2:B:3186:LEU:HD22	1.98	0.46
2:D:590:LEU:HB2	2:D:599:VAL:HG11	1.97	0.46
2:F:2026:ASP:OD1	2:F:2026:ASP:N	2.49	0.46
2:H:3110:LEU:HD11	2:H:3186:LEU:HD22	1.98	0.46
2:D:796:ARG:O	2:D:1619:ARG:NH2	2.45	0.46
2:D:4966:ASP:OD1	2:D:4966:ASP:N	2.46	0.46
2:F:1089:TYR:HD2	2:F:1152:MET:HG3	1.81	0.46
1:G:24:VAL:HG22	1:G:48:LYS:HG2	1.98	0.46
2:B:4816:ILE:HD11	2:D:4846:VAL:HG21	1.97	0.46
2:D:1076:ARG:HB3	2:D:1191:VAL:HG23	1.98	0.46
2:D:1732:SER:O	2:D:2140:ARG:NH1	2.49	0.46
2:F:2166:LEU:HD11	2:F:2206:THR:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:VAL:HG22	1:A:48:LYS:HG2	1.98	0.45
2:B:636:ASN:HB2	2:B:702:TRP:CZ3	2.51	0.45
1:C:24:VAL:HG22	1:C:48:LYS:HG2	1.98	0.45
2:F:221:ARG:NH2	2:F:255:HIS:O	2.44	0.45
2:B:749:ASP:O	2:B:753:PRO:HA	2.17	0.45
2:B:1089:TYR:HD2	2:B:1152:MET:HG3	1.81	0.45
2:D:1828:ASP:N	2:D:1828:ASP:OD1	2.49	0.45
2:F:4816:ILE:HD11	2:H:4846:VAL:HG21	1.97	0.45
2:H:1447:CYS:HB3	2:H:1555:LEU:HB3	1.96	0.45
2:B:815:VAL:O	2:B:1007:TYR:OH	2.30	0.45
2:B:1076:ARG:HB3	2:B:1191:VAL:HG23	1.98	0.45
2:B:1732:SER:O	2:B:2140:ARG:NH1	2.49	0.45
2:B:3356:SER:OG	2:B:3357:HIS:ND1	2.44	0.45
1:E:24:VAL:HG22	1:E:48:LYS:HG2	1.98	0.45
2:F:317:ARG:NH1	2:F:349:GLN:OE1	2.50	0.45
2:H:1478:ASP:OD1	2:H:1482:ASN:N	2.50	0.45
2:D:749:ASP:O	2:D:753:PRO:HA	2.17	0.45
2:D:2166:LEU:HD11	2:D:2206:THR:HG23	1.97	0.45
2:D:3842:LEU:HB2	2:D:3929:SER:HB2	1.97	0.45
2:B:1771:LEU:HD22	2:B:2153:MET:HE2	1.99	0.45
2:B:3671:ASP:OD1	2:B:3671:ASP:N	2.49	0.45
2:H:1732:SER:O	2:H:2140:ARG:NH1	2.49	0.45
2:H:1828:ASP:OD1	2:H:1828:ASP:N	2.49	0.45
2:B:2228:MET:HB2	2:B:2228:MET:HE2	1.80	0.45
2:B:4582:VAL:HG23	2:D:4856:PHE:CE1	2.51	0.45
2:D:1771:LEU:HD22	2:D:2153:MET:HE2	1.99	0.45
2:F:544:LEU:HD21	2:F:578:ILE:HD13	1.97	0.45
2:F:590:LEU:HB2	2:F:599:VAL:HG11	1.97	0.45
2:F:1076:ARG:HB3	2:F:1191:VAL:HG23	1.98	0.45
2:H:1106:ARG:NH1	2:H:1184:ILE:O	2.50	0.45
2:H:3671:ASP:N	2:H:3671:ASP:OD1	2.49	0.45
2:D:317:ARG:NH1	2:D:349:GLN:OE1	2.50	0.45
2:D:1028:ASP:OD1	2:D:1028:ASP:N	2.43	0.45
2:F:622:THR:HG23	2:F:626:LEU:HD12	1.98	0.45
2:F:879:HIS:NE2	2:F:908:VAL:O	2.38	0.45
2:F:1106:ARG:NH1	2:F:1184:ILE:O	2.50	0.45
2:F:1478:ASP:OD1	2:F:1482:ASN:N	2.50	0.45
2:H:749:ASP:O	2:H:753:PRO:HA	2.17	0.45
2:H:1186:ASP:OD1	2:H:1186:ASP:N	2.41	0.45
2:D:23:GLN:NE2	2:D:203:ASN:OD1	2.50	0.45
2:D:952:LYS:HB3	2:D:968:ALA:HB1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:23:GLN:NE2	2:F:203:ASN:OD1	2.50	0.45
2:F:3110:LEU:HD11	2:F:3186:LEU:HD22	1.98	0.45
2:H:590:LEU:HB2	2:H:599:VAL:HG11	1.97	0.45
2:H:2196:ASN:OD1	2:H:2199:ARG:NH2	2.41	0.45
2:H:4878:ASP:OD1	2:H:4878:ASP:N	2.50	0.45
2:H:622:THR:HG23	2:H:626:LEU:HD12	1.98	0.45
2:B:652:ARG:HD3	2:B:773:LEU:HD13	1.99	0.45
2:B:2716:ASP:OD1	2:B:2716:ASP:N	2.45	0.45
2:D:3110:LEU:HD11	2:D:3186:LEU:HD22	1.98	0.45
2:F:749:ASP:O	2:F:753:PRO:HA	2.17	0.45
2:F:1732:SER:O	2:F:2140:ARG:NH1	2.49	0.45
2:B:317:ARG:NH1	2:B:349:GLN:OE1	2.50	0.44
2:B:952:LYS:HB3	2:B:968:ALA:HB1	1.98	0.44
2:D:1106:ARG:NH1	2:D:1184:ILE:O	2.50	0.44
2:B:2026:ASP:OD1	2:B:2026:ASP:N	2.49	0.44
2:B:2461:VAL:O	2:B:2510:TYR:OH	2.34	0.44
2:F:1771:LEU:HD22	2:F:2153:MET:HE2	1.99	0.44
2:F:4878:ASP:OD1	2:F:4878:ASP:N	2.50	0.44
2:H:317:ARG:NH1	2:H:349:GLN:OE1	2.50	0.44
2:H:2026:ASP:OD1	2:H:2026:ASP:N	2.49	0.44
2:B:23:GLN:NE2	2:B:203:ASN:OD1	2.50	0.44
2:B:4878:ASP:OD1	2:B:4878:ASP:N	2.50	0.44
2:D:652:ARG:HD3	2:D:773:LEU:HD13	1.99	0.44
2:D:4878:ASP:OD1	2:D:4878:ASP:N	2.50	0.44
2:H:952:LYS:HB3	2:H:968:ALA:HB1	1.98	0.44
2:F:2165:LEU:HD13	2:F:2178:MET:HG2	2.00	0.44
2:F:2822:THR:HG1	2:F:2938:THR:HG1	1.63	0.44
2:H:1076:ARG:HB3	2:H:1191:VAL:HG23	1.98	0.44
2:H:2389:ASP:OD1	2:H:2389:ASP:N	2.51	0.44
2:F:952:LYS:HB3	2:F:968:ALA:HB1	1.98	0.44
2:H:2165:LEU:HD13	2:H:2178:MET:HG2	2.00	0.44
2:B:882:TRP:O	2:B:885:THR:OG1	2.32	0.44
2:H:1771:LEU:HD22	2:H:2153:MET:HE2	1.99	0.44
2:H:1039:LEU:HD23	2:H:1039:LEU:HA	1.86	0.44
2:B:128:THR:O	2:H:2371:GLU:CA	2.66	0.44
2:B:1106:ARG:NH1	2:B:1184:ILE:O	2.50	0.44
2:F:2282:ASP:HA	2:F:2341:VAL:HG13	2.00	0.44
2:H:23:GLN:NE2	2:H:203:ASN:OD1	2.50	0.44
2:B:2282:ASP:HA	2:B:2341:VAL:HG13	2.00	0.44
2:B:2371:GLU:CA	2:D:128:THR:O	2.66	0.44
2:F:1828:ASP:OD1	2:F:1828:ASP:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:2591:ARG:H	2:F:2591:ARG:HG2	1.68	0.44
2:F:3132:THR:HA	2:F:3136:LEU:HB3	2.00	0.43
2:D:2165:LEU:HD13	2:D:2178:MET:HG2	2.00	0.43
2:H:652:ARG:HD3	2:H:773:LEU:HD13	1.99	0.43
2:H:3132:THR:HA	2:H:3136:LEU:HB3	2.00	0.43
2:D:2711:PRO:HA	2:D:2712:PRO:HD3	1.92	0.43
2:F:709:ASP:OD1	2:F:725:HIS:ND1	2.49	0.43
2:B:3980:LEU:HD13	2:B:3985:LEU:HD22	2.01	0.43
2:F:2371:GLU:CA	2:H:128:THR:O	2.66	0.43
2:H:2359:ARG:HD3	2:H:2359:ARG:HA	1.80	0.43
2:B:2182:ILE:HG22	2:B:2186:MET:HE2	2.01	0.43
2:F:1650:ILE:O	2:F:1653:LEU:HB2	2.19	0.43
2:F:2196:ASN:OD1	2:F:2199:ARG:NH2	2.41	0.43
2:H:2282:ASP:HA	2:H:2341:VAL:HG13	2.00	0.43
2:B:2165:LEU:HD13	2:B:2178:MET:HG2	2.00	0.43
2:D:552:ASP:OD1	2:D:552:ASP:N	2.46	0.43
2:D:1650:ILE:O	2:D:1653:LEU:HB2	2.19	0.43
2:D:3980:LEU:HD13	2:D:3985:LEU:HD22	2.01	0.43
2:F:1112:ASP:OD1	2:F:1112:ASP:N	2.45	0.43
2:F:2182:ILE:HG22	2:F:2186:MET:HE2	2.01	0.43
2:F:3980:LEU:HD13	2:F:3985:LEU:HD22	2.01	0.43
2:B:1650:ILE:O	2:B:1653:LEU:HB2	2.19	0.43
2:D:1478:ASP:OD1	2:D:1482:ASN:N	2.50	0.43
2:D:2371:GLU:CA	2:F:128:THR:O	2.66	0.43
2:F:652:ARG:HD3	2:F:773:LEU:HD13	1.99	0.43
2:H:2624:ARG:HD2	2:H:2906:VAL:HG11	2.01	0.43
2:H:3980:LEU:HD13	2:H:3985:LEU:HD22	2.01	0.43
2:B:221:ARG:NH2	2:B:255:HIS:O	2.44	0.43
2:F:1186:ASP:OD1	2:F:1186:ASP:N	2.41	0.43
2:F:2624:ARG:HD2	2:F:2906:VAL:HG11	2.01	0.43
2:B:1039:LEU:HD23	2:B:1039:LEU:HA	1.86	0.43
2:B:3132:THR:HA	2:B:3136:LEU:HB3	2.00	0.43
2:D:2282:ASP:HA	2:D:2341:VAL:HG13	2.00	0.43
2:F:4966:ASP:OD1	2:F:4966:ASP:N	2.46	0.43
2:H:709:ASP:OD1	2:H:725:HIS:ND1	2.49	0.43
2:H:2182:ILE:HG22	2:H:2186:MET:HE2	2.01	0.43
2:B:1733:GLU:HG2	2:B:2201:LEU:HD23	2.01	0.43
2:D:1676:LEU:HD22	2:D:2167:ILE:HD12	2.01	0.43
2:D:3671:ASP:OD1	2:D:3671:ASP:N	2.49	0.43
2:F:3671:ASP:OD1	2:F:3671:ASP:N	2.49	0.43
2:H:2644:LEU:HD13	2:H:2678:LEU:HD21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2825:LYS:NZ	2:B:2933:ASN:O	2.41	0.42
2:D:3132:THR:HA	2:D:3136:LEU:HB3	2.00	0.42
2:H:1733:GLU:HG2	2:H:2201:LEU:HD23	2.01	0.42
2:B:2752:ASP:O	2:B:2755:ILE:HB	2.20	0.42
2:D:2182:ILE:HG22	2:D:2186:MET:HE2	2.01	0.42
2:D:2624:ARG:HD2	2:D:2906:VAL:HG11	2.01	0.42
2:H:648:ILE:HG23	2:H:814:ALA:HB3	2.01	0.42
2:H:1650:ILE:O	2:H:1653:LEU:HB2	2.19	0.42
2:B:3768:SER:HA	2:B:3771:HIS:CD2	2.54	0.42
2:F:1255:TYR:O	2:F:1275:ARG:NH1	2.53	0.42
2:F:1733:GLU:HG2	2:F:2201:LEU:HD23	2.01	0.42
2:B:2573:GLU:HA	2:B:2576:ALA:HB2	2.02	0.42
2:B:2711:PRO:HA	2:B:2712:PRO:HD3	1.92	0.42
2:F:430:PRO:HA	2:F:431:PRO:HD3	1.96	0.42
2:F:1676:LEU:HD22	2:F:2167:ILE:HD12	2.01	0.42
2:F:3768:SER:HA	2:F:3771:HIS:CD2	2.54	0.42
2:H:3768:SER:HA	2:H:3771:HIS:CD2	2.54	0.42
2:B:985:VAL:HG11	2:B:1040:CYS:HB2	2.02	0.42
2:D:1255:TYR:O	2:D:1275:ARG:NH1	2.53	0.42
2:D:3288:GLY:HA2	2:D:3303:PRO:HB3	2.02	0.42
2:F:2752:ASP:O	2:F:2755:ILE:HB	2.20	0.42
2:H:2228:MET:HE2	2:H:2228:MET:HB2	1.80	0.42
2:B:2624:ARG:HD2	2:B:2906:VAL:HG11	2.01	0.42
2:B:3288:GLY:HA2	2:B:3303:PRO:HB3	2.02	0.42
2:B:4966:ASP:OD1	2:B:4966:ASP:N	2.46	0.42
2:D:1733:GLU:HG2	2:D:2201:LEU:HD23	2.01	0.42
2:F:648:ILE:HG23	2:F:814:ALA:HB3	2.01	0.42
2:F:2644:LEU:HD13	2:F:2678:LEU:HD21	2.01	0.42
2:F:3288:GLY:HA2	2:F:3303:PRO:HB3	2.02	0.42
2:H:2476:ILE:HG23	2:H:2536:LEU:HD21	2.02	0.42
2:H:2752:ASP:O	2:H:2755:ILE:HB	2.20	0.42
2:H:3288:GLY:HA2	2:H:3303:PRO:HB3	2.02	0.42
2:B:3405:LEU:O	2:B:3409:TYR:HB2	2.20	0.42
2:D:221:ARG:NH2	2:D:255:HIS:O	2.44	0.42
2:F:28:VAL:HB	2:F:33:LEU:HD13	2.02	0.42
1:A:80:ASP:OD1	1:A:80:ASP:N	2.48	0.42
2:B:4711:PHE:HA	2:B:4712:PRO:HA	1.89	0.42
2:D:2644:LEU:HD13	2:D:2678:LEU:HD21	2.01	0.42
2:D:3768:SER:HA	2:D:3771:HIS:CD2	2.54	0.42
2:F:2573:GLU:HA	2:F:2576:ALA:HB2	2.02	0.42
2:F:2692:ASP:HB3	2:F:2695:LEU:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:575:LEU:HD12	2:H:609:CYS:HB3	2.02	0.42
2:H:2461:VAL:O	2:H:2510:TYR:OH	2.34	0.42
2:H:3532:LEU:HD23	2:H:3535:LEU:HD12	2.01	0.42
2:B:575:LEU:HD12	2:B:609:CYS:HB3	2.02	0.42
2:B:1255:TYR:O	2:B:1275:ARG:NH1	2.53	0.42
2:B:1676:LEU:HD22	2:B:2167:ILE:HD12	2.01	0.42
2:B:2476:ILE:HG23	2:B:2536:LEU:HD21	2.02	0.42
2:D:879:HIS:NE2	2:D:908:VAL:O	2.38	0.42
2:D:2476:ILE:HG23	2:D:2536:LEU:HD21	2.02	0.42
2:D:3405:LEU:O	2:D:3409:TYR:HB2	2.20	0.42
2:B:648:ILE:HG23	2:B:814:ALA:HB3	2.01	0.42
2:B:1272:LEU:HD22	2:B:1289:LEU:HD11	2.02	0.42
2:B:3948:LYS:HE2	2:B:4009:GLN:HG2	2.02	0.42
2:D:3948:LYS:HE2	2:D:4009:GLN:HG2	2.02	0.42
2:F:4158:PRO:HA	2:F:4161:ARG:HD2	2.02	0.42
2:H:2573:GLU:HA	2:H:2576:ALA:HB2	2.02	0.42
2:D:648:ILE:HG23	2:D:814:ALA:HB3	2.01	0.41
2:F:2476:ILE:HG23	2:F:2536:LEU:HD21	2.02	0.41
2:H:1255:TYR:O	2:H:1275:ARG:NH1	2.53	0.41
2:B:28:VAL:HB	2:B:33:LEU:HD13	2.02	0.41
2:H:700:GLU:OE2	2:H:1458:HIS:NE2	2.53	0.41
2:H:1272:LEU:HD22	2:H:1289:LEU:HD11	2.02	0.41
2:H:3405:LEU:O	2:H:3409:TYR:HB2	2.20	0.41
2:B:2692:ASP:HB3	2:B:2695:LEU:HB3	2.02	0.41
2:B:4127:GLU:O	2:B:4131:ARG:HB2	2.21	0.41
2:D:2573:GLU:HA	2:D:2576:ALA:HB2	2.02	0.41
2:H:985:VAL:HG11	2:H:1040:CYS:HB2	2.02	0.41
2:H:1021:LEU:HD12	2:H:1021:LEU:HA	1.95	0.41
2:H:3948:LYS:HE2	2:H:4009:GLN:HG2	2.02	0.41
2:B:700:GLU:OE2	2:B:1458:HIS:NE2	2.53	0.41
2:B:1478:ASP:OD1	2:B:1482:ASN:N	2.50	0.41
2:B:2242:ILE:HD13	2:B:2242:ILE:HA	1.93	0.41
2:D:2461:VAL:O	2:D:2510:TYR:OH	2.34	0.41
2:D:2582:MET:HE2	2:D:2582:MET:HB3	1.91	0.41
2:D:2752:ASP:O	2:D:2755:ILE:HB	2.20	0.41
2:B:2644:LEU:HD13	2:B:2678:LEU:HD21	2.01	0.41
2:D:1249:PRO:HA	2:D:1250:PRO:HD3	1.98	0.41
2:F:3532:LEU:HD23	2:F:3535:LEU:HD12	2.01	0.41
2:B:3532:LEU:HD23	2:B:3535:LEU:HD12	2.01	0.41
2:D:700:GLU:OE2	2:D:1458:HIS:NE2	2.53	0.41
2:D:985:VAL:HG11	2:D:1040:CYS:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4158:PRO:HA	2:D:4161:ARG:HD2	2.02	0.41
2:F:985:VAL:HG11	2:F:1040:CYS:HB2	2.02	0.41
2:H:28:VAL:HB	2:H:33:LEU:HD13	2.02	0.41
2:H:1676:LEU:HD22	2:H:2167:ILE:HD12	2.01	0.41
2:H:2692:ASP:HB3	2:H:2695:LEU:HB3	2.02	0.41
2:H:3292:PRO:HA	2:H:3293:PRO:HD3	1.90	0.41
2:H:4158:PRO:HA	2:H:4161:ARG:HD2	2.02	0.41
2:D:4995:LEU:HD23	2:D:4995:LEU:HA	1.94	0.41
2:F:774:ASP:OD1	2:F:774:ASP:N	2.54	0.41
2:F:1773:PRO:HA	2:F:1774:PRO:HD3	1.89	0.41
2:F:3948:LYS:HE2	2:F:4009:GLN:HG2	2.02	0.41
2:H:1509:ILE:HD12	2:H:1509:ILE:HA	1.97	0.41
2:H:4127:GLU:O	2:H:4131:ARG:HB2	2.21	0.41
2:D:5032:TYR:HB3	2:D:5035:GLN:HB2	2.03	0.41
2:F:575:LEU:HD12	2:F:609:CYS:HB3	2.02	0.41
2:F:5032:TYR:HB3	2:F:5035:GLN:HB2	2.03	0.41
2:H:882:TRP:O	2:H:885:THR:OG1	2.32	0.41
2:H:2825:LYS:NZ	2:H:2933:ASN:O	2.41	0.41
2:H:3356:SER:OG	2:H:3357:HIS:ND1	2.44	0.41
2:B:71:GLN:HE21	2:B:71:GLN:HB2	1.68	0.41
2:B:3127:GLN:H	2:B:3127:GLN:HG3	1.73	0.41
2:B:3302:PRO:HA	2:B:3303:PRO:HD3	1.98	0.41
2:D:575:LEU:HD12	2:D:609:CYS:HB3	2.02	0.41
2:D:1509:ILE:HD12	2:D:1509:ILE:HA	1.97	0.41
2:D:2692:ASP:HB3	2:D:2695:LEU:HB3	2.02	0.41
2:D:3823:LYS:HD3	2:D:3823:LYS:HA	1.82	0.41
2:F:1272:LEU:HD22	2:F:1289:LEU:HD11	2.02	0.41
2:F:2228:MET:HE2	2:F:2228:MET:HB2	1.80	0.41
2:F:2461:VAL:O	2:F:2510:TYR:OH	2.34	0.41
2:F:3405:LEU:O	2:F:3409:TYR:HB2	2.20	0.41
2:B:1163:THR:HG22	2:B:1168:VAL:HA	2.04	0.41
2:D:4127:GLU:O	2:D:4131:ARG:HB2	2.21	0.41
2:F:700:GLU:OE2	2:F:1458:HIS:NE2	2.53	0.41
2:F:1163:THR:HG22	2:F:1168:VAL:HA	2.04	0.41
2:F:3292:PRO:HA	2:F:3293:PRO:HD3	1.90	0.41
2:D:2856:ASN:OD1	2:D:2858:GLN:NE2	2.43	0.40
2:D:3532:LEU:HD23	2:D:3535:LEU:HD12	2.01	0.40
2:D:4888:TYR:HE1	2:F:4917:ASP:HB2	1.86	0.40
2:D:4911:LEU:HD13	2:D:4911:LEU:HA	1.96	0.40
2:F:71:GLN:HE21	2:F:71:GLN:HB2	1.68	0.40
2:F:336:PRO:HA	2:F:337:PRO:HD3	1.95	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:2587:TYR:O	2:F:2590:SER:OG	2.31	0.40
2:H:2591:ARG:H	2:H:2591:ARG:HG2	1.68	0.40
2:H:5032:TYR:HB3	2:H:5035:GLN:HB2	2.03	0.40
2:B:2301:TYR:HB3	2:B:2331:TYR:CE2	2.57	0.40
2:B:3840:SER:OG	2:B:3877:ASP:OD1	2.38	0.40
2:B:4158:PRO:HA	2:B:4161:ARG:HD2	2.02	0.40
2:B:5032:TYR:HB3	2:B:5035:GLN:HB2	2.03	0.40
2:D:1039:LEU:HD23	2:D:1039:LEU:HA	1.86	0.40
2:D:1272:LEU:HD22	2:D:1289:LEU:HD11	2.02	0.40
2:D:2359:ARG:HD3	2:D:2359:ARG:HA	1.80	0.40
2:F:4888:TYR:HE1	2:H:4917:ASP:HB2	1.86	0.40
2:H:3916:ILE:H	2:H:3916:ILE:HG12	1.60	0.40
2:B:2359:ARG:HA	2:B:2359:ARG:HD3	1.80	0.40
2:F:990:GLU:HG3	2:F:1024:TYR:HB3	2.04	0.40
2:H:815:VAL:O	2:H:1007:TYR:OH	2.30	0.40
2:H:2301:TYR:HB3	2:H:2331:TYR:CE2	2.57	0.40
2:B:2196:ASN:OD1	2:B:2199:ARG:NH2	2.41	0.40
2:D:28:VAL:HB	2:D:33:LEU:HD13	2.02	0.40
2:F:633:LEU:HD13	2:F:1639:LEU:HD11	2.04	0.40
2:B:2763:HIS:NE2	2:B:2792:ARG:O	2.46	0.40
2:B:2793:PRO:O	2:B:2796:THR:OG1	2.37	0.40
2:D:990:GLU:HG3	2:D:1024:TYR:HB3	2.04	0.40
2:D:1163:THR:HG22	2:D:1168:VAL:HA	2.04	0.40
2:D:1699:GLU:HG3	2:D:1810:LYS:HE3	2.04	0.40
2:H:2711:PRO:HA	2:H:2712:PRO:HD3	1.92	0.40
2:H:4182:GLU:OE1	2:H:4983:HIS:NE2	2.53	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	106/110 (96%)	104 (98%)	2 (2%)	0	100	100
1	C	106/110 (96%)	104 (98%)	2 (2%)	0	100	100
1	E	106/110 (96%)	104 (98%)	2 (2%)	0	100	100
1	G	106/110 (96%)	104 (98%)	2 (2%)	0	100	100
2	B	4202/5037 (83%)	4151 (99%)	51 (1%)	0	100	100
2	D	4202/5037 (83%)	4151 (99%)	51 (1%)	0	100	100
2	F	4202/5037 (83%)	4151 (99%)	51 (1%)	0	100	100
2	H	4202/5037 (83%)	4151 (99%)	51 (1%)	0	100	100
All	All	17232/20588 (84%)	17020 (99%)	212 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	87/90 (97%)	84 (97%)	3 (3%)	32	64
1	C	87/90 (97%)	84 (97%)	3 (3%)	32	64
1	E	87/90 (97%)	84 (97%)	3 (3%)	32	64
1	G	87/90 (97%)	84 (97%)	3 (3%)	32	64
2	B	3510/4276 (82%)	3489 (99%)	21 (1%)	78	88
2	D	3510/4276 (82%)	3489 (99%)	21 (1%)	78	88
2	F	3510/4276 (82%)	3489 (99%)	21 (1%)	78	88
2	H	3510/4276 (82%)	3489 (99%)	21 (1%)	78	88
All	All	14388/17464 (82%)	14292 (99%)	96 (1%)	73	87

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	26	HIS

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Mol	Chain	Res	Type
1	A	80	ASP
2	B	35	LEU
2	B	191	VAL
2	B	220	LEU
2	B	280	LEU
2	B	301	VAL
2	B	318	VAL
2	B	458	GLU
2	B	690	GLU
2	B	1520	VAL
2	B	1562	ILE
2	B	1566	LEU
2	B	1760	HIS
2	B	2044	ILE
2	B	2254	LEU
2	B	2667	THR
2	B	2906	VAL
2	B	3409	TYR
2	B	3899	PHE
2	B	3916	ILE
2	B	4178	LEU
2	B	4580	TYR
1	C	5	ILE
1	C	26	HIS
1	C	80	ASP
2	D	35	LEU
2	D	191	VAL
2	D	220	LEU
2	D	280	LEU
2	D	301	VAL
2	D	318	VAL
2	D	458	GLU
2	D	690	GLU
2	D	1520	VAL
2	D	1562	ILE
2	D	1566	LEU
2	D	1760	HIS
2	D	2044	ILE
2	D	2254	LEU
2	D	2667	THR
2	D	2906	VAL
2	D	3409	TYR

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Mol	Chain	Res	Type
2	D	3899	PHE
2	D	3916	ILE
2	D	4178	LEU
2	D	4580	TYR
1	E	5	ILE
1	E	26	HIS
1	E	80	ASP
2	F	35	LEU
2	F	191	VAL
2	F	220	LEU
2	F	280	LEU
2	F	301	VAL
2	F	318	VAL
2	F	458	GLU
2	F	690	GLU
2	F	1520	VAL
2	F	1562	ILE
2	F	1566	LEU
2	F	1760	HIS
2	F	2044	ILE
2	F	2254	LEU
2	F	2667	THR
2	F	2906	VAL
2	F	3409	TYR
2	F	3899	PHE
2	F	3916	ILE
2	F	4178	LEU
2	F	4580	TYR
1	G	5	ILE
1	G	26	HIS
1	G	80	ASP
2	H	35	LEU
2	H	191	VAL
2	H	220	LEU
2	H	280	LEU
2	H	301	VAL
2	H	318	VAL
2	H	458	GLU
2	H	690	GLU
2	H	1520	VAL
2	H	1562	ILE
2	H	1566	LEU

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Mol	Chain	Res	Type
2	H	1760	HIS
2	H	2044	ILE
2	H	2254	LEU
2	H	2667	THR
2	H	2906	VAL
2	H	3409	TYR
2	H	3899	PHE
2	H	3916	ILE
2	H	4178	LEU
2	H	4580	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (181) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
2	B	23	GLN
2	B	71	GLN
2	B	297	GLN
2	B	765	GLN
2	B	911	HIS
2	B	991	ASN
2	B	1220	GLN
2	B	1281	ASN
2	B	1296	GLN
2	B	1532	ASN
2	B	1569	GLN
2	B	1631	GLN
2	B	1824	GLN
2	B	1928	GLN
2	B	1938	GLN
2	B	2011	HIS
2	B	2095	GLN
2	B	2161	GLN
2	B	2260	ASN
2	B	2291	GLN
2	B	2342	ASN
2	B	2620	GLN
2	B	2673	HIS
2	B	2877	GLN
2	B	2993	GLN
2	B	3030	HIS
2	B	3151	GLN

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Mol	Chain	Res	Type
2	B	3462	ASN
2	B	3523	ASN
2	B	3556	ASN
2	B	3560	GLN
2	B	3667	HIS
2	B	3704	HIS
2	B	3734	HIS
2	B	3946	GLN
2	B	3950	ASN
2	B	4020	GLN
2	B	4078	GLN
2	B	4102	GLN
2	B	4133	GLN
2	B	4707	ASN
2	B	4714	ASN
2	B	4833	ASN
2	B	5003	HIS
2	B	5031	GLN
1	C	32	GLN
2	D	23	GLN
2	D	71	GLN
2	D	297	GLN
2	D	765	GLN
2	D	911	HIS
2	D	991	ASN
2	D	1220	GLN
2	D	1281	ASN
2	D	1296	GLN
2	D	1532	ASN
2	D	1569	GLN
2	D	1631	GLN
2	D	1776	HIS
2	D	1824	GLN
2	D	1928	GLN
2	D	1938	GLN
2	D	2095	GLN
2	D	2161	GLN
2	D	2260	ASN
2	D	2291	GLN
2	D	2342	ASN
2	D	2620	GLN
2	D	2673	HIS

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Mol	Chain	Res	Type
2	D	2877	GLN
2	D	2993	GLN
2	D	3030	HIS
2	D	3151	GLN
2	D	3462	ASN
2	D	3523	ASN
2	D	3556	ASN
2	D	3560	GLN
2	D	3667	HIS
2	D	3704	HIS
2	D	3946	GLN
2	D	3950	ASN
2	D	4020	GLN
2	D	4078	GLN
2	D	4102	GLN
2	D	4133	GLN
2	D	4707	ASN
2	D	4714	ASN
2	D	4833	ASN
2	D	5003	HIS
2	D	5031	GLN
1	E	32	GLN
2	F	23	GLN
2	F	71	GLN
2	F	297	GLN
2	F	479	GLN
2	F	765	GLN
2	F	911	HIS
2	F	991	ASN
2	F	1220	GLN
2	F	1281	ASN
2	F	1296	GLN
2	F	1532	ASN
2	F	1569	GLN
2	F	1631	GLN
2	F	1824	GLN
2	F	1928	GLN
2	F	1938	GLN
2	F	2095	GLN
2	F	2161	GLN
2	F	2260	ASN
2	F	2291	GLN

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Mol	Chain	Res	Type
2	F	2342	ASN
2	F	2620	GLN
2	F	2673	HIS
2	F	2877	GLN
2	F	2993	GLN
2	F	3030	HIS
2	F	3151	GLN
2	F	3462	ASN
2	F	3523	ASN
2	F	3556	ASN
2	F	3560	GLN
2	F	3667	HIS
2	F	3704	HIS
2	F	3734	HIS
2	F	3946	GLN
2	F	3950	ASN
2	F	4020	GLN
2	F	4078	GLN
2	F	4102	GLN
2	F	4133	GLN
2	F	4707	ASN
2	F	4714	ASN
2	F	4833	ASN
2	F	5003	HIS
1	G	32	GLN
2	H	23	GLN
2	H	71	GLN
2	H	297	GLN
2	H	479	GLN
2	H	765	GLN
2	H	911	HIS
2	H	991	ASN
2	H	1220	GLN
2	H	1281	ASN
2	H	1296	GLN
2	H	1532	ASN
2	H	1569	GLN
2	H	1631	GLN
2	H	1824	GLN
2	H	1928	GLN
2	H	1938	GLN
2	H	2011	HIS

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Mol	Chain	Res	Type
2	H	2095	GLN
2	H	2161	GLN
2	H	2260	ASN
2	H	2291	GLN
2	H	2342	ASN
2	H	2620	GLN
2	H	2673	HIS
2	H	2877	GLN
2	H	2993	GLN
2	H	3030	HIS
2	H	3151	GLN
2	H	3462	ASN
2	H	3523	ASN
2	H	3556	ASN
2	H	3560	GLN
2	H	3667	HIS
2	H	3704	HIS
2	H	3946	GLN
2	H	3950	ASN
2	H	4020	GLN
2	H	4078	GLN
2	H	4102	GLN
2	H	4133	GLN
2	H	4707	ASN
2	H	4714	ASN
2	H	4833	ASN
2	H	5003	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 8 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	$\#\|Z\| > 2$
5	ATP	B	5303	-	32,33,33	0.26	0	48,52,52	0.28	0
5	ATP	D	5303	-	32,33,33	0.26	0	48,52,52	0.28	0
5	ATP	H	5303	-	32,33,33	0.26	0	48,52,52	0.28	0
5	ATP	F	5303	-	32,33,33	0.26	0	48,52,52	0.28	0

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
5	ATP	B	5303	-	-	8/22/38/38	0/3/3/3
5	ATP	D	5303	-	-	8/22/38/38	0/3/3/3
5	ATP	H	5303	-	-	8/22/38/38	0/3/3/3
5	ATP	F	5303	-	-	8/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	5303	ATP	PB-O3B-PG-O2G
5	B	5303	ATP	PB-O3B-PG-O3G
5	B	5303	ATP	C5'-O5'-PA-O1A
5	B	5303	ATP	C5'-O5'-PA-O2A
5	B	5303	ATP	C5'-O5'-PA-O3A
5	D	5303	ATP	PB-O3B-PG-O2G
5	D	5303	ATP	PB-O3B-PG-O3G

Continued on next page...

Continued from previous page...

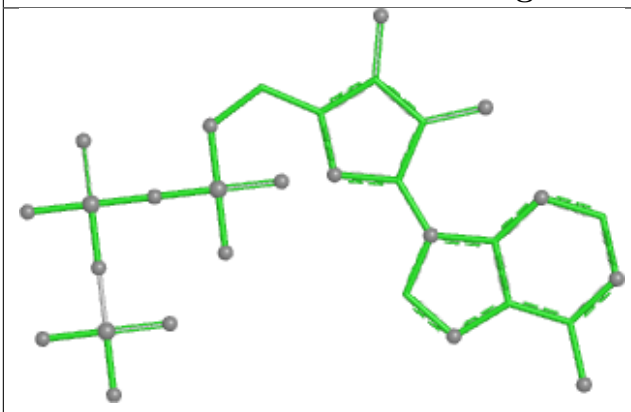
Mol	Chain	Res	Type	Atoms
5	D	5303	ATP	C5'-O5'-PA-O1A
5	D	5303	ATP	C5'-O5'-PA-O2A
5	D	5303	ATP	C5'-O5'-PA-O3A
5	F	5303	ATP	PB-O3B-PG-O2G
5	F	5303	ATP	PB-O3B-PG-O3G
5	F	5303	ATP	C5'-O5'-PA-O1A
5	F	5303	ATP	C5'-O5'-PA-O2A
5	F	5303	ATP	C5'-O5'-PA-O3A
5	H	5303	ATP	PB-O3B-PG-O2G
5	H	5303	ATP	PB-O3B-PG-O3G
5	H	5303	ATP	C5'-O5'-PA-O1A
5	H	5303	ATP	C5'-O5'-PA-O2A
5	H	5303	ATP	C5'-O5'-PA-O3A
5	B	5303	ATP	C4'-C5'-O5'-PA
5	D	5303	ATP	C4'-C5'-O5'-PA
5	F	5303	ATP	C4'-C5'-O5'-PA
5	H	5303	ATP	C4'-C5'-O5'-PA
5	B	5303	ATP	O4'-C4'-C5'-O5'
5	B	5303	ATP	C3'-C4'-C5'-O5'
5	D	5303	ATP	O4'-C4'-C5'-O5'
5	D	5303	ATP	C3'-C4'-C5'-O5'
5	F	5303	ATP	O4'-C4'-C5'-O5'
5	F	5303	ATP	C3'-C4'-C5'-O5'
5	H	5303	ATP	O4'-C4'-C5'-O5'
5	H	5303	ATP	C3'-C4'-C5'-O5'

There are no ring outliers.

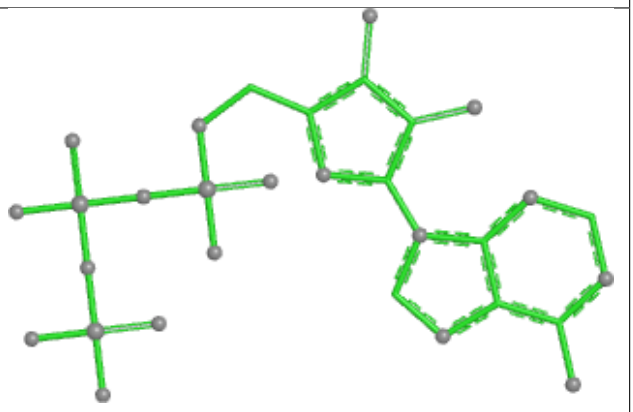
No monomer is involved in short contacts.

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

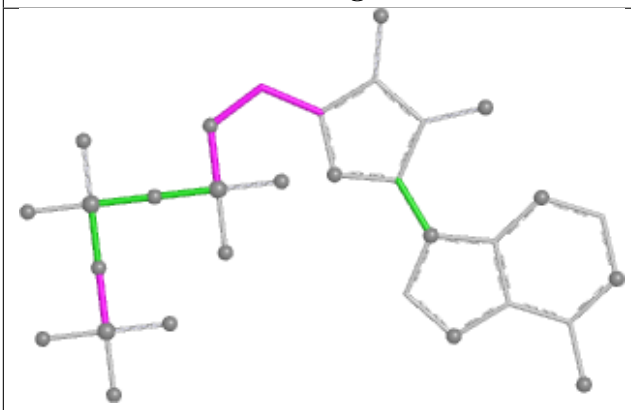
Ligand ATP B 5303



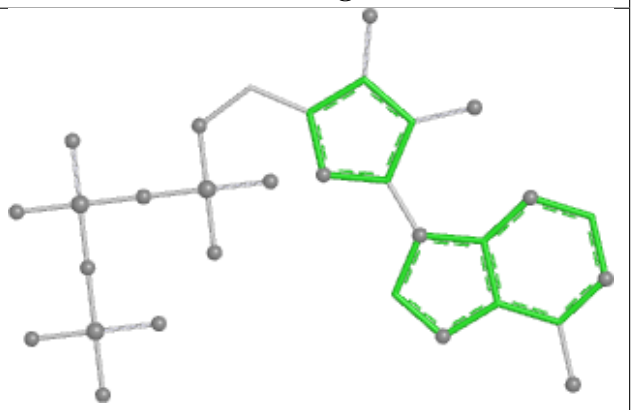
Bond lengths



Bond angles

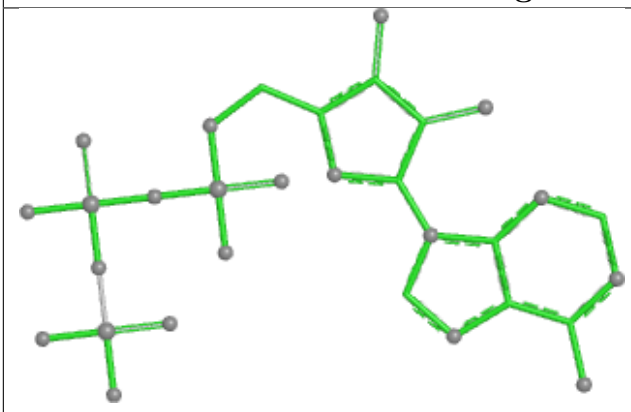


Torsions

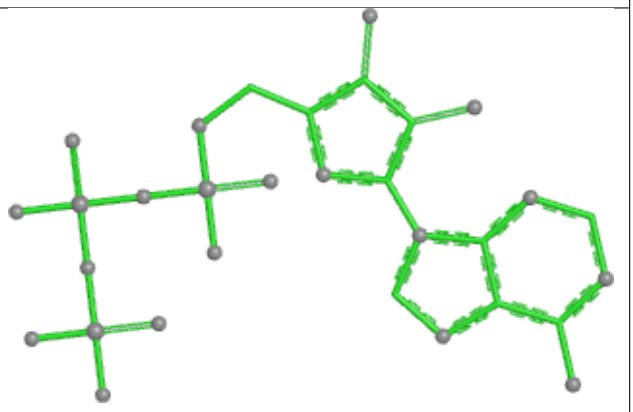


Rings

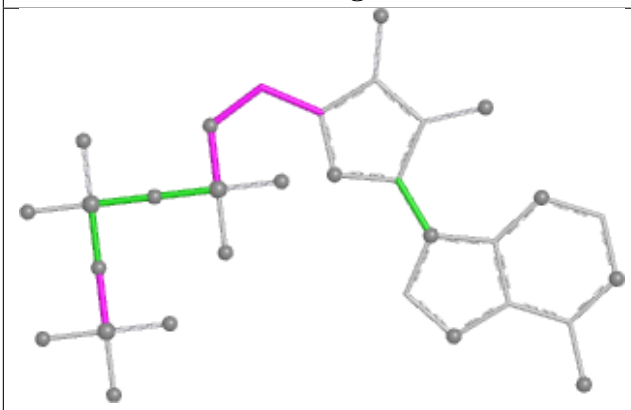
Ligand ATP D 5303



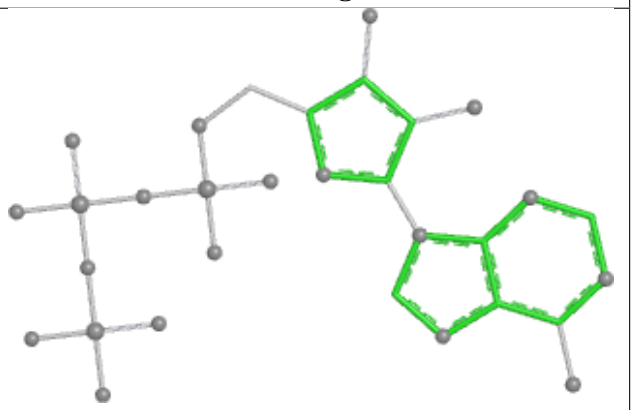
Bond lengths



Bond angles

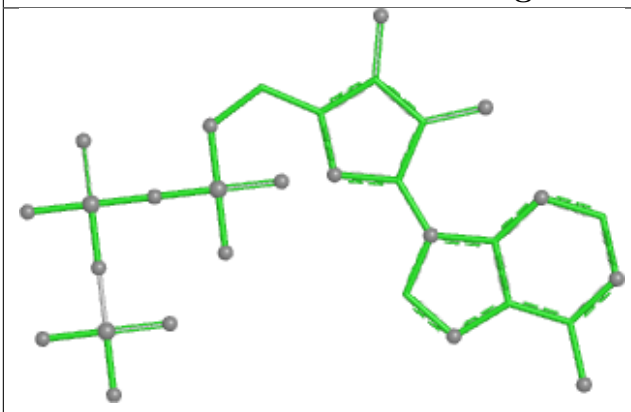


Torsions

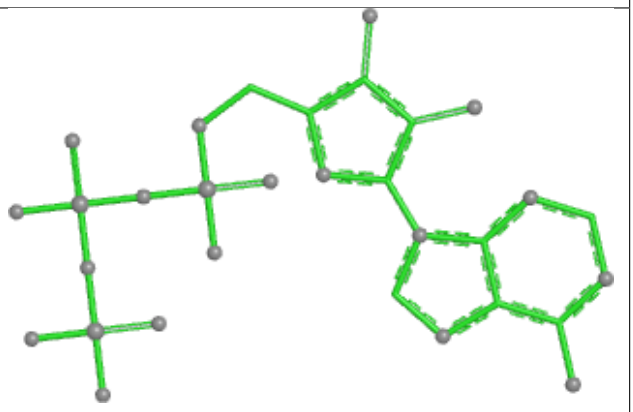


Rings

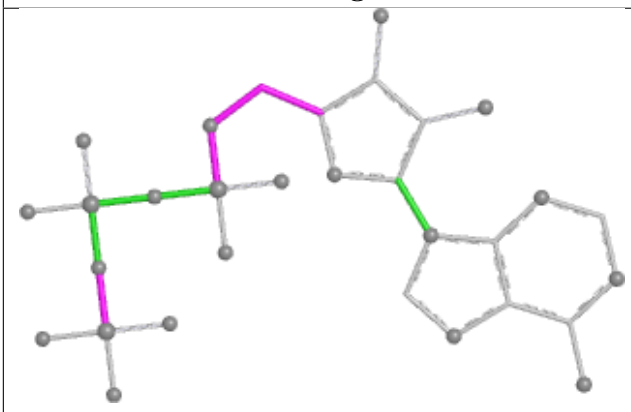
Ligand ATP H 5303



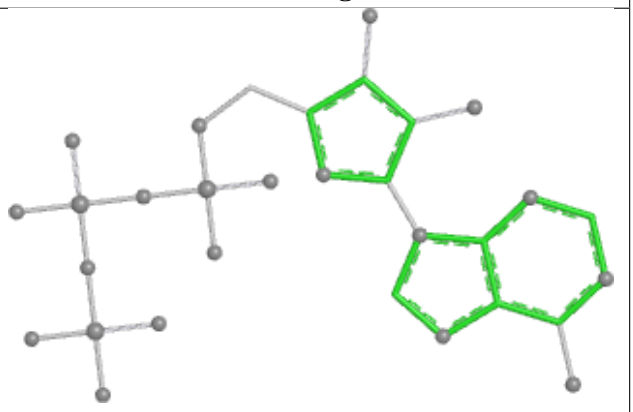
Bond lengths



Bond angles

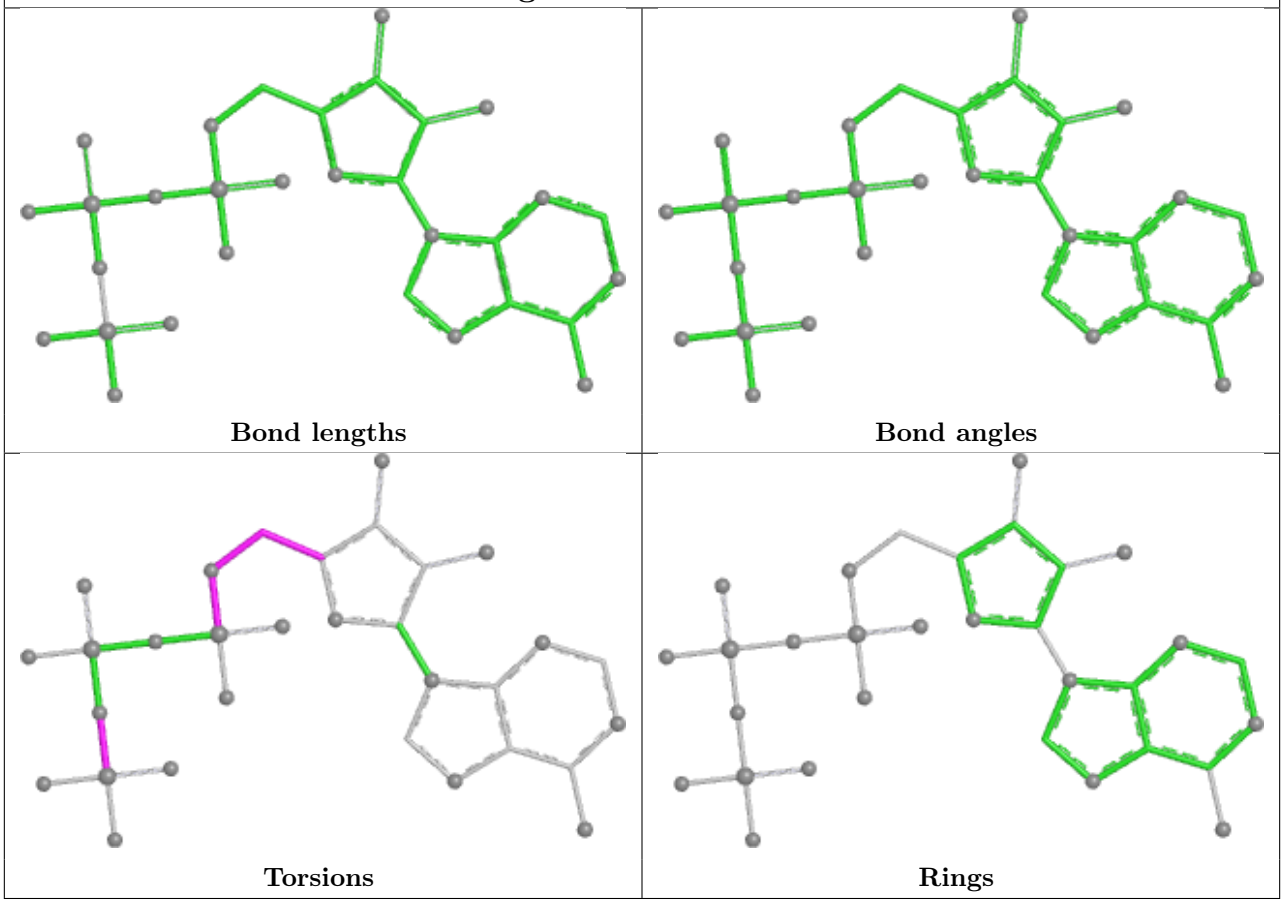


Torsions



Rings

Ligand ATP F 5303



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.

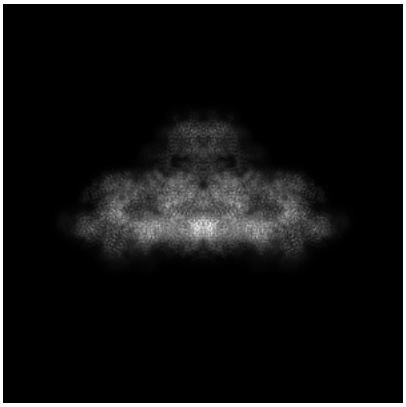
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-73958. These allow visual inspection of the internal detail of the map and identification of artifacts.

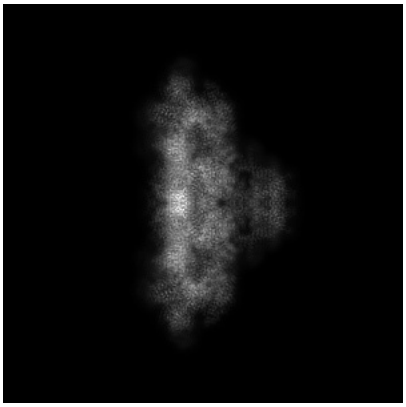
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

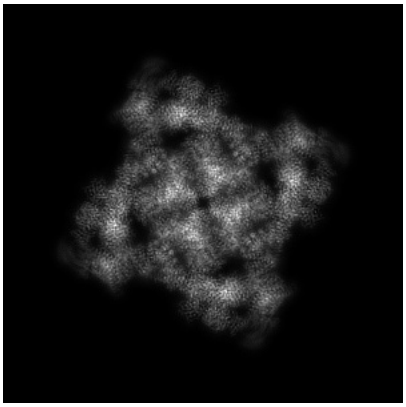
6.1.1 Primary map



X



Y

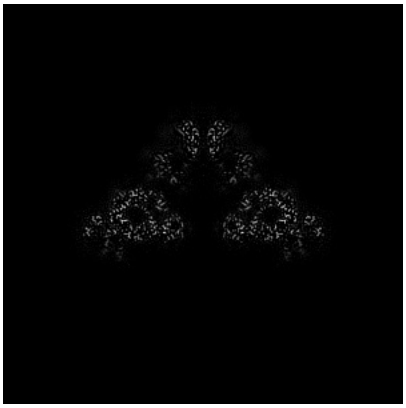


Z

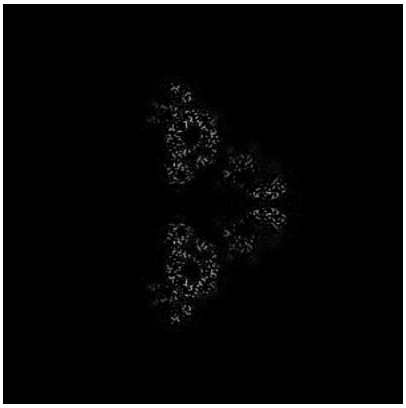
The images above show the map projected in three orthogonal directions.

6.2 Central slices

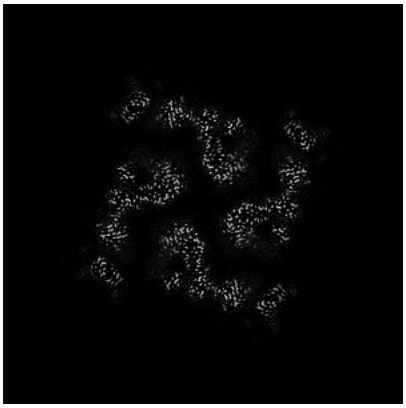
6.2.1 Primary map



X Index: 256



Y Index: 256

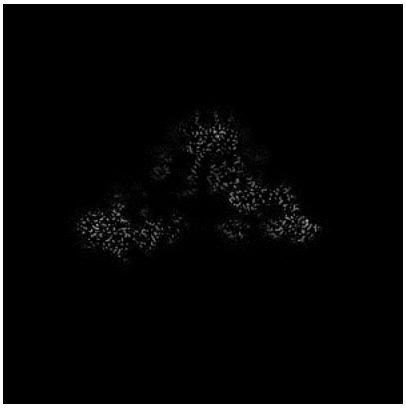


Z Index: 256

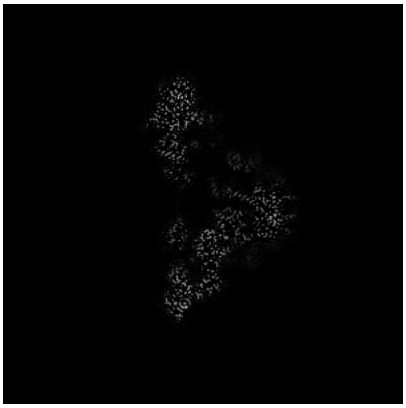
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

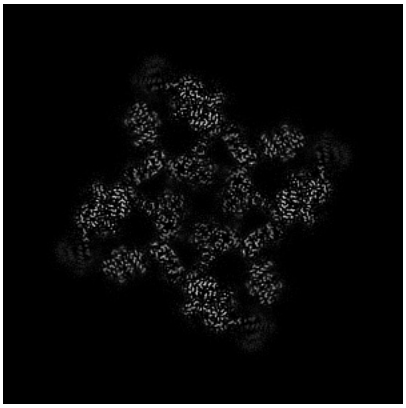
6.3.1 Primary map



X Index: 267



Y Index: 267

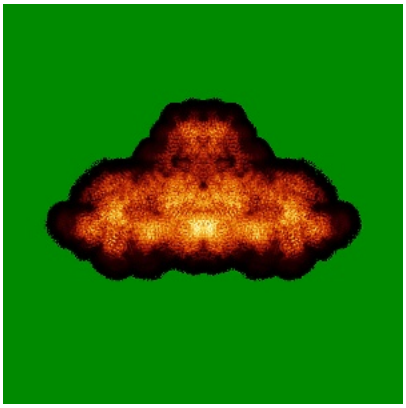


Z Index: 231

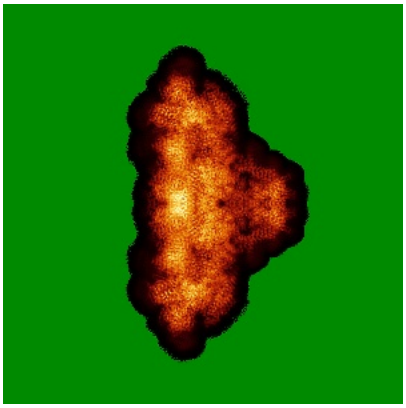
The images above show the largest variance slices of the map in three orthogonal directions.

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

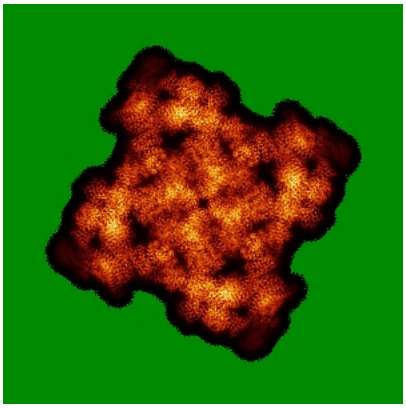
6.4.1 Primary map



X



Y

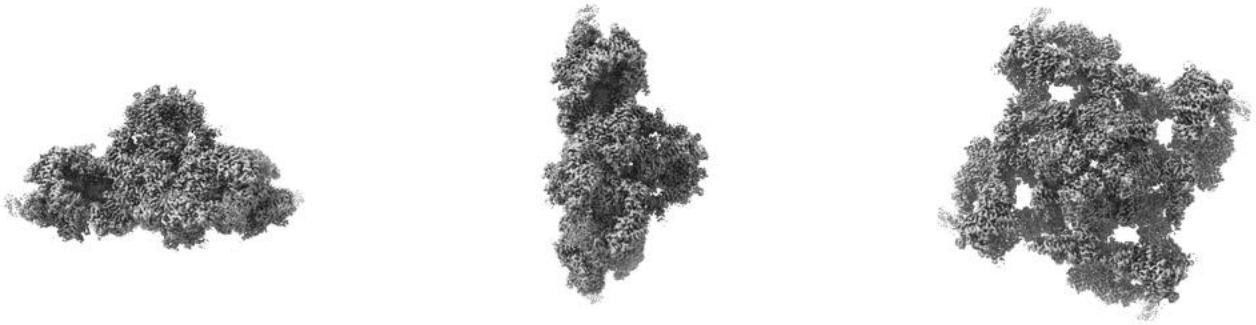


Z

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

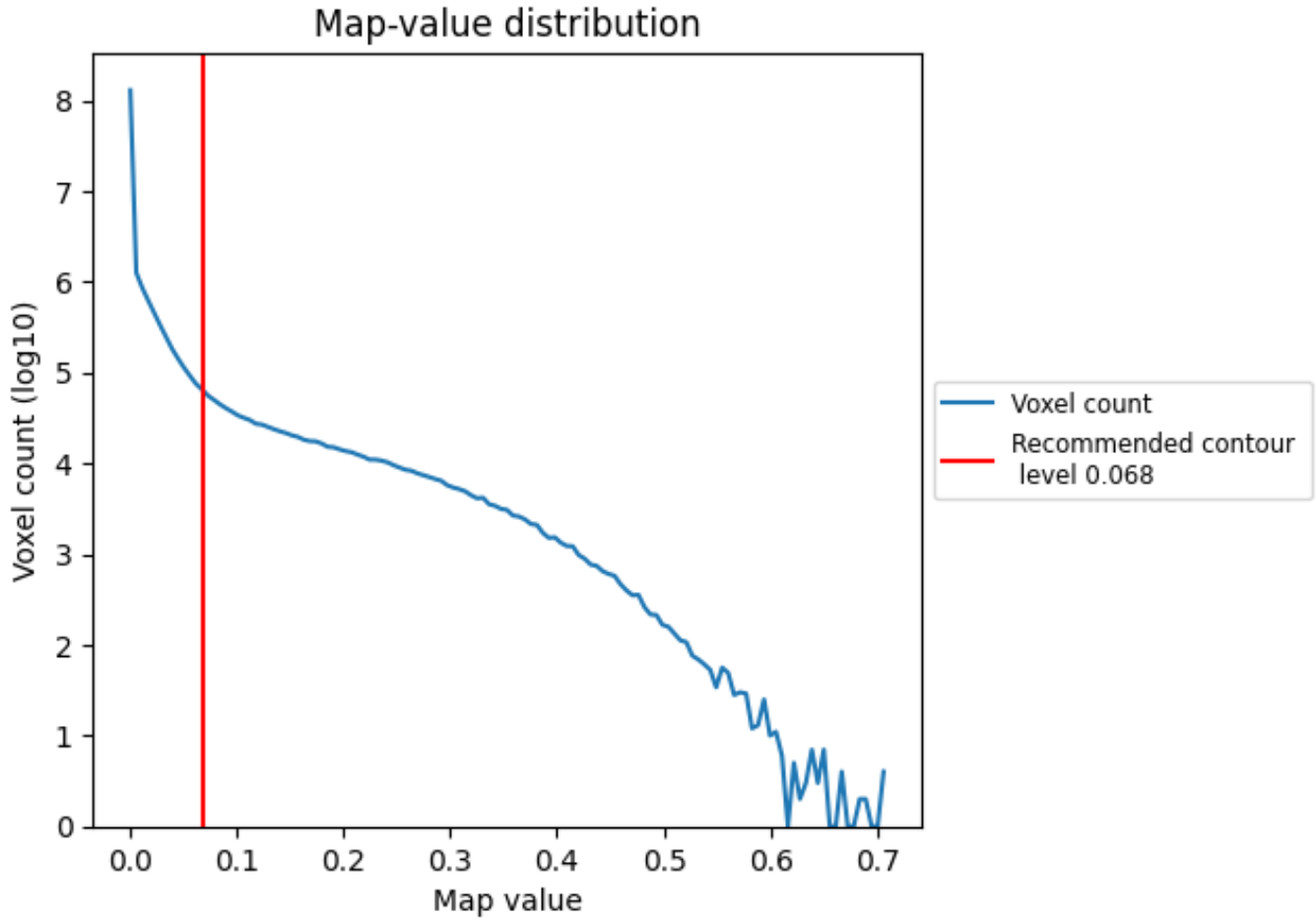
6.6 Mask visualisation (i)

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

7 Map analysis

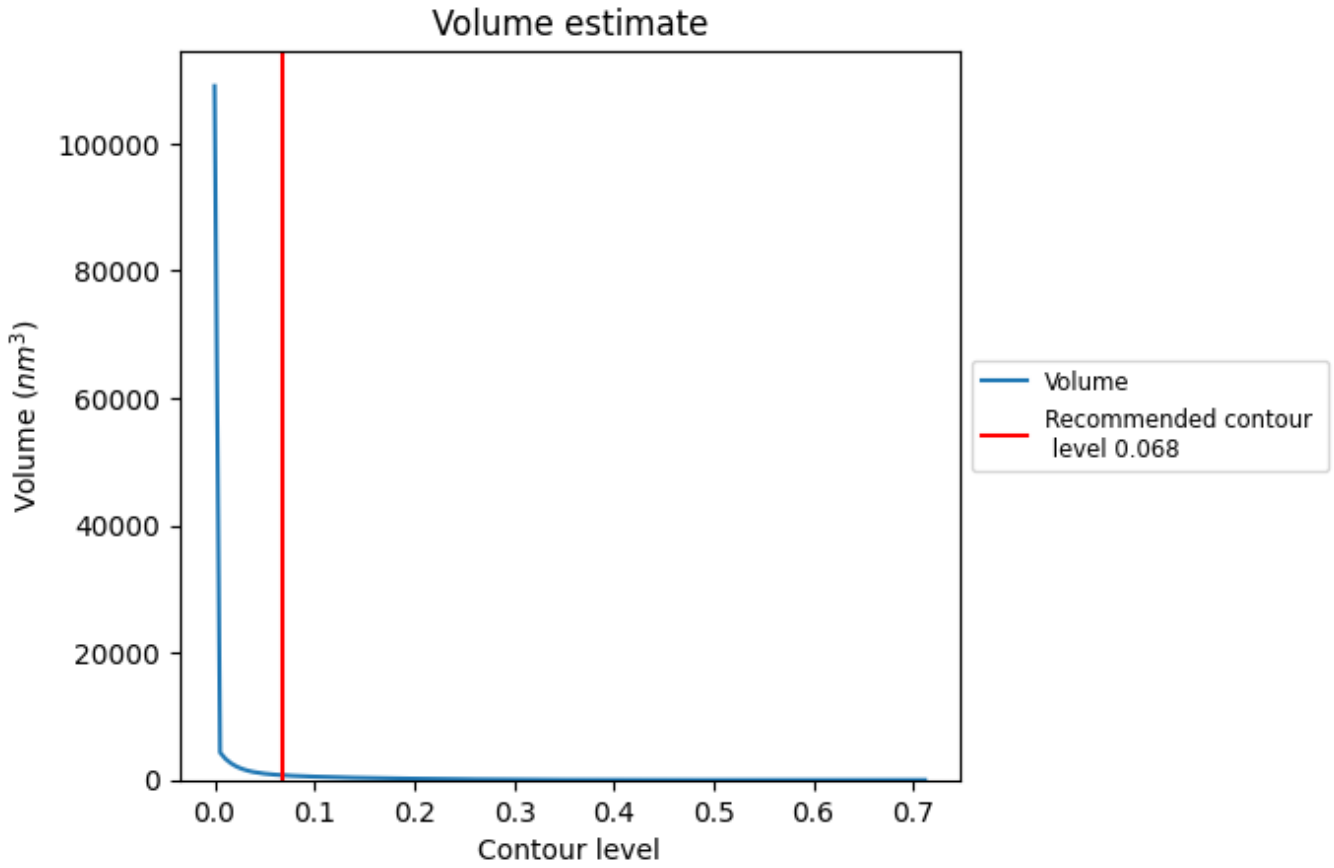
This section contains the results of statistical analysis of the map.

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.

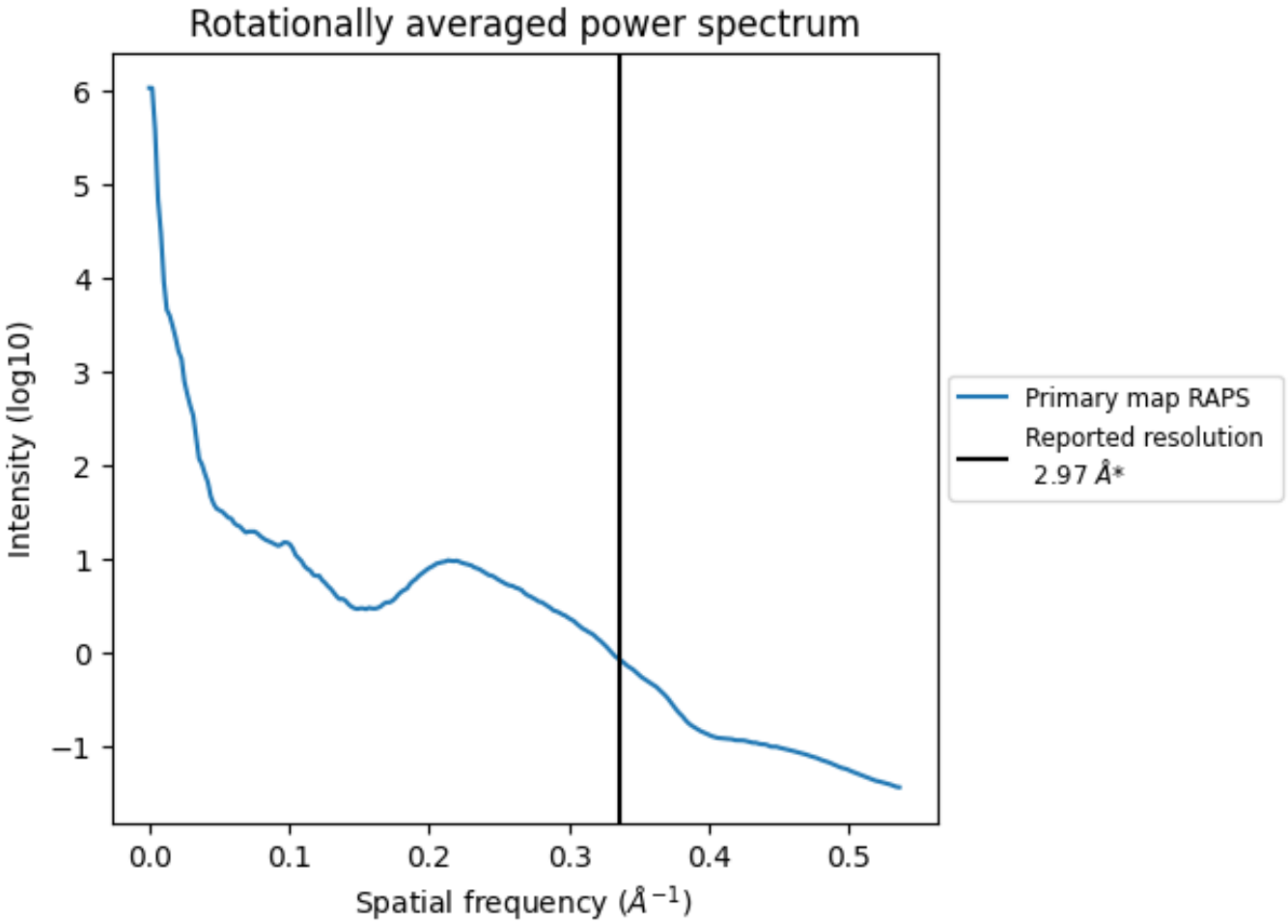
7.2 Volume estimate



The volume at the recommended contour level is 748 nm^3; this corresponds to an approximate mass of 676 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 0.337 Å^{-1}

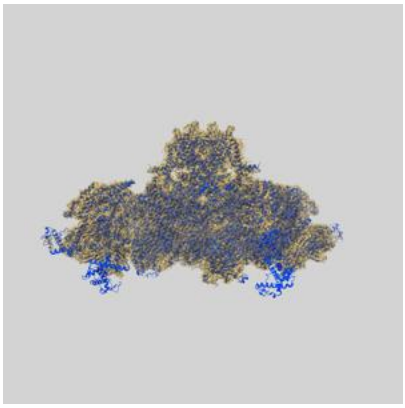
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

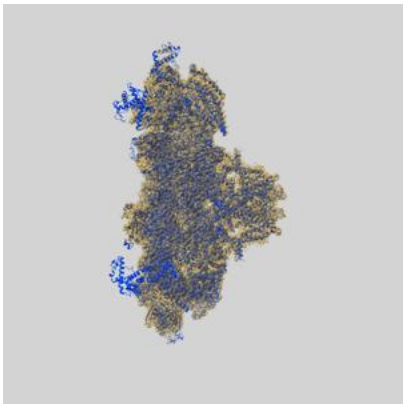
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-73958 and PDB model 9Z9T. Per-residue inclusion information can be found in section 3 on page 7.

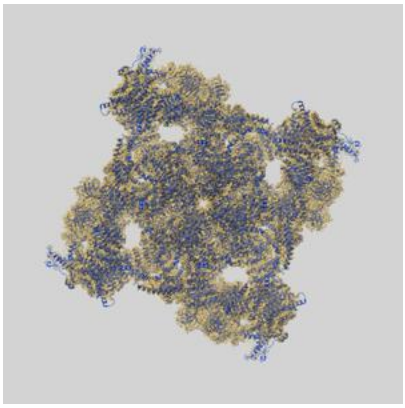
9.1 Map-model overlay



X



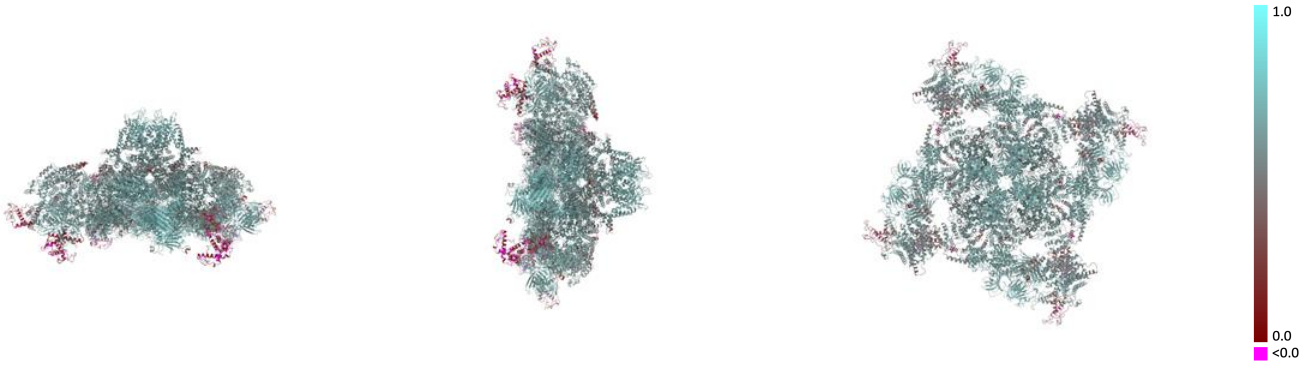
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.068 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

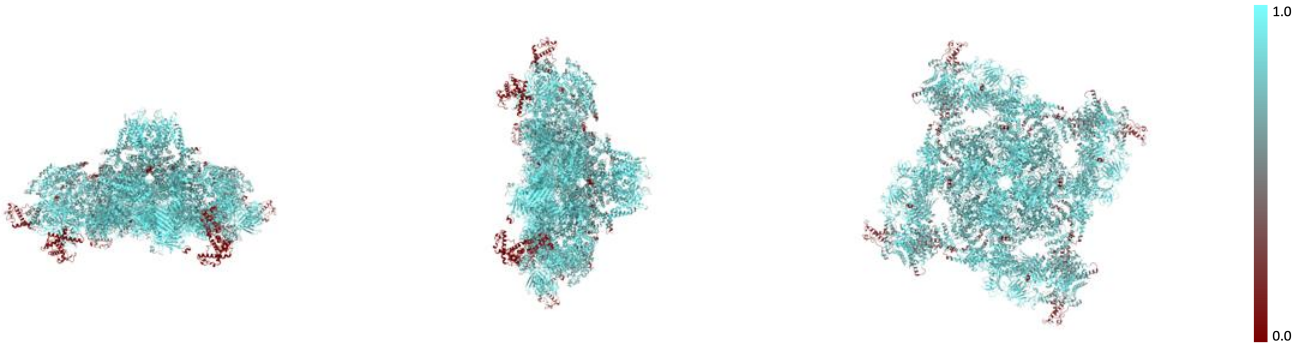
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

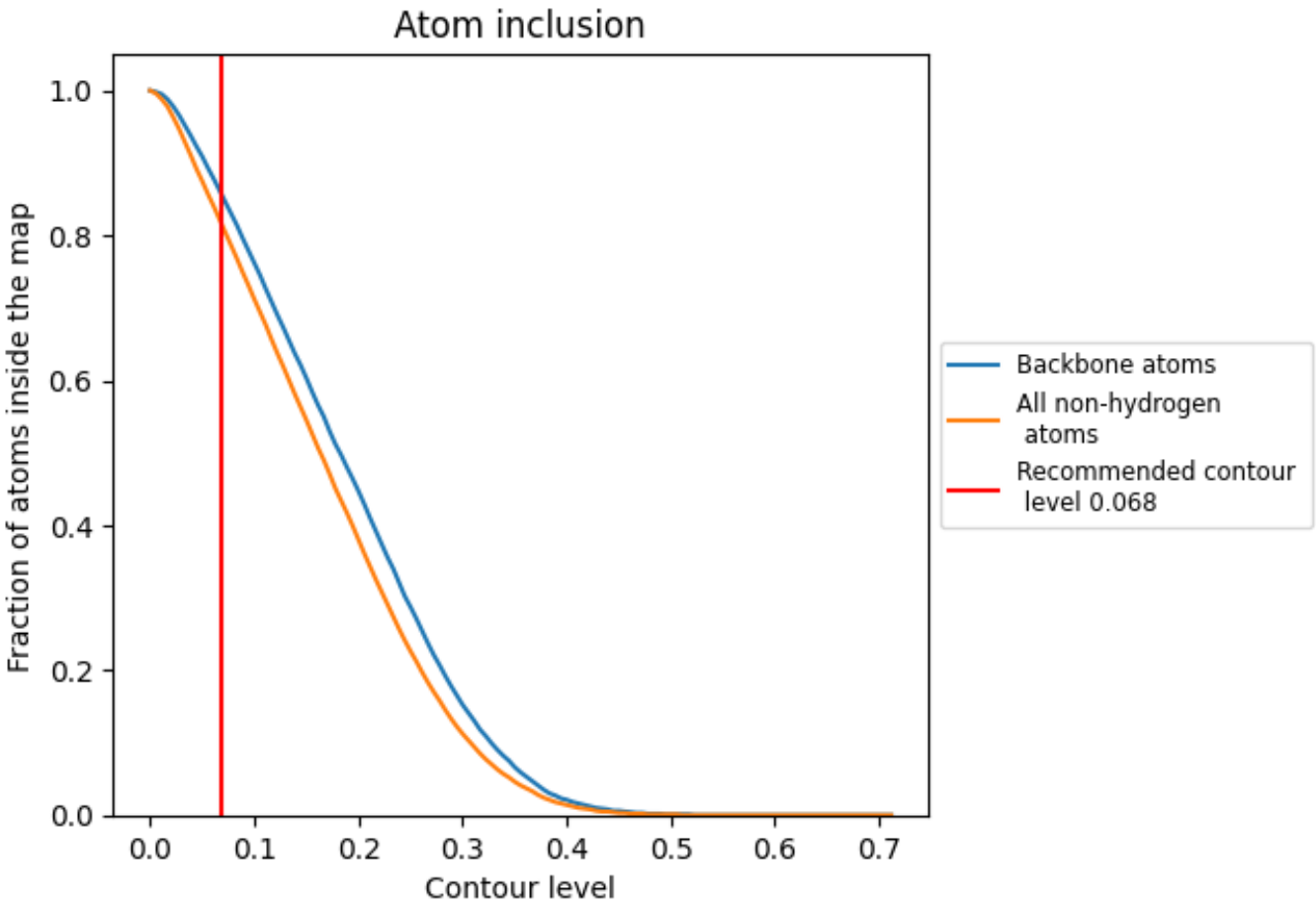
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.068).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 82% 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 (0.068) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8180	0.5790
A	0.9360	0.6500
B	0.8150	0.5770
C	0.9360	0.6520
D	0.8150	0.5770
E	0.9360	0.6500
F	0.8150	0.5770
G	0.9360	0.6500
H	0.8150	0.5770

