Full wwPDB EM Validation Report

Mar 19, 2024 – 11:45 PM JST

PDB ID	:	6JRS
EMDB ID	:	EMD-9880
Title	:	Structure of RyR2 (*F/A/C/L-Ca2+/Ca2+-CaM dataset)
Authors	:	Gong, D.S.; Chi, X.M.; Zhou, G.W.; Huang, G.X.Y.; Lei, J.L.; Yan, N.
Deposited on	:	2019-04-05
Resolution	:	3.70 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

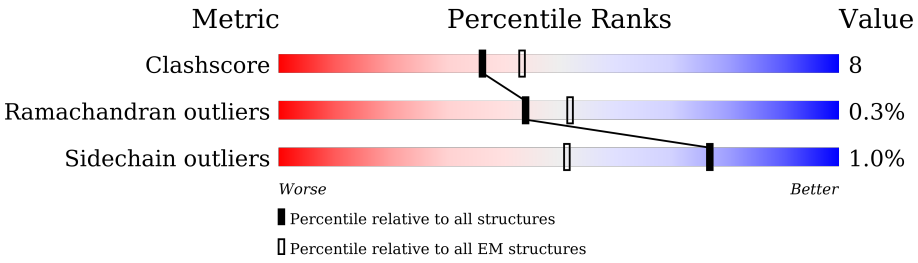
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance

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

The reported resolution of this entry is 3.70 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	4968	7% 56% 14% 30%
1	D	4968	7% 56% 14% 30%
1	G	4968	7% 56% 13% 30%
1	J	4968	7% 56% 14% 30%
2	B	108	82% 17%
2	E	108	82% 17%
2	H	108	83% 16%
2	K	108	83% 16%

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Mol	Chain	Length	Quality of chain
3	C	149	40% 37% 9% 54%
3	F	149	40% 37% 9% 54%
3	I	149	40% 37% 9% 54%
3	L	149	40% 37% 9% 54%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 112168 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 RyR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3488	Total 26650	C 16980	N 4570	O 4941	S 159	0	0
1	D	3488	Total 26650	C 16980	N 4570	O 4941	S 159	0	0
1	G	3488	Total 26650	C 16980	N 4570	O 4941	S 159	0	0
1	J	3488	Total 26650	C 16980	N 4570	O 4941	S 159	0	0

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	107	Total 819	C 516	N 144	O 155	S 4	0	0
2	E	107	Total 819	C 516	N 144	O 155	S 4	0	0
2	H	107	Total 819	C 516	N 144	O 155	S 4	0	0
2	K	107	Total 819	C 516	N 144	O 155	S 4	0	0

- Molecule 3 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	68	Total 524	C 326	N 83	O 110	S 5	0	0
3	F	68	Total 524	C 326	N 83	O 110	S 5	0	0
3	I	68	Total 524	C 326	N 83	O 110	S 5	0	0
3	L	68	Total 524	C 326	N 83	O 110	S 5	0	0

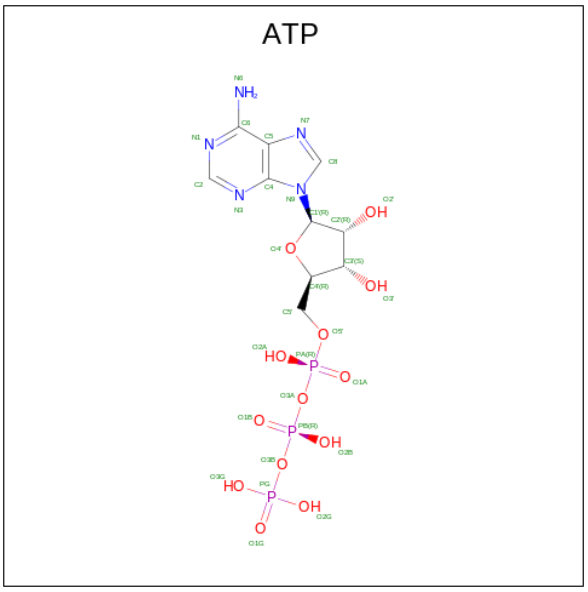
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total Zn 1 1	0
4	D	1	Total Zn 1 1	0
4	G	1	Total Zn 1 1	0
4	J	1	Total Zn 1 1	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

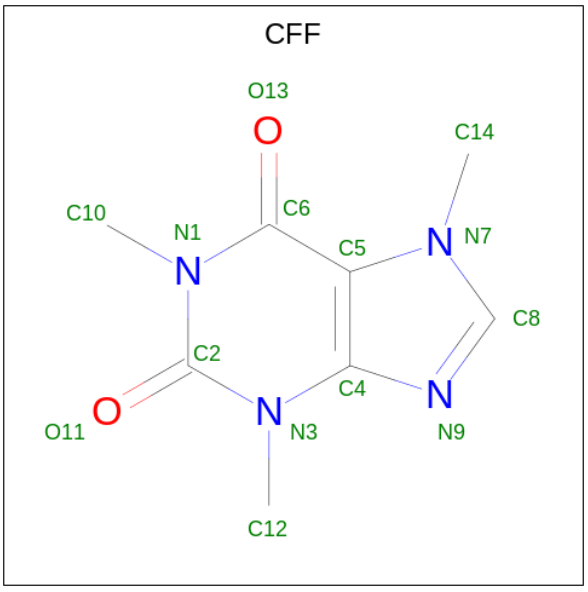
Mol	Chain	Residues	Atoms	AltConf
5	A	1	Total Ca 1 1	0
5	C	2	Total Ca 2 2	0
5	D	1	Total Ca 1 1	0
5	F	2	Total Ca 2 2	0
5	G	1	Total Ca 1 1	0
5	I	2	Total Ca 2 2	0
5	J	1	Total Ca 1 1	0
5	L	2	Total Ca 2 2	0

- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	G	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	J	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 7 is CAFFEINE (three-letter code: CFF) (formula: $C_8H_{10}N_4O_2$).



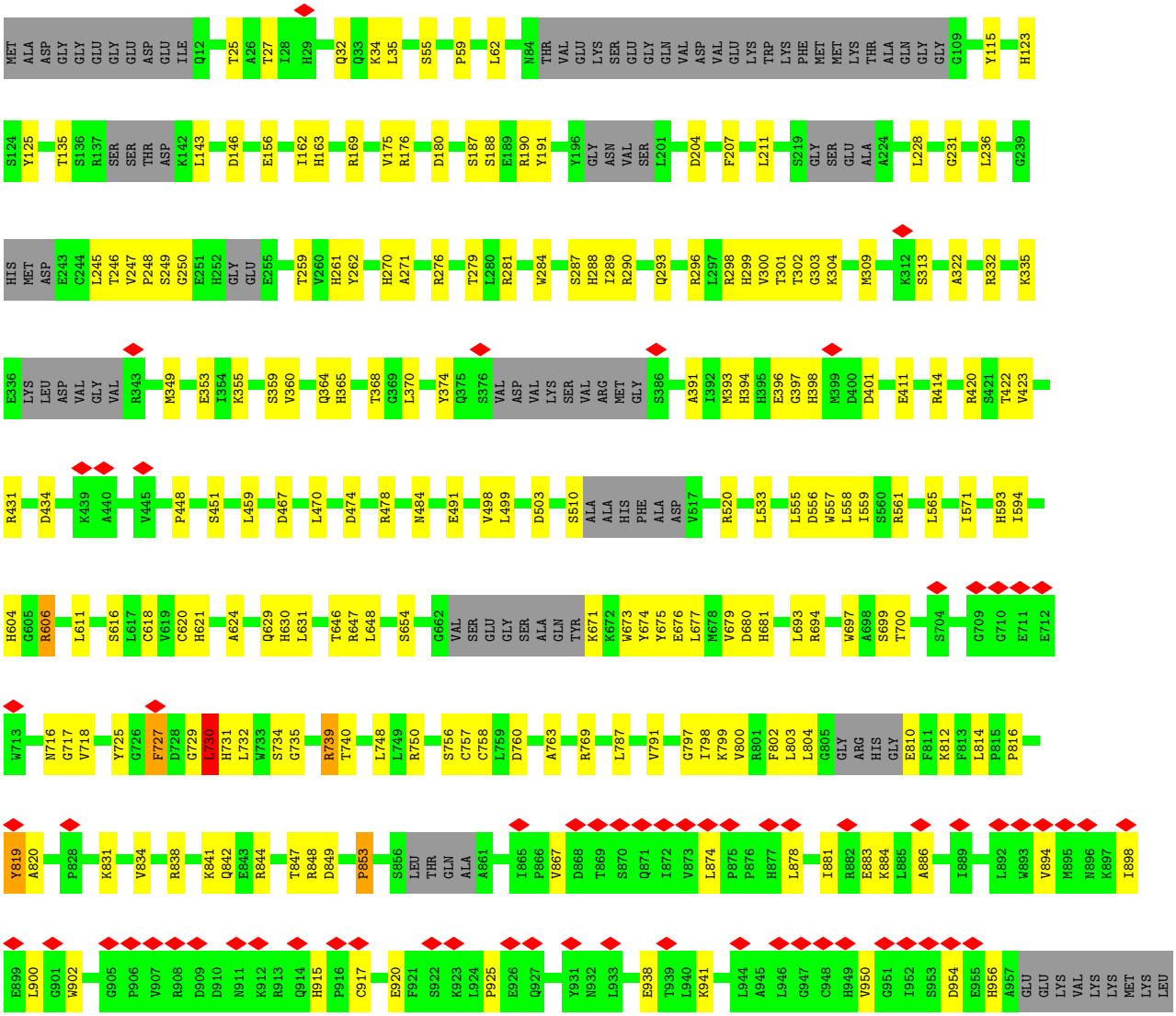
Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	N	O	0
			14	8	4	2	
7	D	1	Total	C	N	O	0
			14	8	4	2	
7	G	1	Total	C	N	O	0
			14	8	4	2	
7	J	1	Total	C	N	O	0
			14	8	4	2	

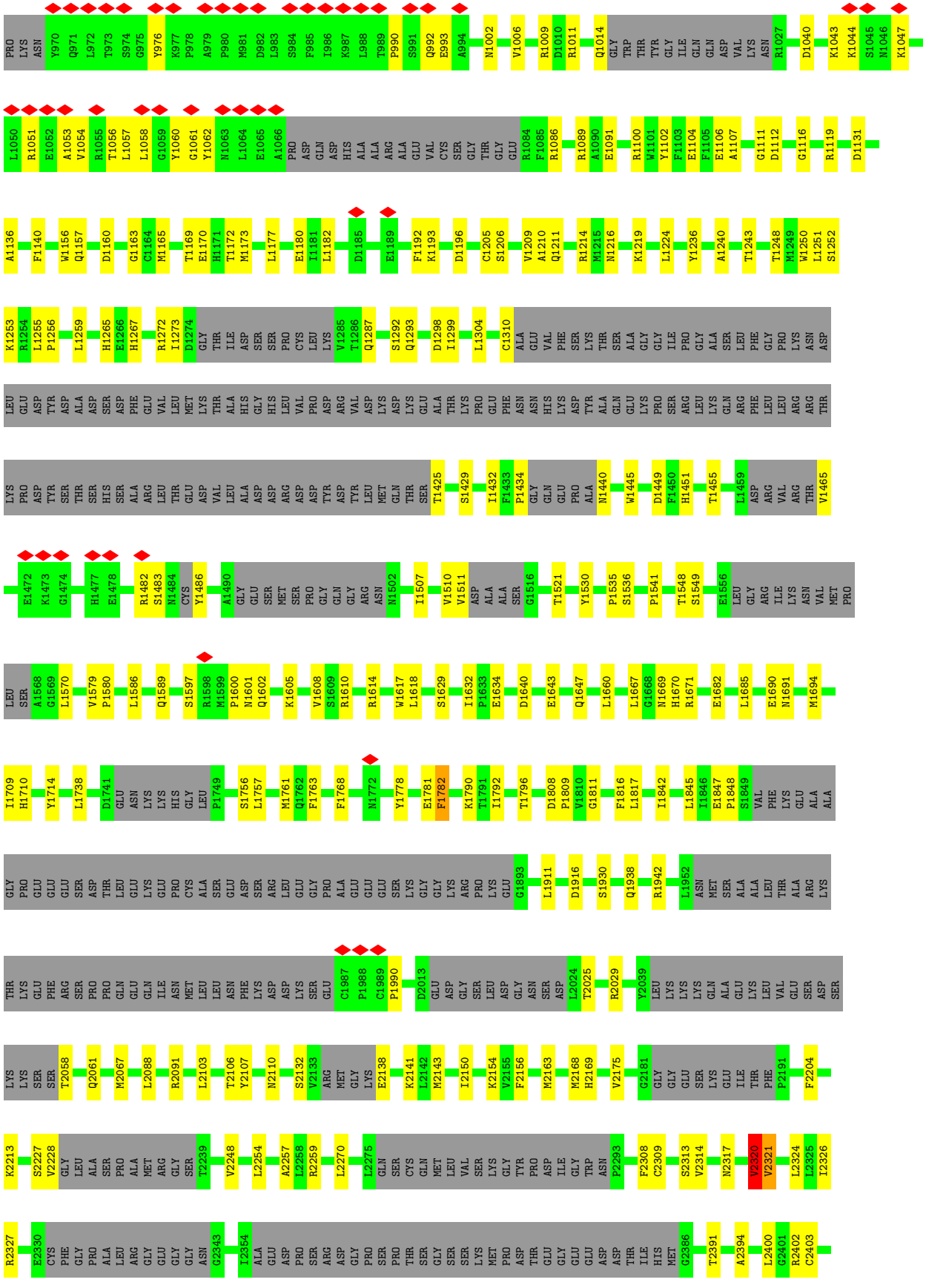
3 Residue-property plots (i)

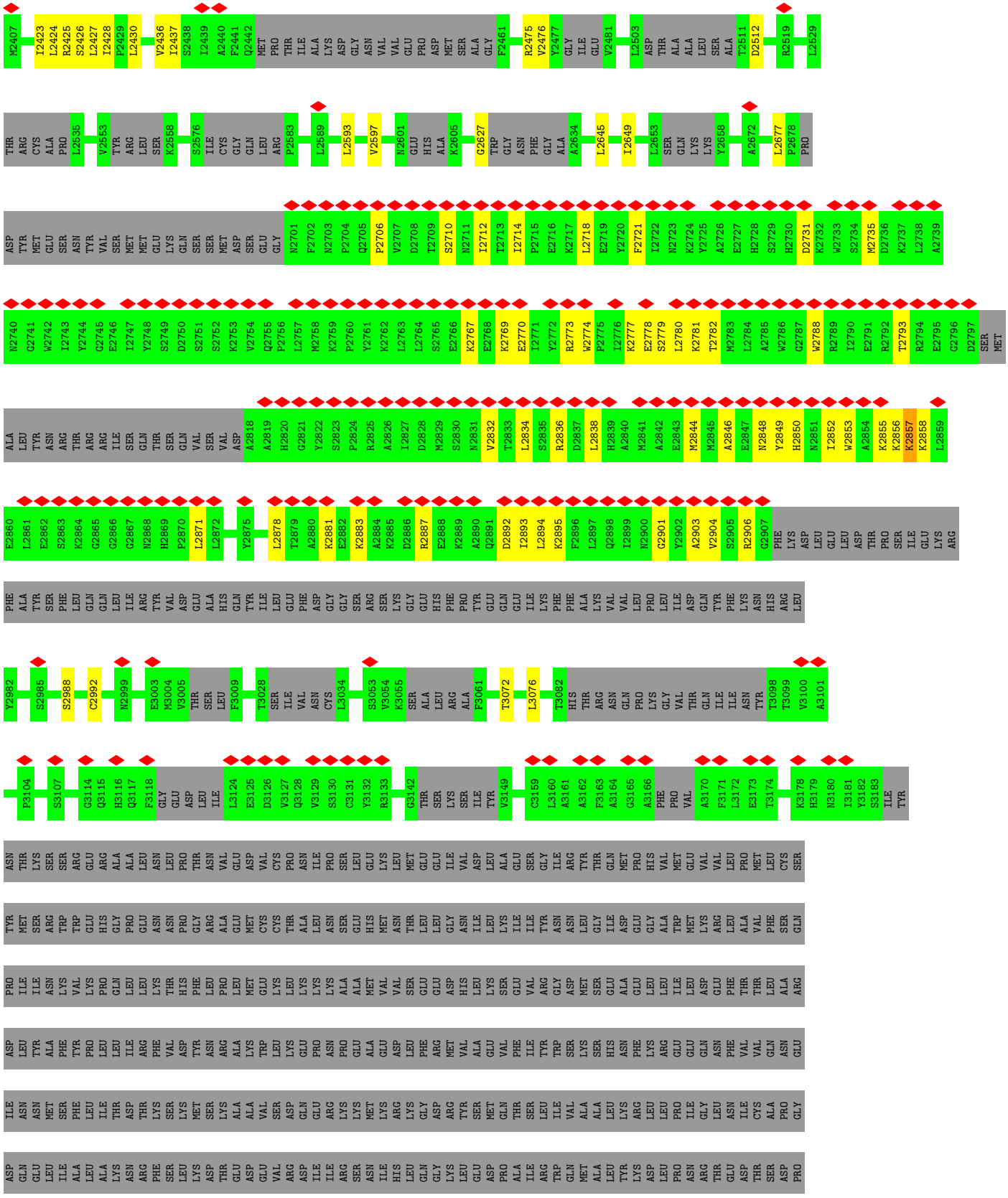
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

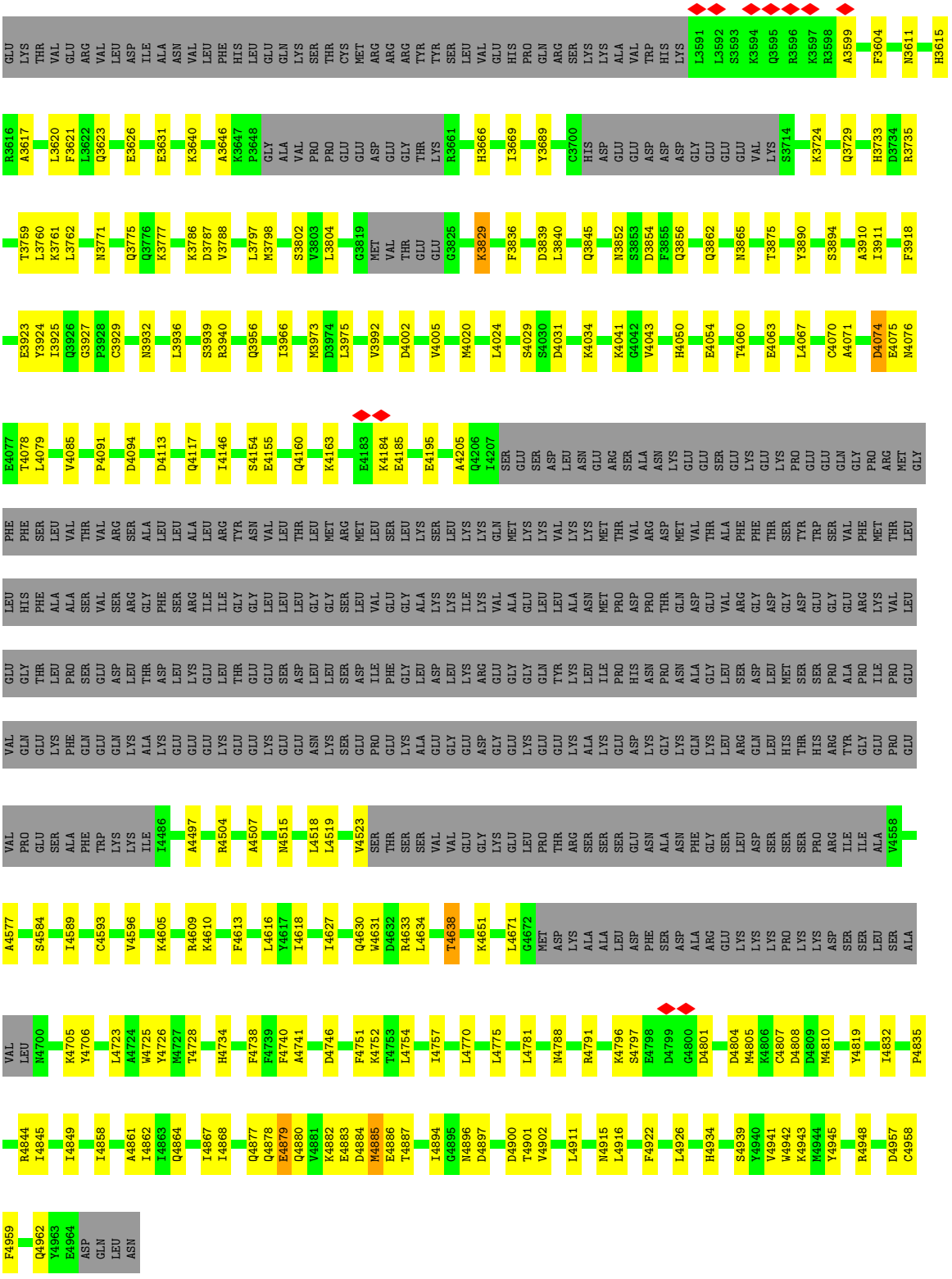
- Molecule 1: RyR2

Chain A:



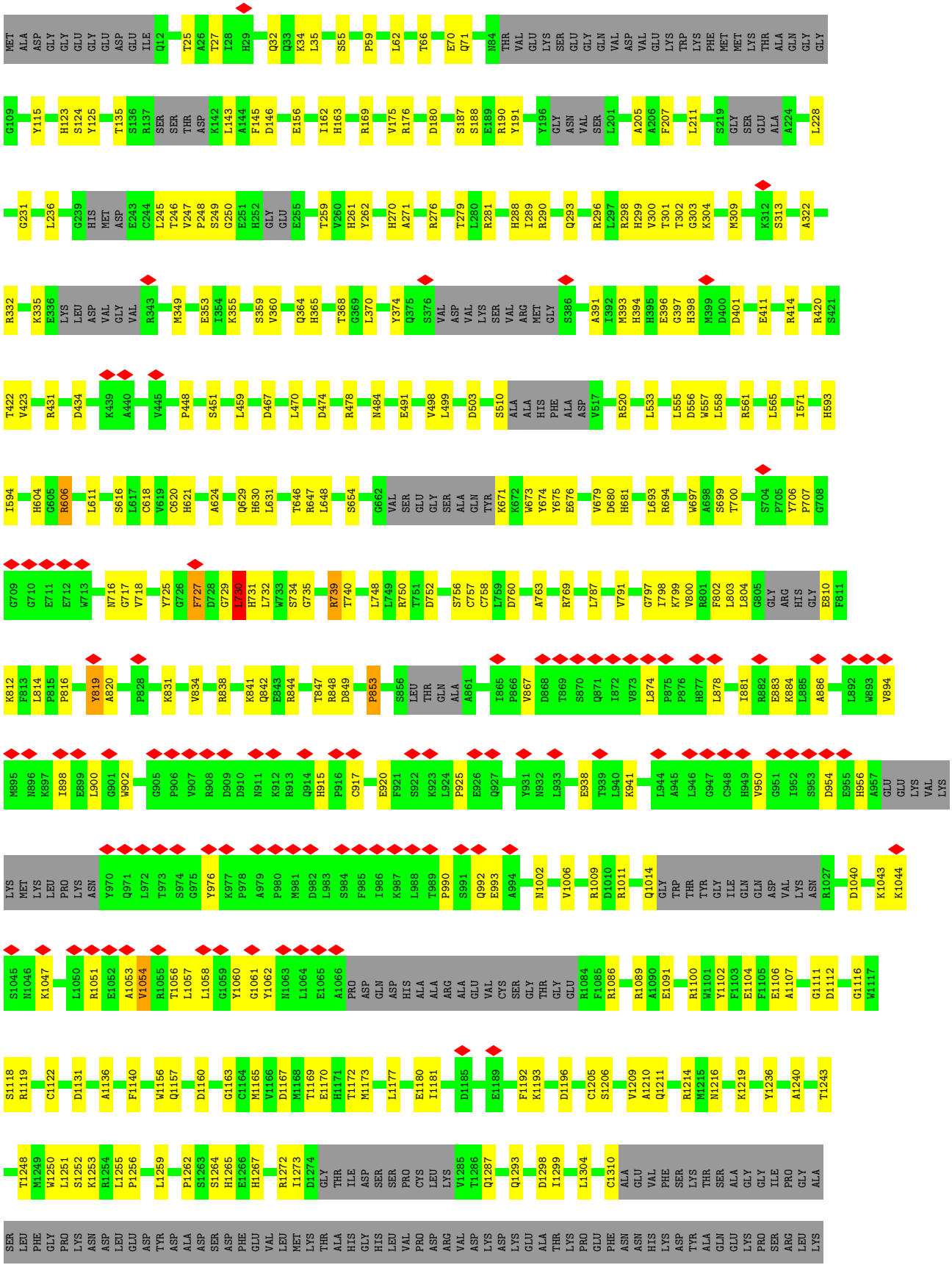


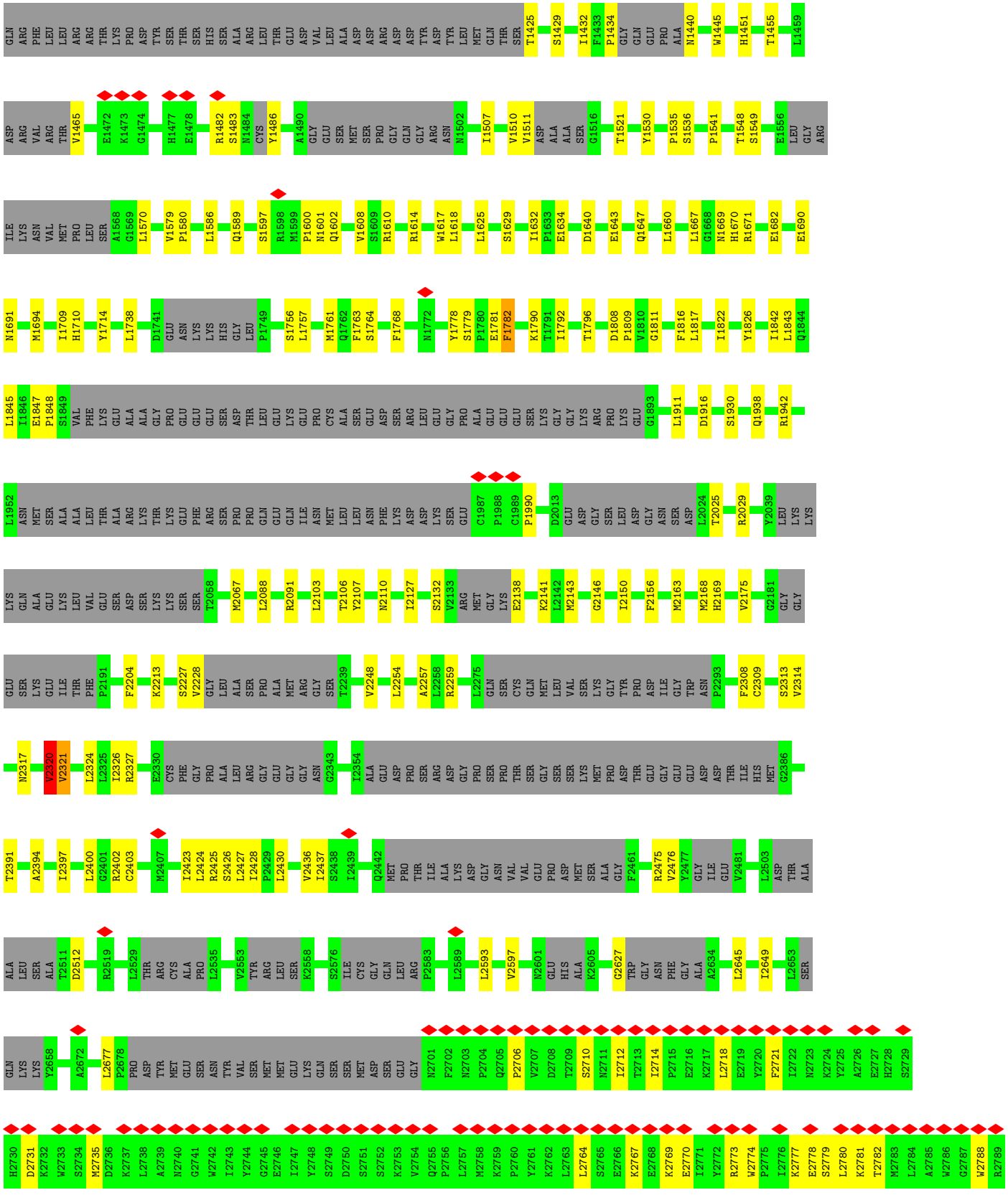


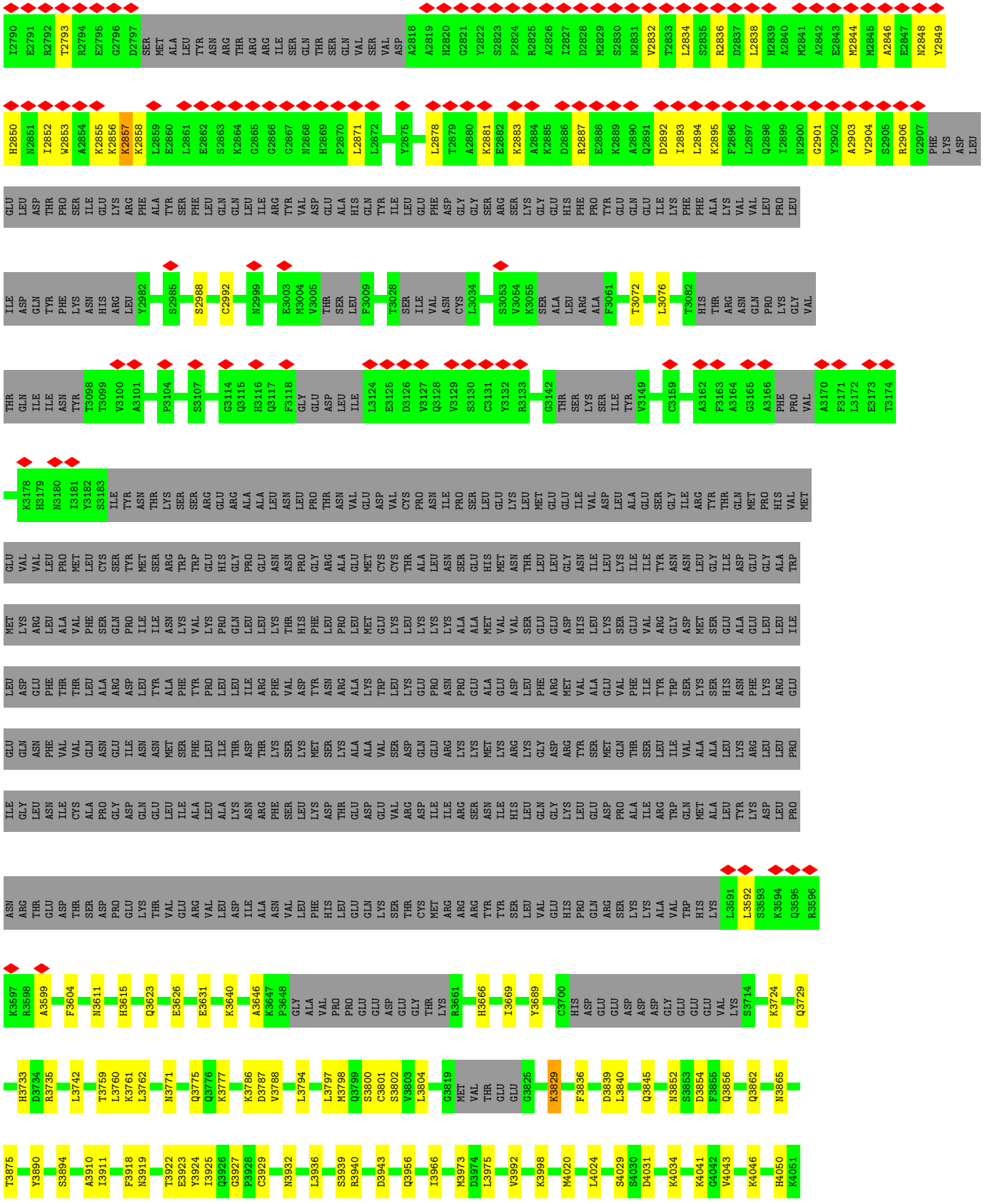


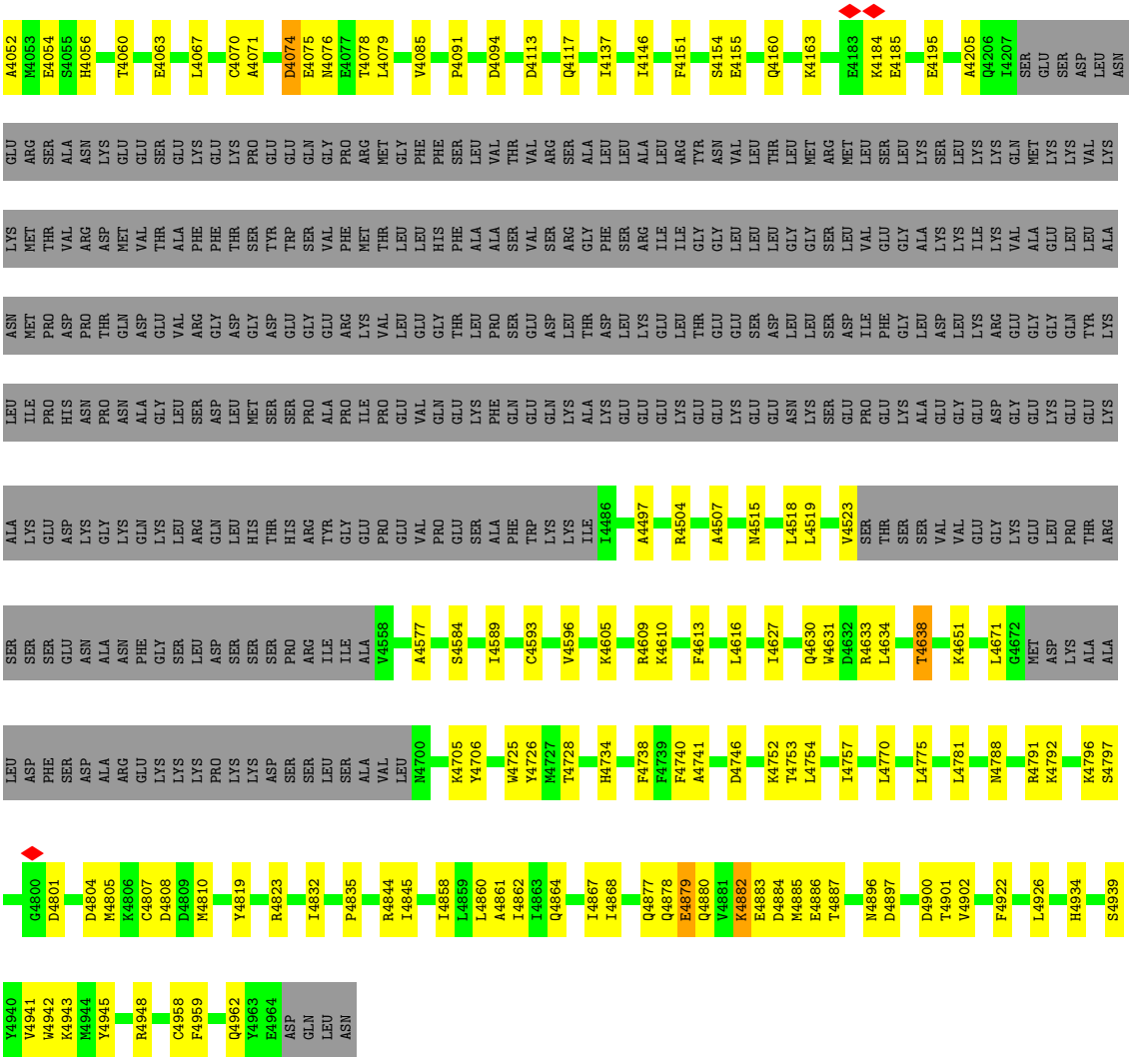
• Molecule 1: RyR2

Chain D:



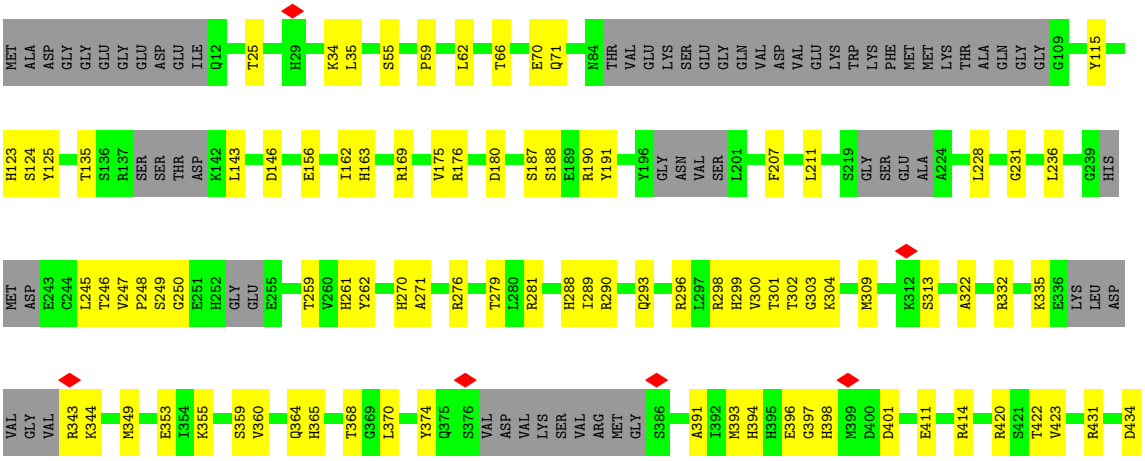


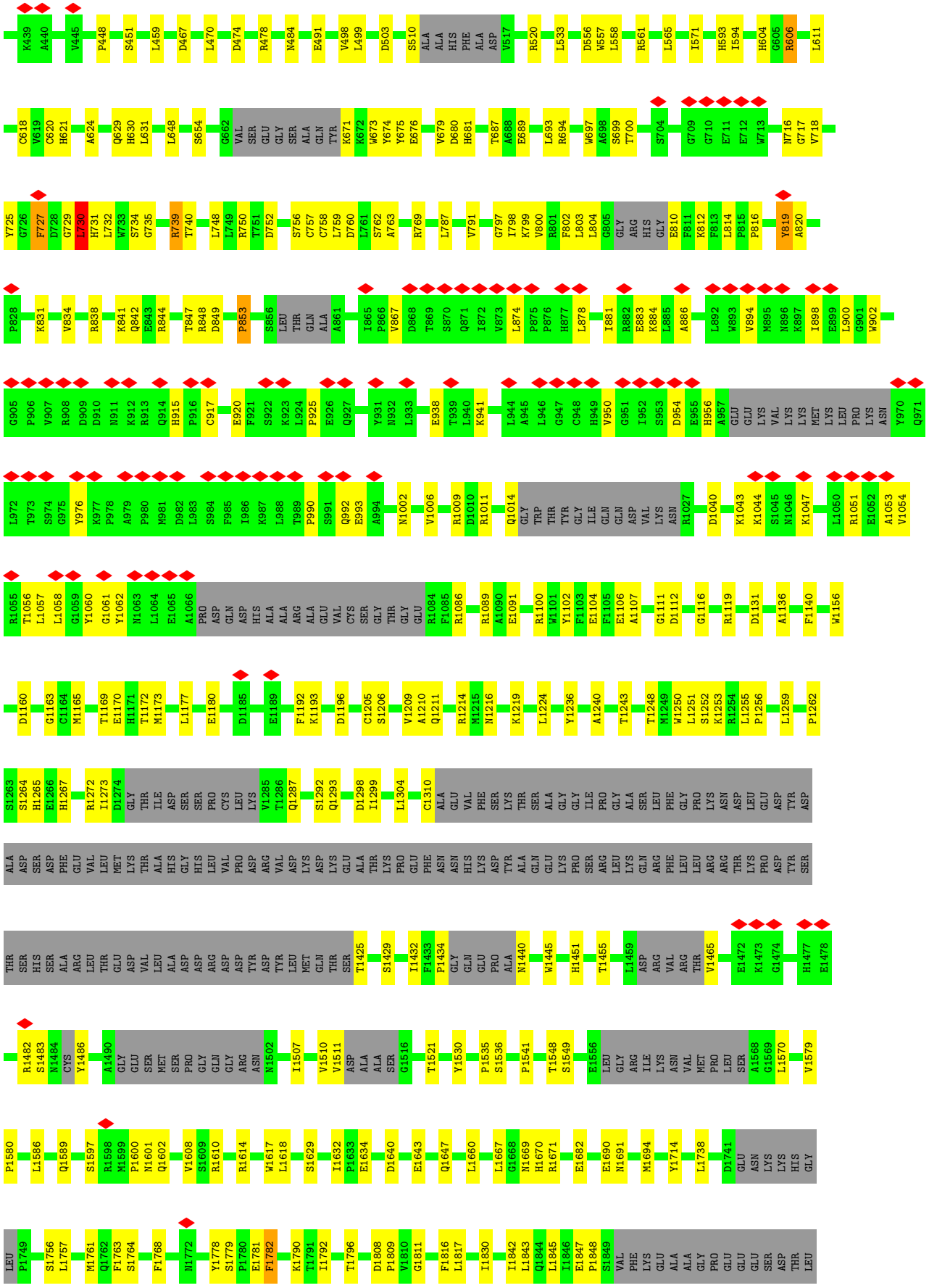

I2790 E2791 R2792 T2793 R2794 E2795 G2796 D2797 SER MET ALA LEU TYR ASN ARG THR ARG ARG ILE SER GLN THR SER GLN VAL SER VAL ASP A2818 A2819 H2820 G2821 Y2822 S2823 P2824 R2825 A2826 I2827 D2828 M2829 S2830 N2831 V2832 T2833 L2834 S2835 R2836 D2837 L2838 H2839 A2840 M2841 A2842 E2843 M2844 M2845 A2846 E2847 N2848 Y2849
H2850 N2851 I2852 W2853 A2854 K2855 K2856 K2857 K2858 L2859 E2860 L2861 E2862 S2863 K2864 G2865 G2866 G2867 N2868 H2869 P2870 L2871 L2872 Y2875 L2878 T2879 A2880 K2881 E2882 K2883 A2884 K2885 D2886 R2887 E2888 K2889 A2890 Q2891 D2892 I2893 L2894 K2895 F2896 L2897 Q2898 I2899 N2900 G2901 Y2902 A2903 V2904 S2905 R2906 G2907 PHE LYS ASP LEU
GLU LEU ASP THR PRO SER ILE GLU LYS ARG PHE ALA TYR SER PHE LEU GLN GLN LEU ILE ARG TYR VAL ASP GLU ALA HIS GLN TYR ILE LEU GLU PHE ASP GLY GLY SER ARG SER LYS GLY GLU HIS PHE PRO TYR GLU GLN GLU ILE LYS PHE PHE ALA LYS VAL VAL LEU PRO LEU
ILE ASP GLN TYR PHE LYS ASN HIS ARG LEU Y2982 S2985 S2988 C2992 N2999 E3003 M3004 V3005 THR SER LEU F3009 T3028 SER ILE VAL ASN CYS L3034 S3053 V3054 K3055 SER ALA LEU ARG ALA F3061 T3072 L3076 T3082 HIS THR ARG ASN GLN PRO LYS GLY VAL
THR GLN ILE ILE ASN TYR T3098 T3099 V3100 A3101 F3104 S3107 G3114 Q3115 H3116 Q3117 F3118 GLY GLU ASP LEU ILE L3124 E3125 D3126 V3127 Q3128 V3129 S3130 C3131 Y3132 R3133 G3142 THR SER LYS SER ILE TYR V3149 C3159 A3162 F3163 A3164 G3165 A3166 PHE PRO VAL A3170 F3171 L3172 E3173 T3174
K3178 H3179 N3180 I3181 Y3182 S3183 ILE TYR ASN THR LYS SER SER ARG GLU GLU ARG ALA ALA LEU ASN LEU PRO THR ASN VAL GLU ASP VAL CYS PRO ASN ILE PRO SER LEU GLU LYS LEU MET GLU GLU ILE VAL ASP LEU ALA GLU SER GLY ILE ARG TYR THR GLN MET PRO HIS VAL MET
GLU VAL VAL LEU PRO MET LEU CYS SER TYR MET SER ARG TRP TRP GLU HIS GLY PRO GLU ASN ASN PRO GLY ARG ALA GLU MET CYS CYS THR ALA LEU ASN SER GLU HIS MET ASN THR LEU LEU GLY ASN ILE LEU LYS ILE ILE TYR ASN ASN LEU GLY ILE ASP GLU GLY ALA TRP
MET LYS ARG LEU ALA VAL PHE SER GLN PRO ILE ILE ASN LYS VAL LYS PRO GLN LEU LEU LYS THR HIS PHE LEU PRO LEU MET GLU LYS LEU LYS LYS LYS ALA ALA MET VAL VAL SER GLU GLU GLU ASP HIS LEU LYS SER GLU VAL ARG GLY ASP MET SER GLU ALA GLU LEU LEU ILE
LEU ASP GLU PHE THR THR LEU ALA ARG ASP LEU TYR ALA PHE TYR PRO LEU LEU ILE ARG PHE VAL ASP TYR ASN ARG ALA ALA LYS TRP LEU LYS GLU PRO ASN PRO GLU ALA ALA GLU ASP LEU PHE ARG MET VAL ALA GLU VAL PHE ILE TYR TRP SER LYS SER HIS ASN PHE LYS ARG GLU
GLU GLN ASN PHE VAL VAL GLN ASN GLU ILE ASN ASN MET SER PHE LEU ILE THR ASP THR LYS SER LYS MET SER LYS ALA ALA VAL ASP SER GLN GLU ARG LYS LYS MET LYS ARG LYS GLY ASP MET GLN THR SER LEU ILE VAL ALA ALA LEU LYS ARG LEU LEU PRO
ILE GLY LEU ASN ILE CYS ALA PRO GLY ASP GLN GLU LEU ILE ALA LEU ALA LYS ASN ARG PHE SER LEU LYS ASP THR GLU ASP GLU VAL ARG ASP ILE ILE ARG SER ASN ILE HIS LEU GLN GLY LYS LEU GLU ASP PRO ALA ILE ARG TRP GLN MET ALA LEU TYR LYS ASP PRO
ASN ARG THR GLU ASP THR SER ASP PRO GLU LYS THR VAL GLU ARG VAL LEU ASP ILE ALA ASN VAL LEU PHE HIS LEU GLU GLN LYS SER THR CYS MET ARG ARG ARG TYR TYR SER LEU VAL GLU HIS PRO GLN ARG SER LYS LYS ALA VAL TRP HIS LYS L3591 L3592 S3593 K3594 Q3595 R3596
K3597 R3598 A3599 F3604 N3611 H3615 Q3623 E3626 E3631 K3640 A3646 K3647 P3648 GLY ALA VAL PRO PRO GLU GLU GLU ASP GLU GLY THR LYS R3661 H3666 I3669 Y3689 C3700 HIS ASP GLU GLU ASP ASP GLY GLU GLU GLU VAL LYS S3714 K3724 Q3729
H3733 R3734 R3735 L3742 T3759 L3760 K3761 L3762 N3771 Q3775 Q3776 K3777 K3786 D3787 V3788 L3794 L3797 M3798 Q3799 S3800 C3801 S3802 V3803 L3804 G3819 MET VAL THR GLU GLU G3825 K3829 F3836 D3839 L3840 Q3845 N3852 S3853 D3854 F3855 Q3856 Q3862 N3865
T3875 Y3890 S3894 A3910 I3911 F3918 N3919 T3922 E3923 Y3924 I3925 Q3926 G3927 P3928 C3929 N3932 L3936 S3939 R3940 D3943 Q3956 I3966 M3973 D3974 L3975 V3992 K3998 M4020 L4024 S4029 S4030 D4031 K4034 K4041 G4042 V4043 K4046 H4050 K4051

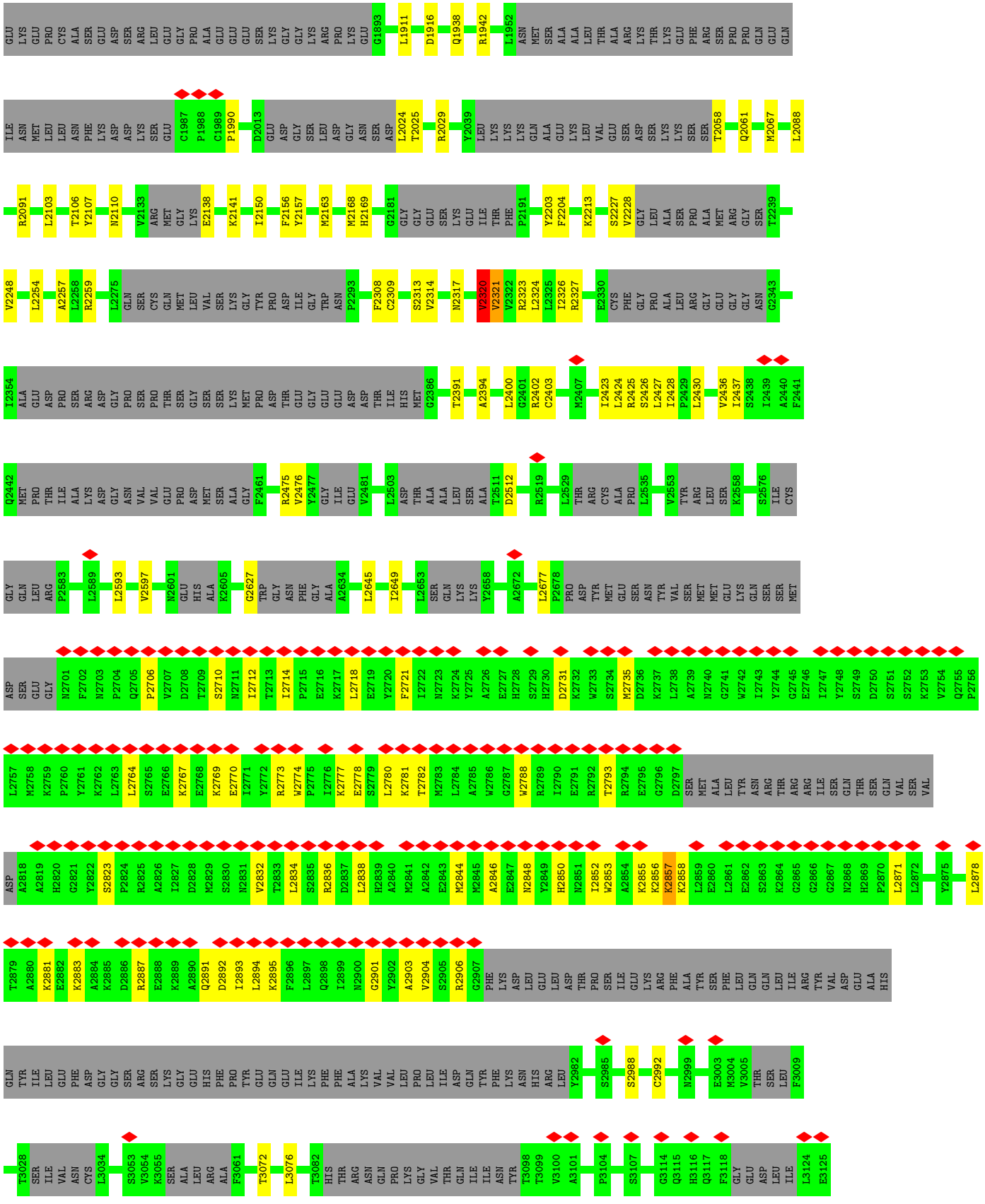


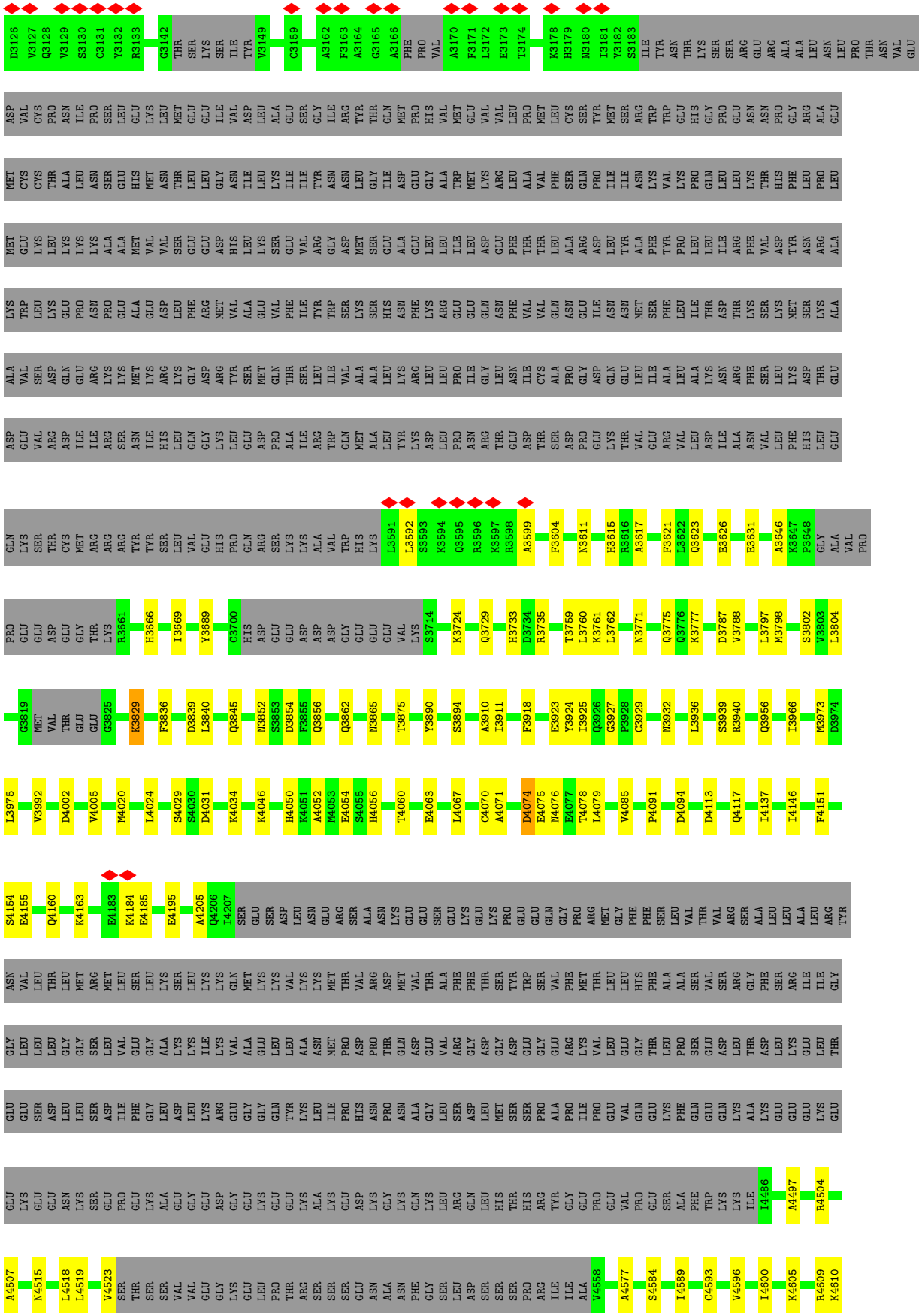
• Molecule 1: RyR2

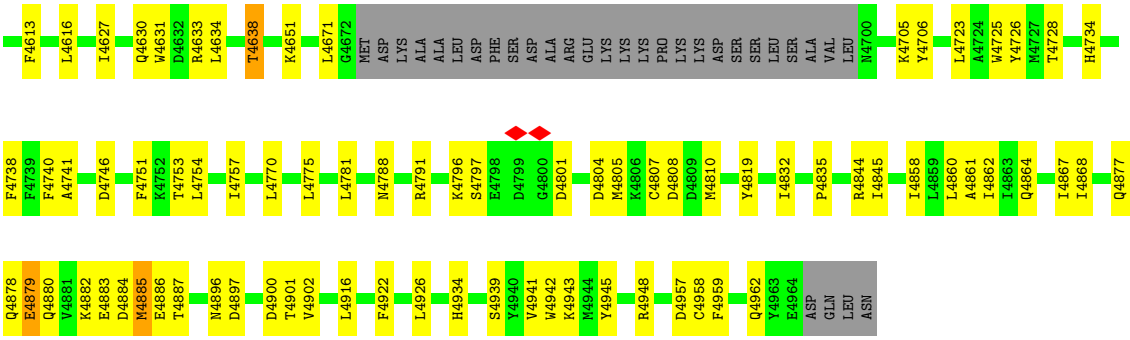
Chain G:

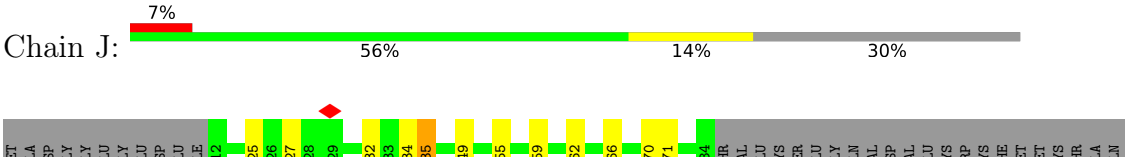



K439 A440 V445 P448 S451 L459 D467 L470 D474 R478 N484 E491 V498 L499 D503 S510 ALA ALA HIS PHE ALA ASP V517 R520 L533 D556 W557 L558 R561 L565 I571 H593 I594 H604 G605 R606 L611
C618 V619 C620 H621 A624 Q629 H630 L631 L648 S654 G662 VAL SER GLU GLY SER ALA GLN TYR K671 K672 W673 Y674 Y675 E676 V679 D680 H681 T687 A688 E689 L693 R694 W697 A698 S699 T700 S704 G709 G710 E711 E712 W713 N716 G717 V718
Y725 G726 F727 D728 G729 L730 H731 L732 W733 S734 G735 R739 T740 L748 L749 R750 T751 D752 S756 C757 C758 L759 D760 L761 S762 A763 R769 L787 V791 G797 I798 K799 V800 R801 F802 L803 L804 G805 GLY ARG HIS GLY E810 F811 K812 F813 L814 P815 P816 Y819 A820
P828 K831 V834 R838 K841 Q842 E843 R844 T847 R848 D849 P853 S856 LEU THR GLN ALA A861 I865 P866 V867 D868 T869 S870 Q871 I872 V873 L874 P875 P876 H877 L878 I881 R882 E883 K884 L885 A886 L892 W893 V894 M895 N896 K897 I898 E899 L900 G901 W902
G905 P906 V907 R908 D909 D910 N911 K912 R913 Q914 H915 P916 C917 E920 F921 S922 K923 L924 P925 E926 Q927 Y931 N932 L933 E938 T939 L940 K941 L944 A945 L946 G947 C948 H949 V950 G951 I952 S953 D954 E955 H956 A957 GLU GLU LYS VAL LYS LYS MET LYS LEU PRO LYS ASN Y970 Q971
L972 T973 S974 G975 Y976 K977 P978 A979 P980 M981 D982 L983 S984 F985 I986 K987 L988 T989 P990 S991 Q992 E993 A994 N1002 V1006 R1009 D1010 R1011 Q1014 GLY TRP THR TYR GLY ILE GLN GLN ASP VAL LYS ASN R1027 D1040 K1043 K1044 S1045 N1046 K1047 L1050 R1051 E1052 A1053 V1054
R1055 T1056 L1057 L1058 G1059 Y1060 G1061 Y1062 N1063 L1064 E1065 A1066 PRO ASP GLN ASP HIS ALA ALA ARG ALA GLU VAL CYS SER GLY THR GLY GLU R1084 F1085 R1086 R1089 A1090 E1091 R1100 W1101 Y1102 F1103 E1104 F1105 E1106 A1107 G1111 D1112 G1116 R1119 D1131 A1136 F1140 W1156
D1160 G1163 C1164 M1165 T1169 E1170 H1171 T1172 M1173 L1177 E1180 D1185 E1189 F1192 K1193 D1196 C1205 S1206 V1209 A1210 Q1211 R1214 M1215 N1216 K1219 L1224 Y1236 A1240 T1243 T1248 M1249 W1250 L1251 S1252 K1253 R1254 L1255 P1256 L1259 P1262
S1263 S1264 H1265 E1266 H1267 R1272 I1273 D1274 GLY THR ILE ASP SER SER PRO CYS LEU LYS V1285 T1286 Q1287 S1292 Q1293 D1298 I1299 L1304 C1310 ALA GLU VAL PHE SER LYS THR SER ALA GLY GLY ILE PRO GLY ALA SER LEU PHE GLY PRO LYS ASN ASP LEU GLU ASP TYR ASP
ALA ASP SER ASP PHE GLU VAL LEU MET LYS THR ALA HIS GLY HIS LEU VAL PRO ASP ARG VAL ASP LYS ASP LYS GLU ALA THR LYS PRO GLU PHE ASN ASN HIS LYS ASP TYR ALA GLN GLU LYS PRO SER ARG LEU LEU LYS GLN ARG PHE LEU LEU ARG ARG THR LYS PRO ASP TYR SER
THR SER HIS SER ALA ARG LEU THR GLU ASP VAL LEU ALA ASP ASP ARG ASP ASP TYR ASP TYR LEU MET GLN THR SER T1425 S1429 I1432 F1433 P1434 GLY GLN GLU PRO ALA N1440 W1445 H1451 T1455 L1459 ASP ARG VAL ARG THR V1465 E1472 K1473 G1474 H1477 E1478
R1482 S1483 N1484 CYS Y1486 A1490 GLY GLU SER MET SER PRO GLY GLN GLY ARG ASN N1502 I1507 V1510 V1511 ASP ALA ALA SER G1516 T1521 Y1530 P1535 S1536 P1541 T1548 S1549 E1556 LEU GLY ARG ILE LYS ASN VAL MET PRO LEU SER A1568 G1569 L1570 V1579
P1580 L1586 Q1589 S1597 R1598 M1599 P1600 N1601 Q1602 V1608 S1609 R1610 R1614 W1617 L1618 S1629 I1632 P1633 E1634 D1640 E1643 Q1647 L1660 L1667 G1668 N1669 H1670 R1671 E1682 E1690 N1691 M1694 Y1714 L1738 D1741 GLU ASN LYS LYS HIS GLY
LEU P1749 S1756 L1757 M1761 Q1762 F1763 S1764 F1768 M1772 Y1778 S1779 P1780 E1781 F1782 K1790 T1791 I1792 T1796 D1808 P1809 V1810 G1811 F1816 L1817 I1830 I1842 L1843 Q1844 L1845 I1846 E1847 P1848 S1849 VAL PHE LYS GLU ALA ALA GLY PRO GLU GLU GLU SER ASP THR LEU



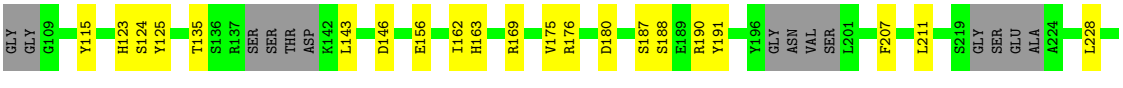


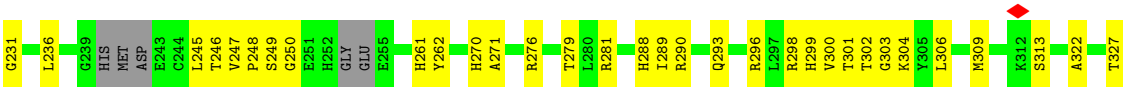


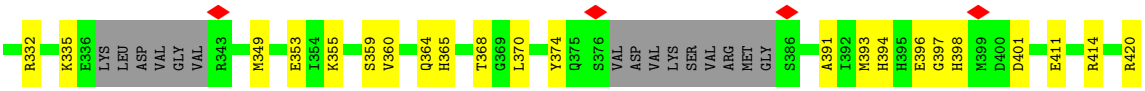


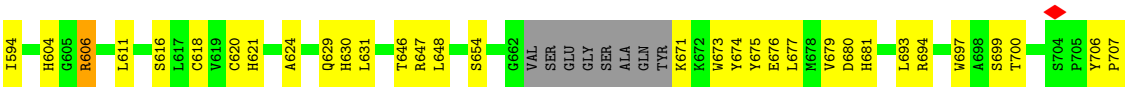
• Molecule 1: RyR2

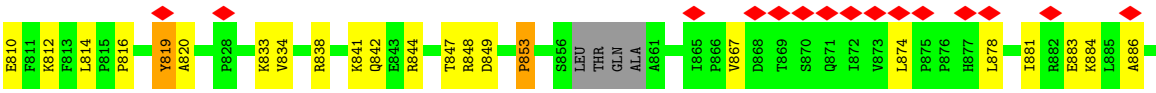
Chain J:

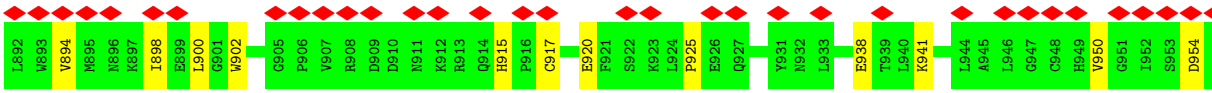


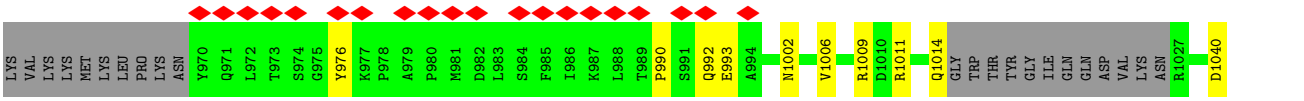


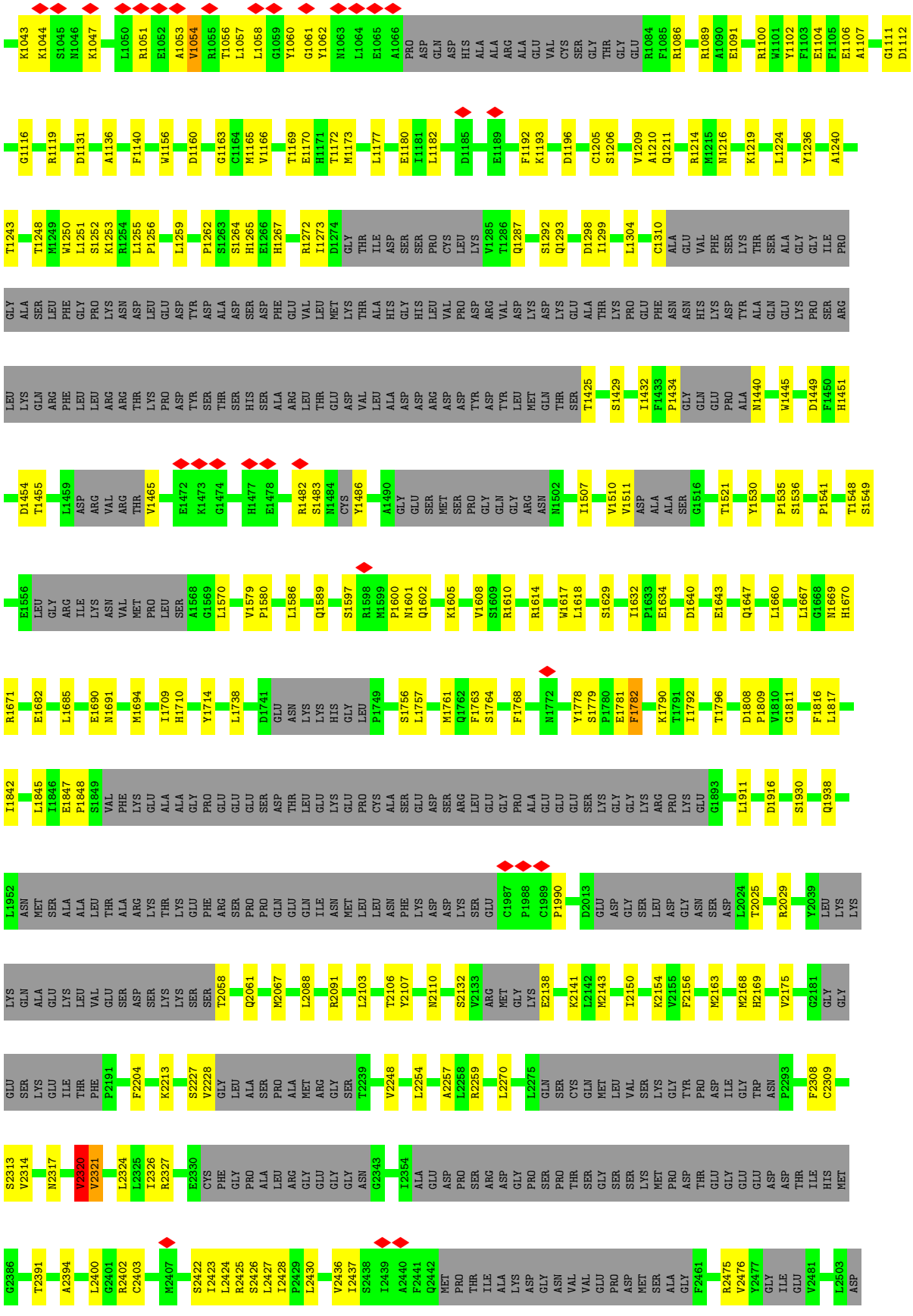


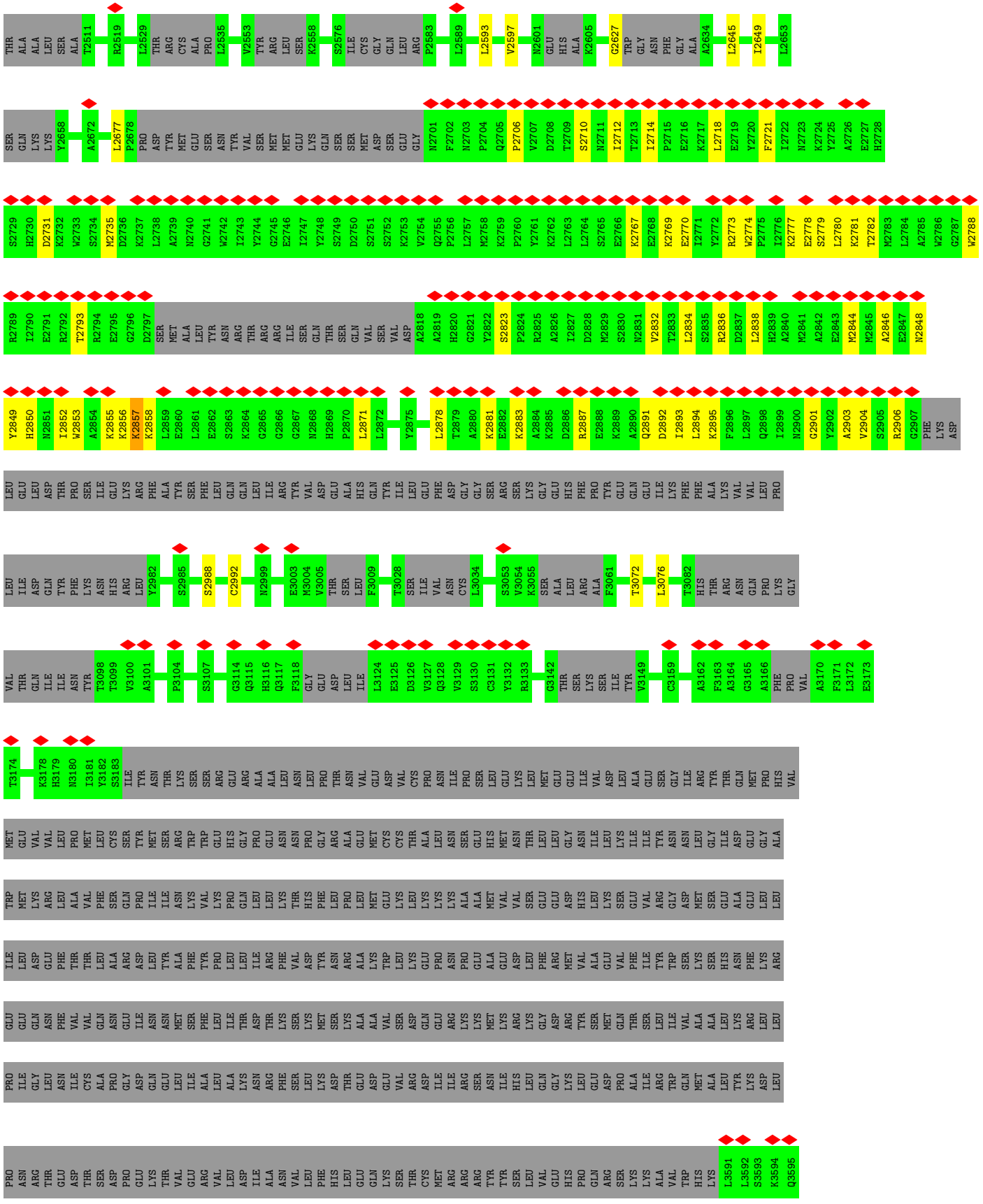


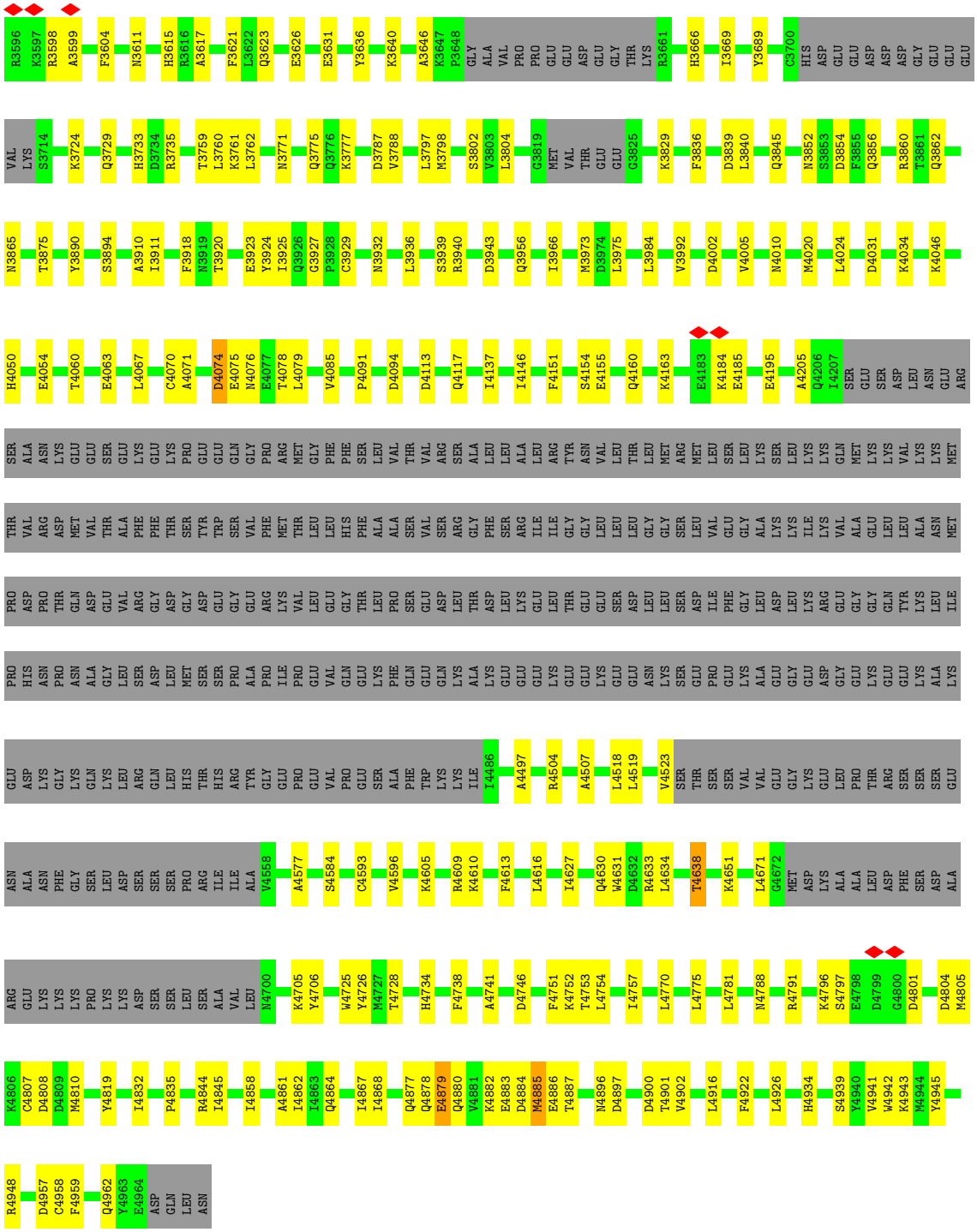






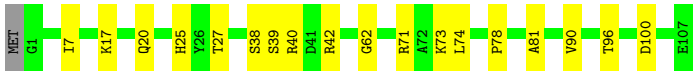



THR ALA ALA LEU SER ALA T2511 R2519 L2529 THR ARG CYS ALA PRO L2535 V2553 TYR ARG LEU SER K2558 S2576 ILE CYS GLY GLN LEU ARG P2583 L2589 L2593 V2597 N2601 GLU HIS ALA K2605 G2627 TRP GLY ASN PHE GLY ALA A2634 L2645 I2649 L2653
SER GLN LYS LYS Y2668 A2672 L2677 P2678 PRO ASP TYR MET GLU SER ASN TYR VAL SER MET MET GLU LYS GLN SER SER MET ASP SER GLU GLY N2701 F2702 N2703 P2704 Q2705 P2706 V2707 D2708 T2709 S2710 N2711 I2712 T2713 I2714 P2715 E2716 K2717 L2718 E2719 Y2720 F2721 I2722 N2723 K2724 Y2725 A2726 E2727 H2728
S2729 H2730 D2731 K2732 W2733 S2734 M2735 D2736 K2737 L2738 A2739 N2740 G2741 W2742 I2743 Y2744 G2745 E2746 I2747 Y2748 S2749 D2750 S2751 S2752 K2753 V2754 Q2755 P2756 L2757 M2758 K2759 P2760 Y2761 K2762 L2763 L2764 S2765 E2766 K2767 E2768 K2769 E2770 I2771 Y2772 R2773 W2774 P2775 I2776 K2777 E2778 S2779 L2780 K2781 T2782 M2783 L2784 A2785 W2786 G2787 W2788
R2789 I2790 E2791 R2792 T2793 R2794 E2795 G2796 D2797 SER MET ALA LEU TYR ASN ARG THR ARG ARG ILE SER GLN THR SER GLN VAL SER VAL ASP A2818 A2819 H2820 G2821 Y2822 S2823 P2824 R2825 A2826 I2827 D2828 M2829 S2830 N2831 V2832 T2833 L2834 S2835 R2836 D2837 L2838 H2839 A2840 M2841 A2842 E2843 M2844 M2845 A2846 E2847 N2848
Y2849 H2850 N2851 I2852 W2853 A2854 K2855 K2856 K2857 K2858 L2859 E2860 L2861 E2862 S2863 K2864 G2865 G2866 G2867 N2868 H2869 P2870 L2871 L2872 Y2875 L2878 T2879 A2880 K2881 E2882 K2883 A2884 K2885 D2886 R2887 E2888 K2889 A2890 Q2891 D2892 I2893 L2894 K2895 F2896 L2897 Q2898 I2899 N2900 G2901 Y2902 A2903 V2904 S2905 R2906 G2907 PHE LYS ASP
LEU GLU LEU ASP THR PRO SER ILE GLU LYS ARG PHE ALA TYR SER PHE LEU GLN GLN LEU ILE ARG TYR VAL ASP GLU ALA HIS GLN TYR ILE LEU GLU PHE ASP GLY GLY SER ARG SER LYS GLY GLU HIS PHE PRO TYR GLU GLN GLN GLU ILE LYS PHE PHE ALA LYS VAL VAL LEU PRO
LEU ILE ASP GLN TYR PHE LYS ASN HIS ARG LEU Y2982 S2985 S2988 C2992 N2999 E3003 M3004 V3005 THR SER LEU F3009 T3028 SER ILE VAL ASN CYS L3034 S3053 V3054 K3055 SER ALA LEU ARG ALA F3061 T3072 L3076 T3082 HIS THR ARG ASN GLN PRO LYS GLY
VAL THR GLN ILE ILE ASN TYR T3098 T3099 V3100 A3101 P3104 S3107 G3114 Q3115 H3116 Q3117 F3118 GLY GLU ASP LEU ILE L3124 E3125 D3126 V3127 Q3128 V3129 S3130 C3131 Y3132 R3133 G3142 THR SER LYS SER ILE TYR V3149 C3159 A3162 F3163 A3164 G3165 A3166 PHE PRO VAL A3170 F3171 L3172 E3173
T3174 K3178 H3179 N3180 I3181 Y3182 S3183 ILE TYR ASN THR LYS SER SER ARG GLU ARG ALA ALA LEU ASN LEU PRO THR ASN VAL GLU GLU ASP VAL CYS PRO ASN ILE PRO SER LEU GLU LYS LEU MET GLU GLU ILE VAL ASP LEU ALA GLU SER GLY ILE ARG TYR THR GLN MET PRO HIS VAL
MET GLU VAL VAL LEU PRO MET LEU CYS SER TYR MET SER ARG TRP TRP GLU HIS GLY PRO GLU ASN ASN PRO GLY ARG ALA ALA GLU MET CYS CYS THR ALA LEU ASN SER GLU HIS MET ASN THR LEU LEU GLY ASN ILE LEU LYS ILE ILE TYR ASN ASN LEU GLY ILE ASP GLU GLY ALA
TRP MET LYS ARG LEU ALA VAL PHE SER GLN PRO ILE ILE ASN LYS VAL LYS PRO GLN LEU LEU LYS THR HIS PHE LEU PRO LEU MET GLU LYS LEU LYS LYS LYS ALA ALA MET VAL VAL SER GLU GLU ASP HIS LEU LYS SER GLU VAL ARG GLY ASP MET SER GLU ALA GLU LEU LEU
ILE LEU ASP GLU PHE THR THR LEU ALA ARG ASP LEU TYR ALA PHE TYR PRO LEU LEU ILE ARG PHE VAL ASP TYR ASN ARG ALA ALA LYS TRP LEU LYS GLU PRO ASN PRO GLU ALA GLU ASP LEU PHE ARG MET VAL ALA GLU VAL PHE ILE TYR TRP SER LYS SER LEU ARG LYS
GLU GLU GLN ASN PHE VAL VAL GLN ASN GLU ILE ASN ASN MET SER PHE LEU ILE THR ASP THR LYS SER LYS MET SER LYS ALA ALA VAL SER ASP GLN GLU ARG LYS LYS MET LYS ARG LYS GLY ASP ARG TYR SER MET GLN THR SER LEU ILE VAL ALA ALA LEU LYS LYS ARG LEU LEU
PRO ILE GLY LEU ASN ILE CYS ALA PRO GLY ASP GLN GLU LEU ILE ALA LEU ALA LYS ASN ARG PHE SER LEU LYS ASP THR GLU ASP GLU VAL ARG ASP ILE ILE ARG SER ASN ILE HIS LEU GLN GLY LYS LEU GLU ASP PRO ALA ILE ARG TRP GLN MET ALA LEU TYR LYS ASP LEU
PRO ASN ARG THR GLU ASP PRO GLU LYS THR VAL GLU ARG VAL LEU ASP ILE ALA ASN VAL LEU PHE HIS LEU GLU GLN LYS SER THR CYS MET ARG ARG ARG TYR TYR SER LEU VAL GLU HIS PRO GLN ARG SER LYS LYS ALA VAL TRP HIS LYS L3591 L3592 S3593 K3594 Q3595



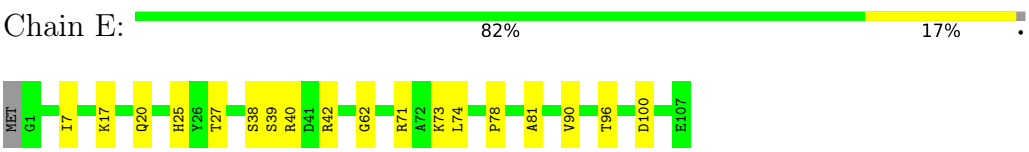
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain B:



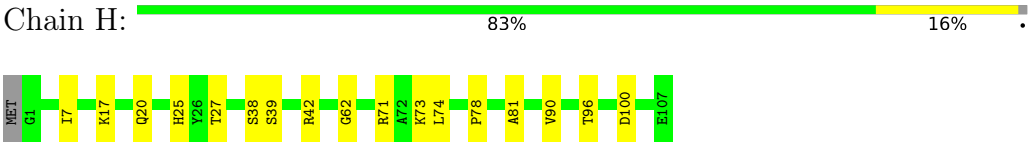
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain E:



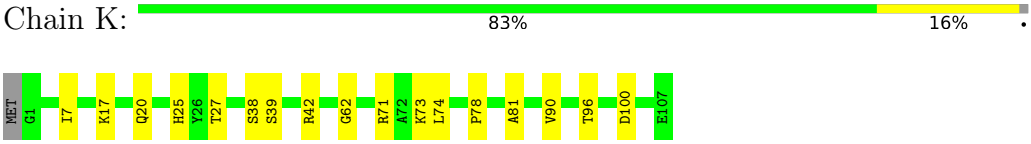
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H:



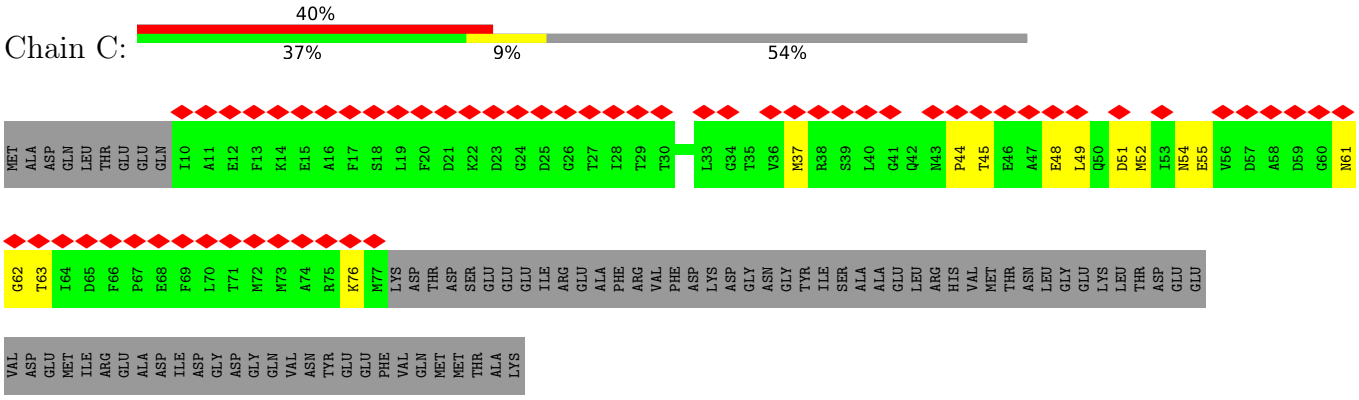
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain K:



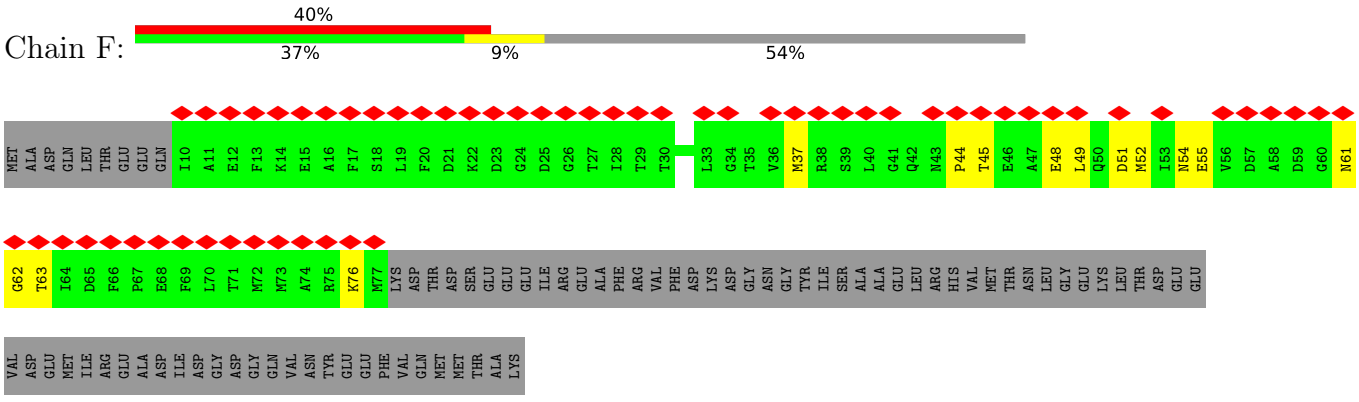
• Molecule 3: Calmodulin-1

Chain C:



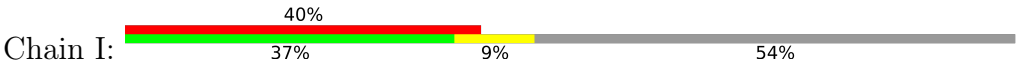
• Molecule 3: Calmodulin-1

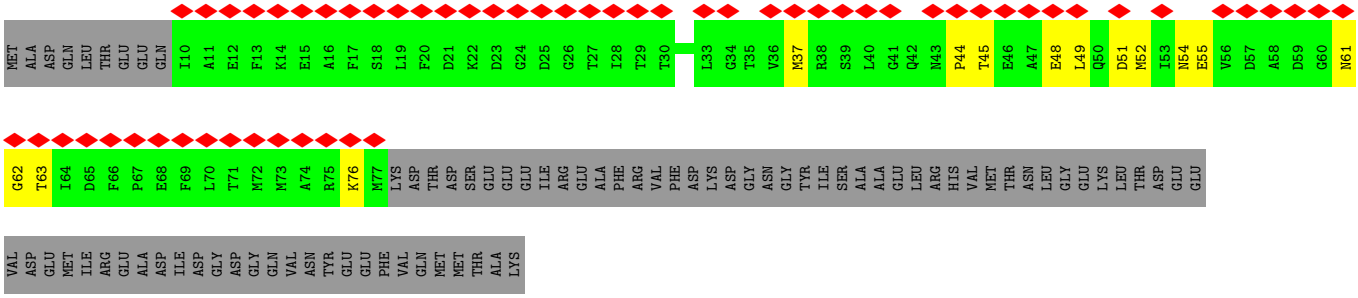
Chain F:



• Molecule 3: Calmodulin-1

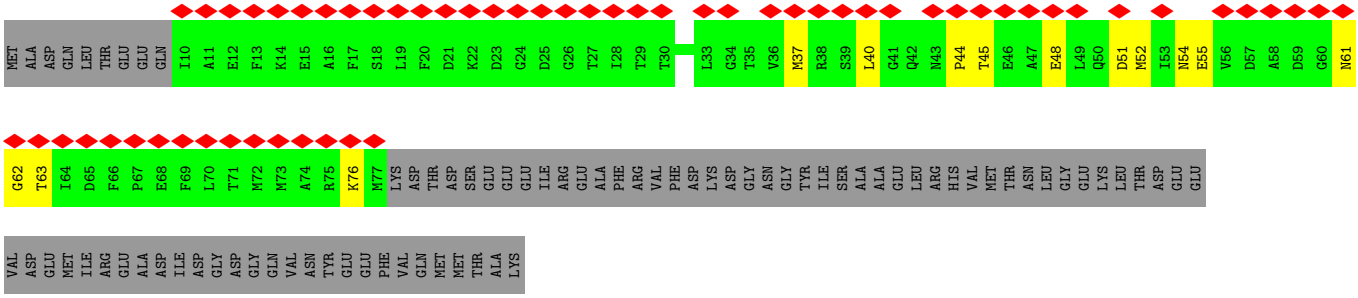
Chain I:





- Molecule 3: Calmodulin-1

Chain L:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	154111	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.182	Depositor
Minimum map value	-0.093	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.021	Depositor
Map size (Å)	436.4, 436.4, 436.4	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.091, 1.091, 1.091	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CFF, CA, ATP, 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	0.47	0/27151	0.60	7/36715 (0.0%)
1	D	0.47	0/27151	0.60	7/36715 (0.0%)
1	G	0.47	0/27151	0.60	7/36715 (0.0%)
1	J	0.47	0/27151	0.60	7/36715 (0.0%)
2	B	0.39	0/835	0.56	0/1123
2	E	0.39	0/835	0.56	0/1123
2	H	0.39	0/835	0.56	0/1123
2	K	0.39	0/835	0.56	0/1123
3	C	0.29	0/530	0.54	0/711
3	F	0.29	0/530	0.54	0/711
3	I	0.29	0/530	0.54	0/711
3	L	0.29	0/530	0.54	0/711
All	All	0.46	0/114064	0.60	28/154196 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	17
1	D	0	17
1	G	0	17
1	J	0	17
All	All	0	68

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1608	VAL	CG1-CB-CG2	-6.65	100.26	110.90
1	D	1608	VAL	CG1-CB-CG2	-6.65	100.26	110.90
1	G	1608	VAL	CG1-CB-CG2	-6.65	100.26	110.90
1	J	1608	VAL	CG1-CB-CG2	-6.64	100.28	110.90
1	A	2403	CYS	C-N-CA	6.51	137.97	121.70
1	D	2403	CYS	C-N-CA	6.51	137.97	121.70
1	J	2403	CYS	C-N-CA	6.51	137.97	121.70
1	G	2403	CYS	C-N-CA	6.51	137.97	121.70
1	D	2430	LEU	CA-CB-CG	6.44	130.10	115.30
1	A	2430	LEU	CA-CB-CG	6.43	130.10	115.30
1	G	2430	LEU	CA-CB-CG	6.43	130.10	115.30
1	J	2430	LEU	CA-CB-CG	6.43	130.10	115.30
1	J	648	LEU	CA-CB-CG	5.86	128.78	115.30
1	A	648	LEU	CA-CB-CG	5.86	128.77	115.30
1	G	648	LEU	CA-CB-CG	5.86	128.77	115.30
1	D	648	LEU	CA-CB-CG	5.84	128.74	115.30
1	A	1738	LEU	CA-CB-CG	5.78	128.60	115.30
1	D	1738	LEU	CA-CB-CG	5.78	128.60	115.30
1	G	1738	LEU	CA-CB-CG	5.78	128.60	115.30
1	J	1738	LEU	CA-CB-CG	5.78	128.60	115.30
1	J	730	LEU	CA-CB-CG	5.51	127.98	115.30
1	A	730	LEU	CA-CB-CG	5.50	127.95	115.30
1	D	730	LEU	CA-CB-CG	5.50	127.95	115.30
1	G	730	LEU	CA-CB-CG	5.50	127.95	115.30
1	A	1259	LEU	CA-CB-CG	5.39	127.70	115.30
1	G	1259	LEU	CA-CB-CG	5.39	127.70	115.30
1	J	1259	LEU	CA-CB-CG	5.39	127.70	115.30
1	D	1259	LEU	CA-CB-CG	5.38	127.67	115.30

There are no chirality outliers.

All (68) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1570	LEU	Peptide
1	A	1579	VAL	Peptide
1	A	1808	ASP	Peptide
1	A	1847	GLU	Peptide
1	A	2248	VAL	Peptide
1	A	2320	VAL	Peptide
1	A	3802	SER	Peptide
1	A	3829	LYS	Peptide
1	A	3925	ILE	Peptide
1	A	4074	ASP	Peptide

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Mol	Chain	Res	Type	Group
1	A	4091	PRO	Peptide
1	A	4163	LYS	Peptide
1	A	729	GLY	Peptide
1	A	739	ARG	Peptide
1	A	816	PRO	Peptide
1	A	819	TYR	Peptide
1	A	838	ARG	Peptide
1	D	1570	LEU	Peptide
1	D	1579	VAL	Peptide
1	D	1808	ASP	Peptide
1	D	1847	GLU	Peptide
1	D	2248	VAL	Peptide
1	D	2320	VAL	Peptide
1	D	3802	SER	Peptide
1	D	3829	LYS	Peptide
1	D	3925	ILE	Peptide
1	D	4074	ASP	Peptide
1	D	4091	PRO	Peptide
1	D	4163	LYS	Peptide
1	D	729	GLY	Peptide
1	D	739	ARG	Peptide
1	D	816	PRO	Peptide
1	D	819	TYR	Peptide
1	D	838	ARG	Peptide
1	G	1570	LEU	Peptide
1	G	1579	VAL	Peptide
1	G	1808	ASP	Peptide
1	G	1847	GLU	Peptide
1	G	2248	VAL	Peptide
1	G	2320	VAL	Peptide
1	G	3802	SER	Peptide
1	G	3829	LYS	Peptide
1	G	3925	ILE	Peptide
1	G	4074	ASP	Peptide
1	G	4091	PRO	Peptide
1	G	4163	LYS	Peptide
1	G	729	GLY	Peptide
1	G	739	ARG	Peptide
1	G	816	PRO	Peptide
1	G	819	TYR	Peptide
1	G	838	ARG	Peptide
1	J	1570	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	J	1579	VAL	Peptide
1	J	1808	ASP	Peptide
1	J	1847	GLU	Peptide
1	J	2248	VAL	Peptide
1	J	2320	VAL	Peptide
1	J	3802	SER	Peptide
1	J	3829	LYS	Peptide
1	J	3925	ILE	Peptide
1	J	4074	ASP	Peptide
1	J	4091	PRO	Peptide
1	J	4163	LYS	Peptide
1	J	729	GLY	Peptide
1	J	739	ARG	Peptide
1	J	816	PRO	Peptide
1	J	819	TYR	Peptide
1	J	838	ARG	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	26650	0	25168	484	0
1	D	26650	0	25168	493	0
1	G	26650	0	25168	475	0
1	J	26650	0	25168	495	0
2	B	819	0	824	13	0
2	E	819	0	824	12	0
2	H	819	0	824	12	0
2	K	819	0	824	12	0
3	C	524	0	503	8	0
3	F	524	0	503	8	0
3	I	524	0	503	8	0
3	L	524	0	503	8	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
4	G	1	0	0	0	0
4	J	1	0	0	0	0
5	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	2	0	0	0	0
5	D	1	0	0	0	0
5	F	2	0	0	0	0
5	G	1	0	0	0	0
5	I	2	0	0	0	0
5	J	1	0	0	0	0
5	L	2	0	0	0	0
6	A	31	0	12	1	0
6	D	31	0	12	0	0
6	G	31	0	12	1	0
6	J	31	0	12	1	0
7	A	14	0	10	1	0
7	D	14	0	10	1	0
7	G	14	0	10	1	0
7	J	14	0	10	1	0
All	All	112168	0	106068	1842	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 8.

All (1842) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:143:LEU:HD22	1:J:2427:LEU:CB	1.57	1.34
1:A:2427:LEU:CB	1:J:143:LEU:HD22	1.56	1.33
1:A:143:LEU:HD22	1:D:2427:LEU:CB	1.58	1.33
1:D:143:LEU:HD22	1:G:2427:LEU:CB	1.55	1.33
1:A:2427:LEU:HB3	1:J:143:LEU:CD2	1.60	1.29
1:D:143:LEU:CD2	1:G:2427:LEU:HB3	1.60	1.29
1:A:143:LEU:CD2	1:D:2427:LEU:HB3	1.62	1.28
1:G:143:LEU:CD2	1:J:2427:LEU:HB3	1.61	1.27
1:D:4788:ASN:ND2	1:G:4738:PHE:HD2	1.42	1.17
1:A:4738:PHE:HD2	1:J:4788:ASN:ND2	1.44	1.14
1:G:4788:ASN:ND2	1:J:4738:PHE:HD2	1.45	1.13
1:A:207:PHE:HD1	1:D:2326:ILE:HD13	1.10	1.11
1:A:2326:ILE:HD13	1:J:207:PHE:HD1	1.11	1.10
1:D:207:PHE:HD1	1:G:2326:ILE:HD13	1.12	1.08
1:G:207:PHE:HD1	1:J:2326:ILE:HD13	1.11	1.08
1:D:4788:ASN:ND2	1:G:4738:PHE:CD2	2.22	1.00
1:D:207:PHE:CD1	1:G:2326:ILE:HB	1.96	1.00
1:A:2326:ILE:HB	1:J:207:PHE:CD1	1.96	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:PHE:CD1	1:D:2326:ILE:HB	1.98	0.99
1:G:207:PHE:CD1	1:J:2326:ILE:HB	1.97	0.98
1:A:207:PHE:CD1	1:D:2326:ILE:HD13	1.97	0.98
1:G:207:PHE:CD1	1:J:2326:ILE:HD13	1.97	0.98
1:A:2326:ILE:HD13	1:J:207:PHE:CD1	1.98	0.98
1:A:4862:ILE:HG22	1:D:4868:ILE:HD12	1.46	0.98
1:D:207:PHE:CD1	1:G:2326:ILE:HD13	1.99	0.97
1:G:4862:ILE:HG22	1:J:4868:ILE:HD12	1.47	0.97
1:A:4868:ILE:HD12	1:J:4862:ILE:HG22	1.48	0.95
1:A:4788:ASN:HD21	1:D:4738:PHE:HE2	1.04	0.93
1:A:2427:LEU:HD12	1:A:2428:ILE:HG22	1.52	0.92
1:A:4738:PHE:CD2	1:J:4788:ASN:ND2	2.25	0.92
1:D:4862:ILE:HG22	1:G:4868:ILE:HD12	1.50	0.92
1:J:2427:LEU:HD12	1:J:2428:ILE:HG22	1.52	0.92
1:D:2427:LEU:HD12	1:D:2428:ILE:HG22	1.52	0.91
1:J:2427:LEU:CD1	1:J:2428:ILE:HG22	2.01	0.90
1:A:2427:LEU:CD1	1:A:2428:ILE:HG22	2.01	0.90
1:G:2427:LEU:HD12	1:G:2428:ILE:HG22	1.52	0.90
1:G:2427:LEU:CD1	1:G:2428:ILE:HG22	2.01	0.89
1:G:4788:ASN:ND2	1:J:4738:PHE:CD2	2.26	0.89
1:D:2427:LEU:CD1	1:D:2428:ILE:HG22	2.01	0.89
1:J:2423:ILE:O	1:J:2427:LEU:HG	1.73	0.88
1:D:2423:ILE:O	1:D:2427:LEU:HG	1.73	0.88
1:G:4770:LEU:O	1:J:4754:LEU:HD21	1.74	0.87
1:A:4770:LEU:O	1:D:4754:LEU:HD21	1.74	0.87
1:G:2423:ILE:O	1:G:2427:LEU:HG	1.73	0.87
1:A:2423:ILE:O	1:A:2427:LEU:HG	1.73	0.86
1:A:4754:LEU:HD21	1:J:4770:LEU:O	1.75	0.86
1:D:4770:LEU:O	1:G:4754:LEU:HD21	1.76	0.85
1:G:4184:LYS:HG3	1:G:4185:GLU:OE1	1.78	0.84
1:D:4184:LYS:HG3	1:D:4185:GLU:OE1	1.78	0.84
1:J:4184:LYS:HG3	1:J:4185:GLU:OE1	1.78	0.83
1:A:4788:ASN:ND2	1:D:4738:PHE:CE2	2.45	0.83
1:A:4184:LYS:HG3	1:A:4185:GLU:OE1	1.78	0.82
1:G:2326:ILE:HD12	1:G:2327:ARG:HG3	1.61	0.82
1:A:2326:ILE:CD1	1:A:2327:ARG:HG3	2.10	0.82
1:A:2326:ILE:HD12	1:A:2327:ARG:HG3	1.60	0.82
1:A:2423:ILE:HG22	1:A:2427:LEU:HD23	1.62	0.82
1:D:2326:ILE:CD1	1:D:2327:ARG:HG3	2.09	0.82
1:D:2326:ILE:HD12	1:D:2327:ARG:HG3	1.60	0.82
1:J:2326:ILE:HD12	1:J:2327:ARG:HG3	1.60	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:2326:ILE:CD1	1:J:2327:ARG:HG3	2.10	0.81
1:G:2423:ILE:HG22	1:G:2427:LEU:HD23	1.62	0.81
1:G:2326:ILE:CD1	1:G:2327:ARG:HG3	2.10	0.81
1:J:2423:ILE:HG22	1:J:2427:LEU:HD23	1.62	0.81
1:D:2423:ILE:HG22	1:D:2427:LEU:HD23	1.62	0.80
1:A:2423:ILE:CG2	1:A:2427:LEU:HD23	2.12	0.79
1:J:2423:ILE:CG2	1:J:2427:LEU:HD23	2.12	0.79
1:G:2423:ILE:CG2	1:G:2427:LEU:HD23	2.12	0.79
2:B:25:HIS:HD1	2:B:39:SER:HG	1.30	0.79
1:D:2423:ILE:CG2	1:D:2427:LEU:HD23	2.12	0.78
1:A:2326:ILE:CD1	1:J:207:PHE:HD1	1.99	0.71
1:D:143:LEU:HD13	1:G:2426:SER:C	2.12	0.70
1:A:4862:ILE:HG22	1:D:4868:ILE:CD1	2.19	0.70
1:A:207:PHE:CD1	1:D:2326:ILE:CD1	2.75	0.70
1:G:4862:ILE:HG22	1:J:4868:ILE:CD1	2.20	0.70
1:G:4796:LYS:NZ	1:G:4807:CYS:SG	2.65	0.69
1:J:4796:LYS:NZ	1:J:4807:CYS:SG	2.65	0.69
1:A:207:PHE:CG	1:D:2326:ILE:HB	2.28	0.69
1:A:4796:LYS:NZ	1:A:4807:CYS:SG	2.65	0.69
1:D:207:PHE:CG	1:G:2326:ILE:HB	2.27	0.69
1:G:1763:PHE:HB3	1:G:1781:GLU:HB3	1.75	0.69
1:D:4796:LYS:NZ	1:D:4807:CYS:SG	2.65	0.69
1:A:207:PHE:HD1	1:D:2326:ILE:CD1	1.99	0.69
1:A:2326:ILE:HB	1:J:207:PHE:CG	2.27	0.69
1:J:1763:PHE:HB3	1:J:1781:GLU:HB3	1.75	0.68
1:A:2426:SER:C	1:J:143:LEU:HD13	2.13	0.68
1:G:207:PHE:CD1	1:J:2326:ILE:CB	2.76	0.68
1:G:143:LEU:HD13	1:J:2426:SER:C	2.14	0.68
1:G:207:PHE:CD1	1:J:2326:ILE:CD1	2.75	0.68
1:A:4868:ILE:CD1	1:J:4862:ILE:HG22	2.21	0.68
1:G:207:PHE:CG	1:J:2326:ILE:HB	2.27	0.68
1:A:143:LEU:HD13	1:D:2426:SER:C	2.15	0.67
1:A:1763:PHE:HB3	1:A:1781:GLU:HB3	1.75	0.67
1:D:207:PHE:CD1	1:G:2326:ILE:CD1	2.76	0.67
1:D:4862:ILE:HG22	1:G:4868:ILE:CD1	2.23	0.67
1:D:190:ARG:NE	1:D:207:PHE:CE2	2.62	0.67
1:G:190:ARG:NE	1:G:207:PHE:CE2	2.62	0.67
1:D:1763:PHE:HB3	1:D:1781:GLU:HB3	1.75	0.67
1:G:4883:GLU:O	1:G:4887:THR:HG22	1.95	0.67
1:A:2326:ILE:CD1	1:J:207:PHE:CD1	2.75	0.66
1:D:143:LEU:HB2	1:G:2427:LEU:HA	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2326:ILE:CB	1:J:207:PHE:CD1	2.76	0.66
1:J:4883:GLU:O	1:J:4887:THR:HG22	1.96	0.66
1:A:190:ARG:NE	1:A:207:PHE:CE2	2.62	0.66
1:J:190:ARG:NE	1:J:207:PHE:CE2	2.62	0.66
1:D:207:PHE:CD1	1:G:2326:ILE:CB	2.76	0.66
1:A:4883:GLU:O	1:A:4887:THR:HG22	1.96	0.66
1:D:143:LEU:HD13	1:G:2427:LEU:N	2.11	0.66
1:D:4879:GLU:OE1	1:D:4879:GLU:HA	1.96	0.65
1:G:4862:ILE:CG2	1:J:4868:ILE:HD12	2.25	0.65
1:A:2427:LEU:HA	1:J:143:LEU:HB2	1.78	0.65
1:A:4879:GLU:OE1	1:A:4879:GLU:HA	1.96	0.65
1:D:4883:GLU:O	1:D:4887:THR:HG22	1.96	0.65
1:G:4879:GLU:OE1	1:G:4879:GLU:HA	1.97	0.65
1:D:2706:PRO:HB3	1:D:2855:LYS:HG3	1.79	0.65
1:G:2706:PRO:HB3	1:G:2855:LYS:HG3	1.79	0.65
1:G:2769:LYS:HG3	1:G:2773:ARG:HB2	1.79	0.65
1:J:2769:LYS:HG3	1:J:2773:ARG:HB2	1.79	0.64
1:G:143:LEU:HB2	1:J:2427:LEU:HA	1.79	0.64
1:A:143:LEU:HB2	1:D:2427:LEU:HA	1.79	0.64
1:A:2769:LYS:HG3	1:A:2773:ARG:HB2	1.79	0.64
1:A:4788:ASN:ND2	1:D:4738:PHE:HE2	1.87	0.64
1:D:2423:ILE:HG22	1:D:2427:LEU:CD2	2.28	0.64
1:D:4638:THR:HG21	1:D:4706:TYR:HB2	1.80	0.64
1:A:2427:LEU:N	1:J:143:LEU:HD13	2.11	0.64
1:J:2706:PRO:HB3	1:J:2855:LYS:HG3	1.79	0.64
1:D:2436:VAL:HG23	1:D:2437:ILE:HG13	1.80	0.64
1:G:1219:LYS:H	1:G:1240:ALA:HB2	1.63	0.64
1:G:2436:VAL:HG23	1:G:2437:ILE:HG13	1.80	0.64
1:J:4879:GLU:OE1	1:J:4879:GLU:HA	1.96	0.64
2:H:17:LYS:HE2	2:H:20:GLN:HE22	1.63	0.64
1:D:4781:LEU:HD11	1:G:4741:ALA:O	1.98	0.64
2:E:17:LYS:HE2	2:E:20:GLN:HE22	1.63	0.64
1:G:143:LEU:HD13	1:J:2427:LEU:N	2.12	0.64
1:J:2436:VAL:HG23	1:J:2437:ILE:HG13	1.80	0.64
1:A:143:LEU:HD13	1:D:2427:LEU:N	2.12	0.64
2:K:17:LYS:HE2	2:K:20:GLN:HE22	1.63	0.64
1:A:4741:ALA:O	1:J:4781:LEU:HD11	1.98	0.64
2:B:17:LYS:HE2	2:B:20:GLN:HE22	1.63	0.63
1:G:3775:GLN:OE1	1:G:3852:ASN:ND2	2.29	0.63
1:G:4781:LEU:HD11	1:J:4741:ALA:O	1.98	0.63
1:A:207:PHE:CD1	1:D:2326:ILE:CB	2.77	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:143:LEU:HG	1:G:143:LEU:O	1.98	0.63
1:J:143:LEU:HG	1:J:143:LEU:O	1.98	0.63
1:D:1682:GLU:HG3	1:D:1782:PHE:HB2	1.81	0.63
1:D:191:TYR:OH	1:G:2327:ARG:HD3	1.98	0.63
1:A:2423:ILE:HG22	1:A:2427:LEU:CD2	2.28	0.63
1:A:2706:PRO:HB3	1:A:2855:LYS:HG3	1.79	0.63
1:J:1682:GLU:HG3	1:J:1782:PHE:HB2	1.81	0.63
1:J:2423:ILE:HG22	1:J:2427:LEU:CD2	2.28	0.63
1:A:2327:ARG:HD3	1:J:191:TYR:OH	1.99	0.63
1:A:2436:VAL:HG23	1:A:2437:ILE:HG13	1.80	0.63
1:A:4638:THR:HG21	1:A:4706:TYR:HB2	1.80	0.63
1:A:4862:ILE:CG2	1:D:4868:ILE:CD1	2.76	0.63
1:A:1102:TYR:HB2	1:A:1165:MET:HG2	1.81	0.63
1:A:1682:GLU:HG3	1:A:1782:PHE:HB2	1.81	0.63
1:A:3729:GLN:OE1	1:A:3771:ASN:ND2	2.32	0.63
1:D:1219:LYS:H	1:D:1240:ALA:HB2	1.63	0.63
1:D:2769:LYS:HG3	1:D:2773:ARG:HB2	1.79	0.63
1:A:143:LEU:HG	1:A:143:LEU:O	1.98	0.63
1:D:143:LEU:HD22	1:G:2427:LEU:CA	2.28	0.63
1:D:1102:TYR:HB2	1:D:1165:MET:HG2	1.81	0.63
1:G:2423:ILE:HG22	1:G:2427:LEU:CD2	2.28	0.63
1:J:1102:TYR:HB2	1:J:1165:MET:HG2	1.81	0.63
1:A:4868:ILE:HD12	1:J:4862:ILE:CG2	2.26	0.63
1:G:1682:GLU:HG3	1:G:1782:PHE:HB2	1.81	0.63
1:J:1219:LYS:H	1:J:1240:ALA:HB2	1.63	0.63
1:D:143:LEU:HG	1:D:143:LEU:O	1.98	0.62
1:G:4070:CYS:SG	1:G:4071:ALA:N	2.72	0.62
1:A:4070:CYS:SG	1:A:4071:ALA:N	2.72	0.62
1:A:4862:ILE:CG2	1:D:4868:ILE:HD12	2.23	0.62
1:G:191:TYR:OH	1:J:2327:ARG:HD3	2.00	0.62
1:G:1102:TYR:HB2	1:G:1165:MET:HG2	1.81	0.62
1:G:4862:ILE:CG2	1:J:4868:ILE:CD1	2.77	0.62
1:J:4638:THR:HG21	1:J:4706:TYR:HB2	1.80	0.62
1:A:1219:LYS:H	1:A:1240:ALA:HB2	1.63	0.62
1:D:4070:CYS:SG	1:D:4071:ALA:N	2.72	0.62
1:J:3729:GLN:OE1	1:J:3771:ASN:ND2	2.32	0.62
1:J:3775:GLN:OE1	1:J:3852:ASN:ND2	2.29	0.62
1:D:4791:ARG:NH2	1:G:4523:VAL:HG21	2.14	0.62
1:J:810:GLU:OE1	1:J:812:LYS:NZ	2.33	0.62
1:A:2427:LEU:CA	1:J:143:LEU:HD22	2.29	0.62
1:J:4070:CYS:SG	1:J:4071:ALA:N	2.72	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:810:GLU:OE1	1:D:812:LYS:NZ	2.33	0.62
1:A:3854:ASP:OD1	1:A:3854:ASP:N	2.33	0.61
1:A:4788:ASN:ND2	1:D:4738:PHE:CD2	2.68	0.61
1:D:3939:SER:OG	1:D:3940:ARG:N	2.33	0.61
1:G:810:GLU:OE1	1:G:812:LYS:NZ	2.33	0.61
1:J:3939:SER:OG	1:J:3940:ARG:N	2.33	0.61
1:D:3729:GLN:OE1	1:D:3771:ASN:ND2	2.32	0.61
1:D:3775:GLN:OE1	1:D:3852:ASN:ND2	2.28	0.61
1:G:3729:GLN:OE1	1:G:3771:ASN:ND2	2.32	0.61
1:G:4638:THR:HG21	1:G:4706:TYR:HB2	1.80	0.61
1:A:4781:LEU:HD11	1:D:4741:ALA:O	2.00	0.61
1:A:4868:ILE:CD1	1:J:4862:ILE:CG2	2.78	0.61
1:A:810:GLU:OE1	1:A:812:LYS:NZ	2.33	0.61
1:D:4862:ILE:CG2	1:G:4868:ILE:HD12	2.27	0.61
1:G:954:ASP:HB2	1:G:1061:GLY:HA3	1.83	0.61
1:G:4858:ILE:HD12	1:J:4867:ILE:HG21	1.82	0.61
1:A:3939:SER:OG	1:A:3940:ARG:N	2.33	0.61
1:A:4523:VAL:HG21	1:J:4791:ARG:NH2	2.16	0.61
1:G:1425:THR:N	1:G:1510:VAL:O	2.34	0.61
1:J:1425:THR:N	1:J:1510:VAL:O	2.34	0.61
1:A:143:LEU:HD22	1:D:2427:LEU:HB3	0.71	0.61
1:D:4788:ASN:OD1	1:G:4738:PHE:CE2	2.54	0.61
1:J:335:LYS:NZ	1:J:398:HIS:O	2.33	0.60
1:D:4862:ILE:CG2	1:G:4868:ILE:CD1	2.79	0.60
1:D:335:LYS:NZ	1:D:398:HIS:O	2.33	0.60
1:A:954:ASP:HB2	1:A:1061:GLY:HA3	1.83	0.60
1:G:618:CYS:HB2	1:G:629:GLN:HG2	1.84	0.60
1:G:1272:ARG:HH11	1:G:1586:LEU:HD21	1.67	0.60
2:H:62:GLY:HA3	2:H:74:LEU:HD21	1.82	0.60
1:A:3775:GLN:OE1	1:A:3852:ASN:ND2	2.29	0.60
2:E:62:GLY:HA3	2:E:74:LEU:HD21	1.82	0.60
1:J:954:ASP:HB2	1:J:1061:GLY:HA3	1.83	0.60
1:A:191:TYR:OH	1:D:2327:ARG:HD3	2.01	0.60
1:D:954:ASP:HB2	1:D:1061:GLY:HA3	1.83	0.60
1:D:1792:ILE:HG23	1:D:1842:ILE:HD13	1.84	0.60
1:G:881:ILE:HA	1:G:884:LYS:HD2	1.84	0.60
1:G:2427:LEU:HD11	1:G:2428:ILE:HG22	1.84	0.60
1:G:3939:SER:OG	1:G:3940:ARG:N	2.33	0.60
1:G:4791:ARG:NH2	1:J:4523:VAL:HG21	2.17	0.60
1:A:697:TRP:NE1	1:A:757:CYS:SG	2.75	0.60
1:A:1792:ILE:HG23	1:A:1842:ILE:HD13	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1425:THR:N	1:D:1510:VAL:O	2.34	0.60
1:G:697:TRP:NE1	1:G:757:CYS:SG	2.75	0.60
1:J:1205:CYS:SG	1:J:1206:SER:N	2.75	0.60
1:D:2425:ARG:NH2	1:D:2476:VAL:O	2.35	0.60
1:A:1205:CYS:SG	1:A:1206:SER:N	2.75	0.59
1:A:4738:PHE:CE2	1:J:4788:ASN:OD1	2.55	0.59
1:D:2838:LEU:HD12	1:D:2904:VAL:HG11	1.84	0.59
1:G:2838:LEU:HD12	1:G:2904:VAL:HG11	1.84	0.59
1:J:881:ILE:HA	1:J:884:LYS:HD2	1.84	0.59
1:J:2425:ARG:NH2	1:J:2476:VAL:O	2.35	0.59
1:A:1425:THR:N	1:A:1510:VAL:O	2.34	0.59
1:D:143:LEU:HD22	1:G:2427:LEU:HB3	0.69	0.59
1:G:2782:THR:OG1	1:G:2848:ASN:ND2	2.36	0.59
1:J:2782:THR:OG1	1:J:2848:ASN:ND2	2.36	0.59
2:K:62:GLY:HA3	2:K:74:LEU:HD21	1.82	0.59
1:A:207:PHE:O	1:D:2327:ARG:HG2	2.03	0.59
1:A:881:ILE:HA	1:A:884:LYS:HD2	1.84	0.59
2:B:62:GLY:HA3	2:B:74:LEU:HD21	1.82	0.59
1:G:2425:ARG:NH2	1:G:2476:VAL:O	2.35	0.59
1:J:618:CYS:HB2	1:J:629:GLN:HG2	1.84	0.59
1:D:618:CYS:HB2	1:D:629:GLN:HG2	1.84	0.59
1:G:1792:ILE:HG23	1:G:1842:ILE:HD13	1.84	0.59
1:G:3854:ASP:OD1	1:G:3854:ASP:N	2.33	0.59
1:J:1006:VAL:HA	1:J:1009:ARG:HD3	1.85	0.59
1:J:2838:LEU:HD12	1:J:2904:VAL:HG11	1.84	0.59
1:A:2425:ARG:NH2	1:A:2476:VAL:O	2.35	0.59
1:A:2782:THR:OG1	1:A:2848:ASN:ND2	2.36	0.59
1:D:1205:CYS:SG	1:D:1206:SER:N	2.75	0.59
1:D:3761:LYS:NZ	1:D:3839:ASP:OD2	2.36	0.59
1:D:4858:ILE:HD12	1:G:4867:ILE:HG21	1.84	0.59
1:J:697:TRP:NE1	1:J:757:CYS:SG	2.75	0.59
1:J:1272:ARG:HH11	1:J:1586:LEU:HD21	1.67	0.59
1:G:1205:CYS:SG	1:G:1206:SER:N	2.75	0.59
1:G:4113:ASP:O	1:G:4117:GLN:NE2	2.36	0.59
1:G:4957:ASP:OD1	1:G:4957:ASP:N	2.34	0.59
1:A:1272:ARG:HH11	1:A:1586:LEU:HD21	1.67	0.59
1:A:2327:ARG:HG2	1:J:207:PHE:O	2.02	0.59
1:G:335:LYS:NZ	1:G:398:HIS:O	2.33	0.59
1:D:2782:THR:OG1	1:D:2848:ASN:ND2	2.36	0.59
1:G:207:PHE:O	1:J:2327:ARG:HG2	2.02	0.59
1:G:231:GLY:O	1:G:276:ARG:NH1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3761:LYS:NZ	1:G:3839:ASP:OD2	2.36	0.59
1:J:4024:LEU:HG	1:J:4085:VAL:HG12	1.85	0.59
1:A:618:CYS:HB2	1:A:629:GLN:HG2	1.84	0.59
1:A:2838:LEU:HD12	1:A:2904:VAL:HG11	1.84	0.59
1:A:4791:ARG:NH2	1:D:4523:VAL:HG21	2.17	0.59
1:A:4858:ILE:HD12	1:D:4867:ILE:HG21	1.84	0.59
1:A:4867:ILE:HG21	1:J:4858:ILE:HD12	1.83	0.59
2:B:7:ILE:HB	2:B:71:ARG:HG3	1.85	0.59
1:D:697:TRP:NE1	1:D:757:CYS:SG	2.75	0.59
2:E:7:ILE:HB	2:E:71:ARG:HG3	1.85	0.59
1:J:231:GLY:O	1:J:276:ARG:NH1	2.35	0.59
1:D:881:ILE:HA	1:D:884:LYS:HD2	1.84	0.58
1:D:1272:ARG:HH11	1:D:1586:LEU:HD21	1.67	0.58
1:D:2779:SER:HG	1:D:2849:TYR:HH	1.49	0.58
1:G:4788:ASN:OD1	1:J:4738:PHE:CE2	2.56	0.58
1:J:2427:LEU:HD11	1:J:2428:ILE:HG22	1.84	0.58
1:J:4113:ASP:O	1:J:4117:GLN:NE2	2.36	0.58
1:A:1100:ARG:HH12	1:A:1170:GLU:H	1.51	0.58
1:A:2326:ILE:HG21	1:J:207:PHE:CE1	2.38	0.58
1:G:207:PHE:CE1	1:J:2326:ILE:HG21	2.38	0.58
1:J:1792:ILE:HG23	1:J:1842:ILE:HD13	1.84	0.58
1:D:207:PHE:CE1	1:G:2326:ILE:HG21	2.38	0.58
1:D:867:VAL:O	1:D:1002:ASN:ND2	2.36	0.58
1:G:694:ARG:NH1	1:G:716:ASN:O	2.35	0.58
1:J:694:ARG:NH1	1:J:716:ASN:O	2.35	0.58
2:K:7:ILE:HB	2:K:71:ARG:HG3	1.85	0.58
1:A:207:PHE:CE1	1:D:2326:ILE:HG21	2.39	0.58
1:A:1916:ASP:OD1	1:A:2091:ARG:NH1	2.37	0.58
1:D:503:ASP:OD1	1:D:561:ARG:NH2	2.37	0.58
1:G:867:VAL:O	1:G:1002:ASN:ND2	2.37	0.58
1:J:867:VAL:O	1:J:1002:ASN:ND2	2.37	0.58
1:A:180:ASP:HB3	1:A:211:LEU:HD12	1.86	0.58
1:A:231:GLY:O	1:A:276:ARG:NH1	2.35	0.58
1:A:1106:GLU:HB3	1:A:1214:ARG:HB2	1.86	0.58
1:D:231:GLY:O	1:D:276:ARG:NH1	2.35	0.58
1:D:4577:ALA:O	1:D:4734:HIS:NE2	2.35	0.58
1:A:4113:ASP:O	1:A:4117:GLN:NE2	2.36	0.58
2:H:7:ILE:HB	2:H:71:ARG:HG3	1.85	0.58
1:A:3761:LYS:NZ	1:A:3839:ASP:OD2	2.36	0.58
1:D:180:ASP:HB3	1:D:211:LEU:HD12	1.86	0.58
1:D:207:PHE:O	1:G:2327:ARG:HG2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1250:TRP:HE1	1:D:1602:GLN:HG3	1.68	0.58
1:J:734:SER:OG	1:J:739:ARG:NH1	2.37	0.58
1:D:734:SER:OG	1:D:739:ARG:NH1	2.37	0.58
1:D:4808:ASP:HB2	1:G:4523:VAL:CG1	2.34	0.58
1:G:1250:TRP:HE1	1:G:1602:GLN:HG3	1.68	0.58
1:J:1100:ARG:HH12	1:J:1170:GLU:H	1.51	0.58
1:A:867:VAL:O	1:A:1002:ASN:ND2	2.37	0.58
1:A:1482:ARG:NH1	1:A:1530:TYR:O	2.37	0.58
1:A:4523:VAL:CG1	1:J:4808:ASP:HB2	2.34	0.58
1:G:207:PHE:HB3	1:J:2326:ILE:HD12	1.86	0.58
1:G:734:SER:OG	1:G:739:ARG:NH1	2.37	0.58
1:G:1006:VAL:HA	1:G:1009:ARG:HD3	1.85	0.58
1:G:4808:ASP:HB2	1:J:4523:VAL:CG1	2.34	0.58
1:J:180:ASP:HB3	1:J:211:LEU:HD12	1.86	0.58
1:J:834:VAL:H	1:J:1614:ARG:HH22	1.51	0.58
1:A:1006:VAL:HA	1:A:1009:ARG:HD3	1.85	0.57
1:A:3599:ALA:HB1	3:C:76:LYS:HE2	1.86	0.57
1:D:3599:ALA:HB1	3:F:76:LYS:HE2	1.86	0.57
1:D:4094:ASP:OD1	1:D:4094:ASP:N	2.33	0.57
1:D:4113:ASP:O	1:D:4117:GLN:NE2	2.36	0.57
1:G:503:ASP:OD1	1:G:561:ARG:NH2	2.37	0.57
1:G:510:SER:O	1:G:520:ARG:NH2	2.37	0.57
1:D:1006:VAL:HA	1:D:1009:ARG:HD3	1.85	0.57
1:D:1482:ARG:NH1	1:D:1530:TYR:O	2.37	0.57
1:G:1916:ASP:OD1	1:G:2091:ARG:NH1	2.37	0.57
1:G:4024:LEU:HG	1:G:4085:VAL:HG12	1.85	0.57
1:J:1304:LEU:HB2	1:J:1541:PRO:HG2	1.87	0.57
1:J:1482:ARG:NH1	1:J:1530:TYR:O	2.37	0.57
1:A:143:LEU:HD22	1:D:2427:LEU:CA	2.31	0.57
1:D:834:VAL:H	1:D:1614:ARG:HH22	1.51	0.57
1:G:180:ASP:HB3	1:G:211:LEU:HD12	1.86	0.57
1:A:694:ARG:NH1	1:A:716:ASN:O	2.35	0.57
1:G:1482:ARG:NH1	1:G:1530:TYR:O	2.37	0.57
1:G:4195:GLU:OE1	1:G:4948:ARG:NH2	2.37	0.57
1:A:4788:ASN:OD1	1:D:4738:PHE:CD2	2.57	0.57
1:D:510:SER:O	1:D:520:ARG:NH2	2.37	0.57
1:D:4024:LEU:HG	1:D:4085:VAL:HG12	1.85	0.57
2:E:38:SER:OG	2:E:39:SER:N	2.37	0.57
1:J:3761:LYS:NZ	1:J:3839:ASP:OD2	2.36	0.57
1:A:1250:TRP:HE1	1:A:1602:GLN:HG3	1.68	0.57
1:A:4195:GLU:OE1	1:A:4948:ARG:NH2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1916:ASP:OD1	1:D:2091:ARG:NH1	2.37	0.57
1:G:1172:THR:HG22	1:G:1193:LYS:HG2	1.87	0.57
1:J:1916:ASP:OD1	1:J:2091:ARG:NH1	2.37	0.57
1:A:4024:LEU:HG	1:A:4085:VAL:HG12	1.85	0.57
1:G:1106:GLU:HB3	1:G:1214:ARG:HB2	1.86	0.57
2:H:38:SER:OG	2:H:39:SER:N	2.37	0.57
1:J:510:SER:O	1:J:520:ARG:NH2	2.37	0.57
1:J:1106:GLU:HB3	1:J:1214:ARG:HB2	1.86	0.57
1:J:1250:TRP:HE1	1:J:1602:GLN:HG3	1.68	0.57
2:K:38:SER:OG	2:K:39:SER:N	2.37	0.57
1:A:1304:LEU:HB2	1:A:1541:PRO:HG2	1.87	0.57
1:D:4845:ILE:HD12	1:G:4819:TYR:CD1	2.40	0.57
1:G:556:ASP:OD1	1:G:593:HIS:NE2	2.38	0.57
1:A:510:SER:O	1:A:520:ARG:NH2	2.37	0.56
1:A:556:ASP:OD1	1:A:593:HIS:NE2	2.38	0.56
1:A:3862:GLN:HE21	1:A:3865:ASN:HD22	1.53	0.56
1:D:3862:GLN:HE21	1:D:3865:ASN:HD22	1.53	0.56
1:A:834:VAL:H	1:A:1614:ARG:HH22	1.51	0.56
1:D:1100:ARG:HH12	1:D:1170:GLU:H	1.51	0.56
1:J:1172:THR:HG22	1:J:1193:LYS:HG2	1.87	0.56
1:A:467:ASP:N	1:A:467:ASP:OD1	2.38	0.56
1:A:734:SER:OG	1:A:739:ARG:NH1	2.37	0.56
1:A:756:SER:HB2	1:A:769:ARG:HB2	1.87	0.56
1:A:2326:ILE:HD12	1:J:207:PHE:HB3	1.87	0.56
1:D:1304:LEU:HB2	1:D:1541:PRO:HG2	1.87	0.56
1:D:4195:GLU:OE1	1:D:4948:ARG:NH2	2.37	0.56
1:G:834:VAL:H	1:G:1614:ARG:HH22	1.51	0.56
1:G:1100:ARG:HH12	1:G:1170:GLU:H	1.51	0.56
1:A:1172:THR:HG22	1:A:1193:LYS:HG2	1.87	0.56
2:B:38:SER:OG	2:B:39:SER:N	2.37	0.56
1:J:2883:LYS:O	1:J:2887:ARG:N	2.37	0.56
1:J:4195:GLU:OE1	1:J:4948:ARG:NH2	2.37	0.56
1:A:2427:LEU:HD11	1:A:2428:ILE:HG22	1.84	0.56
1:A:2712:ILE:O	1:A:2781:LYS:NZ	2.35	0.56
1:D:694:ARG:NH1	1:D:716:ASN:O	2.35	0.56
1:D:3856:GLN:O	1:D:3932:ASN:ND2	2.39	0.56
1:G:3862:GLN:HE21	1:G:3865:ASN:HD22	1.53	0.56
1:D:207:PHE:HB3	1:G:2326:ILE:HD12	1.87	0.56
1:D:748:LEU:HB2	1:D:750:ARG:HG3	1.88	0.56
1:J:503:ASP:OD1	1:J:561:ARG:NH2	2.37	0.56
1:J:3862:GLN:HE21	1:J:3865:ASN:HD22	1.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:PHE:HB3	1:D:2326:ILE:HD12	1.86	0.56
1:A:3856:GLN:O	1:A:3932:ASN:ND2	2.39	0.56
1:D:1106:GLU:HB3	1:D:1214:ARG:HB2	1.86	0.56
1:G:3599:ALA:HB1	3:I:76:LYS:HE2	1.86	0.56
1:G:4094:ASP:OD1	1:G:4094:ASP:N	2.33	0.56
1:J:1465:VAL:N	1:J:1483:SER:O	2.39	0.56
1:J:2793:THR:HG23	1:J:2903:ALA:HB2	1.88	0.56
1:A:2779:SER:HG	1:A:2849:TYR:HH	1.51	0.56
1:G:2793:THR:HG23	1:G:2903:ALA:HB2	1.88	0.56
1:J:2779:SER:HG	1:J:2849:TYR:HH	1.54	0.56
1:J:3599:ALA:HB1	3:L:76:LYS:HE2	1.86	0.56
1:A:1465:VAL:N	1:A:1483:SER:O	2.39	0.56
1:A:4808:ASP:HB2	1:D:4523:VAL:CG1	2.36	0.56
1:A:4819:TYR:CD1	1:J:4845:ILE:HD12	2.41	0.56
1:D:756:SER:HB2	1:D:769:ARG:HB2	1.87	0.56
1:D:2427:LEU:HD11	1:D:2428:ILE:HG22	1.84	0.56
1:G:143:LEU:HD22	1:J:2427:LEU:CA	2.30	0.56
1:G:4020:MET:HB3	1:G:4067:LEU:HD21	1.88	0.56
1:A:4845:ILE:HD12	1:D:4819:TYR:CD1	2.41	0.55
1:D:2326:ILE:HD11	1:D:2327:ARG:HG3	1.88	0.55
1:D:2883:LYS:O	1:D:2887:ARG:N	2.37	0.55
1:A:503:ASP:OD1	1:A:561:ARG:NH2	2.37	0.55
1:A:2892:ASP:HA	1:A:2895:LYS:HB2	1.88	0.55
1:D:4031:ASP:HA	1:D:4034:LYS:HB2	1.89	0.55
3:F:51:ASP:O	3:F:55:GLU:N	2.39	0.55
1:G:4858:ILE:HD12	1:J:4867:ILE:CG2	2.37	0.55
1:J:2712:ILE:O	1:J:2781:LYS:NZ	2.35	0.55
1:J:2892:ASP:HA	1:J:2895:LYS:HB2	1.88	0.55
1:A:748:LEU:HB2	1:A:750:ARG:HG3	1.88	0.55
1:D:2025:THR:O	1:D:2029:ARG:NH1	2.40	0.55
1:G:1304:LEU:HB2	1:G:1541:PRO:HG2	1.87	0.55
1:J:2326:ILE:HD11	1:J:2327:ARG:HG3	1.89	0.55
1:J:3854:ASP:OD1	1:J:3854:ASP:N	2.33	0.55
1:A:1432:ILE:HG22	1:A:1434:PRO:HD2	1.89	0.55
1:D:1172:THR:HG22	1:D:1193:LYS:HG2	1.87	0.55
1:G:2427:LEU:HD12	1:G:2428:ILE:N	2.22	0.55
1:G:3623:GLN:NE2	1:G:3626:GLU:OE2	2.40	0.55
1:J:1112:ASP:H	1:J:1211:GLN:HE21	1.55	0.55
1:A:188:SER:OG	1:A:190:ARG:NH2	2.36	0.55
1:A:2793:THR:HG23	1:A:2903:ALA:HB2	1.88	0.55
1:A:4020:MET:HB3	1:A:4067:LEU:HD21	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3623:GLN:NE2	1:D:3626:GLU:OE2	2.40	0.55
1:G:474:ASP:OD1	1:G:478:ARG:NH1	2.40	0.55
1:G:4146:ILE:H	1:G:4962:GLN:HE22	1.54	0.55
1:J:3856:GLN:O	1:J:3932:ASN:ND2	2.39	0.55
1:A:2025:THR:O	1:A:2029:ARG:NH1	2.40	0.55
1:J:1643:GLU:O	1:J:1647:GLN:NE2	2.40	0.55
1:J:4146:ILE:H	1:J:4962:GLN:HE22	1.54	0.55
1:A:1643:GLU:O	1:A:1647:GLN:NE2	2.40	0.55
1:D:2892:ASP:HA	1:D:2895:LYS:HB2	1.88	0.55
1:G:2025:THR:O	1:G:2029:ARG:NH1	2.40	0.55
1:G:4031:ASP:HA	1:G:4034:LYS:HB2	1.89	0.55
1:A:3623:GLN:NE2	1:A:3626:GLU:OE2	2.40	0.55
1:D:394:HIS:CD2	1:D:397:GLY:H	2.25	0.55
1:D:1930:SER:O	1:D:1930:SER:OG	2.24	0.55
1:D:2257:ALA:O	1:D:2259:ARG:NH1	2.40	0.55
1:D:2793:THR:HG23	1:D:2903:ALA:HB2	1.88	0.55
1:G:2892:ASP:HA	1:G:2895:LYS:HB2	1.88	0.55
1:G:3856:GLN:O	1:G:3932:ASN:ND2	2.39	0.55
1:J:748:LEU:HB2	1:J:750:ARG:HG3	1.88	0.55
1:J:2427:LEU:HD12	1:J:2428:ILE:N	2.22	0.55
1:J:4518:LEU:HD21	1:J:4738:PHE:CD1	2.42	0.55
1:A:2257:ALA:O	1:A:2259:ARG:NH1	2.40	0.55
1:A:4577:ALA:O	1:A:4734:HIS:NE2	2.35	0.55
1:G:4577:ALA:O	1:G:4734:HIS:NE2	2.35	0.55
1:G:4926:LEU:HD13	1:G:4942:TRP:HB2	1.89	0.55
1:J:756:SER:HB2	1:J:769:ARG:HB2	1.87	0.55
1:J:4926:LEU:HD13	1:J:4942:TRP:HB2	1.89	0.55
3:L:51:ASP:O	3:L:55:GLU:N	2.39	0.55
1:D:699:SER:OG	1:D:700:THR:N	2.40	0.55
1:D:1432:ILE:HG22	1:D:1434:PRO:HD2	1.89	0.55
1:G:2257:ALA:O	1:G:2259:ARG:NH1	2.40	0.55
1:G:4845:ILE:HD12	1:J:4819:TYR:CD1	2.42	0.55
1:J:556:ASP:OD1	1:J:593:HIS:NE2	2.38	0.55
1:J:2025:THR:O	1:J:2029:ARG:NH1	2.40	0.55
1:J:3623:GLN:NE2	1:J:3626:GLU:OE2	2.40	0.55
1:A:474:ASP:OD1	1:A:478:ARG:NH1	2.40	0.54
1:A:1112:ASP:H	1:A:1211:GLN:HE21	1.55	0.54
1:A:4867:ILE:CG2	1:J:4858:ILE:HD12	2.37	0.54
1:D:1465:VAL:N	1:D:1483:SER:O	2.39	0.54
1:G:748:LEU:HB2	1:G:750:ARG:HG3	1.88	0.54
1:J:394:HIS:CD2	1:J:397:GLY:H	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1589:GLN:NE2	1:A:1634:GLU:OE2	2.40	0.54
1:A:1756:SER:OG	1:A:1757:LEU:N	2.40	0.54
1:D:676:GLU:HB2	1:D:803:LEU:HB2	1.89	0.54
1:G:290:ARG:H	1:G:293:GLN:HE22	1.55	0.54
1:J:290:ARG:H	1:J:293:GLN:HE22	1.56	0.54
1:J:1432:ILE:HG22	1:J:1434:PRO:HD2	1.89	0.54
1:A:699:SER:OG	1:A:700:THR:N	2.40	0.54
1:A:2645:LEU:O	1:A:2649:ILE:N	2.40	0.54
1:A:4146:ILE:H	1:A:4962:GLN:HE22	1.54	0.54
1:D:1589:GLN:NE2	1:D:1634:GLU:OE2	2.40	0.54
1:D:4518:LEU:HD21	1:D:4738:PHE:CD1	2.42	0.54
1:G:756:SER:HB2	1:G:769:ARG:HB2	1.87	0.54
1:G:1465:VAL:N	1:G:1483:SER:O	2.39	0.54
1:J:1589:GLN:NE2	1:J:1634:GLU:OE2	2.40	0.54
1:J:4154:SER:OG	1:J:4155:GLU:N	2.41	0.54
1:A:290:ARG:H	1:A:293:GLN:HE22	1.56	0.54
1:D:2427:LEU:HD12	1:D:2428:ILE:N	2.22	0.54
1:D:4020:MET:HB3	1:D:4067:LEU:HD21	1.88	0.54
1:G:228:LEU:HB3	1:G:289:ILE:HD12	1.89	0.54
1:G:676:GLU:HB2	1:G:803:LEU:HB2	1.89	0.54
1:J:2317:ASN:HA	1:J:2320:VAL:HG12	1.90	0.54
1:J:2423:ILE:HG23	1:J:2427:LEU:HD23	1.89	0.54
1:J:4020:MET:HB3	1:J:4067:LEU:HD21	1.88	0.54
1:J:4577:ALA:O	1:J:4734:HIS:NE2	2.35	0.54
1:A:2423:ILE:HG23	1:A:2427:LEU:HD23	1.89	0.54
1:D:300:VAL:O	1:D:420:ARG:NE	2.34	0.54
1:D:556:ASP:OD1	1:D:593:HIS:NE2	2.38	0.54
1:D:1756:SER:OG	1:D:1757:LEU:N	2.40	0.54
1:A:2317:ASN:HA	1:A:2320:VAL:HG12	1.90	0.54
1:A:2893:ILE:HG13	1:A:2894:LEU:HG	1.90	0.54
1:D:290:ARG:H	1:D:293:GLN:HE22	1.55	0.54
1:D:4858:ILE:HD12	1:G:4867:ILE:CG2	2.37	0.54
1:G:4154:SER:OG	1:G:4155:GLU:N	2.41	0.54
1:J:115:TYR:HE2	1:J:175:VAL:HA	1.73	0.54
1:J:699:SER:OG	1:J:700:THR:N	2.40	0.54
1:A:394:HIS:CD2	1:A:397:GLY:H	2.25	0.54
1:A:4031:ASP:HA	1:A:4034:LYS:HB2	1.89	0.54
3:C:51:ASP:O	3:C:55:GLU:N	2.39	0.54
1:G:115:TYR:HE2	1:G:175:VAL:HA	1.73	0.54
1:G:2326:ILE:HD11	1:G:2327:ARG:HG3	1.89	0.54
3:I:51:ASP:O	3:I:55:GLU:N	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:467:ASP:N	1:J:467:ASP:OD1	2.38	0.54
1:J:676:GLU:HB2	1:J:803:LEU:HB2	1.89	0.54
1:J:2257:ALA:O	1:J:2259:ARG:NH1	2.40	0.54
1:A:411:GLU:OE2	1:A:484:ASN:ND2	2.41	0.54
1:A:1445:TRP:O	1:A:1486:TYR:N	2.41	0.54
1:D:1119:ARG:NH2	1:D:1196:ASP:O	2.40	0.54
1:D:2893:ILE:HG13	1:D:2894:LEU:HG	1.90	0.54
1:G:394:HIS:CD2	1:G:397:GLY:H	2.25	0.54
1:G:699:SER:OG	1:G:700:THR:N	2.40	0.54
1:G:1432:ILE:HG22	1:G:1434:PRO:HD2	1.89	0.54
1:G:1756:SER:OG	1:G:1757:LEU:N	2.40	0.54
1:J:2321:VAL:HG12	1:J:2324:LEU:HD12	1.90	0.54
1:J:2423:ILE:O	1:J:2427:LEU:CG	2.54	0.54
1:A:2326:ILE:HD11	1:A:2327:ARG:HG3	1.89	0.54
1:A:2427:LEU:HD12	1:A:2428:ILE:N	2.22	0.54
1:A:4094:ASP:OD1	1:A:4094:ASP:N	2.33	0.54
1:A:4518:LEU:HD21	1:A:4738:PHE:CD1	2.42	0.54
1:D:474:ASP:OD1	1:D:478:ARG:NH1	2.40	0.54
1:D:2317:ASN:HA	1:D:2320:VAL:HG12	1.89	0.54
1:D:4146:ILE:H	1:D:4962:GLN:HE22	1.54	0.54
1:G:62:LEU:HB3	1:G:276:ARG:HH21	1.73	0.54
1:G:143:LEU:HD22	1:J:2427:LEU:HB3	0.70	0.54
1:G:1112:ASP:H	1:G:1211:GLN:HE21	1.55	0.54
1:G:2317:ASN:HA	1:G:2320:VAL:HG12	1.90	0.54
1:J:3733:HIS:O	1:J:3777:LYS:NZ	2.40	0.54
1:J:4031:ASP:HA	1:J:4034:LYS:HB2	1.89	0.54
1:A:62:LEU:HB3	1:A:276:ARG:HH21	1.73	0.54
1:D:1112:ASP:H	1:D:1211:GLN:HE21	1.55	0.54
1:D:3733:HIS:O	1:D:3777:LYS:NZ	2.40	0.54
1:G:2844:MET:O	1:G:2848:ASN:N	2.40	0.54
1:J:411:GLU:OE2	1:J:484:ASN:ND2	2.41	0.54
1:J:474:ASP:OD1	1:J:478:ARG:NH1	2.40	0.54
1:J:2893:ILE:HG13	1:J:2894:LEU:HG	1.90	0.54
1:D:1643:GLU:O	1:D:1647:GLN:NE2	2.40	0.53
1:G:2893:ILE:HG13	1:G:2894:LEU:HG	1.90	0.53
1:A:2321:VAL:HG12	1:A:2324:LEU:HD12	1.90	0.53
1:D:4926:LEU:HD13	1:D:4942:TRP:HB2	1.89	0.53
1:G:1589:GLN:NE2	1:G:1634:GLU:OE2	2.40	0.53
1:D:115:TYR:HE2	1:D:175:VAL:HA	1.73	0.53
1:D:411:GLU:OE2	1:D:484:ASN:ND2	2.41	0.53
1:D:499:LEU:HD22	1:D:557:TRP:HZ3	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3845:GLN:HG3	1:D:3923:GLU:HG3	1.90	0.53
1:G:4060:THR:OG1	1:G:4063:GLU:OE2	2.27	0.53
1:A:115:TYR:HE2	1:A:175:VAL:HA	1.73	0.53
1:A:4926:LEU:HD13	1:A:4942:TRP:HB2	1.89	0.53
1:D:62:LEU:HB3	1:D:276:ARG:HH21	1.73	0.53
1:D:228:LEU:HB3	1:D:289:ILE:HD12	1.89	0.53
1:D:1445:TRP:O	1:D:1486:TYR:N	2.41	0.53
1:D:2138:GLU:O	1:D:2141:LYS:NZ	2.37	0.53
1:G:4518:LEU:HD21	1:G:4738:PHE:CD1	2.43	0.53
1:A:2593:LEU:O	1:A:2597:VAL:N	2.42	0.53
1:D:188:SER:OG	1:D:190:ARG:NH2	2.36	0.53
1:G:1643:GLU:O	1:G:1647:GLN:NE2	2.40	0.53
1:G:2645:LEU:O	1:G:2649:ILE:N	2.40	0.53
1:J:654:SER:HB3	1:J:791:VAL:HG12	1.91	0.53
1:A:676:GLU:HB2	1:A:803:LEU:HB2	1.89	0.53
1:A:4154:SER:OG	1:A:4155:GLU:N	2.41	0.53
1:J:671:LYS:N	1:J:819:TYR:O	2.42	0.53
1:J:1445:TRP:O	1:J:1486:TYR:N	2.41	0.53
1:J:3787:ASP:O	1:J:3865:ASN:ND2	2.42	0.53
1:A:629:GLN:OE1	1:A:1669:ASN:ND2	2.42	0.53
1:A:4060:THR:OG1	1:A:4063:GLU:OE2	2.27	0.53
1:D:671:LYS:N	1:D:819:TYR:O	2.42	0.53
1:D:847:THR:OG1	1:D:1216:ASN:OD1	2.27	0.53
1:D:3956:GLN:NE2	1:D:3973:MET:SD	2.82	0.53
1:G:300:VAL:O	1:G:420:ARG:NE	2.34	0.53
1:G:2150:ILE:HG21	1:G:2168:MET:HE1	1.90	0.53
1:A:335:LYS:HZ3	1:A:401:ASP:HB2	1.74	0.53
1:A:335:LYS:NZ	1:A:398:HIS:O	2.33	0.53
1:A:2150:ILE:HG21	1:A:2168:MET:HE1	1.90	0.53
1:A:2883:LYS:O	1:A:2887:ARG:N	2.37	0.53
1:A:4858:ILE:HD12	1:D:4867:ILE:CG2	2.38	0.53
1:D:2844:MET:O	1:D:2848:ASN:N	2.40	0.53
1:G:654:SER:HB3	1:G:791:VAL:HG12	1.91	0.53
1:G:411:GLU:OE2	1:G:484:ASN:ND2	2.41	0.53
1:G:1445:TRP:O	1:G:1486:TYR:N	2.41	0.53
1:J:62:LEU:HB3	1:J:276:ARG:HH21	1.73	0.53
1:D:420:ARG:HA	1:D:423:VAL:HB	1.91	0.53
1:D:4154:SER:OG	1:D:4155:GLU:N	2.41	0.53
1:G:207:PHE:HD1	1:J:2326:ILE:CD1	1.99	0.53
1:G:2423:ILE:HG23	1:G:2427:LEU:HD23	1.89	0.53
1:J:629:GLN:OE1	1:J:1669:ASN:ND2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:LEU:HB3	1:A:289:ILE:HD12	1.89	0.52
1:A:4957:ASP:OD1	1:A:4957:ASP:N	2.34	0.52
1:G:188:SER:OG	1:G:190:ARG:NH2	2.36	0.52
1:G:680:ASP:O	1:G:799:LYS:NZ	2.41	0.52
1:G:847:THR:OG1	1:G:1216:ASN:OD1	2.27	0.52
1:G:3733:HIS:O	1:G:3777:LYS:NZ	2.40	0.52
1:G:3787:ASP:O	1:G:3865:ASN:ND2	2.42	0.52
1:J:499:LEU:HD22	1:J:557:TRP:HZ3	1.74	0.52
1:J:2844:MET:O	1:J:2848:ASN:N	2.40	0.52
1:A:671:LYS:N	1:A:819:TYR:O	2.42	0.52
1:A:1293:GLN:NE2	1:A:1548:THR:O	2.43	0.52
1:A:3787:ASP:O	1:A:3865:ASN:ND2	2.42	0.52
1:D:2321:VAL:HG12	1:D:2324:LEU:HD12	1.90	0.52
1:G:629:GLN:OE1	1:G:1669:ASN:ND2	2.42	0.52
1:G:2593:LEU:O	1:G:2597:VAL:N	2.42	0.52
1:J:228:LEU:HB3	1:J:289:ILE:HD12	1.89	0.52
1:A:847:THR:OG1	1:A:1216:ASN:OD1	2.27	0.52
1:D:1811:GLY:HA3	1:D:1816:PHE:HB2	1.92	0.52
1:D:4060:THR:OG1	1:D:4063:GLU:OE2	2.27	0.52
1:G:2423:ILE:O	1:G:2427:LEU:CG	2.54	0.52
1:G:3845:GLN:HG3	1:G:3923:GLU:HG3	1.90	0.52
1:J:1938:GLN:HG3	1:J:3611:ASN:HA	1.91	0.52
1:J:3845:GLN:HG3	1:J:3923:GLU:HG3	1.90	0.52
1:A:499:LEU:HD22	1:A:557:TRP:HZ3	1.74	0.52
1:A:1811:GLY:HA3	1:A:1816:PHE:HB2	1.92	0.52
3:C:61:ASN:ND2	3:C:63:THR:O	2.43	0.52
1:D:2150:ILE:HG21	1:D:2168:MET:HE1	1.90	0.52
1:G:2321:VAL:HG12	1:G:2324:LEU:HD12	1.90	0.52
1:G:3956:GLN:NE2	1:G:3973:MET:SD	2.82	0.52
1:J:2150:ILE:HG21	1:J:2168:MET:HE1	1.90	0.52
1:J:2593:LEU:O	1:J:2597:VAL:N	2.42	0.52
1:J:2645:LEU:O	1:J:2649:ILE:N	2.40	0.52
1:A:1938:GLN:HG3	1:A:3611:ASN:HA	1.91	0.52
1:A:2427:LEU:HB3	1:J:143:LEU:HD22	0.69	0.52
1:D:467:ASP:N	1:D:467:ASP:OD1	2.38	0.52
1:D:654:SER:HB3	1:D:791:VAL:HG12	1.91	0.52
1:D:2645:LEU:O	1:D:2649:ILE:N	2.40	0.52
1:D:2712:ILE:O	1:D:2781:LYS:NZ	2.35	0.52
1:G:420:ARG:HA	1:G:423:VAL:HB	1.91	0.52
1:G:499:LEU:HD22	1:G:557:TRP:HZ3	1.74	0.52
1:G:620:CYS:SG	1:G:621:HIS:N	2.82	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1293:GLN:NE2	1:G:1548:THR:O	2.43	0.52
1:G:3875:THR:HG21	1:G:3924:TYR:HE2	1.75	0.52
1:A:3875:THR:HG21	1:A:3924:TYR:HE2	1.75	0.52
1:D:629:GLN:OE1	1:D:1669:ASN:ND2	2.42	0.52
1:G:671:LYS:N	1:G:819:TYR:O	2.42	0.52
1:J:420:ARG:HA	1:J:423:VAL:HB	1.91	0.52
1:J:680:ASP:O	1:J:799:LYS:NZ	2.41	0.52
1:D:207:PHE:HD1	1:G:2326:ILE:CD1	2.00	0.52
1:D:1938:GLN:HG3	1:D:3611:ASN:HA	1.91	0.52
1:D:3787:ASP:O	1:D:3865:ASN:ND2	2.42	0.52
1:G:467:ASP:N	1:G:467:ASP:OD1	2.38	0.52
1:G:4630:GLN:OE1	1:G:4633:ARG:NH2	2.43	0.52
1:J:1293:GLN:NE2	1:J:1548:THR:O	2.43	0.52
1:A:300:VAL:O	1:A:420:ARG:NE	2.34	0.52
1:D:2423:ILE:HG23	1:D:2427:LEU:HD23	1.89	0.52
1:D:2832:VAL:O	1:D:2895:LYS:NZ	2.38	0.52
1:A:3956:GLN:NE2	1:A:3973:MET:SD	2.82	0.52
1:D:1293:GLN:NE2	1:D:1548:THR:O	2.43	0.52
1:D:2423:ILE:O	1:D:2427:LEU:CG	2.54	0.52
3:F:61:ASN:ND2	3:F:63:THR:O	2.43	0.52
1:A:4634:LEU:O	1:A:4705:LYS:NZ	2.43	0.52
1:D:4630:GLN:OE1	1:D:4633:ARG:NH2	2.43	0.52
1:G:1811:GLY:HA3	1:G:1816:PHE:HB2	1.92	0.52
1:G:4634:LEU:O	1:G:4705:LYS:NZ	2.43	0.52
3:I:61:ASN:ND2	3:I:63:THR:O	2.43	0.52
1:J:3956:GLN:NE2	1:J:3973:MET:SD	2.82	0.52
1:A:654:SER:HB3	1:A:791:VAL:HG12	1.91	0.51
1:A:4630:GLN:OE1	1:A:4633:ARG:NH2	2.43	0.51
1:D:1440:ASN:N	1:D:1440:ASN:OD1	2.43	0.51
1:D:2593:LEU:O	1:D:2597:VAL:N	2.42	0.51
1:D:3875:THR:HG21	1:D:3924:TYR:HE2	1.75	0.51
1:G:681:HIS:ND1	1:G:797:GLY:O	2.44	0.51
1:G:956:HIS:HA	1:G:1060:TYR:HB3	1.92	0.51
1:J:620:CYS:SG	1:J:621:HIS:N	2.82	0.51
1:J:1209:VAL:N	1:J:1211:GLN:OE1	2.43	0.51
1:J:1811:GLY:HA3	1:J:1816:PHE:HB2	1.92	0.51
1:J:4634:LEU:O	1:J:4705:LYS:NZ	2.43	0.51
3:L:61:ASN:ND2	3:L:63:THR:O	2.43	0.51
1:A:1209:VAL:N	1:A:1211:GLN:OE1	2.43	0.51
1:A:3845:GLN:HG3	1:A:3923:GLU:HG3	1.90	0.51
1:D:680:ASP:O	1:D:799:LYS:NZ	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:300:VAL:O	1:J:420:ARG:NE	2.34	0.51
1:J:847:THR:OG1	1:J:1216:ASN:OD1	2.27	0.51
1:A:420:ARG:HA	1:A:423:VAL:HB	1.91	0.51
1:A:1440:ASN:N	1:A:1440:ASN:OD1	2.43	0.51
1:D:681:HIS:ND1	1:D:797:GLY:O	2.44	0.51
1:G:245:LEU:HD12	1:G:262:TYR:HE1	1.75	0.51
1:G:4497:ALA:HB2	1:G:4593:CYS:HB2	1.93	0.51
1:A:2138:GLU:O	1:A:2141:LYS:NZ	2.37	0.51
1:A:4497:ALA:HB2	1:A:4593:CYS:HB2	1.93	0.51
2:E:7:ILE:HD11	2:E:73:LYS:HB2	1.93	0.51
1:G:1440:ASN:N	1:G:1440:ASN:OD1	2.43	0.51
1:J:1756:SER:OG	1:J:1757:LEU:N	2.40	0.51
1:J:4094:ASP:OD1	1:J:4094:ASP:N	2.33	0.51
1:A:288:HIS:ND1	1:A:349:MET:O	2.37	0.51
1:A:618:CYS:O	1:A:629:GLN:NE2	2.38	0.51
1:G:1938:GLN:HG3	1:G:3611:ASN:HA	1.91	0.51
1:J:3875:THR:HG21	1:J:3924:TYR:HE2	1.75	0.51
1:J:4497:ALA:HB2	1:J:4593:CYS:HB2	1.93	0.51
1:J:4630:GLN:OE1	1:J:4633:ARG:NH2	2.43	0.51
1:A:4958:CYS:SG	1:A:4959:PHE:N	2.84	0.51
1:D:1429:SER:HA	1:D:1507:ILE:HG12	1.93	0.51
2:E:25:HIS:ND1	2:E:39:SER:OG	2.40	0.51
1:A:611:LEU:HD22	1:A:1660:LEU:HD22	1.92	0.51
1:D:731:HIS:HB2	1:D:740:THR:HA	1.93	0.51
1:D:1053:ALA:O	1:D:1056:THR:OG1	2.29	0.51
1:D:4497:ALA:HB2	1:D:4593:CYS:HB2	1.93	0.51
1:D:3788:VAL:HG22	1:D:3865:ASN:HB3	1.93	0.51
1:G:700:THR:HG22	1:G:787:LEU:H	1.76	0.51
1:G:1053:ALA:O	1:G:1056:THR:OG1	2.29	0.51
1:G:2213:LYS:HA	1:G:2254:LEU:HD21	1.93	0.51
1:J:1119:ARG:NH2	1:J:1196:ASP:O	2.40	0.51
1:J:1440:ASN:N	1:J:1440:ASN:OD1	2.43	0.51
1:A:245:LEU:HD12	1:A:262:TYR:HE1	1.75	0.51
1:A:3798:MET:HG2	1:A:3840:LEU:HD21	1.92	0.51
1:G:674:TYR:HE2	1:G:814:LEU:HB2	1.76	0.51
1:G:2883:LYS:O	1:G:2887:ARG:N	2.37	0.51
1:J:674:TYR:HE2	1:J:814:LEU:HB2	1.76	0.51
1:J:2213:LYS:HA	1:J:2254:LEU:HD21	1.93	0.51
1:A:620:CYS:SG	1:A:621:HIS:N	2.82	0.51
1:A:2423:ILE:O	1:A:2427:LEU:CG	2.54	0.51
1:D:956:HIS:HA	1:D:1060:TYR:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:611:LEU:HD22	1:G:1660:LEU:HD22	1.92	0.51
1:G:2712:ILE:O	1:G:2781:LYS:NZ	2.35	0.51
2:H:7:ILE:HD11	2:H:73:LYS:HB2	1.93	0.51
1:J:2832:VAL:O	1:J:2895:LYS:NZ	2.38	0.51
1:A:681:HIS:ND1	1:A:797:GLY:O	2.44	0.50
1:A:920:GLU:OE2	1:A:976:TYR:OH	2.29	0.50
1:D:4634:LEU:O	1:D:4705:LYS:NZ	2.43	0.50
1:G:4897:ASP:OD1	1:G:4897:ASP:N	2.43	0.50
1:J:188:SER:OG	1:J:190:ARG:NH2	2.36	0.50
1:J:190:ARG:NE	1:J:207:PHE:CZ	2.79	0.50
1:J:681:HIS:ND1	1:J:797:GLY:O	2.44	0.50
1:J:1429:SER:HA	1:J:1507:ILE:HG12	1.93	0.50
1:A:680:ASP:O	1:A:799:LYS:NZ	2.41	0.50
1:A:956:HIS:HA	1:A:1060:TYR:HB3	1.92	0.50
1:A:1429:SER:HA	1:A:1507:ILE:HG12	1.93	0.50
1:A:3797:LEU:HD22	1:A:3836:PHE:HZ	1.77	0.50
2:B:7:ILE:HD11	2:B:73:LYS:HB2	1.93	0.50
1:D:355:LYS:O	1:D:359:SER:OG	2.27	0.50
1:D:674:TYR:HE2	1:D:814:LEU:HB2	1.76	0.50
1:D:1298:ASP:OD1	1:D:1298:ASP:N	2.44	0.50
1:G:3788:VAL:HG22	1:G:3865:ASN:HB3	1.93	0.50
1:J:700:THR:HG22	1:J:787:LEU:H	1.76	0.50
1:G:4797:SER:OG	1:G:4805:MET:N	2.45	0.50
1:J:956:HIS:HA	1:J:1060:TYR:HB3	1.92	0.50
1:J:1434:PRO:HB2	1:J:1440:ASN:HD21	1.76	0.50
1:A:1434:PRO:HB2	1:A:1440:ASN:HD21	1.76	0.50
1:A:1449:ASP:OD1	1:A:1449:ASP:N	2.45	0.50
1:D:394:HIS:HD2	1:D:396:GLU:H	1.59	0.50
1:D:920:GLU:OE2	1:D:976:TYR:OH	2.29	0.50
1:D:3927:GLY:O	1:D:3929:CYS:N	2.44	0.50
1:G:920:GLU:OE2	1:G:976:TYR:OH	2.29	0.50
1:G:1091:GLU:OE1	1:G:1248:THR:OG1	2.30	0.50
1:J:245:LEU:HD12	1:J:262:TYR:HE1	1.75	0.50
1:J:611:LEU:HD22	1:J:1660:LEU:HD22	1.92	0.50
1:A:190:ARG:NE	1:A:207:PHE:CZ	2.80	0.50
1:A:271:ALA:O	1:A:301:THR:OG1	2.25	0.50
1:A:2213:LYS:HA	1:A:2254:LEU:HD21	1.93	0.50
1:D:3798:MET:HG2	1:D:3840:LEU:HD21	1.92	0.50
2:E:27:THR:HG23	2:E:100:ASP:HB3	1.93	0.50
1:G:1119:ARG:NH2	1:G:1196:ASP:O	2.40	0.50
1:G:1209:VAL:N	1:G:1211:GLN:OE1	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1053:ALA:O	1:J:1056:THR:OG1	2.29	0.50
1:J:4958:CYS:SG	1:J:4959:PHE:N	2.84	0.50
1:A:673:TRP:HA	1:A:820:ALA:HB3	1.94	0.50
1:A:674:TYR:HE2	1:A:814:LEU:HB2	1.76	0.50
1:A:700:THR:HG22	1:A:787:LEU:H	1.76	0.50
1:A:1091:GLU:OE1	1:A:1248:THR:OG1	2.30	0.50
2:B:27:THR:HG23	2:B:100:ASP:HB3	1.93	0.50
1:D:1209:VAL:N	1:D:1211:GLN:OE1	2.43	0.50
1:A:355:LYS:O	1:A:359:SER:OG	2.27	0.50
1:D:190:ARG:NE	1:D:207:PHE:CZ	2.80	0.50
1:G:3798:MET:HG2	1:G:3840:LEU:HD21	1.92	0.50
1:J:731:HIS:HB2	1:J:740:THR:HA	1.93	0.50
1:J:1298:ASP:OD1	1:J:1298:ASP:N	2.44	0.50
1:J:2793:THR:OG1	1:J:2901:GLY:O	2.29	0.50
1:J:3798:MET:HG2	1:J:3840:LEU:HD21	1.92	0.50
2:K:7:ILE:HD11	2:K:73:LYS:HB2	1.93	0.50
1:D:2213:LYS:HA	1:D:2254:LEU:HD21	1.93	0.50
1:G:394:HIS:HD2	1:G:396:GLU:H	1.59	0.50
1:G:1298:ASP:OD1	1:G:1298:ASP:N	2.44	0.50
1:G:1434:PRO:HB2	1:G:1440:ASN:HD21	1.76	0.50
1:G:2832:VAL:O	1:G:2895:LYS:NZ	2.38	0.50
2:H:25:HIS:ND1	2:H:39:SER:OG	2.40	0.50
1:J:920:GLU:OE2	1:J:976:TYR:OH	2.29	0.50
1:J:3797:LEU:HD22	1:J:3836:PHE:HZ	1.77	0.50
1:A:3733:HIS:O	1:A:3777:LYS:NZ	2.40	0.50
1:D:245:LEU:HD12	1:D:262:TYR:HE1	1.75	0.50
1:D:611:LEU:HD22	1:D:1660:LEU:HD22	1.92	0.50
1:D:700:THR:HG22	1:D:787:LEU:H	1.76	0.50
1:D:2132:SER:O	1:D:2132:SER:OG	2.30	0.50
1:G:731:HIS:HB2	1:G:740:THR:HA	1.93	0.50
1:G:3927:GLY:O	1:G:3929:CYS:N	2.45	0.50
1:G:4958:CYS:SG	1:G:4959:PHE:N	2.84	0.50
1:J:1449:ASP:OD1	1:J:1449:ASP:N	2.45	0.50
1:A:1044:LYS:HA	1:A:1047:LYS:HB2	1.94	0.49
1:D:431:ARG:HA	1:D:434:ASP:HB2	1.94	0.49
1:G:249:SER:OG	1:G:250:GLY:N	2.45	0.49
1:G:1429:SER:HA	1:G:1507:ILE:HG12	1.93	0.49
1:A:3927:GLY:O	1:A:3929:CYS:N	2.45	0.49
1:D:673:TRP:HA	1:D:820:ALA:HB3	1.94	0.49
1:D:3800:SER:OG	1:D:3801:CYS:N	2.44	0.49
2:H:27:THR:HG23	2:H:100:ASP:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1044:LYS:HA	1:J:1047:LYS:HB2	1.94	0.49
1:A:394:HIS:HD2	1:A:396:GLU:H	1.59	0.49
1:D:335:LYS:HZ3	1:D:401:ASP:HB2	1.78	0.49
1:J:1091:GLU:OE1	1:J:1248:THR:OG1	2.30	0.49
1:A:1930:SER:O	1:A:1930:SER:OG	2.24	0.49
1:A:2838:LEU:HD21	1:A:2894:LEU:HB2	1.94	0.49
1:A:3788:VAL:HG22	1:A:3865:ASN:HB3	1.93	0.49
1:D:2793:THR:OG1	1:D:2901:GLY:O	2.29	0.49
1:D:2838:LEU:HD21	1:D:2894:LEU:HB2	1.94	0.49
1:D:3797:LEU:HD22	1:D:3836:PHE:HZ	1.77	0.49
1:G:190:ARG:NE	1:G:207:PHE:CZ	2.80	0.49
1:J:394:HIS:HD2	1:J:396:GLU:H	1.59	0.49
1:J:431:ARG:HA	1:J:434:ASP:HB2	1.94	0.49
1:J:3604:PHE:HB2	3:L:52:MET:HG2	1.95	0.49
1:A:1265:HIS:CD2	1:A:1267:HIS:H	2.31	0.49
1:D:1058:LEU:HA	1:D:1062:TYR:H	1.78	0.49
1:G:431:ARG:HA	1:G:434:ASP:HB2	1.94	0.49
1:G:673:TRP:HA	1:G:820:ALA:HB3	1.94	0.49
1:G:4078:THR:OG1	1:G:4079:LEU:N	2.46	0.49
1:J:3788:VAL:HG22	1:J:3865:ASN:HB3	1.93	0.49
1:J:4922:PHE:HE2	1:J:4941:VAL:HG11	1.77	0.49
1:A:731:HIS:HB2	1:A:740:THR:HA	1.93	0.49
1:D:288:HIS:ND1	1:D:349:MET:O	2.37	0.49
1:D:1044:LYS:HA	1:D:1047:LYS:HB2	1.94	0.49
1:D:3646:ALA:HB1	1:D:3735:ARG:HH22	1.78	0.49
1:D:3759:THR:O	1:D:3759:THR:OG1	2.28	0.49
1:G:618:CYS:O	1:G:629:GLN:NE2	2.38	0.49
1:G:2838:LEU:HD21	1:G:2894:LEU:HB2	1.94	0.49
1:J:279:THR:HG22	1:J:281:ARG:H	1.78	0.49
1:J:2731:ASP:O	1:J:2735:MET:N	2.44	0.49
1:J:2838:LEU:HD21	1:J:2894:LEU:HB2	1.94	0.49
1:J:4060:THR:OG1	1:J:4063:GLU:OE2	2.27	0.49
1:A:2710:SER:HA	1:A:2781:LYS:HD3	1.93	0.49
1:A:4605:LYS:HG3	1:A:4609:ARG:HH21	1.77	0.49
1:D:1434:PRO:HB2	1:D:1440:ASN:HD21	1.76	0.49
1:D:2710:SER:HA	1:D:2781:LYS:HD3	1.93	0.49
1:D:4958:CYS:SG	1:D:4959:PHE:N	2.84	0.49
1:G:279:THR:HG22	1:G:281:ARG:H	1.78	0.49
1:G:1044:LYS:HA	1:G:1047:LYS:HB2	1.94	0.49
1:J:3646:ALA:HB1	1:J:3735:ARG:HH22	1.78	0.49
2:K:27:THR:HG23	2:K:100:ASP:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1911:LEU:HB2	1:A:2088:LEU:HD21	1.95	0.49
1:A:3604:PHE:HB2	3:C:52:MET:HG2	1.95	0.49
1:A:4922:PHE:HE2	1:A:4941:VAL:HG11	1.77	0.49
1:D:1091:GLU:OE1	1:D:1248:THR:OG1	2.30	0.49
1:D:2731:ASP:O	1:D:2735:MET:N	2.44	0.49
1:D:3604:PHE:HB2	3:F:52:MET:HG2	1.95	0.49
1:D:4797:SER:OG	1:D:4805:MET:N	2.45	0.49
1:D:4862:ILE:HD11	1:G:4757:ILE:HD13	1.93	0.49
1:G:844:ARG:NH1	1:G:849:ASP:OD1	2.46	0.49
1:G:2793:THR:OG1	1:G:2901:GLY:O	2.29	0.49
1:A:125:TYR:O	1:A:414:ARG:NH1	2.46	0.49
1:D:279:THR:HG22	1:D:281:ARG:H	1.78	0.49
1:G:248:PRO:HD3	1:G:261:HIS:CD2	2.48	0.49
1:G:3604:PHE:HB2	3:I:52:MET:HG2	1.95	0.49
1:G:3646:ALA:HB1	1:G:3735:ARG:HH22	1.78	0.49
1:J:125:TYR:O	1:J:414:ARG:NH1	2.46	0.49
1:J:248:PRO:HD3	1:J:261:HIS:CD2	2.48	0.49
1:J:1930:SER:O	1:J:1930:SER:OG	2.24	0.49
1:J:2774:TRP:HA	1:J:2777:LYS:HG2	1.95	0.49
1:J:4078:THR:OG1	1:J:4079:LEU:N	2.46	0.49
1:J:4957:ASP:OD1	1:J:4957:ASP:N	2.34	0.49
1:A:844:ARG:NH1	1:A:849:ASP:OD1	2.46	0.49
1:A:1298:ASP:OD1	1:A:1298:ASP:N	2.44	0.49
1:A:4757:ILE:HD13	1:J:4862:ILE:HD11	1.94	0.49
1:D:606:ARG:HH21	1:D:1632:ILE:HG23	1.78	0.49
1:G:1911:LEU:HB2	1:G:2088:LEU:HD21	1.95	0.49
1:G:2138:GLU:O	1:G:2141:LYS:NZ	2.37	0.49
1:G:3797:LEU:HD22	1:G:3836:PHE:HZ	1.77	0.49
1:J:3927:GLY:O	1:J:3929:CYS:N	2.45	0.49
1:A:1210:ALA:N	1:A:1211:GLN:OE1	2.46	0.48
1:A:2774:TRP:HA	1:A:2777:LYS:HG2	1.95	0.48
1:A:2844:MET:O	1:A:2848:ASN:N	2.40	0.48
1:A:4797:SER:OG	1:A:4805:MET:N	2.45	0.48
1:D:125:TYR:O	1:D:414:ARG:NH1	2.46	0.48
1:D:1210:ALA:N	1:D:1211:GLN:OE1	2.46	0.48
1:D:4922:PHE:HE2	1:D:4941:VAL:HG11	1.77	0.48
1:G:1058:LEU:HA	1:G:1062:TYR:H	1.78	0.48
1:G:2852:ILE:O	1:G:2856:LYS:N	2.44	0.48
1:J:1058:LEU:HA	1:J:1062:TYR:H	1.78	0.48
1:D:2834:LEU:HD21	1:D:2838:LEU:HD22	1.95	0.48
1:G:1629:SER:HA	1:G:1640:ASP:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4605:LYS:HG3	1:G:4609:ARG:HH21	1.77	0.48
1:J:673:TRP:HA	1:J:820:ALA:HB3	1.94	0.48
1:J:1210:ALA:N	1:J:1211:GLN:OE1	2.46	0.48
1:A:143:LEU:HD23	1:A:207:PHE:CE2	2.49	0.48
1:A:2314:VAL:HG23	1:A:2317:ASN:HB2	1.95	0.48
1:D:618:CYS:O	1:D:629:GLN:NE2	2.38	0.48
1:G:125:TYR:O	1:G:414:ARG:NH1	2.46	0.48
1:G:143:LEU:HD23	1:G:207:PHE:CE2	2.49	0.48
1:G:1210:ALA:N	1:G:1211:GLN:OE1	2.46	0.48
1:G:4922:PHE:HE2	1:G:4941:VAL:HG11	1.77	0.48
1:J:143:LEU:HD23	1:J:207:PHE:CE2	2.49	0.48
1:J:1011:ARG:HA	1:J:1014:GLN:HB3	1.95	0.48
1:J:1691:ASN:HB3	1:J:1694:MET:HG3	1.96	0.48
1:A:431:ARG:HA	1:A:434:ASP:HB2	1.94	0.48
1:D:248:PRO:HD3	1:D:261:HIS:CD2	2.48	0.48
1:D:1691:ASN:HB3	1:D:1694:MET:HG3	1.95	0.48
1:D:1911:LEU:HB2	1:D:2088:LEU:HD21	1.95	0.48
1:G:1265:HIS:CD2	1:G:1267:HIS:H	2.31	0.48
1:J:727:PHE:H	1:J:730:LEU:HD13	1.78	0.48
1:J:894:VAL:O	1:J:898:ILE:N	2.47	0.48
1:J:1911:LEU:HB2	1:J:2088:LEU:HD21	1.95	0.48
1:J:2314:VAL:HG23	1:J:2317:ASN:HB2	1.95	0.48
1:J:2710:SER:HA	1:J:2781:LYS:HD3	1.93	0.48
1:A:894:VAL:O	1:A:898:ILE:N	2.47	0.48
1:D:844:ARG:NH1	1:D:849:ASP:OD1	2.46	0.48
1:D:4074:ASP:O	1:D:4076:ASN:N	2.47	0.48
1:G:727:PHE:H	1:G:730:LEU:HD13	1.78	0.48
1:G:2731:ASP:O	1:G:2735:MET:N	2.44	0.48
1:G:2834:LEU:HD21	1:G:2838:LEU:HD22	1.95	0.48
1:J:1265:HIS:CD2	1:J:1267:HIS:H	2.31	0.48
1:J:1292:SER:O	1:J:1292:SER:OG	2.32	0.48
1:J:4605:LYS:HG3	1:J:4609:ARG:HH21	1.77	0.48
1:A:248:PRO:HD3	1:A:261:HIS:CD2	2.48	0.48
1:A:606:ARG:HH21	1:A:1632:ILE:HG23	1.78	0.48
1:D:4897:ASP:OD1	1:D:4897:ASP:N	2.43	0.48
1:J:844:ARG:NH1	1:J:849:ASP:OD1	2.46	0.48
1:A:727:PHE:H	1:A:730:LEU:HD13	1.78	0.48
1:A:1086:ARG:HH11	1:A:1251:LEU:HD12	1.79	0.48
1:D:620:CYS:SG	1:D:621:HIS:N	2.82	0.48
1:D:1629:SER:HA	1:D:1640:ASP:HA	1.95	0.48
1:G:2710:SER:HA	1:G:2781:LYS:HD3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:355:LYS:O	1:J:359:SER:OG	2.27	0.48
1:J:422:THR:HG21	1:J:459:LEU:HD11	1.96	0.48
2:K:25:HIS:ND1	2:K:39:SER:OG	2.40	0.48
1:D:1265:HIS:CD2	1:D:1267:HIS:H	2.31	0.48
1:G:207:PHE:CE1	1:J:2326:ILE:CG2	2.97	0.48
1:G:332:ARG:NE	1:G:364:GLN:OE1	2.47	0.48
1:G:606:ARG:HH21	1:G:1632:ILE:HG23	1.78	0.48
1:G:4862:ILE:HD11	1:J:4757:ILE:HD13	1.95	0.48
1:J:249:SER:OG	1:J:250:GLY:N	2.45	0.48
1:J:2132:SER:O	1:J:2132:SER:OG	2.30	0.48
1:A:249:SER:OG	1:A:250:GLY:N	2.45	0.48
1:A:1011:ARG:HA	1:A:1014:GLN:HB3	1.95	0.48
1:A:1058:LEU:HA	1:A:1062:TYR:H	1.78	0.48
1:A:2731:ASP:O	1:A:2735:MET:N	2.44	0.48
1:D:143:LEU:HD23	1:D:207:PHE:CE2	2.49	0.48
1:D:2774:TRP:HA	1:D:2777:LYS:HG2	1.95	0.48
1:D:4900:ASP:O	1:D:4902:VAL:N	2.47	0.48
1:G:55:SER:O	1:G:296:ARG:NH2	2.41	0.48
1:G:725:TYR:HD1	1:G:732:LEU:HB3	1.79	0.48
1:J:4900:ASP:O	1:J:4902:VAL:N	2.47	0.48
1:A:717:GLY:O	1:A:735:GLY:N	2.47	0.48
1:A:3724:LYS:HB3	1:A:3724:LYS:HE2	1.69	0.48
1:G:2774:TRP:HA	1:G:2777:LYS:HG2	1.95	0.48
1:J:1629:SER:HA	1:J:1640:ASP:HA	1.95	0.48
2:K:78:PRO:HA	2:K:81:ALA:HB3	1.96	0.48
1:A:302:THR:OG1	1:A:304:LYS:NZ	2.47	0.47
1:A:1116:GLY:HA3	1:A:1136:ALA:HA	1.96	0.47
1:A:2326:ILE:CG2	1:J:207:PHE:CE1	2.97	0.47
1:A:4074:ASP:O	1:A:4076:ASN:N	2.47	0.47
1:A:4804:ASP:OD1	1:A:4804:ASP:N	2.47	0.47
1:D:725:TYR:HD1	1:D:732:LEU:HB3	1.79	0.47
1:D:3854:ASP:OD1	1:D:3854:ASP:N	2.33	0.47
1:G:1177:LEU:N	1:G:1180:GLU:O	2.44	0.47
1:J:302:THR:OG1	1:J:304:LYS:NZ	2.47	0.47
1:A:207:PHE:CE1	1:D:2326:ILE:CG2	2.97	0.47
1:A:725:TYR:HD1	1:A:732:LEU:HB3	1.79	0.47
1:A:1629:SER:HA	1:A:1640:ASP:HA	1.95	0.47
1:A:2834:LEU:HD21	1:A:2838:LEU:HD22	1.95	0.47
1:A:3646:ALA:HB1	1:A:3735:ARG:HH22	1.78	0.47
1:A:4900:ASP:O	1:A:4902:VAL:N	2.47	0.47
1:D:249:SER:OG	1:D:250:GLY:N	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2314:VAL:HG23	1:D:2317:ASN:HB2	1.95	0.47
1:D:4605:LYS:HG3	1:D:4609:ARG:HH21	1.77	0.47
1:G:762:SER:O	1:G:762:SER:OG	2.33	0.47
1:G:1691:ASN:HB3	1:G:1694:MET:HG3	1.95	0.47
1:G:4900:ASP:O	1:G:4902:VAL:N	2.47	0.47
1:J:1116:GLY:HA3	1:J:1136:ALA:HA	1.96	0.47
1:A:279:THR:HG22	1:A:281:ARG:H	1.78	0.47
1:D:727:PHE:H	1:D:730:LEU:HD13	1.78	0.47
1:D:4804:ASP:OD1	1:D:4804:ASP:N	2.47	0.47
1:G:1011:ARG:HA	1:G:1014:GLN:HB3	1.95	0.47
2:H:78:PRO:HA	2:H:81:ALA:HB3	1.96	0.47
1:J:394:HIS:HD2	1:J:397:GLY:H	1.62	0.47
1:J:725:TYR:HD1	1:J:732:LEU:HB3	1.79	0.47
1:J:4804:ASP:N	1:J:4804:ASP:OD1	2.47	0.47
1:D:332:ARG:NE	1:D:364:GLN:OE1	2.47	0.47
2:E:78:PRO:HA	2:E:81:ALA:HB3	1.96	0.47
1:G:2427:LEU:HD12	1:G:2428:ILE:CG2	2.35	0.47
1:G:4074:ASP:O	1:G:4076:ASN:N	2.47	0.47
1:J:1219:LYS:HD3	1:J:1243:THR:HG23	1.96	0.47
1:J:2834:LEU:HD21	1:J:2838:LEU:HD22	1.95	0.47
1:J:2852:ILE:O	1:J:2856:LYS:N	2.44	0.47
1:A:332:ARG:NE	1:A:364:GLN:OE1	2.47	0.47
1:A:422:THR:HG21	1:A:459:LEU:HD11	1.96	0.47
1:A:1089:ARG:HH22	1:A:1600:PRO:HG3	1.80	0.47
1:A:1173:MET:HB3	1:A:1192:PHE:HB2	1.96	0.47
1:A:1691:ASN:HB3	1:A:1694:MET:HG3	1.95	0.47
1:D:422:THR:HG21	1:D:459:LEU:HD11	1.96	0.47
1:G:394:HIS:HD2	1:G:397:GLY:H	1.62	0.47
1:J:1086:ARG:HH11	1:J:1251:LEU:HD12	1.79	0.47
1:A:1119:ARG:NH2	1:A:1196:ASP:O	2.40	0.47
1:D:298:ARG:HE	1:D:303:GLY:HA2	1.80	0.47
1:D:717:GLY:O	1:D:735:GLY:N	2.47	0.47
1:D:1011:ARG:HA	1:D:1014:GLN:HB3	1.95	0.47
1:D:1173:MET:HB3	1:D:1192:PHE:HB2	1.96	0.47
1:D:2400:LEU:HD12	1:D:2424:LEU:HD22	1.97	0.47
1:D:3966:ILE:HD12	1:D:3966:ILE:HA	1.80	0.47
1:G:2314:VAL:HG23	1:G:2317:ASN:HB2	1.95	0.47
3:I:54:ASN:ND2	3:I:62:GLY:O	2.47	0.47
1:J:4074:ASP:O	1:J:4076:ASN:N	2.47	0.47
1:A:1053:ALA:O	1:A:1056:THR:OG1	2.29	0.47
1:A:1510:VAL:HG12	1:A:1511:VAL:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:78:PRO:HA	2:B:81:ALA:HB3	1.96	0.47
1:D:1140:PHE:HB2	1:D:1156:TRP:HE1	1.79	0.47
1:G:271:ALA:O	1:G:301:THR:OG1	2.25	0.47
1:G:302:THR:OG1	1:G:304:LYS:NZ	2.47	0.47
1:G:355:LYS:O	1:G:359:SER:OG	2.27	0.47
1:G:1089:ARG:HH22	1:G:1600:PRO:HG3	1.80	0.47
1:G:1116:GLY:HA3	1:G:1136:ALA:HA	1.96	0.47
1:G:1714:TYR:CZ	1:G:1761:MET:HB3	2.50	0.47
1:J:993:GLU:O	1:J:1051:ARG:NE	2.46	0.47
1:J:1089:ARG:HH22	1:J:1600:PRO:HG3	1.80	0.47
1:J:1104:GLU:HA	1:J:1163:GLY:HA2	1.97	0.47
1:J:1140:PHE:HB2	1:J:1156:TRP:HE1	1.79	0.47
1:J:2627:GLY:HA3	1:J:2677:LEU:HA	1.97	0.47
1:J:4797:SER:OG	1:J:4805:MET:N	2.45	0.47
1:A:1140:PHE:HB2	1:A:1156:TRP:HE1	1.79	0.47
1:A:1219:LYS:HD3	1:A:1243:THR:HG23	1.96	0.47
1:D:1086:ARG:HH11	1:D:1251:LEU:HD12	1.79	0.47
1:D:1104:GLU:HA	1:D:1163:GLY:HA2	1.97	0.47
1:D:1253:LYS:HD3	1:D:1601:ASN:HD21	1.80	0.47
3:F:54:ASN:ND2	3:F:62:GLY:O	2.47	0.47
1:G:422:THR:HG21	1:G:459:LEU:HD11	1.96	0.47
1:G:4507:ALA:O	1:G:4726:TYR:OH	2.33	0.47
1:G:4804:ASP:N	1:G:4804:ASP:OD1	2.47	0.47
1:J:332:ARG:NE	1:J:364:GLN:OE1	2.47	0.47
1:J:606:ARG:HH21	1:J:1632:ILE:HG23	1.78	0.47
1:J:717:GLY:O	1:J:735:GLY:N	2.47	0.47
1:J:1510:VAL:HG12	1:J:1511:VAL:HG23	1.97	0.47
1:J:1714:TYR:CZ	1:J:1761:MET:HB3	2.50	0.47
1:A:55:SER:O	1:A:296:ARG:NH2	2.41	0.47
1:D:207:PHE:CE1	1:G:2326:ILE:CG2	2.97	0.47
1:D:802:PHE:HB2	1:D:1617:TRP:HB2	1.97	0.47
1:D:1219:LYS:HD3	1:D:1243:THR:HG23	1.96	0.47
1:G:681:HIS:HB3	1:G:798:ILE:HA	1.97	0.47
1:G:1292:SER:O	1:G:1292:SER:OG	2.32	0.47
1:G:4627:ILE:O	1:G:4631:TRP:N	2.46	0.47
1:A:123:HIS:HD2	1:A:125:TYR:H	1.63	0.47
1:A:1104:GLU:HA	1:A:1163:GLY:HA2	1.97	0.47
1:A:2627:GLY:HA3	1:A:2677:LEU:HA	1.97	0.47
1:A:4507:ALA:O	1:A:4726:TYR:OH	2.33	0.47
1:D:123:HIS:HD2	1:D:125:TYR:H	1.63	0.47
1:D:1116:GLY:HA3	1:D:1136:ALA:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4078:THR:OG1	1:D:4079:LEU:N	2.46	0.47
1:G:717:GLY:O	1:G:735:GLY:N	2.47	0.47
1:G:802:PHE:HB2	1:G:1617:TRP:HB2	1.97	0.47
1:G:1253:LYS:HD3	1:G:1601:ASN:HD21	1.80	0.47
1:J:370:LEU:HB2	1:J:393:MET:HB3	1.97	0.47
1:J:1131:ASP:OD1	1:J:1131:ASP:N	2.48	0.47
1:A:1253:LYS:HD3	1:A:1601:ASN:HD21	1.80	0.46
1:D:681:HIS:HB3	1:D:798:ILE:HA	1.97	0.46
1:D:1131:ASP:OD1	1:D:1131:ASP:N	2.48	0.46
1:G:299:HIS:CD2	1:G:302:THR:HG22	2.50	0.46
1:G:2627:GLY:HA3	1:G:2677:LEU:HA	1.97	0.46
1:J:4584:SER:O	1:J:4584:SER:OG	2.33	0.46
1:A:2400:LEU:HD12	1:A:2424:LEU:HD22	1.97	0.46
1:G:143:LEU:HD23	1:G:207:PHE:HE2	1.80	0.46
1:G:298:ARG:HE	1:G:303:GLY:HA2	1.80	0.46
1:G:894:VAL:O	1:G:898:ILE:N	2.47	0.46
1:J:1173:MET:HB3	1:J:1192:PHE:HB2	1.96	0.46
1:J:3920:THR:O	1:J:3920:THR:OG1	2.32	0.46
1:A:1714:TYR:CZ	1:A:1761:MET:HB3	2.50	0.46
1:A:4638:THR:O	1:A:4651:LYS:NZ	2.39	0.46
1:D:370:LEU:HB2	1:D:393:MET:HB3	1.97	0.46
1:D:1272:ARG:HD2	1:D:1586:LEU:HD21	1.98	0.46
1:G:1086:ARG:HH11	1:G:1251:LEU:HD12	1.79	0.46
1:G:1104:GLU:HA	1:G:1163:GLY:HA2	1.97	0.46
1:G:1173:MET:HB3	1:G:1192:PHE:HB2	1.96	0.46
1:J:143:LEU:HD23	1:J:207:PHE:HE2	1.80	0.46
3:L:54:ASN:ND2	3:L:62:GLY:O	2.47	0.46
1:A:693:LEU:HD22	1:A:798:ILE:HG21	1.98	0.46
1:A:1272:ARG:HD2	1:A:1586:LEU:HD21	1.98	0.46
1:A:4078:THR:OG1	1:A:4079:LEU:N	2.46	0.46
1:A:4584:SER:O	1:A:4584:SER:OG	2.33	0.46
1:D:894:VAL:O	1:D:898:ILE:N	2.47	0.46
1:G:1140:PHE:HB2	1:G:1156:TRP:HE1	1.79	0.46
1:G:1219:LYS:HD3	1:G:1243:THR:HG23	1.96	0.46
1:J:298:ARG:HE	1:J:303:GLY:HA2	1.80	0.46
1:D:1510:VAL:HG12	1:D:1511:VAL:HG23	1.97	0.46
1:D:1714:TYR:CZ	1:D:1761:MET:HB3	2.50	0.46
1:G:123:HIS:HD2	1:G:125:TYR:H	1.63	0.46
1:G:1510:VAL:HG12	1:G:1511:VAL:HG23	1.97	0.46
1:A:2832:VAL:O	1:A:2895:LYS:NZ	2.38	0.46
1:A:4861:ALA:HB2	1:D:4864:GLN:HE21	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:38:SER:O	2:B:42:ARG:NH1	2.49	0.46
3:C:54:ASN:ND2	3:C:62:GLY:O	2.47	0.46
1:D:302:THR:OG1	1:D:304:LYS:NZ	2.47	0.46
1:D:1089:ARG:HH22	1:D:1600:PRO:HG3	1.80	0.46
1:D:2427:LEU:HD12	1:D:2428:ILE:CG2	2.35	0.46
1:D:2627:GLY:HA3	1:D:2677:LEU:HA	1.97	0.46
1:D:3072:THR:O	1:D:3076:LEU:N	2.49	0.46
1:D:4515:ASN:ND2	1:D:4740:PHE:O	2.33	0.46
1:G:4861:ALA:HB2	1:J:4864:GLN:HE21	1.81	0.46
1:J:693:LEU:HD22	1:J:798:ILE:HG21	1.98	0.46
1:J:1272:ARG:HD2	1:J:1586:LEU:HD21	1.98	0.46
1:A:298:ARG:HE	1:A:303:GLY:HA2	1.80	0.46
1:G:1272:ARG:HD2	1:G:1586:LEU:HD21	1.98	0.46
1:J:190:ARG:CZ	1:J:207:PHE:CZ	2.99	0.46
1:J:2400:LEU:HD12	1:J:2424:LEU:HD22	1.97	0.46
1:J:3072:THR:O	1:J:3076:LEU:N	2.49	0.46
1:A:190:ARG:CZ	1:A:207:PHE:CZ	2.99	0.46
1:A:2777:LYS:NZ	1:A:2778:GLU:OE2	2.49	0.46
2:B:78:PRO:HD3	2:B:96:THR:HG22	1.98	0.46
1:G:2400:LEU:HD12	1:G:2424:LEU:HD22	1.97	0.46
1:G:2777:LYS:NZ	1:G:2778:GLU:OE2	2.49	0.46
1:J:66:THR:OG1	1:J:124:SER:OG	2.29	0.46
1:J:123:HIS:HD2	1:J:125:TYR:H	1.63	0.46
1:J:2777:LYS:NZ	1:J:2778:GLU:OE2	2.49	0.46
1:J:4507:ALA:O	1:J:4726:TYR:OH	2.33	0.46
1:A:259:THR:HG1	1:A:261:HIS:CE1	2.30	0.46
1:A:299:HIS:CD2	1:A:302:THR:HG22	2.50	0.46
1:A:3072:THR:O	1:A:3076:LEU:N	2.49	0.46
1:D:992:GLN:HB2	1:D:1054:VAL:HG11	1.98	0.46
1:D:1299:ILE:HG13	1:D:1455:THR:HG23	1.98	0.46
2:E:78:PRO:HD3	2:E:96:THR:HG22	1.98	0.46
1:G:993:GLU:O	1:G:1051:ARG:NE	2.46	0.46
1:J:802:PHE:HB2	1:J:1617:TRP:HB2	1.97	0.46
1:J:4050:HIS:ND1	1:J:4054:GLU:OE2	2.48	0.46
1:A:370:LEU:HB2	1:A:393:MET:HB3	1.97	0.46
1:A:4862:ILE:HD11	1:D:4757:ILE:HD13	1.96	0.46
1:D:1118:SER:HG	1:D:1122:CYS:HG	1.63	0.46
1:D:1310:CYS:HB2	1:D:1536:SER:HA	1.98	0.46
1:D:4808:ASP:HB2	1:G:4523:VAL:HG12	1.97	0.46
2:E:38:SER:O	2:E:42:ARG:NH1	2.49	0.46
1:G:1670:HIS:ND1	1:G:1778:TYR:O	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:2313:SER:OG	1:G:2402:ARG:O	2.31	0.46
1:A:394:HIS:HD2	1:A:397:GLY:H	1.62	0.45
1:A:681:HIS:HB3	1:A:798:ILE:HA	1.97	0.45
1:D:4507:ALA:O	1:D:4726:TYR:OH	2.33	0.45
1:D:4725:TRP:HA	1:D:4728:THR:HG22	1.98	0.45
1:G:4589:ILE:HD13	1:G:4589:ILE:HA	1.83	0.45
1:J:1310:CYS:HB2	1:J:1536:SER:HA	1.98	0.45
1:J:2143:MET:HE1	1:J:2175:VAL:HG21	1.98	0.45
1:J:3724:LYS:HB3	1:J:3724:LYS:HE2	1.69	0.45
1:A:802:PHE:HB2	1:A:1617:TRP:HB2	1.97	0.45
1:A:878:LEU:HA	1:A:881:ILE:HB	1.98	0.45
1:A:1299:ILE:HG13	1:A:1455:THR:HG23	1.98	0.45
1:D:236:LEU:HD22	1:D:245:LEU:HD13	1.98	0.45
1:D:2777:LYS:NZ	1:D:2778:GLU:OE2	2.49	0.45
1:D:3911:ILE:HG23	1:D:3975:LEU:HD22	1.98	0.45
1:G:370:LEU:HB2	1:G:393:MET:HB3	1.97	0.45
1:G:878:LEU:HA	1:G:881:ILE:HB	1.98	0.45
1:G:4725:TRP:HA	1:G:4728:THR:HG22	1.99	0.45
1:J:681:HIS:HB3	1:J:798:ILE:HA	1.97	0.45
1:J:1253:LYS:HD3	1:J:1601:ASN:HD21	1.80	0.45
2:K:38:SER:O	2:K:42:ARG:NH1	2.49	0.45
1:A:27:THR:OG1	1:A:32:GLN:OE1	2.26	0.45
1:D:394:HIS:HD2	1:D:397:GLY:H	1.62	0.45
1:D:993:GLU:O	1:D:1051:ARG:NE	2.46	0.45
1:D:2106:THR:OG1	1:D:2107:TYR:N	2.50	0.45
1:D:2852:ILE:O	1:D:2856:LYS:N	2.44	0.45
1:D:3666:HIS:HD2	1:D:3735:ARG:HG3	1.82	0.45
1:D:4775:LEU:HD12	1:D:4775:LEU:HA	1.82	0.45
1:G:236:LEU:HD22	1:G:245:LEU:HD13	1.98	0.45
1:G:630:HIS:CE1	1:G:1671:ARG:HD3	2.52	0.45
1:J:236:LEU:HD22	1:J:245:LEU:HD13	1.98	0.45
1:J:1299:ILE:HG13	1:J:1455:THR:HG23	1.98	0.45
2:K:78:PRO:HD3	2:K:96:THR:HG22	1.98	0.45
1:A:993:GLU:O	1:A:1051:ARG:NE	2.46	0.45
1:D:630:HIS:CE1	1:D:1671:ARG:HD3	2.52	0.45
1:D:878:LEU:HA	1:D:881:ILE:HB	1.98	0.45
1:G:3072:THR:O	1:G:3076:LEU:N	2.49	0.45
1:J:2110:ASN:HB3	1:J:3615:HIS:CE1	2.52	0.45
1:A:2106:THR:OG1	1:A:2107:TYR:N	2.50	0.45
1:A:2132:SER:O	1:A:2132:SER:OG	2.30	0.45
1:A:2852:ILE:O	1:A:2856:LYS:N	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3911:ILE:HG23	1:A:3975:LEU:HD22	1.98	0.45
1:A:4725:TRP:HA	1:A:4728:THR:HG22	1.99	0.45
1:D:27:THR:OG1	1:D:32:GLN:OE1	2.26	0.45
1:D:271:ALA:O	1:D:301:THR:OG1	2.25	0.45
1:D:374:TYR:HA	1:D:391:ALA:HA	1.99	0.45
1:G:1299:ILE:HG13	1:G:1455:THR:HG23	1.98	0.45
1:G:4050:HIS:ND1	1:G:4054:GLU:OE2	2.48	0.45
1:J:374:TYR:HA	1:J:391:ALA:HA	1.99	0.45
1:J:2106:THR:OG1	1:J:2107:TYR:N	2.50	0.45
1:J:2846:ALA:O	1:J:2850:HIS:N	2.50	0.45
1:A:1310:CYS:HB2	1:A:1536:SER:HA	1.98	0.45
1:A:1670:HIS:ND1	1:A:1778:TYR:O	2.49	0.45
1:A:2110:ASN:HB3	1:A:3615:HIS:CE1	2.52	0.45
1:A:2143:MET:HE1	1:A:2175:VAL:HG21	1.98	0.45
1:A:3631:GLU:OE1	1:A:3631:GLU:N	2.48	0.45
1:D:55:SER:O	1:D:296:ARG:NH2	2.41	0.45
1:D:299:HIS:CD2	1:D:302:THR:HG22	2.50	0.45
1:D:1670:HIS:ND1	1:D:1778:TYR:O	2.49	0.45
1:D:4880:GLN:OE1	1:D:4880:GLN:HA	2.17	0.45
1:G:1131:ASP:OD1	1:G:1131:ASP:N	2.48	0.45
2:H:38:SER:O	2:H:42:ARG:NH1	2.49	0.45
1:A:2793:THR:OG1	1:A:2901:GLY:O	2.29	0.45
1:A:3666:HIS:HD2	1:A:3735:ARG:HG3	1.82	0.45
1:A:4627:ILE:O	1:A:4631:TRP:N	2.46	0.45
1:A:4880:GLN:OE1	1:A:4880:GLN:HA	2.17	0.45
1:D:190:ARG:CZ	1:D:207:PHE:CZ	2.99	0.45
1:D:3631:GLU:OE1	1:D:3631:GLU:N	2.48	0.45
1:G:1310:CYS:HB2	1:G:1536:SER:HA	1.98	0.45
1:G:2767:LYS:HD2	1:G:2767:LYS:HA	1.73	0.45
1:G:3911:ILE:HG23	1:G:3975:LEU:HD22	1.98	0.45
1:G:4880:GLN:OE1	1:G:4880:GLN:HA	2.17	0.45
1:A:143:LEU:HD23	1:A:207:PHE:HE2	1.80	0.45
1:D:874:LEU:HD21	1:D:941:LYS:HA	1.99	0.45
1:D:1057:LEU:O	1:D:1061:GLY:N	2.50	0.45
1:D:4627:ILE:O	1:D:4631:TRP:N	2.46	0.45
1:G:1057:LEU:O	1:G:1061:GLY:N	2.50	0.45
1:J:4725:TRP:HA	1:J:4728:THR:HG22	1.99	0.45
1:J:4880:GLN:OE1	1:J:4880:GLN:HA	2.17	0.45
1:A:236:LEU:HD22	1:A:245:LEU:HD13	1.98	0.45
1:A:374:TYR:HA	1:A:391:ALA:HA	1.99	0.45
1:A:992:GLN:HB2	1:A:1054:VAL:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2270:LEU:HD23	1:A:2270:LEU:HA	1.84	0.45
1:D:3724:LYS:HB3	1:D:3724:LYS:HE2	1.69	0.45
1:G:992:GLN:HB2	1:G:1054:VAL:HG21	1.98	0.45
1:G:3666:HIS:HD2	1:G:3735:ARG:HG3	1.82	0.45
1:G:4775:LEU:HD12	1:G:4775:LEU:HA	1.82	0.45
1:J:299:HIS:CD2	1:J:302:THR:HG22	2.50	0.45
1:J:1111:GLY:HA3	1:J:1211:GLN:HE21	1.82	0.45
1:J:1670:HIS:ND1	1:J:1778:TYR:O	2.49	0.45
1:A:1111:GLY:HA3	1:A:1211:GLN:HE21	1.82	0.45
1:A:1131:ASP:N	1:A:1131:ASP:OD1	2.48	0.45
1:D:365:HIS:HD2	1:D:368:THR:HG23	1.82	0.45
1:D:1177:LEU:N	1:D:1180:GLU:O	2.44	0.45
1:D:2110:ASN:HB3	1:D:3615:HIS:CE1	2.52	0.45
1:D:2857:LYS:HE3	1:D:2858:LYS:HD2	1.99	0.45
1:G:190:ARG:CZ	1:G:207:PHE:CZ	2.99	0.45
1:G:2853:TRP:HA	1:G:2856:LYS:HB2	1.99	0.45
1:G:4808:ASP:HB2	1:J:4523:VAL:HG12	1.99	0.45
1:J:992:GLN:HB2	1:J:1054:VAL:HG11	1.98	0.45
1:J:2853:TRP:HA	1:J:2856:LYS:HB2	1.99	0.45
1:A:270:HIS:ND1	1:A:491:GLU:OE1	2.51	0.44
1:A:594:ILE:HD12	1:A:631:LEU:HD23	2.00	0.44
1:A:2846:ALA:O	1:A:2850:HIS:N	2.50	0.44
1:D:270:HIS:ND1	1:D:491:GLU:OE1	2.51	0.44
1:D:4810:MET:HB3	1:G:4519:LEU:O	2.16	0.44
1:G:374:TYR:HA	1:G:391:ALA:HA	1.99	0.44
1:J:618:CYS:O	1:J:629:GLN:NE2	2.38	0.44
1:J:1177:LEU:N	1:J:1180:GLU:O	2.44	0.44
1:J:4945:TYR:OH	7:J:6003:CFF:H81	2.17	0.44
1:A:630:HIS:CE1	1:A:1671:ARG:HD3	2.52	0.44
1:A:874:LEU:HD21	1:A:941:LYS:HA	1.99	0.44
1:A:1614:ARG:HA	1:A:1614:ARG:HD3	1.83	0.44
1:A:2853:TRP:HA	1:A:2856:LYS:HB2	1.99	0.44
1:A:4864:GLN:HE21	1:J:4861:ALA:HB2	1.82	0.44
1:A:4943:LYS:HB3	1:A:4943:LYS:HE2	1.81	0.44
1:D:693:LEU:HD22	1:D:798:ILE:HG21	1.98	0.44
1:D:4050:HIS:ND1	1:D:4054:GLU:OE2	2.48	0.44
1:G:693:LEU:HD22	1:G:798:ILE:HG21	1.98	0.44
1:G:2110:ASN:HB3	1:G:3615:HIS:CE1	2.52	0.44
1:G:2857:LYS:HE3	1:G:2858:LYS:HD2	2.00	0.44
1:G:3724:LYS:HB3	1:G:3724:LYS:HE2	1.69	0.44
1:G:4515:ASN:ND2	1:G:4740:PHE:O	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4638:THR:O	1:G:4651:LYS:NZ	2.39	0.44
2:H:78:PRO:HD3	2:H:96:THR:HG22	1.98	0.44
1:J:594:ILE:HD12	1:J:631:LEU:HD23	2.00	0.44
1:J:2156:PHE:HD1	1:J:2163:MET:HG2	1.82	0.44
1:J:2871:LEU:HG	1:J:2878:LEU:HD21	2.00	0.44
1:J:2891:GLN:O	1:J:2895:LYS:N	2.48	0.44
1:A:616:SER:O	1:A:616:SER:OG	2.35	0.44
1:A:734:SER:OG	1:A:734:SER:O	2.36	0.44
1:A:2714:ILE:HD13	1:A:2780:LEU:HD11	2.00	0.44
1:A:2767:LYS:HD2	1:A:2767:LYS:HA	1.73	0.44
1:A:3762:LEU:HD12	1:A:3762:LEU:HA	1.83	0.44
1:A:4945:TYR:OH	7:A:6003:CFF:H81	2.17	0.44
1:D:143:LEU:HD23	1:D:207:PHE:HE2	1.80	0.44
1:D:1169:THR:OG1	1:D:1170:GLU:N	2.51	0.44
1:D:2391:THR:HA	1:D:2394:ALA:HB3	1.99	0.44
1:D:2714:ILE:HD13	1:D:2780:LEU:HD11	2.00	0.44
1:G:470:LEU:HD12	1:G:470:LEU:HA	1.87	0.44
1:G:2024:LEU:HB3	1:G:2025:THR:H	1.47	0.44
1:G:4945:TYR:OH	7:G:6003:CFF:H81	2.17	0.44
1:J:270:HIS:ND1	1:J:491:GLU:OE1	2.51	0.44
1:J:878:LEU:HA	1:J:881:ILE:HB	1.98	0.44
1:J:3666:HIS:HD2	1:J:3735:ARG:HG3	1.82	0.44
1:J:3911:ILE:HG23	1:J:3975:LEU:HD22	1.98	0.44
1:J:4627:ILE:O	1:J:4631:TRP:N	2.46	0.44
1:J:4897:ASP:N	1:J:4897:ASP:OD1	2.43	0.44
1:A:4934:HIS:HB3	1:A:4939:SER:HB2	2.00	0.44
1:D:757:CYS:SG	1:D:758:CYS:N	2.90	0.44
1:D:1111:GLY:HA3	1:D:1211:GLN:HE21	1.82	0.44
1:D:2767:LYS:HA	1:D:2767:LYS:HD2	1.73	0.44
1:D:2846:ALA:O	1:D:2850:HIS:N	2.50	0.44
1:D:2853:TRP:HA	1:D:2856:LYS:HB2	1.99	0.44
1:D:4589:ILE:HD13	1:D:4589:ILE:HA	1.83	0.44
1:G:188:SER:O	1:G:190:ARG:NH2	2.51	0.44
1:G:2846:ALA:O	1:G:2850:HIS:N	2.50	0.44
1:G:3966:ILE:HD12	1:G:3966:ILE:HA	1.80	0.44
1:J:365:HIS:HD2	1:J:368:THR:HG23	1.82	0.44
1:J:630:HIS:CE1	1:J:1671:ARG:HD3	2.52	0.44
1:J:1169:THR:OG1	1:J:1170:GLU:N	2.51	0.44
1:A:2857:LYS:HE3	1:A:2858:LYS:HD2	2.00	0.44
1:D:842:GLN:H	1:D:848:ARG:HD3	1.83	0.44
1:J:2270:LEU:HD23	1:J:2270:LEU:HA	1.84	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:4638:THR:O	1:J:4651:LYS:NZ	2.39	0.44
1:A:900:LEU:HB3	1:A:902:TRP:CD1	2.53	0.44
1:D:2227:SER:OG	1:D:2228:VAL:N	2.51	0.44
1:D:4788:ASN:CG	1:G:4738:PHE:CD2	2.88	0.44
1:G:270:HIS:ND1	1:G:491:GLU:OE1	2.51	0.44
1:G:1111:GLY:HA3	1:G:1211:GLN:HE21	1.82	0.44
1:G:2156:PHE:HD1	1:G:2163:MET:HG2	1.82	0.44
1:J:762:SER:O	1:J:762:SER:OG	2.33	0.44
1:D:2156:PHE:HD1	1:D:2163:MET:HG2	1.82	0.44
1:J:27:THR:OG1	1:J:32:GLN:OE1	2.26	0.44
1:J:3640:LYS:HA	1:J:3640:LYS:HD2	1.81	0.44
1:A:1057:LEU:O	1:A:1061:GLY:N	2.50	0.44
1:A:4519:LEU:O	1:J:4810:MET:HB3	2.18	0.44
1:A:4523:VAL:HG12	1:J:4808:ASP:HB2	1.98	0.44
1:G:624:ALA:HB2	1:G:1667:LEU:HD12	2.00	0.44
1:J:900:LEU:HB3	1:J:902:TRP:CD1	2.53	0.44
1:J:1057:LEU:O	1:J:1061:GLY:N	2.50	0.44
1:J:2714:ILE:HD13	1:J:2780:LEU:HD11	2.00	0.44
1:J:2857:LYS:HE3	1:J:2858:LYS:HD2	1.99	0.44
1:J:4934:HIS:HB3	1:J:4939:SER:HB2	2.00	0.44
1:A:1169:THR:OG1	1:A:1170:GLU:N	2.51	0.44
1:A:1757:LEU:HD12	1:A:1757:LEU:HA	1.88	0.44
1:A:2227:SER:OG	1:A:2228:VAL:N	2.51	0.44
1:A:4738:PHE:CD2	1:J:4788:ASN:CG	2.89	0.44
1:A:4775:LEU:HD12	1:A:4775:LEU:HA	1.82	0.44
1:A:4897:ASP:OD1	1:A:4897:ASP:N	2.43	0.44
1:D:734:SER:OG	1:D:734:SER:O	2.36	0.44
1:G:594:ILE:HD12	1:G:631:LEU:HD23	2.00	0.44
1:G:757:CYS:SG	1:G:758:CYS:N	2.90	0.44
1:G:831:LYS:HE3	1:G:831:LYS:HB2	1.80	0.44
1:G:2714:ILE:HD13	1:G:2780:LEU:HD11	2.00	0.44
1:J:558:LEU:HD23	1:J:558:LEU:HA	1.88	0.44
1:J:1224:LEU:HD23	1:J:1224:LEU:HA	1.85	0.44
1:J:2138:GLU:O	1:J:2141:LYS:NZ	2.37	0.44
1:J:4752:LYS:HD2	1:J:4752:LYS:HA	1.75	0.44
1:A:365:HIS:HD2	1:A:368:THR:HG23	1.82	0.43
1:A:757:CYS:SG	1:A:758:CYS:N	2.90	0.43
1:A:1610:ARG:HE	1:A:1610:ARG:HB3	1.64	0.43
1:A:3786:LYS:HE2	1:A:3786:LYS:HB3	1.79	0.43
2:B:17:LYS:N	2:B:20:GLN:OE1	2.50	0.43
1:D:169:ARG:HH21	1:D:176:ARG:HH11	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4792:LYS:H	1:D:4792:LYS:HG2	1.57	0.43
1:G:1169:THR:OG1	1:G:1170:GLU:N	2.51	0.43
1:G:4046:LYS:HB2	1:G:4046:LYS:HE3	1.81	0.43
1:J:757:CYS:SG	1:J:758:CYS:N	2.90	0.43
1:A:2871:LEU:HG	1:A:2878:LEU:HD21	2.00	0.43
1:A:4613:PHE:HE2	1:A:4948:ARG:HD2	1.83	0.43
1:D:900:LEU:HB3	1:D:902:TRP:CD1	2.53	0.43
1:D:4584:SER:O	1:D:4584:SER:OG	2.33	0.43
1:D:4934:HIS:HB3	1:D:4939:SER:HB2	2.00	0.43
1:G:3762:LEU:HD12	1:G:3762:LEU:HA	1.83	0.43
1:G:4613:PHE:HE2	1:G:4948:ARG:HD2	1.83	0.43
1:J:188:SER:O	1:J:190:ARG:NH2	2.51	0.43
1:A:188:SER:O	1:A:190:ARG:NH2	2.51	0.43
1:A:938:GLU:HA	1:A:941:LYS:HG3	2.00	0.43
1:A:1224:LEU:HD23	1:A:1224:LEU:HA	1.85	0.43
1:A:3804:LEU:HD13	1:A:3910:ALA:HB2	2.00	0.43
1:A:4801:ASP:N	1:A:4801:ASP:OD1	2.51	0.43
1:D:594:ILE:HD12	1:D:631:LEU:HD23	2.00	0.43
1:J:3631:GLU:OE1	1:J:3631:GLU:N	2.48	0.43
1:A:677:LEU:HD23	1:A:677:LEU:HA	1.87	0.43
1:D:4801:ASP:OD1	1:D:4801:ASP:N	2.51	0.43
1:G:335:LYS:HZ3	1:G:401:ASP:HB2	1.83	0.43
1:G:365:HIS:HD2	1:G:368:THR:HG23	1.82	0.43
1:G:874:LEU:HD21	1:G:941:LYS:HA	1.99	0.43
1:G:2871:LEU:HG	1:G:2878:LEU:HD21	2.00	0.43
1:J:616:SER:O	1:J:616:SER:OG	2.35	0.43
1:J:1764:SER:OG	1:J:1779:SER:O	2.36	0.43
1:A:2103:LEU:HA	1:A:2106:THR:HG22	2.00	0.43
1:A:2156:PHE:HD1	1:A:2163:MET:HG2	1.82	0.43
1:A:2391:THR:HA	1:A:2394:ALA:HB3	1.99	0.43
1:D:3760:LEU:HD23	1:D:3760:LEU:HA	1.78	0.43
1:G:123:HIS:CD2	1:G:125:TYR:H	2.37	0.43
1:G:2227:SER:OG	1:G:2228:VAL:N	2.51	0.43
1:G:2308:PHE:HE1	1:G:2475:ARG:HH22	1.67	0.43
1:G:4943:LYS:HB3	1:G:4943:LYS:HE2	1.81	0.43
1:J:335:LYS:HZ3	1:J:401:ASP:HB2	1.83	0.43
1:J:734:SER:OG	1:J:734:SER:O	2.36	0.43
1:J:874:LEU:HD21	1:J:941:LYS:HA	1.99	0.43
1:J:2391:THR:HA	1:J:2394:ALA:HB3	1.99	0.43
1:J:2427:LEU:HD12	1:J:2428:ILE:CG2	2.35	0.43
1:J:3804:LEU:HD13	1:J:3910:ALA:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:4613:PHE:HE2	1:J:4948:ARG:HD2	1.83	0.43
1:A:2308:PHE:HE1	1:A:2475:ARG:HH22	1.67	0.43
1:A:4845:ILE:CD1	1:D:4819:TYR:CD1	3.02	0.43
1:D:188:SER:O	1:D:190:ARG:NH2	2.51	0.43
1:D:4835:PRO:HG3	1:D:4844:ARG:HG2	2.01	0.43
1:D:4845:ILE:CD1	1:G:4819:TYR:CD1	3.01	0.43
1:D:4945:TYR:OH	7:D:6003:CFF:H81	2.17	0.43
1:G:2391:THR:HA	1:G:2394:ALA:HB3	1.99	0.43
1:G:3804:LEU:HD13	1:G:3910:ALA:HB2	2.00	0.43
1:G:3890:TYR:O	1:G:3894:SER:N	2.52	0.43
1:J:169:ARG:HH21	1:J:176:ARG:HH11	1.66	0.43
1:J:2227:SER:OG	1:J:2228:VAL:N	2.51	0.43
1:J:4801:ASP:OD1	1:J:4801:ASP:N	2.51	0.43
3:L:45:THR:HG23	3:L:48:GLU:H	1.84	0.43
1:A:25:THR:HG22	1:A:34:LYS:HA	2.01	0.43
1:A:4894:ILE:HD13	1:A:4894:ILE:HA	1.89	0.43
1:D:679:VAL:HA	1:D:800:VAL:HG23	2.01	0.43
1:G:1690:GLU:HG2	1:G:1790:LYS:HE3	2.01	0.43
1:G:4788:ASN:CG	1:J:4738:PHE:CD2	2.90	0.43
1:J:1842:ILE:HD12	1:J:1845:LEU:HD23	2.01	0.43
1:J:2103:LEU:HA	1:J:2106:THR:HG22	2.00	0.43
1:J:4504:ARG:NH1	1:J:4746:ASP:OD1	2.52	0.43
1:J:4775:LEU:HD12	1:J:4775:LEU:HA	1.82	0.43
1:A:123:HIS:CD2	1:A:125:TYR:H	2.37	0.43
1:A:207:PHE:HB3	1:D:2326:ILE:CD1	2.49	0.43
1:A:1112:ASP:H	1:A:1211:GLN:NE2	2.17	0.43
3:C:45:THR:HG23	3:C:48:GLU:H	1.84	0.43
1:D:4504:ARG:NH1	1:D:4746:ASP:OD1	2.52	0.43
1:D:4791:ARG:HH22	1:G:4523:VAL:HG21	1.83	0.43
1:D:4861:ALA:HB2	1:G:4864:GLN:HE21	1.84	0.43
1:G:842:GLN:H	1:G:848:ARG:HD3	1.83	0.43
1:G:1764:SER:OG	1:G:1779:SER:O	2.36	0.43
1:G:4835:PRO:HG3	1:G:4844:ARG:HG2	2.01	0.43
1:J:799:LYS:HB2	1:J:1618:LEU:HD11	2.00	0.43
1:A:842:GLN:H	1:A:848:ARG:HD3	1.83	0.43
1:A:1177:LEU:N	1:A:1180:GLU:O	2.44	0.43
1:A:1690:GLU:HG2	1:A:1790:LYS:HE3	2.01	0.43
1:D:624:ALA:HB2	1:D:1667:LEU:HD12	2.00	0.43
1:D:4613:PHE:HE2	1:D:4948:ARG:HD2	1.83	0.43
1:G:679:VAL:HA	1:G:800:VAL:HG23	2.01	0.43
1:G:900:LEU:HB3	1:G:902:TRP:CD1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:938:GLU:HA	1:G:941:LYS:HG3	2.00	0.43
1:G:1255:LEU:HD22	1:G:1451:HIS:HB2	2.01	0.43
1:J:679:VAL:HA	1:J:800:VAL:HG23	2.01	0.43
1:J:706:TYR:HA	1:J:707:PRO:HD3	1.85	0.43
1:J:2770:GLU:HA	1:J:2773:ARG:HB3	2.01	0.43
1:J:2988:SER:O	1:J:2992:CYS:N	2.52	0.43
1:J:4835:PRO:HG3	1:J:4844:ARG:HG2	2.01	0.43
1:A:1255:LEU:HD22	1:A:1451:HIS:HB2	2.01	0.43
1:A:2718:LEU:HA	1:A:2721:PHE:HB3	2.01	0.43
1:A:3760:LEU:HD23	1:A:3760:LEU:HA	1.78	0.43
1:A:4835:PRO:HG3	1:A:4844:ARG:HG2	2.01	0.43
1:G:1040:ASP:HA	1:G:1043:LYS:HB2	2.01	0.43
1:G:4934:HIS:HB3	1:G:4939:SER:HB2	2.00	0.43
1:J:25:THR:HG22	1:J:34:LYS:HA	2.01	0.43
1:J:135:THR:OG1	1:J:146:ASP:OD2	2.36	0.43
1:J:842:GLN:H	1:J:848:ARG:HD3	1.83	0.43
1:J:1107:ALA:HB3	1:J:1160:ASP:HB2	2.01	0.43
1:J:1255:LEU:HD22	1:J:1451:HIS:HB2	2.01	0.43
1:J:1614:ARG:HA	1:J:1614:ARG:HD3	1.83	0.43
1:J:2718:LEU:HA	1:J:2721:PHE:HB3	2.01	0.43
1:A:135:THR:OG1	1:A:146:ASP:OD2	2.36	0.42
1:A:760:ASP:HB3	1:A:763:ALA:HB3	2.01	0.42
1:A:1842:ILE:HD12	1:A:1845:LEU:HD23	2.01	0.42
1:A:2777:LYS:HE2	1:A:2781:LYS:HE3	2.01	0.42
1:A:3617:ALA:O	1:A:3621:PHE:N	2.51	0.42
1:D:1255:LEU:HD22	1:D:1451:HIS:HB2	2.01	0.42
1:D:2718:LEU:HA	1:D:2721:PHE:HB3	2.01	0.42
1:D:2770:GLU:HA	1:D:2773:ARG:HB3	2.01	0.42
1:D:3592:LEU:HD23	1:D:3592:LEU:HA	1.91	0.42
1:D:4610:LYS:HD3	1:D:4616:LEU:HD22	2.01	0.42
1:G:498:VAL:HG23	1:G:533:LEU:HD22	2.01	0.42
1:G:2106:THR:OG1	1:G:2107:TYR:N	2.50	0.42
1:G:4885:MET:O	6:G:6002:ATP:H1'	2.18	0.42
1:J:938:GLU:HA	1:J:941:LYS:HG3	2.00	0.42
1:J:2308:PHE:HE1	1:J:2475:ARG:HH22	1.67	0.42
1:A:1086:ARG:NH1	1:A:1252:SER:O	2.53	0.42
1:A:2326:ILE:CD1	1:J:207:PHE:HB3	2.50	0.42
1:A:2770:GLU:HA	1:A:2773:ARG:HB3	2.01	0.42
1:A:4610:LYS:HD3	1:A:4616:LEU:HD22	2.01	0.42
1:D:25:THR:HG22	1:D:34:LYS:HA	2.01	0.42
1:D:555:LEU:HD23	1:D:555:LEU:HA	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:799:LYS:HB2	1:D:1618:LEU:HD11	2.00	0.42
1:D:915:HIS:CE1	1:D:917:CYS:HB2	2.54	0.42
1:D:3804:LEU:HD13	1:D:3910:ALA:HB2	2.00	0.42
1:G:915:HIS:CE1	1:G:917:CYS:HB2	2.54	0.42
1:G:2718:LEU:HA	1:G:2721:PHE:HB3	2.01	0.42
1:G:2770:GLU:HA	1:G:2773:ARG:HB3	2.01	0.42
1:G:4584:SER:O	1:G:4584:SER:OG	2.33	0.42
1:G:4723:LEU:HD13	1:G:4723:LEU:HA	1.88	0.42
1:G:4810:MET:HB3	1:J:4519:LEU:O	2.19	0.42
1:J:1040:ASP:HA	1:J:1043:LYS:HB2	2.01	0.42
1:J:1112:ASP:H	1:J:1211:GLN:NE2	2.17	0.42
1:J:1685:LEU:HD23	1:J:1685:LEU:HA	1.88	0.42
1:J:2317:ASN:HA	1:J:2317:ASN:HD22	1.66	0.42
1:J:3759:THR:O	1:J:3759:THR:OG1	2.28	0.42
1:A:915:HIS:CE1	1:A:917:CYS:HB2	2.54	0.42
1:A:1605:LYS:HA	1:A:1605:LYS:HD3	1.83	0.42
1:A:4504:ARG:NH1	1:A:4746:ASP:OD1	2.52	0.42
1:A:4589:ILE:HD13	1:A:4589:ILE:HA	1.83	0.42
1:D:1764:SER:OG	1:D:1779:SER:O	2.36	0.42
1:D:2169:HIS:HB3	1:D:2204:PHE:CE2	2.55	0.42
1:D:2871:LEU:HG	1:D:2878:LEU:HD21	1.99	0.42
3:F:45:THR:HG23	3:F:48:GLU:H	1.84	0.42
1:G:4610:LYS:HD3	1:G:4616:LEU:HD22	2.01	0.42
1:G:4753:THR:O	1:G:4753:THR:OG1	2.34	0.42
1:J:306:LEU:O	1:J:327:THR:OG1	2.32	0.42
1:J:624:ALA:HB2	1:J:1667:LEU:HD12	2.00	0.42
1:J:1709:ILE:HD13	1:J:1709:ILE:HA	1.92	0.42
1:J:4610:LYS:HD3	1:J:4616:LEU:HD22	2.01	0.42
1:A:309:MET:O	1:A:313:SER:N	2.53	0.42
1:A:624:ALA:HB2	1:A:1667:LEU:HD12	2.00	0.42
1:A:4050:HIS:ND1	1:A:4054:GLU:OE2	2.48	0.42
1:D:1112:ASP:H	1:D:1211:GLN:NE2	2.17	0.42
1:D:2397:ILE:HD13	1:D:2397:ILE:HA	1.88	0.42
1:D:2788:TRP:NE1	1:D:2906:ARG:O	2.53	0.42
1:D:4770:LEU:HD13	1:G:4751:PHE:CD1	2.55	0.42
1:G:169:ARG:HH21	1:G:176:ARG:HH11	1.66	0.42
1:G:675:TYR:HB2	1:G:804:LEU:HD21	2.01	0.42
1:G:2169:HIS:HB3	1:G:2204:PHE:CE2	2.55	0.42
1:G:4160:GLN:HE22	1:G:4205:ALA:HA	1.85	0.42
1:G:4504:ARG:NH1	1:G:4746:ASP:OD1	2.52	0.42
1:G:4651:LYS:HG2	1:G:4671:LEU:HD23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:17:LYS:N	2:H:20:GLN:OE1	2.50	0.42
1:J:498:VAL:HG23	1:J:533:LEU:HD22	2.01	0.42
1:J:1690:GLU:HG2	1:J:1790:LYS:HE3	2.01	0.42
1:A:169:ARG:HH21	1:A:176:ARG:HH11	1.66	0.42
1:A:1107:ALA:HB3	1:A:1160:ASP:HB2	2.01	0.42
1:A:1256:PRO:HB3	1:A:1597:SER:HA	2.02	0.42
1:A:2788:TRP:NE1	1:A:2906:ARG:O	2.53	0.42
1:D:470:LEU:HD12	1:D:470:LEU:HA	1.87	0.42
1:D:616:SER:O	1:D:616:SER:OG	2.34	0.42
1:D:760:ASP:HB3	1:D:763:ALA:HB3	2.01	0.42
1:D:1086:ARG:NH1	1:D:1252:SER:O	2.53	0.42
1:D:2308:PHE:HE1	1:D:2475:ARG:HH22	1.67	0.42
1:D:3919:ASN:O	1:D:3922:THR:OG1	2.32	0.42
1:D:4518:LEU:HD21	1:D:4738:PHE:CE1	2.54	0.42
1:G:343:ARG:HB3	1:G:344:LYS:H	1.60	0.42
1:G:883:GLU:HA	1:G:886:ALA:HB3	2.02	0.42
1:G:1224:LEU:HD23	1:G:1224:LEU:HA	1.85	0.42
1:G:1610:ARG:HE	1:G:1610:ARG:HB3	1.64	0.42
1:G:4052:ALA:O	1:G:4056:HIS:ND1	2.52	0.42
3:I:45:THR:HG23	3:I:48:GLU:H	1.84	0.42
1:J:246:THR:HG22	1:J:247:VAL:H	1.84	0.42
1:J:271:ALA:O	1:J:301:THR:OG1	2.25	0.42
1:J:3890:TYR:O	1:J:3894:SER:N	2.52	0.42
1:A:59:PRO:HD3	1:A:322:ALA:HB3	2.01	0.42
1:A:246:THR:HG22	1:A:247:VAL:H	1.84	0.42
1:A:470:LEU:HD12	1:A:470:LEU:HA	1.87	0.42
1:A:555:LEU:HD23	1:A:555:LEU:HA	1.87	0.42
1:A:679:VAL:HA	1:A:800:VAL:HG23	2.01	0.42
1:A:3829:LYS:HE3	1:A:3829:LYS:HB3	1.83	0.42
1:A:3890:TYR:O	1:A:3894:SER:N	2.52	0.42
1:A:4518:LEU:HD21	1:A:4738:PHE:CE1	2.55	0.42
1:D:259:THR:HG1	1:D:261:HIS:CE1	2.31	0.42
1:D:1690:GLU:HG2	1:D:1790:LYS:HE3	2.01	0.42
1:G:59:PRO:HD3	1:G:322:ALA:HB3	2.01	0.42
1:J:883:GLU:HA	1:J:886:ALA:HB3	2.02	0.42
1:J:2788:TRP:NE1	1:J:2906:ARG:O	2.53	0.42
1:A:228:LEU:HD23	1:A:228:LEU:HA	1.91	0.42
1:A:284:TRP:O	1:A:287:SER:OG	2.31	0.42
1:A:1157:GLN:N	1:A:1160:ASP:OD2	2.42	0.42
1:A:4867:ILE:HG21	1:J:4858:ILE:CD1	2.49	0.42
1:D:3640:LYS:HA	1:D:3640:LYS:HD2	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3890:TYR:O	1:D:3894:SER:N	2.52	0.42
1:D:4858:ILE:CD1	1:G:4867:ILE:HG21	2.50	0.42
1:G:1086:ARG:NH1	1:G:1252:SER:O	2.53	0.42
1:G:1112:ASP:H	1:G:1211:GLN:NE2	2.17	0.42
1:G:3592:LEU:HD23	1:G:3592:LEU:HA	1.91	0.42
1:G:3631:GLU:OE1	1:G:3631:GLU:N	2.48	0.42
1:J:675:TYR:HB2	1:J:804:LEU:HD21	2.01	0.42
1:A:290:ARG:HA	1:A:353:GLU:HG2	2.02	0.42
1:A:831:LYS:HE3	1:A:831:LYS:HB2	1.80	0.42
1:A:2154:LYS:HB2	1:A:2154:LYS:HE2	1.79	0.42
1:A:4819:TYR:CD1	1:J:4845:ILE:CD1	3.02	0.42
1:D:883:GLU:HA	1:D:886:ALA:HB3	2.02	0.42
1:D:938:GLU:HA	1:D:941:LYS:HG3	2.00	0.42
1:D:1610:ARG:HE	1:D:1610:ARG:HB3	1.64	0.42
1:D:1843:LEU:HD23	1:D:1843:LEU:HA	1.93	0.42
1:D:2103:LEU:HA	1:D:2106:THR:HG22	2.00	0.42
1:D:2988:SER:O	1:D:2992:CYS:N	2.52	0.42
1:D:4943:LYS:HE2	1:D:4943:LYS:HB3	1.81	0.42
1:G:25:THR:HG22	1:G:34:LYS:HA	2.01	0.42
1:G:162:ILE:O	1:G:163:HIS:ND1	2.53	0.42
1:G:799:LYS:HB2	1:G:1618:LEU:HD11	2.00	0.42
1:G:1107:ALA:HB3	1:G:1160:ASP:HB2	2.01	0.42
1:G:1165:MET:HB3	1:G:1236:TYR:CE1	2.55	0.42
1:G:1842:ILE:HD12	1:G:1845:LEU:HD23	2.01	0.42
1:G:2788:TRP:NE1	1:G:2906:ARG:O	2.53	0.42
1:G:2823:SER:O	1:G:2823:SER:OG	2.37	0.42
3:I:37:MET:HG2	3:I:44:PRO:HG3	2.02	0.42
1:J:309:MET:O	1:J:313:SER:N	2.53	0.42
1:J:677:LEU:HD23	1:J:677:LEU:HA	1.87	0.42
1:J:915:HIS:CE1	1:J:917:CYS:HB2	2.54	0.42
1:J:1086:ARG:NH1	1:J:1252:SER:O	2.53	0.42
1:J:1256:PRO:HB3	1:J:1597:SER:HA	2.02	0.42
1:J:4160:GLN:HE22	1:J:4205:ALA:HA	1.85	0.42
1:A:1292:SER:O	1:A:1292:SER:OG	2.32	0.42
1:A:4515:ASN:ND2	1:A:4740:PHE:O	2.33	0.42
1:D:309:MET:O	1:D:313:SER:N	2.53	0.42
1:D:2313:SER:OG	1:D:2402:ARG:O	2.31	0.42
1:D:4046:LYS:HE3	1:D:4046:LYS:HB2	1.81	0.42
1:G:2067:MET:HE1	1:G:2088:LEU:HD23	2.02	0.42
1:G:2103:LEU:HA	1:G:2106:THR:HG22	2.00	0.42
1:G:4845:ILE:CD1	1:J:4819:TYR:CD1	3.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:559:ILE:H	1:J:559:ILE:HG13	1.72	0.42
1:J:1165:MET:HB3	1:J:1236:TYR:CE1	2.55	0.42
1:J:2313:SER:OG	1:J:2402:ARG:O	2.31	0.42
1:J:2422:SER:O	1:J:2426:SER:OG	2.33	0.42
1:J:3617:ALA:O	1:J:3621:PHE:N	2.51	0.42
1:J:3762:LEU:HD12	1:J:3762:LEU:HA	1.83	0.42
1:J:4046:LYS:HE3	1:J:4046:LYS:HB2	1.81	0.42
1:J:4885:MET:O	6:J:6002:ATP:H1'	2.20	0.42
1:A:853:PRO:HD2	1:A:1209:VAL:HA	2.02	0.42
1:A:883:GLU:HA	1:A:886:ALA:HB3	2.02	0.42
1:A:1768:PHE:HE1	2:B:90:VAL:HG21	1.85	0.42
1:A:2427:LEU:HD12	1:A:2428:ILE:CG2	2.35	0.42
1:D:1107:ALA:HB3	1:D:1160:ASP:HB2	2.01	0.42
1:D:2764:LEU:HD23	1:D:2764:LEU:HA	1.91	0.42
1:D:3794:LEU:HD23	1:D:3794:LEU:HA	1.81	0.42
1:G:448:PRO:HB2	1:G:451:SER:HB3	2.02	0.42
1:G:4600:ILE:HD13	1:G:4600:ILE:HA	1.88	0.42
1:J:59:PRO:HD3	1:J:322:ALA:HB3	2.01	0.42
1:J:290:ARG:HA	1:J:353:GLU:HG2	2.02	0.42
1:J:760:ASP:HB3	1:J:763:ALA:HB3	2.01	0.42
1:J:2067:MET:HE1	1:J:2088:LEU:HD23	2.02	0.42
1:J:2777:LYS:HE2	1:J:2781:LYS:HE3	2.02	0.42
1:J:4943:LYS:HE2	1:J:4943:LYS:HB3	1.81	0.42
1:A:2313:SER:OG	1:A:2402:ARG:O	2.31	0.41
1:D:59:PRO:HD3	1:D:322:ALA:HB3	2.01	0.41
1:D:123:HIS:CD2	1:D:125:TYR:H	2.37	0.41
1:D:162:ILE:O	1:D:163:HIS:ND1	2.53	0.41
1:D:498:VAL:HG23	1:D:533:LEU:HD22	2.01	0.41
1:D:706:TYR:HA	1:D:707:PRO:HD3	1.85	0.41
1:D:1040:ASP:HA	1:D:1043:LYS:HB2	2.01	0.41
1:D:1256:PRO:HB3	1:D:1597:SER:HA	2.02	0.41
1:D:1809:PRO:HB2	1:D:1817:LEU:HD22	2.02	0.41
1:D:1842:ILE:HD12	1:D:1845:LEU:HD23	2.01	0.41
1:D:2259:ARG:HA	1:D:2259:ARG:HD3	1.87	0.41
1:D:4638:THR:O	1:D:4651:LYS:NZ	2.39	0.41
1:G:66:THR:OG1	1:G:124:SER:OG	2.29	0.41
1:G:246:THR:HG22	1:G:247:VAL:H	1.84	0.41
1:G:1843:LEU:HD23	1:G:1843:LEU:HA	1.93	0.41
1:G:4858:ILE:CD1	1:J:4867:ILE:HG21	2.49	0.41
1:J:1809:PRO:HB2	1:J:1817:LEU:HD22	2.02	0.41
2:K:17:LYS:N	2:K:20:GLN:OE1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:ILE:O	1:A:163:HIS:ND1	2.53	0.41
1:A:1040:ASP:HA	1:A:1043:LYS:HB2	2.01	0.41
1:A:1165:MET:HB3	1:A:1236:TYR:CE1	2.55	0.41
1:A:4885:MET:O	6:A:6002:ATP:H1'	2.21	0.41
2:B:40:ARG:H	2:B:40:ARG:HG2	1.64	0.41
1:D:448:PRO:HB2	1:D:451:SER:HB3	2.02	0.41
1:D:1157:GLN:N	1:D:1160:ASP:OD2	2.42	0.41
1:D:1165:MET:HB3	1:D:1236:TYR:CE1	2.55	0.41
1:D:3786:LYS:HB3	1:D:3786:LYS:HE2	1.79	0.41
1:D:3829:LYS:HE3	1:D:3829:LYS:HB3	1.83	0.41
1:D:4752:LYS:HA	1:D:4752:LYS:HD2	1.75	0.41
1:G:309:MET:O	1:G:313:SER:N	2.53	0.41
1:G:4801:ASP:OD1	1:G:4801:ASP:N	2.51	0.41
1:J:1610:ARG:HE	1:J:1610:ARG:HB3	1.64	0.41
1:J:4651:LYS:HG2	1:J:4671:LEU:HD23	2.01	0.41
1:A:498:VAL:HG23	1:A:533:LEU:HD22	2.01	0.41
1:A:1685:LEU:HA	1:A:1685:LEU:HD23	1.88	0.41
1:A:3669:ILE:HD12	1:A:3735:ARG:HB3	2.02	0.41
1:A:4911:LEU:O	1:A:4915:ASN:ND2	2.42	0.41
1:D:156:GLU:HG3	1:D:187:SER:HB3	2.02	0.41
1:D:1757:LEU:HD12	1:D:1757:LEU:HA	1.88	0.41
1:D:1822:ILE:O	1:D:1826:TYR:N	2.47	0.41
1:G:1256:PRO:HB3	1:G:1597:SER:HA	2.02	0.41
1:G:1809:PRO:HB2	1:G:1817:LEU:HD22	2.02	0.41
1:G:2891:GLN:O	1:G:2895:LYS:N	2.48	0.41
1:G:4896:ASN:O	1:G:4900:ASP:HB2	2.20	0.41
1:J:143:LEU:O	1:J:143:LEU:CG	2.68	0.41
1:J:1182:LEU:HD23	1:J:1182:LEU:HA	1.90	0.41
1:A:799:LYS:HB2	1:A:1618:LEU:HD11	2.00	0.41
1:A:1809:PRO:HB2	1:A:1817:LEU:HD22	2.02	0.41
1:A:1942:ARG:HG3	1:A:3611:ASN:HB2	2.02	0.41
1:A:3640:LYS:HA	1:A:3640:LYS:HD2	1.81	0.41
1:A:4896:ASN:O	1:A:4900:ASP:HB2	2.20	0.41
1:D:135:THR:OG1	1:D:146:ASP:OD2	2.36	0.41
1:D:246:THR:HG22	1:D:247:VAL:H	1.84	0.41
1:D:290:ARG:HA	1:D:353:GLU:HG2	2.02	0.41
1:D:1091:GLU:HG3	1:D:1250:TRP:CH2	2.55	0.41
1:D:2777:LYS:HE2	1:D:2781:LYS:HE3	2.02	0.41
1:D:3689:TYR:HE2	1:D:3759:THR:HB	1.86	0.41
1:G:558:LEU:HD22	1:G:571:ILE:HG12	2.03	0.41
1:G:2512:ASP:N	1:G:2512:ASP:OD1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:123:HIS:CD2	1:J:125:TYR:H	2.37	0.41
1:J:4518:LEU:HD21	1:J:4738:PHE:CE1	2.55	0.41
1:A:558:LEU:HD23	1:A:558:LEU:HA	1.88	0.41
1:A:565:LEU:HD22	1:A:604:HIS:HE1	1.86	0.41
1:A:2058:THR:N	1:A:2061:GLN:OE1	2.54	0.41
1:A:2169:HIS:HB3	1:A:2204:PHE:CE2	2.55	0.41
1:A:4651:LYS:HG2	1:A:4671:LEU:HD23	2.01	0.41
1:D:831:LYS:HB2	1:D:831:LYS:HE3	1.80	0.41
1:D:2143:MET:HE1	1:D:2175:VAL:HG21	2.01	0.41
1:D:4052:ALA:O	1:D:4056:HIS:ND1	2.52	0.41
1:G:760:ASP:HB3	1:G:763:ALA:HB3	2.01	0.41
1:G:1273:ILE:HD11	1:G:1287:GLN:HB2	2.03	0.41
1:G:2764:LEU:HD23	1:G:2764:LEU:HA	1.91	0.41
1:G:2777:LYS:HE2	1:G:2781:LYS:HE3	2.01	0.41
1:G:2988:SER:O	1:G:2992:CYS:N	2.52	0.41
1:J:555:LEU:HD23	1:J:555:LEU:HA	1.87	0.41
1:J:2169:HIS:HB3	1:J:2204:PHE:CE2	2.55	0.41
1:J:2823:SER:O	1:J:2823:SER:OG	2.37	0.41
3:L:37:MET:HG2	3:L:44:PRO:HG3	2.02	0.41
1:A:448:PRO:HB2	1:A:451:SER:HB3	2.02	0.41
1:A:1182:LEU:HD23	1:A:1182:LEU:HA	1.91	0.41
1:A:4041:LYS:HB3	1:A:4043:VAL:HG12	2.02	0.41
1:A:4160:GLN:HE22	1:A:4205:ALA:HA	1.85	0.41
1:A:4618:ILE:HD13	1:A:4618:ILE:HA	1.87	0.41
1:D:675:TYR:HB2	1:D:804:LEU:HD21	2.01	0.41
1:D:1548:THR:OG1	1:D:1549:SER:N	2.54	0.41
1:D:1625:LEU:HD23	1:D:1625:LEU:HA	1.90	0.41
1:D:1768:PHE:HE1	2:E:90:VAL:HG21	1.85	0.41
1:D:1796:THR:HG22	1:D:1845:LEU:HD11	2.03	0.41
1:D:1942:ARG:HG3	1:D:3611:ASN:HB2	2.02	0.41
1:D:4160:GLN:HE22	1:D:4205:ALA:HA	1.85	0.41
3:F:49:LEU:HD12	3:F:49:LEU:HA	1.92	0.41
1:G:288:HIS:ND1	1:G:349:MET:O	2.37	0.41
1:G:1768:PHE:HE1	2:H:90:VAL:HG21	1.85	0.41
1:G:1796:THR:HG22	1:G:1845:LEU:HD11	2.03	0.41
1:G:2058:THR:N	1:G:2061:GLN:OE1	2.54	0.41
1:G:4137:ILE:HG23	1:G:4151:PHE:HE1	1.86	0.41
1:G:4770:LEU:HD13	1:J:4751:PHE:CD1	2.56	0.41
1:J:558:LEU:HD22	1:J:571:ILE:HG12	2.03	0.41
1:J:2058:THR:N	1:J:2061:GLN:OE1	2.54	0.41
1:J:3669:ILE:HD12	1:J:3735:ARG:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1548:THR:OG1	1:A:1549:SER:N	2.54	0.41
1:A:4751:PHE:CD1	1:J:4770:LEU:HD13	2.55	0.41
1:A:4808:ASP:HB2	1:D:4523:VAL:HG12	2.01	0.41
1:D:228:LEU:HD23	1:D:228:LEU:HA	1.91	0.41
1:D:853:PRO:HD2	1:D:1209:VAL:HA	2.03	0.41
1:D:1273:ILE:HD11	1:D:1287:GLN:HB2	2.03	0.41
1:D:4041:LYS:HB3	1:D:4043:VAL:HG12	2.02	0.41
1:D:4753:THR:O	1:D:4753:THR:OG1	2.34	0.41
3:F:37:MET:HG2	3:F:44:PRO:HG3	2.02	0.41
1:G:734:SER:OG	1:G:734:SER:O	2.36	0.41
1:G:3689:TYR:HE2	1:G:3759:THR:HB	1.86	0.41
1:J:162:ILE:O	1:J:163:HIS:ND1	2.53	0.41
1:J:288:HIS:ND1	1:J:349:MET:O	2.37	0.41
1:J:853:PRO:HD2	1:J:1209:VAL:HA	2.02	0.41
1:J:2767:LYS:HD2	1:J:2767:LYS:HA	1.73	0.41
1:J:3636:TYR:HD1	1:J:3636:TYR:HA	1.78	0.41
1:J:4896:ASN:O	1:J:4900:ASP:HB2	2.20	0.41
1:A:675:TYR:HB2	1:A:804:LEU:HD21	2.01	0.41
1:A:4029:SER:HA	1:A:4034:LYS:HE2	2.02	0.41
1:A:4723:LEU:HD13	1:A:4723:LEU:HA	1.88	0.41
1:A:4810:MET:HB3	1:D:4519:LEU:O	2.20	0.41
1:A:4845:ILE:HD12	1:D:4819:TYR:CG	2.55	0.41
1:D:2512:ASP:N	1:D:2512:ASP:OD1	2.54	0.41
1:D:3742:LEU:HD12	1:D:3742:LEU:HA	1.89	0.41
1:D:3762:LEU:HA	1:D:3762:LEU:HD12	1.83	0.41
1:G:259:THR:HG1	1:G:261:HIS:CE1	2.33	0.41
1:G:3759:THR:O	1:G:3759:THR:OG1	2.28	0.41
1:G:3829:LYS:HB3	1:G:3829:LYS:HE3	1.83	0.41
1:J:1091:GLU:HG3	1:J:1250:TRP:CH2	2.56	0.41
1:J:1548:THR:OG1	1:J:1549:SER:N	2.54	0.41
1:J:3966:ILE:HA	1:J:3966:ILE:HD12	1.80	0.41
1:J:4753:THR:O	1:J:4753:THR:OG1	2.34	0.41
1:A:1796:THR:HG22	1:A:1845:LEU:HD11	2.03	0.41
1:A:3689:TYR:HE2	1:A:3759:THR:HB	1.86	0.41
1:D:70:GLU:HG3	1:D:71:GLN:HG3	2.03	0.41
1:D:1181:ILE:H	1:D:1181:ILE:HG13	1.74	0.41
1:D:1710:HIS:CD2	1:D:1782:PHE:HB3	2.56	0.41
1:D:2067:MET:HE1	1:D:2088:LEU:HD23	2.03	0.41
1:D:3998:LYS:HB2	1:D:3998:LYS:HE3	1.85	0.41
1:D:4651:LYS:HG2	1:D:4671:LEU:HD23	2.01	0.41
1:D:4896:ASN:O	1:D:4900:ASP:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:156:GLU:HG3	1:G:187:SER:HB3	2.02	0.41
1:G:693:LEU:HD22	1:G:798:ILE:HD13	2.03	0.41
1:G:1262:PRO:HG2	1:G:1264:SER:H	1.86	0.41
1:G:3617:ALA:O	1:G:3621:PHE:N	2.51	0.41
3:I:49:LEU:HD12	3:I:49:LEU:HA	1.92	0.41
1:J:35:LEU:H	1:J:35:LEU:HG	1.75	0.41
1:J:448:PRO:HB2	1:J:451:SER:HB3	2.02	0.41
1:J:693:LEU:HD22	1:J:798:ILE:HD13	2.03	0.41
1:J:3760:LEU:HD23	1:J:3760:LEU:HA	1.78	0.41
1:A:1709:ILE:HD13	1:A:1709:ILE:HA	1.92	0.41
1:A:2988:SER:O	1:A:2992:CYS:N	2.52	0.41
1:D:1167:ASP:OD1	1:D:1236:TYR:OH	2.28	0.41
1:G:70:GLU:HG3	1:G:71:GLN:HG3	2.03	0.41
1:G:290:ARG:HA	1:G:353:GLU:HG2	2.02	0.41
1:G:2323:ARG:HE	1:G:2323:ARG:HB3	1.71	0.41
1:J:55:SER:O	1:J:296:ARG:NH2	2.41	0.41
1:J:156:GLU:HG3	1:J:187:SER:HB3	2.02	0.41
1:J:565:LEU:HD22	1:J:604:HIS:HE1	1.86	0.41
1:J:833:LYS:HE2	1:J:833:LYS:HB2	1.90	0.41
1:J:1796:THR:HG22	1:J:1845:LEU:HD11	2.03	0.41
1:J:4010:ASN:OD1	1:J:4010:ASN:N	2.41	0.41
1:A:558:LEU:HD22	1:A:571:ILE:HG12	2.03	0.40
1:A:4788:ASN:CG	1:D:4738:PHE:CD2	2.94	0.40
1:D:1709:ILE:HD13	1:D:1709:ILE:HA	1.92	0.40
1:D:3669:ILE:HD12	1:D:3735:ARG:HB3	2.02	0.40
2:E:40:ARG:H	2:E:40:ARG:HG2	1.64	0.40
1:G:1091:GLU:HG3	1:G:1250:TRP:CH2	2.56	0.40
1:G:1548:THR:OG1	1:G:1549:SER:N	2.54	0.40
1:G:4029:SER:HA	1:G:4034:LYS:HE2	2.02	0.40
1:J:35:LEU:HD13	1:J:49:LEU:HD22	2.03	0.40
1:J:673:TRP:N	1:J:759:LEU:O	2.51	0.40
1:J:1768:PHE:HE1	2:K:90:VAL:HG21	1.85	0.40
1:J:3689:TYR:HE2	1:J:3759:THR:HB	1.86	0.40
1:A:204:ASP:N	1:A:204:ASP:OD1	2.55	0.40
1:A:1091:GLU:HG3	1:A:1250:TRP:CH2	2.56	0.40
1:D:558:LEU:HD22	1:D:571:ILE:HG12	2.03	0.40
1:D:752:ASP:N	1:D:752:ASP:OD1	2.55	0.40
1:D:3943:ASP:OD1	1:D:3943:ASP:N	2.54	0.40
1:D:4845:ILE:HD12	1:G:4819:TYR:CG	2.56	0.40
1:D:4882:LYS:HZ3	1:D:4882:LYS:HG2	1.82	0.40
1:G:673:TRP:N	1:G:759:LEU:O	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4808:ASP:HB2	1:J:4523:VAL:HG11	2.04	0.40
1:J:752:ASP:N	1:J:752:ASP:OD1	2.55	0.40
1:J:1454:ASP:OD1	1:J:1454:ASP:N	2.54	0.40
1:J:1605:LYS:HA	1:J:1605:LYS:HD3	1.83	0.40
1:J:4002:ASP:HA	1:J:4005:VAL:HG22	2.02	0.40
1:A:156:GLU:HG3	1:A:187:SER:HB3	2.02	0.40
1:A:646:THR:OG1	1:A:647:ARG:N	2.55	0.40
1:A:1710:HIS:CD2	1:A:1782:PHE:HB3	2.56	0.40
1:A:2067:MET:HE1	1:A:2088:LEU:HD23	2.03	0.40
1:A:2259:ARG:HD3	1:A:2259:ARG:HA	1.87	0.40
1:A:3620:LEU:HD23	1:A:3620:LEU:HA	1.93	0.40
1:A:4752:LYS:HD2	1:A:4752:LYS:HA	1.75	0.40
1:D:145:PHE:O	1:D:205:ALA:N	2.51	0.40
1:D:646:THR:OG1	1:D:647:ARG:N	2.55	0.40
1:D:1262:PRO:HG2	1:D:1264:SER:H	1.86	0.40
1:D:1614:ARG:HA	1:D:1614:ARG:HD3	1.83	0.40
1:G:135:THR:OG1	1:G:146:ASP:OD2	2.36	0.40
1:G:3669:ILE:HD12	1:G:3735:ARG:HB3	2.02	0.40
1:J:70:GLU:HG3	1:J:71:GLN:HG3	2.03	0.40
1:J:646:THR:OG1	1:J:647:ARG:N	2.55	0.40
1:J:1262:PRO:HG2	1:J:1264:SER:H	1.86	0.40
1:J:1710:HIS:CD2	1:J:1782:PHE:HB3	2.56	0.40
1:J:2154:LYS:HB2	1:J:2154:LYS:HE2	1.79	0.40
1:A:559:ILE:H	1:A:559:ILE:HG13	1.72	0.40
1:A:2512:ASP:OD1	1:A:2512:ASP:N	2.54	0.40
1:A:3966:ILE:HD12	1:A:3966:ILE:HA	1.80	0.40
1:A:4002:ASP:HA	1:A:4005:VAL:HG22	2.02	0.40
1:A:4849:ILE:HD13	1:D:4823:ARG:HD3	2.04	0.40
3:C:37:MET:HG2	3:C:44:PRO:HG3	2.02	0.40
1:D:66:THR:OG1	1:D:124:SER:OG	2.29	0.40
1:D:1255:LEU:HD23	1:D:1255:LEU:HA	1.91	0.40
1:D:4029:SER:HA	1:D:4034:LYS:HE2	2.02	0.40
1:G:355:LYS:HE3	1:G:355:LYS:HB3	1.91	0.40
1:G:565:LEU:HD22	1:G:604:HIS:HE1	1.86	0.40
1:G:853:PRO:HD2	1:G:1209:VAL:HA	2.02	0.40
1:G:3760:LEU:HD23	1:G:3760:LEU:HA	1.78	0.40
1:J:35:LEU:HD13	1:J:49:LEU:HD13	2.04	0.40
1:J:355:LYS:HE3	1:J:355:LYS:HB3	1.91	0.40
1:J:3598:ARG:HG2	3:L:40:LEU:HD11	2.04	0.40
1:J:3860:ARG:HH11	1:J:3860:ARG:HD3	1.76	0.40
1:A:1273:ILE:HD11	1:A:1287:GLN:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4819:TYR:CG	1:J:4845:ILE:HD12	2.56	0.40
3:C:49:LEU:HD12	3:C:49:LEU:HA	1.92	0.40
1:D:565:LEU:HD22	1:D:604:HIS:HE1	1.86	0.40
1:D:2127:ILE:HD11	1:D:2146:GLY:HA3	2.04	0.40
1:D:4137:ILE:HG23	1:D:4151:PHE:HE1	1.86	0.40
1:D:4860:LEU:HD12	1:D:4860:LEU:HA	1.84	0.40
1:G:687:THR:OG1	1:G:689:GLU:O	2.40	0.40
1:G:752:ASP:N	1:G:752:ASP:OD1	2.55	0.40
1:G:1830:ILE:H	1:G:1830:ILE:HG13	1.72	0.40
1:G:1942:ARG:HG3	1:G:3611:ASN:HB2	2.02	0.40
1:G:2157:TYR:HE1	1:G:2203:TYR:HE2	1.70	0.40
1:G:4002:ASP:HA	1:G:4005:VAL:HG22	2.02	0.40
1:G:4845:ILE:HD12	1:J:4819:TYR:CG	2.57	0.40
1:G:4860:LEU:HD12	1:G:4860:LEU:HA	1.84	0.40
1:J:1166:VAL:HG22	1:J:1173:MET:HG3	2.04	0.40
1:J:1273:ILE:HD11	1:J:1287:GLN:HB2	2.03	0.40
1:J:3943:ASP:N	1:J:3943:ASP:OD1	2.54	0.40
1:J:3984:LEU:HA	1:J:3984:LEU:HD23	1.93	0.40
1:J:4137:ILE:HG23	1:J:4151:PHE:HE1	1.86	0.40
1:J:4627:ILE:H	1:J:4627:ILE:HG12	1.66	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	3366/4968 (68%)	2925 (87%)	429 (13%)	12 (0%)	34	69
1	D	3366/4968 (68%)	2927 (87%)	428 (13%)	11 (0%)	41	74
1	G	3366/4968 (68%)	2925 (87%)	429 (13%)	12 (0%)	34	69
1	J	3366/4968 (68%)	2927 (87%)	427 (13%)	12 (0%)	34	69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	105/108 (97%)	97 (92%)	8 (8%)	0	100	100
2	E	105/108 (97%)	97 (92%)	8 (8%)	0	100	100
2	H	105/108 (97%)	97 (92%)	8 (8%)	0	100	100
2	K	105/108 (97%)	97 (92%)	8 (8%)	0	100	100
3	C	66/149 (44%)	63 (96%)	3 (4%)	0	100	100
3	F	66/149 (44%)	63 (96%)	3 (4%)	0	100	100
3	I	66/149 (44%)	63 (96%)	3 (4%)	0	100	100
3	L	66/149 (44%)	63 (96%)	3 (4%)	0	100	100
All	All	14148/20900 (68%)	12344 (87%)	1757 (12%)	47 (0%)	44	74

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2321	VAL
1	A	4901	THR
1	D	2321	VAL
1	D	4901	THR
1	G	2321	VAL
1	G	4901	THR
1	J	2321	VAL
1	J	4901	THR
1	A	4075	GLU
1	D	4075	GLU
1	G	4075	GLU
1	J	4075	GLU
1	A	730	LEU
1	A	853	PRO
1	A	1580	PRO
1	A	2309	CYS
1	D	730	LEU
1	D	853	PRO
1	D	1580	PRO
1	D	2309	CYS
1	G	730	LEU
1	G	853	PRO
1	G	1580	PRO
1	G	2309	CYS
1	J	730	LEU
1	J	853	PRO

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Mol	Chain	Res	Type
1	J	1580	PRO
1	J	2309	CYS
1	A	1848	PRO
1	A	1990	PRO
1	A	4916	LEU
1	D	1848	PRO
1	D	1990	PRO
1	G	1848	PRO
1	G	1990	PRO
1	G	4916	LEU
1	J	1848	PRO
1	J	1990	PRO
1	J	4916	LEU
1	A	1535	PRO
1	A	2320	VAL
1	D	1535	PRO
1	D	2320	VAL
1	G	1535	PRO
1	G	2320	VAL
1	J	1535	PRO
1	J	2320	VAL

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	2677/4355 (62%)	2650 (99%)	27 (1%)	76 86
1	D	2678/4355 (62%)	2650 (99%)	28 (1%)	76 86
1	G	2677/4355 (62%)	2650 (99%)	27 (1%)	76 86
1	J	2678/4355 (62%)	2650 (99%)	28 (1%)	76 86
2	B	88/89 (99%)	88 (100%)	0	100 100
2	E	88/89 (99%)	88 (100%)	0	100 100
2	H	88/89 (99%)	88 (100%)	0	100 100
2	K	88/89 (99%)	88 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	C	57/127 (45%)	57 (100%)	0	100 100
3	F	57/127 (45%)	57 (100%)	0	100 100
3	I	57/127 (45%)	57 (100%)	0	100 100
3	L	57/127 (45%)	57 (100%)	0	100 100
All	All	11290/18284 (62%)	11180 (99%)	110 (1%)	77 86

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	LEU
1	A	360	VAL
1	A	606	ARG
1	A	718	VAL
1	A	727	PHE
1	A	841	LYS
1	A	925	PRO
1	A	950	VAL
1	A	990	PRO
1	A	1521	THR
1	A	1782	PHE
1	A	2836	ARG
1	A	2857	LYS
1	A	2881	LYS
1	A	3918	PHE
1	A	3936	LEU
1	A	3992	VAL
1	A	4596	VAL
1	A	4638	THR
1	A	4832	ILE
1	A	4877	GLN
1	A	4878	GLN
1	A	4879	GLU
1	A	4882	LYS
1	A	4884	ASP
1	A	4885	MET
1	A	4886	GLU
1	D	35	LEU
1	D	360	VAL
1	D	606	ARG
1	D	718	VAL
1	D	727	PHE

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Mol	Chain	Res	Type
1	D	841	LYS
1	D	925	PRO
1	D	950	VAL
1	D	990	PRO
1	D	1054	VAL
1	D	1521	THR
1	D	1782	PHE
1	D	2836	ARG
1	D	2857	LYS
1	D	2881	LYS
1	D	3918	PHE
1	D	3936	LEU
1	D	3992	VAL
1	D	4596	VAL
1	D	4638	THR
1	D	4832	ILE
1	D	4877	GLN
1	D	4878	GLN
1	D	4879	GLU
1	D	4882	LYS
1	D	4884	ASP
1	D	4885	MET
1	D	4886	GLU
1	G	35	LEU
1	G	360	VAL
1	G	606	ARG
1	G	718	VAL
1	G	727	PHE
1	G	841	LYS
1	G	925	PRO
1	G	950	VAL
1	G	990	PRO
1	G	1521	THR
1	G	1782	PHE
1	G	2836	ARG
1	G	2857	LYS
1	G	2881	LYS
1	G	3918	PHE
1	G	3936	LEU
1	G	3992	VAL
1	G	4596	VAL
1	G	4638	THR

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Mol	Chain	Res	Type
1	G	4832	ILE
1	G	4877	GLN
1	G	4878	GLN
1	G	4879	GLU
1	G	4882	LYS
1	G	4884	ASP
1	G	4885	MET
1	G	4886	GLU
1	J	35	LEU
1	J	360	VAL
1	J	606	ARG
1	J	718	VAL
1	J	727	PHE
1	J	841	LYS
1	J	925	PRO
1	J	950	VAL
1	J	990	PRO
1	J	1054	VAL
1	J	1521	THR
1	J	1782	PHE
1	J	2836	ARG
1	J	2857	LYS
1	J	2881	LYS
1	J	3918	PHE
1	J	3936	LEU
1	J	3992	VAL
1	J	4596	VAL
1	J	4638	THR
1	J	4832	ILE
1	J	4877	GLN
1	J	4878	GLN
1	J	4879	GLU
1	J	4882	LYS
1	J	4884	ASP
1	J	4885	MET
1	J	4886	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (167) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	123	HIS

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Mol	Chain	Res	Type
1	A	293	GLN
1	A	365	HIS
1	A	394	HIS
1	A	476	GLN
1	A	484	ASN
1	A	490	GLN
1	A	550	GLN
1	A	651	HIS
1	A	746	GLN
1	A	890	HIS
1	A	1265	HIS
1	A	1267	HIS
1	A	1294	ASN
1	A	1440	ASN
1	A	1554	GLN
1	A	1906	GLN
1	A	1918	GLN
1	A	2061	GLN
1	A	2196	ASN
1	A	2225	ASN
1	A	2317	ASN
1	A	2848	ASN
1	A	3595	GLN
1	A	3623	GLN
1	A	3635	HIS
1	A	3865	ASN
1	A	3906	ASN
1	A	3961	GLN
1	A	3990	ASN
1	A	3993	ASN
1	A	4109	HIS
1	A	4172	GLN
1	A	4490	GLN
1	A	4494	ASN
1	A	4788	ASN
1	A	4864	GLN
1	A	4934	HIS
1	A	4962	GLN
2	B	31	GLN
3	C	50	GLN
3	C	54	ASN
1	D	54	ASN

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Mol	Chain	Res	Type
1	D	123	HIS
1	D	293	GLN
1	D	365	HIS
1	D	394	HIS
1	D	476	GLN
1	D	484	ASN
1	D	490	GLN
1	D	550	GLN
1	D	651	HIS
1	D	746	GLN
1	D	890	HIS
1	D	1265	HIS
1	D	1267	HIS
1	D	1294	ASN
1	D	1440	ASN
1	D	1554	GLN
1	D	1906	GLN
1	D	1918	GLN
1	D	2061	GLN
1	D	2196	ASN
1	D	2225	ASN
1	D	2317	ASN
1	D	2848	ASN
1	D	3595	GLN
1	D	3623	GLN
1	D	3635	HIS
1	D	3865	ASN
1	D	3906	ASN
1	D	3961	GLN
1	D	3990	ASN
1	D	3993	ASN
1	D	4109	HIS
1	D	4172	GLN
1	D	4490	GLN
1	D	4494	ASN
1	D	4864	GLN
1	D	4934	HIS
1	D	4962	GLN
2	E	31	GLN
3	F	50	GLN
3	F	54	ASN
1	G	54	ASN

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Mol	Chain	Res	Type
1	G	123	HIS
1	G	293	GLN
1	G	365	HIS
1	G	394	HIS
1	G	476	GLN
1	G	484	ASN
1	G	490	GLN
1	G	550	GLN
1	G	651	HIS
1	G	746	GLN
1	G	890	HIS
1	G	1265	HIS
1	G	1267	HIS
1	G	1294	ASN
1	G	1440	ASN
1	G	1554	GLN
1	G	1906	GLN
1	G	1918	GLN
1	G	2061	GLN
1	G	2196	ASN
1	G	2225	ASN
1	G	2317	ASN
1	G	2848	ASN
1	G	3595	GLN
1	G	3623	GLN
1	G	3635	HIS
1	G	3865	ASN
1	G	3906	ASN
1	G	3961	GLN
1	G	3990	ASN
1	G	3993	ASN
1	G	4109	HIS
1	G	4172	GLN
1	G	4490	GLN
1	G	4494	ASN
1	G	4864	GLN
1	G	4934	HIS
1	G	4962	GLN
3	I	50	GLN
3	I	54	ASN
1	J	54	ASN
1	J	123	HIS

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Mol	Chain	Res	Type
1	J	365	HIS
1	J	394	HIS
1	J	476	GLN
1	J	484	ASN
1	J	490	GLN
1	J	550	GLN
1	J	651	HIS
1	J	746	GLN
1	J	890	HIS
1	J	1265	HIS
1	J	1267	HIS
1	J	1294	ASN
1	J	1440	ASN
1	J	1554	GLN
1	J	1906	GLN
1	J	1918	GLN
1	J	2061	GLN
1	J	2196	ASN
1	J	2225	ASN
1	J	2317	ASN
1	J	2848	ASN
1	J	3595	GLN
1	J	3623	GLN
1	J	3635	HIS
1	J	3865	ASN
1	J	3906	ASN
1	J	3961	GLN
1	J	3990	ASN
1	J	3993	ASN
1	J	4109	HIS
1	J	4172	GLN
1	J	4490	GLN
1	J	4494	ASN
1	J	4864	GLN
1	J	4934	HIS
1	J	4962	GLN
2	K	31	GLN
3	L	50	GLN
3	L	54	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 24 ligands modelled in this entry, 16 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
7	CFF	D	6003	-	8,15,15	2.91	4 (50%)	8,23,23	1.34	1 (12%)
6	ATP	A	6002	-	26,33,33	0.91	0	31,52,52	1.67	5 (16%)
6	ATP	J	6002	-	26,33,33	0.91	0	31,52,52	1.67	5 (16%)
6	ATP	D	6002	-	26,33,33	0.92	0	31,52,52	1.67	5 (16%)
7	CFF	A	6003	-	8,15,15	2.91	4 (50%)	8,23,23	1.35	1 (12%)
7	CFF	G	6003	-	8,15,15	2.91	4 (50%)	8,23,23	1.35	1 (12%)
6	ATP	G	6002	-	26,33,33	0.91	0	31,52,52	1.67	5 (16%)
7	CFF	J	6003	-	8,15,15	2.91	4 (50%)	8,23,23	1.35	1 (12%)

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
7	CFF	D	6003	-	-	-	0/2/2/2
6	ATP	A	6002	-	-	6/18/38/38	0/3/3/3
6	ATP	J	6002	-	-	6/18/38/38	0/3/3/3
6	ATP	D	6002	-	-	6/18/38/38	0/3/3/3
7	CFF	A	6003	-	-	-	0/2/2/2
7	CFF	G	6003	-	-	-	0/2/2/2
6	ATP	G	6002	-	-	6/18/38/38	0/3/3/3
7	CFF	J	6003	-	-	-	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	6003	CFF	C5-C4	-5.00	1.32	1.39
7	D	6003	CFF	C5-C4	-5.00	1.32	1.39
7	G	6003	CFF	C5-C4	-5.00	1.32	1.39
7	J	6003	CFF	C5-C4	-5.00	1.32	1.39
7	A	6003	CFF	C6-N1	-4.92	1.31	1.38
7	D	6003	CFF	C6-N1	-4.92	1.31	1.38
7	G	6003	CFF	C6-N1	-4.92	1.31	1.38
7	J	6003	CFF	C6-N1	-4.92	1.31	1.38
7	A	6003	CFF	C5-C6	-2.67	1.36	1.41
7	G	6003	CFF	C5-C6	-2.67	1.36	1.41
7	J	6003	CFF	C5-C6	-2.67	1.36	1.41
7	D	6003	CFF	C5-C6	-2.65	1.36	1.41
7	D	6003	CFF	O13-C6	-2.63	1.18	1.24
7	A	6003	CFF	O13-C6	-2.61	1.18	1.24
7	G	6003	CFF	O13-C6	-2.61	1.18	1.24
7	J	6003	CFF	O13-C6	-2.61	1.18	1.24

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	6002	ATP	N3-C2-N1	-4.12	122.24	128.68
6	D	6002	ATP	N3-C2-N1	-4.12	122.24	128.68
6	G	6002	ATP	N3-C2-N1	-4.12	122.24	128.68
6	J	6002	ATP	N3-C2-N1	-4.12	122.24	128.68
6	G	6002	ATP	PA-O3A-PB	-3.75	119.94	132.83
6	A	6002	ATP	PA-O3A-PB	-3.75	119.95	132.83
6	J	6002	ATP	PA-O3A-PB	-3.75	119.95	132.83
6	D	6002	ATP	PA-O3A-PB	-3.75	119.96	132.83
6	A	6002	ATP	PB-O3B-PG	-3.56	120.60	132.83
6	J	6002	ATP	PB-O3B-PG	-3.56	120.60	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	6002	ATP	PB-O3B-PG	-3.56	120.61	132.83
6	G	6002	ATP	PB-O3B-PG	-3.55	120.63	132.83
6	A	6002	ATP	C3'-C2'-C1'	3.50	106.25	100.98
6	D	6002	ATP	C3'-C2'-C1'	3.50	106.25	100.98
6	G	6002	ATP	C3'-C2'-C1'	3.50	106.25	100.98
6	J	6002	ATP	C3'-C2'-C1'	3.50	106.25	100.98
7	D	6003	CFF	C14-N7-C8	-2.77	112.12	125.43
7	A	6003	CFF	C14-N7-C8	-2.76	112.15	125.43
7	G	6003	CFF	C14-N7-C8	-2.76	112.15	125.43
7	J	6003	CFF	C14-N7-C8	-2.76	112.15	125.43
6	A	6002	ATP	C2-N1-C6	2.20	122.51	118.75
6	D	6002	ATP	C2-N1-C6	2.20	122.51	118.75
6	G	6002	ATP	C2-N1-C6	2.20	122.51	118.75
6	J	6002	ATP	C2-N1-C6	2.20	122.51	118.75

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	6002	ATP	C5'-O5'-PA-O2A
6	A	6002	ATP	C3'-C4'-C5'-O5'
6	D	6002	ATP	C5'-O5'-PA-O2A
6	D	6002	ATP	C3'-C4'-C5'-O5'
6	G	6002	ATP	C5'-O5'-PA-O2A
6	G	6002	ATP	C3'-C4'-C5'-O5'
6	J	6002	ATP	C5'-O5'-PA-O2A
6	J	6002	ATP	C3'-C4'-C5'-O5'
6	A	6002	ATP	O4'-C4'-C5'-O5'
6	D	6002	ATP	O4'-C4'-C5'-O5'
6	G	6002	ATP	O4'-C4'-C5'-O5'
6	J	6002	ATP	O4'-C4'-C5'-O5'
6	A	6002	ATP	PB-O3A-PA-O5'
6	D	6002	ATP	PB-O3A-PA-O5'
6	G	6002	ATP	PB-O3A-PA-O5'
6	J	6002	ATP	PB-O3A-PA-O5'
6	A	6002	ATP	C5'-O5'-PA-O3A
6	D	6002	ATP	C5'-O5'-PA-O3A
6	G	6002	ATP	C5'-O5'-PA-O3A
6	J	6002	ATP	C5'-O5'-PA-O3A
6	A	6002	ATP	C5'-O5'-PA-O1A
6	D	6002	ATP	C5'-O5'-PA-O1A
6	G	6002	ATP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
6	J	6002	ATP	C5'-O5'-PA-O1A

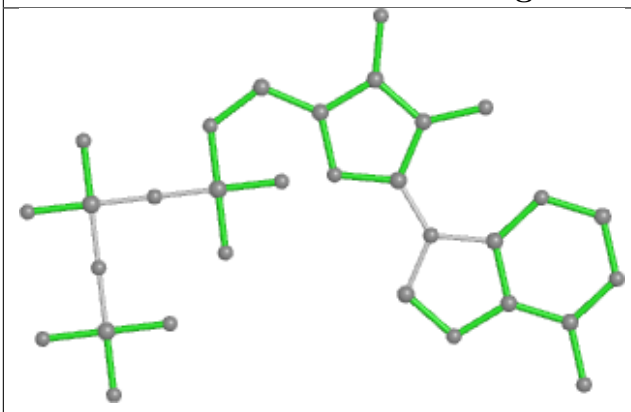
There are no ring outliers.

7 monomers are involved in 7 short contacts:

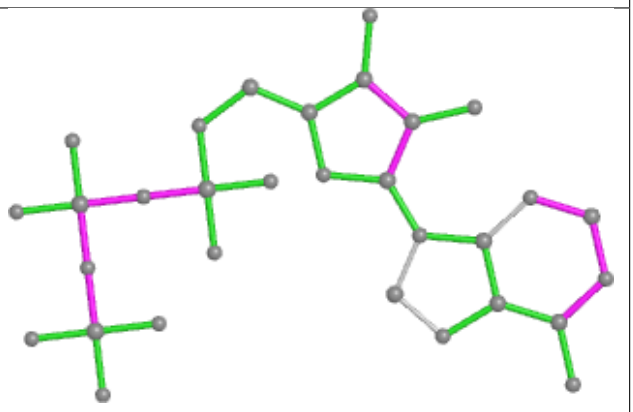
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	6003	CFF	1	0
6	A	6002	ATP	1	0
6	J	6002	ATP	1	0
7	A	6003	CFF	1	0
7	G	6003	CFF	1	0
6	G	6002	ATP	1	0
7	J	6003	CFF	1	0

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

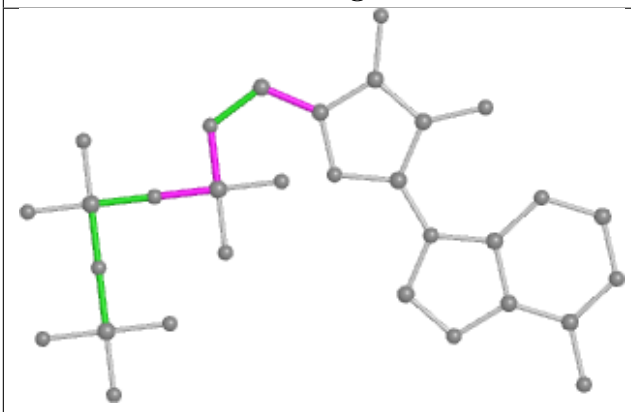
Ligand ATP A 6002



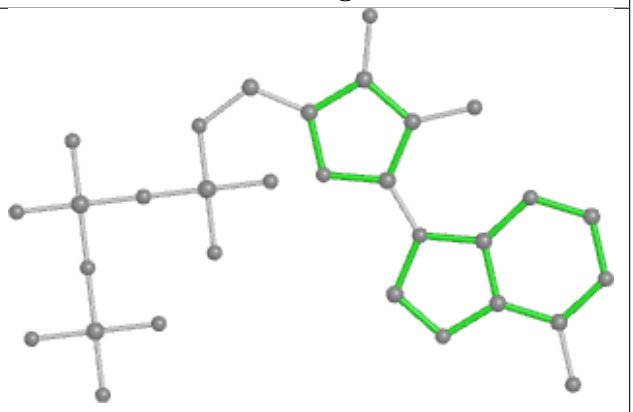
Bond lengths



Bond angles

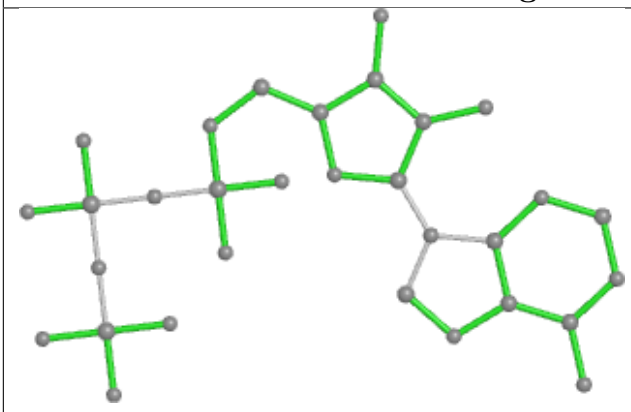


Torsions

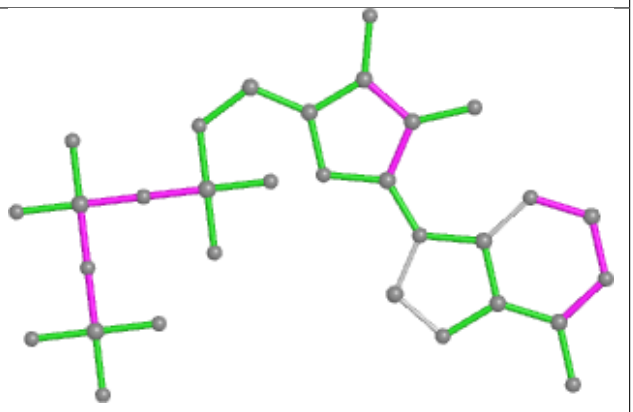


Rings

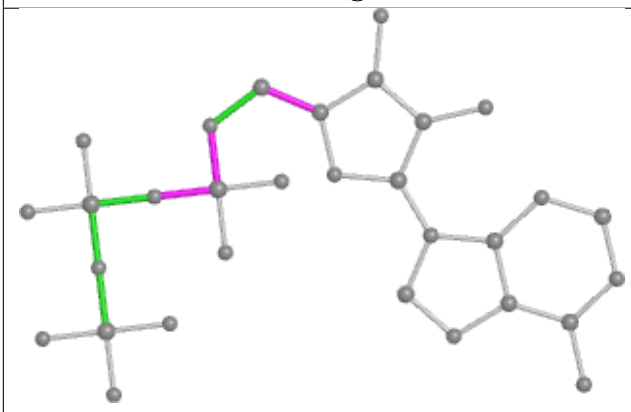
Ligand ATP J 6002



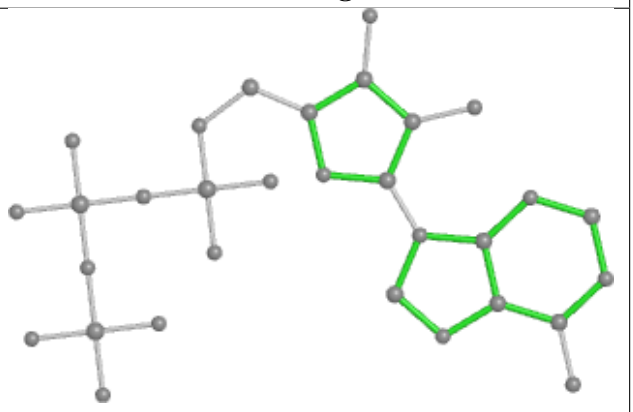
Bond lengths



Bond angles

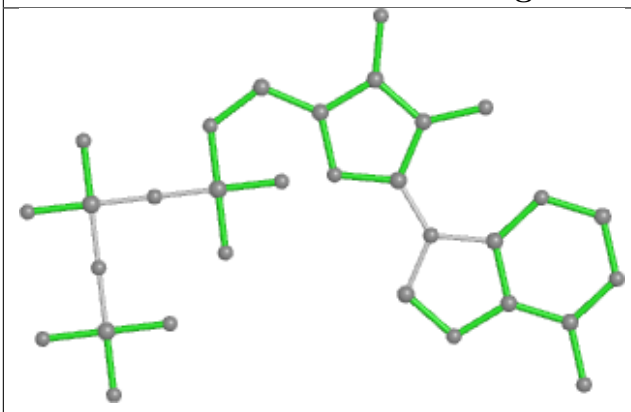


Torsions

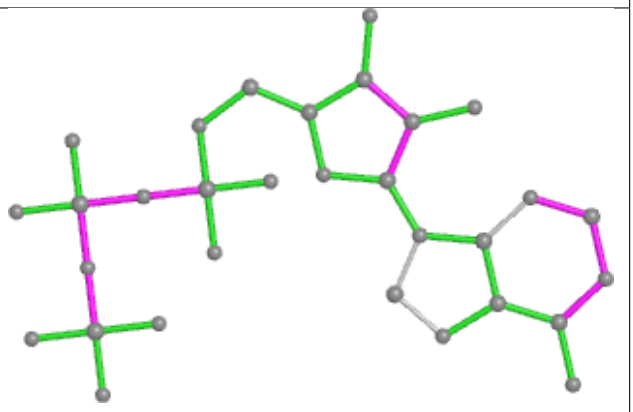


Rings

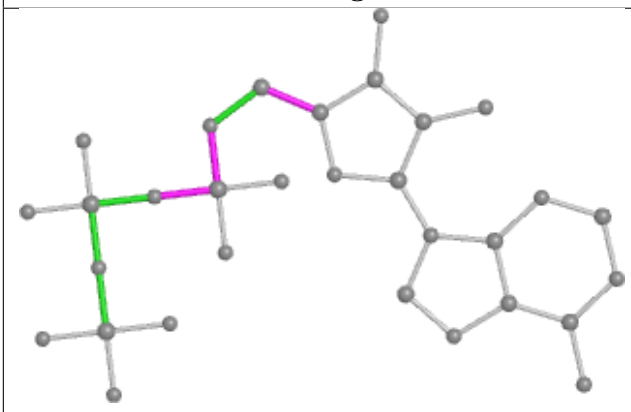
Ligand ATP D 6002



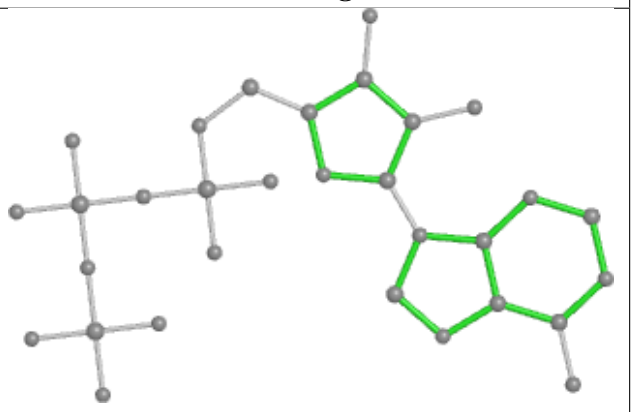
Bond lengths



Bond angles

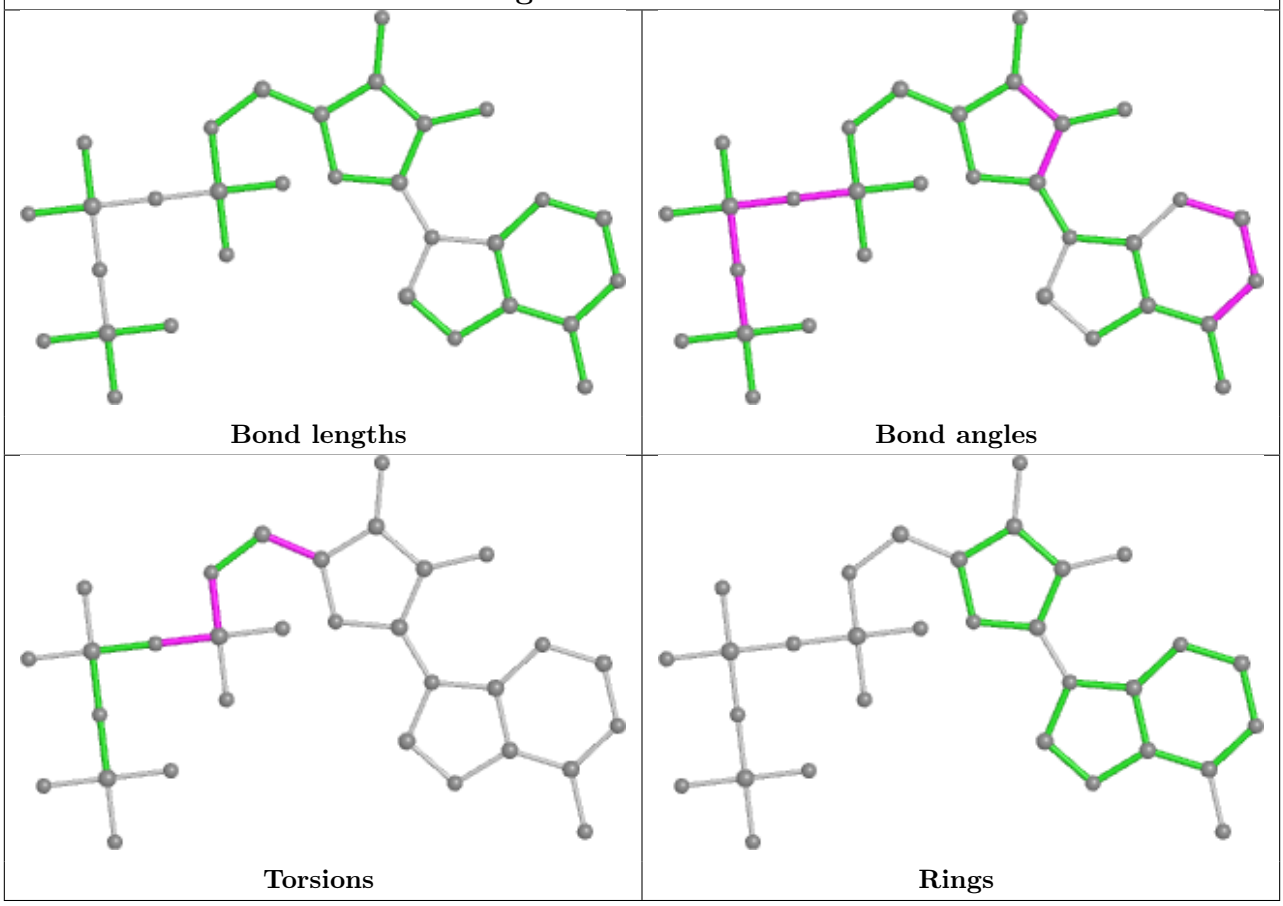


Torsions



Rings

Ligand ATP G 6002



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.

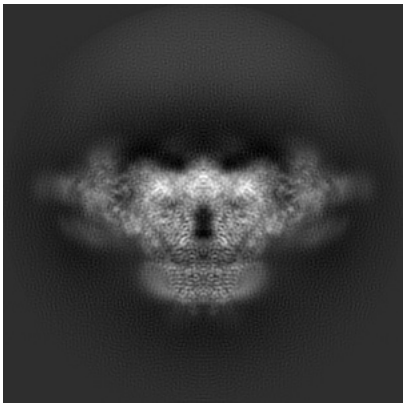
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-9880. These allow visual inspection of the internal detail of the map and identification of artifacts.

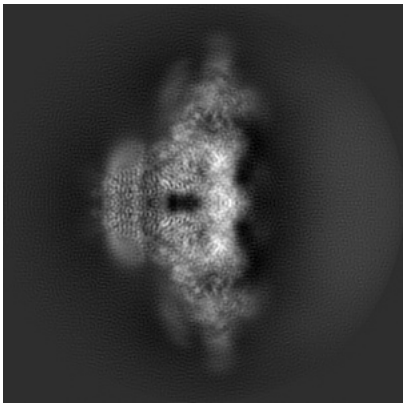
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

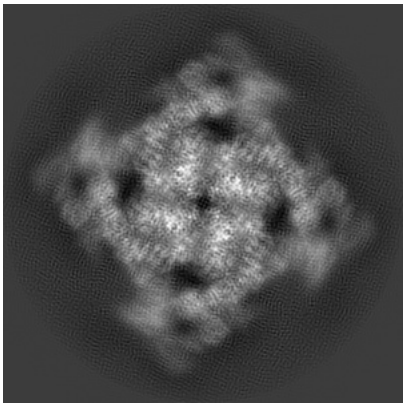
6.1.1 Primary map



X



Y



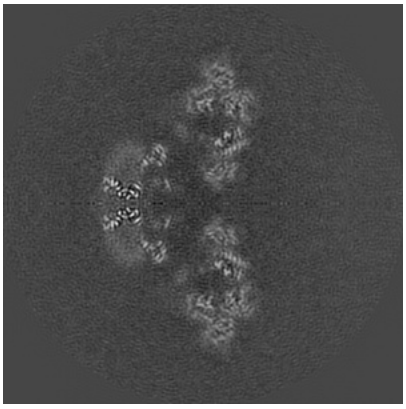
Z

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

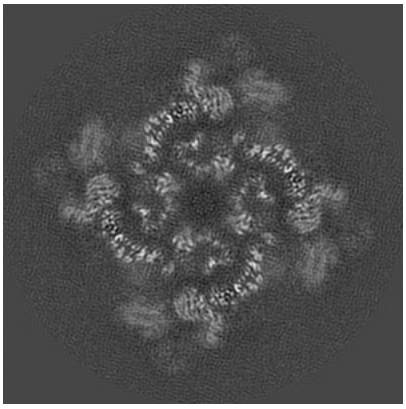
6.2 Central slices

6.2.1 Primary map

X Index: 200



Y Index: 200

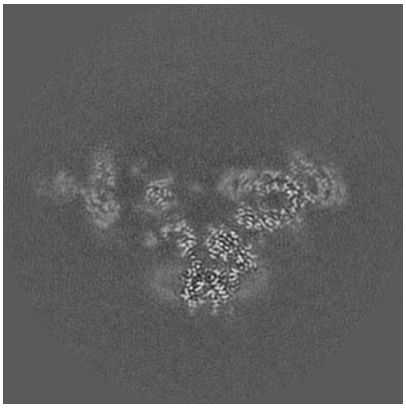


Z Index: 200

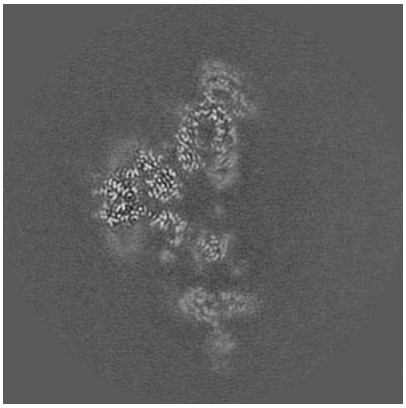
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

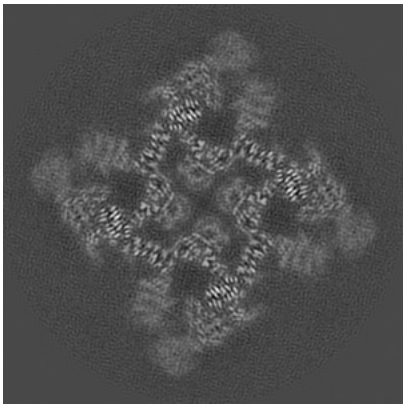
6.3.1 Primary map



X Index: 187



Y Index: 213

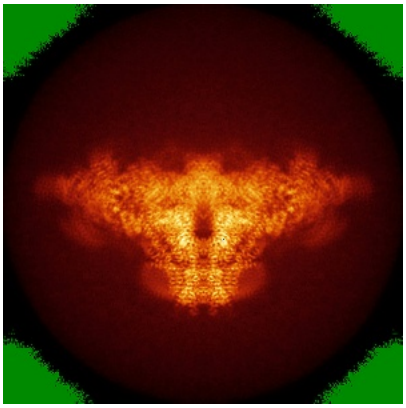


Z Index: 212

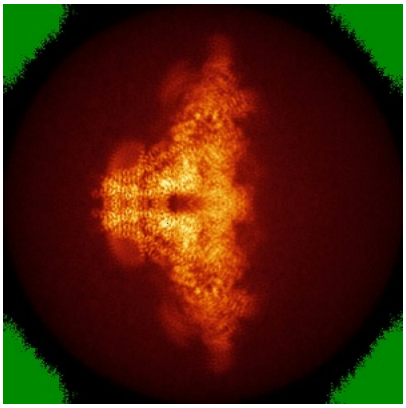
The images above show the largest variance slices of the map in three orthogonal directions.

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

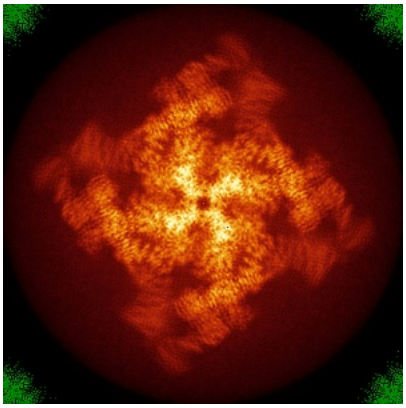
6.4.1 Primary map



X



Y

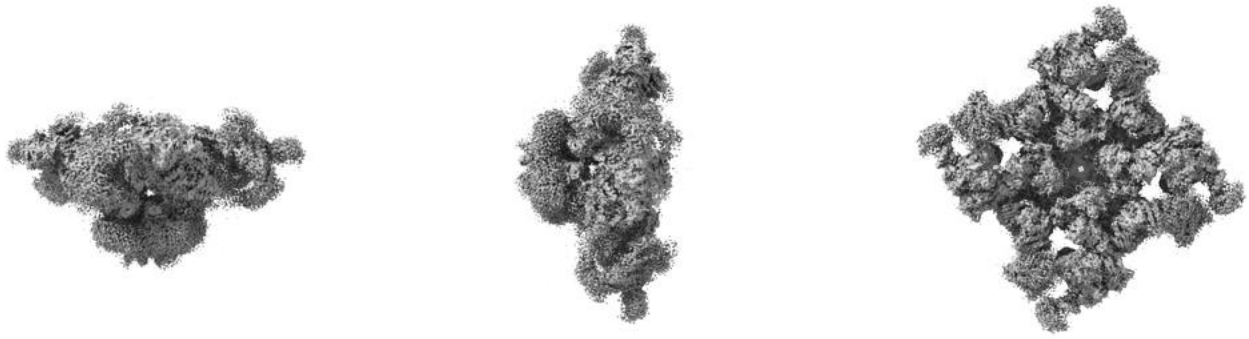


Z

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

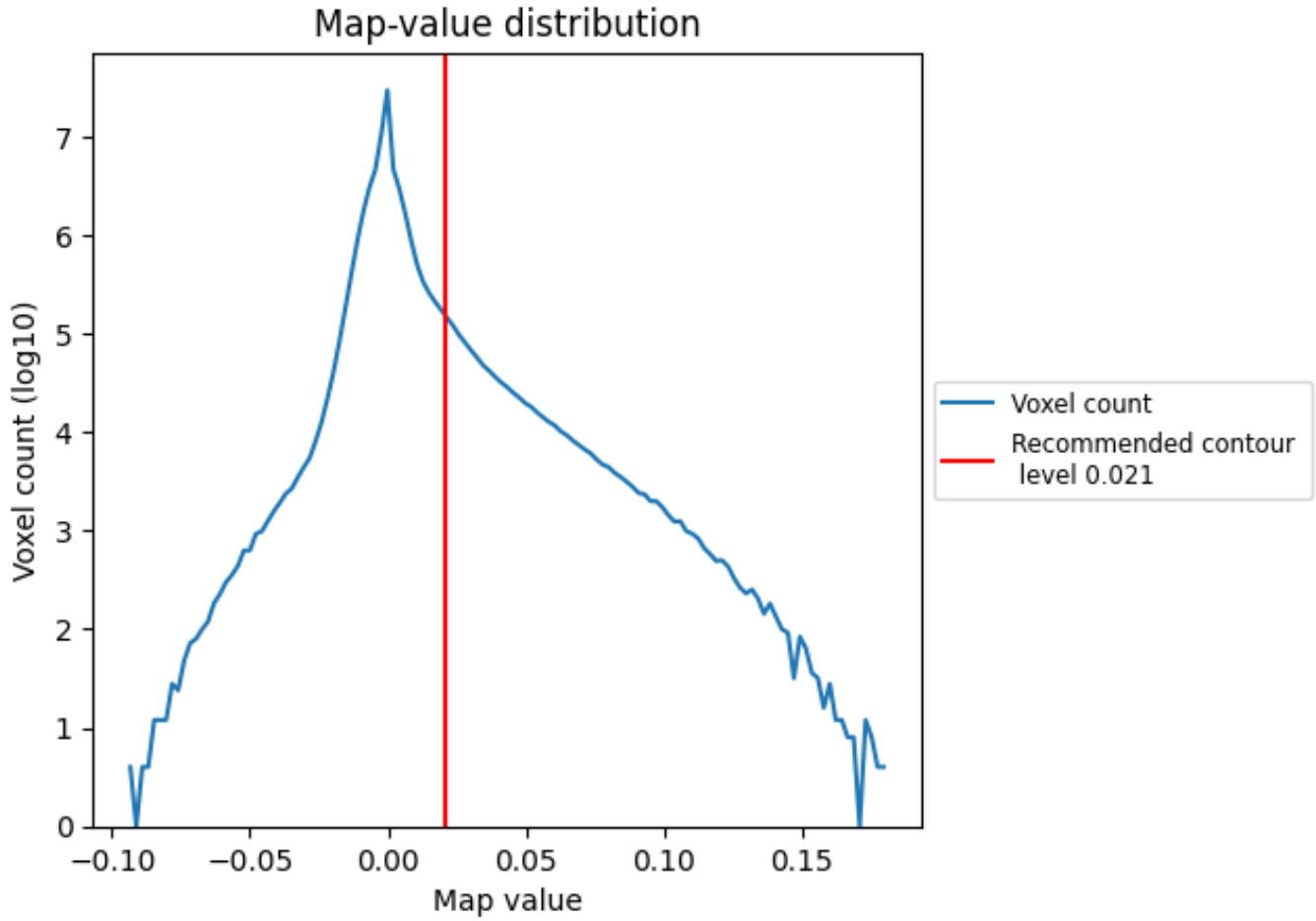
6.6 Mask visualisation (i)

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

7 Map analysis

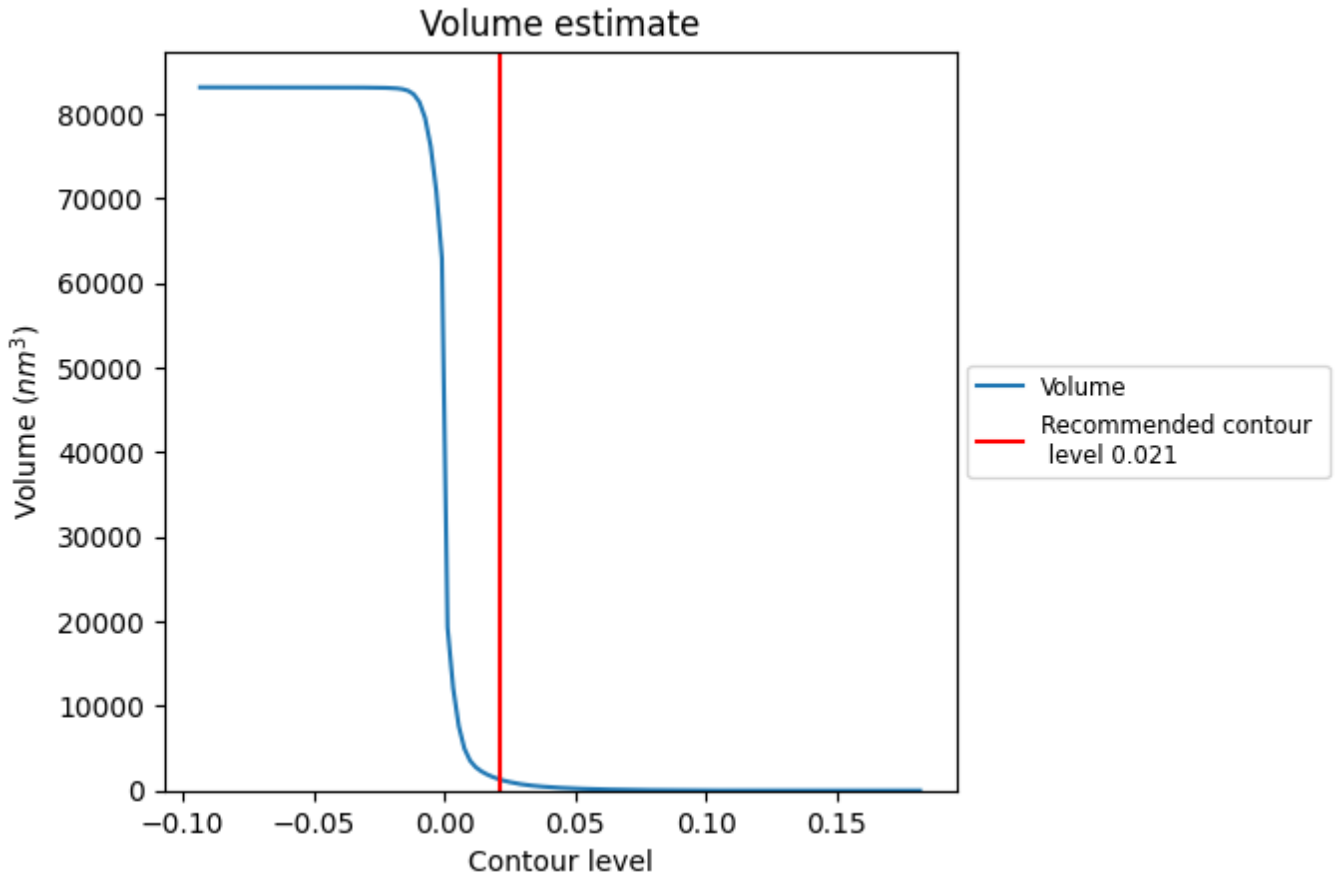
This section contains the results of statistical analysis of the map.

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.

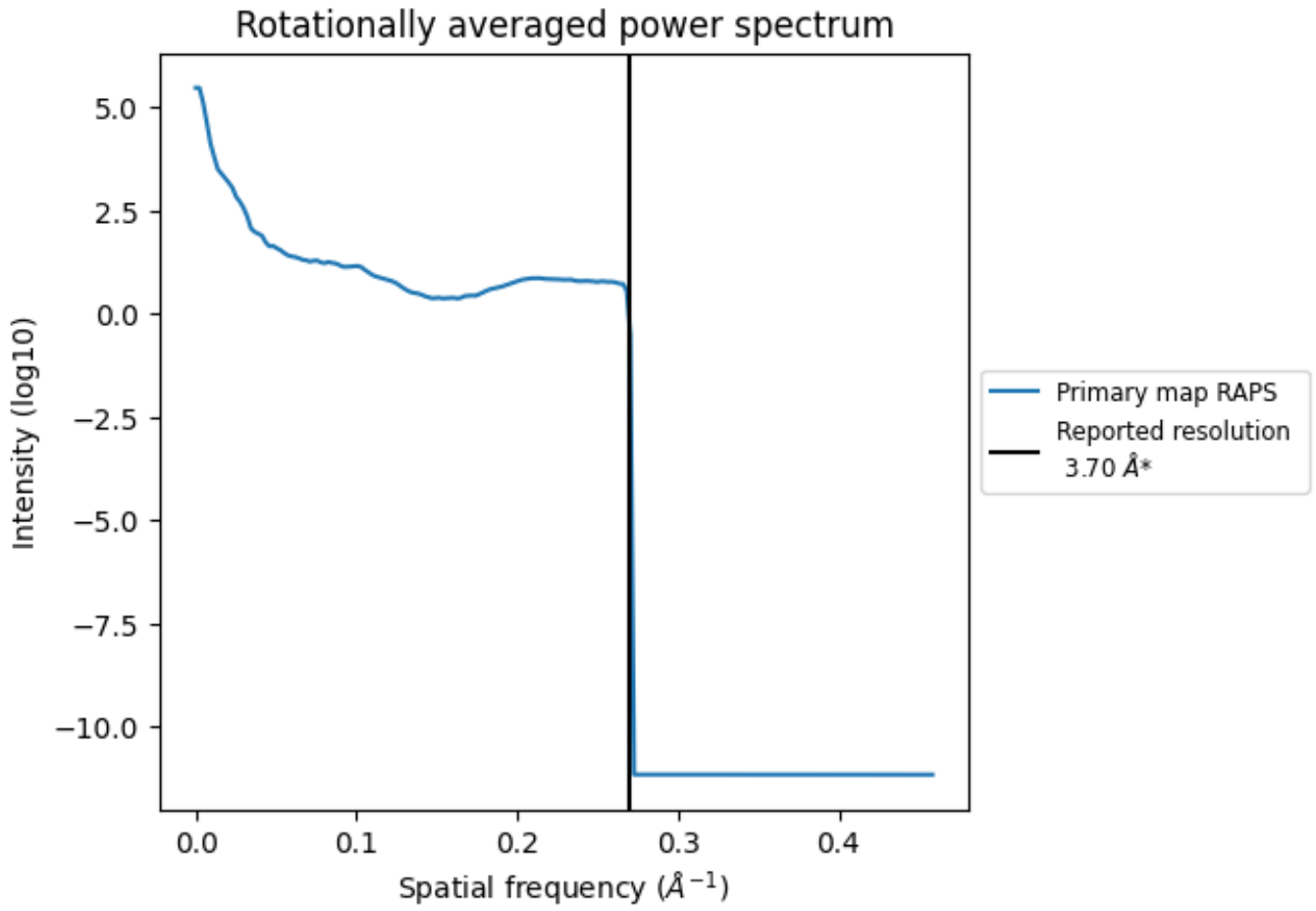
7.2 Volume estimate



The volume at the recommended contour level is 1340 nm^3; this corresponds to an approximate mass of 1210 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)

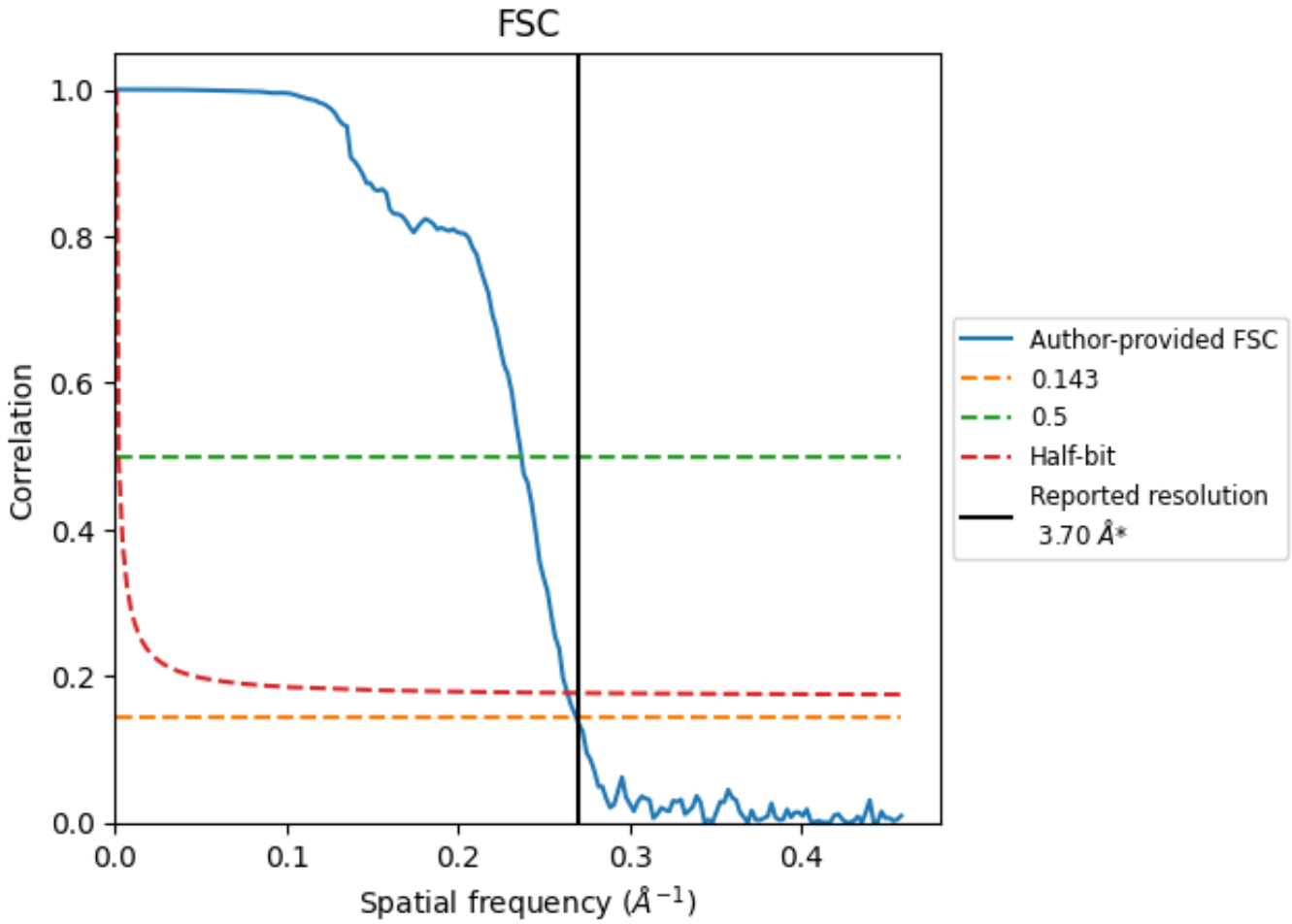


*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

8.2 Resolution estimates (i)

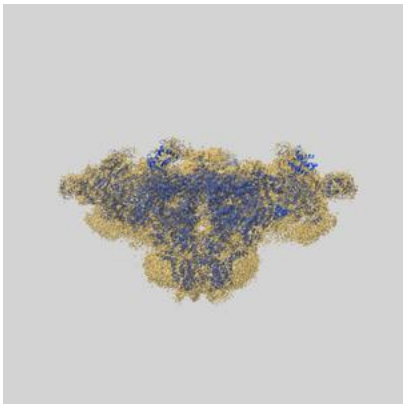
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.72	4.22	3.79
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

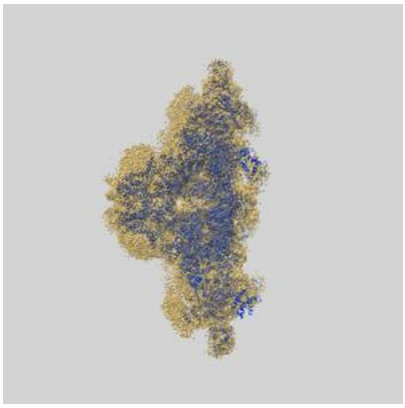
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-9880 and PDB model 6JRS. Per-residue inclusion information can be found in section 3 on page 8.

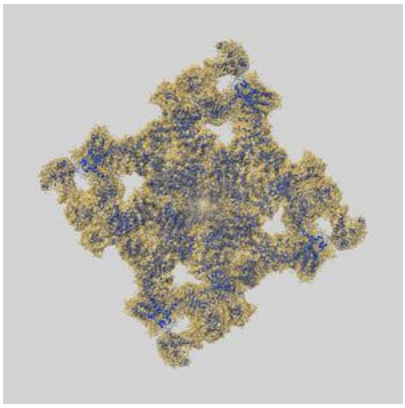
9.1 Map-model overlay



X



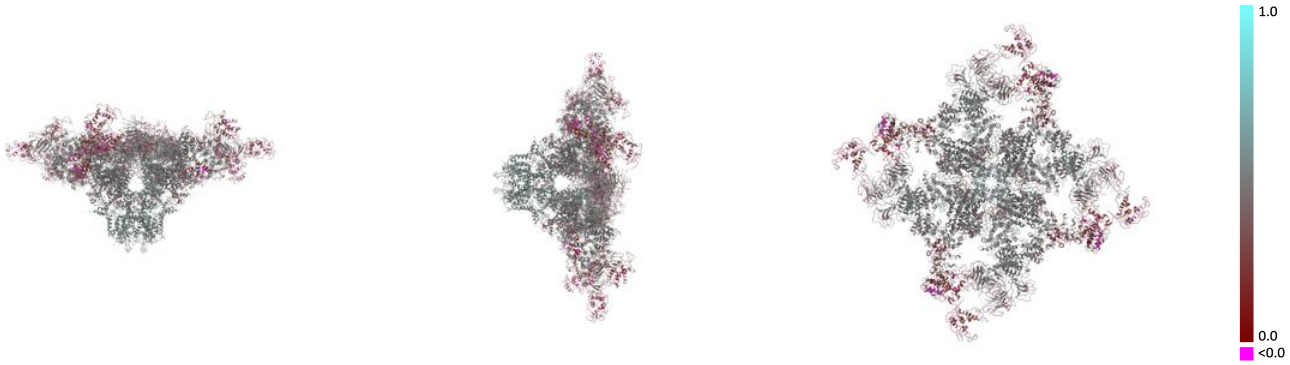
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.021 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.

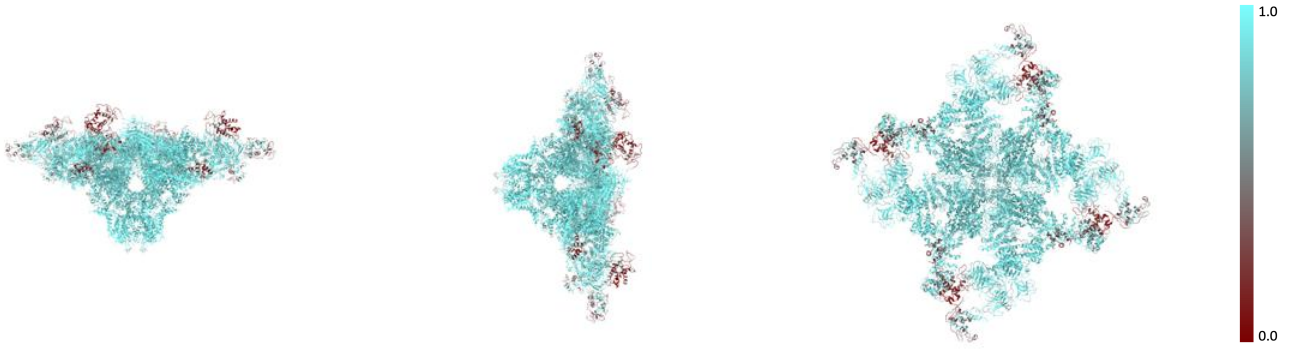
9.2 Q-score mapped to coordinate model (i)



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.

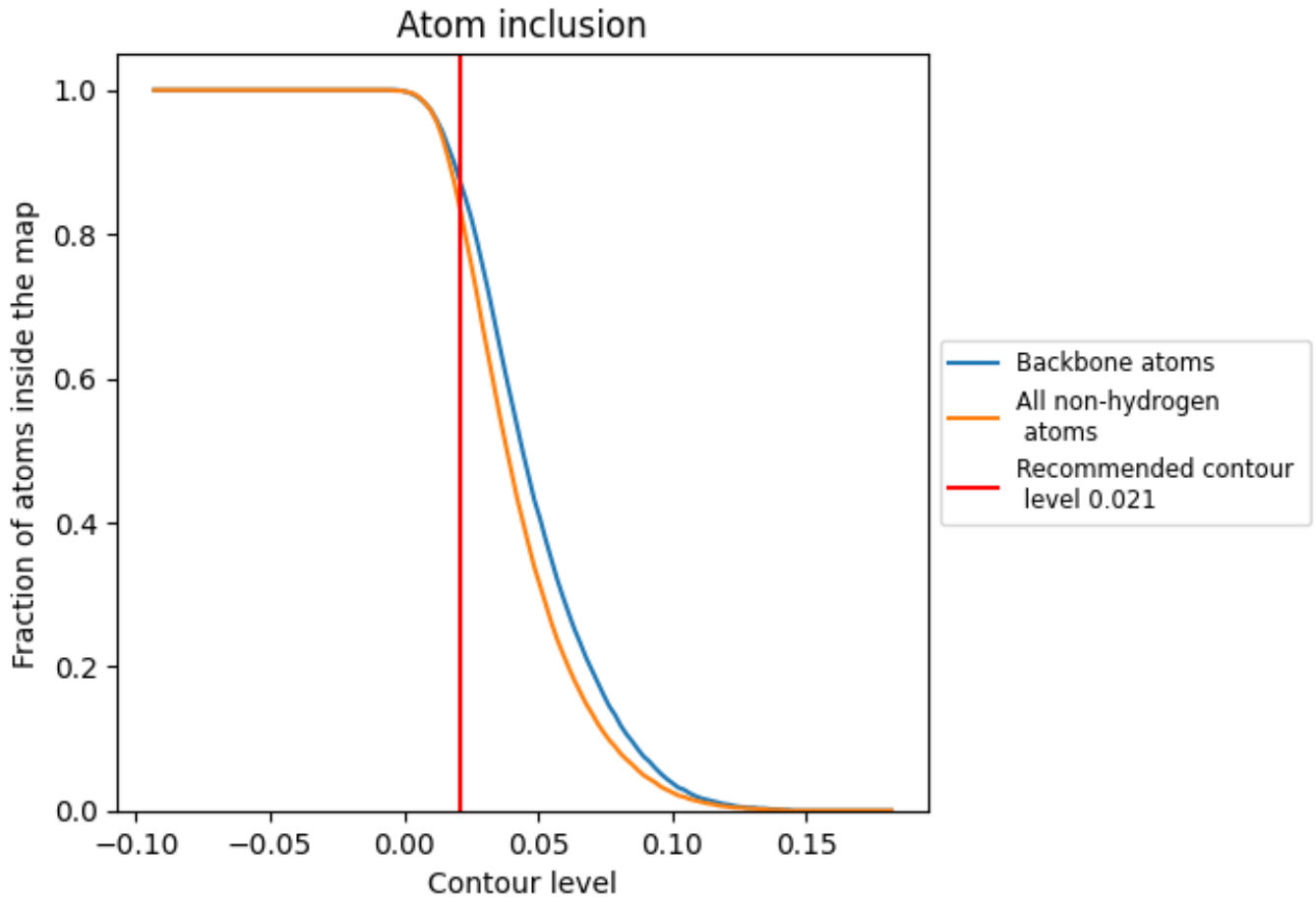
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.021).

9.4 Atom inclusion (i)



At the recommended contour level, 87% of all backbone atoms, 83% 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 (0.021) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8320	0.4210
A	0.8420	0.4240
B	0.9010	0.4500
C	0.2030	0.2530
D	0.8430	0.4240
E	0.9010	0.4470
F	0.2050	0.2570
G	0.8420	0.4240
H	0.9060	0.4470
I	0.2050	0.2560
J	0.8430	0.4230
K	0.9000	0.4460
L	0.2010	0.2520