Full wwPDB EM Validation Report ⓘ

Nov 11, 2026 – 12:51 PM EST

PDB ID	:	9Z9V / pdb_00009z9v
EMDB ID	:	EMD-73960
Title	:	Open-state rabbit RyR1 with activating ligands (Ca2+/ATP) and S107
Authors	:	Chen, Y.S.; Hu, R.B.; Van Petegem, F.
Deposited on	:	2025-11-18
Resolution	:	2.91 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:

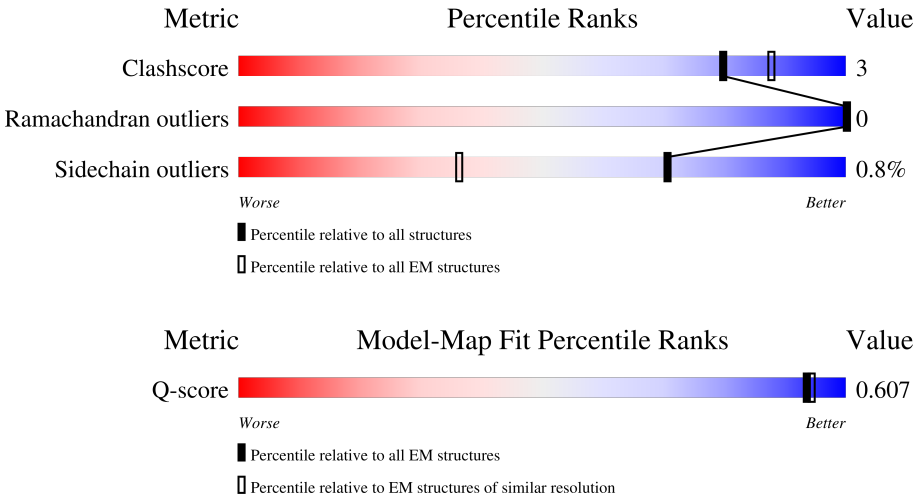
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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 2.91 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.



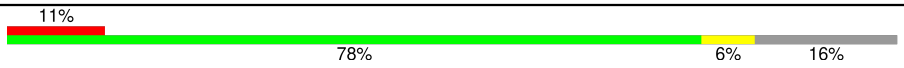
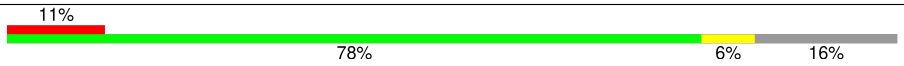
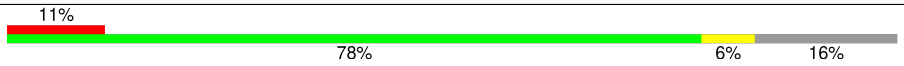
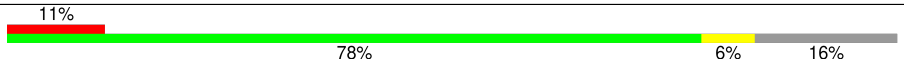
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12972 (2.41 - 3.41)

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	86% 12%
1	C	110	85% 13%
1	E	110	85% 13%
1	G	110	86% 12%

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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

There are 5 unique types of molecules in this entry. The entry contains 136040 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
			815	514	144	153	4		
1	C	108	Total	C	N	O	S	0	0
			815	514	144	153	4		
1	E	108	Total	C	N	O	S	0	0
			815	514	144	153	4		
1	G	108	Total	C	N	O	S	0	0
			815	514	144	153	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	3	0
			33162	21189	5743	6004	226		
2	D	4246	Total	C	N	O	S	3	0
			33162	21189	5743	6004	226		
2	F	4246	Total	C	N	O	S	3	0
			33162	21189	5743	6004	226		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	4246	Total 33162	C 21189	N 5743	O 6004	S 226	3	0

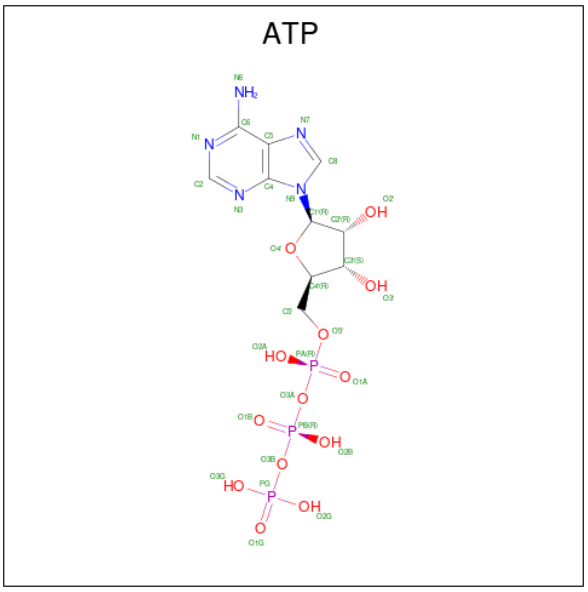
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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	

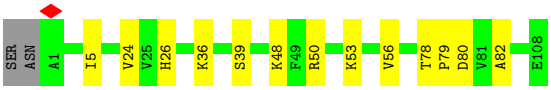
3 Residue-property plots (i)

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:

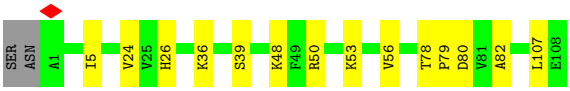




• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain C:

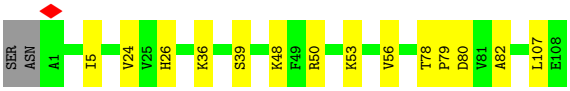




• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain E:

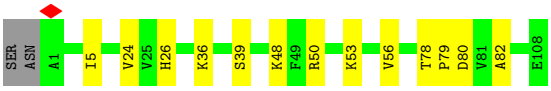




• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain G:

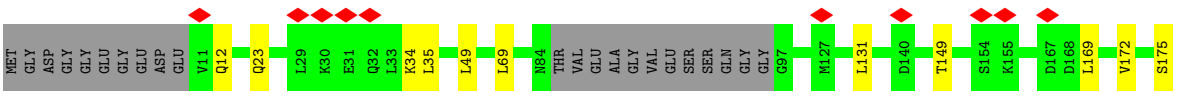


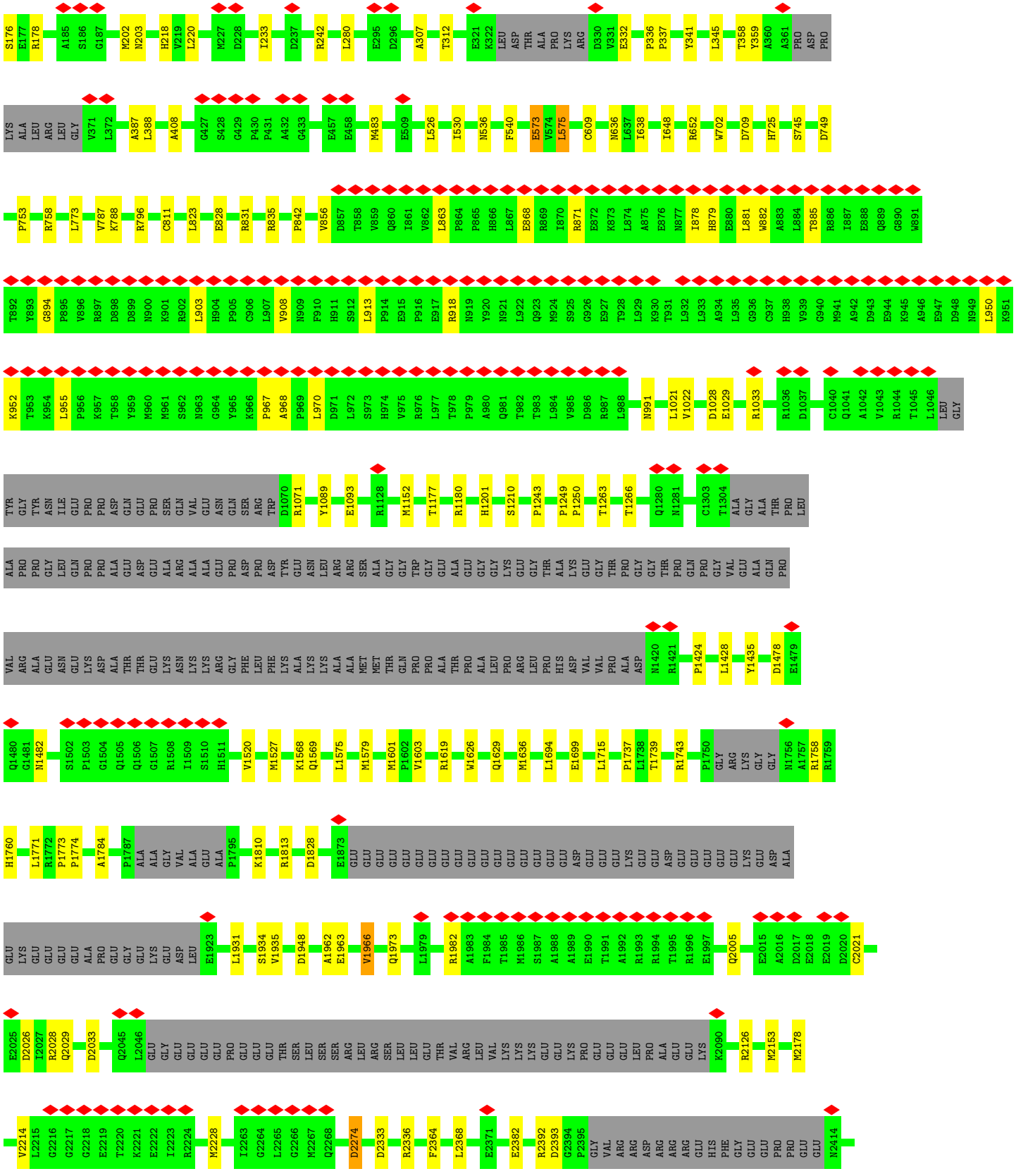


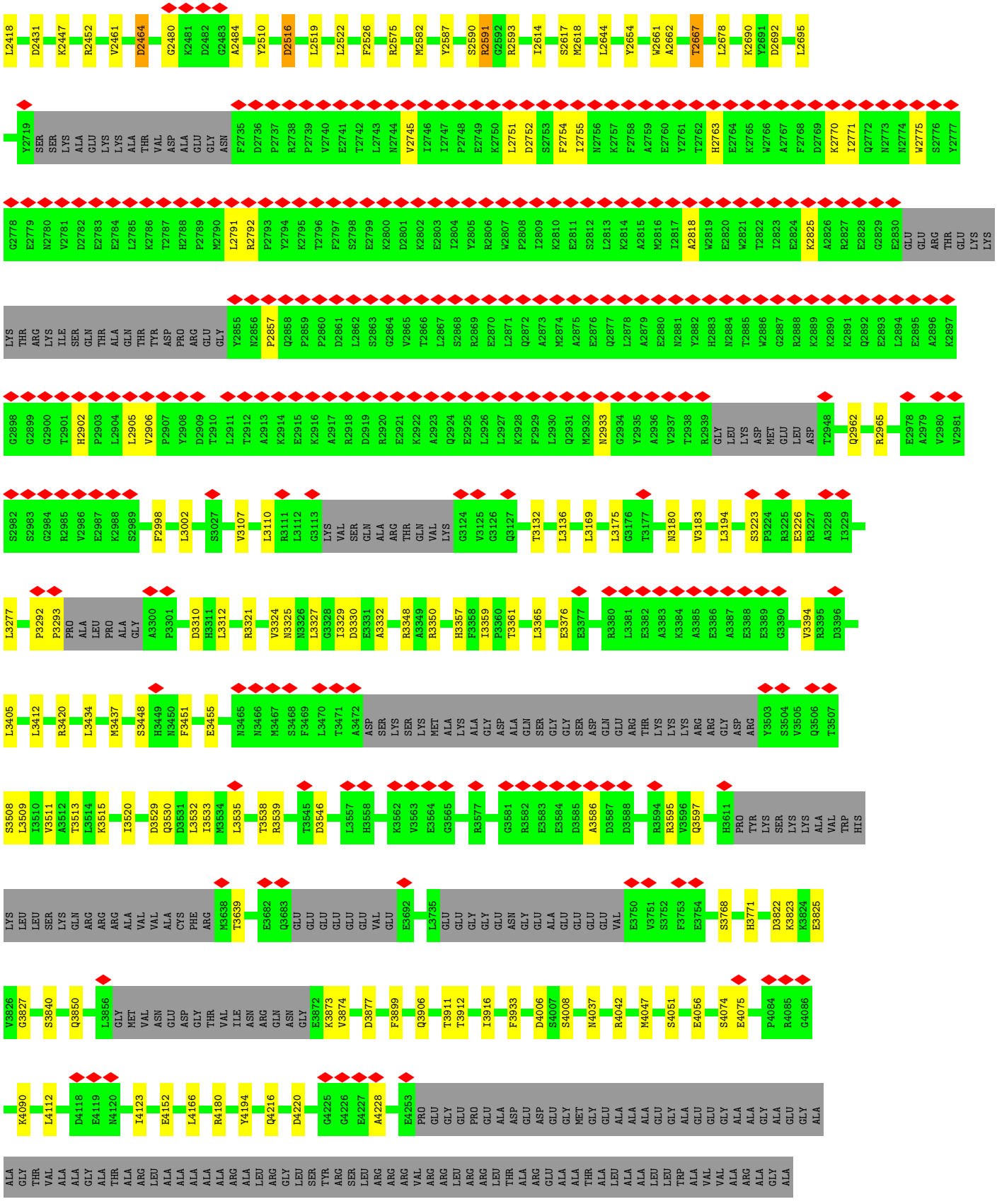
• Molecule 2: Ryanodine receptor 1

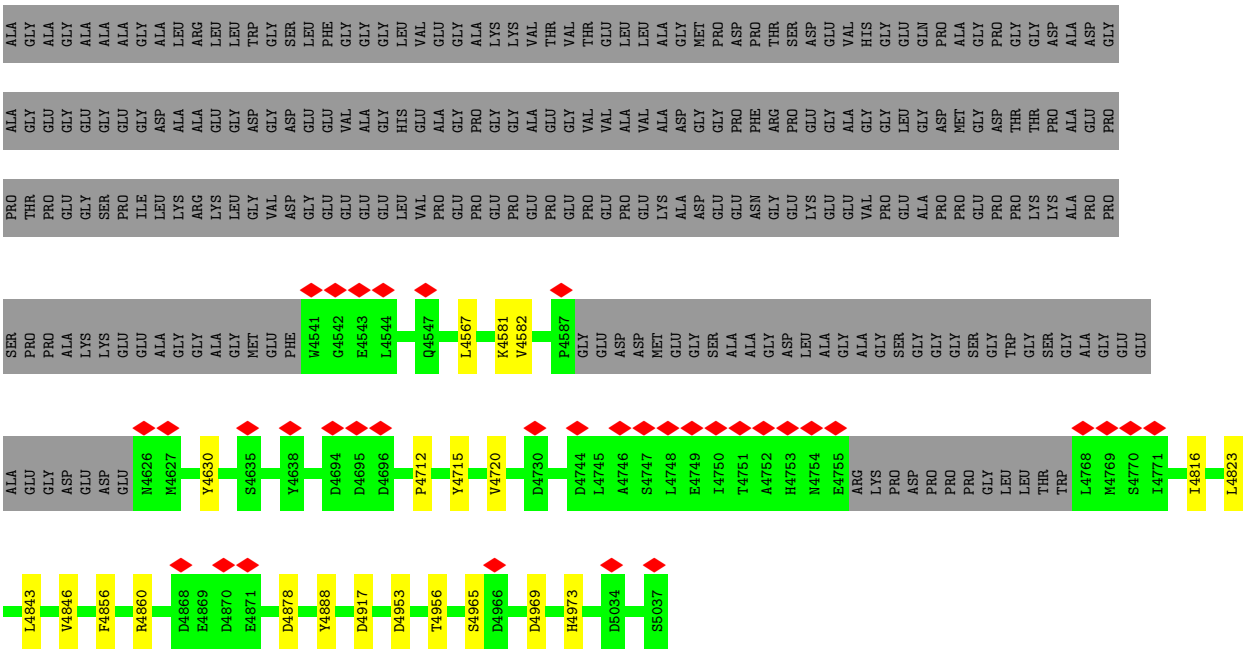
Chain B:






S176 E177 R178 A185 S186 G187 M202 N203 H218 V219 L220 M227 D228 I233 D237 R242 L280 E295 D296 A307 T312 E321 K322 LEU ASP THR ALA PRO LYS ARG D330 V331 E332 P336 P337 Y341 L345 T358 Y359 A360 A361 PRO ASP PRO
LYS ALA LEU ARG LEU GLY V371 L372 A387 L388 A408 G427 S428 G429 P430 P431 A432 G433 E457 E458 M483 E509 L526 I530 N536 F540 E573 V574 L575 C609 M636 L637 I638 I648 R652 W702 D709 H725 S745 D749
P753 R758 L773 V787 K788 R796 C811 L823 E828 R831 R835 P842 V856 D857 T858 V859 Q860 I861 V862 L863 P864 P865 H866 L867 E868 R869 I870 R871 E872 K873 L874 A875 E876 M877 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 K930 T931 L932 L933 A934 L935 G936 C937 H938 V939 G940 M941 A942 D943 E944 K945 A946 E947 D948 N949 L950 K951
K952 T953 K954 L955 P956 K957 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 L1021 V1022 D1028 E1029 R1033 R1036 D1037 C1040 Q1041 A1042 V1043 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 R1071 Y1089 E1093 R1128 M1152 T1177 R1180 H1201 S1210 P1243 P1249 P1250 T1263 T1266 Q1280 N1281 C1303 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 THR PRO ALA LEU PRO ARG LEU PRO HIS ASP VAL VAL PRO ALA ASP N1420 R1421 P1424 L1428 Y1435 D1478 E1479
Q1480 G1481 N1482 S1502 P1503 G1504 Q1505 Q1506 G1507 R1508 I1509 S1510 H1511 V1520 M1527 K1568 Q1569 L1575 M1579 M1601 P1602 V1603 R1619 W1626 Q1629 M1636 L1694 E1699 L1715 P1737 L1738 T1739 R1743 P1750 GLY ARG LYS GLY GLY N1756 A1757 R1758 R1759
H1760 L1771 R1772 P1773 P1774 A1784 P1787 ALA ALA GLY VAL ALA GLU ALA P1795 K1810 R1813 D1828 E1873 GLU GLU GLU

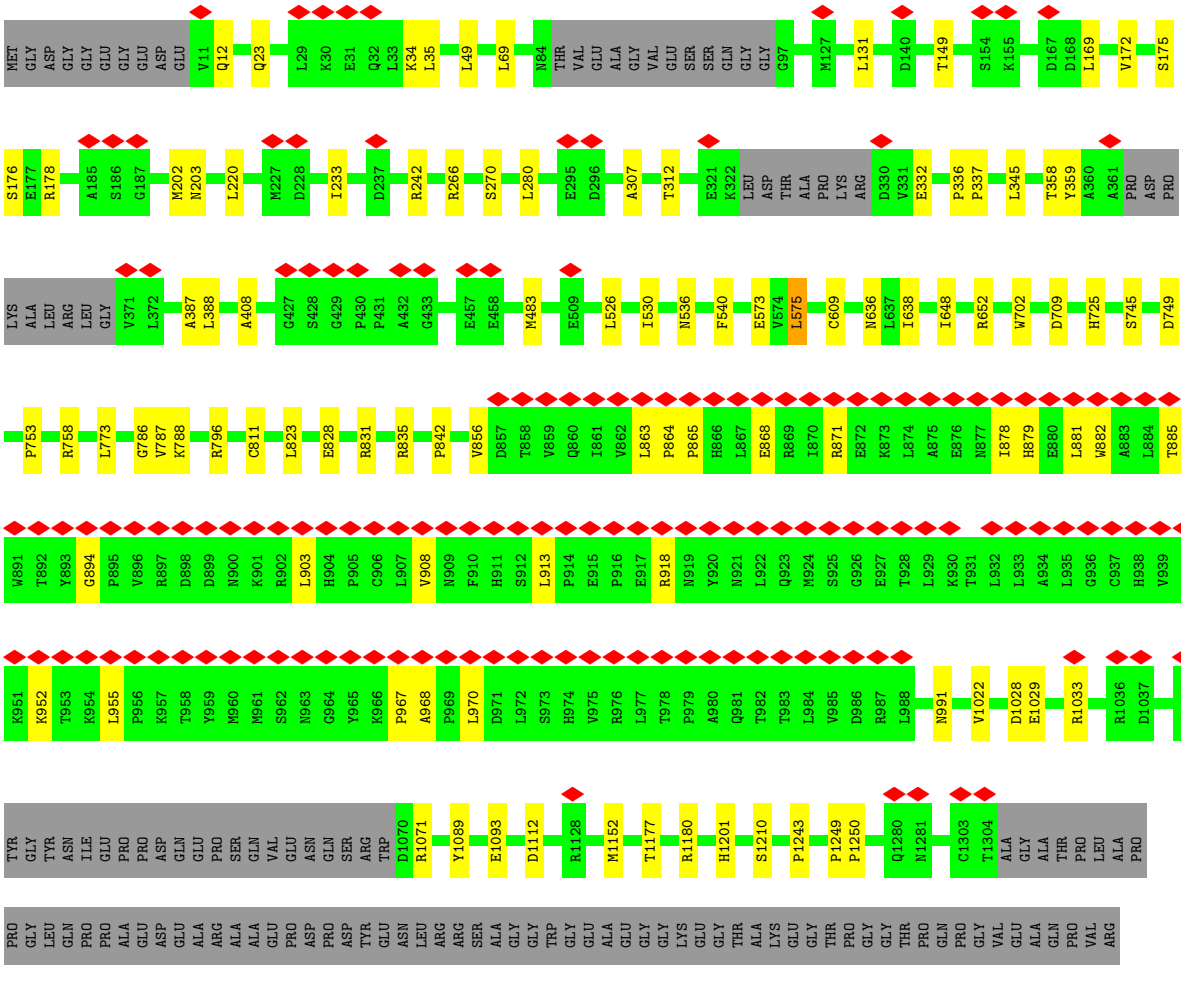

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Y2719 SER SER LYS ALA GLU LYS LYS ALA THR VAL ASP ALA GLU GLY ASN F2735 D2736 P2737 R2738 P2739 V2740 E2741 T2742 L2743 N2744 V2745 I2746 I2747 P2748 E2749 K2750 L2751 D2752 S2753 F2754 I2755 N2756 K2757 F2758 A2759 E2760 Y2761 T2762 H2763 E2764 K2765 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 Q2962 R2965 E2978 A2979 V2980 V2981
S2982 S2983 G2984 R2985 V2986 E2987 K2988 S2989 F2998 L3002 S3027 V3107 L3110 R3111 L3112 G3113 LYS VAL SER GLN ALA ARG THR GLN VAL LYS G3124 V3125 G3126 Q3127 T3132 L3136 L3169 L3175 G3176 T3177 N3180 V3183 L3194 S3223 P3224 R3225 E3226 R3227 A3228 I3229
L3277 P3292 P3293 PRO ALA LEU PRO ALA GLY A3300 P3301 D3310 H3311 L3312 R3321 V3324 N3325 N3326 L3327 G3328 I3329 D3330 E3331 A3332 R3348 A3349 R3350 H3357 F3358 I3359 P3360 T3361 L3365 E3376 E3377 R3380 L3381 E3382 A3383 K3384 A3385 E3386 A3387 E3388 E3389 G3390 V3394 R3395 D3396
L3405 L3412 R3420 L3434 M3437 S3448 H3449 N3450 F3451 E3455 N3465 N3466 M3467 S3468 F3469 L3470 T3471 A3472 ASP SER LYS SER LYS MET ALA LYS ALA GLY ASP ALA GLN SER GLY GLY SER ASP GLN GLU ARG THR LYS LYS ARG ARG GLY ASP ARG Y3503 S3504 V3505 Q3506 T3507
S3508 L3509 T3510 V3511 A3512 T3513 L3514 K3515 I3520 D3529 Q3530 D3531 L3532 I3533 M3534 L3535 T3538 R3539 T3545 D3546 L3557 H3558 K3562 V3563 E3564 G3565 R3577 G3581 R3582 E3583 E3584 D3585 A3586 D3587 D3588 R3594 R3595 V3596 Q3597 H3611 PRO TYR LYS SER LYS LYS ALA VAL TRP HIS
LYS LEU LEU SER LYS GLN ARG ARG ARG ALA VAL VAL VAL ALA CYS PHE ARG M3638 T3639 E3682 Q3683 GLU GLU GLU GLU GLU GLU VAL GLU E3692 L3735 GLU GLU GLY GLY GLU ASN GLY GLU GLU ALA GLU GLU GLU GLU VAL E3750 V3751 S3752 F3753 E3754 S3768 H3771 D3822 K3823 K3824 E3825
V3826 G3827 S3840 Q3850 L3856 GLY MET VAL ASN GLU ASP GLY THR VAL ILE ASN ARG GLN ASN GLY E3872 K3873 V3874 D3877 F3899 Q3906 T3911 T3912 I3916 F3933 D4006 S4007 S4008 N4037 R4042 M4047 S4051 E4056 S4074 E4075 P4084 R4085 G4086
K4090 L4112 D4118 E4119 N4120 I4123 E4152 L4166 R4180 Y4194 Q4216 D4220 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 GLU GLU GLY ALA ALA ALA GLY ALA GLU GLY ALA
ALA GLY THR VAL ALA ALA GLY ALA THR ALA ARG LEU ALA ALA ALA ALA ARG ALA LEU 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 ALA ALA ALA LEU LEU TRP ALA VAL VAL ALA ARG ALA ALA GLY ALA

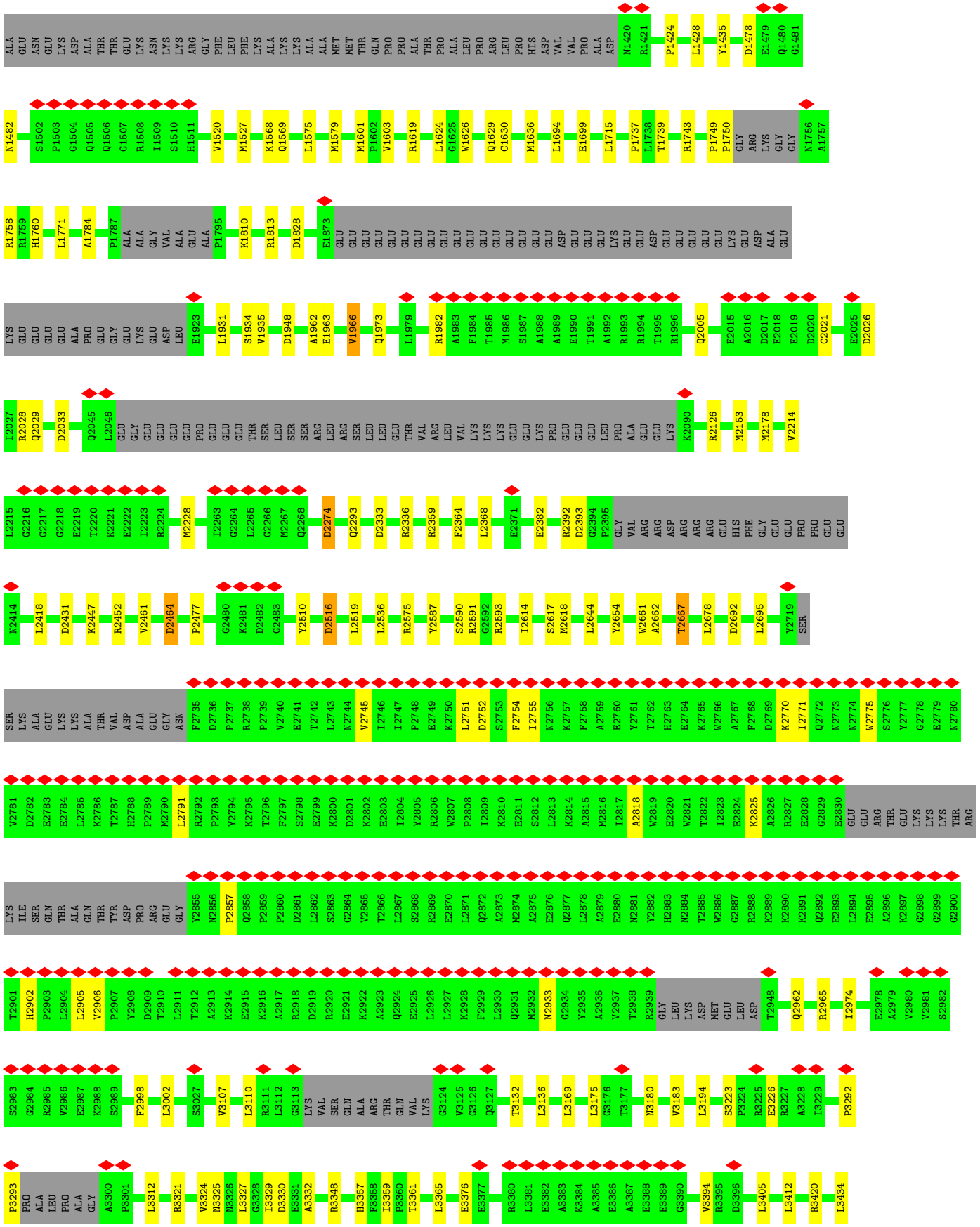


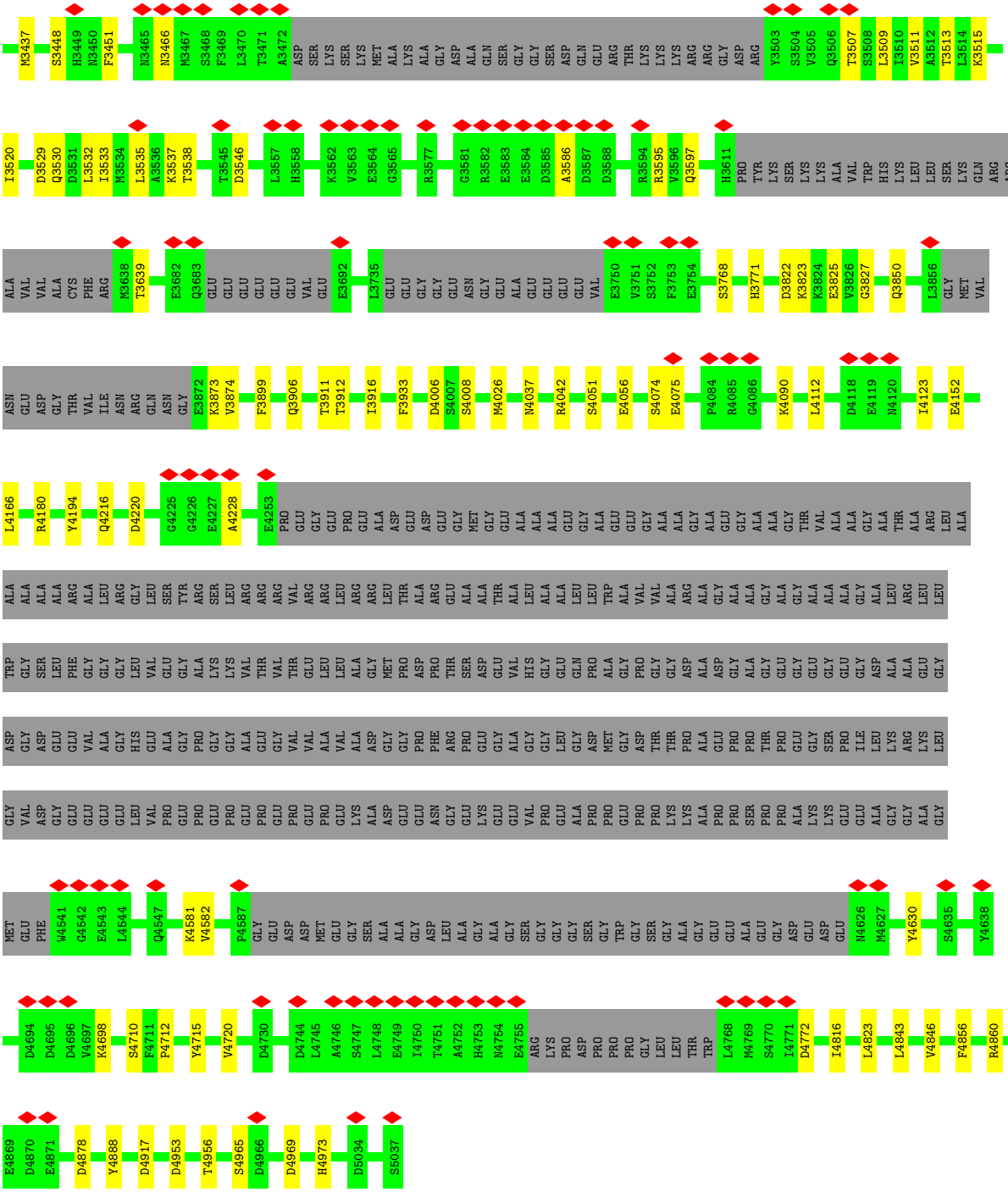
• Molecule 2: Ryanodine receptor 1

Chain D:





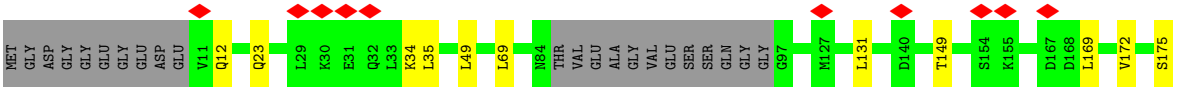

ALA GLU ASN GLU LYS ASP ALA THR THR GLU LYS ASN LYS LYS ARG GLY PHE LEU PHE LYS ALA LYS LYS ALA ALA MET MET THR GLN PRO PRO ALA THR PRO ALA LEU PRO ARG LEU PRO HIS ASP VAL VAL PRO ALA ASP
N1420 R1421 P1424 L1428 Y1435 D1478 E1479 Q1480 G1481
N1482 S1502 P1503 G1504 Q1505 Q1506 G1507 R1508 I1509 S1510 H1511 V1520 M1527 K1568 Q1569 L1575 M1579 M1601 P1602 V1603 R1619 L1624 G1625 W1626 Q1629 C1630 M1636 L1694 E1699 L1715 P1737 L1738 T1739 R1743 P1749 P1750 GLY ARG LYS GLY GLY N1756 A1757
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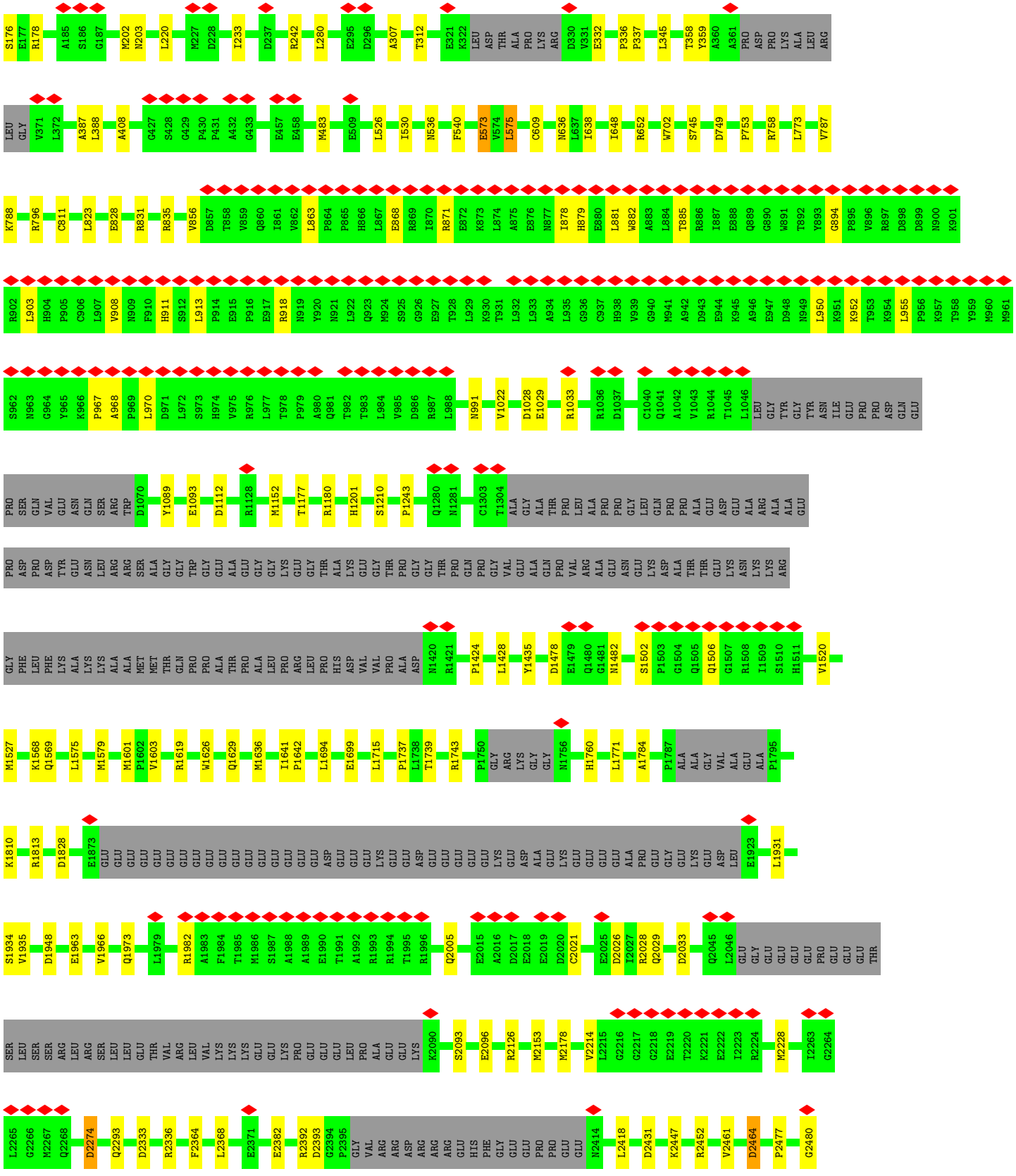


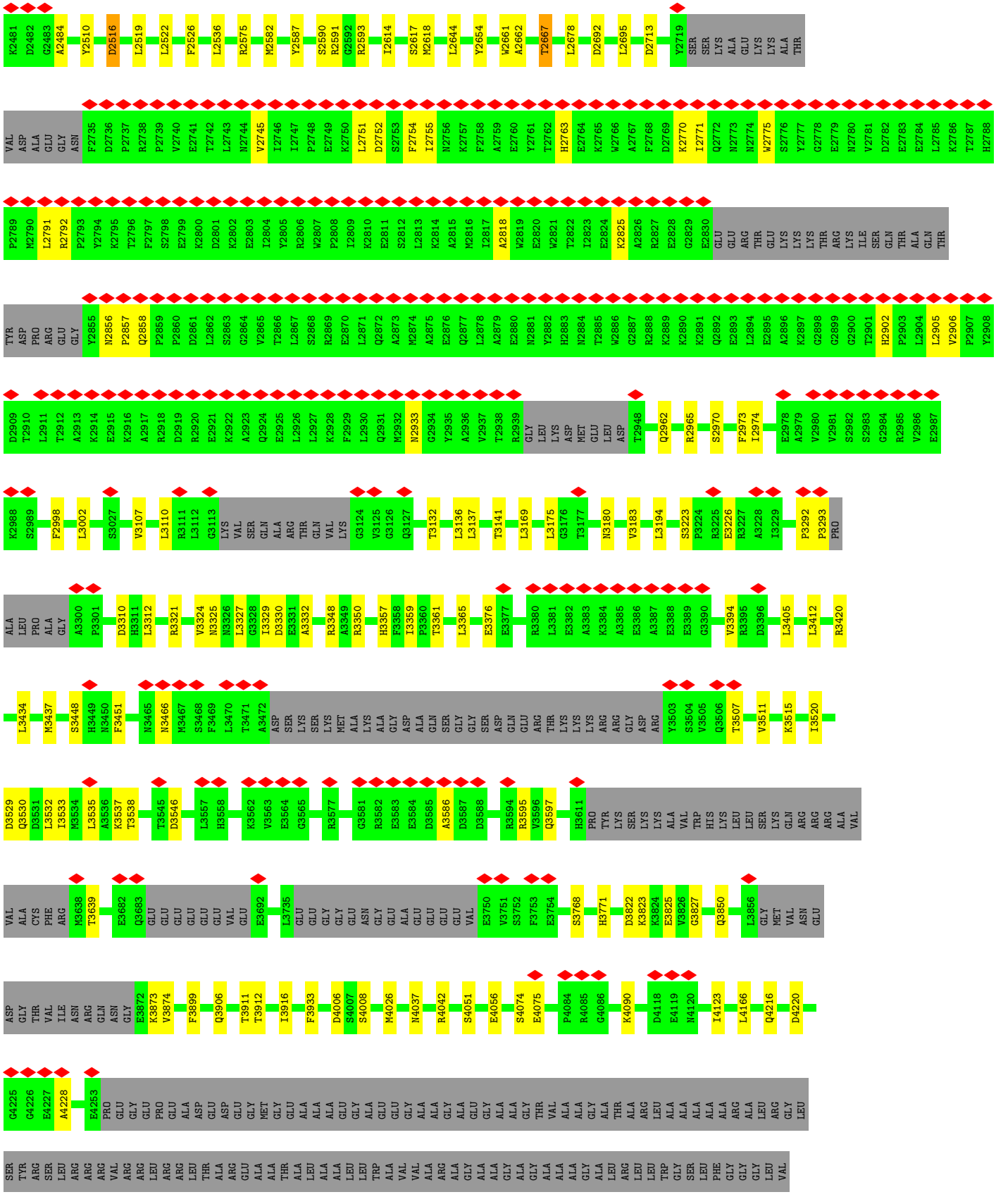
• Molecule 2: Ryanodine receptor 1

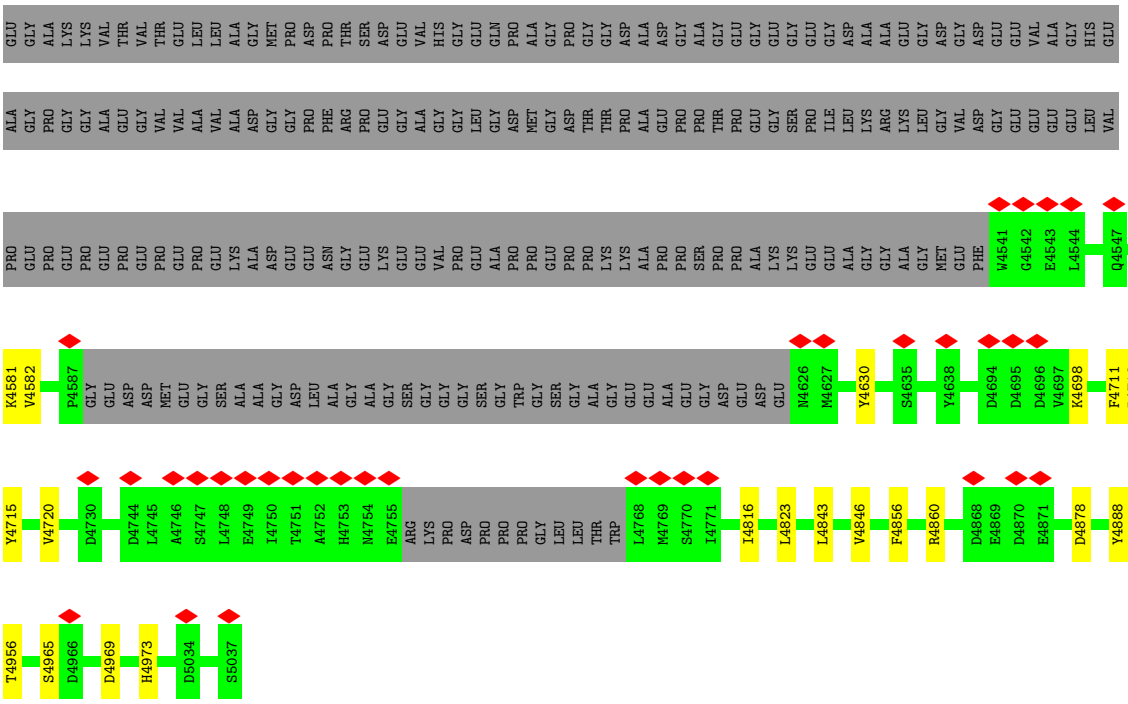
Chain F:






S176 E177 R178 A185 S186 G187 M202 N203 L220 M227 D228 I233 D237 R242 L280 E295 D296 A307 T312 E321 K322 LEU ASP THR ALA PRO LYS ARG D330 V331 E332 P336 P337 L345 T358 Y359 A360 A361 PRO ASP PRO LYS ALA LEU ARG
LEU GLY V371 L372 A387 L388 A408 G427 S428 G429 P430 P431 A432 G433 E457 E458 M483 E509 L526 I530 N536 F540 E573 V574 L575 C609 N636 L637 I638 I648 R652 W702 S745 D749 P753 R758 L773 V787
K788 R796 C811 L823 E828 R831 R835 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 K930 T931 L932 L933 A934 L935 G936 C937 H938 V939 G940 M941 A942 D943 E944 K945 A946 E947 D948 N949 L950 K951 K952 T953 K954 L955 P956 K957 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 V1022 D1028 E1029 R1033 R1036 D1037 C1040 Q1041 A1042 V1043 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 Y1089 E1093 D1112 R1128 M1152 T1177 R1180 H1201 S1210 P1243 Q1280 N1281 C1303 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 R1421 P1424 L1428 Y1435 D1478 E1479 Q1480 G1481 N1482 S1502 P1503 G1504 Q1505 Q1506 G1507 R1508 I1509 S1510 H1511 V1520
M1527 K1568 Q1569 L1575 M1579 M1601 P1602 V1603 R1619 W1626 Q1629 M1636 I1641 P1642 L1694 E1699 L1715 P1737 L1738 T1739 R1743 P1750 GLY ARG LYS GLY GLY N1756 H1760 L1771 A1784 P1787 ALA ALA GLY VAL ALA GLU ALA P1795
K1810 R1813 D1828 E1873 GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU ASP GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU

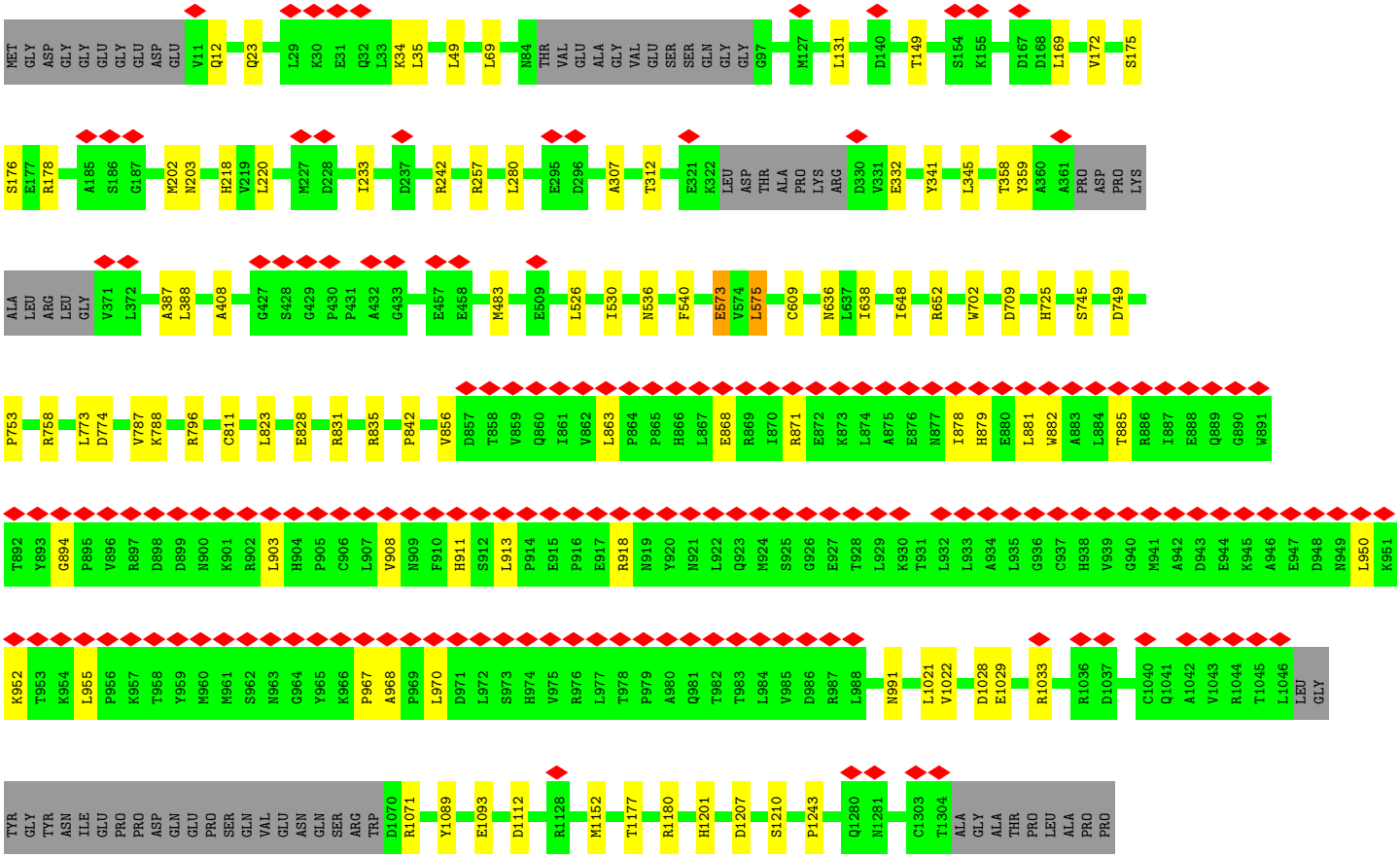

K2481 D2482 G2483 A2484 Y2510 D2516 L2519 L2522 F2526 L2536 R2575 M2582 Y2587 S2590 R2591 G2592 R2593 I2614 S2617 M2618 L2644 Y2654 W2661 A2662 T2667 L2678 D2692 L2695 D2713 Y2719 SER SER LYS ALA GLU LYS LYS ALA THR
VAL ASP ALA GLU GLY ASN F2735 D2736 P2737 R2738 P2739 V2740 E2741 T2742 L2743 N2744 V2745 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 Q2962 R2965 S2970 F2973 I2974 E2978 A2979 V2980 V2981 S2982 S2983 G2984 R2985 V2986 E2987
K2988 S2989 F2998 L3002 S3027 V3107 L3110 R3111 L3112 G3113 LYS VAL SER GLN ALA ARG THR GLN VAL LYS G3124 V3125 G3126 Q3127 T3132 L3136 L3137 T3141 L3169 L3175 G3176 T3177 N3180 V3183 L3194 S3223 P3224 R3225 E3226 R3227 A3228 I3229 P3292 P3293 PRO
ALA LEU PRO ALA GLY A3300 P3301 D3310 H3311 L3312 R3321 V3324 N3325 N3326 L3327 G3328 I3329 D3330 E3331 A3332 R3348 A3349 R3350 H3357 F3358 I3359 P3360 T3361 L3365 E3376 E3377 R3380 L3381 E3382 A3383 K3384 A3385 E3386 A3387 E3388 E3389 G3390 V3394 R3395 D3396 L3405 L3412 R3420
L3434 M3437 S3448 H3449 N3450 F3451 N3465 N3466 M3467 S3468 F3469 L3470 T3471 A3472 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 T3507 V3511 K3515 I3520
D3529 Q3530 D3531 L3532 I3533 M3534 L3535 A3536 K3537 T3538 T3545 D3546 L3557 H3558 K3562 V3563 E3564 G3565 R3577 G3581 R3582 E3583 E3584 D3585 A3586 D3587 D3588 R3594 R3595 V3596 Q3597 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 T3639 E3682 Q3683 GLU GLU GLU GLU GLU VAL GLU E3692 L3735 GLU GLY GLY GLU ASN GLY GLU ALA GLU GLU GLU GLU VAL E3750 V3751 S3752 F3753 E3754 S3768 H3771 D3822 K3823 K3824 E3825 V3826 G3827 Q3850 L3856 GLY MET VAL ASN GLU
ASP GLY THR VAL ILE ASN ARG GLN ASN GLY E3872 K3873 V3874 F3899 Q3906 T3911 T3912 I3916 F3933 D4006 S4007 S4008 M4026 N4037 R4042 S4051 E4056 S4074 E4075 P4084 R4085 G4086 K4090 D4118 E4119 N4120 I4123 L4166 Q4216 D4220
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 ALA ALA ALA GLY ALA GLU ALA ALA ALA GLY THR VAL ALA ALA ALA GLY ALA THR ALA ARG LEU ALA ALA ALA ARG LEU LEU TRP GLY SER LEU PHE GLY GLY GLY LEU VAL
SER TYR ARG SER LEU ARG ARG ARG VAL ARG ARG LEU ARG ARG LEU THR ALA ARG GLU ALA ALA THR ALA LEU ALA ALA ALA LEU LEU TRP ALA VAL VAL ALA ARG ALA GLY ALA ALA GLY ALA GLY ALA LEU ARG LEU LEU TRP GLY SER LEU PHE GLY GLY GLY LEU VAL

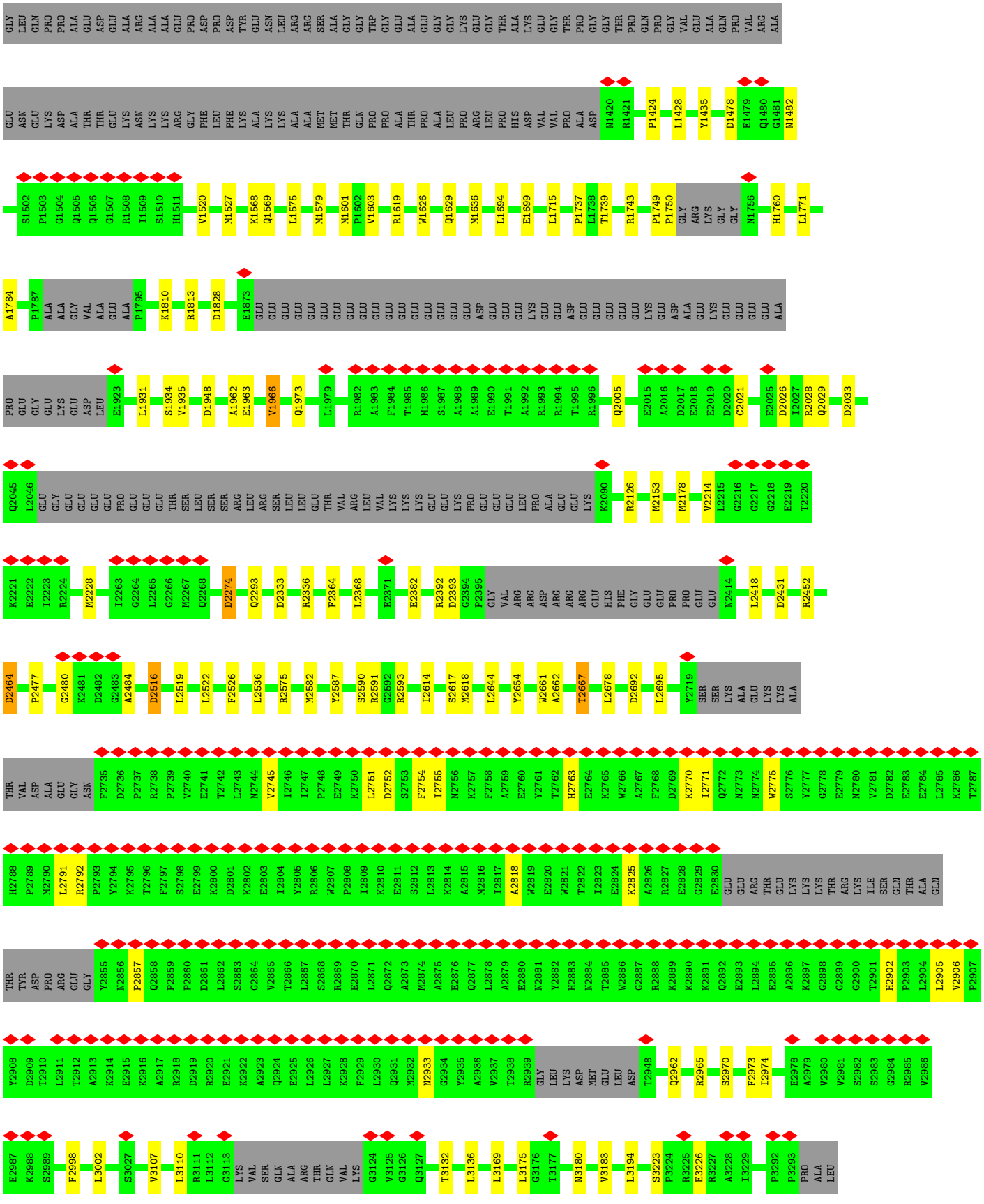


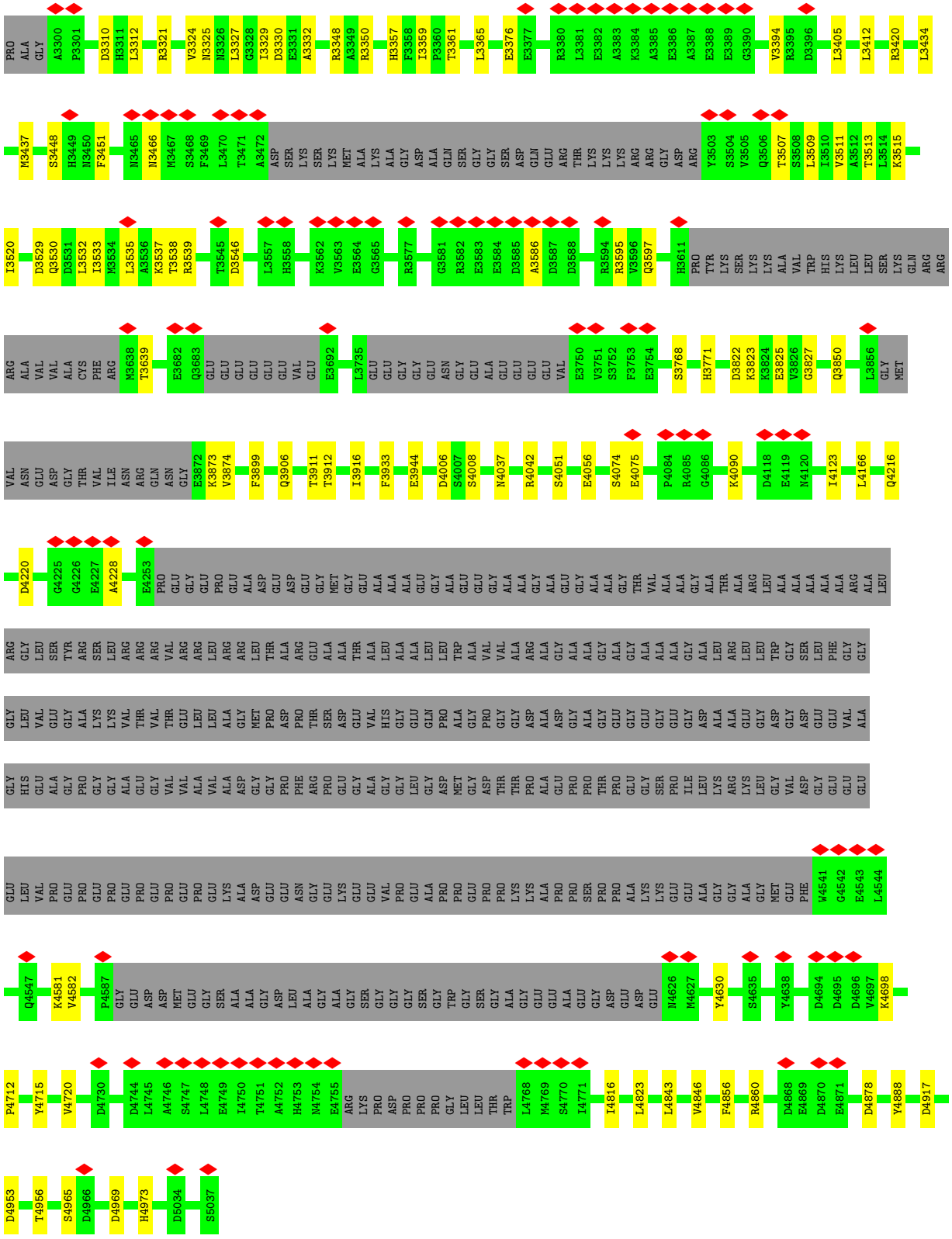
• Molecule 2: Ryanodine receptor 1

Chain H:






GLY LEU GLN PRO PRO ALA GLU ASP GLU ALA ARG ALA ALA GLU PRO ASP PRO ASP TYR GLU ASN LEU ALA 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 R1421 P1424 L1428 Y1435 D1478 E1479 Q1480 G1481 N1482
S1502 P1503 G1504 Q1505 Q1506 G1507 R1508 I1509 S1510 H1511 V1520 M1527 K1568 Q1569 L1575 M1579 M1601 P1602 V1603 R1619 W1626 Q1629 M1636 L1694 E1699 L1715 P1737 L1738 T1739 R1743 P1749 P1750 GLY ARG LYS GLY GLY N1766 H1760 L1771
A1784 P1787 ALA ALA GLY VAL ALA GLU ALA P1795 K1810 R1813 D1828 E1873 GLU GLU GLU


PRO ALA GLY A4300 P3301 D3310 H3311 L3312 R3321 V3324 N3325 N3326 L3327 G3328 I3329 D3330 E3331 A3332 R3348 A3349 R3350 H3357 F3358 I3359 P3360 T3361 L3365 E3376 E3377 R3380 L3381 E3382 A3383 K3384 A3385 E3386 A3387 E3388 E3389 G3390 V3394 R3395 D3396 L3405 L3412 R3420 L3434
M3437 S3448 H3449 N3450 F3451 N3465 N3466 M3467 S3468 F3469 L3470 T3471 A3472 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 T3507 S3508 L3509 I3510 V3511 A3512 T3513 L3514 K3515
I3520 D3529 Q3530 D3531 L3532 I3533 M3534 L3535 A3536 K3537 T3538 R3539 T3545 D3546 L3557 H3558 K3562 V3563 E3564 G3565 R3577 G3581 R3582 E3583 E3584 D3585 A3586 D3587 D3588 R3594 R3595 V3596 Q3597 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 T3639 E3682 Q3683 GLU GLU GLU GLU GLU VAL GLU E3692 L3735 GLU GLU GLY GLY GLU ASN GLY GLU ALA GLU GLU GLU VAL E3750 V3751 S3752 F3753 E3754 S3768 H3771 D3822 K3823 K3824 E3825 V3826 G3827 Q3850 L3856 GLY MET
VAL ASN GLU ASP GLY THR VAL ILE ASN ARG GLN ASN GLY E3872 K3873 V3874 F3899 Q3906 T3911 T3912 I3916 F3933 E3944 D4006 S4007 S4008 N4037 R4042 S4051 E4056 S4074 E4075 P4084 R4085 G4086 K4090 D4118 E4119 N4120 I4123 L4166 Q4216
D4220 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 GLY ALA GLU GLU GLY ALA GLU GLY ALA ALA GLY THR VAL ALA ALA GLY ALA THR ALA ARG LEU ALA ALA ALA ALA ALA ALA LEU
ARG GLY LEU SER TYR ARG SER LEU ARG ARG VAL ARG ARG LEU ARG ARG LEU THR ALA ARG GLU ALA LEU LEU ALA ALA ARG LEU LEU TRP ALA VAL VAL ALA ARG ALA GLY ALA ALA GLY ALA GLY ALA LEU ARG LEU LEU TRP GLY SER LEU PHE GLY GLY
GLY LEU VAL GLU GLY ALA LYS LYS VAL THR VAL THR GLU LEU LEU ALA GLY MET PRO ASP PRO THR SER ASP GLU VAL HIS GLY GLU GLN PRO ALA GLY PRO GLY GLY ASP ALA ASP GLY ALA ALA GLY GLU GLY GLU GLY GLU GLY GLU ASP ALA ALA GLU GLY ASP GLU GLU VAL ALA
GLY HIS GLU ALA GLY PRO GLY GLY ALA GLU GLY VAL VAL ALA ALA VAL ALA ASP GLY GLY 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 GLY SER PRO ILE LEU LYS ARG LYS LEU GLY VAL ASP GLY GLU GLU GLU
GLU LEU VAL PRO GLU PRO GLU PRO GLU PRO GLU PRO GLU PRO GLU PRO GLU LYS ALA ASP GLU GLU ASN GLY GLU LYS GLU GLU VAL PRO GLU GLU ALA PRO PRO GLU PRO PRO LYS LYS ALA PRO PRO SER PRO PRO ALA LYS LYS GLU GLU ALA GLY GLY ALA LEU GLU PHE W4541 G4542 E4543 L4544
Q4547 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 GLU ALA ASP GLU N4626 M4627 Y4630 S4635 Y4638 D4694 D4695 D4696 V4697 K4698
P4712 Y4715 V4720 D4730 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 I4771 I4816 L4823 L4843 V4846 F4856 R4860 D4868 E4869 D4870 E4871 D4878 Y4888 D4917
D4953 T4956 S4965 D4966 D4969 H4973 D5034 S5037

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	138818	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	0.734	Depositor
Minimum map value	0.000	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.078	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, ZN, CA

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	0.24	0/831	0.40	0/1121
1	C	0.24	0/831	0.40	0/1121
1	E	0.24	0/831	0.40	0/1121
1	G	0.24	0/831	0.40	0/1121
2	B	0.23	0/33920	0.38	0/46016
2	D	0.23	0/33920	0.38	0/46016
2	F	0.23	0/33920	0.38	0/46016
2	H	0.23	0/33920	0.38	0/46016
All	All	0.23	0/139004	0.38	0/188548

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	815	0	814	6	0
1	C	815	0	814	7	0
1	E	815	0	814	7	0
1	G	815	0	814	6	0
2	B	33162	0	32378	194	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	33162	0	32378	189	0
2	F	33162	0	32378	189	0
2	H	33162	0	32378	190	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	136040	0	132816	733	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 3.

All (733) 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:B:4856:PHE:CZ	2:H:4582:VAL:HG23	2.24	0.73
2:D:4582:VAL:HG23	2:F:4856:PHE:CZ	2.24	0.72
2:F:4582:VAL:HG23	2:H:4856:PHE:CZ	2.24	0.72
2:B:4582:VAL:HG23	2:D:4856:PHE:CZ	2.24	0.72
1:E:50:ARG:HE	1:E:53:LYS:HG3	1.57	0.69
1:A:50:ARG:HE	1:A:53:LYS:HG3	1.57	0.69
2:D:868:GLU:O	2:D:871:ARG:HB3	1.93	0.69
2:F:868:GLU:O	2:F:871:ARG:HB3	1.93	0.68
2:D:2452:ARG:HG3	2:F:175:SER:O	1.93	0.68
2:H:868:GLU:O	2:H:871:ARG:HB3	1.93	0.68
2:B:175:SER:O	2:H:2452:ARG:HG3	1.93	0.68
2:B:2452:ARG:HG3	2:D:175:SER:O	1.93	0.68
1:C:50:ARG:HE	1:C:53:LYS:HG3	1.57	0.68
2:F:2452:ARG:HG3	2:H:175:SER:O	1.93	0.68
1:G:50:ARG:HE	1:G:53:LYS:HG3	1.57	0.67
2:B:868:GLU:O	2:B:871:ARG:HB3	1.93	0.67
2:F:2214:VAL:HG21	2:F:2228:MET:HG2	1.77	0.66
2:H:2214:VAL:HG21	2:H:2228:MET:HG2	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2214:VAL:HG21	2:B:2228:MET:HG2	1.77	0.65
2:D:2214:VAL:HG21	2:D:2228:MET:HG2	1.77	0.65
2:F:3107:VAL:HG22	2:F:3175:LEU:HD22	1.79	0.64
2:B:3107:VAL:HG22	2:B:3175:LEU:HD22	1.79	0.64
2:H:3324:VAL:HA	2:H:3327:LEU:HG	1.80	0.64
2:D:3324:VAL:HA	2:D:3327:LEU:HG	1.80	0.63
2:B:3324:VAL:HA	2:B:3327:LEU:HG	1.80	0.63
2:H:3107:VAL:HG22	2:H:3175:LEU:HD22	1.79	0.63
2:D:3107:VAL:HG22	2:D:3175:LEU:HD22	1.79	0.63
2:F:3324:VAL:HA	2:F:3327:LEU:HG	1.80	0.63
2:H:1520:VAL:HG12	2:H:1527:MET:HG2	1.81	0.63
2:F:4630:TYR:OH	2:H:4860:ARG:NH1	2.30	0.63
2:F:1520:VAL:HG12	2:F:1527:MET:HG2	1.81	0.63
2:B:3312:LEU:HD22	2:B:3348:ARG:HG3	1.80	0.62
2:D:1520:VAL:HG12	2:D:1527:MET:HG2	1.81	0.62
2:B:1520:VAL:HG12	2:B:1527:MET:HG2	1.81	0.62
2:B:4860:ARG:NH1	2:H:4630:TYR:OH	2.30	0.62
2:D:3312:LEU:HD22	2:D:3348:ARG:HG3	1.80	0.62
2:D:4630:TYR:OH	2:F:4860:ARG:NH1	2.30	0.62
2:H:3312:LEU:HD22	2:H:3348:ARG:HG3	1.80	0.61
2:D:4582:VAL:CG2	2:F:4856:PHE:CZ	2.84	0.61
2:B:4582:VAL:CG2	2:D:4856:PHE:CZ	2.84	0.61
2:B:4630:TYR:OH	2:D:4860:ARG:NH1	2.30	0.61
2:H:856:VAL:H	2:H:991:ASN:HD21	1.49	0.61
2:B:835:ARG:NH2	2:B:1210:SER:O	2.34	0.61
2:B:856:VAL:H	2:B:991:ASN:HD21	1.49	0.61
2:D:856:VAL:H	2:D:991:ASN:HD21	1.49	0.61
2:F:856:VAL:H	2:F:991:ASN:HD21	1.49	0.61
2:F:3312:LEU:HD22	2:F:3348:ARG:HG3	1.80	0.61
2:H:3324:VAL:HG11	2:H:3361:THR:HG22	1.83	0.60
2:B:4856:PHE:CZ	2:H:4582:VAL:CG2	2.84	0.60
2:F:4582:VAL:CG2	2:H:4856:PHE:CZ	2.84	0.60
2:D:2178:MET:HB3	2:D:2228:MET:HE1	1.84	0.60
2:B:4888:TYR:OH	2:D:4917:ASP:OD2	2.17	0.60
2:F:3825:GLU:HG2	2:F:3827:GLY:H	1.67	0.60
2:B:2178:MET:HB3	2:B:2228:MET:HE1	1.84	0.60
2:H:3825:GLU:HG2	2:H:3827:GLY:H	1.67	0.60
2:F:835:ARG:NH2	2:F:1210:SER:O	2.34	0.60
2:B:3825:GLU:HG2	2:B:3827:GLY:H	1.67	0.60
2:F:3324:VAL:HG11	2:F:3361:THR:HG22	1.83	0.59
2:D:3825:GLU:HG2	2:D:3827:GLY:H	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:3906:GLN:H	2:H:3912:THR:HG23	1.68	0.59
1:A:79:PRO:HA	1:A:82:ALA:HB3	1.84	0.59
2:B:3324:VAL:HG11	2:B:3361:THR:HG22	1.83	0.59
2:H:2178:MET:HB3	2:H:2228:MET:HE1	1.84	0.59
2:B:3906:GLN:H	2:B:3912:THR:HG23	1.68	0.59
2:F:3906:GLN:H	2:F:3912:THR:HG23	1.68	0.58
2:D:4888:TYR:OH	2:F:4917:ASP:OD2	2.17	0.58
2:H:788:LYS:HG2	2:H:1629:GLN:HG3	1.85	0.58
2:D:788:LYS:HG2	2:D:1629:GLN:HG3	1.85	0.58
2:D:3324:VAL:HG11	2:D:3361:THR:HG22	1.83	0.58
1:G:79:PRO:HA	1:G:82:ALA:HB3	1.84	0.58
2:F:2178:MET:HB3	2:F:2228:MET:HE1	1.84	0.58
2:B:4917:ASP:OD2	2:H:4888:TYR:OH	2.17	0.58
2:H:835:ARG:NH2	2:H:1210:SER:O	2.34	0.58
2:B:788:LYS:HG2	2:B:1629:GLN:HG3	1.85	0.58
2:D:3906:GLN:H	2:D:3912:THR:HG23	1.68	0.58
1:C:79:PRO:HA	1:C:82:ALA:HB3	1.84	0.57
2:F:3321:ARG:NH1	2:F:3325:ASN:OD1	2.38	0.57
2:D:863:LEU:HD23	2:D:871:ARG:HH21	1.70	0.57
1:E:79:PRO:HA	1:E:82:ALA:HB3	1.84	0.57
2:H:3321:ARG:NH1	2:H:3325:ASN:OD1	2.38	0.57
2:B:3321:ARG:NH1	2:B:3325:ASN:OD1	2.38	0.57
2:B:4037:ASN:O	2:B:4042:ARG:NH1	2.38	0.56
2:F:788:LYS:HG2	2:F:1629:GLN:HG3	1.85	0.56
2:F:2029:GLN:NE2	2:F:2033:ASP:OD1	2.39	0.56
2:D:2029:GLN:NE2	2:D:2033:ASP:OD1	2.39	0.56
2:D:3321:ARG:NH1	2:D:3325:ASN:OD1	2.38	0.56
2:H:863:LEU:HD23	2:H:871:ARG:HH21	1.70	0.56
2:B:863:LEU:HD23	2:B:871:ARG:HH21	1.70	0.56
2:B:3110:LEU:O	2:B:3180:ASN:ND2	2.39	0.56
2:H:2029:GLN:NE2	2:H:2033:ASP:OD1	2.39	0.56
2:F:4888:TYR:OH	2:H:4917:ASP:OD2	2.17	0.56
2:H:4037:ASN:O	2:H:4042:ARG:NH1	2.38	0.56
2:B:2029:GLN:NE2	2:B:2033:ASP:OD1	2.39	0.56
2:D:3132:THR:HA	2:D:3136:LEU:HB3	1.88	0.56
2:D:4037:ASN:O	2:D:4042:ARG:NH1	2.38	0.56
2:H:3110:LEU:O	2:H:3180:ASN:ND2	2.39	0.56
2:D:835:ARG:NH2	2:D:1210:SER:O	2.34	0.56
2:D:3110:LEU:O	2:D:3180:ASN:ND2	2.39	0.55
2:F:863:LEU:HD23	2:F:871:ARG:HH21	1.70	0.55
2:F:4037:ASN:O	2:F:4042:ARG:NH1	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2654:TYR:O	2:D:2667:THR:OG1	2.24	0.55
2:F:3110:LEU:O	2:F:3180:ASN:ND2	2.39	0.55
2:F:3132:THR:HA	2:F:3136:LEU:HB3	1.88	0.55
2:F:3822:ASP:OD2	2:F:3823:LYS:NZ	2.40	0.55
2:H:2654:TYR:O	2:H:2667:THR:OG1	2.24	0.55
2:H:3132:THR:HA	2:H:3136:LEU:HB3	1.88	0.55
2:D:1743:ARG:NH1	2:D:1963:GLU:OE2	2.37	0.55
2:B:2654:TYR:O	2:B:2667:THR:OG1	2.24	0.54
2:B:3132:THR:HA	2:B:3136:LEU:HB3	1.88	0.54
2:H:3822:ASP:OD2	2:H:3823:LYS:NZ	2.40	0.54
2:B:3822:ASP:OD2	2:B:3823:LYS:NZ	2.40	0.54
2:D:3822:ASP:OD2	2:D:3823:LYS:NZ	2.40	0.54
2:H:1699:GLU:OE2	2:H:1813:ARG:NH2	2.40	0.54
2:F:131:LEU:O	2:F:178:ARG:NE	2.41	0.54
2:F:1699:GLU:OE2	2:F:1813:ARG:NH2	2.40	0.54
2:H:131:LEU:O	2:H:178:ARG:NE	2.41	0.54
2:D:2692:ASP:HB3	2:D:2695:LEU:HB3	1.89	0.54
2:D:131:LEU:O	2:D:178:ARG:NE	2.41	0.54
2:H:2382:GLU:OE2	2:H:2392:ARG:NH2	2.40	0.54
2:B:131:LEU:O	2:B:178:ARG:NE	2.41	0.54
2:B:1743:ARG:NH1	2:B:1963:GLU:OE2	2.37	0.54
2:B:2393:ASP:OD1	2:B:2418:LEU:N	2.41	0.54
2:H:1028:ASP:OD1	2:H:1028:ASP:N	2.41	0.54
2:H:2393:ASP:OD1	2:H:2418:LEU:N	2.41	0.54
2:B:2692:ASP:HB3	2:B:2695:LEU:HB3	1.89	0.53
2:B:3365:LEU:HD13	2:B:3405:LEU:HD23	1.90	0.53
2:B:2902:HIS:HB3	2:B:2905:LEU:HG	1.90	0.53
2:F:2654:TYR:O	2:F:2667:THR:OG1	2.24	0.53
2:B:913:LEU:O	2:B:918:ARG:NH2	2.42	0.53
2:F:3365:LEU:HD13	2:F:3405:LEU:HD23	1.90	0.53
2:H:913:LEU:O	2:H:918:ARG:NH2	2.42	0.53
2:D:913:LEU:O	2:D:918:ARG:NH2	2.42	0.53
2:D:879:HIS:NE2	2:D:908:VAL:O	2.41	0.53
2:B:1478:ASP:OD1	2:B:1482:ASN:N	2.42	0.53
2:D:3365:LEU:HD13	2:D:3405:LEU:HD23	1.90	0.53
2:F:12:GLN:NE2	2:F:332:GLU:O	2.38	0.53
2:F:2382:GLU:OE2	2:F:2392:ARG:NH2	2.40	0.53
2:H:1931:LEU:HD22	2:H:1935:VAL:HG11	1.91	0.53
2:D:1478:ASP:OD1	2:D:1482:ASN:N	2.42	0.53
2:B:879:HIS:NE2	2:B:908:VAL:O	2.41	0.53
2:B:1931:LEU:HD22	2:B:1935:VAL:HG11	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1931:LEU:HD22	2:F:1935:VAL:HG11	1.91	0.53
2:H:2962:GLN:OE1	2:H:2965:ARG:NH1	2.42	0.53
2:B:749:ASP:O	2:B:753:PRO:HA	2.09	0.52
2:D:1931:LEU:HD22	2:D:1935:VAL:HG11	1.91	0.52
2:D:2902:HIS:HB3	2:D:2905:LEU:HG	1.90	0.52
2:B:638:ILE:HD11	2:B:1636:MET:HE2	1.91	0.52
2:F:749:ASP:O	2:F:753:PRO:HA	2.09	0.52
2:F:913:LEU:O	2:F:918:ARG:NH2	2.42	0.52
2:F:2825:LYS:NZ	2:F:2933:ASN:O	2.40	0.52
2:H:1478:ASP:OD1	2:H:1482:ASN:N	2.42	0.52
2:H:2692:ASP:HB3	2:H:2695:LEU:HB3	1.89	0.52
2:D:638:ILE:HD11	2:D:1636:MET:HE2	1.91	0.52
2:D:2382:GLU:OE2	2:D:2392:ARG:NH2	2.40	0.52
2:D:2962:GLN:OE1	2:D:2965:ARG:NH1	2.42	0.52
2:F:1028:ASP:OD1	2:F:1028:ASP:N	2.41	0.52
2:F:2770:LYS:HB3	2:F:2775:TRP:HB2	1.92	0.52
2:B:2962:GLN:OE1	2:B:2965:ARG:NH1	2.42	0.52
2:D:749:ASP:O	2:D:753:PRO:HA	2.09	0.52
2:F:2692:ASP:HB3	2:F:2695:LEU:HB3	1.89	0.52
2:H:2770:LYS:HB3	2:H:2775:TRP:HB2	1.92	0.52
2:H:3365:LEU:HD13	2:H:3405:LEU:HD23	1.90	0.52
2:B:1028:ASP:OD1	2:B:1028:ASP:N	2.41	0.52
2:F:2393:ASP:OD1	2:F:2418:LEU:N	2.41	0.52
2:D:2393:ASP:OD1	2:D:2418:LEU:N	2.41	0.52
2:D:2770:LYS:HB3	2:D:2775:TRP:HB2	1.92	0.52
2:F:2902:HIS:HB3	2:F:2905:LEU:HG	1.90	0.52
2:H:2902:HIS:HB3	2:H:2905:LEU:HG	1.90	0.52
2:B:1699:GLU:OE2	2:B:1813:ARG:NH2	2.40	0.52
2:F:1743:ARG:NH1	2:F:1963:GLU:OE2	2.37	0.52
2:F:1478:ASP:OD1	2:F:1482:ASN:N	2.42	0.52
2:B:2464:ASP:N	2:B:2464:ASP:OD1	2.42	0.51
2:F:638:ILE:HD11	2:F:1636:MET:HE2	1.91	0.51
2:H:12:GLN:NE2	2:H:332:GLU:O	2.38	0.51
2:H:4074:SER:OG	2:H:4075:GLU:N	2.43	0.51
2:F:2962:GLN:OE1	2:F:2965:ARG:NH1	2.42	0.51
2:H:638:ILE:HD11	2:H:1636:MET:HE2	1.91	0.51
2:H:749:ASP:O	2:H:753:PRO:HA	2.09	0.51
2:H:2825:LYS:NZ	2:H:2933:ASN:O	2.40	0.51
2:H:1743:ARG:NH1	2:H:1963:GLU:OE2	2.37	0.51
2:D:4074:SER:OG	2:D:4075:GLU:N	2.43	0.51
2:F:950:LEU:HD13	2:F:970:LEU:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:950:LEU:HD13	2:B:970:LEU:HD13	1.92	0.51
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	1.92	0.51
2:B:4074:SER:OG	2:B:4075:GLU:N	2.43	0.51
2:F:2464:ASP:OD1	2:F:2464:ASP:N	2.42	0.51
2:H:2464:ASP:OD1	2:H:2464:ASP:N	2.42	0.51
2:B:4216:GLN:NE2	2:B:4220:ASP:OD1	2.44	0.51
2:D:1177:THR:O	2:D:1180:ARG:NH2	2.44	0.51
2:B:1177:THR:O	2:B:1180:ARG:NH2	2.44	0.51
2:F:4216:GLN:NE2	2:F:4220:ASP:OD1	2.44	0.51
2:F:1177:THR:O	2:F:1180:ARG:NH2	2.44	0.50
2:B:2382:GLU:OE2	2:B:2392:ARG:NH2	2.40	0.50
2:D:950:LEU:HD13	2:D:970:LEU:HD13	1.92	0.50
2:H:950:LEU:HD13	2:H:970:LEU:HD13	1.92	0.50
2:B:955:LEU:HD12	2:B:967:PRO:HG2	1.93	0.50
2:D:4216:GLN:NE2	2:D:4220:ASP:OD1	2.44	0.50
2:F:879:HIS:NE2	2:F:908:VAL:O	2.41	0.50
2:D:2825:LYS:NZ	2:D:2933:ASN:O	2.40	0.50
2:F:4074:SER:OG	2:F:4075:GLU:N	2.43	0.50
2:H:1177:THR:O	2:H:1180:ARG:NH2	2.44	0.50
2:H:879:HIS:NE2	2:H:908:VAL:O	2.41	0.50
2:B:1243:PRO:HA	2:B:1601:MET:O	2.12	0.50
2:D:796:ARG:O	2:D:1619:ARG:NH2	2.40	0.50
2:F:1699:GLU:HG3	2:F:1810:LYS:HE3	1.94	0.50
2:D:955:LEU:HD12	2:D:967:PRO:HG2	1.93	0.50
2:H:4216:GLN:NE2	2:H:4220:ASP:OD1	2.44	0.50
2:D:1243:PRO:HA	2:D:1601:MET:O	2.12	0.49
2:D:1699:GLU:HG3	2:D:1810:LYS:HE3	1.94	0.49
2:D:2464:ASP:N	2:D:2464:ASP:OD1	2.42	0.49
2:F:358:THR:OG1	2:F:359:TYR:N	2.45	0.49
2:D:4816:ILE:CD1	2:F:4846:VAL:HG21	2.43	0.49
2:H:796:ARG:O	2:H:1619:ARG:NH2	2.40	0.49
2:H:3329:ILE:HD11	2:H:3332:ALA:HB2	1.95	0.49
2:D:3107:VAL:HG13	2:D:3175:LEU:HD13	1.95	0.49
2:F:955:LEU:HD12	2:F:967:PRO:HG2	1.93	0.49
1:A:24:VAL:HG22	1:A:48:LYS:HG2	1.95	0.49
2:B:1694:LEU:HB3	2:B:1715:LEU:HD12	1.95	0.49
1:C:24:VAL:HG22	1:C:48:LYS:HG2	1.95	0.49
2:H:1243:PRO:HA	2:H:1601:MET:O	2.12	0.49
2:B:1089:TYR:HD1	2:B:1152:MET:HG3	1.78	0.49
2:D:358:THR:OG1	2:D:359:TYR:N	2.45	0.49
2:H:358:THR:OG1	2:H:359:TYR:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:3107:VAL:HG13	2:H:3175:LEU:HD13	1.95	0.49
2:B:3329:ILE:HD11	2:B:3332:ALA:HB2	1.95	0.49
2:H:955:LEU:HD12	2:H:967:PRO:HG2	1.93	0.49
2:F:3329:ILE:HD11	2:F:3332:ALA:HB2	1.95	0.49
2:H:1089:TYR:HD1	2:H:1152:MET:HG3	1.78	0.49
2:H:1694:LEU:HB3	2:H:1715:LEU:HD12	1.95	0.49
2:B:4816:ILE:CD1	2:D:4846:VAL:HG21	2.43	0.49
2:F:1694:LEU:HB3	2:F:1715:LEU:HD12	1.95	0.49
2:H:2644:LEU:HD13	2:H:2678:LEU:HD21	1.95	0.49
2:D:3329:ILE:HD11	2:D:3332:ALA:HB2	1.95	0.48
2:D:4006:ASP:OD2	2:D:4008:SER:OG	2.25	0.48
2:F:4816:ILE:CD1	2:H:4846:VAL:HG21	2.43	0.48
1:G:24:VAL:HG22	1:G:48:LYS:HG2	1.95	0.48
2:H:2745:VAL:HG21	2:H:2818:ALA:HB2	1.95	0.48
2:B:4846:VAL:HG21	2:H:4816:ILE:CD1	2.43	0.48
2:D:1089:TYR:HD1	2:D:1152:MET:HG3	1.78	0.48
1:E:24:VAL:HG22	1:E:48:LYS:HG2	1.95	0.48
2:B:1699:GLU:HG3	2:B:1810:LYS:HE3	1.94	0.48
2:D:1699:GLU:OE2	2:D:1813:ARG:NH2	2.40	0.48
2:F:1243:PRO:HA	2:F:1601:MET:O	2.12	0.48
2:F:3107:VAL:HG13	2:F:3175:LEU:HD13	1.95	0.48
2:H:1699:GLU:HG3	2:H:1810:LYS:HE3	1.94	0.48
2:D:1694:LEU:HB3	2:D:1715:LEU:HD12	1.95	0.48
2:B:2644:LEU:HD13	2:B:2678:LEU:HD21	1.95	0.48
2:D:176:SER:OG	2:D:178:ARG:NH1	2.38	0.48
2:D:1028:ASP:OD1	2:D:1028:ASP:N	2.41	0.48
2:F:176:SER:OG	2:F:178:ARG:NH1	2.38	0.48
2:F:1089:TYR:HD1	2:F:1152:MET:HG3	1.78	0.48
2:H:2770:LYS:HG3	2:H:2791:LEU:HD21	1.96	0.48
2:B:2745:VAL:HG21	2:B:2818:ALA:HB2	1.95	0.48
2:B:3107:VAL:HG13	2:B:3175:LEU:HD13	1.95	0.48
2:F:796:ARG:O	2:F:1619:ARG:NH2	2.40	0.48
2:B:2771:ILE:HD11	2:B:2857:PRO:HD2	1.96	0.48
2:H:2771:ILE:HD11	2:H:2857:PRO:HD2	1.96	0.48
2:H:3511:VAL:HG12	2:H:3515:LYS:HE2	1.96	0.48
2:B:2770:LYS:HG3	2:B:2791:LEU:HD21	1.96	0.48
2:B:3511:VAL:HG12	2:B:3515:LYS:HE2	1.96	0.48
2:D:2771:ILE:HD11	2:D:2857:PRO:HD2	1.96	0.48
2:B:2591:ARG:H	2:B:2591:ARG:HG2	1.57	0.47
2:F:952:LYS:HD3	2:F:968:ALA:HB1	1.95	0.47
2:F:1575:LEU:HD13	2:F:1579:MET:HE3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:176:SER:OG	2:B:178:ARG:NH1	2.38	0.47
2:B:952:LYS:HD3	2:B:968:ALA:HB1	1.95	0.47
2:D:1575:LEU:HD13	2:D:1579:MET:HE3	1.96	0.47
2:F:2745:VAL:HG21	2:F:2818:ALA:HB2	1.95	0.47
2:F:2771:ILE:HD11	2:F:2857:PRO:HD2	1.96	0.47
2:B:2026:ASP:OD1	2:B:2026:ASP:N	2.47	0.47
2:H:952:LYS:HD3	2:H:968:ALA:HB1	1.95	0.47
2:B:796:ARG:O	2:B:1619:ARG:NH2	2.40	0.47
2:B:4856:PHE:CE1	2:H:4582:VAL:HG23	2.50	0.47
2:D:2745:VAL:HG21	2:D:2818:ALA:HB2	1.95	0.47
2:F:4582:VAL:HG23	2:H:4856:PHE:CE1	2.50	0.47
2:H:882:TRP:O	2:H:885:THR:OG1	2.32	0.47
2:D:2644:LEU:HD13	2:D:2678:LEU:HD21	1.95	0.47
2:D:2770:LYS:HG3	2:D:2791:LEU:HD21	1.96	0.47
2:H:2364:PHE:HB3	2:H:2368:LEU:HB2	1.96	0.47
2:D:12:GLN:NE2	2:D:332:GLU:O	2.38	0.47
2:D:952:LYS:HD3	2:D:968:ALA:HB1	1.95	0.47
2:F:1973:GLN:NE2	2:F:2005:GLN:OE1	2.40	0.47
2:H:2026:ASP:OD1	2:H:2026:ASP:N	2.47	0.47
2:F:23:GLN:HG2	2:F:34:LYS:HE3	1.97	0.47
2:F:636:ASN:HB2	2:F:702:TRP:CZ3	2.50	0.47
2:H:23:GLN:HG2	2:H:34:LYS:HE3	1.97	0.47
2:H:1575:LEU:HD13	2:H:1579:MET:HE3	1.96	0.47
2:B:1575:LEU:HD13	2:B:1579:MET:HE3	1.96	0.47
2:B:2364:PHE:HB3	2:B:2368:LEU:HB2	1.96	0.47
2:B:2825:LYS:NZ	2:B:2933:ASN:O	2.40	0.47
2:B:2998:PHE:HA	2:B:3002:LEU:HD12	1.97	0.47
2:D:652:ARG:HD3	2:D:773:LEU:HD13	1.97	0.47
2:F:2644:LEU:HD13	2:F:2678:LEU:HD21	1.95	0.47
2:F:2770:LYS:HG3	2:F:2791:LEU:HD21	1.96	0.47
2:F:2998:PHE:HA	2:F:3002:LEU:HD12	1.97	0.47
2:H:3412:LEU:HD11	2:H:3434:LEU:HD21	1.97	0.47
2:B:23:GLN:NE2	2:B:203:ASN:OD1	2.48	0.47
2:B:4006:ASP:OD2	2:B:4008:SER:OG	2.25	0.47
2:D:2364:PHE:HB3	2:D:2368:LEU:HB2	1.96	0.47
2:F:1737:PRO:HB2	2:F:1739:THR:HG23	1.97	0.47
2:H:2998:PHE:HA	2:H:3002:LEU:HD12	1.97	0.47
2:D:23:GLN:NE2	2:D:203:ASN:OD1	2.48	0.46
2:F:3412:LEU:HD11	2:F:3434:LEU:HD21	1.97	0.46
2:H:3535:LEU:O	2:H:3538:THR:OG1	2.30	0.46
2:H:1973:GLN:NE2	2:H:2005:GLN:OE1	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:2005:GLN:NE2	2:H:3639:THR:O	2.48	0.46
2:B:2587:TYR:O	2:B:2590:SER:OG	2.30	0.46
2:B:4090:LYS:HG2	2:B:4123:ILE:HD11	1.97	0.46
2:D:2005:GLN:NE2	2:D:3639:THR:O	2.48	0.46
2:D:3412:LEU:HD11	2:D:3434:LEU:HD21	1.97	0.46
2:D:4090:LYS:HG2	2:D:4123:ILE:HD11	1.97	0.46
2:F:23:GLN:NE2	2:F:203:ASN:OD1	2.48	0.46
2:F:1948:ASP:OD1	2:F:2126:ARG:NH2	2.45	0.46
2:H:23:GLN:NE2	2:H:203:ASN:OD1	2.48	0.46
2:H:894:GLY:HA3	2:H:903:LEU:HB3	1.97	0.46
2:B:23:GLN:HG2	2:B:34:LYS:HE3	1.97	0.46
2:B:3412:LEU:HD11	2:B:3434:LEU:HD21	1.97	0.46
2:D:23:GLN:HG2	2:D:34:LYS:HE3	1.97	0.46
2:D:1029:GLU:HB3	2:D:1033:ARG:HH21	1.81	0.46
2:D:4953:ASP:HA	2:D:4956:THR:HG22	1.98	0.46
1:G:78:THR:OG1	1:G:80:ASP:OD1	2.29	0.46
2:H:1948:ASP:OD1	2:H:2126:ARG:NH2	2.45	0.46
2:B:636:ASN:HB2	2:B:702:TRP:CZ3	2.50	0.46
2:B:652:ARG:HD3	2:B:773:LEU:HD13	1.97	0.46
2:B:4582:VAL:HG23	2:D:4856:PHE:CE1	2.50	0.46
2:B:4965:SER:O	2:B:4969:ASP:HB2	2.16	0.46
2:D:408:ALA:HB2	2:D:483:MET:HE1	1.98	0.46
2:D:1568:LYS:NZ	2:D:1569:GLN:O	2.45	0.46
2:D:3511:VAL:HG12	2:D:3515:LYS:HE2	1.96	0.46
2:F:2026:ASP:OD1	2:F:2026:ASP:N	2.47	0.46
2:F:2587:TYR:O	2:F:2590:SER:OG	2.30	0.46
2:H:2274:ASP:OD1	2:H:2274:ASP:N	2.48	0.46
2:H:4090:LYS:HG2	2:H:4123:ILE:HD11	1.97	0.46
2:D:69:LEU:HD21	2:D:202:MET:HE1	1.98	0.46
2:D:2026:ASP:OD1	2:D:2026:ASP:N	2.47	0.46
2:D:2274:ASP:N	2:D:2274:ASP:OD1	2.48	0.46
2:D:2998:PHE:HA	2:D:3002:LEU:HD12	1.97	0.46
2:D:3509:LEU:O	2:D:3513:THR:OG1	2.33	0.46
2:F:69:LEU:HD21	2:F:202:MET:HE1	1.98	0.46
2:F:4090:LYS:HG2	2:F:4123:ILE:HD11	1.97	0.46
2:H:408:ALA:HB2	2:H:483:MET:HE1	1.98	0.46
2:B:894:GLY:HA3	2:B:903:LEU:HB3	1.97	0.46
2:D:4582:VAL:HG23	2:F:4856:PHE:CE1	2.50	0.46
2:F:882:TRP:O	2:F:885:THR:OG1	2.32	0.46
2:F:3511:VAL:HG12	2:F:3515:LYS:HE2	1.96	0.46
2:F:4965:SER:O	2:F:4969:ASP:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:4712:PRO:HB2	2:H:4715:TYR:HB3	1.98	0.46
2:B:408:ALA:HB2	2:B:483:MET:HE1	1.98	0.46
2:F:652:ARG:HD3	2:F:773:LEU:HD13	1.97	0.46
2:F:2274:ASP:N	2:F:2274:ASP:OD1	2.48	0.46
2:H:69:LEU:HD21	2:H:202:MET:HE1	1.98	0.46
2:H:176:SER:OG	2:H:178:ARG:NH1	2.38	0.46
2:H:709:ASP:OD1	2:H:725:HIS:ND1	2.40	0.46
2:B:69:LEU:HD21	2:B:202:MET:HE1	1.98	0.46
2:B:2582:MET:HE2	2:B:2582:MET:HB3	1.86	0.46
2:F:1029:GLU:HB3	2:F:1033:ARG:HH21	1.81	0.46
2:F:4712:PRO:HB2	2:F:4715:TYR:HB3	1.98	0.46
2:F:4953:ASP:HA	2:F:4956:THR:HG22	1.98	0.46
2:H:1029:GLU:HB3	2:H:1033:ARG:HH21	1.81	0.46
2:B:1737:PRO:HB2	2:B:1739:THR:HG23	1.97	0.46
2:D:307:ALA:HB1	2:D:312:THR:HG21	1.98	0.46
2:D:636:ASN:HB2	2:D:702:TRP:CZ3	2.50	0.46
2:D:3586:ALA:HB1	2:D:3595:ARG:HH12	1.81	0.46
2:F:307:ALA:HB1	2:F:312:THR:HG21	1.98	0.45
2:H:526:LEU:HD11	2:H:540:PHE:HZ	1.82	0.45
2:H:636:ASN:HB2	2:H:702:TRP:CZ3	2.50	0.45
2:B:2005:GLN:NE2	2:B:3639:THR:O	2.48	0.45
2:B:3359:ILE:HG23	2:B:3437:MET:HE1	1.99	0.45
2:B:3376:GLU:HB2	2:B:3394:VAL:HG11	1.99	0.45
2:B:3586:ALA:HB1	2:B:3595:ARG:HH12	1.81	0.45
2:D:3376:GLU:HB2	2:D:3394:VAL:HG11	1.99	0.45
2:F:2364:PHE:HB3	2:F:2368:LEU:HB2	1.96	0.45
2:H:3359:ILE:HG23	2:H:3437:MET:HE1	1.99	0.45
2:H:4965:SER:O	2:H:4969:ASP:HB2	2.16	0.45
2:D:526:LEU:HD11	2:D:540:PHE:HZ	1.82	0.45
2:F:2005:GLN:NE2	2:F:3639:THR:O	2.48	0.45
2:D:894:GLY:HA3	2:D:903:LEU:HB3	1.97	0.45
2:D:3359:ILE:HG23	2:D:3437:MET:HE1	1.99	0.45
2:H:652:ARG:HD3	2:H:773:LEU:HD13	1.97	0.45
2:H:3310:ASP:OD1	2:H:3350:ARG:NH2	2.49	0.45
2:B:526:LEU:HD11	2:B:540:PHE:HZ	1.82	0.45
2:D:4816:ILE:HD11	2:F:4846:VAL:HG21	1.99	0.45
2:F:408:ALA:HB2	2:F:483:MET:HE1	1.98	0.45
2:F:3359:ILE:HG23	2:F:3437:MET:HE1	1.99	0.45
2:H:1737:PRO:HB2	2:H:1739:THR:HG23	1.97	0.45
2:B:307:ALA:HB1	2:B:312:THR:HG21	1.98	0.45
2:B:4878:ASP:HB3	2:H:4581:LYS:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1737:PRO:HB2	2:D:1739:THR:HG23	1.97	0.45
2:D:4712:PRO:HB2	2:D:4715:TYR:HB3	1.98	0.45
2:D:4965:SER:O	2:D:4969:ASP:HB2	2.16	0.45
2:F:233:ILE:HD12	2:F:242:ARG:HB3	1.99	0.45
2:F:894:GLY:HA3	2:F:903:LEU:HB3	1.97	0.45
2:F:2480:GLY:N	2:F:2484:ALA:O	2.42	0.45
2:F:3535:LEU:O	2:F:3538:THR:OG1	2.30	0.45
2:D:4090:LYS:HZ2	2:D:4112:LEU:HD22	1.81	0.45
2:H:3586:ALA:HB1	2:H:3595:ARG:HH12	1.81	0.45
2:B:4712:PRO:HB2	2:B:4715:TYR:HB3	1.98	0.45
2:F:4816:ILE:HD11	2:H:4846:VAL:HG21	1.99	0.45
2:H:2614:ILE:HG23	2:H:2618:MET:HE3	1.99	0.45
2:H:4953:ASP:HA	2:H:4956:THR:HG22	1.98	0.45
2:B:4090:LYS:HZ2	2:B:4112:LEU:HD22	1.81	0.45
2:B:4581:LYS:HG2	2:D:4878:ASP:HB3	1.98	0.45
2:D:2293:GLN:H	2:D:2293:GLN:HG3	1.64	0.45
2:F:3310:ASP:OD1	2:F:3350:ARG:NH2	2.49	0.45
2:F:3376:GLU:HB2	2:F:3394:VAL:HG11	1.99	0.45
2:B:1029:GLU:HB3	2:B:1033:ARG:HH21	1.81	0.45
2:B:573:GLU:H	2:B:573:GLU:HG3	1.57	0.44
2:B:2751:LEU:O	2:B:2754:PHE:HB3	2.17	0.44
2:B:4953:ASP:HA	2:B:4956:THR:HG22	1.98	0.44
2:F:1424:PRO:O	2:F:1428:LEU:HB2	2.17	0.44
2:F:2614:ILE:HG23	2:F:2618:MET:HE3	1.99	0.44
2:H:307:ALA:HB1	2:H:312:THR:HG21	1.98	0.44
2:H:774:ASP:OD1	2:H:774:ASP:N	2.46	0.44
2:H:1568:LYS:NZ	2:H:1569:GLN:O	2.45	0.44
2:H:3546:ASP:OD2	2:H:3597:GLN:NE2	2.51	0.44
2:B:2274:ASP:OD1	2:B:2274:ASP:N	2.48	0.44
2:B:2333:ASP:OD1	2:B:2336:ARG:NH2	2.48	0.44
2:B:3330:ASP:OD1	2:B:3330:ASP:N	2.50	0.44
2:D:3546:ASP:OD2	2:D:3597:GLN:NE2	2.51	0.44
2:F:526:LEU:HD11	2:F:540:PHE:HZ	1.82	0.44
2:H:2751:LEU:O	2:H:2754:PHE:HB3	2.17	0.44
1:E:78:THR:OG1	1:E:80:ASP:OD1	2.29	0.44
2:F:3537:LYS:HE2	2:F:3537:LYS:HB3	1.86	0.44
2:F:3586:ALA:HB1	2:F:3595:ARG:HH12	1.81	0.44
2:H:233:ILE:HD12	2:H:242:ARG:HB3	1.99	0.44
2:H:3376:GLU:HB2	2:H:3394:VAL:HG11	1.99	0.44
2:B:218:HIS:ND1	2:B:341:TYR:OH	2.42	0.44
2:D:233:ILE:HD12	2:D:242:ARG:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:2021:CYS:HB3	2:F:2028:ARG:HH21	1.83	0.44
2:F:2752:ASP:O	2:F:2755:ILE:HB	2.18	0.44
2:H:1424:PRO:O	2:H:1428:LEU:HB2	2.17	0.44
2:B:1263:THR:OG1	2:B:1266:THR:OG1	2.31	0.44
2:B:2461:VAL:O	2:B:2510:TYR:OH	2.35	0.44
2:D:4581:LYS:HG2	2:F:4878:ASP:HB3	1.98	0.44
2:F:3546:ASP:OD2	2:F:3597:GLN:NE2	2.51	0.44
2:F:4581:LYS:HG2	2:H:4878:ASP:HB3	1.98	0.44
2:H:823:LEU:HD11	2:H:1626:TRP:HB3	2.00	0.44
2:D:648:ILE:HD13	2:D:811:CYS:HB3	2.00	0.44
2:D:745:SER:HB2	2:D:758:ARG:HB2	2.00	0.44
2:B:336:PRO:HA	2:B:337:PRO:HD3	1.89	0.44
2:B:358:THR:OG1	2:B:359:TYR:N	2.45	0.44
2:B:709:ASP:OD1	2:B:725:HIS:ND1	2.40	0.44
2:B:3546:ASP:OD2	2:B:3597:GLN:NE2	2.51	0.44
2:B:4846:VAL:HG21	2:H:4816:ILE:HD11	1.99	0.44
2:F:823:LEU:HD11	2:F:1626:TRP:HB3	2.00	0.44
2:B:878:ILE:HD13	2:B:881:LEU:HD12	2.00	0.44
2:B:3535:LEU:O	2:B:3538:THR:OG1	2.30	0.44
2:D:2751:LEU:O	2:D:2754:PHE:HB3	2.17	0.44
2:F:2333:ASP:OD1	2:F:2336:ARG:NH2	2.48	0.44
2:H:149:THR:HG23	2:H:172:VAL:HB	2.00	0.44
2:H:648:ILE:HD13	2:H:811:CYS:HB3	2.00	0.44
2:H:1771:LEU:HD22	2:H:2153:MET:HE2	1.99	0.44
2:H:3330:ASP:N	2:H:3330:ASP:OD1	2.50	0.44
2:B:1568:LYS:NZ	2:B:1569:GLN:O	2.45	0.43
2:B:2021:CYS:HB3	2:B:2028:ARG:HH21	1.83	0.43
2:D:35:LEU:HD13	2:D:49:LEU:HD13	2.00	0.43
2:D:2752:ASP:O	2:D:2755:ILE:HB	2.18	0.43
2:D:3357:HIS:O	2:D:3361:THR:HG23	2.18	0.43
2:D:4056:GLU:HG2	2:D:4166:LEU:HD13	2.00	0.43
2:F:2519:LEU:HD13	2:F:2575:ARG:HG3	2.00	0.43
2:F:3357:HIS:O	2:F:3361:THR:HG23	2.18	0.43
2:B:2614:ILE:HG23	2:B:2618:MET:HE3	1.99	0.43
2:B:3357:HIS:O	2:B:3361:THR:HG23	2.18	0.43
1:C:78:THR:OG1	1:C:80:ASP:OD1	2.29	0.43
2:D:878:ILE:HD13	2:D:881:LEU:HD12	2.00	0.43
2:D:3535:LEU:O	2:D:3538:THR:OG1	2.30	0.43
2:F:1771:LEU:HD22	2:F:2153:MET:HE2	1.99	0.43
2:F:2751:LEU:O	2:F:2754:PHE:HB3	2.17	0.43
2:H:2021:CYS:HB3	2:H:2028:ARG:HH21	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:233:ILE:HD12	2:B:242:ARG:HB3	1.99	0.43
2:B:1424:PRO:O	2:B:1428:LEU:HB2	2.17	0.43
2:B:3455:GLU:OE2	2:B:3508:SER:OG	2.33	0.43
2:B:4056:GLU:HG2	2:B:4166:LEU:HD13	2.00	0.43
2:D:1424:PRO:O	2:D:1428:LEU:HB2	2.17	0.43
2:D:3529:ASP:O	2:D:3532:LEU:HB2	2.18	0.43
2:F:745:SER:HB2	2:F:758:ARG:HB2	2.00	0.43
2:F:1828:ASP:OD1	2:F:1828:ASP:N	2.52	0.43
2:F:2661:TRP:CD1	2:F:2662:ALA:H	2.37	0.43
2:H:878:ILE:HD13	2:H:881:LEU:HD12	2.00	0.43
2:H:3223:SER:HB2	2:H:3226:GLU:HG3	2.01	0.43
2:B:2752:ASP:O	2:B:2755:ILE:HB	2.18	0.43
2:D:1771:LEU:HD22	2:D:2153:MET:HE2	1.99	0.43
2:F:1568:LYS:NZ	2:F:1569:GLN:O	2.45	0.43
2:F:3223:SER:HB2	2:F:3226:GLU:HG3	2.01	0.43
2:F:3330:ASP:OD1	2:F:3330:ASP:N	2.50	0.43
2:F:3529:ASP:O	2:F:3532:LEU:HB2	2.18	0.43
2:F:3530:GLN:O	2:F:3533:ILE:HB	2.18	0.43
2:H:2228:MET:HE2	2:H:2228:MET:HB2	1.84	0.43
2:H:2661:TRP:CD1	2:H:2662:ALA:H	2.37	0.43
2:B:35:LEU:HD13	2:B:49:LEU:HD13	2.00	0.43
2:B:2519:LEU:HD13	2:B:2575:ARG:HG3	2.00	0.43
2:B:3223:SER:HB2	2:B:3226:GLU:HG3	2.01	0.43
2:B:3529:ASP:O	2:B:3532:LEU:HB2	2.18	0.43
2:B:4816:ILE:HD11	2:D:4846:VAL:HG21	1.99	0.43
2:D:2461:VAL:O	2:D:2510:TYR:OH	2.35	0.43
2:D:2614:ILE:HG23	2:D:2618:MET:HE3	1.99	0.43
2:F:149:THR:HG23	2:F:172:VAL:HB	2.00	0.43
2:F:573:GLU:H	2:F:573:GLU:HG3	1.57	0.43
2:H:530:ILE:HG22	2:H:536:ASN:HB3	2.01	0.43
2:B:2661:TRP:CD1	2:B:2662:ALA:H	2.37	0.43
2:B:3310:ASP:OD1	2:B:3350:ARG:NH2	2.49	0.43
2:D:709:ASP:OD1	2:D:725:HIS:ND1	2.40	0.43
2:D:823:LEU:HD11	2:D:1626:TRP:HB3	2.00	0.43
2:D:1948:ASP:OD1	2:D:2126:ARG:NH2	2.45	0.43
2:D:2021:CYS:HB3	2:D:2028:ARG:HH21	1.83	0.43
2:D:2519:LEU:HD13	2:D:2575:ARG:HG3	2.00	0.43
2:D:3530:GLN:O	2:D:3533:ILE:HB	2.18	0.43
2:F:4006:ASP:OD2	2:F:4008:SER:OG	2.25	0.43
2:H:2021:CYS:O	2:H:2028:ARG:NH2	2.52	0.43
2:B:3180:ASN:HB2	2:B:3183:VAL:HG23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:336:PRO:HA	2:D:337:PRO:HD3	1.89	0.43
2:D:2661:TRP:CD1	2:D:2662:ALA:H	2.37	0.43
1:E:56:VAL:HA	2:F:1784:ALA:HA	2.00	0.43
1:G:56:VAL:HA	2:H:1784:ALA:HA	2.00	0.43
2:B:149:THR:HG23	2:B:172:VAL:HB	2.00	0.43
2:B:2021:CYS:O	2:B:2028:ARG:NH2	2.52	0.43
2:D:2333:ASP:OD1	2:D:2336:ARG:NH2	2.48	0.43
2:F:2021:CYS:O	2:F:2028:ARG:NH2	2.52	0.43
2:H:35:LEU:HD13	2:H:49:LEU:HD13	2.00	0.43
2:H:745:SER:HB2	2:H:758:ARG:HB2	2.00	0.43
2:H:2752:ASP:O	2:H:2755:ILE:HB	2.18	0.43
2:H:3530:GLN:O	2:H:3533:ILE:HB	2.18	0.43
2:H:3768:SER:HA	2:H:3771:HIS:CD2	2.54	0.43
2:B:823:LEU:HD11	2:B:1626:TRP:HB3	2.00	0.43
2:B:1758:ARG:HD2	2:B:1758:ARG:HA	1.86	0.43
2:B:1948:ASP:OD1	2:B:2126:ARG:NH2	2.45	0.43
2:B:3530:GLN:O	2:B:3533:ILE:HB	2.18	0.43
2:D:1112:ASP:OD1	2:D:1112:ASP:N	2.52	0.43
2:F:3180:ASN:HB2	2:F:3183:VAL:HG23	2.01	0.43
2:H:2480:GLY:N	2:H:2484:ALA:O	2.42	0.43
2:H:2763:HIS:NE2	2:H:2792:ARG:O	2.52	0.43
2:H:3537:LYS:HE2	2:H:3537:LYS:HB3	1.86	0.43
2:B:648:ILE:HD13	2:B:811:CYS:HB3	2.00	0.43
2:B:1771:LEU:HD22	2:B:2153:MET:HE2	1.99	0.43
2:B:4152:GLU:OE2	2:B:4180:ARG:NH1	2.50	0.43
2:B:4581:LYS:HE2	2:B:4581:LYS:HB3	1.87	0.43
2:D:1828:ASP:N	2:D:1828:ASP:OD1	2.52	0.43
2:D:1973:GLN:NE2	2:D:2005:GLN:OE1	2.40	0.43
2:F:2461:VAL:O	2:F:2510:TYR:OH	2.35	0.43
2:H:233:ILE:O	2:H:257:ARG:NH1	2.47	0.43
2:H:3529:ASP:O	2:H:3532:LEU:HB2	2.18	0.43
2:H:4006:ASP:OD2	2:H:4008:SER:OG	2.25	0.43
2:B:1773:PRO:HA	2:B:1774:PRO:HD3	1.88	0.42
2:B:1828:ASP:N	2:B:1828:ASP:OD1	2.52	0.42
2:B:2447:LYS:HB3	2:B:2447:LYS:HE2	1.79	0.42
2:D:882:TRP:O	2:D:885:THR:OG1	2.32	0.42
2:D:3223:SER:HB2	2:D:3226:GLU:HG3	2.01	0.42
2:F:35:LEU:HD13	2:F:49:LEU:HD13	2.00	0.42
2:F:4581:LYS:HE2	2:F:4581:LYS:HB3	1.87	0.42
2:F:4698:LYS:HE2	2:F:4698:LYS:HB3	1.87	0.42
2:H:2293:GLN:H	2:H:2293:GLN:HG3	1.64	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:530:ILE:HG22	2:B:536:ASN:HB3	2.01	0.42
2:D:1982:ARG:HD3	2:D:1982:ARG:HA	1.83	0.42
2:D:3768:SER:HA	2:D:3771:HIS:CD2	2.54	0.42
2:D:4698:LYS:HE2	2:D:4698:LYS:HB3	1.87	0.42
2:F:648:ILE:HD13	2:F:811:CYS:HB3	2.00	0.42
2:H:1828:ASP:OD1	2:H:1828:ASP:N	2.52	0.42
1:A:36:LYS:HE3	1:A:39:SER:HB2	2.01	0.42
2:B:745:SER:HB2	2:B:758:ARG:HB2	2.00	0.42
2:D:149:THR:HG23	2:D:172:VAL:HB	2.00	0.42
2:D:2336:ARG:HD3	2:D:2431:ASP:HB3	2.01	0.42
2:F:1982:ARG:HA	2:F:1982:ARG:HD3	1.83	0.42
2:F:3466:ASN:ND2	2:F:3507:THR:O	2.45	0.42
2:F:3768:SER:HA	2:F:3771:HIS:CD2	2.54	0.42
2:F:4026:MET:HE2	2:F:4026:MET:HB3	1.95	0.42
2:H:1435:TYR:HB3	2:H:1575:LEU:HG	2.01	0.42
2:H:3357:HIS:O	2:H:3361:THR:HG23	2.18	0.42
2:H:3850:GLN:HB2	2:H:3873:LYS:HD2	2.01	0.42
2:B:1435:TYR:HB3	2:B:1575:LEU:HG	2.01	0.42
2:D:2021:CYS:O	2:D:2028:ARG:NH2	2.52	0.42
2:F:530:ILE:HG22	2:F:536:ASN:HB3	2.01	0.42
2:F:4056:GLU:HG2	2:F:4166:LEU:HD13	2.00	0.42
2:B:345:LEU:HB3	2:B:387:ALA:HB1	2.01	0.42
2:B:3292:PRO:HA	2:B:3293:PRO:HD3	1.94	0.42
1:C:56:VAL:HA	2:D:1784:ALA:HA	2.00	0.42
2:D:530:ILE:HG22	2:D:536:ASN:HB3	2.01	0.42
2:D:3466:ASN:ND2	2:D:3507:THR:O	2.45	0.42
2:F:878:ILE:HD13	2:F:881:LEU:HD12	2.00	0.42
2:F:2763:HIS:NE2	2:F:2792:ARG:O	2.52	0.42
2:H:2519:LEU:HD13	2:H:2575:ARG:HG3	2.00	0.42
2:H:4056:GLU:HG2	2:H:4166:LEU:HD13	2.00	0.42
2:B:12:GLN:NE2	2:B:332:GLU:O	2.38	0.42
2:B:3277:LEU:HD23	2:B:3277:LEU:HA	1.85	0.42
2:B:3768:SER:HA	2:B:3771:HIS:CD2	2.54	0.42
2:D:266:ARG:O	2:D:270:SER:OG	2.34	0.42
2:F:336:PRO:HA	2:F:337:PRO:HD3	1.89	0.42
2:F:2336:ARG:HD3	2:F:2431:ASP:HB3	2.01	0.42
2:F:3448:SER:HB2	2:F:3451:PHE:HB2	2.02	0.42
2:H:3420:ARG:HG3	2:H:3520:ILE:HD11	2.02	0.42
2:B:575:LEU:HD12	2:B:609:CYS:HB3	2.02	0.42
2:B:2228:MET:HE2	2:B:2228:MET:HB2	1.84	0.42
2:D:575:LEU:HD12	2:D:609:CYS:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:864:PRO:HA	2:D:865:PRO:HD3	1.89	0.42
2:F:2447:LYS:HB3	2:F:2447:LYS:HE2	1.79	0.42
2:F:3420:ARG:HG3	2:F:3520:ILE:HD11	2.02	0.42
2:H:1093:GLU:HB3	2:H:1201:HIS:HB3	2.02	0.42
2:B:1093:GLU:HB3	2:B:1201:HIS:HB3	2.02	0.42
2:B:2480:GLY:N	2:B:2484:ALA:O	2.42	0.42
2:B:2516:ASP:OD1	2:B:2516:ASP:N	2.53	0.42
2:D:3180:ASN:HB2	2:D:3183:VAL:HG23	2.01	0.42
2:D:1435:TYR:HB3	2:D:1575:LEU:HG	2.01	0.42
2:D:2228:MET:HB2	2:D:2228:MET:HE2	1.84	0.42
2:F:3850:GLN:HB2	2:F:3873:LYS:HD2	2.01	0.42
2:H:3944:GLU:H	2:H:3944:GLU:HG3	1.72	0.42
2:B:1021:LEU:HD12	2:B:1021:LEU:HA	1.94	0.41
2:B:1973:GLN:NE2	2:B:2005:GLN:OE1	2.40	0.41
2:D:4152:GLU:OE1	2:D:4194:TYR:OH	2.32	0.41
2:D:4581:LYS:HE2	2:D:4581:LYS:HB3	1.87	0.41
2:D:4710:SER:OG	2:D:4772:ASP:OD2	2.28	0.41
2:H:2516:ASP:OD1	2:H:2516:ASP:N	2.53	0.41
2:H:3448:SER:HB2	2:H:3451:PHE:HB2	2.02	0.41
1:A:56:VAL:HA	2:B:1784:ALA:HA	2.00	0.41
2:B:1962:ALA:O	2:B:1966:VAL:HB	2.20	0.41
2:B:4843:LEU:HD22	2:H:4823:LEU:HD22	2.02	0.41
2:D:1093:GLU:HB3	2:D:1201:HIS:HB3	2.02	0.41
2:D:3448:SER:HB2	2:D:3451:PHE:HB2	2.02	0.41
2:F:575:LEU:HD12	2:F:609:CYS:HB3	2.02	0.41
2:F:1435:TYR:HB3	2:F:1575:LEU:HG	2.01	0.41
2:F:1575:LEU:HD23	2:F:1575:LEU:HA	1.93	0.41
2:F:3137:LEU:O	2:F:3141:THR:OG1	2.32	0.41
2:H:3539:ARG:HA	2:H:3539:ARG:HD3	1.87	0.41
2:B:3850:GLN:HB2	2:B:3873:LYS:HD2	2.01	0.41
2:D:828:GLU:OE2	2:D:831:ARG:NH2	2.53	0.41
2:D:1249:PRO:HA	2:D:1250:PRO:HD3	1.93	0.41
2:D:2477:PRO:HD2	2:D:2536:LEU:HD11	2.02	0.41
2:D:3330:ASP:OD1	2:D:3330:ASP:N	2.50	0.41
2:D:3850:GLN:HB2	2:D:3873:LYS:HD2	2.01	0.41
1:E:36:LYS:HE3	1:E:39:SER:HB2	2.01	0.41
2:F:1093:GLU:HB3	2:F:1201:HIS:HB3	2.02	0.41
2:H:1962:ALA:O	2:H:1966:VAL:HB	2.20	0.41
2:H:2336:ARG:HD3	2:H:2431:ASP:HB3	2.01	0.41
2:B:4152:GLU:OE1	2:B:4194:TYR:OH	2.32	0.41
2:F:2856:ASN:OD1	2:F:2858:GLN:NE2	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:36:LYS:HE3	1:G:39:SER:HB2	2.01	0.41
2:H:345:LEU:HB3	2:H:387:ALA:HB1	2.01	0.41
2:B:828:GLU:OE2	2:B:831:ARG:NH2	2.53	0.41
2:B:1249:PRO:HA	2:B:1250:PRO:HD3	1.93	0.41
2:B:4228:ALA:HB1	2:H:4973:HIS:NE2	2.36	0.41
2:B:4823:LEU:HD22	2:D:4843:LEU:HD22	2.02	0.41
2:D:2447:LYS:HE2	2:D:2447:LYS:HB3	1.79	0.41
2:F:176:SER:HG	2:F:178:ARG:HH11	1.65	0.41
2:H:218:HIS:ND1	2:H:341:TYR:OH	2.42	0.41
2:H:3180:ASN:HB2	2:H:3183:VAL:HG23	2.01	0.41
2:H:3823:LYS:HD3	2:H:3823:LYS:HA	1.86	0.41
2:B:4888:TYR:HE1	2:D:4917:ASP:HB2	1.86	0.41
2:B:4917:ASP:HB2	2:H:4888:TYR:HE1	1.86	0.41
1:C:36:LYS:HE3	1:C:39:SER:HB2	2.01	0.41
2:D:3537:LYS:HE2	2:D:3537:LYS:HB3	1.86	0.41
2:H:573:GLU:H	2:H:573:GLU:HG3	1.57	0.41
2:H:575:LEU:HD12	2:H:609:CYS:HB3	2.02	0.41
2:D:2359:ARG:HD3	2:D:2359:ARG:HA	1.92	0.41
2:F:828:GLU:OE2	2:F:831:ARG:NH2	2.53	0.41
2:F:1112:ASP:OD1	2:F:1112:ASP:N	2.52	0.41
2:F:2293:GLN:H	2:F:2293:GLN:HG3	1.64	0.41
2:F:2477:PRO:HD2	2:F:2536:LEU:HD11	2.02	0.41
2:F:2516:ASP:OD1	2:F:2516:ASP:N	2.53	0.41
2:H:1112:ASP:OD1	2:H:1112:ASP:N	2.52	0.41
2:H:2333:ASP:OD1	2:H:2336:ARG:NH2	2.48	0.41
2:B:2336:ARG:HD3	2:B:2431:ASP:HB3	2.01	0.41
2:B:4973:HIS:NE2	2:D:4228:ALA:HB1	2.36	0.41
2:D:4152:GLU:OE2	2:D:4180:ARG:NH1	2.50	0.41
2:F:345:LEU:HB3	2:F:387:ALA:HB1	2.01	0.41
2:F:1641:ILE:HA	2:F:1642:PRO:HD3	1.93	0.41
2:H:842:PRO:HG3	2:H:1071:ARG:O	2.21	0.41
2:H:1749:PRO:HA	2:H:1750:PRO:HD3	1.94	0.41
2:H:4698:LYS:HB3	2:H:4698:LYS:HE2	1.87	0.41
1:A:78:THR:OG1	1:A:80:ASP:OD1	2.29	0.41
2:B:175:SER:O	2:H:2452:ARG:CG	2.67	0.41
2:B:1982:ARG:HD3	2:B:1982:ARG:HA	1.83	0.41
2:B:2690:LYS:HE2	2:B:2690:LYS:HB3	1.92	0.41
2:B:3169:LEU:HD12	2:B:3194:LEU:HD11	2.03	0.41
2:B:3840:SER:OG	2:B:3877:ASP:OD1	2.34	0.41
2:D:1749:PRO:HA	2:D:1750:PRO:HD3	1.94	0.41
2:D:2587:TYR:O	2:D:2590:SER:OG	2.30	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3169:LEU:HD12	2:D:3194:LEU:HD11	2.03	0.41
2:D:4888:TYR:HE1	2:F:4917:ASP:HB2	1.86	0.41
2:F:2713:ASP:OD1	2:F:2713:ASP:N	2.51	0.41
2:F:2974:ILE:HD13	2:F:2974:ILE:HA	1.93	0.41
2:F:4711:PHE:HA	2:F:4712:PRO:HA	1.93	0.41
2:F:4888:TYR:HE1	2:H:4917:ASP:HB2	1.86	0.41
2:F:4973:HIS:NE2	2:H:4228:ALA:HB1	2.36	0.41
2:H:1207:ASP:O	2:H:1210:SER:OG	2.35	0.41
2:H:2477:PRO:HD2	2:H:2536:LEU:HD11	2.02	0.41
2:H:2522:LEU:HA	2:H:2526:PHE:HB2	2.03	0.41
2:H:3509:LEU:O	2:H:3513:THR:OG1	2.33	0.41
2:B:3448:SER:HB2	2:B:3451:PHE:HB2	2.02	0.41
2:B:3539:ARG:HA	2:B:3539:ARG:HD3	1.87	0.41
2:D:345:LEU:HB3	2:D:387:ALA:HB1	2.01	0.41
2:D:786:GLY:N	2:D:1630:CYS:O	2.48	0.41
2:F:3292:PRO:HA	2:F:3293:PRO:HD3	1.94	0.41
2:H:2582:MET:HE2	2:H:2582:MET:HB3	1.86	0.41
2:H:2974:ILE:HD13	2:H:2974:ILE:HA	1.93	0.41
2:H:3466:ASN:ND2	2:H:3507:THR:O	2.45	0.41
2:B:842:PRO:HG3	2:B:1071:ARG:O	2.21	0.40
2:B:2452:ARG:CG	2:D:175:SER:O	2.67	0.40
2:B:3823:LYS:HA	2:B:3823:LYS:HD3	1.86	0.40
2:D:842:PRO:HG3	2:D:1071:ARG:O	2.21	0.40
2:D:1624:LEU:HD23	2:D:1624:LEU:HA	1.96	0.40
2:D:2974:ILE:HD13	2:D:2974:ILE:HA	1.93	0.40
1:E:107:LEU:HD23	1:E:107:LEU:HA	1.88	0.40
2:F:911:HIS:O	2:F:918:ARG:NH2	2.54	0.40
2:H:2587:TYR:O	2:H:2590:SER:OG	2.30	0.40
2:B:2522:LEU:HA	2:B:2526:PHE:HB2	2.03	0.40
2:B:4567:LEU:HD11	2:B:4816:ILE:HG22	2.04	0.40
2:D:4823:LEU:HD22	2:F:4843:LEU:HD22	2.02	0.40
2:D:4973:HIS:NE2	2:F:4228:ALA:HB1	2.36	0.40
2:F:1502:SER:O	2:F:1506:GLN:N	2.52	0.40
2:F:2093:SER:HB3	2:F:2096:GLU:HG3	2.03	0.40
2:F:2452:ARG:CG	2:H:175:SER:O	2.67	0.40
2:F:3169:LEU:HD12	2:F:3194:LEU:HD11	2.03	0.40
2:F:4823:LEU:HD22	2:H:4843:LEU:HD22	2.02	0.40
2:H:3169:LEU:HD12	2:H:3194:LEU:HD11	2.03	0.40
2:B:4047:MET:HE3	2:B:4047:MET:HB3	1.92	0.40
1:C:107:LEU:HD23	1:C:107:LEU:HA	1.88	0.40
2:D:2516:ASP:OD1	2:D:2516:ASP:N	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3420:ARG:HG3	2:D:3520:ILE:HD11	2.02	0.40
2:F:2522:LEU:HA	2:F:2526:PHE:HB2	2.03	0.40
2:F:2970:SER:HA	2:F:2973:PHE:CE2	2.57	0.40
2:H:1021:LEU:HD12	2:H:1021:LEU:HA	1.94	0.40
2:B:882:TRP:O	2:B:885:THR:OG1	2.32	0.40
2:B:3420:ARG:HG3	2:B:3520:ILE:HD11	2.02	0.40
2:D:1758:ARG:HD2	2:D:1758:ARG:HA	1.86	0.40
2:H:828:GLU:OE2	2:H:831:ARG:NH2	2.53	0.40
2:H:878:ILE:HD13	2:H:878:ILE:HA	1.91	0.40
2:B:2763:HIS:NE2	2:B:2792:ARG:O	2.52	0.40
2:B:3509:LEU:O	2:B:3513:THR:OG1	2.33	0.40
2:D:1962:ALA:O	2:D:1966:VAL:HB	2.20	0.40
2:D:3292:PRO:HA	2:D:3293:PRO:HD3	1.94	0.40
2:D:4026:MET:HE2	2:D:4026:MET:HB3	1.95	0.40
2:F:2582:MET:HE2	2:F:2582:MET:HB3	1.86	0.40
2:H:911:HIS:O	2:H:918:ARG:NH2	2.54	0.40
2:H:2770:LYS:HA	2:H:2770:LYS:HD3	1.90	0.40
2:H:2970:SER:HA	2:H:2973:PHE:CE2	2.57	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	4201/5037 (83%)	4139 (98%)	62 (2%)	0	100	100
2	D	4201/5037 (83%)	4139 (98%)	62 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	4201/5037 (83%)	4139 (98%)	62 (2%)	0	100	100
2	H	4201/5037 (83%)	4139 (98%)	62 (2%)	0	100	100
All	All	17228/20588 (84%)	16972 (98%)	256 (2%)	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	86/90 (96%)	84 (98%)	2 (2%)	44	74
1	C	86/90 (96%)	84 (98%)	2 (2%)	44	74
1	E	86/90 (96%)	84 (98%)	2 (2%)	44	74
1	G	86/90 (96%)	84 (98%)	2 (2%)	44	74
2	B	3490/4276 (82%)	3463 (99%)	27 (1%)	73	89
2	D	3490/4276 (82%)	3463 (99%)	27 (1%)	73	89
2	F	3490/4276 (82%)	3463 (99%)	27 (1%)	73	89
2	H	3490/4276 (82%)	3463 (99%)	27 (1%)	73	89
All	All	14304/17464 (82%)	14188 (99%)	116 (1%)	70	89

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	26	HIS
2	B	169	LEU
2	B	220	LEU
2	B	280	LEU
2	B	388	LEU
2	B	573	GLU
2	B	575	LEU
2	B	787	VAL

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Mol	Chain	Res	Type
2	B	1022	VAL
2	B	1603	VAL
2	B	1760	HIS
2	B	1934	SER
2	B	1966	VAL
2	B	2274	ASP
2	B	2464	ASP
2	B	2516	ASP
2	B	2591	ARG
2	B	2593	ARG
2	B	2617	SER
2	B	2667	THR
2	B	2906	VAL
2	B	3874	VAL
2	B	3899	PHE
2	B	3911	THR
2	B	3916	ILE
2	B	3933	PHE
2	B	4051	SER
2	B	4720	VAL
1	C	5	ILE
1	C	26	HIS
2	D	169	LEU
2	D	220	LEU
2	D	280	LEU
2	D	388	LEU
2	D	573	GLU
2	D	575	LEU
2	D	787	VAL
2	D	1022	VAL
2	D	1603	VAL
2	D	1760	HIS
2	D	1934	SER
2	D	1966	VAL
2	D	2274	ASP
2	D	2464	ASP
2	D	2516	ASP
2	D	2591	ARG
2	D	2593	ARG
2	D	2617	SER
2	D	2667	THR
2	D	2906	VAL

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Mol	Chain	Res	Type
2	D	3874	VAL
2	D	3899	PHE
2	D	3911	THR
2	D	3916	ILE
2	D	3933	PHE
2	D	4051	SER
2	D	4720	VAL
1	E	5	ILE
1	E	26	HIS
2	F	169	LEU
2	F	220	LEU
2	F	280	LEU
2	F	388	LEU
2	F	573	GLU
2	F	575	LEU
2	F	787	VAL
2	F	1022	VAL
2	F	1603	VAL
2	F	1760	HIS
2	F	1934	SER
2	F	1966	VAL
2	F	2274	ASP
2	F	2464	ASP
2	F	2516	ASP
2	F	2591	ARG
2	F	2593	ARG
2	F	2617	SER
2	F	2667	THR
2	F	2906	VAL
2	F	3874	VAL
2	F	3899	PHE
2	F	3911	THR
2	F	3916	ILE
2	F	3933	PHE
2	F	4051	SER
2	F	4720	VAL
1	G	5	ILE
1	G	26	HIS
2	H	169	LEU
2	H	220	LEU
2	H	280	LEU
2	H	388	LEU

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Mol	Chain	Res	Type
2	H	573	GLU
2	H	575	LEU
2	H	787	VAL
2	H	1022	VAL
2	H	1603	VAL
2	H	1760	HIS
2	H	1934	SER
2	H	1966	VAL
2	H	2274	ASP
2	H	2464	ASP
2	H	2516	ASP
2	H	2591	ARG
2	H	2593	ARG
2	H	2617	SER
2	H	2667	THR
2	H	2906	VAL
2	H	3874	VAL
2	H	3899	PHE
2	H	3911	THR
2	H	3916	ILE
2	H	3933	PHE
2	H	4051	SER
2	H	4720	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (204) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
2	B	23	GLN
2	B	32	GLN
2	B	44	ASN
2	B	105	HIS
2	B	203	ASN
2	B	658	GLN
2	B	812	HIS
2	B	838	HIS
2	B	866	HIS
2	B	981	GLN
2	B	991	ASN
2	B	1281	ASN
2	B	1296	GLN
2	B	1299	GLN

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Mol	Chain	Res	Type
2	B	1480	GLN
2	B	1569	GLN
2	B	1586	ASN
2	B	1691	GLN
2	B	1928	GLN
2	B	1938	GLN
2	B	2092	GLN
2	B	2260	ASN
2	B	2342	ASN
2	B	2599	GLN
2	B	2620	GLN
2	B	2634	ASN
2	B	2773	ASN
2	B	2877	GLN
2	B	3149	GLN
2	B	3234	ASN
2	B	3313	ASN
2	B	3462	ASN
2	B	3555	ASN
2	B	3608	GLN
2	B	3667	HIS
2	B	3704	HIS
2	B	3734	HIS
2	B	3927	GLN
2	B	3946	GLN
2	B	3950	ASN
2	B	3994	HIS
2	B	4020	GLN
2	B	4054	ASN
2	B	4078	GLN
2	B	4100	GLN
2	B	4102	GLN
2	B	4223	ASN
2	B	4707	ASN
2	B	4714	ASN
2	B	4833	ASN
2	B	4949	GLN
1	C	32	GLN
2	D	23	GLN
2	D	32	GLN
2	D	105	HIS
2	D	203	ASN

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Mol	Chain	Res	Type
2	D	658	GLN
2	D	812	HIS
2	D	838	HIS
2	D	866	HIS
2	D	981	GLN
2	D	991	ASN
2	D	1281	ASN
2	D	1296	GLN
2	D	1299	GLN
2	D	1480	GLN
2	D	1569	GLN
2	D	1586	ASN
2	D	1691	GLN
2	D	1928	GLN
2	D	1938	GLN
2	D	2092	GLN
2	D	2260	ASN
2	D	2342	ASN
2	D	2599	GLN
2	D	2620	GLN
2	D	2634	ASN
2	D	2773	ASN
2	D	2877	GLN
2	D	3149	GLN
2	D	3234	ASN
2	D	3313	ASN
2	D	3462	ASN
2	D	3555	ASN
2	D	3608	GLN
2	D	3667	HIS
2	D	3704	HIS
2	D	3734	HIS
2	D	3927	GLN
2	D	3946	GLN
2	D	3950	ASN
2	D	3994	HIS
2	D	4020	GLN
2	D	4054	ASN
2	D	4078	GLN
2	D	4100	GLN
2	D	4102	GLN
2	D	4223	ASN

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Mol	Chain	Res	Type
2	D	4707	ASN
2	D	4714	ASN
2	D	4728	HIS
2	D	4833	ASN
2	D	4949	GLN
2	D	4987	ASN
1	E	32	GLN
2	F	23	GLN
2	F	32	GLN
2	F	105	HIS
2	F	203	ASN
2	F	658	GLN
2	F	838	HIS
2	F	866	HIS
2	F	981	GLN
2	F	991	ASN
2	F	1281	ASN
2	F	1299	GLN
2	F	1480	GLN
2	F	1545	ASN
2	F	1569	GLN
2	F	1586	ASN
2	F	1691	GLN
2	F	1928	GLN
2	F	1938	GLN
2	F	2003	GLN
2	F	2092	GLN
2	F	2342	ASN
2	F	2599	GLN
2	F	2620	GLN
2	F	2634	ASN
2	F	2877	GLN
2	F	2976	HIS
2	F	2991	HIS
2	F	3234	ASN
2	F	3313	ASN
2	F	3462	ASN
2	F	3555	ASN
2	F	3597	GLN
2	F	3667	HIS
2	F	3704	HIS
2	F	3734	HIS

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Mol	Chain	Res	Type
2	F	3927	GLN
2	F	3946	GLN
2	F	3950	ASN
2	F	3994	HIS
2	F	4020	GLN
2	F	4054	ASN
2	F	4078	GLN
2	F	4100	GLN
2	F	4102	GLN
2	F	4223	ASN
2	F	4707	ASN
2	F	4833	ASN
2	F	4949	GLN
1	G	32	GLN
2	H	23	GLN
2	H	32	GLN
2	H	105	HIS
2	H	203	ASN
2	H	658	GLN
2	H	812	HIS
2	H	838	HIS
2	H	866	HIS
2	H	981	GLN
2	H	991	ASN
2	H	1281	ASN
2	H	1299	GLN
2	H	1480	GLN
2	H	1532	ASN
2	H	1545	ASN
2	H	1569	GLN
2	H	1586	ASN
2	H	1691	GLN
2	H	1928	GLN
2	H	1938	GLN
2	H	2003	GLN
2	H	2092	GLN
2	H	2342	ASN
2	H	2599	GLN
2	H	2620	GLN
2	H	2634	ASN
2	H	2773	ASN
2	H	2877	GLN

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Mol	Chain	Res	Type
2	H	3234	ASN
2	H	3313	ASN
2	H	3462	ASN
2	H	3555	ASN
2	H	3597	GLN
2	H	3667	HIS
2	H	3704	HIS
2	H	3734	HIS
2	H	3927	GLN
2	H	3946	GLN
2	H	3950	ASN
2	H	3994	HIS
2	H	4020	GLN
2	H	4054	ASN
2	H	4078	GLN
2	H	4100	GLN
2	H	4102	GLN
2	H	4223	ASN
2	H	4707	ASN
2	H	4833	ASN
2	H	4987	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no 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	0.29	0	48,52,52	0.32	0
5	ATP	F	5303	-	32,33,33	0.29	0	48,52,52	0.32	0
5	ATP	H	5303	-	32,33,33	0.29	0	48,52,52	0.32	0
5	ATP	D	5303	-	32,33,33	0.29	0	48,52,52	0.32	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	-	-	11/22/38/38	0/3/3/3
5	ATP	F	5303	-	-	11/22/38/38	0/3/3/3
5	ATP	H	5303	-	-	11/22/38/38	0/3/3/3
5	ATP	D	5303	-	-	11/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	B	5303	ATP	C4'-C5'-O5'-PA
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	D	5303	ATP	C4'-C5'-O5'-PA
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	F	5303	ATP	C4'-C5'-O5'-PA
5	H	5303	ATP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
5	H	5303	ATP	C5'-O5'-PA-O2A
5	H	5303	ATP	C5'-O5'-PA-O3A
5	H	5303	ATP	C4'-C5'-O5'-PA
5	B	5303	ATP	O4'-C4'-C5'-O5'
5	D	5303	ATP	O4'-C4'-C5'-O5'
5	F	5303	ATP	O4'-C4'-C5'-O5'
5	H	5303	ATP	O4'-C4'-C5'-O5'
5	B	5303	ATP	C3'-C4'-C5'-O5'
5	D	5303	ATP	C3'-C4'-C5'-O5'
5	F	5303	ATP	C3'-C4'-C5'-O5'
5	H	5303	ATP	C3'-C4'-C5'-O5'
5	B	5303	ATP	O4'-C1'-N9-C8
5	D	5303	ATP	O4'-C1'-N9-C8
5	F	5303	ATP	O4'-C1'-N9-C8
5	H	5303	ATP	O4'-C1'-N9-C8
5	B	5303	ATP	PG-O3B-PB-O3A
5	D	5303	ATP	PG-O3B-PB-O3A
5	F	5303	ATP	PG-O3B-PB-O3A
5	H	5303	ATP	PG-O3B-PB-O3A
5	B	5303	ATP	PG-O3B-PB-O1B
5	D	5303	ATP	PG-O3B-PB-O1B
5	F	5303	ATP	PG-O3B-PB-O1B
5	H	5303	ATP	PG-O3B-PB-O1B
5	B	5303	ATP	O4'-C1'-N9-C4
5	D	5303	ATP	O4'-C1'-N9-C4
5	F	5303	ATP	O4'-C1'-N9-C4
5	H	5303	ATP	O4'-C1'-N9-C4
5	B	5303	ATP	PG-O3B-PB-O2B
5	D	5303	ATP	PG-O3B-PB-O2B
5	F	5303	ATP	PG-O3B-PB-O2B
5	H	5303	ATP	PG-O3B-PB-O2B

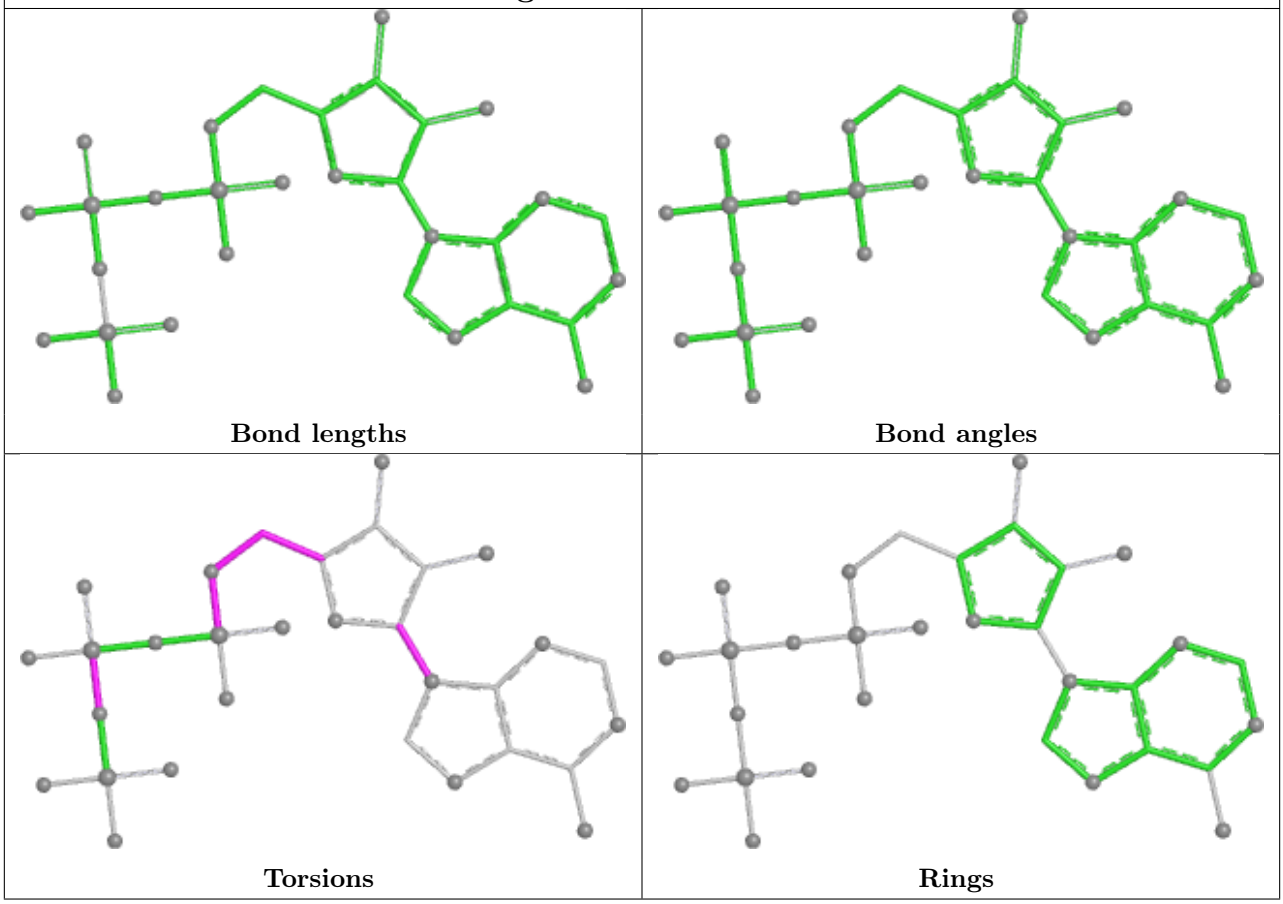
There are no ring outliers.

No monomer is involved in short contacts.

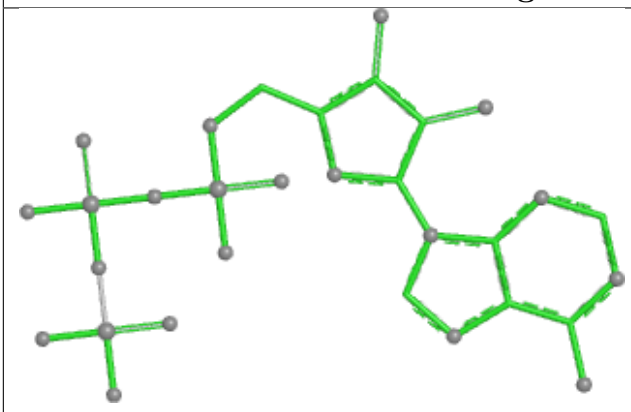
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

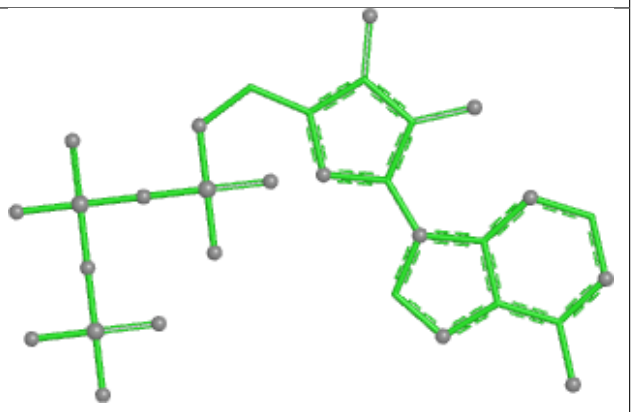
Ligand ATP B 5303



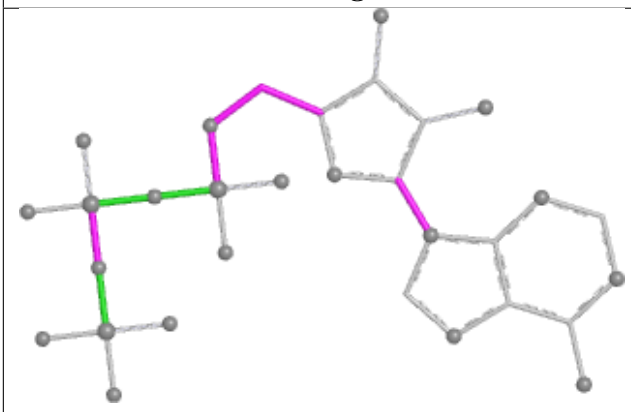
Ligand ATP F 5303



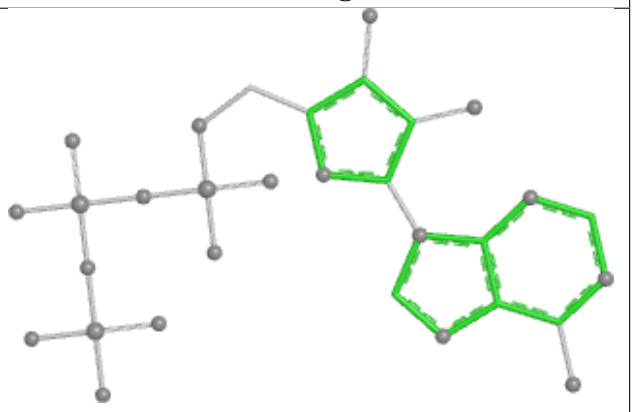
Bond lengths



Bond angles

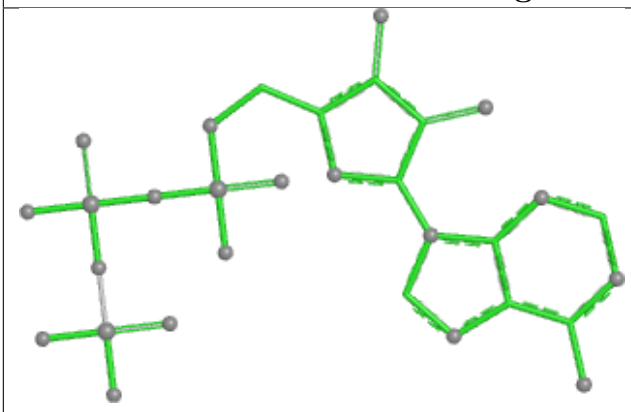


Torsions

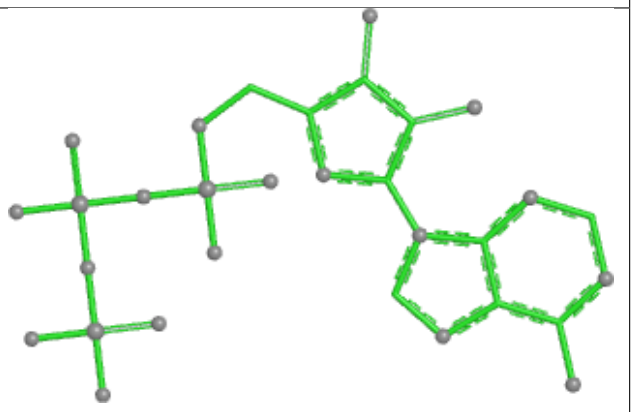


Rings

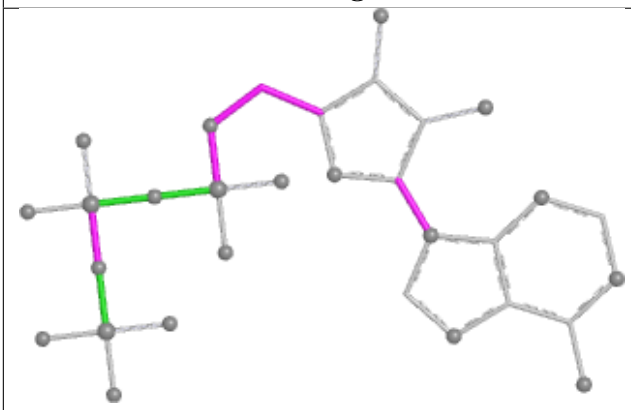
Ligand ATP H 5303



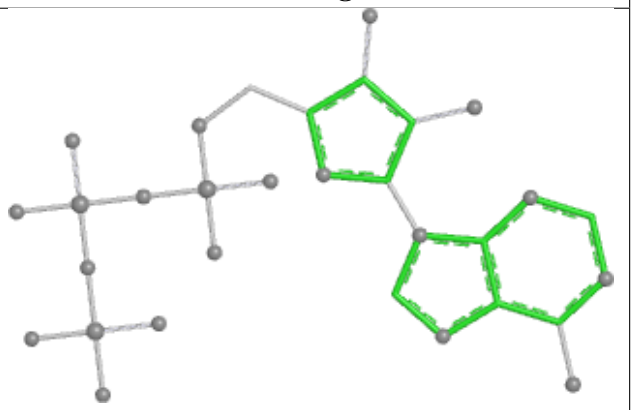
Bond lengths



Bond angles

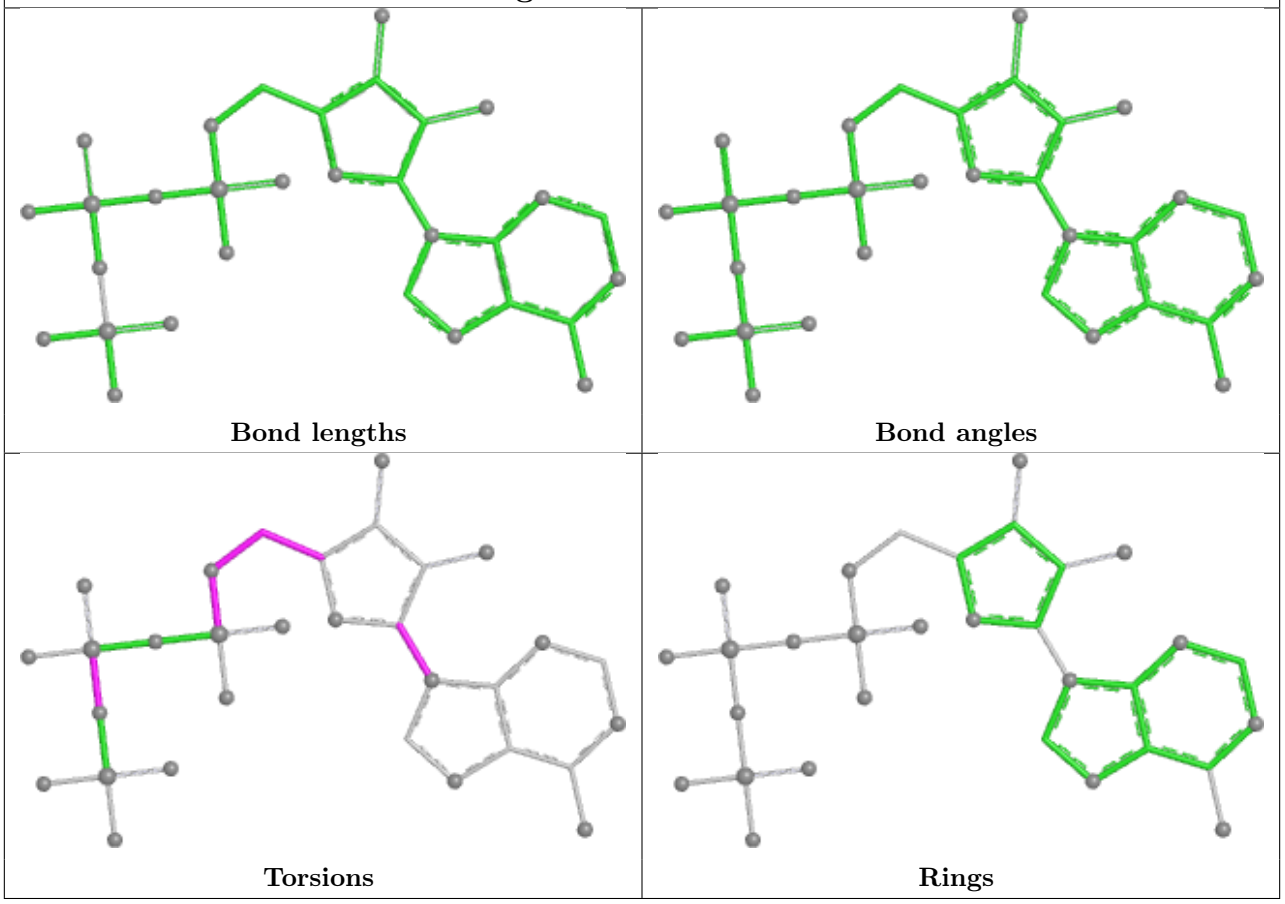


Torsions



Rings

Ligand ATP D 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.

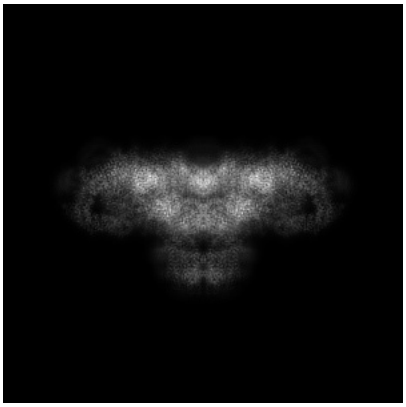
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-73960. These allow visual inspection of the internal detail of the map and identification of artifacts.

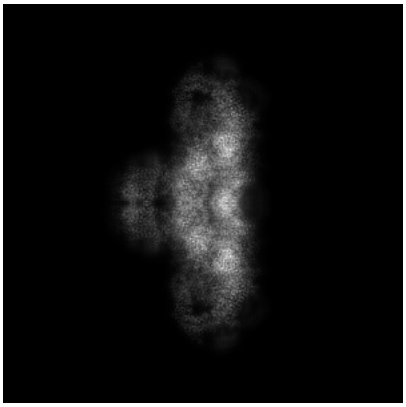
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

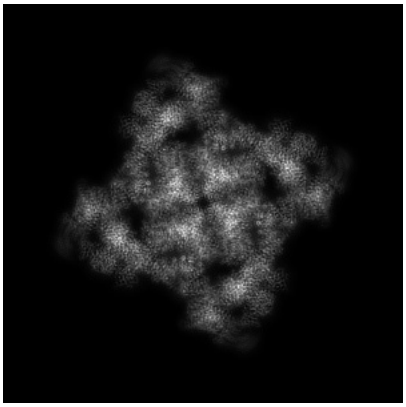
6.1.1 Primary map



X



Y



Z

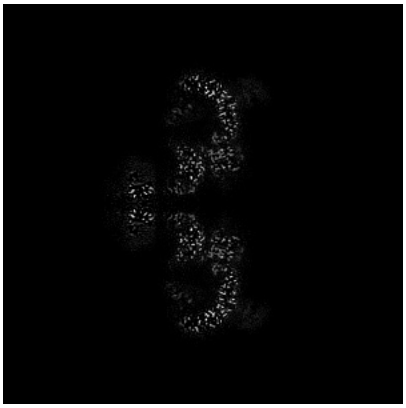
The images above show the map projected in three orthogonal directions.

6.2 Central slices

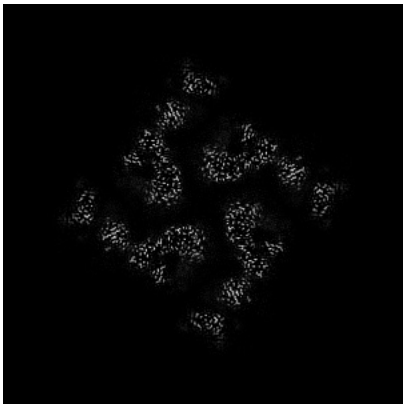
6.2.1 Primary map



X Index: 256



Y Index: 256

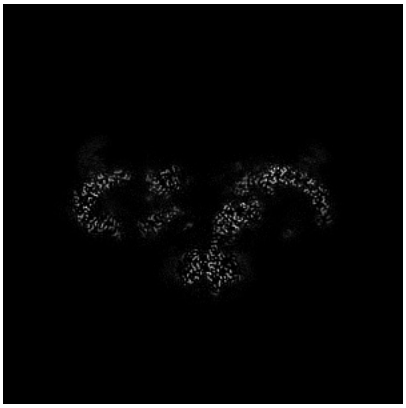


Z Index: 256

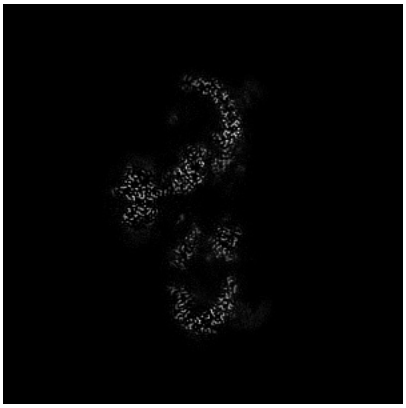
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

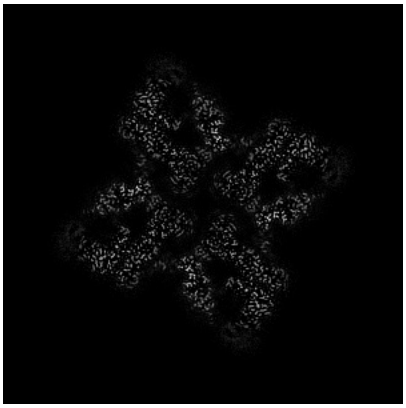
6.3.1 Primary map



X Index: 263



Y Index: 249

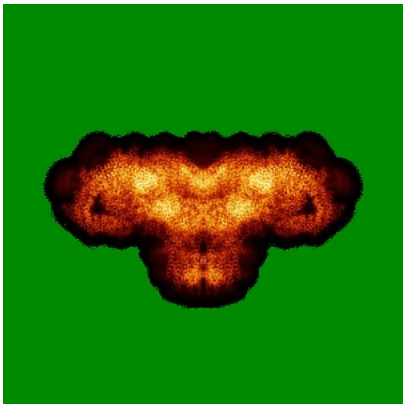


Z Index: 291

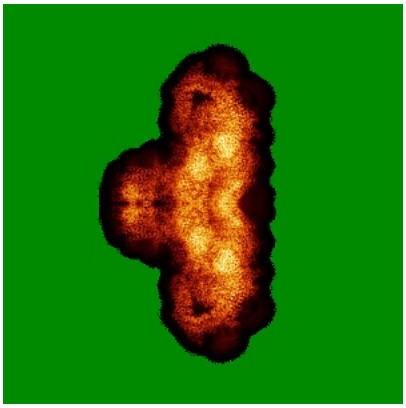
The images above show the largest variance slices of the map in three orthogonal directions.

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

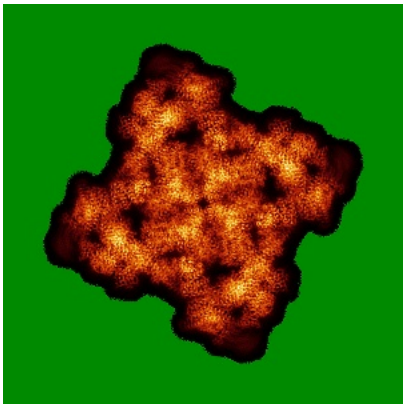
6.4.1 Primary map



X



Y

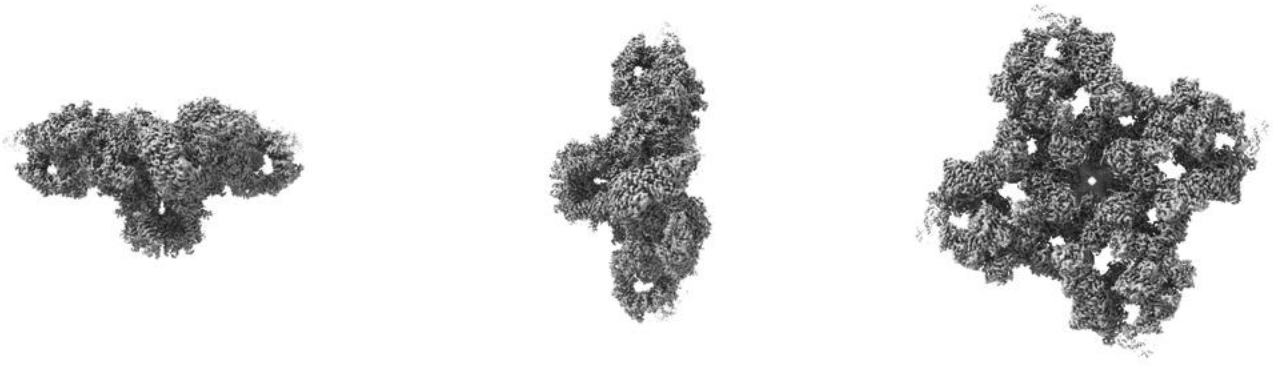


Z

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

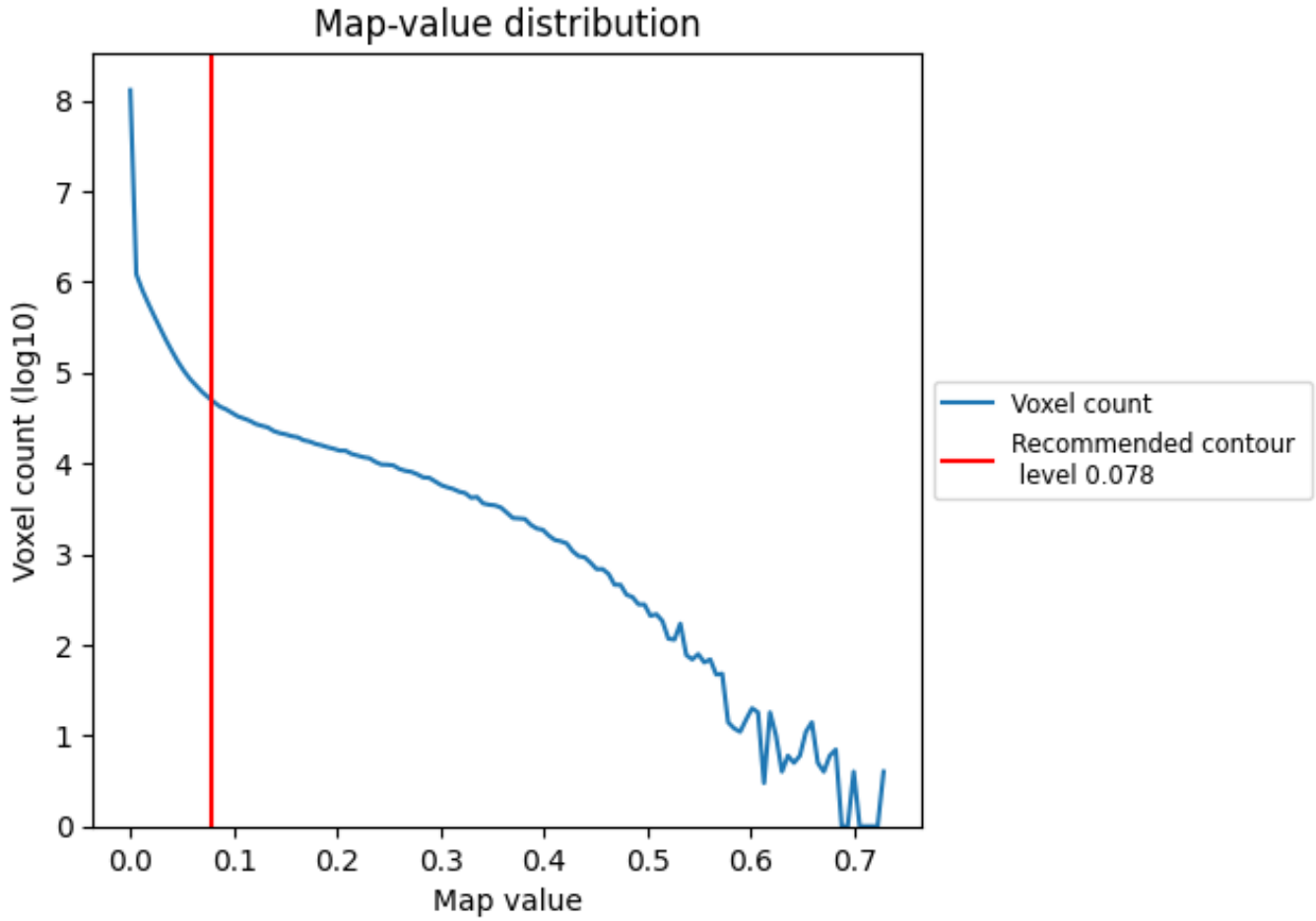
6.6 Mask visualisation (i)

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

7 Map analysis

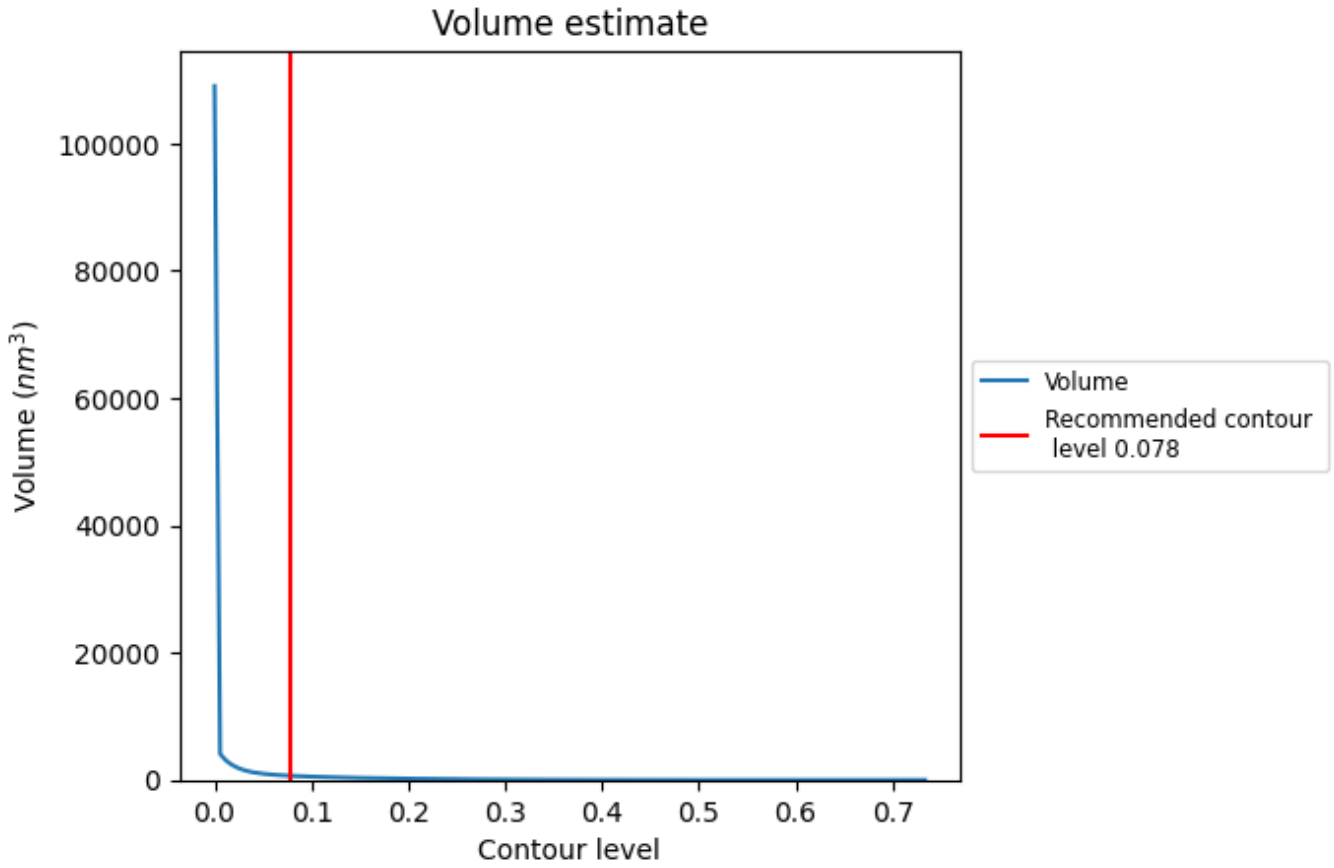
This section contains the results of statistical analysis of the map.

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.

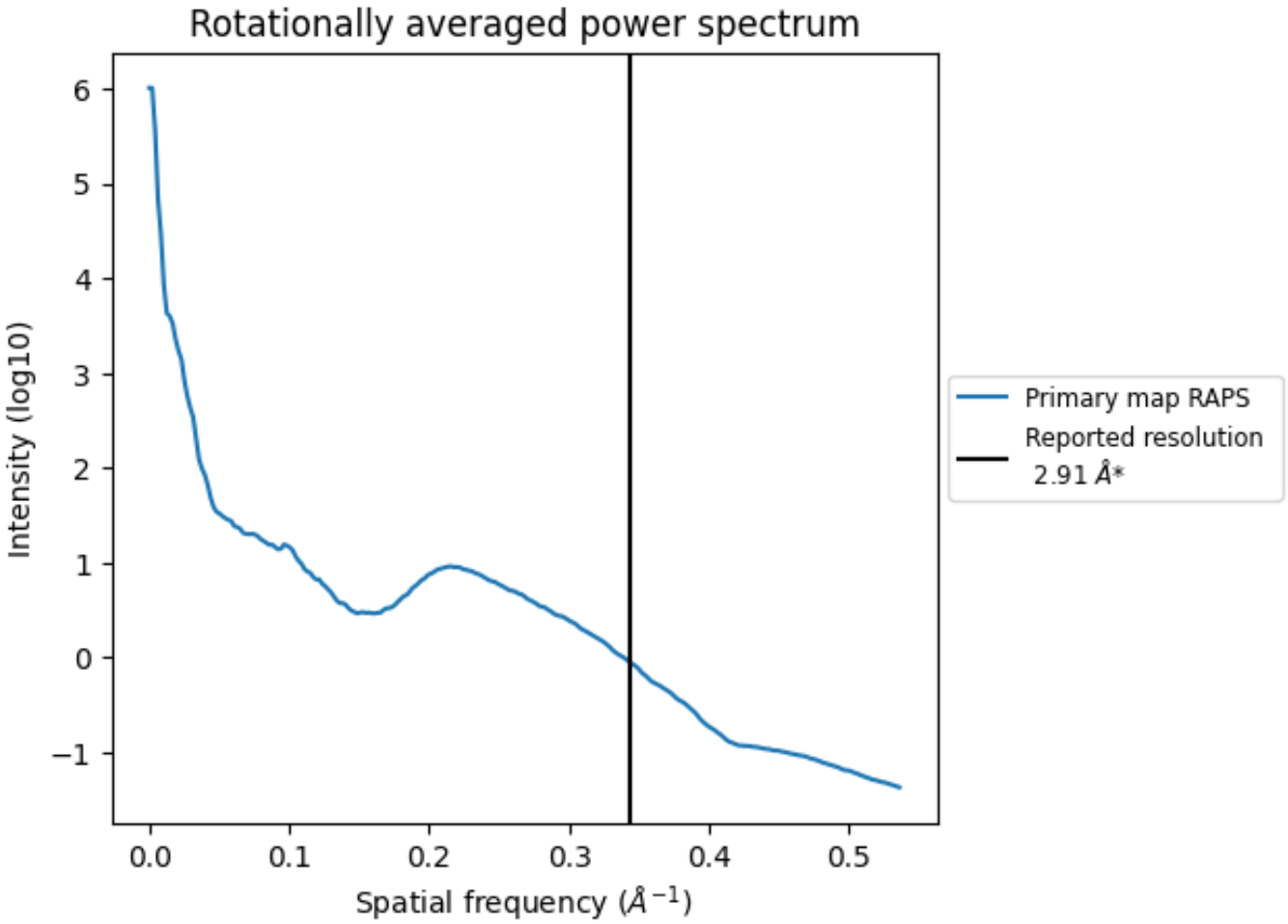
7.2 Volume estimate



The volume at the recommended contour level is 659 nm^3; this corresponds to an approximate mass of 595 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 0.344 Å^{-1}

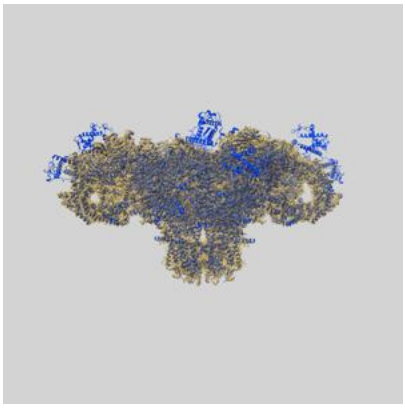
8 Fourier-Shell correlation (i)

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

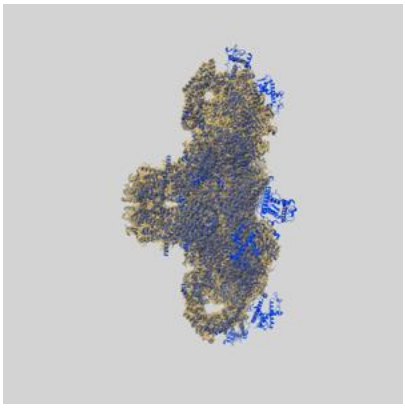
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-73960 and PDB model 9Z9V. Per-residue inclusion information can be found in section 3 on page 7.

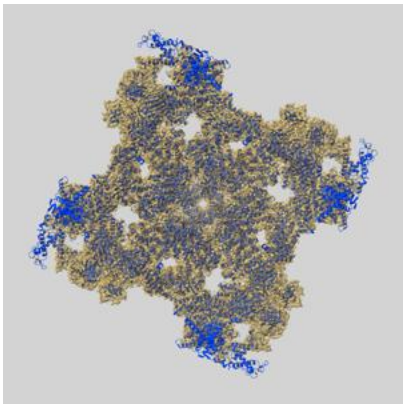
9.1 Map-model overlay



X



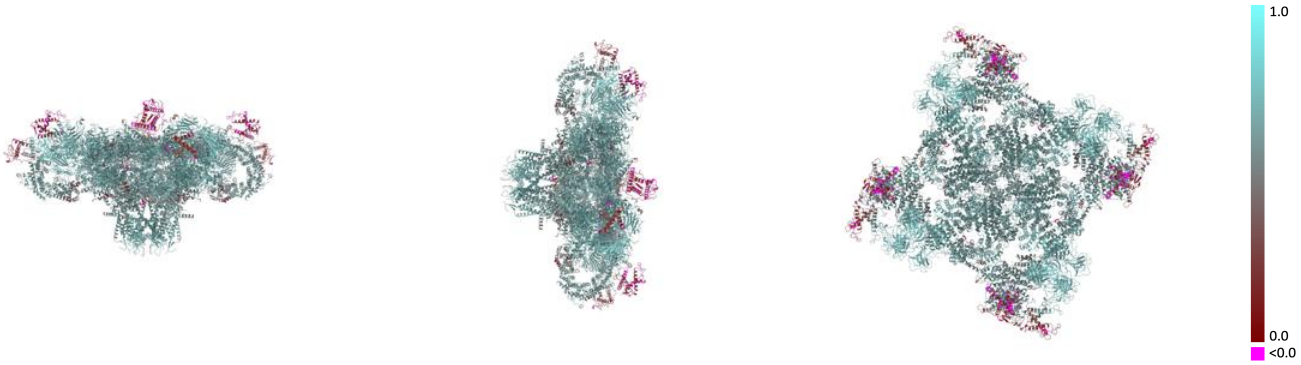
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.078 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.

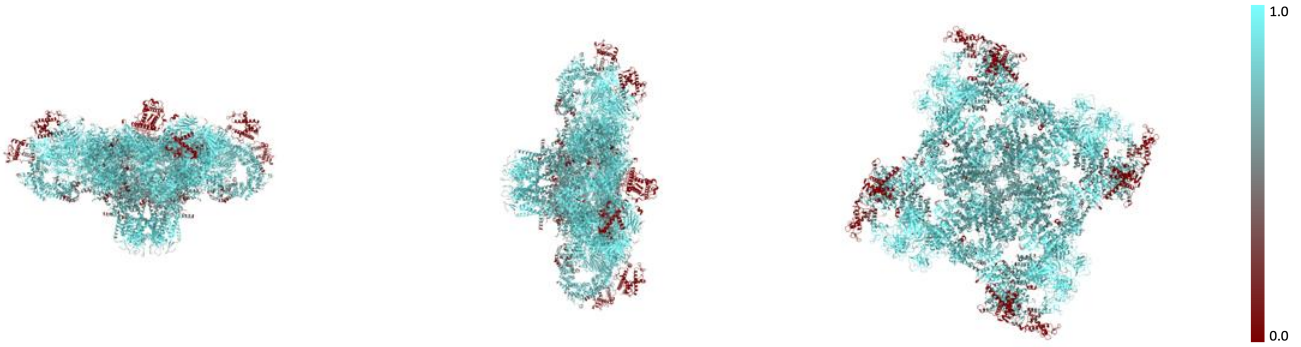
9.2 Q-score mapped to coordinate model (i)



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.

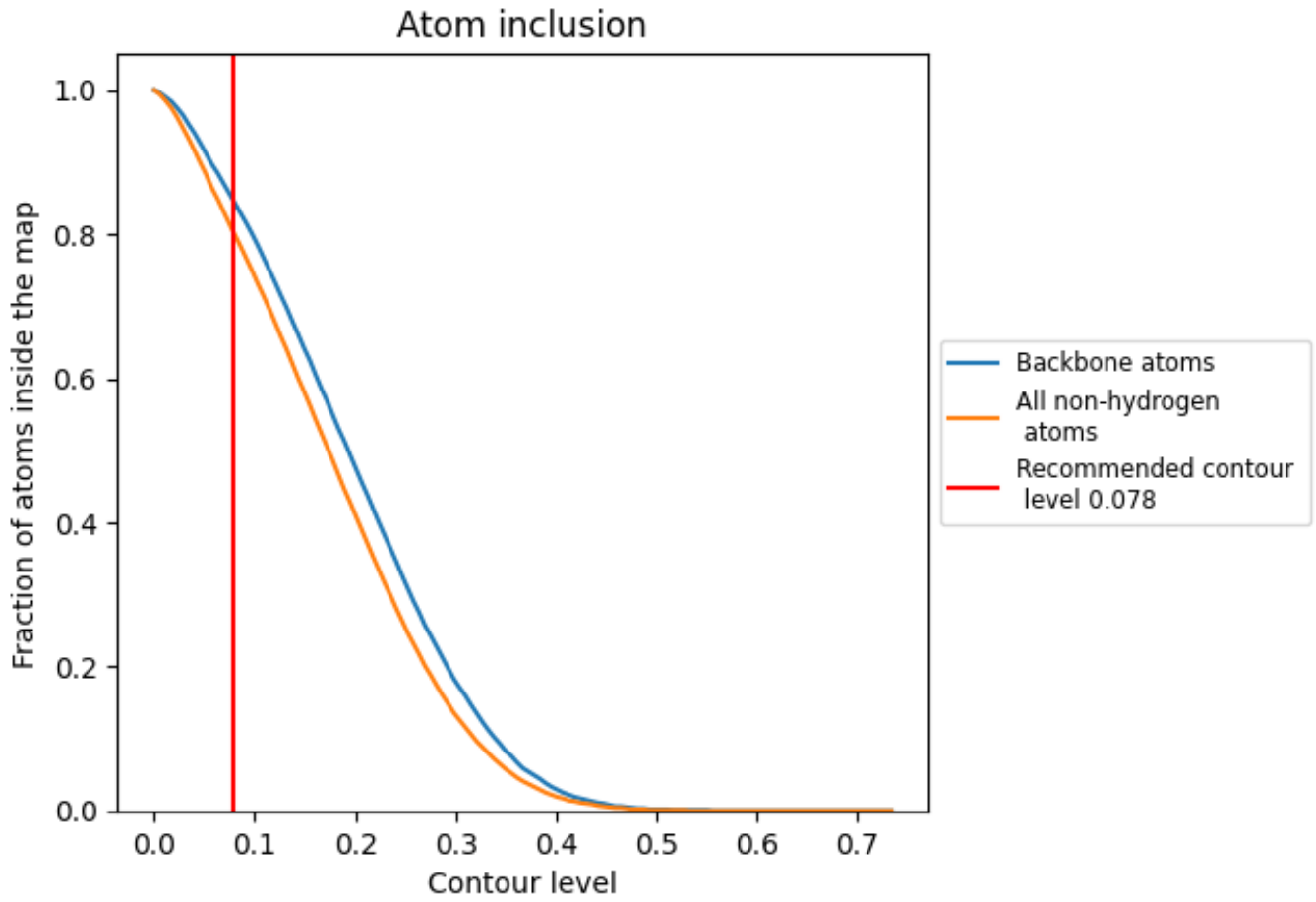
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.078).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 80% 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 (0.078) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8050	0.6070
A	0.9230	0.6780
B	0.8020	0.6050
C	0.9240	0.6770
D	0.8020	0.6060
E	0.9240	0.6770
F	0.8030	0.6050
G	0.9230	0.6760
H	0.8020	0.6050

