Full wwPDB EM Validation Report

Jul 10, 2023 – 07:48 PM EDT

PDB ID	:	8SEN
EMDB ID	:	EMD-40422
Title	:	Cryo-EM Structure of RyR1
Authors	:	Cholak, S.; Saville, J.W.; Zhu, X.; Berezuk, A.M.; Tuttle, K.S.; Haji-Ghassemi, O.; Van Petegem, F.; Subramaniam, S.
Deposited on	:	2023-04-10
Resolution	:	3.49 Å(reported)

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

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

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

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

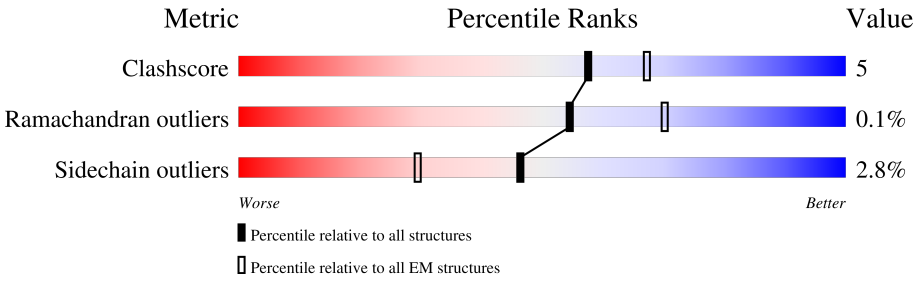
EMDB validation analysis	:	0.0.1.dev50
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

1 Overall quality at a glance

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

The reported resolution of this entry is 3.49 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	5037	16% 73% 14% 13%
1	B	5037	16% 73% 14% 13%
1	C	5037	16% 73% 13% 13%
1	D	5037	16% 73% 13% 13%
2	E	350	25% 6% 69%
2	F	350	24% 6% 69%
2	G	350	24% 6% 69%
2	H	350	25% 6% 69%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 142960 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4378	Total 34921	C 22217	N 6025	O 6443	S 236	9	0
1	B	4378	Total 34921	C 22217	N 6025	O 6443	S 236	9	0
1	C	4378	Total 34921	C 22217	N 6025	O 6443	S 236	9	0
1	D	4378	Total 34921	C 22217	N 6025	O 6443	S 236	9	0

- Molecule 2 is a protein called Glutathione S-transferase class-mu 26 kDa isozyme,Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	107	Total 818	C 516	N 144	O 154	S 4	0	0
2	F	107	Total 818	C 516	N 144	O 154	S 4	0	0
2	G	107	Total 818	C 516	N 144	O 154	S 4	0	0
2	H	107	Total 818	C 516	N 144	O 154	S 4	0	0

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-242	MET	-	expression tag	UNP P08515
E	-241	LYS	-	expression tag	UNP P08515
E	-240	SER	-	expression tag	UNP P08515
E	-239	SER	-	expression tag	UNP P08515
E	-238	HIS	-	expression tag	UNP P08515
E	-237	HIS	-	expression tag	UNP P08515
E	-236	HIS	-	expression tag	UNP P08515
E	-235	HIS	-	expression tag	UNP P08515

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-234	HIS	-	expression tag	UNP P08515
E	-233	HIS	-	expression tag	UNP P08515
E	-232	GLY	-	expression tag	UNP P08515
E	-231	SER	-	expression tag	UNP P08515
E	-230	SER	-	expression tag	UNP P08515
E	-11	GLY	-	linker	UNP P08515
E	-10	ILE	-	linker	UNP P08515
E	-9	GLU	-	linker	UNP P08515
E	-8	GLU	-	linker	UNP P08515
E	-7	ASN	-	linker	UNP P08515
E	-6	LEU	-	linker	UNP P08515
E	-5	TYR	-	linker	UNP P08515
E	-4	PHE	-	linker	UNP P08515
E	-3	GLN	-	linker	UNP P08515
E	-2	SER	-	linker	UNP P08515
E	-1	ASN	-	linker	UNP P08515
E	0	ALA	-	linker	UNP P08515
F	-242	MET	-	expression tag	UNP P08515
F	-241	LYS	-	expression tag	UNP P08515
F	-240	SER	-	expression tag	UNP P08515
F	-239	SER	-	expression tag	UNP P08515
F	-238	HIS	-	expression tag	UNP P08515
F	-237	HIS	-	expression tag	UNP P08515
F	-236	HIS	-	expression tag	UNP P08515
F	-235	HIS	-	expression tag	UNP P08515
F	-234	HIS	-	expression tag	UNP P08515
F	-233	HIS	-	expression tag	UNP P08515
F	-232	GLY	-	expression tag	UNP P08515
F	-231	SER	-	expression tag	UNP P08515
F	-230	SER	-	expression tag	UNP P08515
F	-11	GLY	-	linker	UNP P08515
F	-10	ILE	-	linker	UNP P08515
F	-9	GLU	-	linker	UNP P08515
F	-8	GLU	-	linker	UNP P08515
F	-7	ASN	-	linker	UNP P08515
F	-6	LEU	-	linker	UNP P08515
F	-5	TYR	-	linker	UNP P08515
F	-4	PHE	-	linker	UNP P08515
F	-3	GLN	-	linker	UNP P08515
F	-2	SER	-	linker	UNP P08515
F	-1	ASN	-	linker	UNP P08515
F	0	ALA	-	linker	UNP P08515

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-242	MET	-	expression tag	UNP P08515
G	-241	LYS	-	expression tag	UNP P08515
G	-240	SER	-	expression tag	UNP P08515
G	-239	SER	-	expression tag	UNP P08515
G	-238	HIS	-	expression tag	UNP P08515
G	-237	HIS	-	expression tag	UNP P08515
G	-236	HIS	-	expression tag	UNP P08515
G	-235	HIS	-	expression tag	UNP P08515
G	-234	HIS	-	expression tag	UNP P08515
G	-233	HIS	-	expression tag	UNP P08515
G	-232	GLY	-	expression tag	UNP P08515
G	-231	SER	-	expression tag	UNP P08515
G	-230	SER	-	expression tag	UNP P08515
G	-11	GLY	-	linker	UNP P08515
G	-10	ILE	-	linker	UNP P08515
G	-9	GLU	-	linker	UNP P08515
G	-8	GLU	-	linker	UNP P08515
G	-7	ASN	-	linker	UNP P08515
G	-6	LEU	-	linker	UNP P08515
G	-5	TYR	-	linker	UNP P08515
G	-4	PHE	-	linker	UNP P08515
G	-3	GLN	-	linker	UNP P08515
G	-2	SER	-	linker	UNP P08515
G	-1	ASN	-	linker	UNP P08515
G	0	ALA	-	linker	UNP P08515
H	-242	MET	-	expression tag	UNP P08515
H	-241	LYS	-	expression tag	UNP P08515
H	-240	SER	-	expression tag	UNP P08515
H	-239	SER	-	expression tag	UNP P08515
H	-238	HIS	-	expression tag	UNP P08515
H	-237	HIS	-	expression tag	UNP P08515
H	-236	HIS	-	expression tag	UNP P08515
H	-235	HIS	-	expression tag	UNP P08515
H	-234	HIS	-	expression tag	UNP P08515
H	-233	HIS	-	expression tag	UNP P08515
H	-232	GLY	-	expression tag	UNP P08515
H	-231	SER	-	expression tag	UNP P08515
H	-230	SER	-	expression tag	UNP P08515
H	-11	GLY	-	linker	UNP P08515
H	-10	ILE	-	linker	UNP P08515
H	-9	GLU	-	linker	UNP P08515
H	-8	GLU	-	linker	UNP P08515

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-7	ASN	-	linker	UNP P08515
H	-6	LEU	-	linker	UNP P08515
H	-5	TYR	-	linker	UNP P08515
H	-4	PHE	-	linker	UNP P08515
H	-3	GLN	-	linker	UNP P08515
H	-2	SER	-	linker	UNP P08515
H	-1	ASN	-	linker	UNP P08515
H	0	ALA	-	linker	UNP P08515

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

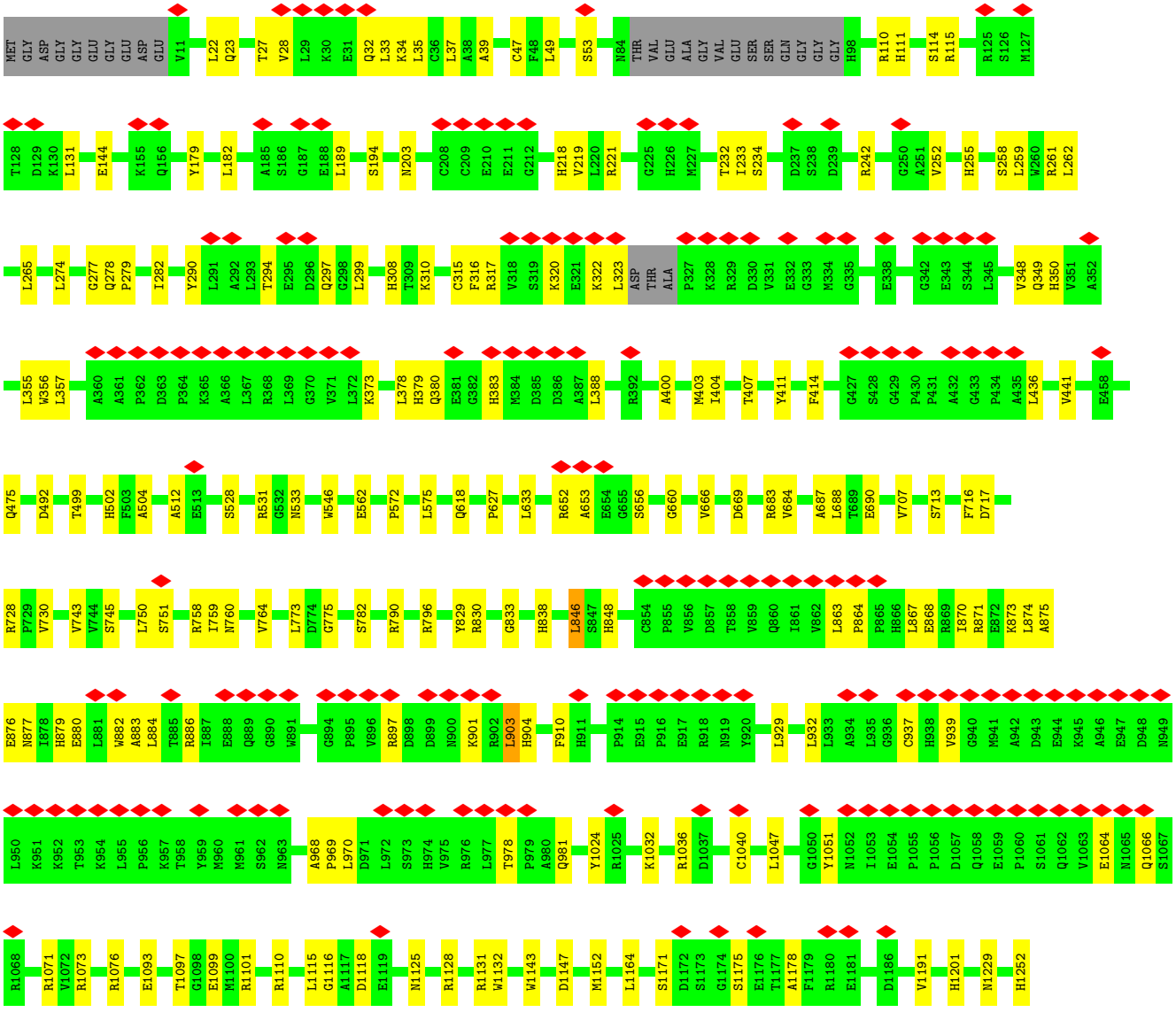
Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total Zn 1 1	0
3	B	1	Total Zn 1 1	0
3	C	1	Total Zn 1 1	0
3	D	1	Total Zn 1 1	0

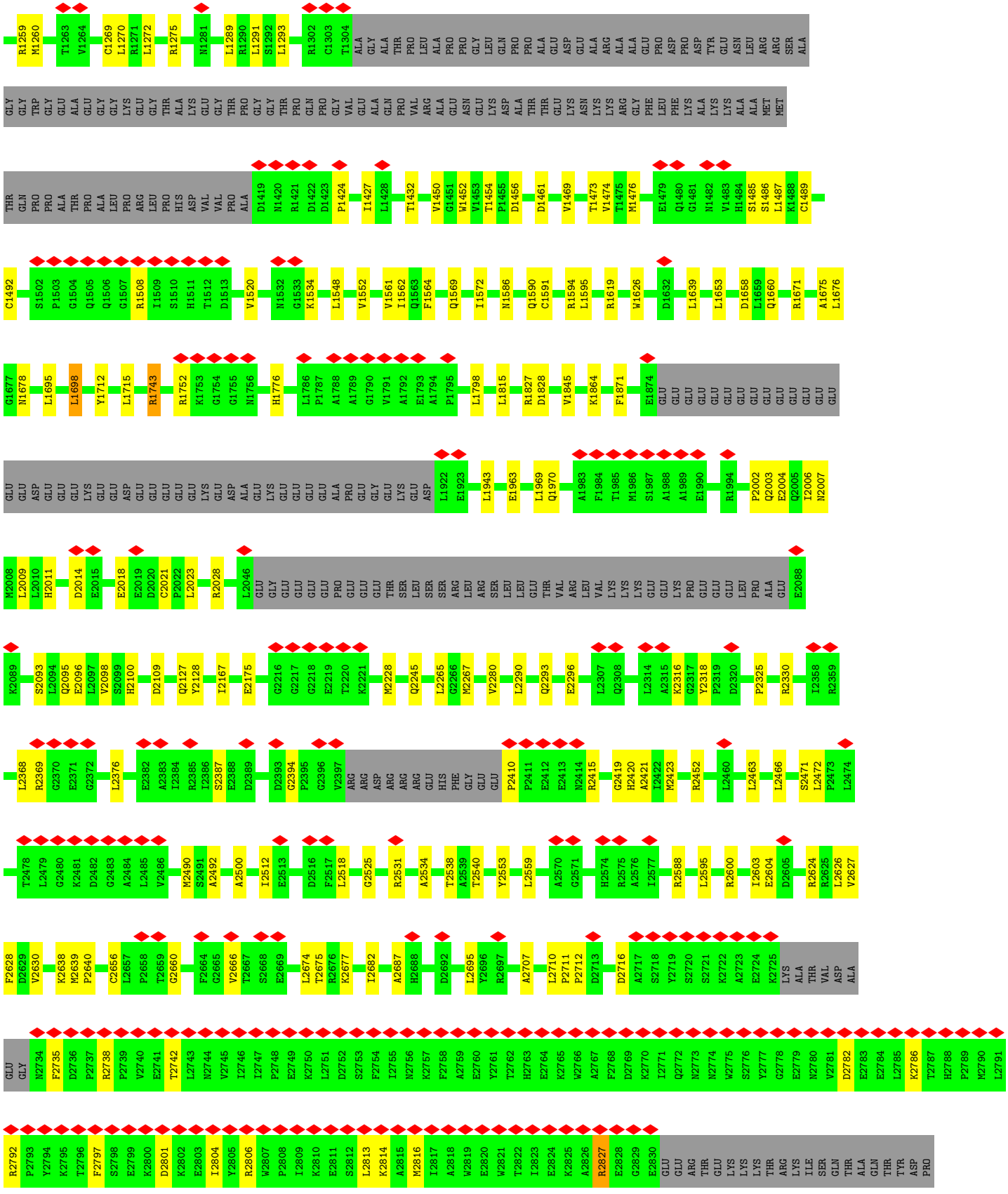
3 Residue-property plots (i)

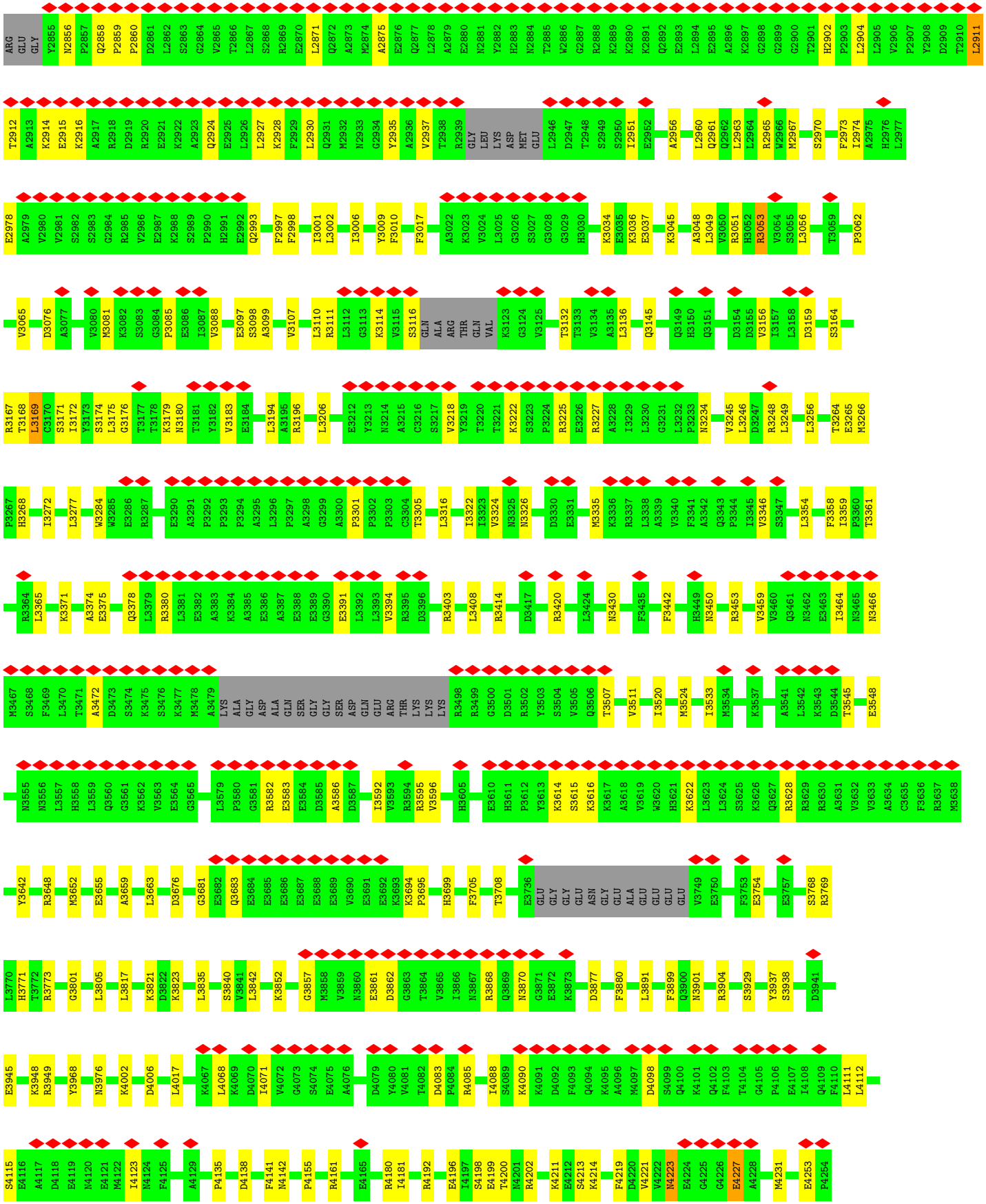
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

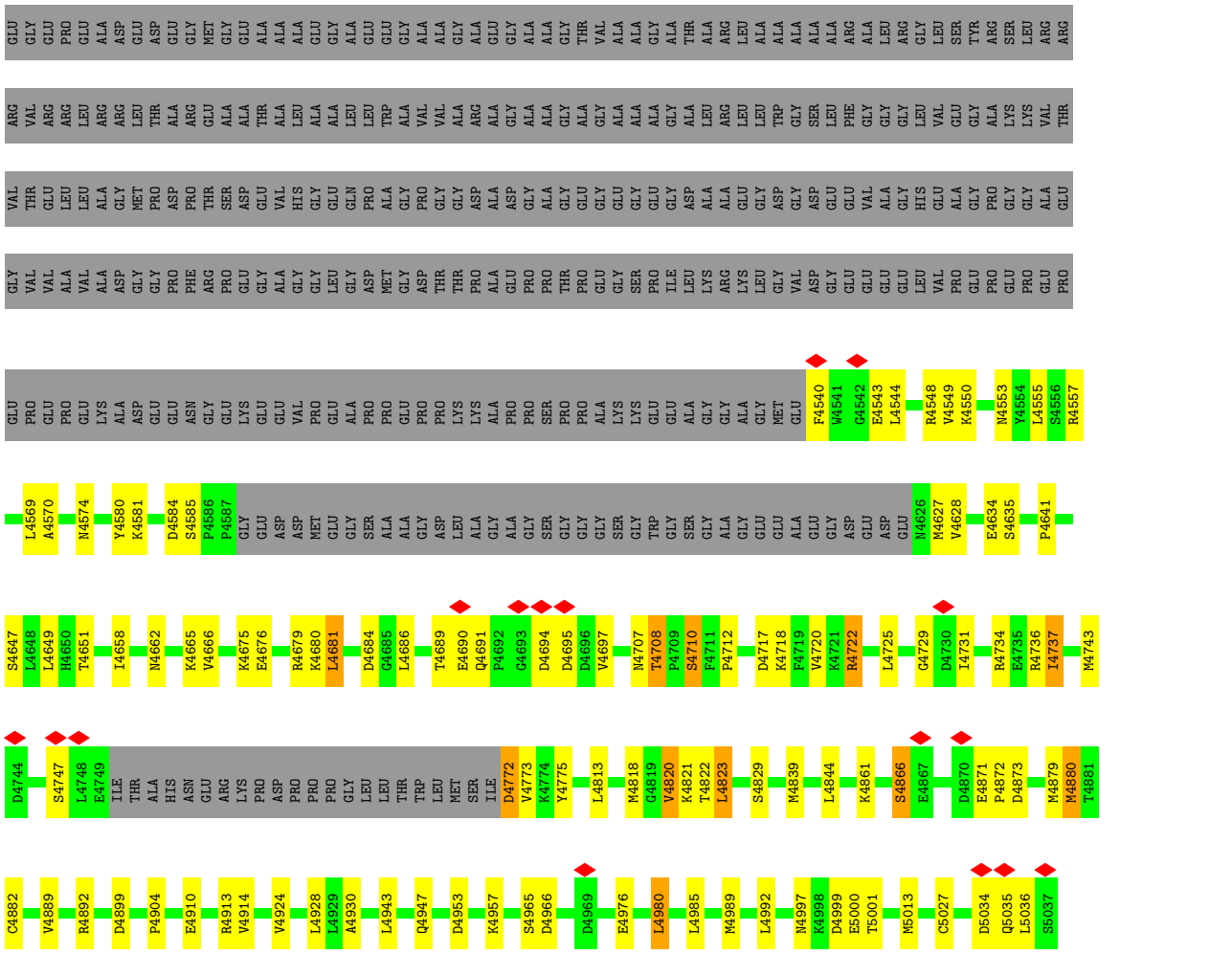
- Molecule 1: Ryanodine receptor 1

Chain A:



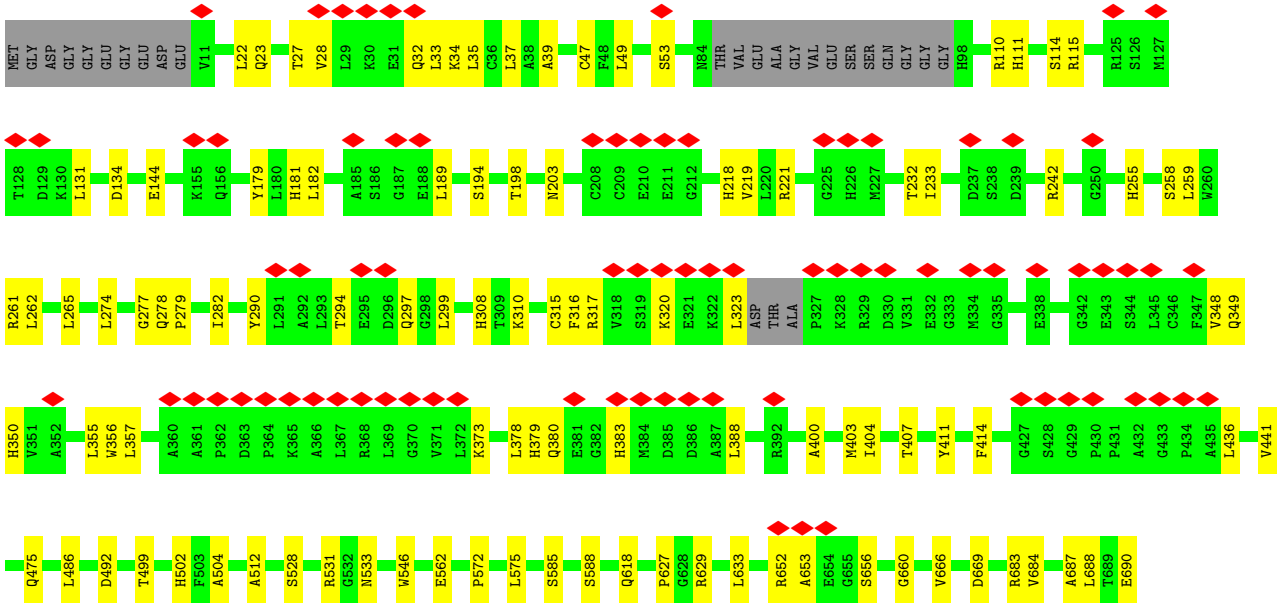

R1259 M1260 T1263 V1264 C1269 L1270 R1271 L1272 R1275 N1281 L1289 R1290 L1291 S1292 L1293 R1302 C1303 T1304 ALA GLY ALA THR PRO LEU ALA PRO PRO GLY GLU LEU GLN PRO PRO ALA GLU ASP GLU ALA ARG ALA ALA GLU PRO ASP PRO ASP TYR GLU ASN LEU ARG ARG SER ALA
GLY GLY TRP GLY GLU ALA GLU GLY GLY LYS GLU GLY THR ALA LYS GLU GLY THR PRO GLY GLY THR PRO GLN PRO GLY VAL GLU ALA GLN PRO VAL ARG ALA GLU ASN GLU LYS ASP ALA THR THR GLU LYS ASN LYS LYS ARG GLY PHE LEU PHE LYS ALA LYS LYS ALA ALA MET MET
THR GLN PRO PRO ALA THR PRO ALA LEU PRO ARG LEU PRO HIS ASP VAL VAL PRO ALA D1419 N1420 R1421 D1422 D1423 P1424 I1427 L1428 T1432 V1450 G1451 W1452 V1453 T1454 P1455 D1456 D1461 V1469 T1473 V1474 T1475 M1476 E1479 Q1480 G1481 N1482 V1483 H1484 S1485 S1486 L1487 K1488 C1489
C1492 S1502 P1503 G1504 Q1505 Q1506 G1507 R1508 I1509 S1510 H1511 T1512 D1513 V1520 N1532 G1533 K1534 L1548 V1552 V1561 I1562 Q1563 F1564 Q1569 I1572 N1586 Q1590 C1591 R1594 L1595 R1619 W1626 D1632 L1639 L1653 D1658 L1659 Q1660 R1671 A1675 L1676
G1677 N1678 L1695 L1698 Y1712 L1715 R1743 R1752 K1753 G1754 G1755 N1756 H1776 L1786 P1787 A1788 A1789 G1790 V1791 A1792 E1793 A1794 P1795 L1798 L1815 R1827 D1828 V1845 K1864 F1871 E1874 GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU
GLU GLU ASP GLU GLU GLU LYS GLU GLU ASP GLU GLU GLU LYS GLU ASP ALA GLU LYS GLU GLU GLU GLU ALA PRO GLU GLY GLU LYS GLU ASP L1922 E1923 L1943 E1963 L1969 Q1970 A1983 F1984 T1985 M1986 S1987 A1988 A1989 E1990 R1994 P2002 Q2003 E2004 Q2005 I2006 N2007
M2008 L2009 L2010 H2011 D2014 E2015 E2018 E2019 D2020 C2021 P2022 L2023 R2028 L2046 GLU GLY GLU GLU GLU GLU PRO GLU GLU GLU THR SER LEU SER SER ARG LEU ARG SER LEU LEU GLU THR VAL ARG LEU VAL LYS LYS LYS GLU GLU LYS PRO GLU GLU GLU LEU PRO ALA GLU E2088
K2089 S2093 L2094 Q2095 E2096 L2097 V2098 S2099 H2100 D2109 Q2127 Y2128 I2167 E2175 G2216 G2217 G2218 E2219 T2220 K2221 M2228 Q2245 L2265 G2266 M2267 V2280 L2290 Q2293 E2296 L2307 Q2308 L2314 A2315 K2316 G2317 Y2318 P2319 D2320 P2325 R2330 I2358 R2359
L2368 R2369 G2370 E2371 G2372 L2376 E2382 A2383 I2384 R2385 I2386 S2387 E2388 D2389 D2393 G2394 P2395 G2396 V2397 ARG ARG ASP ARG ARG ARG GLU HIS PHE GLY GLU GLU P2410 P2411 E2412 E2413 N2414 R2415 G2419 H2420 A2421 I2422 M2423 R2452 L2460 L2463 L2466 S2471 L2472 P2473 L2474
T2478 L2479 G2480 K2481 D2482 G2483 A2484 L2485 V2486 M2490 S2491 A2492 A2500 I2512 E2513 D2516 F2517 L2518 G2525 R2531 A2534 T2538 A2539 T2540 Y2553 L2559 A2570 G2571 H2574 R2575 A2576 I2577 R2588 L2595 R2600 I2603 E2604 D2605 R2624 R2625 L2626 V2627
F2628 D2629 V2630 K2638 M2639 P2640 C2656 L2657 P2658 T2659 G2660 F2664 G2665 V2666 T2667 S2668 E2669 L2674 T2675 R2676 K2677 I2682 A2687 H2688 D2692 L2695 Y2696 R2697 A2707 L2710 P2711 P2712 D2713 D2716 A2717 S2718 Y2719 S2720 S2721 K2722 A2723 E2724 K2725 LYS ALA THR VAL ASP ALA
GLU GLY N2734 F2735 D2736 P2737 R2738 P2739 V2740 E2741 T2742 L2743 N2744 V2745 I2746 I2747 P2748 E2749 K2750 L2751 D2752 S2753 F2754 I2755 N2756 K2757 F2758 A2759 E2760 Y2761 T2762 H2763 E2764 K2765 W2766 A2767 F2768 D2769 K2770 I2771 Q2772 N2773 N2774 W2775 S2776 Y2777 G2778 E2779 N2780 V2781 D2782 E2783 E2784 L2785 K2786 T2787 H2788 P2789 M2790 L2791
R2792 P2793 Y2794 K2795 T2796 F2797 S2798 E2799 K2800 D2801 K2802 E2803 I2804 Y2805 R2806 W2807 P2808 I2809 K2810 E2811 S2812 L2813 K2814 A2815 M2816 I2817 A2818 W2819 E2820 W2821 T2822 I2823 E2824 K2825 A2826 R2827 E2828 G2829 E2830 GLU GLU ARG THR GLU LYS LYS LYS THR ARG LYS ILE SER GLN THR ALA GLN THR TYR ASP PRO

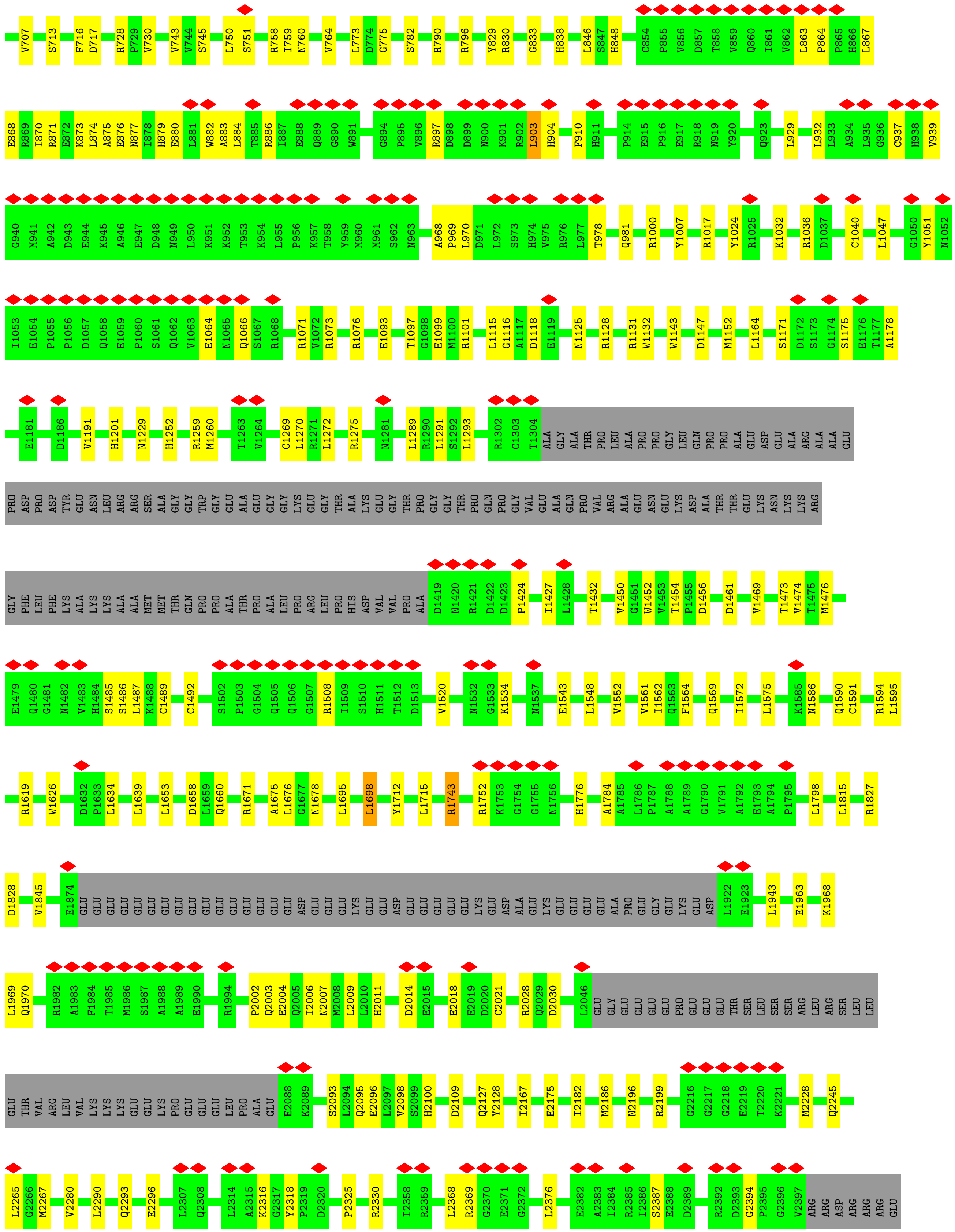


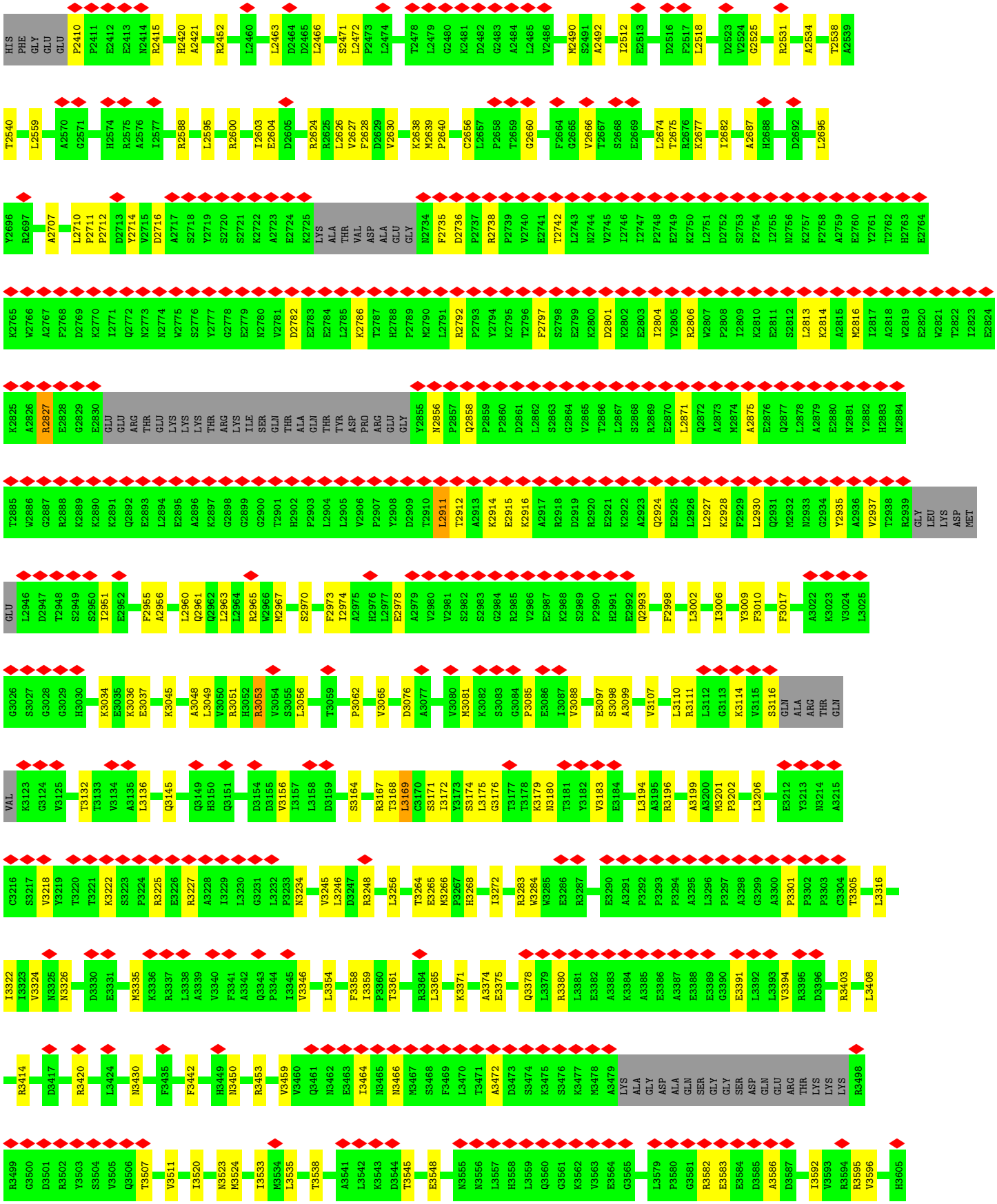


• Molecule 1: Ryanodine receptor 1

Chain B:




V707 S713 F716 D717 R728 P729 V730 V743 V744 S745 L750 S751 R758 I759 N760 V764 L773 D774 G775 S782 R790 R796 Y829 R830 G833 H838 L846 S847 H848 C854 P855 V856 D857 T858 V859 Q860 I861 V862 L863 P864 P865 H866 L867
E868 R869 I870 R871 E872 K873 L874 A875 E876 N877 I878 H879 E880 L881 W882 A883 L884 T885 R886 I887 E888 Q889 G890 W891 G894 P895 V896 R897 D898 D899 N900 K901 R902 L903 H904 F910 H911 P914 E915 P916 E917 R918 N919 Y920 Q923 L929 L932 L933 A934 L935 G936 C937 H938 V939
G940 M941 A942 D943 E944 K945 A946 E947 D948 N949 L950 K951 K952 T953 K954 L955 P956 K957 T958 Y959 M960 M961 S962 N963 A968 P969 L970 D971 L972 S973 H974 V975 R976 L977 T978 Q981 R1000 Y1007 R1017 Y1024 R1025 K1032 R1036 D1037 C1040 L1047 G1050 Y1051 N1052
I1053 E1054 P1055 P1056 D1057 Q1058 E1059 P1060 S1061 Q1062 V1063 E1064 N1065 Q1066 S1067 R1068 R1071 V1072 R1073 R1076 E1093 T1097 G1098 E1099 M1100 R1101 L1115 G1116 A1117 D1118 E1119 N1125 R1128 R1131 W1132 W1143 D1147 M1152 L1164 S1171 D1172 S1173 G1174 S1175 E1176 T1177 A1178
E1181 D1186 V1191 H1201 N1229 H1252 R1259 M1260 T1263 V1264 C1269 L1270 R1271 L1272 R1275 N1281 L1289 R1290 L1291 S1292 L1293 R1302 C1303 T1304 ALA GLY ALA THR PRO LEU ALA PRO PRO GLY LEU GLN PRO PRO ALA GLU ASP GLU ALA ARG ALA ALA GLU
PRO ASP PRO ASP TYR GLU ASN LEU ARG ARG SER ALA GLY GLY TRP GLY GLU ALA GLU GLY GLY LYS GLU GLY THR ALA LYS GLU GLY THR PRO GLY GLY THR PRO GLN PRO GLY VAL GLU ALA GLN PRO VAL ARG ALA GLU ASN GLU LYS ASP ALA THR THR GLU LYS ASN LYS LYS ARG
GLY PHE LEU PHE LYS ALA LYS LYS ALA ALA MET MET THR GLN PRO PRO ALA THR PRO ALA LEU PRO ARG LEU PRO HIS ASP VAL VAL PRO ALA D1419 N1420 R1421 D1422 D1423 P1424 I1427 L1428 T1432 V1450 G1451 W1452 V1453 T1454 P1455 D1456 D1461 V1469 T1473 V1474 T1475 M1476
E1479 Q1480 G1481 N1482 V1483 H1484 S1485 S1486 L1487 K1488 C1489 C1492 S1502 P1503 G1504 Q1505 Q1506 G1507 R1508 I1509 S1510 H1511 T1512 D1513 V1520 N1532 G1533 K1534 N1537 E1543 L1548 V1552 V1561 I1562 Q1563 F1564 Q1569 I1572 L1575 K1585 N1586 Q1590 C1591 R1594 L1595
R1619 W1626 D1632 P1633 L1634 L1639 L1653 D1658 L1659 Q1660 R1671 A1675 L1676 G1677 N1678 L1695 L1698 Y1712 L1715 R1743 R1752 K1753 G1754 G1755 N1756 H1776 A1784 A1785 L1786 P1787 A1788 A1789 G1790 V1791 A1792 E1793 A1794 P1795 L1798 L1815 R1827
D1828 V1845 E1874 GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU ASP GLU GLU GLU LYS GLU GLU ASP GLU GLU GLU GLU GLU GLU LYS GLU ASP ALA GLU LYS GLU GLU GLU GLU ALA PRO GLU GLY GLU LYS GLU ASP L1922 E1923 L1943 E1963 K1968
L1969 Q1970 R1982 A1983 F1984 T1985 M1986 S1987 A1988 A1989 E1990 R1994 P2002 Q2003 E2004 Q2005 I2006 N2007 M2008 L2009 L2010 H2011 D2014 E2015 E2018 E2019 D2020 C2021 R2028 Q2029 D2030 L2046 GLU GLY GLU GLU GLU GLU PRO GLU GLU GLU THR SER LEU SER SER ARG LEU ARG SER LEU LEU
GLU THR VAL ARG LEU VAL LYS LYS LYS GLU GLU LYS PRO GLU GLU GLU LEU PRO ALA GLU E2088 K2089 S2093 L2094 Q2095 E2096 L2097 V2098 S2099 H2100 D2109 Q2127 Y2128 I2167 E2175 I2182 M2186 N2196 R2199 G2216 G2217 G2218 E2219 T2220 K2221 M2228 Q2245
L2265 G2266 M2267 V2280 L2290 Q2293 E2296 L2307 Q2308 L2314 A2315 K2316 G2317 Y2318 P2319 D2320 P2325 R2330 I2358 R2359 L2368 R2369 G2370 E2371 G2372 L2376 E2382 A2383 I2384 R2385 I2386 S2387 E2388 D2389 R2392 D2393 G2394 P2395 G2396 V2397 ARG ARG ASP ARG ARG ARG GLU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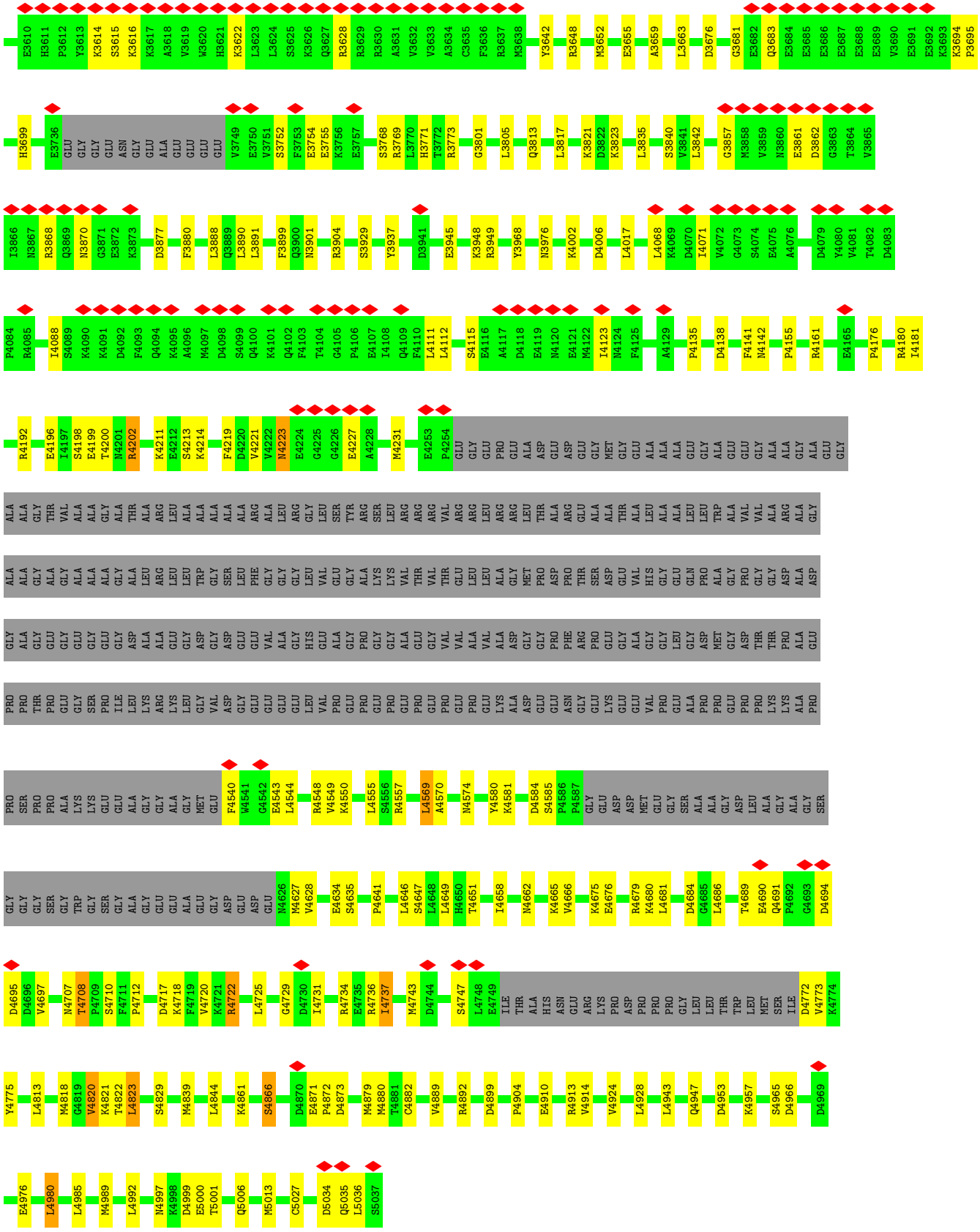
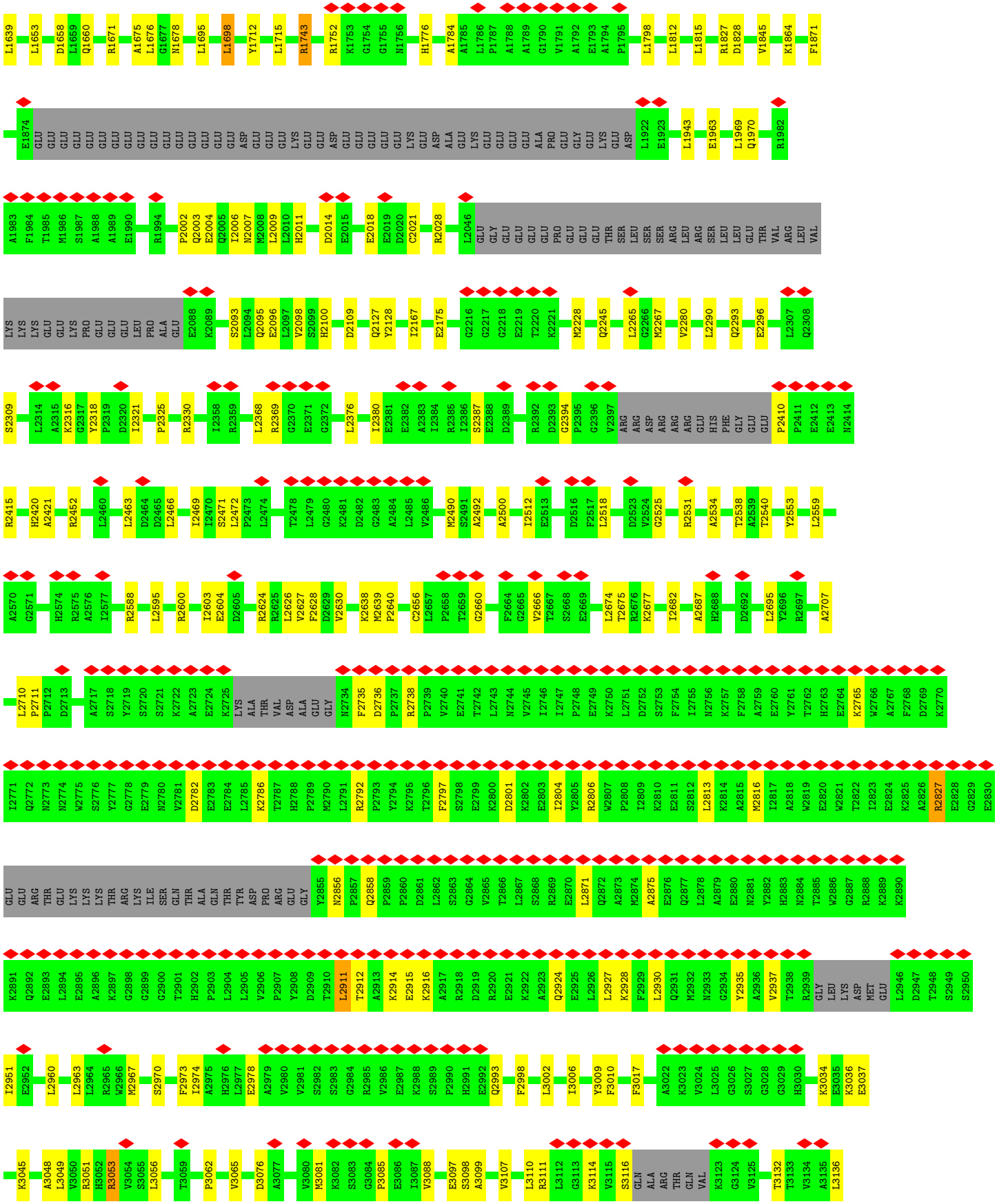
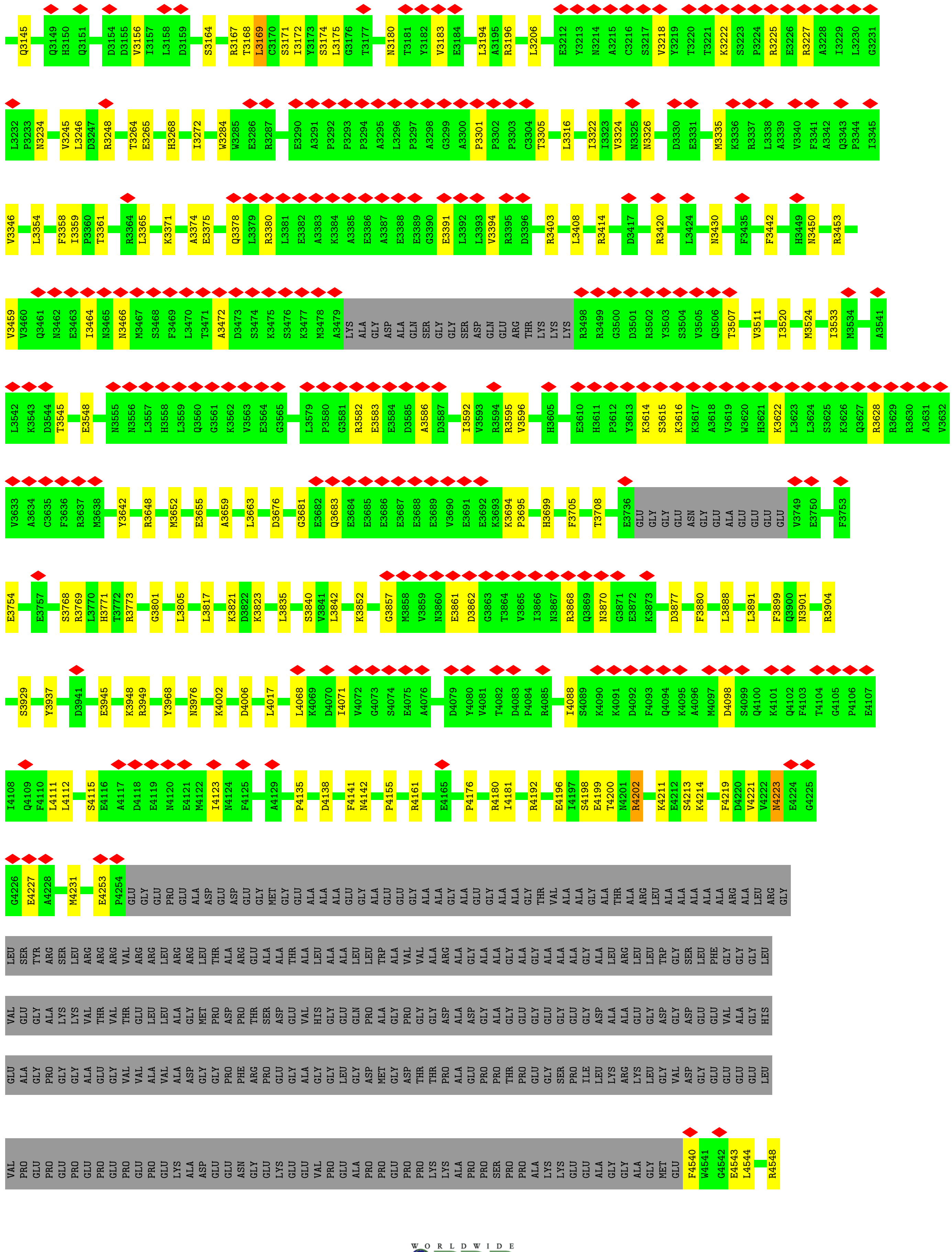


• Molecule 1: Ryanodine receptor 1

Chain C:

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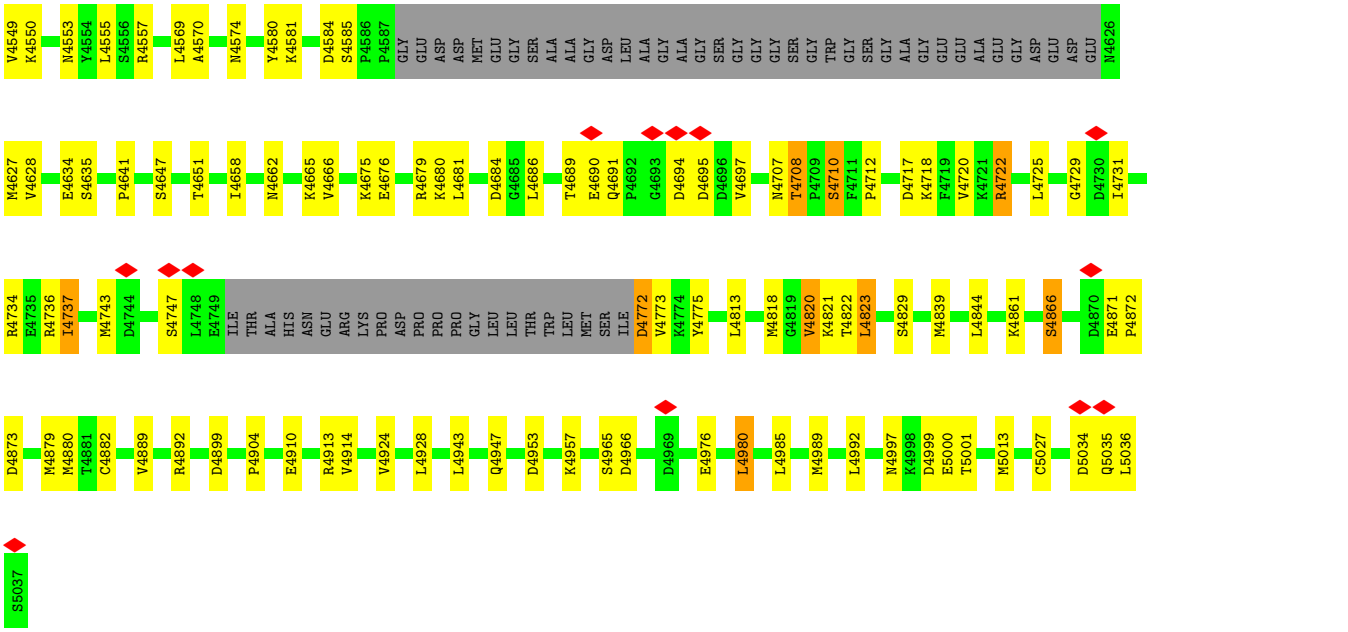
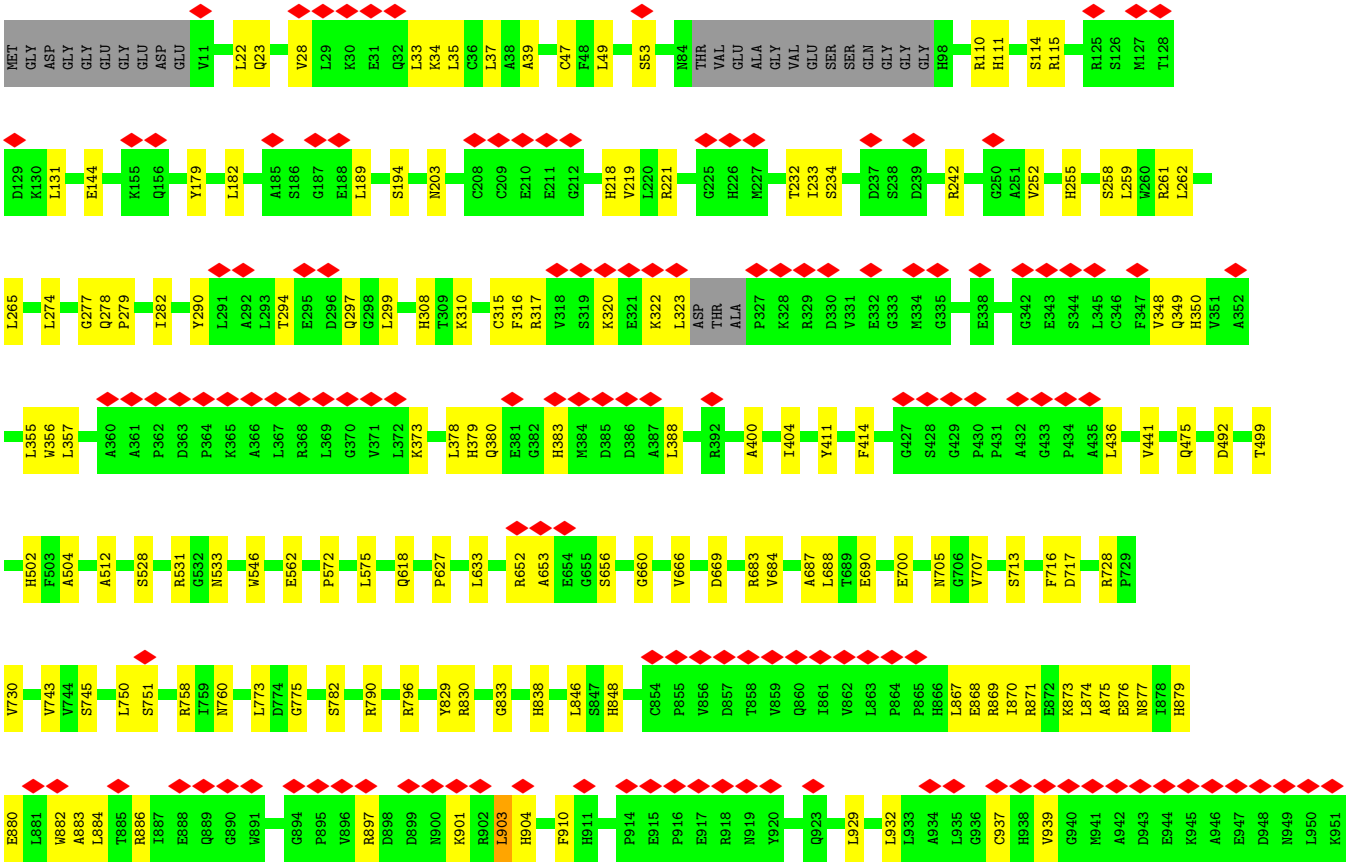
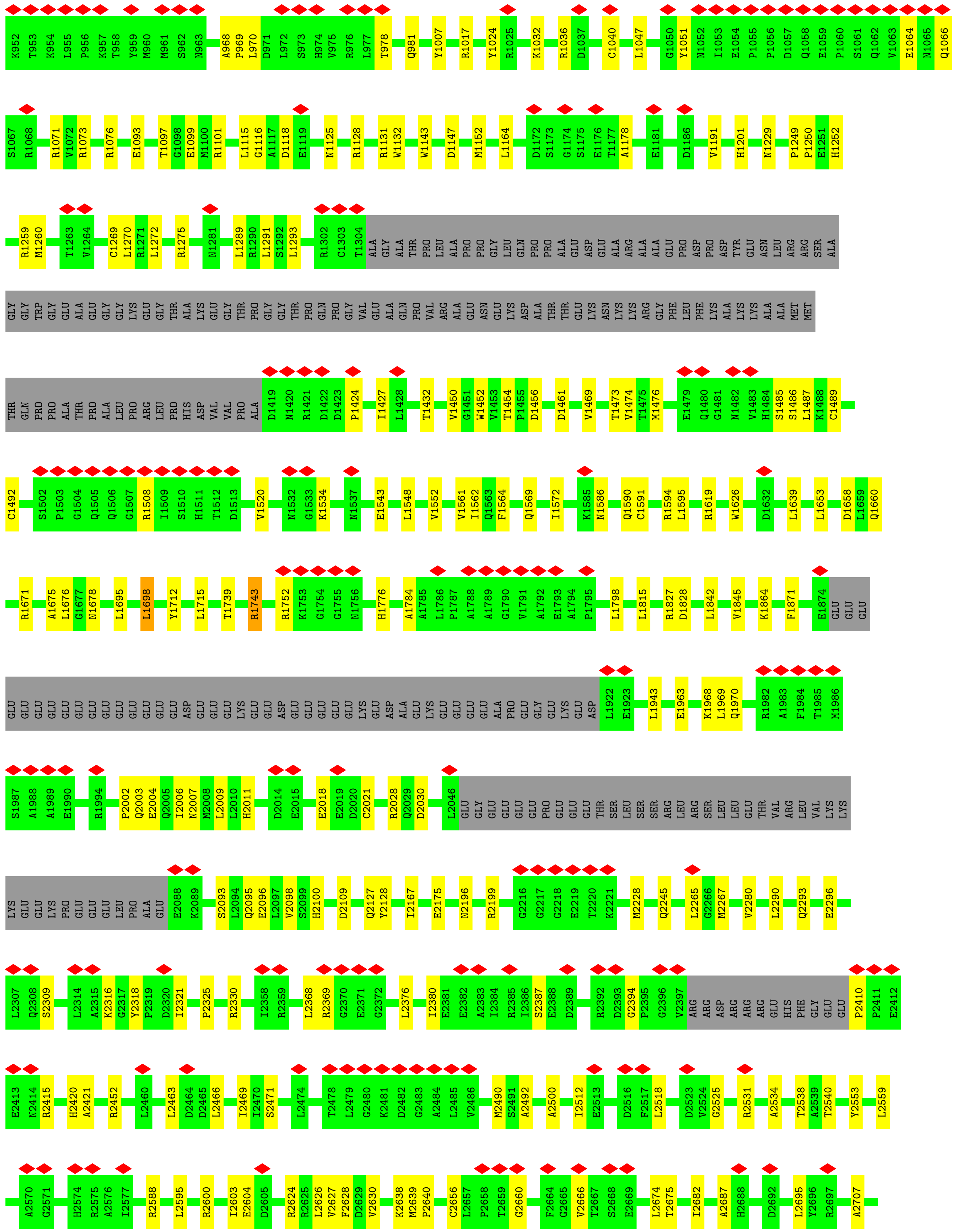
GLU ALA GLY PRO GLY GLY ALA GLU GLY VAL VAL ALA VAL ALA ASP GLY GLY PRO PHE ARG PRO GLU GLY ALA GLY GLY LEU GLY ASP MET GLY ASP THR THR PRO ALA GLU PRO PRO THR PRO GLU GLY SER PRO ILE LEU LYS ARG LYS LEU GLY VAL ASP GLY GLU GLU GLU GLU LEU
VAL PRO GLU PRO GLU PRO GLU PRO GLU PRO GLU PRO GLU LYS ALA ASP GLU GLU ASN GLY GLU LYS GLU GLU VAL PRO GLU ALA PRO PRO GLU PRO PRO LYS LYS ALA PRO PRO SER PRO PRO ALA LYS LYS GLU GLU ALA GLY GLY ALA GLY MET GLU F4540 W4541 G4542 E4543 L4544 R4548



• Molecule 1: Ryanodine receptor 1

Chain D:

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R1259 M1260 T1263 V1264 C1269 L1270 R1271 L1272 R1275 N1281 L1289 R1290 L1291 S1292 L1293 R1302 C1303 T1304 ALA GLY ALA THR PRO LEU ALA PRO PRO GLY LEU GLN PRO PRO ALA GLU ASP GLU ALA ARG ALA ALA GLU PRO ASP PRO ASP TYR GLU ASN LEU ARG ARG SER ALA
GLY GLY TRP GLY GLU ALA GLU GLY GLY LYS GLU GLY THR ALA LYS GLU GLY THR PRO GLY GLY THR PRO GLN PRO GLY VAL GLU ALA GLN PRO VAL ARG ALA GLU ASN GLU LYS ASP ALA THR THR GLU LYS ASN LYS LYS ARG GLY PHE LEU PHE LYS ALA LYS LYS ALA ALA MET MET
THR GLN PRO PRO ALA THR PRO ALA LEU PRO ARG LEU PRO HIS ASP VAL VAL PRO ALA D1419 N1420 R1421 D1422 D1423 P1424 I1427 L1428 T1432 V1450 G1451 W1452 V1453 T1454 P1455 D1456 D1461 V1469 T1473 V1474 T1475 M1476 E1479 Q1480 G1481 N1482 V1483 H1484 S1485 S1486 L1487 K1488 C1489
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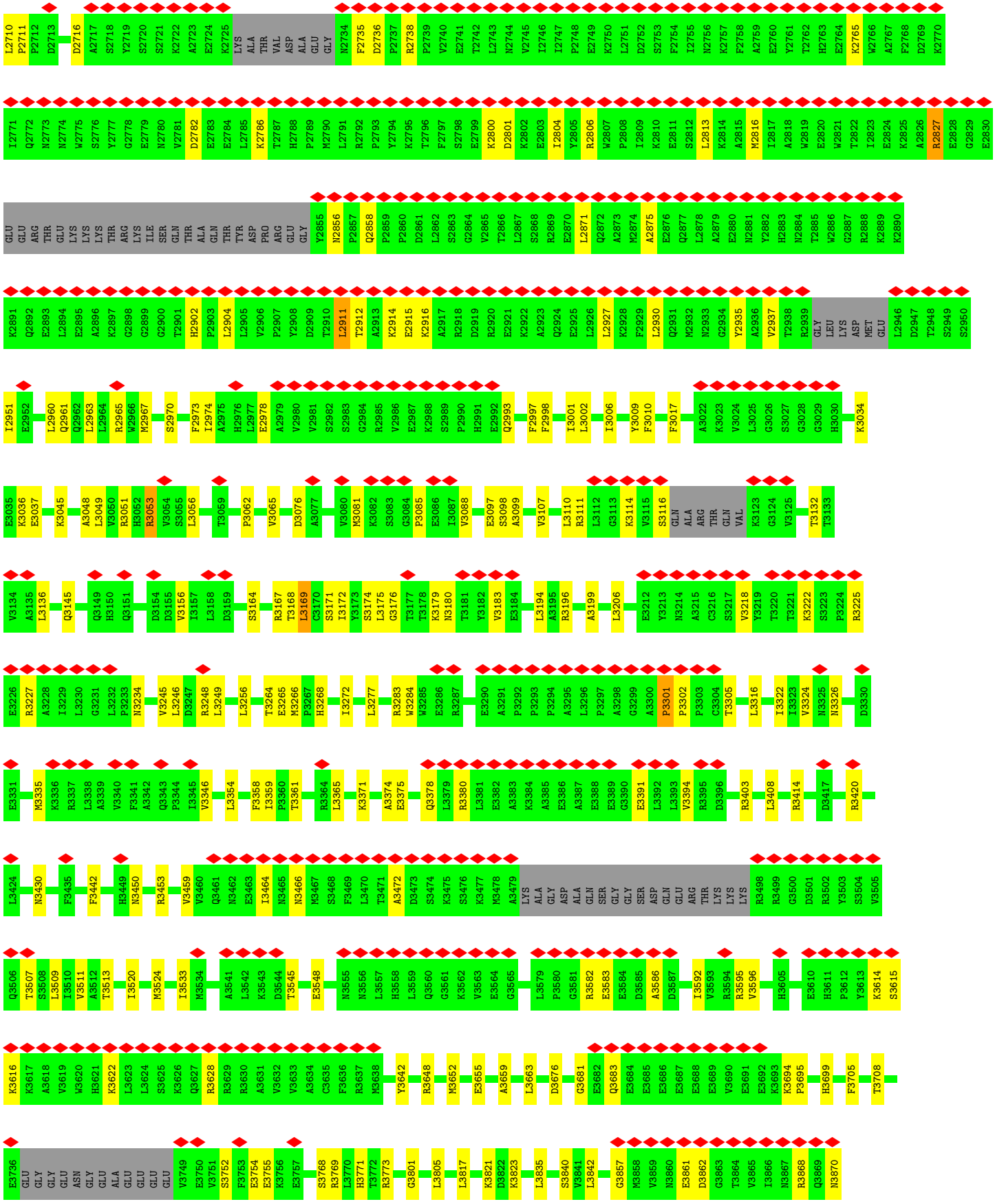
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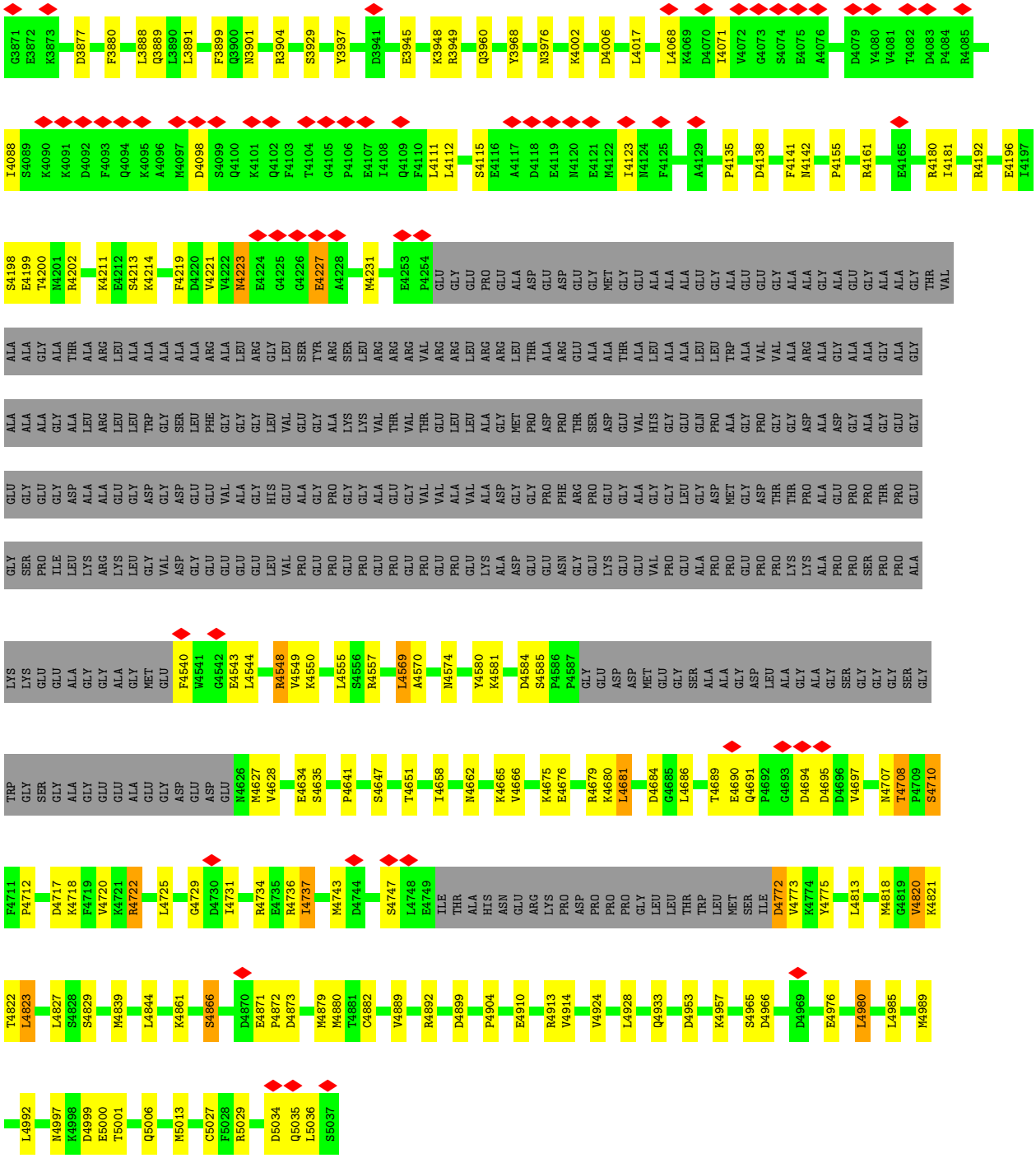
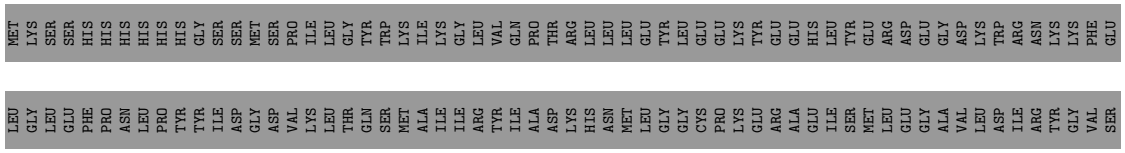
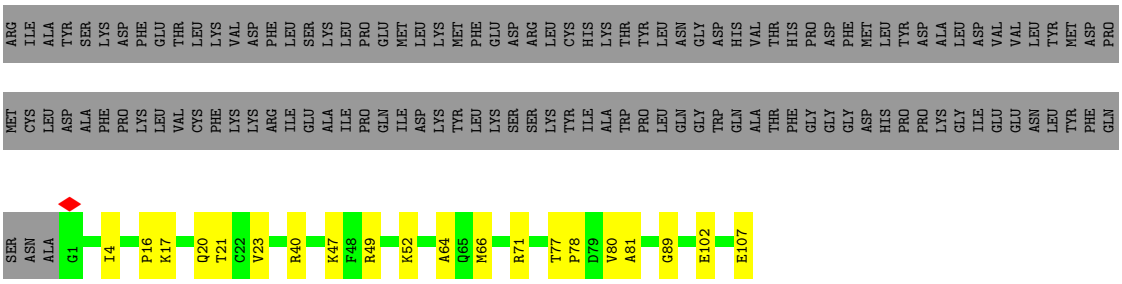
L3424 N3430 F3435 F3442 H3449 N3450 R3453 V3459 V3460 Q3461 N3462 E3463 I3464 N3465 N3466 M3467 S3468 F3469 L3470 T3471 A3472 D3473 S3474 K3475 S3476 K3477 M3478 A3479 LYS ALA GLY ASP ALA GLN SER GLY GLY SER ASP GLN GLU ARG THR LYS LYS LYS R3498 R3499 G3500 D3501 R3502 Y3503 S3504 V3505
Q3506 T3507 S3508 L3509 I3510 V3511 A3512 T3513 I3520 M3524 I3533 M3534 A3541 L3542 K3543 D3544 T3545 E3548 N3555 N3556 L3557 H3558 L3559 Q3560 G3561 K3562 V3563 E3564 G3565 L3579 P3580 G3581 R3582 E3583 E3584 D3585 A3586 D3587 I3592 V3593 R3594 R3595 V3596 H3605 E3610 H3611 P3612 Y3613 K3614 S3615
K3616 K3617 A3618 V3619 W3620 H3621 K3622 L3623 L3624 S3625 K3626 Q3627 R3628 R3629 R3630 A3631 V3632 V3633 A3634 C3635 F3636 R3637 M3638 Y3642 R3648 M3652 E3655 A3659 L3663 D3676 G3681 E3682 Q3683 E3684 E3685 E3686 E3687 E3688 E3689 V3690 E3691 E3692 K3693 K3694 P3695 H3699 F3705 T3708
E3736 GLU GLY GLY GLU ASN GLY GLU ALA GLU GLU GLU V3749 E3750 V3751 S3752 F3753 E3754 E3755 K3756 E3757 S3768 R3769 L3770 H3771 T3772 R3773 G3801 L3805 L3817 K3821 D3822 K3823 L3835 S3840 V3841 L3842 G3857 M3858 V3859 N3860 E3861 D3862 G3863 T3864 V3865 I3866 N3867 R3868 Q3869 N3870



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

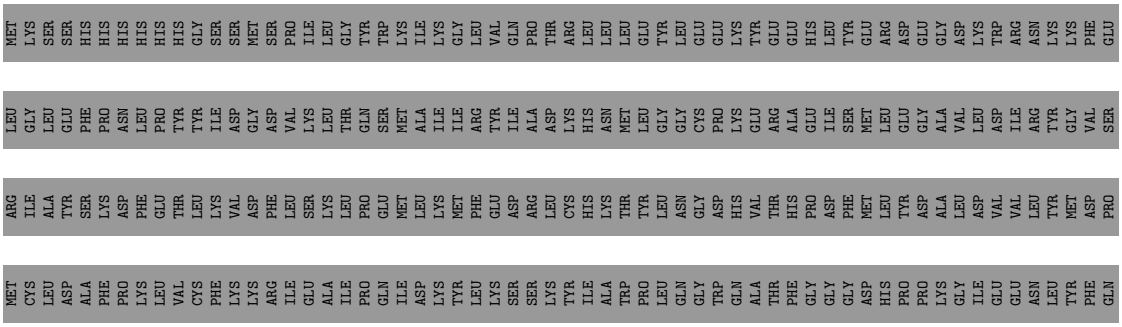
Chain E:





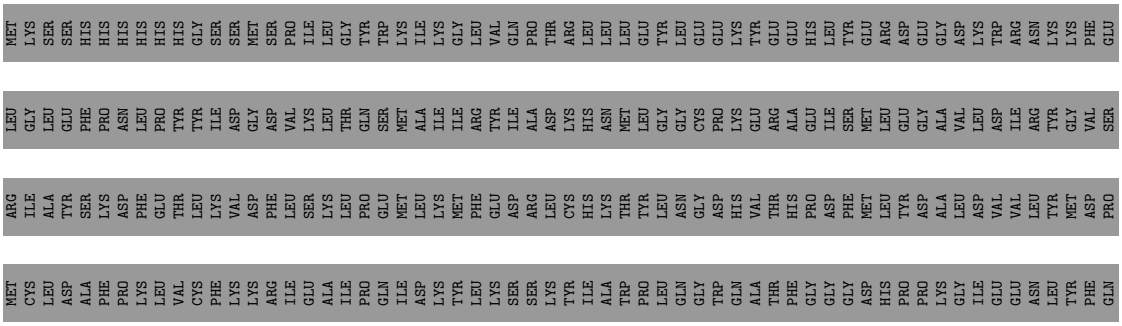
• Molecule 2: Glutathione S-transferase class-mu 26 kDa isozyme,Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F:



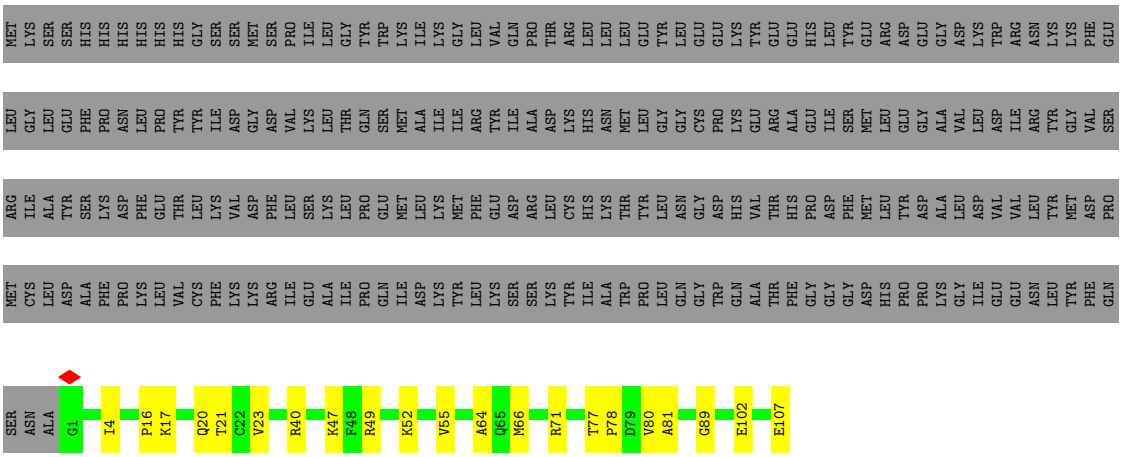
• Molecule 2: Glutathione S-transferase class-mu 26 kDa isozyme,Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain G:



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

Chain H:


MET LYS SER SER HIS HIS HIS HIS HIS HIS GLY SER SER MET SER PRO ILE LEU GLY TYR TRP LYS ILE LYS GLY LEU VAL GLN PRO THR ARG LEU LEU LEU GLU TYR LEU GLU GLU LYS TYR GLU GLU HIS LEU TYR GLU ARG ASP GLU GLY ASP LYS TRP ARG ASN LYS LYS PHE GLU
LEU GLY LEU GLU PHE PRO ASN LEU PRO TYR TYR ILE ASP GLY ASP VAL LYS LEU THR GLN SER MET ALA ILE ILE ARG TYR ILE ALA ASP LYS HIS ASN MET LEU GLY GLY CYS PRO LYS GLU ARG ALA GLU ILE SER MET LEU GLU GLU GLY ALA VAL LEU ASP ILE ARG TYR GLY VAL SER
ARG ILE ALA TYR SER LYS ASP PHE GLU THR LEU LYS VAL ASP PHE LEU SER LYS LEU PRO GLU MET LEU LYS MET PHE GLU ASP ARG LEU CYS HIS LYS THR TYR LEU ASN GLY ASP HIS VAL THR HIS PRO ASP PHE MET LEU TYR ASP ALA LEU VAL VAL LEU TYR MET ASP PRO
MET CYS LEU ASP ALA PHE PRO LYS LEU VAL CYS PHE LYS LYS ARG ILE GLU ALA ILE PRO GLN ILE ASP LYS TYR LEU LYS SER SER LYS TYR ILE ALA TRP PRO LEU GLN GLY TRP GLN ALA THR PHE GLY GLY GLY ASP HIS PRO PRO LYS GLY ILE GLU GLU ASN LEU TYR PHE GLN
SER ASN ALA G1 I4 P16 K17 Q20 T21 C22 V23 R40 K47 F48 R49 K52 V55 A64 Q65 M66 R71 T77 P78 D79 V80 A81 G89 E102 E107

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	45876	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.402	Depositor
Minimum map value	-0.437	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.075	Depositor
Recommended contour level	0.428	Depositor
Map size (Å)	515.2, 515.2, 515.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.288, 1.288, 1.288	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.32	0/35738	0.63	10/48398 (0.0%)
1	B	0.32	0/35738	0.63	10/48398 (0.0%)
1	C	0.32	0/35738	0.63	10/48398 (0.0%)
1	D	0.32	0/35738	0.63	10/48398 (0.0%)
2	E	0.32	0/834	0.62	0/1123
2	F	0.32	0/834	0.62	0/1123
2	G	0.32	0/834	0.62	0/1123
2	H	0.32	0/834	0.62	0/1123
All	All	0.32	0/146288	0.63	40/198084 (0.0%)

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	3301	PRO	N-CD-CG	-7.38	92.12	103.20
1	B	3301	PRO	N-CD-CG	-7.38	92.13	103.20
1	C	3301	PRO	N-CD-CG	-7.38	92.13	103.20
1	D	3301	PRO	N-CD-CG	-7.38	92.13	103.20
1	A	3301	PRO	CA-N-CD	-6.90	101.85	111.50
1	B	3301	PRO	CA-N-CD	-6.87	101.89	111.50
1	C	3301	PRO	CA-N-CD	-6.87	101.89	111.50
1	D	3301	PRO	CA-N-CD	-6.87	101.89	111.50
1	B	1698	LEU	CA-CB-CG	6.78	130.89	115.30
1	C	1698	LEU	CA-CB-CG	6.77	130.88	115.30
1	D	1698	LEU	CA-CB-CG	6.77	130.88	115.30
1	A	1698	LEU	CA-CB-CG	6.77	130.87	115.30
1	A	903	LEU	CA-CB-CG	6.48	130.21	115.30
1	B	903	LEU	CA-CB-CG	6.46	130.16	115.30
1	C	903	LEU	CA-CB-CG	6.46	130.16	115.30
1	D	903	LEU	CA-CB-CG	6.46	130.16	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	131	LEU	CA-CB-CG	5.79	128.61	115.30
1	C	131	LEU	CA-CB-CG	5.79	128.61	115.30
1	D	131	LEU	CA-CB-CG	5.79	128.61	115.30
1	A	131	LEU	CA-CB-CG	5.76	128.54	115.30
1	B	3169	LEU	CA-CB-CG	5.43	127.79	115.30
1	C	3169	LEU	CA-CB-CG	5.43	127.79	115.30
1	D	3169	LEU	CA-CB-CG	5.43	127.79	115.30
1	A	3169	LEU	CA-CB-CG	5.41	127.75	115.30
1	B	2267	MET	CA-CB-CG	5.39	122.46	113.30
1	C	2267	MET	CA-CB-CG	5.39	122.46	113.30
1	D	2267	MET	CA-CB-CG	5.39	122.46	113.30
1	A	2267	MET	CA-CB-CG	5.39	122.46	113.30
1	B	2911	LEU	CA-CB-CG	5.31	127.51	115.30
1	C	2911	LEU	CA-CB-CG	5.31	127.51	115.30
1	D	2911	LEU	CA-CB-CG	5.31	127.51	115.30
1	A	2911	LEU	CA-CB-CG	5.28	127.45	115.30
1	B	182	LEU	CA-CB-CG	5.26	127.40	115.30
1	C	182	LEU	CA-CB-CG	5.26	127.40	115.30
1	D	182	LEU	CA-CB-CG	5.26	127.40	115.30
1	A	182	LEU	CA-CB-CG	5.26	127.39	115.30
1	A	1152	MET	CA-CB-CG	5.02	121.84	113.30
1	B	1152	MET	CA-CB-CG	5.01	121.82	113.30
1	C	1152	MET	CA-CB-CG	5.01	121.82	113.30
1	D	1152	MET	CA-CB-CG	5.01	121.82	113.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	34921	0	34541	354	0
1	B	34921	0	34541	351	0
1	C	34921	0	34541	343	0
1	D	34921	0	34541	354	0
2	E	818	0	824	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	818	0	824	13	0
2	G	818	0	824	13	0
2	H	818	0	824	12	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
All	All	142960	0	141460	1433	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 5.

All (1433) 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:A:1561:VAL:HG12	1:A:1562:ILE:HG12	1.73	0.71
1:C:1561:VAL:HG12	1:C:1562:ILE:HG12	1.73	0.71
1:B:1561:VAL:HG12	1:B:1562:ILE:HG12	1.73	0.71
1:D:3114:LYS:HD3	1:D:3116:SER:H	1.56	0.70
1:D:1561:VAL:HG12	1:D:1562:ILE:HG12	1.73	0.70
1:A:3114:LYS:HD3	1:A:3116:SER:H	1.56	0.70
1:B:3114:LYS:HD3	1:B:3116:SER:H	1.56	0.70
1:C:3114:LYS:HD3	1:C:3116:SER:H	1.56	0.69
1:A:4904:PRO:HB3	1:A:4913:ARG:HG2	1.76	0.68
1:D:4904:PRO:HB3	1:D:4913:ARG:HG2	1.76	0.67
1:A:2875:ALA:HB2	1:A:2927:LEU:HD22	1.77	0.67
1:B:2875:ALA:HB2	1:B:2927:LEU:HD22	1.77	0.66
1:C:4904:PRO:HB3	1:C:4913:ARG:HG2	1.76	0.66
1:C:2875:ALA:HB2	1:C:2927:LEU:HD22	1.77	0.66
1:B:4904:PRO:HB3	1:B:4913:ARG:HG2	1.76	0.66
1:C:1116:GLY:HA3	1:C:1132:TRP:HB3	1.78	0.66
1:D:1116:GLY:HA3	1:D:1132:TRP:HB3	1.78	0.66
1:D:2875:ALA:HB2	1:D:2927:LEU:HD22	1.77	0.65
1:B:666:VAL:HG21	1:B:684:VAL:HG21	1.79	0.65
1:D:666:VAL:HG21	1:D:684:VAL:HG21	1.79	0.65
1:B:1116:GLY:HA3	1:B:1132:TRP:HB3	1.78	0.65
1:C:666:VAL:HG21	1:C:684:VAL:HG21	1.79	0.65
1:D:981:GLN:HG2	1:D:1047:LEU:HD11	1.78	0.65
1:C:981:GLN:HG2	1:C:1047:LEU:HD11	1.78	0.65
1:A:35:LEU:HD13	1:A:49:LEU:HD13	1.79	0.65
1:A:1116:GLY:HA3	1:A:1132:TRP:HB3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:LEU:HD13	1:D:49:LEU:HD13	1.79	0.64
1:A:666:VAL:HG21	1:A:684:VAL:HG21	1.79	0.64
1:D:1476:MET:HB2	1:D:1485:SER:HB3	1.80	0.64
1:B:1476:MET:HB2	1:B:1485:SER:HB3	1.80	0.64
1:A:1476:MET:HB2	1:A:1485:SER:HB3	1.80	0.64
1:B:35:LEU:HD13	1:B:49:LEU:HD13	1.79	0.64
1:B:981:GLN:HG2	1:B:1047:LEU:HD11	1.78	0.64
1:C:23:GLN:OE1	1:C:203:ASN:ND2	2.31	0.64
1:D:23:GLN:OE1	1:D:203:ASN:ND2	2.31	0.64
1:A:981:GLN:HG2	1:A:1047:LEU:HD11	1.78	0.63
1:B:23:GLN:OE1	1:B:203:ASN:ND2	2.31	0.63
1:C:1476:MET:HB2	1:C:1485:SER:HB3	1.80	0.63
1:C:35:LEU:HD13	1:C:49:LEU:HD13	1.79	0.63
1:A:23:GLN:OE1	1:A:203:ASN:ND2	2.31	0.63
1:B:3459:VAL:HG13	1:B:3464:ILE:HB	1.81	0.63
1:A:3459:VAL:HG13	1:A:3464:ILE:HB	1.81	0.62
1:C:1024:TYR:O	1:C:1032:LYS:NZ	2.33	0.62
1:B:1024:TYR:O	1:B:1032:LYS:NZ	2.33	0.62
1:C:3459:VAL:HG13	1:C:3464:ILE:HB	1.81	0.62
1:A:978:THR:OG1	1:A:981:GLN:OE1	2.18	0.62
1:A:34:LYS:H	1:A:53:SER:HB3	1.66	0.61
1:B:317:ARG:NH1	1:B:349:GLN:OE1	2.34	0.61
1:B:978:THR:OG1	1:B:981:GLN:OE1	2.18	0.61
1:D:3459:VAL:HG13	1:D:3464:ILE:HB	1.81	0.61
1:A:317:ARG:NH1	1:A:349:GLN:OE1	2.34	0.61
1:B:34:LYS:H	1:B:53:SER:HB3	1.66	0.61
1:D:1024:TYR:O	1:D:1032:LYS:NZ	2.33	0.61
1:C:317:ARG:NH1	1:C:349:GLN:OE1	2.34	0.61
1:C:3524:MET:HA	1:C:3582:ARG:HH22	1.65	0.61
1:A:688:LEU:HD23	1:A:690:GLU:H	1.66	0.61
1:A:3172:ILE:HD11	1:A:3194:LEU:HD13	1.83	0.61
1:D:1569:GLN:HB2	1:D:1572:ILE:HD12	1.83	0.61
1:D:3524:MET:HA	1:D:3582:ARG:HH22	1.65	0.61
1:D:4138:ASP:O	1:D:4142:ASN:ND2	2.33	0.61
1:A:3335:MET:SD	1:A:3403:ARG:NH1	2.74	0.61
1:B:3172:ILE:HD11	1:B:3194:LEU:HD13	1.83	0.61
1:B:3335:MET:SD	1:B:3403:ARG:NH1	2.74	0.61
1:D:317:ARG:NH1	1:D:349:GLN:OE1	2.34	0.61
1:A:4892:ARG:NH1	1:B:4899:ASP:OD1	2.34	0.61
1:C:3681:GLY:O	1:C:3683:GLN:NE2	2.34	0.60
1:D:978:THR:OG1	1:D:981:GLN:OE1	2.18	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1569:GLN:HB2	1:A:1572:ILE:HD12	1.83	0.60
1:A:3524:MET:HA	1:A:3582:ARG:HH22	1.65	0.60
1:B:3524:MET:HA	1:B:3582:ARG:HH22	1.65	0.60
1:C:1131:ARG:NH1	1:C:1178:ALA:O	2.34	0.60
1:D:3172:ILE:HD11	1:D:3194:LEU:HD13	1.83	0.60
1:A:1024:TYR:O	1:A:1032:LYS:NZ	2.33	0.60
1:B:3681:GLY:O	1:B:3683:GLN:NE2	2.34	0.60
1:C:978:THR:OG1	1:C:981:GLN:OE1	2.18	0.60
1:C:2175:GLU:HG3	1:C:2228:MET:HB2	1.82	0.60
1:C:3335:MET:SD	1:C:3403:ARG:NH1	2.74	0.60
1:D:34:LYS:H	1:D:53:SER:HB3	1.66	0.60
1:D:1131:ARG:NH1	1:D:1178:ALA:O	2.34	0.60
1:B:1569:GLN:HB2	1:B:1572:ILE:HD12	1.83	0.60
1:B:688:LEU:HD23	1:B:690:GLU:H	1.65	0.60
1:B:1064:GLU:O	1:B:1071:ARG:NH2	2.32	0.60
1:C:34:LYS:H	1:C:53:SER:HB3	1.66	0.60
1:B:2175:GLU:HG3	1:B:2228:MET:HB2	1.82	0.60
1:C:1252:HIS:O	1:C:1275:ARG:NH2	2.34	0.60
1:A:2175:GLU:HG3	1:A:2228:MET:HB2	1.82	0.60
1:A:1131:ARG:NH1	1:A:1178:ALA:O	2.35	0.59
1:A:3681:GLY:O	1:A:3683:GLN:NE2	2.34	0.59
1:D:2175:GLU:HG3	1:D:2228:MET:HB2	1.82	0.59
1:C:688:LEU:HD23	1:C:690:GLU:H	1.65	0.59
1:C:1569:GLN:HB2	1:C:1572:ILE:HD12	1.83	0.59
1:C:3172:ILE:HD11	1:C:3194:LEU:HD13	1.83	0.59
1:A:1064:GLU:O	1:A:1071:ARG:NH2	2.32	0.59
1:D:688:LEU:HD23	1:D:690:GLU:H	1.65	0.59
1:D:317:ARG:HD3	1:D:323:LEU:HD23	1.84	0.59
1:B:1131:ARG:NH1	1:B:1178:ALA:O	2.34	0.59
1:D:3681:GLY:O	1:D:3683:GLN:NE2	2.34	0.59
1:A:897:ARG:HB2	1:A:903:LEU:HD11	1.85	0.59
1:A:3324:VAL:HG11	1:A:3361:THR:HG22	1.85	0.59
1:B:745:SER:HB2	1:B:758:ARG:HB2	1.85	0.59
1:C:3354:LEU:HA	1:C:3358:PHE:HB2	1.85	0.59
1:A:317:ARG:HD3	1:A:323:LEU:HD23	1.84	0.58
1:B:1101:ARG:NH1	1:B:1115:LEU:O	2.36	0.58
1:C:3324:VAL:HG11	1:C:3361:THR:HG22	1.85	0.58
1:D:1101:ARG:NH1	1:D:1115:LEU:O	2.36	0.58
1:C:1101:ARG:NH1	1:C:1115:LEU:O	2.36	0.58
1:D:897:ARG:HB2	1:D:903:LEU:HD11	1.85	0.58
1:B:317:ARG:HD3	1:B:323:LEU:HD23	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:317:ARG:HD3	1:C:323:LEU:HD23	1.84	0.58
1:C:728:ARG:NH2	1:C:1489:CYS:SG	2.77	0.58
1:D:745:SER:HB2	1:D:758:ARG:HB2	1.85	0.58
1:D:3335:MET:SD	1:D:3403:ARG:NH1	2.74	0.58
1:A:745:SER:HB2	1:A:758:ARG:HB2	1.85	0.58
1:A:3533:ILE:HD13	1:A:3596:VAL:HG13	1.85	0.58
1:B:1252:HIS:O	1:B:1275:ARG:NH2	2.34	0.58
1:D:3354:LEU:HA	1:D:3358:PHE:HB2	1.85	0.58
1:A:728:ARG:NH2	1:A:1489:CYS:SG	2.77	0.58
1:B:728:ARG:NH2	1:B:1489:CYS:SG	2.77	0.58
1:D:728:ARG:NH2	1:D:1489:CYS:SG	2.77	0.58
1:B:3354:LEU:HA	1:B:3358:PHE:HB2	1.85	0.58
1:D:2093:SER:OG	1:D:2096:GLU:OE1	2.21	0.58
1:A:1101:ARG:NH1	1:A:1115:LEU:O	2.36	0.58
1:C:1064:GLU:O	1:C:1071:ARG:NH2	2.32	0.58
1:C:4138:ASP:O	1:C:4142:ASN:ND2	2.33	0.58
1:D:1252:HIS:O	1:D:1275:ARG:NH2	2.34	0.58
1:C:3533:ILE:HD13	1:C:3596:VAL:HG13	1.85	0.58
1:D:3324:VAL:HG11	1:D:3361:THR:HG22	1.85	0.57
1:B:3324:VAL:HG11	1:B:3361:THR:HG22	1.85	0.57
1:D:3533:ILE:HD13	1:D:3596:VAL:HG13	1.85	0.57
1:A:2624:ARG:HH12	1:A:2911:LEU:HA	1.70	0.57
1:C:897:ARG:HB2	1:C:903:LEU:HD11	1.85	0.57
1:A:3354:LEU:HA	1:A:3358:PHE:HB2	1.85	0.57
1:A:3937:TYR:O	1:A:4002:LYS:NZ	2.38	0.57
1:B:1943:LEU:HD13	1:B:2098:VAL:HG22	1.87	0.57
1:D:3284:TRP:HB3	1:D:3305:THR:HG21	1.87	0.57
1:A:2630:VAL:HG12	1:A:2682:ILE:HD11	1.87	0.57
1:B:897:ARG:HB2	1:B:903:LEU:HD11	1.85	0.57
1:D:2630:VAL:HG12	1:D:2682:ILE:HD11	1.87	0.57
1:B:475:GLN:NE2	1:B:528:SER:O	2.38	0.57
1:C:745:SER:HB2	1:C:758:ARG:HB2	1.85	0.57
1:C:2624:ARG:HH12	1:C:2911:LEU:HA	1.70	0.57
1:C:3284:TRP:HB3	1:C:3305:THR:HG21	1.87	0.57
1:D:1097:THR:HA	1:D:1143:TRP:HE1	1.70	0.57
1:A:3017:PHE:O	1:A:3036:LYS:NZ	2.38	0.57
1:B:3533:ILE:HD13	1:B:3596:VAL:HG13	1.85	0.57
1:C:2630:VAL:HG12	1:C:2682:ILE:HD11	1.87	0.57
1:D:1698:LEU:HD21	1:D:1715:LEU:HD13	1.86	0.57
1:B:3017:PHE:O	1:B:3036:LYS:NZ	2.38	0.57
1:C:475:GLN:NE2	1:C:528:SER:O	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:475:GLN:NE2	1:D:528:SER:O	2.38	0.57
1:A:475:GLN:NE2	1:A:528:SER:O	2.38	0.56
1:B:1698:LEU:HD21	1:B:1715:LEU:HD13	1.86	0.56
1:B:4866:SER:HB2	1:B:4873:ASP:H	1.70	0.56
1:D:3937:TYR:O	1:D:4002:LYS:NZ	2.38	0.56
1:B:882:TRP:O	1:B:886:ARG:NH1	2.38	0.56
1:B:2630:VAL:HG12	1:B:2682:ILE:HD11	1.87	0.56
1:D:1943:LEU:HD13	1:D:2098:VAL:HG22	1.87	0.56
1:A:882:TRP:O	1:A:886:ARG:NH1	2.38	0.56
1:B:3937:TYR:O	1:B:4002:LYS:NZ	2.38	0.56
1:C:1698:LEU:HD21	1:C:1715:LEU:HD13	1.86	0.56
1:D:2624:ARG:HH12	1:D:2911:LEU:HA	1.70	0.56
1:B:1097:THR:HA	1:B:1143:TRP:HE1	1.70	0.56
1:C:1097:THR:HA	1:C:1143:TRP:HE1	1.70	0.56
1:C:3937:TYR:O	1:C:4002:LYS:NZ	2.38	0.56
1:D:1064:GLU:O	1:D:1071:ARG:NH2	2.32	0.56
1:D:1259:ARG:NH2	1:D:1591:CYS:SG	2.79	0.56
1:A:1698:LEU:HD21	1:A:1715:LEU:HD13	1.86	0.56
1:B:3006:ILE:O	1:B:3010:PHE:HB2	2.06	0.56
1:D:867:LEU:HD13	1:D:929:LEU:HB3	1.88	0.56
1:A:867:LEU:HD13	1:A:929:LEU:HB3	1.88	0.56
1:C:882:TRP:O	1:C:886:ARG:NH1	2.38	0.56
1:A:1097:THR:HA	1:A:1143:TRP:HE1	1.70	0.56
1:A:1252:HIS:O	1:A:1275:ARG:NH2	2.34	0.56
1:C:867:LEU:HD13	1:C:929:LEU:HB3	1.88	0.56
1:C:1259:ARG:NH2	1:C:1591:CYS:SG	2.79	0.56
1:D:882:TRP:O	1:D:886:ARG:NH1	2.38	0.56
1:A:1943:LEU:HD13	1:A:2098:VAL:HG22	1.87	0.56
1:A:2093:SER:OG	1:A:2096:GLU:OE1	2.21	0.56
1:A:3769:ARG:O	1:A:3773:ARG:NH1	2.39	0.56
1:B:3284:TRP:HB3	1:B:3305:THR:HG21	1.87	0.56
1:C:1943:LEU:HD13	1:C:2098:VAL:HG22	1.87	0.56
2:G:40:ARG:NH2	2:G:102:GLU:OE1	2.39	0.56
1:B:2624:ARG:HH12	1:B:2911:LEU:HA	1.70	0.56
1:B:4138:ASP:O	1:B:4142:ASN:ND2	2.33	0.56
1:C:3017:PHE:O	1:C:3036:LYS:NZ	2.38	0.56
1:A:1259:ARG:NH2	1:A:1591:CYS:SG	2.79	0.56
1:A:3006:ILE:O	1:A:3010:PHE:HB2	2.06	0.56
1:A:3945:GLU:OE1	1:A:3949:ARG:NH1	2.40	0.56
1:A:4866:SER:HB2	1:A:4873:ASP:H	1.70	0.56
1:A:475:GLN:OE1	1:A:533:ASN:ND2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3051:ARG:O	1:A:3053:ARG:NE	2.35	0.55
1:A:3284:TRP:HB3	1:A:3305:THR:HG21	1.87	0.55
1:B:357:LEU:HD11	1:B:388:LEU:HD11	1.89	0.55
1:B:475:GLN:OE1	1:B:533:ASN:ND2	2.39	0.55
1:B:3107:VAL:HG21	1:B:3171:SER:HB2	1.88	0.55
1:C:4866:SER:HB2	1:C:4873:ASP:H	1.70	0.55
1:D:357:LEU:HD11	1:D:388:LEU:HD11	1.89	0.55
1:D:3206:LEU:HB3	1:D:3246:LEU:HB2	1.88	0.55
1:B:3206:LEU:HB3	1:B:3246:LEU:HB2	1.88	0.55
1:B:294:THR:HG23	1:B:297:GLN:H	1.72	0.55
1:D:1653:LEU:O	1:D:1660:GLN:NE2	2.40	0.55
2:E:40:ARG:NH2	2:E:102:GLU:OE1	2.39	0.55
1:A:357:LEU:HD11	1:A:388:LEU:HD11	1.89	0.55
1:A:1653:LEU:O	1:A:1660:GLN:NE2	2.39	0.55
1:B:1259:ARG:NH2	1:B:1591:CYS:SG	2.79	0.55
1:B:3769:ARG:O	1:B:3773:ARG:NH1	2.39	0.55
1:C:357:LEU:HD11	1:C:388:LEU:HD11	1.89	0.55
1:C:4214:LYS:HD2	1:C:4985:LEU:HD11	1.89	0.55
1:D:2368:LEU:HD11	1:D:2376:LEU:HD12	1.88	0.55
1:D:3107:VAL:HG21	1:D:3171:SER:HB2	1.88	0.55
1:A:2538:THR:HG23	1:A:2540:THR:H	1.71	0.55
1:A:2960:LEU:HD23	1:A:2963:LEU:HD12	1.88	0.55
1:C:110:ARG:HH21	1:C:115:ARG:HB3	1.72	0.55
1:C:2538:THR:HG23	1:C:2540:THR:H	1.71	0.55
1:D:3051:ARG:O	1:D:3053:ARG:NE	2.35	0.55
1:D:4866:SER:HB2	1:D:4873:ASP:H	1.70	0.55
2:F:40:ARG:NH2	2:F:102:GLU:OE1	2.39	0.55
2:H:40:ARG:NH2	2:H:102:GLU:OE1	2.39	0.55
1:B:867:LEU:HD13	1:B:929:LEU:HB3	1.88	0.55
1:B:2960:LEU:HD23	1:B:2963:LEU:HD12	1.88	0.55
1:D:4068:LEU:HD22	1:D:4111:LEU:HD11	1.89	0.55
1:D:4214:LYS:HD2	1:D:4985:LEU:HD11	1.89	0.55
1:B:1260:MET:HB2	1:B:1269:CYS:HB2	1.89	0.55
1:C:3006:ILE:O	1:C:3010:PHE:HB2	2.06	0.55
1:D:683:ARG:HG2	1:D:717:ASP:HB3	1.89	0.55
1:A:4214:LYS:HD2	1:A:4985:LEU:HD11	1.89	0.55
1:C:2368:LEU:HD11	1:C:2376:LEU:HD12	1.88	0.55
1:C:2912:THR:O	1:C:2916:LYS:HB2	2.07	0.55
1:C:3206:LEU:HB3	1:C:3246:LEU:HB2	1.88	0.55
1:A:499:THR:HG23	1:A:502:HIS:H	1.72	0.55
1:A:4068:LEU:HD22	1:A:4111:LEU:HD11	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2368:LEU:HD11	1:B:2376:LEU:HD12	1.88	0.55
1:B:3945:GLU:OE1	1:B:3949:ARG:NH1	2.40	0.55
1:C:707:VAL:HG23	1:C:782:SER:HB3	1.89	0.55
1:D:707:VAL:HG23	1:D:782:SER:HB3	1.89	0.55
1:D:3006:ILE:O	1:D:3010:PHE:HB2	2.06	0.55
1:A:683:ARG:HG2	1:A:717:ASP:HB3	1.89	0.54
1:A:1260:MET:HB2	1:A:1269:CYS:HB2	1.89	0.54
1:A:2018:GLU:OE1	1:A:2028:ARG:NH1	2.40	0.54
1:A:3107:VAL:HG21	1:A:3171:SER:HB2	1.88	0.54
1:A:3145:GLN:OE1	1:A:3196:ARG:NE	2.40	0.54
1:A:3206:LEU:HB3	1:A:3246:LEU:HB2	1.88	0.54
1:B:707:VAL:HG23	1:B:782:SER:HB3	1.89	0.54
1:C:683:ARG:HG2	1:C:717:ASP:HB3	1.89	0.54
1:C:1653:LEU:O	1:C:1660:GLN:NE2	2.40	0.54
1:C:2018:GLU:OE1	1:C:2028:ARG:NH1	2.40	0.54
1:D:1272:LEU:HD22	1:D:1289:LEU:HD11	1.90	0.54
1:D:3145:GLN:OE1	1:D:3196:ARG:NE	2.40	0.54
1:A:2368:LEU:HD11	1:A:2376:LEU:HD12	1.88	0.54
1:B:4214:LYS:HD2	1:B:4985:LEU:HD11	1.89	0.54
1:C:232:THR:HG22	1:C:258:SER:HB3	1.89	0.54
1:C:1260:MET:HB2	1:C:1269:CYS:HB2	1.89	0.54
1:C:3145:GLN:OE1	1:C:3196:ARG:NE	2.40	0.54
1:A:233:ILE:HD12	1:A:242:ARG:HB3	1.90	0.54
1:A:707:VAL:HG23	1:A:782:SER:HB3	1.89	0.54
1:A:886:ARG:HE	1:A:904:HIS:HB2	1.72	0.54
1:A:1272:LEU:HD22	1:A:1289:LEU:HD11	1.90	0.54
1:A:2912:THR:O	1:A:2916:LYS:HB2	2.07	0.54
1:B:499:THR:HG23	1:B:502:HIS:H	1.72	0.54
1:B:886:ARG:HE	1:B:904:HIS:HB2	1.72	0.54
1:D:232:THR:HG22	1:D:258:SER:HB3	1.89	0.54
1:D:294:THR:HG23	1:D:297:GLN:H	1.72	0.54
1:D:1260:MET:HB2	1:D:1269:CYS:HB2	1.89	0.54
1:B:1653:LEU:O	1:B:1660:GLN:NE2	2.40	0.54
1:D:499:THR:HG23	1:D:502:HIS:H	1.72	0.54
1:D:3945:GLU:OE1	1:D:3949:ARG:NH1	2.40	0.54
1:A:2595:LEU:O	1:A:2600:ARG:NH2	2.41	0.54
1:A:4138:ASP:O	1:A:4142:ASN:ND2	2.33	0.54
1:B:2018:GLU:OE1	1:B:2028:ARG:NH1	2.40	0.54
1:B:2595:LEU:O	1:B:2600:ARG:NH2	2.41	0.54
1:B:2912:THR:O	1:B:2916:LYS:HB2	2.07	0.54
1:C:475:GLN:OE1	1:C:533:ASN:ND2	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:THR:HG23	1:A:297:GLN:H	1.72	0.54
1:B:110:ARG:HH21	1:B:115:ARG:HB3	1.72	0.54
1:C:1272:LEU:HD22	1:C:1289:LEU:HD11	1.90	0.54
1:C:2960:LEU:HD23	1:C:2963:LEU:HD12	1.88	0.54
1:D:110:ARG:HH21	1:D:115:ARG:HB3	1.72	0.54
1:D:2538:THR:HG23	1:D:2540:THR:H	1.71	0.54
1:D:2960:LEU:HD23	1:D:2963:LEU:HD12	1.88	0.54
1:D:3048:ALA:O	1:D:3053:ARG:NH2	2.41	0.54
1:A:3414:ARG:HE	1:A:3472:ALA:HB3	1.73	0.54
1:B:683:ARG:HG2	1:B:717:ASP:HB3	1.89	0.54
1:C:1454:THR:OG1	1:C:1456:ASP:OD1	2.24	0.54
1:D:3769:ARG:O	1:D:3773:ARG:NH1	2.39	0.54
2:E:17:LYS:HE3	2:E:20:GLN:HE22	1.73	0.54
1:B:3048:ALA:O	1:B:3053:ARG:NH2	2.41	0.54
1:B:3145:GLN:OE1	1:B:3196:ARG:NE	2.40	0.54
1:C:2093:SER:OG	1:C:2096:GLU:OE1	2.21	0.54
1:C:3048:ALA:O	1:C:3053:ARG:NH2	2.41	0.54
1:C:3051:ARG:O	1:C:3053:ARG:NE	2.35	0.54
1:C:3414:ARG:HE	1:C:3472:ALA:HB3	1.73	0.54
1:D:475:GLN:OE1	1:D:533:ASN:ND2	2.39	0.54
1:D:1270:LEU:HB2	1:D:1564:PHE:HB2	1.90	0.54
1:D:2912:THR:O	1:D:2916:LYS:HB2	2.07	0.54
1:C:499:THR:HG23	1:C:502:HIS:H	1.72	0.54
1:C:4068:LEU:HD22	1:C:4111:LEU:HD11	1.89	0.54
2:F:17:LYS:HE3	2:F:20:GLN:HE22	1.73	0.54
1:B:1272:LEU:HD22	1:B:1289:LEU:HD11	1.90	0.54
1:C:3945:GLU:OE1	1:C:3949:ARG:NH1	2.40	0.54
1:D:233:ILE:HD12	1:D:242:ARG:HB3	1.89	0.54
1:D:3017:PHE:O	1:D:3036:LYS:NZ	2.38	0.54
2:H:17:LYS:HE3	2:H:20:GLN:HE22	1.73	0.54
1:B:3414:ARG:HE	1:B:3472:ALA:HB3	1.73	0.53
1:B:4068:LEU:HD22	1:B:4111:LEU:HD11	1.89	0.53
1:C:294:THR:HG23	1:C:297:GLN:H	1.72	0.53
1:C:3659:ALA:HA	1:C:3663:LEU:HD12	1.89	0.53
1:D:3414:ARG:HE	1:D:3472:ALA:HB3	1.73	0.53
1:A:110:ARG:HH21	1:A:115:ARG:HB3	1.72	0.53
1:A:1270:LEU:HB2	1:A:1564:PHE:HB2	1.90	0.53
1:B:1270:LEU:HB2	1:B:1564:PHE:HB2	1.90	0.53
1:B:2093:SER:OG	1:B:2096:GLU:OE1	2.21	0.53
1:C:3107:VAL:HG21	1:C:3171:SER:HB2	1.88	0.53
1:A:4570:ALA:O	1:A:4574:ASN:ND2	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1469:VAL:HG13	1:B:1492:CYS:HB3	1.91	0.53
1:B:2538:THR:HG23	1:B:2540:THR:H	1.71	0.53
1:B:4570:ALA:O	1:B:4574:ASN:ND2	2.40	0.53
1:C:1270:LEU:HB2	1:C:1564:PHE:HB2	1.90	0.53
1:C:2595:LEU:O	1:C:2600:ARG:NH2	2.41	0.53
1:D:1469:VAL:HG13	1:D:1492:CYS:HB3	1.91	0.53
1:D:2018:GLU:OE1	1:D:2028:ARG:NH1	2.40	0.53
1:C:1469:VAL:HG13	1:C:1492:CYS:HB3	1.91	0.53
1:C:4570:ALA:O	1:C:4574:ASN:ND2	2.40	0.53
1:D:886:ARG:HE	1:D:904:HIS:HB2	1.72	0.53
1:D:4570:ALA:O	1:D:4574:ASN:ND2	2.40	0.53
1:A:232:THR:HG22	1:A:258:SER:HB3	1.89	0.53
1:A:1469:VAL:HG13	1:A:1492:CYS:HB3	1.91	0.53
1:A:2534:ALA:O	1:A:2588:ARG:NH1	2.42	0.53
1:A:3048:ALA:O	1:A:3053:ARG:NH2	2.41	0.53
1:D:2595:LEU:O	1:D:2600:ARG:NH2	2.41	0.53
1:D:3111:ARG:NH2	1:D:3174:SER:OG	2.42	0.53
2:G:17:LYS:HE3	2:G:20:GLN:HE22	1.73	0.53
1:A:627:PRO:HD3	2:E:89:GLY:HA2	1.89	0.53
1:A:1450:VAL:HG22	1:A:1552:VAL:HG22	1.91	0.53
1:B:3659:ALA:HA	1:B:3663:LEU:HD12	1.89	0.53
1:C:886:ARG:HE	1:C:904:HIS:HB2	1.72	0.53
1:D:350:HIS:HB2	1:D:378:LEU:HD21	1.91	0.53
1:A:3111:ARG:NH2	1:A:3174:SER:OG	2.42	0.53
1:B:232:THR:HG22	1:B:258:SER:HB3	1.89	0.53
2:H:78:PRO:HA	2:H:81:ALA:HB3	1.91	0.53
1:A:3659:ALA:HA	1:A:3663:LEU:HD12	1.90	0.53
1:B:3111:ARG:NH2	1:B:3174:SER:OG	2.42	0.53
1:C:3769:ARG:O	1:C:3773:ARG:NH1	2.39	0.53
1:D:2534:ALA:O	1:D:2588:ARG:NH1	2.42	0.53
1:C:233:ILE:HD12	1:C:242:ARG:HB3	1.89	0.53
1:C:2534:ALA:O	1:C:2588:ARG:NH1	2.42	0.53
1:C:4112:LEU:O	1:C:4115:SER:OG	2.26	0.53
1:B:233:ILE:HD12	1:B:242:ARG:HB3	1.89	0.53
1:B:1450:VAL:HG22	1:B:1552:VAL:HG22	1.91	0.53
1:C:4068:LEU:HA	1:C:4071:ILE:HB	1.91	0.53
1:D:3659:ALA:HA	1:D:3663:LEU:HD12	1.89	0.53
1:C:320:LYS:NZ	1:C:383:HIS:O	2.42	0.52
1:C:3111:ARG:NH2	1:C:3174:SER:OG	2.42	0.52
1:B:3442:PHE:HE1	1:B:3511:VAL:HG12	1.75	0.52
2:E:78:PRO:HA	2:E:81:ALA:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:HIS:HB2	1:A:378:LEU:HD21	1.91	0.52
1:B:1454:THR:OG1	1:B:1456:ASP:OD1	2.24	0.52
1:C:2628:PHE:HE2	1:C:2735:PHE:HA	1.74	0.52
1:B:2628:PHE:HE2	1:B:2735:PHE:HA	1.74	0.52
1:C:1450:VAL:HG22	1:C:1552:VAL:HG22	1.91	0.52
1:C:4088:ILE:O	1:C:4123:ILE:N	2.43	0.52
1:D:2021:CYS:O	1:D:2028:ARG:NH2	2.42	0.52
1:A:2021:CYS:O	1:A:2028:ARG:NH2	2.42	0.52
1:A:3442:PHE:HE1	1:A:3511:VAL:HG12	1.75	0.52
1:A:4088:ILE:O	1:A:4123:ILE:N	2.43	0.52
1:C:2021:CYS:O	1:C:2028:ARG:NH2	2.42	0.52
1:D:3442:PHE:HE1	1:D:3511:VAL:HG12	1.75	0.52
1:A:4112:LEU:O	1:A:4115:SER:OG	2.26	0.52
1:B:350:HIS:HB2	1:B:378:LEU:HD21	1.91	0.52
1:B:4088:ILE:O	1:B:4123:ILE:N	2.43	0.52
1:C:492:ASP:OD1	1:C:546:TRP:NE1	2.42	0.52
1:D:2628:PHE:HE2	1:D:2735:PHE:HA	1.74	0.52
2:G:78:PRO:HA	2:G:81:ALA:HB3	1.91	0.52
1:B:2021:CYS:O	1:B:2028:ARG:NH2	2.42	0.52
1:D:1671:ARG:O	1:D:1675:ALA:HB2	2.10	0.52
1:A:2628:PHE:HE2	1:A:2735:PHE:HA	1.74	0.52
1:A:4068:LEU:HA	1:A:4071:ILE:HB	1.91	0.52
1:B:504:ALA:HB2	1:B:512:ALA:HB2	1.92	0.52
1:B:2967:MET:HE2	1:B:3045:LYS:HB3	1.92	0.52
1:B:3051:ARG:O	1:B:3053:ARG:NE	2.35	0.52
1:D:1450:VAL:HG22	1:D:1552:VAL:HG22	1.91	0.52
1:D:4088:ILE:O	1:D:4123:ILE:N	2.43	0.52
2:F:71:ARG:HG2	2:F:102:GLU:HB2	1.92	0.52
1:A:1815:LEU:HD22	1:A:1845:VAL:HG21	1.92	0.52
1:B:1815:LEU:HD22	1:B:1845:VAL:HG21	1.92	0.52
1:D:1676:LEU:HD22	1:D:2167:ILE:HD12	1.92	0.52
2:E:71:ARG:HG2	2:E:102:GLU:HB2	1.92	0.52
1:B:2534:ALA:O	1:B:2588:ARG:NH1	2.42	0.51
1:C:111:HIS:ND1	1:C:114:SER:OG	2.39	0.51
1:C:350:HIS:HB2	1:C:378:LEU:HD21	1.91	0.51
1:C:1676:LEU:HD22	1:C:2167:ILE:HD12	1.92	0.51
1:A:320:LYS:NZ	1:A:383:HIS:O	2.42	0.51
1:B:2604:GLU:HG2	1:B:2639:MET:HG3	1.92	0.51
1:C:1658:ASP:OD1	1:C:1658:ASP:N	2.44	0.51
1:D:1658:ASP:OD1	1:D:1658:ASP:N	2.44	0.51
2:F:78:PRO:HA	2:F:81:ALA:HB3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2109:ASP:HA	1:A:3694:LYS:HD2	1.93	0.51
1:A:2967:MET:HE2	1:A:3045:LYS:HB3	1.92	0.51
1:B:1671:ARG:O	1:B:1675:ALA:HB2	2.10	0.51
1:D:2109:ASP:HA	1:D:3694:LYS:HD2	1.93	0.51
1:A:1676:LEU:HD22	1:A:2167:ILE:HD12	1.92	0.51
1:B:1969:LEU:HD11	1:B:2009:LEU:HD13	1.93	0.51
1:C:504:ALA:HB2	1:C:512:ALA:HB2	1.92	0.51
1:C:1969:LEU:HD11	1:C:2009:LEU:HD13	1.93	0.51
1:D:504:ALA:HB2	1:D:512:ALA:HB2	1.92	0.51
1:C:1815:LEU:HD22	1:C:1845:VAL:HG21	1.92	0.51
1:D:1969:LEU:HD11	1:D:2009:LEU:HD13	1.93	0.51
1:C:1864:LYS:NZ	1:C:1871:PHE:O	2.39	0.51
1:D:2827:ARG:NH2	1:D:2935:TYR:OH	2.44	0.51
1:A:743:VAL:HB	1:A:760:ASN:HA	1.93	0.51
1:A:1671:ARG:O	1:A:1675:ALA:HB2	2.10	0.51
1:A:1969:LEU:HD11	1:A:2009:LEU:HD13	1.93	0.51
1:B:1658:ASP:N	1:B:1658:ASP:OD1	2.44	0.51
1:B:1676:LEU:HD22	1:B:2167:ILE:HD12	1.92	0.51
1:C:743:VAL:HB	1:C:760:ASN:HA	1.93	0.51
1:C:3442:PHE:HE1	1:C:3511:VAL:HG12	1.75	0.51
1:D:4689:THR:HG22	1:D:4690:GLU:HG3	1.93	0.51
1:D:4729:GLY:HA2	1:D:4737:ILE:HG13	1.93	0.51
2:H:71:ARG:HG2	2:H:102:GLU:HB2	1.92	0.51
1:A:2604:GLU:HG2	1:A:2639:MET:HG3	1.92	0.51
1:A:4689:THR:HG22	1:A:4690:GLU:HG3	1.93	0.51
1:C:1695:LEU:HA	1:C:1698:LEU:HG	1.93	0.51
1:D:320:LYS:NZ	1:D:383:HIS:O	2.42	0.51
1:D:1815:LEU:HD22	1:D:1845:VAL:HG21	1.92	0.51
1:D:3842:LEU:HB2	1:D:3929:SER:HB2	1.93	0.51
1:D:4068:LEU:HA	1:D:4071:ILE:HB	1.91	0.51
2:F:21:THR:N	2:F:107:GLU:OE2	2.44	0.51
1:B:403:MET:O	1:B:407:THR:OG1	2.23	0.51
1:B:4068:LEU:HA	1:B:4071:ILE:HB	1.91	0.51
1:C:2624:ARG:NH2	1:C:2915:GLU:OE2	2.44	0.51
1:C:3545:THR:HG22	1:C:3548:GLU:HG3	1.93	0.51
1:C:4680:LYS:HD2	1:C:4686:LEU:HD22	1.92	0.51
1:C:4689:THR:HG22	1:C:4690:GLU:HG3	1.93	0.51
1:D:111:HIS:ND1	1:D:114:SER:OG	2.39	0.51
1:B:2827:ARG:NH2	1:B:2935:TYR:OH	2.44	0.51
1:B:4689:THR:HG22	1:B:4690:GLU:HG3	1.93	0.51
1:D:492:ASP:OD1	1:D:546:TRP:NE1	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2624:ARG:NH2	1:D:2915:GLU:OE2	2.44	0.51
1:A:2624:ARG:NH2	1:A:2915:GLU:OE2	2.44	0.50
1:A:2827:ARG:NH2	1:A:2935:TYR:OH	2.44	0.50
1:C:1291:LEU:HD13	1:C:1595:LEU:HD11	1.94	0.50
1:C:2109:ASP:HA	1:C:3694:LYS:HD2	1.93	0.50
1:C:3628:ARG:NH2	1:C:3857:GLY:O	2.45	0.50
1:D:2604:GLU:HG2	1:D:2639:MET:HG3	1.92	0.50
2:G:21:THR:N	2:G:107:GLU:OE2	2.44	0.50
1:B:1695:LEU:HA	1:B:1698:LEU:HG	1.93	0.50
1:C:1671:ARG:O	1:C:1675:ALA:HB2	2.10	0.50
1:D:3628:ARG:NH2	1:D:3857:GLY:O	2.45	0.50
1:A:504:ALA:HB2	1:A:512:ALA:HB2	1.92	0.50
1:A:3628:ARG:NH2	1:A:3857:GLY:O	2.45	0.50
1:A:3835:LEU:HD22	1:A:3880:PHE:HZ	1.76	0.50
1:A:4729:GLY:HA2	1:A:4737:ILE:HG13	1.93	0.50
1:B:320:LYS:NZ	1:B:383:HIS:O	2.42	0.50
1:B:3545:THR:HG22	1:B:3548:GLU:HG3	1.93	0.50
1:C:1093:GLU:HB3	1:C:1201:HIS:HB3	1.94	0.50
1:C:2856:ASN:ND2	1:C:2858:GLN:OE1	2.44	0.50
1:A:2856:ASN:ND2	1:A:2858:GLN:OE1	2.44	0.50
1:B:355:LEU:HD22	1:B:380:GLN:HA	1.94	0.50
1:B:3901:ASN:OD1	1:B:3904:ARG:NH1	2.36	0.50
1:C:2604:GLU:HG2	1:C:2639:MET:HG3	1.92	0.50
1:D:218:HIS:O	1:D:261:ARG:HA	2.12	0.50
1:D:2394:GLY:HA3	1:D:2415:ARG:HH21	1.77	0.50
1:A:355:LEU:HD22	1:A:380:GLN:HA	1.94	0.50
1:A:492:ASP:OD1	1:A:546:TRP:NE1	2.42	0.50
1:A:1291:LEU:HD13	1:A:1595:LEU:HD11	1.94	0.50
1:B:2109:ASP:HA	1:B:3694:LYS:HD2	1.93	0.50
1:B:2624:ARG:NH2	1:B:2915:GLU:OE2	2.44	0.50
1:B:2856:ASN:ND2	1:B:2858:GLN:OE1	2.44	0.50
1:C:218:HIS:O	1:C:261:ARG:HA	2.12	0.50
1:C:2967:MET:HE2	1:C:3045:LYS:HB3	1.93	0.50
1:C:3835:LEU:HD22	1:C:3880:PHE:HZ	1.76	0.50
1:D:743:VAL:HB	1:D:760:ASN:HA	1.93	0.50
1:D:1698:LEU:HA	1:D:1712:TYR:HE1	1.77	0.50
1:D:4680:LYS:HD2	1:D:4686:LEU:HD22	1.92	0.50
2:E:21:THR:N	2:E:107:GLU:OE2	2.44	0.50
1:A:1093:GLU:HB3	1:A:1201:HIS:HB3	1.94	0.50
1:A:1099:GLU:OE2	1:A:1125:ASN:ND2	2.42	0.50
1:A:2394:GLY:HA3	1:A:2415:ARG:HH21	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2490:MET:SD	1:A:2490:MET:N	2.85	0.50
1:B:4729:GLY:HA2	1:B:4737:ILE:HG13	1.93	0.50
1:D:3545:THR:HG22	1:D:3548:GLU:HG3	1.93	0.50
1:A:2003:GLN:NE2	1:A:3655:GLU:OE2	2.45	0.50
1:B:4112:LEU:O	1:B:4115:SER:OG	2.26	0.50
1:C:355:LEU:HD22	1:C:380:GLN:HA	1.94	0.50
1:C:1698:LEU:HA	1:C:1712:TYR:HE1	1.77	0.50
1:C:4924:VAL:HA	1:C:4928:LEU:HD12	1.94	0.50
2:G:71:ARG:HG2	2:G:102:GLU:HB2	1.92	0.50
1:A:1229:ASN:HB2	1:A:1827:ARG:HG3	1.94	0.50
1:A:1695:LEU:HA	1:A:1698:LEU:HG	1.93	0.50
1:B:4680:LYS:HD2	1:B:4686:LEU:HD22	1.92	0.50
1:B:4924:VAL:HA	1:B:4928:LEU:HD12	1.94	0.50
1:D:3835:LEU:HD22	1:D:3880:PHE:HZ	1.76	0.50
1:A:3545:THR:HG22	1:A:3548:GLU:HG3	1.93	0.50
1:B:3628:ARG:NH2	1:B:3857:GLY:O	2.45	0.50
1:D:707:VAL:HG13	1:D:713:SER:HB2	1.94	0.50
1:D:2003:GLN:NE2	1:D:3655:GLU:OE2	2.45	0.50
1:D:2856:ASN:ND2	1:D:2858:GLN:OE1	2.44	0.50
2:H:21:THR:N	2:H:107:GLU:OE2	2.44	0.50
1:A:707:VAL:HG13	1:A:713:SER:HB2	1.94	0.49
1:B:2394:GLY:HA3	1:B:2415:ARG:HH21	1.77	0.49
1:B:3842:LEU:HB2	1:B:3929:SER:HB2	1.93	0.49
1:C:2003:GLN:NE2	1:C:3655:GLU:OE2	2.45	0.49
1:C:2394:GLY:HA3	1:C:2415:ARG:HH21	1.77	0.49
1:C:2827:ARG:NH2	1:C:2935:TYR:OH	2.44	0.49
1:A:218:HIS:O	1:A:261:ARG:HA	2.12	0.49
1:B:3450:ASN:OD1	1:B:3453:ARG:NH1	2.39	0.49
1:C:3840:SER:OG	1:C:3877:ASP:OD1	2.26	0.49
1:D:1291:LEU:HD13	1:D:1595:LEU:HD11	1.94	0.49
1:A:3842:LEU:HB2	1:A:3929:SER:HB2	1.93	0.49
1:B:218:HIS:O	1:B:261:ARG:HA	2.12	0.49
1:A:932:LEU:HB3	1:A:937:CYS:HB3	1.94	0.49
1:A:4680:LYS:HD2	1:A:4686:LEU:HD22	1.92	0.49
1:B:743:VAL:HB	1:B:760:ASN:HA	1.93	0.49
1:B:932:LEU:HB3	1:B:937:CYS:HB3	1.94	0.49
1:B:3097:GLU:OE1	1:B:3167:ARG:NH2	2.46	0.49
1:D:355:LEU:HD22	1:D:380:GLN:HA	1.94	0.49
1:D:2967:MET:HE2	1:D:3045:LYS:HB3	1.94	0.49
1:A:2128:TYR:OH	1:A:3676:ASP:OD2	2.31	0.49
1:B:1291:LEU:HD13	1:B:1595:LEU:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2128:TYR:OH	1:C:3676:ASP:OD2	2.31	0.49
1:D:1229:ASN:HB2	1:D:1827:ARG:HG3	1.94	0.49
1:A:3817:LEU:HD11	1:A:3821:LYS:HE3	1.95	0.49
1:A:4924:VAL:HA	1:A:4928:LEU:HD12	1.93	0.49
1:B:870:ILE:HG13	1:B:874:LEU:HD23	1.95	0.49
1:B:2245:GLN:NE2	1:B:3861:GLU:OE1	2.46	0.49
1:B:3835:LEU:HD22	1:B:3880:PHE:HZ	1.76	0.49
1:C:1586:ASN:ND2	1:C:1590:GLN:OE1	2.46	0.49
1:C:3097:GLU:OE1	1:C:3167:ARG:NH2	2.46	0.49
1:D:1093:GLU:HB3	1:D:1201:HIS:HB3	1.94	0.49
1:A:870:ILE:HG13	1:A:874:LEU:HD23	1.95	0.49
1:A:3583:GLU:HB2	1:A:3586:ALA:HB2	1.95	0.49
1:B:1093:GLU:HB3	1:B:1201:HIS:HB3	1.94	0.49
1:B:1586:ASN:ND2	1:B:1590:GLN:OE1	2.46	0.49
1:B:2003:GLN:NE2	1:B:3655:GLU:OE2	2.45	0.49
1:B:2128:TYR:OH	1:B:3676:ASP:OD2	2.31	0.49
1:C:348:VAL:HB	1:C:357:LEU:HD22	1.95	0.49
1:C:3817:LEU:HD11	1:C:3821:LYS:HE3	1.95	0.49
1:D:932:LEU:HB3	1:D:937:CYS:HB3	1.94	0.49
1:D:1695:LEU:HA	1:D:1698:LEU:HG	1.93	0.49
1:A:2245:GLN:NE2	1:A:3861:GLU:OE1	2.46	0.49
1:C:932:LEU:HB3	1:C:937:CYS:HB3	1.94	0.49
1:D:348:VAL:HB	1:D:357:LEU:HD22	1.95	0.49
1:D:4924:VAL:HA	1:D:4928:LEU:HD12	1.94	0.49
1:A:3097:GLU:OE1	1:A:3167:ARG:NH2	2.46	0.49
1:A:4976:GLU:O	1:A:4980:LEU:HB2	2.13	0.49
1:D:277:GLY:HA2	1:D:315:CYS:HB3	1.95	0.49
1:D:2387:SER:OG	1:D:2492:ALA:O	2.31	0.49
1:D:2490:MET:SD	1:D:2490:MET:N	2.85	0.49
1:A:277:GLY:HA2	1:A:315:CYS:HB3	1.95	0.49
1:A:3862:ASP:OD1	1:A:3862:ASP:N	2.46	0.49
1:C:707:VAL:HG13	1:C:713:SER:HB2	1.94	0.49
1:C:3227:ARG:NH1	1:C:3234:ASN:OD1	2.46	0.49
1:C:3842:LEU:HB2	1:C:3929:SER:HB2	1.93	0.49
1:C:3862:ASP:N	1:C:3862:ASP:OD1	2.46	0.49
1:C:4976:GLU:O	1:C:4980:LEU:HB2	2.13	0.49
1:D:2128:TYR:OH	1:D:3676:ASP:OD2	2.31	0.49
1:D:3097:GLU:OE1	1:D:3167:ARG:NH2	2.46	0.49
1:A:3227:ARG:NH1	1:A:3234:ASN:OD1	2.46	0.48
1:B:660:GLY:HA2	1:B:750:LEU:HD12	1.95	0.48
1:B:3583:GLU:HB2	1:B:3586:ALA:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3968:TYR:O	1:B:3976:ASN:ND2	2.42	0.48
1:B:4976:GLU:O	1:B:4980:LEU:HB2	2.13	0.48
1:C:2410:PRO:HB3	1:C:2415:ARG:HB3	1.95	0.48
1:C:4729:GLY:HA2	1:C:4737:ILE:HG13	1.93	0.48
1:D:1454:THR:OG1	1:D:1456:ASP:OD1	2.24	0.48
1:D:3227:ARG:NH1	1:D:3234:ASN:OD1	2.46	0.48
1:B:652:ARG:NH1	1:B:751:SER:O	2.46	0.48
1:B:707:VAL:HG13	1:B:713:SER:HB2	1.94	0.48
1:B:2410:PRO:HB3	1:B:2415:ARG:HB3	1.95	0.48
1:B:3817:LEU:HD11	1:B:3821:LYS:HE3	1.95	0.48
1:C:2974:ILE:HD13	1:C:3049:LEU:HD12	1.95	0.48
1:C:4017:LEU:HD13	1:C:4135:PRO:HB2	1.95	0.48
1:D:660:GLY:HA2	1:D:750:LEU:HD12	1.95	0.48
1:D:1586:ASN:ND2	1:D:1590:GLN:OE1	2.46	0.48
1:A:1698:LEU:HA	1:A:1712:TYR:HE1	1.77	0.48
1:A:2387:SER:OG	1:A:2492:ALA:O	2.31	0.48
1:B:277:GLY:HA2	1:B:315:CYS:HB3	1.95	0.48
1:B:1698:LEU:HA	1:B:1712:TYR:HE1	1.77	0.48
1:B:2280:VAL:HG21	1:B:2290:LEU:HD12	1.95	0.48
1:B:3371:LYS:NZ	1:B:3375:GLU:OE2	2.45	0.48
1:C:2280:VAL:HG21	1:C:2290:LEU:HD12	1.95	0.48
1:D:627:PRO:HD3	2:H:89:GLY:HA2	1.96	0.48
1:D:1293:LEU:HD11	1:D:1594:ARG:HD3	1.95	0.48
1:D:2978:GLU:OE2	1:D:3053:ARG:NH1	2.43	0.48
1:D:3817:LEU:HD11	1:D:3821:LYS:HE3	1.95	0.48
1:B:2974:ILE:HD13	1:B:3049:LEU:HD12	1.95	0.48
1:C:870:ILE:HG13	1:C:874:LEU:HD23	1.95	0.48
1:C:1229:ASN:HB2	1:C:1827:ARG:HG3	1.94	0.48
1:C:3901:ASN:OD1	1:C:3904:ARG:NH1	2.36	0.48
1:D:28:VAL:HG22	1:D:33:LEU:HD22	1.96	0.48
1:D:652:ARG:NH1	1:D:751:SER:O	2.46	0.48
1:D:875:ALA:O	1:D:879:HIS:ND1	2.47	0.48
1:A:1293:LEU:HD11	1:A:1594:ARG:HD3	1.95	0.48
1:B:1293:LEU:HD11	1:B:1594:ARG:HD3	1.95	0.48
1:D:1743[A]:ARG:NH1	1:D:1963:GLU:OE2	2.47	0.48
1:A:868:GLU:HA	1:A:871:ARG:HB2	1.96	0.48
1:B:1743[A]:ARG:NH1	1:B:1963:GLU:OE2	2.47	0.48
1:C:277:GLY:HA2	1:C:315:CYS:HB3	1.95	0.48
1:C:652:ARG:NH1	1:C:751:SER:O	2.46	0.48
1:A:572:PRO:HA	1:A:575:LEU:HD13	1.96	0.48
1:A:1658:ASP:OD1	1:A:1658:ASP:N	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2325:PRO:HB2	1:B:2421:ALA:HB1	1.96	0.48
1:B:3256:LEU:HB3	1:B:3266:MET:HE1	1.96	0.48
1:C:875:ALA:O	1:C:879:HIS:ND1	2.47	0.48
1:C:2245:GLN:NE2	1:C:3861:GLU:OE1	2.46	0.48
1:D:3322:ILE:O	1:D:3326:ASN:ND2	2.37	0.48
1:A:348:VAL:HB	1:A:357:LEU:HD22	1.95	0.48
1:A:1586:ASN:ND2	1:A:1590:GLN:OE1	2.46	0.48
1:A:3371:LYS:NZ	1:A:3375:GLU:OE2	2.45	0.48
1:C:3583:GLU:HB2	1:C:3586:ALA:HB2	1.95	0.48
1:D:3583:GLU:HB2	1:D:3586:ALA:HB2	1.95	0.48
1:D:4976:GLU:O	1:D:4980:LEU:HB2	2.13	0.48
1:A:111:HIS:ND1	1:A:114:SER:OG	2.39	0.48
1:B:492:ASP:OD1	1:B:546:TRP:NE1	2.42	0.48
1:B:875:ALA:O	1:B:879:HIS:ND1	2.47	0.48
1:B:2387:SER:OG	1:B:2492:ALA:O	2.31	0.48
1:B:4017:LEU:HD13	1:B:4135:PRO:HB2	1.95	0.48
1:C:1743[A]:ARG:NH1	1:C:1963:GLU:OE2	2.47	0.48
1:C:2325:PRO:HB2	1:C:2421:ALA:HB1	1.96	0.48
1:D:221:ARG:NH2	1:D:255:HIS:O	2.46	0.48
1:A:1743[A]:ARG:NH1	1:A:1963:GLU:OE2	2.46	0.48
1:A:2410:PRO:HB3	1:A:2415:ARG:HB3	1.95	0.48
1:A:3968:TYR:O	1:A:3976:ASN:ND2	2.41	0.48
1:B:299:LEU:HD13	1:B:378:LEU:HD22	1.96	0.48
1:B:2871:LEU:HG	1:B:2927:LEU:HD21	1.95	0.48
1:B:2998:PHE:HD1	1:B:3002:LEU:HD22	1.79	0.48
1:C:627:PRO:HD3	2:G:89:GLY:HA2	1.96	0.48
1:C:1293:LEU:HD11	1:C:1594:ARG:HD3	1.95	0.48
1:C:3450:ASN:OD1	1:C:3453:ARG:NH1	2.39	0.48
1:D:868:GLU:HA	1:D:871:ARG:HB2	1.96	0.48
1:D:2420:HIS:HB2	1:D:2492:ALA:HA	1.96	0.48
1:D:3840:SER:OG	1:D:3877:ASP:OD1	2.26	0.48
1:A:28:VAL:HG22	1:A:33:LEU:HD22	1.96	0.47
1:A:4722:ARG:H	1:A:4722:ARG:HG2	1.43	0.47
1:B:2813:LEU:HA	1:B:2816:MET:HG3	1.97	0.47
1:C:28:VAL:HG22	1:C:33:LEU:HD22	1.96	0.47
1:C:868:GLU:HA	1:C:871:ARG:HB2	1.96	0.47
1:C:1118:ASP:OD1	1:C:1118:ASP:N	2.47	0.47
1:D:870:ILE:HG13	1:D:874:LEU:HD23	1.95	0.47
1:D:2245:GLN:NE2	1:D:3861:GLU:OE1	2.46	0.47
1:D:2974:ILE:HD13	1:D:3049:LEU:HD12	1.95	0.47
1:A:2974:ILE:HD13	1:A:3049:LEU:HD12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4017:LEU:HD13	1:A:4135:PRO:HB2	1.95	0.47
1:B:884:LEU:HB2	1:B:969:PRO:HD3	1.96	0.47
1:B:1118:ASP:N	1:B:1118:ASP:OD1	2.47	0.47
1:B:1229:ASN:HB2	1:B:1827:ARG:HG3	1.94	0.47
1:D:299:LEU:HD13	1:D:378:LEU:HD22	1.96	0.47
1:D:796:ARG:O	1:D:1619:ARG:NH2	2.46	0.47
1:D:2816:MET:HE1	1:D:2937:VAL:HG21	1.96	0.47
1:A:652:ARG:NH1	1:A:751:SER:O	2.46	0.47
1:A:875:ALA:O	1:A:879:HIS:ND1	2.47	0.47
1:A:2280:VAL:HG21	1:A:2290:LEU:HD12	1.95	0.47
1:A:2813:LEU:HA	1:A:2816:MET:HG3	1.96	0.47
1:A:3420:ARG:HG3	1:A:3520:ILE:HD11	1.97	0.47
1:B:348:VAL:HB	1:B:357:LEU:HD22	1.95	0.47
1:B:868:GLU:HA	1:B:871:ARG:HB2	1.96	0.47
1:B:3380:ARG:HH22	1:B:3394:VAL:HG21	1.79	0.47
1:B:3420:ARG:HG3	1:B:3520:ILE:HD11	1.97	0.47
1:C:299:LEU:HD13	1:C:378:LEU:HD22	1.96	0.47
1:C:1653:LEU:HD23	1:C:1660:GLN:HA	1.97	0.47
1:C:2387:SER:OG	1:C:2492:ALA:O	2.31	0.47
1:C:2813:LEU:HA	1:C:2816:MET:HG3	1.97	0.47
1:C:2998:PHE:HD1	1:C:3002:LEU:HD22	1.79	0.47
1:D:2998:PHE:HD1	1:D:3002:LEU:HD22	1.79	0.47
1:D:3420:ARG:HG3	1:D:3520:ILE:HD11	1.97	0.47
1:D:4017:LEU:HD13	1:D:4135:PRO:HB2	1.95	0.47
1:A:299:LEU:HD13	1:A:378:LEU:HD22	1.96	0.47
1:A:2420:HIS:HB2	1:A:2492:ALA:HA	1.96	0.47
1:A:3132:THR:HA	1:A:3136:LEU:HB3	1.96	0.47
1:B:28:VAL:HG22	1:B:33:LEU:HD22	1.96	0.47
1:B:572:PRO:HA	1:B:575:LEU:HD13	1.96	0.47
1:B:3862:ASP:OD1	1:B:3862:ASP:N	2.46	0.47
1:C:660:GLY:HA2	1:C:750:LEU:HD12	1.95	0.47
1:C:2978:GLU:OE2	1:C:3053:ARG:NH1	2.43	0.47
1:D:274:LEU:HD23	1:D:278:GLN:HE21	1.79	0.47
1:D:1118:ASP:N	1:D:1118:ASP:OD1	2.47	0.47
1:D:2410:PRO:HB3	1:D:2415:ARG:HB3	1.95	0.47
1:A:3180:ASN:HB2	1:A:3183:VAL:HG23	1.97	0.47
1:A:3380:ARG:HH22	1:A:3394:VAL:HG21	1.79	0.47
1:B:3227:ARG:NH1	1:B:3234:ASN:OD1	2.46	0.47
1:D:572:PRO:HA	1:D:575:LEU:HD13	1.96	0.47
1:D:2280:VAL:HG21	1:D:2290:LEU:HD12	1.95	0.47
1:D:3862:ASP:OD1	1:D:3862:ASP:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:LEU:HD23	1:A:278:GLN:HE21	1.79	0.47
1:A:2463:LEU:HA	1:A:2466:LEU:HD12	1.97	0.47
1:A:2871:LEU:HG	1:A:2927:LEU:HD21	1.95	0.47
1:A:4710:SER:OG	1:A:4772:ASP:OD2	2.32	0.47
1:B:2420:HIS:HB2	1:B:2492:ALA:HA	1.96	0.47
1:B:2490:MET:SD	1:B:2490:MET:N	2.85	0.47
1:C:322:LYS:HZ1	1:C:356:TRP:HE1	1.61	0.47
1:C:572:PRO:HA	1:C:575:LEU:HD13	1.96	0.47
1:C:2490:MET:SD	1:C:2490:MET:N	2.85	0.47
1:C:2660:GLY:HA3	1:C:2666:VAL:HG22	1.97	0.47
1:C:2871:LEU:HG	1:C:2927:LEU:HD21	1.95	0.47
1:D:2463:LEU:HA	1:D:2466:LEU:HD12	1.97	0.47
1:D:2660:GLY:HA3	1:D:2666:VAL:HG22	1.97	0.47
1:D:2871:LEU:HG	1:D:2927:LEU:HD21	1.95	0.47
1:D:3037:GLU:HG2	1:D:3085:PRO:HD3	1.97	0.47
1:D:3380:ARG:HH22	1:D:3394:VAL:HG21	1.79	0.47
1:D:3450:ASN:OD1	1:D:3453:ARG:NH1	2.39	0.47
1:A:3037:GLU:HG2	1:A:3085:PRO:HD3	1.97	0.47
1:A:4006:ASP:N	1:A:4006:ASP:OD1	2.48	0.47
1:C:3380:ARG:HH22	1:C:3394:VAL:HG21	1.79	0.47
1:D:277:GLY:N	1:D:316:PHE:O	2.43	0.47
1:B:627:PRO:HD3	2:F:89:GLY:HA2	1.96	0.47
1:B:4006:ASP:OD1	1:B:4006:ASP:N	2.47	0.47
1:C:221:ARG:NH2	1:C:255:HIS:O	2.46	0.47
1:C:884:LEU:HB2	1:C:969:PRO:HD3	1.96	0.47
1:A:660:GLY:HA2	1:A:750:LEU:HD12	1.95	0.47
1:A:1776:HIS:HB3	1:A:1798:LEU:HD13	1.97	0.47
1:B:1653:LEU:HD23	1:B:1660:GLN:HA	1.97	0.47
1:B:2512:ILE:HG21	1:B:2518:LEU:HD13	1.97	0.47
1:C:2452:ARG:NH1	1:D:144:GLU:OE1	2.48	0.47
1:C:3420:ARG:HG3	1:C:3520:ILE:HD11	1.97	0.47
1:D:2325:PRO:HB2	1:D:2421:ALA:HB1	1.96	0.47
1:D:4006:ASP:N	1:D:4006:ASP:OD1	2.47	0.47
1:D:4112:LEU:O	1:D:4115:SER:OG	2.26	0.47
1:A:144:GLU:OE1	1:D:2452:ARG:NH1	2.48	0.46
1:A:2325:PRO:HB2	1:A:2421:ALA:HB1	1.96	0.46
1:B:277:GLY:N	1:B:316:PHE:O	2.43	0.46
1:B:2463:LEU:HA	1:B:2466:LEU:HD12	1.97	0.46
1:C:531:ARG:NH2	1:C:562:GLU:OE2	2.40	0.46
1:C:3037:GLU:HG2	1:C:3085:PRO:HD3	1.97	0.46
1:D:1784:ALA:HA	2:H:55:VAL:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4823:LEU:HD12	1:D:4823:LEU:HA	1.85	0.46
1:A:1653:LEU:HD23	1:A:1660:GLN:HA	1.97	0.46
1:B:3037:GLU:HG2	1:B:3085:PRO:HD3	1.97	0.46
1:B:3840:SER:OG	1:B:3877:ASP:OD1	2.26	0.46
1:D:3180:ASN:HB2	1:D:3183:VAL:HG23	1.97	0.46
1:A:618:GLN:OE1	1:A:1678:ASN:ND2	2.39	0.46
1:A:884:LEU:HB2	1:A:969:PRO:HD3	1.97	0.46
1:A:2660:GLY:HA3	1:A:2666:VAL:HG22	1.96	0.46
1:A:2998:PHE:HD1	1:A:3002:LEU:HD22	1.80	0.46
1:A:3081:MET:HG3	1:A:3156:VAL:HA	1.98	0.46
1:A:4823:LEU:HD12	1:A:4823:LEU:HA	1.85	0.46
1:B:179:TYR:N	1:B:194:SER:O	2.49	0.46
1:B:1784:ALA:HA	2:F:55:VAL:HA	1.97	0.46
1:B:2816:MET:HE1	1:B:2937:VAL:HG21	1.97	0.46
1:B:3081:MET:HG3	1:B:3156:VAL:HA	1.97	0.46
1:B:3085:PRO:HD2	1:B:3088:VAL:HB	1.98	0.46
1:C:274:LEU:HD23	1:C:278:GLN:HE21	1.79	0.46
1:C:3945:GLU:HA	1:C:3948:LYS:HE2	1.98	0.46
1:C:4892:ARG:NH1	1:D:4899:ASP:OD1	2.49	0.46
1:D:2813:LEU:HA	1:D:2816:MET:HG3	1.97	0.46
1:A:299:LEU:HD22	1:A:378:LEU:HB2	1.98	0.46
1:A:1970:GLN:HG2	1:A:3642:TYR:HA	1.97	0.46
1:B:1147:ASP:HB3	1:B:1164:LEU:HD11	1.98	0.46
1:B:1970:GLN:HG2	1:B:3642:TYR:HA	1.96	0.46
1:B:2677:LYS:HB3	1:B:2677:LYS:HE2	1.73	0.46
1:B:3132:THR:HA	1:B:3136:LEU:HB3	1.96	0.46
1:C:2420:HIS:HB2	1:C:2492:ALA:HA	1.96	0.46
1:C:2801:ASP:HA	1:C:2804:ILE:HG12	1.97	0.46
1:C:3180:ASN:HB2	1:C:3183:VAL:HG23	1.97	0.46
1:C:3968:TYR:O	1:C:3976:ASN:ND2	2.42	0.46
1:D:1099:GLU:OE2	1:D:1125:ASN:ND2	2.41	0.46
1:D:1776:HIS:HB3	1:D:1798:LEU:HD13	1.98	0.46
1:B:3365:LEU:HD21	1:B:3408:LEU:HD12	1.97	0.46
1:D:3081:MET:HG3	1:D:3156:VAL:HA	1.97	0.46
1:D:3176:GLY:O	1:D:3179:LYS:NZ	2.43	0.46
2:F:49:ARG:HG3	2:F:52:LYS:HD3	1.98	0.46
1:A:2316:LYS:HE2	1:A:2318:TYR:HE1	1.81	0.46
1:A:3085:PRO:HD2	1:A:3088:VAL:HB	1.98	0.46
1:B:355:LEU:HB2	1:B:378:LEU:HG	1.98	0.46
1:C:2512:ILE:HG21	1:C:2518:LEU:HD13	1.97	0.46
1:C:3085:PRO:HD2	1:C:3088:VAL:HB	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:633:LEU:HD13	1:D:1639:LEU:HD21	1.98	0.46
1:B:2452:ARG:NH1	1:C:144:GLU:OE1	2.48	0.46
1:C:2316:LYS:HE2	1:C:2318:TYR:HE1	1.81	0.46
1:C:3365:LEU:HD21	1:C:3408:LEU:HD12	1.97	0.46
1:C:4722:ARG:H	1:C:4722:ARG:HG2	1.43	0.46
1:D:884:LEU:HB2	1:D:969:PRO:HD3	1.96	0.46
1:A:1454:THR:OG1	1:A:1456:ASP:OD1	2.24	0.46
1:A:3159:ASP:OD1	1:A:3159:ASP:N	2.49	0.46
1:A:3176:GLY:O	1:A:3179:LYS:NZ	2.43	0.46
1:C:179:TYR:N	1:C:194:SER:O	2.49	0.46
1:C:633:LEU:HD13	1:C:1639:LEU:HD21	1.98	0.46
1:C:1147:ASP:HB3	1:C:1164:LEU:HD11	1.98	0.46
1:C:1970:GLN:HG2	1:C:3642:TYR:HA	1.96	0.46
1:C:2265:LEU:HB3	1:C:2330:ARG:HD2	1.98	0.46
1:C:2463:LEU:HA	1:C:2466:LEU:HD12	1.97	0.46
1:C:3132:THR:HA	1:C:3136:LEU:HB3	1.96	0.46
1:D:2316:LYS:HE2	1:D:2318:TYR:HE1	1.81	0.46
1:A:2265:LEU:HB3	1:A:2330:ARG:HD2	1.98	0.46
1:B:3180:ASN:HB2	1:B:3183:VAL:HG23	1.97	0.46
1:B:3945:GLU:HA	1:B:3948:LYS:HE2	1.98	0.46
1:B:4155:PRO:O	1:B:4161:ARG:NH2	2.45	0.46
1:C:355:LEU:HB2	1:C:378:LEU:HG	1.98	0.46
1:D:355:LEU:HB2	1:D:378:LEU:HG	1.98	0.46
1:A:355:LEU:HB2	1:A:378:LEU:HG	1.98	0.46
1:A:3365:LEU:HD21	1:A:3408:LEU:HD12	1.97	0.46
1:B:274:LEU:HD23	1:B:278:GLN:HE21	1.79	0.46
1:B:2316:LYS:HE2	1:B:2318:TYR:HE1	1.81	0.46
1:B:3823:LYS:HA	1:B:3823:LYS:HD3	1.75	0.46
1:B:4176:PRO:O	1:B:4202:ARG:NH1	2.45	0.46
1:B:4675:LYS:O	1:B:4679:ARG:HG2	2.17	0.46
1:C:2816:MET:HE1	1:C:2937:VAL:HG21	1.97	0.46
1:C:4155:PRO:O	1:C:4161:ARG:NH2	2.45	0.46
1:A:221:ARG:NH2	1:A:255:HIS:O	2.46	0.45
1:A:3450:ASN:OD1	1:A:3453:ARG:NH1	2.40	0.45
1:C:1036:ARG:O	1:C:1040:CYS:HB2	2.16	0.45
1:C:4675:LYS:O	1:C:4679:ARG:HG2	2.17	0.45
1:D:299:LEU:HD22	1:D:378:LEU:HB2	1.98	0.45
1:D:1653:LEU:HD23	1:D:1660:GLN:HA	1.97	0.45
1:D:3132:THR:HA	1:D:3136:LEU:HB3	1.96	0.45
1:D:4141:PHE:CE2	1:D:4196:GLU:HG2	2.52	0.45
1:A:179:TYR:N	1:A:194:SER:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2801:ASP:HA	1:A:2804:ILE:HG12	1.97	0.45
1:A:3256:LEU:HB3	1:A:3266:MET:HE1	1.98	0.45
1:B:299:LEU:HD22	1:B:378:LEU:HB2	1.98	0.45
1:B:1776:HIS:HB3	1:B:1798:LEU:HD13	1.98	0.45
1:B:2660:GLY:HA3	1:B:2666:VAL:HG22	1.97	0.45
1:B:4820:VAL:HG22	1:B:4823:LEU:HB2	1.98	0.45
1:C:411:TYR:HE1	1:C:441:VAL:HG13	1.82	0.45
1:C:796:ARG:O	1:C:1619:ARG:NH2	2.46	0.45
1:C:4006:ASP:OD1	1:C:4006:ASP:N	2.47	0.45
1:D:1147:ASP:HB3	1:D:1164:LEU:HD11	1.98	0.45
1:D:1970:GLN:HG2	1:D:3642:TYR:HA	1.96	0.45
1:D:2265:LEU:HB3	1:D:2330:ARG:HD2	1.98	0.45
1:D:2716:ASP:OD1	1:D:2716:ASP:N	2.45	0.45
1:D:3945:GLU:HA	1:D:3948:LYS:HE2	1.98	0.45
2:H:49:ARG:HG3	2:H:52:LYS:HD3	1.98	0.45
1:A:653:ALA:HB3	1:A:656:SER:HB2	1.99	0.45
1:A:1147:ASP:HB3	1:A:1164:LEU:HD11	1.98	0.45
1:B:1036:ARG:O	1:B:1040:CYS:HB2	2.16	0.45
1:B:2109:ASP:OD1	1:B:2109:ASP:N	2.50	0.45
1:C:1784:ALA:HA	2:G:55:VAL:HA	1.97	0.45
1:C:2014:ASP:OD1	1:C:2014:ASP:N	2.45	0.45
1:C:3371:LYS:NZ	1:C:3375:GLU:OE2	2.45	0.45
1:A:2002:PRO:O	1:A:2006:ILE:HD12	2.17	0.45
1:A:2816:MET:HE1	1:A:2937:VAL:HG21	1.99	0.45
1:A:4141:PHE:CE2	1:A:4196:GLU:HG2	2.52	0.45
1:B:863:LEU:HA	1:B:864:PRO:HD3	1.85	0.45
1:B:2002:PRO:O	1:B:2006:ILE:HD12	2.17	0.45
1:B:3359:ILE:HD11	1:B:3430:ASN:HB3	1.99	0.45
1:C:22:LEU:HD12	1:C:37:LEU:HD12	1.99	0.45
1:C:1776:HIS:HB3	1:C:1798:LEU:HD13	1.98	0.45
1:C:2109:ASP:OD1	1:C:2109:ASP:N	2.50	0.45
1:D:411:TYR:HE1	1:D:441:VAL:HG13	1.82	0.45
1:D:3823:LYS:HA	1:D:3823:LYS:HD3	1.75	0.45
1:D:4820:VAL:HG22	1:D:4823:LEU:HB2	1.98	0.45
1:A:356:TRP:O	1:A:379:HIS:N	2.50	0.45
1:A:403:MET:O	1:A:407:THR:OG1	2.23	0.45
1:A:633:LEU:HD13	1:A:1639:LEU:HD21	1.98	0.45
1:A:2782:ASP:OD1	1:A:2782:ASP:N	2.50	0.45
1:B:4892:ARG:NH1	1:C:4899:ASP:OD1	2.49	0.45
1:C:3081:MET:HG3	1:C:3156:VAL:HA	1.97	0.45
1:D:22:LEU:HD12	1:D:37:LEU:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:653:ALA:HB3	1:D:656:SER:HB2	1.99	0.45
1:D:2512:ILE:HG21	1:D:2518:LEU:HD13	1.97	0.45
1:D:3817:LEU:HD13	1:D:3899:PHE:HD1	1.82	0.45
1:A:219:VAL:HG12	1:A:259:LEU:HD12	1.99	0.45
1:A:4675:LYS:O	1:A:4679:ARG:HG2	2.16	0.45
1:B:633:LEU:HD13	1:B:1639:LEU:HD21	1.98	0.45
1:C:2765:LYS:HA	1:C:2765:LYS:HD3	1.80	0.45
1:D:1036:ARG:O	1:D:1040:CYS:HB2	2.16	0.45
1:D:2002:PRO:O	1:D:2006:ILE:HD12	2.17	0.45
1:D:3085:PRO:HD2	1:D:3088:VAL:HB	1.98	0.45
1:C:299:LEU:HD22	1:C:378:LEU:HB2	1.98	0.45
1:C:3817:LEU:HD13	1:C:3899:PHE:HD1	1.82	0.45
1:D:179:TYR:N	1:D:194:SER:O	2.49	0.45
1:D:2109:ASP:N	1:D:2109:ASP:OD1	2.50	0.45
1:A:2512:ILE:HG21	1:A:2518:LEU:HD13	1.97	0.45
1:A:4930:ALA:HB2	1:D:4933:GLN:HG2	1.99	0.45
1:B:884:LEU:HD13	1:B:968:ALA:H	1.82	0.45
1:B:2265:LEU:HB3	1:B:2330:ARG:HD2	1.98	0.45
1:B:2801:ASP:HA	1:B:2804:ILE:HG12	1.97	0.45
1:B:4722:ARG:HE	1:B:4722:ARG:HB3	1.43	0.45
1:C:3206:LEU:HD13	1:C:3246:LEU:HD13	1.99	0.45
1:D:2801:ASP:HA	1:D:2804:ILE:HG12	1.97	0.45
1:D:3359:ILE:HD11	1:D:3430:ASN:HB3	1.99	0.45
1:A:3945:GLU:HA	1:A:3948:LYS:HE2	1.98	0.45
1:C:219:VAL:HG12	1:C:259:LEU:HD12	1.99	0.45
1:C:4141:PHE:CE2	1:C:4196:GLU:HG2	2.52	0.45
1:D:219:VAL:HG12	1:D:259:LEU:HD12	1.99	0.45
2:F:23:VAL:HG13	2:F:47:LYS:HG2	1.99	0.45
2:G:49:ARG:HG3	2:G:52:LYS:HD3	1.98	0.45
1:A:884:LEU:HD13	1:A:968:ALA:H	1.82	0.45
1:A:1474:VAL:O	1:A:1486:SER:HA	2.17	0.45
1:A:3817:LEU:HD13	1:A:3899:PHE:HD1	1.82	0.45
1:A:3840:SER:OG	1:A:3877:ASP:OD1	2.26	0.45
1:B:221:ARG:NH2	1:B:255:HIS:O	2.46	0.45
1:B:411:TYR:HE1	1:B:441:VAL:HG13	1.82	0.45
1:B:3176:GLY:O	1:B:3179:LYS:NZ	2.43	0.45
1:B:3206:LEU:HD13	1:B:3246:LEU:HD13	1.99	0.45
1:B:3245:VAL:HG23	1:B:3248:ARG:H	1.82	0.45
1:C:356:TRP:O	1:C:379:HIS:N	2.50	0.45
1:C:4710:SER:OG	1:C:4772:ASP:OD2	2.32	0.45
1:D:1474:VAL:O	1:D:1486:SER:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1864:LYS:NZ	1:D:1871:PHE:O	2.39	0.45
1:D:3206:LEU:HD13	1:D:3246:LEU:HD13	1.99	0.45
1:D:3245:VAL:HG23	1:D:3248:ARG:H	1.82	0.45
1:A:411:TYR:HE1	1:A:441:VAL:HG13	1.82	0.44
1:B:618:GLN:OE1	1:B:1678:ASN:ND2	2.39	0.44
1:B:653:ALA:HB3	1:B:656:SER:HB2	1.99	0.44
1:B:3374:ALA:O	1:B:3378:GLN:NE2	2.50	0.44
1:A:22:LEU:HD12	1:A:37:LEU:HD12	1.99	0.44
1:A:400:ALA:O	1:A:404:ILE:HD12	2.17	0.44
1:B:22:LEU:HD12	1:B:37:LEU:HD12	1.99	0.44
1:B:400:ALA:O	1:B:404:ILE:HD12	2.17	0.44
1:B:2716:ASP:OD1	1:B:2716:ASP:N	2.45	0.44
1:C:1099:GLU:OE2	1:C:1125:ASN:ND2	2.41	0.44
1:C:3245:VAL:HG23	1:C:3248:ARG:H	1.82	0.44
1:C:3374:ALA:O	1:C:3378:GLN:NE2	2.50	0.44
1:D:3968:TYR:O	1:D:3976:ASN:ND2	2.42	0.44
1:D:4675:LYS:O	1:D:4679:ARG:HG2	2.17	0.44
1:A:1118:ASP:OD1	1:A:1118:ASP:N	2.47	0.44
1:A:2293:GLN:HA	1:A:2296:GLU:HB2	2.00	0.44
1:B:4141:PHE:CE2	1:B:4196:GLU:HG2	2.52	0.44
1:C:716:PHE:HE1	1:C:730:VAL:HG21	1.82	0.44
1:C:1474:VAL:O	1:C:1486:SER:HA	2.17	0.44
1:C:3036:LYS:NZ	1:C:3076:ASP:OD2	2.37	0.44
1:D:356:TRP:O	1:D:379:HIS:N	2.50	0.44
1:D:2293:GLN:HA	1:D:2296:GLU:HB2	2.00	0.44
1:D:3365:LEU:HD21	1:D:3408:LEU:HD12	1.97	0.44
1:D:3801:GLY:O	1:D:3805:LEU:HB2	2.18	0.44
1:D:4710:SER:OG	1:D:4772:ASP:OD2	2.32	0.44
2:E:23:VAL:HG13	2:E:47:LYS:HG2	1.99	0.44
1:A:796:ARG:O	1:A:1619:ARG:NH2	2.46	0.44
1:A:1036:ARG:O	1:A:1040:CYS:HB2	2.16	0.44
1:A:2927:LEU:HD12	1:A:2930:LEU:HD12	1.99	0.44
1:A:3053:ARG:HA	1:A:3056:LEU:HD13	1.99	0.44
1:A:3053:ARG:HG3	1:A:3056:LEU:HD22	2.00	0.44
1:A:3359:ILE:HD11	1:A:3430:ASN:HB3	1.99	0.44
1:A:3801:GLY:O	1:A:3805:LEU:HB2	2.18	0.44
1:B:219:VAL:HG12	1:B:259:LEU:HD12	1.99	0.44
1:C:884:LEU:HD13	1:C:968:ALA:H	1.82	0.44
1:C:4820:VAL:HG22	1:C:4823:LEU:HB2	1.98	0.44
1:D:3036:LYS:NZ	1:D:3076:ASP:OD2	2.37	0.44
2:E:49:ARG:HG3	2:E:52:LYS:HD3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1171:SER:HG	1:A:1175:SER:HG	1.57	0.44
1:A:2677:LYS:HE2	1:A:2677:LYS:HB3	1.73	0.44
1:A:3245:VAL:HG23	1:A:3248:ARG:H	1.82	0.44
1:B:356:TRP:O	1:B:379:HIS:N	2.50	0.44
1:B:2782:ASP:N	1:B:2782:ASP:OD1	2.50	0.44
1:C:1000:ARG:HA	1:C:1000:ARG:HD3	1.81	0.44
1:C:3053:ARG:HA	1:C:3056:LEU:HD13	1.99	0.44
1:C:3582:ARG:HA	1:C:3582:ARG:HD3	1.79	0.44
1:D:400:ALA:O	1:D:404:ILE:HD12	2.17	0.44
1:D:3168:THR:O	1:D:3172:ILE:HG12	2.18	0.44
1:D:4827:LEU:HD23	1:D:4827:LEU:HA	1.88	0.44
1:A:35:LEU:HD11	1:A:189:LEU:HD23	2.00	0.44
1:A:716:PHE:HE1	1:A:730:VAL:HG21	1.82	0.44
1:B:3053:ARG:HG3	1:B:3056:LEU:HD22	1.99	0.44
1:B:3801:GLY:O	1:B:3805:LEU:HB2	2.18	0.44
1:B:3817:LEU:HD13	1:B:3899:PHE:HD1	1.82	0.44
1:C:400:ALA:O	1:C:404:ILE:HD12	2.17	0.44
1:C:1269:CYS:HA	1:C:1564:PHE:O	2.18	0.44
1:C:2951:ILE:HG21	1:C:3034:LYS:HD2	2.00	0.44
1:D:308:HIS:HD2	1:D:310:LYS:HB3	1.82	0.44
1:D:884:LEU:HD13	1:D:968:ALA:H	1.82	0.44
1:D:3374:ALA:O	1:D:3378:GLN:NE2	2.50	0.44
2:H:23:VAL:HG13	2:H:47:LYS:HG2	1.99	0.44
1:A:939:VAL:HB	1:A:1051:TYR:HB3	2.00	0.44
1:A:2095:GLN:HA	1:A:2127:GLN:HE21	1.83	0.44
1:A:2452:ARG:NH1	1:B:144:GLU:OE1	2.51	0.44
1:A:2626:LEU:HD22	1:A:2640:PRO:HB3	1.99	0.44
1:B:1474:VAL:O	1:B:1486:SER:HA	2.17	0.44
1:C:2095:GLN:HA	1:C:2127:GLN:HE21	1.83	0.44
1:C:2471:SER:HA	1:C:2525:GLY:HA2	2.00	0.44
1:C:2638:LYS:HE2	1:C:2695:LEU:HD13	1.99	0.44
1:D:716:PHE:HE1	1:D:730:VAL:HG21	1.82	0.44
1:A:2109:ASP:N	1:A:2109:ASP:OD1	2.50	0.44
1:A:2471:SER:HA	1:A:2525:GLY:HA2	2.00	0.44
1:A:2951:ILE:HG21	1:A:3034:LYS:HD2	2.00	0.44
1:A:3374:ALA:O	1:A:3378:GLN:NE2	2.50	0.44
1:A:4820:VAL:HG22	1:A:4823:LEU:HB2	1.98	0.44
1:B:308:HIS:HD2	1:B:310:LYS:HB3	1.82	0.44
1:B:716:PHE:HE1	1:B:730:VAL:HG21	1.82	0.44
1:B:1269:CYS:HA	1:B:1564:PHE:O	2.18	0.44
1:B:1968:LYS:NZ	1:B:2030:ASP:OD2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2095:GLN:HA	1:B:2127:GLN:HE21	1.83	0.44
1:B:2196:ASN:OD1	1:B:2199:ARG:NH2	2.47	0.44
1:B:2951:ILE:HG21	1:B:3034:LYS:HD2	2.00	0.44
1:B:3322:ILE:O	1:B:3326:ASN:ND2	2.37	0.44
1:B:3868:ARG:HH11	1:B:3870:ASN:HB3	1.83	0.44
1:C:308:HIS:HD2	1:C:310:LYS:HB3	1.82	0.44
1:C:653:ALA:HB3	1:C:656:SER:HB2	1.99	0.44
1:C:3868:ARG:HH11	1:C:3870:ASN:HB3	1.83	0.44
1:D:3218:VAL:O	1:D:3222:LYS:HB2	2.18	0.44
1:A:308:HIS:HD2	1:A:310:LYS:HB3	1.82	0.44
1:C:2626:LEU:HD22	1:C:2640:PRO:HB3	2.00	0.44
1:C:3110:LEU:HB3	1:C:3175:LEU:HD11	2.00	0.44
1:D:2638:LYS:HE2	1:D:2695:LEU:HD13	1.99	0.44
1:D:2782:ASP:OD1	1:D:2782:ASP:N	2.50	0.44
1:A:3168:THR:O	1:A:3172:ILE:HG12	2.18	0.43
1:A:3218:VAL:O	1:A:3222:LYS:HB2	2.18	0.43
1:A:3901:ASN:OD1	1:A:3904:ARG:NH1	2.36	0.43
1:B:3264:THR:OG1	1:B:3265:GLU:OE1	2.36	0.43
1:D:2951:ILE:HG21	1:D:3034:LYS:HD2	2.00	0.43
1:A:322:LYS:HZ1	1:A:356:TRP:HE1	1.66	0.43
1:B:35:LEU:HD11	1:B:189:LEU:HD23	2.00	0.43
1:B:939:VAL:HB	1:B:1051:TYR:HB3	2.00	0.43
1:B:1099:GLU:OE2	1:B:1125:ASN:ND2	2.41	0.43
1:B:2626:LEU:HD22	1:B:2640:PRO:HB3	2.00	0.43
1:B:2970:SER:HA	1:B:2973:PHE:CE2	2.54	0.43
1:C:3218:VAL:O	1:C:3222:LYS:HB2	2.18	0.43
1:C:3359:ILE:HD11	1:C:3430:ASN:HB3	1.99	0.43
1:D:939:VAL:HB	1:D:1051:TYR:HB3	2.00	0.43
2:G:23:VAL:HG13	2:G:47:LYS:HG2	1.99	0.43
1:A:3110:LEU:HB3	1:A:3175:LEU:HD11	2.00	0.43
1:A:3206:LEU:HD13	1:A:3246:LEU:HD13	1.99	0.43
1:A:3823:LYS:HD3	1:A:3823:LYS:HA	1.75	0.43
1:A:4155:PRO:O	1:A:4161:ARG:NH2	2.45	0.43
1:B:585:SER:O	1:B:588:SER:OG	2.29	0.43
1:B:3218:VAL:O	1:B:3222:LYS:HB2	2.18	0.43
1:C:2002:PRO:O	1:C:2006:ILE:HD12	2.17	0.43
1:D:3371:LYS:NZ	1:D:3375:GLU:OE2	2.45	0.43
1:D:4722:ARG:H	1:D:4722:ARG:HG2	1.43	0.43
1:A:3466:ASN:HB3	1:A:3507:THR:HB	2.00	0.43
1:B:796:ARG:O	1:B:1619:ARG:NH2	2.46	0.43
1:B:2927:LEU:HD12	1:B:2930:LEU:HD12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3582:ARG:HA	1:B:3582:ARG:HD3	1.79	0.43
1:C:863:LEU:HA	1:C:864:PRO:HD3	1.85	0.43
1:C:3168:THR:O	1:C:3172:ILE:HG12	2.18	0.43
1:D:728:ARG:NH2	1:D:1543:GLU:OE2	2.36	0.43
1:D:1424:PRO:HA	1:D:1427:ILE:HG22	2.01	0.43
1:D:2626:LEU:HD22	1:D:2640:PRO:HB3	2.00	0.43
1:D:3053:ARG:HG3	1:D:3056:LEU:HD22	1.99	0.43
1:D:4155:PRO:O	1:D:4161:ARG:NH2	2.45	0.43
2:F:77:THR:HG22	2:F:80:VAL:HG22	2.00	0.43
1:A:775:GLY:H	1:A:848:HIS:CE1	2.37	0.43
1:B:111:HIS:ND1	1:B:114:SER:OG	2.39	0.43
1:B:282:ILE:O	1:B:290:TYR:HA	2.19	0.43
1:B:775:GLY:H	1:B:848:HIS:CE1	2.37	0.43
1:B:2559:LEU:HD13	1:B:2603:ILE:HG13	2.00	0.43
1:B:3110:LEU:HB3	1:B:3175:LEU:HD11	2.00	0.43
1:B:3164:SER:HA	1:B:3167:ARG:HE	1.83	0.43
1:B:3168:THR:O	1:B:3172:ILE:HG12	2.18	0.43
1:C:3801:GLY:O	1:C:3805:LEU:HB2	2.18	0.43
1:D:531:ARG:NH2	1:D:562:GLU:OE2	2.40	0.43
1:D:2687:ALA:O	1:D:2993:GLN:NE2	2.52	0.43
1:D:3110:LEU:HB3	1:D:3175:LEU:HD11	2.00	0.43
1:D:3868:ARG:HH11	1:D:3870:ASN:HB3	1.83	0.43
1:A:3099:ALA:HA	1:A:3136:LEU:HD21	2.00	0.43
1:B:3466:ASN:HB3	1:B:3507:THR:HB	2.00	0.43
1:C:790:ARG:HA	1:C:1626:TRP:O	2.19	0.43
1:C:1424:PRO:HA	1:C:1427:ILE:HG22	2.01	0.43
1:C:2736:ASP:OD1	1:C:2736:ASP:N	2.47	0.43
1:C:2970:SER:HA	1:C:2973:PHE:CE2	2.54	0.43
1:C:3053:ARG:HG3	1:C:3056:LEU:HD22	1.99	0.43
1:C:4722:ARG:HE	1:C:4722:ARG:HB3	1.43	0.43
1:D:322:LYS:HZ1	1:D:356:TRP:HE1	1.67	0.43
1:D:790:ARG:HA	1:D:1626:TRP:O	2.19	0.43
2:E:77:THR:HG22	2:E:80:VAL:HG22	2.00	0.43
1:A:3051:ARG:HH21	1:A:3098:SER:HB3	1.83	0.43
1:A:3768:SER:HA	1:A:3771:HIS:CD2	2.54	0.43
1:B:3051:ARG:HH21	1:B:3098:SER:HB3	1.84	0.43
1:B:3752:SER:OG	1:B:3755:GLU:OE1	2.36	0.43
1:C:939:VAL:HB	1:C:1051:TYR:HB3	2.00	0.43
1:C:2627:VAL:HG21	1:C:2674:LEU:HG	2.00	0.43
1:D:35:LEU:HD11	1:D:189:LEU:HD23	2.00	0.43
1:D:3888:LEU:HD23	1:D:3888:LEU:HA	1.88	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4227:GLU:H	1:D:4227:GLU:HG3	1.57	0.43
1:A:282:ILE:O	1:A:290:TYR:HA	2.19	0.43
1:A:531:ARG:NH2	1:A:562:GLU:OE2	2.40	0.43
1:A:877:ASN:HA	1:A:970:LEU:H	1.84	0.43
1:A:2970:SER:HA	1:A:2973:PHE:CE2	2.54	0.43
1:A:3164:SER:HA	1:A:3167:ARG:HE	1.83	0.43
1:A:3868:ARG:HH11	1:A:3870:ASN:HB3	1.83	0.43
1:C:876:GLU:HG2	1:C:910:PHE:CE2	2.54	0.43
1:C:1452:TRP:HB3	1:C:1548:LEU:HB3	2.01	0.43
1:C:2293:GLN:HA	1:C:2296:GLU:HB2	2.00	0.43
1:C:3164:SER:HA	1:C:3167:ARG:HE	1.83	0.43
1:C:4823:LEU:HD12	1:C:4823:LEU:HA	1.85	0.43
1:D:618:GLN:OE1	1:D:1678:ASN:ND2	2.39	0.43
1:D:876:GLU:HG2	1:D:910:PHE:CE2	2.54	0.43
1:D:2559:LEU:HD13	1:D:2603:ILE:HG13	2.00	0.43
1:D:2927:LEU:HD12	1:D:2930:LEU:HD12	1.99	0.43
1:D:3199:ALA:O	1:D:3283:ARG:NE	2.46	0.43
1:D:3648:ARG:O	1:D:3652:MET:HG2	2.19	0.43
1:A:1424:PRO:HA	1:A:1427:ILE:HG22	2.01	0.43
1:B:876:GLU:HG2	1:B:910:PHE:CE2	2.54	0.43
1:B:1452:TRP:HB3	1:B:1548:LEU:HB3	2.01	0.43
1:B:2293:GLN:HA	1:B:2296:GLU:HB2	2.00	0.43
1:B:2687:ALA:O	1:B:2993:GLN:NE2	2.52	0.43
1:B:3053:ARG:HA	1:B:3056:LEU:HD13	1.99	0.43
1:C:1066:GLN:NE2	1:C:1461:ASP:OD1	2.52	0.43
1:C:1076:ARG:HB3	1:C:1191:VAL:HG23	2.01	0.43
1:D:1076:ARG:HB3	1:D:1191:VAL:HG23	2.01	0.43
1:D:3053:ARG:HA	1:D:3056:LEU:HD13	1.99	0.43
1:D:3264:THR:OG1	1:D:3265:GLU:OE1	2.36	0.43
1:A:876:GLU:HG2	1:A:910:PHE:CE2	2.54	0.43
1:A:1066:GLN:NE2	1:A:1461:ASP:OD1	2.52	0.43
1:A:2627:VAL:HG21	1:A:2674:LEU:HG	2.00	0.43
1:A:3264:THR:OG1	1:A:3265:GLU:OE1	2.36	0.43
1:B:880:GLU:HB3	1:B:883:ALA:HB3	2.01	0.43
1:B:2014:ASP:N	1:B:2014:ASP:OD1	2.45	0.43
1:B:2638:LYS:HE2	1:B:2695:LEU:HD13	1.99	0.43
1:B:2675:THR:HB	1:B:2710:LEU:HD21	2.00	0.43
1:C:1171:SER:HG	1:C:1175:SER:HG	1.59	0.43
1:C:1812:LEU:HD23	1:C:1812:LEU:HA	1.88	0.43
1:C:2927:LEU:HD12	1:C:2930:LEU:HD12	1.99	0.43
1:C:3466:ASN:HB3	1:C:3507:THR:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3648:ARG:O	1:C:3652:MET:HG2	2.19	0.43
1:D:1066:GLN:NE2	1:D:1461:ASP:OD1	2.52	0.43
1:D:1269:CYS:HA	1:D:1564:PHE:O	2.18	0.43
1:D:1828:ASP:N	1:D:1828:ASP:OD1	2.52	0.43
1:D:2627:VAL:HG21	1:D:2674:LEU:HG	2.00	0.43
1:D:2736:ASP:OD1	1:D:2736:ASP:N	2.47	0.43
1:D:3051:ARG:HH21	1:D:3098:SER:HB3	1.84	0.43
1:D:3099:ALA:HA	1:D:3136:LEU:HD21	2.00	0.43
1:D:3169:LEU:HD23	1:D:3194:LEU:HD11	2.01	0.43
1:D:3466:ASN:HB3	1:D:3507:THR:HB	2.00	0.43
1:D:3901:ASN:OD1	1:D:3904:ARG:NH1	2.36	0.43
1:A:262:LEU:HD13	1:A:274:LEU:HD11	2.01	0.42
1:A:1473:THR:HA	1:A:1487:LEU:O	2.19	0.42
1:A:2638:LYS:HE2	1:A:2695:LEU:HD13	1.99	0.42
1:B:3648:ARG:O	1:B:3652:MET:HG2	2.19	0.42
1:B:4646:LEU:HD23	1:B:4646:LEU:HA	1.87	0.42
1:C:618:GLN:OE1	1:C:1678:ASN:ND2	2.39	0.42
1:C:873:LYS:HG2	1:C:970:LEU:HD13	2.01	0.42
1:C:2559:LEU:HD13	1:C:2603:ILE:HG13	2.00	0.42
1:C:2687:ALA:O	1:C:2993:GLN:NE2	2.52	0.42
1:C:2782:ASP:OD1	1:C:2782:ASP:N	2.50	0.42
1:D:2095:GLN:HA	1:D:2127:GLN:HE21	1.83	0.42
1:A:1269:CYS:HA	1:A:1564:PHE:O	2.18	0.42
1:A:3648:ARG:O	1:A:3652:MET:HG2	2.19	0.42
1:B:1066:GLN:NE2	1:B:1461:ASP:OD1	2.52	0.42
1:B:1076:ARG:HB3	1:B:1191:VAL:HG23	2.01	0.42
1:B:2471:SER:HA	1:B:2525:GLY:HA2	2.00	0.42
1:D:2970:SER:HA	1:D:2973:PHE:CE2	2.54	0.42
1:D:3171:SER:O	1:D:3174:SER:OG	2.30	0.42
1:D:3768:SER:HA	1:D:3771:HIS:CD2	2.54	0.42
1:A:1452:TRP:HB3	1:A:1548:LEU:HB3	2.01	0.42
1:A:3062:PRO:HA	1:A:3065:VAL:HG22	2.01	0.42
1:A:4253:GLU:OE2	1:A:4553:ASN:ND2	2.46	0.42
1:B:2712:PRO:O	1:B:2956:ALA:N	2.52	0.42
1:B:3199:ALA:O	1:B:3283:ARG:NE	2.46	0.42
1:C:3051:ARG:HH21	1:C:3098:SER:HB3	1.84	0.42
1:C:3099:ALA:HA	1:C:3136:LEU:HD21	2.00	0.42
1:C:3264:THR:OG1	1:C:3265:GLU:OE1	2.36	0.42
1:D:3754:GLU:HB2	1:D:4718:LYS:HD3	2.02	0.42
2:H:77:THR:HG22	2:H:80:VAL:HG22	2.00	0.42
1:A:2472:LEU:HD23	1:A:2472:LEU:HA	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:652:ARG:HB3	1:B:773:LEU:HD12	2.02	0.42
1:B:728:ARG:NH2	1:B:1543:GLU:OE2	2.36	0.42
1:B:3768:SER:HA	1:B:3771:HIS:CD2	2.54	0.42
1:C:35:LEU:HD11	1:C:189:LEU:HD23	2.00	0.42
1:C:282:ILE:O	1:C:290:TYR:HA	2.19	0.42
1:D:262:LEU:HD13	1:D:274:LEU:HD11	2.02	0.42
1:D:2265:LEU:O	1:D:2330:ARG:NH1	2.53	0.42
1:D:2675:THR:HB	1:D:2710:LEU:HD21	2.00	0.42
1:D:3268:HIS:O	1:D:3272:ILE:HB	2.19	0.42
1:D:3582:ARG:HD3	1:D:3582:ARG:HA	1.79	0.42
1:A:27:THR:OG1	1:A:32:GLN:OE1	2.30	0.42
1:A:790:ARG:HA	1:A:1626:TRP:O	2.19	0.42
1:A:1432:THR:HA	1:A:1520:VAL:O	2.19	0.42
1:A:2559:LEU:HD13	1:A:2603:ILE:HG13	2.00	0.42
1:A:2687:ALA:O	1:A:2993:GLN:NE2	2.52	0.42
1:B:669:ASP:OD1	1:B:790:ARG:NH1	2.53	0.42
1:B:1424:PRO:HA	1:B:1427:ILE:HG22	2.01	0.42
1:B:1473:THR:HA	1:B:1487:LEU:O	2.19	0.42
1:B:3062:PRO:HA	1:B:3065:VAL:HG22	2.01	0.42
1:B:3099:ALA:HA	1:B:3136:LEU:HD21	2.00	0.42
1:C:585:SER:O	1:C:588:SER:OG	2.29	0.42
1:C:877:ASN:HA	1:C:970:LEU:H	1.84	0.42
1:C:3768:SER:HA	1:C:3771:HIS:CD2	2.54	0.42
1:D:652:ARG:HB3	1:D:773:LEU:HD12	2.02	0.42
1:D:669:ASP:OD1	1:D:790:ARG:NH1	2.53	0.42
1:D:833:GLY:HA3	1:D:838:HIS:CD2	2.55	0.42
1:D:3752:SER:OG	1:D:3755:GLU:OE1	2.36	0.42
1:D:4098:ASP:OD1	1:D:4098:ASP:N	2.53	0.42
1:D:4681:LEU:HD12	1:D:4681:LEU:HA	1.87	0.42
1:A:1828:ASP:OD1	1:A:1828:ASP:N	2.52	0.42
1:A:3582:ARG:HA	1:A:3582:ARG:HD3	1.79	0.42
1:A:4161:ARG:HD3	1:A:4161:ARG:HA	1.85	0.42
1:B:265:LEU:HD13	1:B:279:PRO:HB2	2.02	0.42
1:B:873:LYS:HG2	1:B:970:LEU:HD13	2.01	0.42
1:B:1432:THR:HA	1:B:1520:VAL:O	2.19	0.42
1:B:2265:LEU:O	1:B:2330:ARG:NH1	2.53	0.42
1:C:829:TYR:HB3	1:C:1073:ARG:HH11	1.85	0.42
1:C:2265:LEU:O	1:C:2330:ARG:NH1	2.53	0.42
1:C:3169:LEU:HD23	1:C:3194:LEU:HD11	2.01	0.42
1:C:3268:HIS:O	1:C:3272:ILE:HB	2.19	0.42
1:D:282:ILE:O	1:D:290:TYR:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1452:TRP:HB3	1:D:1548:LEU:HB3	2.01	0.42
1:A:3169:LEU:HD23	1:A:3194:LEU:HD11	2.01	0.42
1:A:3754:GLU:HB2	1:A:4718:LYS:HD3	2.02	0.42
1:B:790:ARG:HA	1:B:1626:TRP:O	2.19	0.42
1:B:2627:VAL:HG21	1:B:2674:LEU:HG	2.00	0.42
1:B:2736:ASP:OD1	1:B:2736:ASP:N	2.47	0.42
1:B:4722:ARG:H	1:B:4722:ARG:HG2	1.43	0.42
1:B:5006:GLN:H	1:B:5006:GLN:HG2	1.64	0.42
1:C:3322:ILE:O	1:C:3326:ASN:ND2	2.37	0.42
1:D:265:LEU:HD13	1:D:279:PRO:HB2	2.02	0.42
1:D:873:LYS:HG2	1:D:970:LEU:HD13	2.01	0.42
1:A:669:ASP:OD1	1:A:790:ARG:NH1	2.53	0.42
1:A:1076:ARG:HB3	1:A:1191:VAL:HG23	2.01	0.42
1:B:877:ASN:HA	1:B:970:LEU:H	1.84	0.42
1:B:1007:TYR:O	1:B:1017:ARG:NH2	2.52	0.42
1:B:3316:LEU:HD11	1:B:3346:VAL:HA	2.02	0.42
1:B:3535:LEU:O	1:B:3538:THR:OG1	2.33	0.42
1:B:3754:GLU:HB2	1:B:4718:LYS:HD3	2.02	0.42
1:C:486:LEU:HD12	1:C:486:LEU:HA	1.95	0.42
1:C:775:GLY:H	1:C:848:HIS:CE1	2.37	0.42
1:C:2675:THR:HB	1:C:2710:LEU:HD21	2.00	0.42
1:C:3888:LEU:HD23	1:C:3888:LEU:HA	1.88	0.42
1:D:3164:SER:HA	1:D:3167:ARG:HE	1.83	0.42
1:D:3316:LEU:HD11	1:D:3346:VAL:HA	2.02	0.42
2:F:4:ILE:HD11	2:F:66:MET:HB3	2.02	0.42
1:A:265:LEU:HD13	1:A:279:PRO:HB2	2.02	0.42
1:A:880:GLU:HB3	1:A:883:ALA:HB3	2.01	0.42
1:A:2265:LEU:O	1:A:2330:ARG:NH1	2.53	0.42
1:A:2675:THR:HB	1:A:2710:LEU:HD21	2.01	0.42
1:A:2716:ASP:OD1	1:A:2716:ASP:N	2.45	0.42
1:A:3268:HIS:O	1:A:3272:ILE:HB	2.19	0.42
1:A:3322:ILE:O	1:A:3326:ASN:ND2	2.36	0.42
1:B:262:LEU:HD13	1:B:274:LEU:HD11	2.02	0.42
1:B:629:ARG:NH1	2:F:90:VAL:O	2.43	0.42
1:B:833:GLY:HA3	1:B:838:HIS:CD2	2.55	0.42
1:B:1000:ARG:HA	1:B:1000:ARG:HD3	1.81	0.42
1:B:3888:LEU:HD23	1:B:3888:LEU:HA	1.88	0.42
1:B:4708:THR:HG21	1:B:4775:TYR:HB2	2.01	0.42
1:C:652:ARG:HB3	1:C:773:LEU:HD12	2.02	0.42
1:C:669:ASP:OD1	1:C:790:ARG:NH1	2.53	0.42
1:C:833:GLY:HA3	1:C:838:HIS:CD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1007:TYR:O	1:C:1017:ARG:NH2	2.52	0.42
1:C:4910:GLU:O	1:C:4914:VAL:HG13	2.20	0.42
1:D:877:ASN:HA	1:D:970:LEU:H	1.84	0.42
1:D:880:GLU:HB3	1:D:883:ALA:HB3	2.01	0.42
1:D:3301:PRO:HA	1:D:3302:PRO:HD3	1.86	0.42
1:D:4910:GLU:O	1:D:4914:VAL:HG13	2.20	0.42
1:A:846:LEU:HD22	1:A:846:LEU:HA	1.91	0.42
1:A:2707:ALA:HB1	1:A:3009:TYR:HD1	1.85	0.42
1:A:4899:ASP:OD1	1:D:4892:ARG:NH1	2.53	0.42
1:A:4910:GLU:O	1:A:4914:VAL:HG13	2.20	0.42
1:B:486:LEU:HD12	1:B:486:LEU:HA	1.95	0.42
1:B:2707:ALA:HB1	1:B:3009:TYR:HD1	1.85	0.42
1:B:4155:PRO:HG3	1:B:5036:LEU:HD23	2.02	0.42
1:C:262:LEU:HD13	1:C:274:LEU:HD11	2.02	0.42
1:C:2677:LYS:HE2	1:C:2677:LYS:HB3	1.73	0.42
1:C:3380:ARG:NH2	1:C:3391:GLU:OE1	2.53	0.42
1:C:3852:LYS:HE3	1:C:3852:LYS:HB3	1.93	0.42
1:D:1473:THR:HA	1:D:1487:LEU:O	2.19	0.42
1:D:2471:SER:HA	1:D:2525:GLY:HA2	2.00	0.42
2:G:77:THR:HG22	2:G:80:VAL:HG22	2.00	0.42
1:A:3132:THR:HG23	1:A:3136:LEU:HD23	2.02	0.41
1:A:4227:GLU:H	1:A:4227:GLU:HG3	1.57	0.41
1:B:2656:CYS:HA	1:B:2711:PRO:HG3	2.02	0.41
1:B:3132:THR:HG23	1:B:3136:LEU:HD23	2.02	0.41
1:B:3268:HIS:O	1:B:3272:ILE:HB	2.19	0.41
1:B:4910:GLU:O	1:B:4914:VAL:HG13	2.20	0.41
1:C:1432:THR:HA	1:C:1520:VAL:O	2.19	0.41
1:C:2656:CYS:HA	1:C:2711:PRO:HG3	2.02	0.41
1:C:2707:ALA:HB1	1:C:3009:TYR:HD1	1.85	0.41
1:C:4708:THR:HG21	1:C:4775:TYR:HB2	2.01	0.41
1:D:3380:ARG:NH2	1:D:3391:GLU:OE1	2.53	0.41
1:D:4722:ARG:HE	1:D:4722:ARG:HB3	1.43	0.41
1:A:2004:GLU:HA	1:A:2007:ASN:HB2	2.02	0.41
1:A:3852:LYS:HE3	1:A:3852:LYS:HB3	1.93	0.41
1:A:4098:ASP:OD1	1:A:4098:ASP:N	2.53	0.41
1:B:39:ALA:HB2	1:B:47:CYS:HA	2.02	0.41
1:B:181:HIS:ND1	1:B:198:THR:OG1	2.40	0.41
1:B:2004:GLU:HA	1:B:2007:ASN:HB2	2.03	0.41
1:B:2978:GLU:OE2	1:B:3053:ARG:NH1	2.43	0.41
1:B:3169:LEU:HD23	1:B:3194:LEU:HD11	2.01	0.41
1:B:3380:ARG:NH2	1:B:3391:GLU:OE1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3592:ILE:HA	1:B:3595:ARG:HG2	2.03	0.41
1:C:39:ALA:HB2	1:C:47:CYS:HA	2.02	0.41
1:C:687:ALA:HA	1:C:713:SER:HA	2.03	0.41
1:C:880:GLU:HB3	1:C:883:ALA:HB3	2.01	0.41
1:C:3062:PRO:HA	1:C:3065:VAL:HG22	2.01	0.41
1:C:3754:GLU:HB2	1:C:4718:LYS:HD3	2.02	0.41
1:D:1968:LYS:NZ	1:D:2030:ASP:OD2	2.50	0.41
1:A:4155:PRO:HG3	1:A:5036:LEU:HD23	2.02	0.41
1:B:1634:LEU:HD23	1:B:1634:LEU:HA	1.93	0.41
1:B:3813:GLN:NE2	1:B:3890:LEU:O	2.53	0.41
1:C:1828:ASP:OD1	1:C:1828:ASP:N	2.52	0.41
1:C:3592:ILE:HA	1:C:3595:ARG:HG2	2.03	0.41
1:D:775:GLY:H	1:D:848:HIS:CE1	2.37	0.41
1:D:2656:CYS:HA	1:D:2711:PRO:HG3	2.02	0.41
1:D:3889:GLN:OE1	1:D:3960:GLN:NE2	2.53	0.41
1:A:39:ALA:HB2	1:A:47:CYS:HA	2.02	0.41
1:A:652:ARG:HB3	1:A:773:LEU:HD12	2.02	0.41
1:B:3201:MET:HA	1:B:3202:PRO:HD3	1.98	0.41
1:C:134:ASP:OD1	1:C:134:ASP:N	2.46	0.41
1:C:265:LEU:HD13	1:C:279:PRO:HB2	2.02	0.41
1:D:2707:ALA:HB1	1:D:3009:TYR:HD1	1.85	0.41
1:D:2765:LYS:HA	1:D:2765:LYS:HD3	1.80	0.41
1:A:232:THR:HG21	1:A:252:VAL:HG12	2.03	0.41
1:A:833:GLY:HA3	1:A:838:HIS:CD2	2.55	0.41
1:A:873:LYS:HG2	1:A:970:LEU:HD13	2.01	0.41
1:A:2014:ASP:N	1:A:2014:ASP:OD1	2.45	0.41
1:A:2961:GLN:O	1:A:2965:ARG:HG3	2.21	0.41
1:B:134:ASP:OD1	1:B:134:ASP:N	2.46	0.41
1:B:1171:SER:HG	1:B:1175:SER:HG	1.58	0.41
1:B:1575:LEU:HD23	1:B:1575:LEU:HA	1.95	0.41
1:B:1828:ASP:N	1:B:1828:ASP:OD1	2.52	0.41
1:B:2924:GLN:O	1:B:2928:LYS:HG2	2.21	0.41
1:B:4943:LEU:O	1:B:4947:GLN:HG2	2.21	0.41
1:C:1473:THR:HA	1:C:1487:LEU:O	2.19	0.41
1:C:2309:SER:OG	1:C:2321:ILE:O	2.34	0.41
1:C:3132:THR:HG23	1:C:3136:LEU:HD23	2.02	0.41
1:C:4098:ASP:OD1	1:C:4098:ASP:N	2.53	0.41
1:D:687:ALA:HA	1:D:713:SER:HA	2.03	0.41
1:D:1432:THR:HA	1:D:1520:VAL:O	2.19	0.41
1:D:2800:LYS:HB2	1:D:2800:LYS:HE2	1.89	0.41
1:D:4708:THR:HG21	1:D:4775:TYR:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4708:THR:HG21	1:A:4775:TYR:HB2	2.02	0.41
1:B:27:THR:OG1	1:B:32:GLN:OE1	2.30	0.41
1:B:4219:PHE:O	1:B:4223:ASN:HB2	2.21	0.41
1:C:759:ILE:HG22	1:C:764:VAL:HG22	2.03	0.41
1:C:4253:GLU:OE2	1:C:4553:ASN:ND2	2.46	0.41
1:D:259:LEU:HD13	1:D:259:LEU:HA	1.95	0.41
1:D:3062:PRO:HA	1:D:3065:VAL:HG22	2.01	0.41
1:A:863:LEU:HA	1:A:864:PRO:HD3	1.86	0.41
1:A:2924:GLN:O	1:A:2928:LYS:HG2	2.21	0.41
1:B:759:ILE:HG22	1:B:764:VAL:HG22	2.03	0.41
1:B:829:TYR:HB3	1:B:1073:ARG:HH11	1.85	0.41
1:B:838:HIS:CE1	1:B:1201:HIS:HB2	2.56	0.41
1:C:2004:GLU:HA	1:C:2007:ASN:HB2	2.03	0.41
1:C:2380:ILE:HD13	1:C:2380:ILE:HA	1.96	0.41
1:C:3695:PRO:HB3	1:C:3699:HIS:CD2	2.56	0.41
1:C:3705:PHE:HA	1:C:3708:THR:HG22	2.03	0.41
1:C:3823:LYS:HA	1:C:3823:LYS:HD3	1.75	0.41
1:C:4155:PRO:HG3	1:C:5036:LEU:HD23	2.02	0.41
1:C:4176:PRO:O	1:C:4202:ARG:NH1	2.45	0.41
1:D:414:PHE:HE1	1:D:436:LEU:HD13	1.85	0.41
1:D:3592:ILE:HA	1:D:3595:ARG:HG2	2.03	0.41
1:A:1864:LYS:NZ	1:A:1871:PHE:O	2.39	0.41
1:A:2500:ALA:HB2	1:A:2553:TYR:HD1	1.86	0.41
1:A:2712:PRO:O	1:A:2956:ALA:N	2.52	0.41
1:A:4943:LEU:O	1:A:4947:GLN:HG2	2.21	0.41
1:B:2472:LEU:HD23	1:B:2472:LEU:HA	1.87	0.41
1:B:2742:THR:HB	1:B:2814:LYS:HB3	2.03	0.41
1:B:4569:LEU:HD12	1:B:4569:LEU:HA	1.95	0.41
1:C:277:GLY:N	1:C:316:PHE:O	2.43	0.41
1:C:2472:LEU:HD23	1:C:2472:LEU:HA	1.87	0.41
1:C:4161:ARG:HA	1:C:4161:ARG:HD3	1.86	0.41
1:D:1007:TYR:O	1:D:1017:ARG:NH2	2.52	0.41
1:D:3509:LEU:O	1:D:3513:THR:OG1	2.30	0.41
2:G:4:ILE:HD11	2:G:66:MET:HB3	2.02	0.41
1:A:414:PHE:HE1	1:A:436:LEU:HD13	1.85	0.41
1:A:829:TYR:HB3	1:A:1073:ARG:HH11	1.85	0.41
1:A:3036:LYS:NZ	1:A:3076:ASP:OD2	2.37	0.41
1:A:3380:ARG:NH2	1:A:3391:GLU:OE1	2.53	0.41
1:A:3695:PRO:HB3	1:A:3699:HIS:CD2	2.56	0.41
1:A:3891:LEU:HB3	1:A:3899:PHE:CE2	2.56	0.41
1:A:4681:LEU:HD12	1:A:4681:LEU:HA	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4880:MET:HE2	1:A:4880:MET:HB2	2.00	0.41
1:B:414:PHE:HE1	1:B:436:LEU:HD13	1.85	0.41
1:B:2792:ARG:HB2	1:B:2797:PHE:HD1	1.86	0.41
1:B:3036:LYS:NZ	1:B:3076:ASP:OD2	2.37	0.41
1:C:414:PHE:HE1	1:C:436:LEU:HD13	1.85	0.41
1:C:629:ARG:NH1	2:G:90:VAL:O	2.43	0.41
1:C:2007:ASN:O	1:C:2011:HIS:HB2	2.21	0.41
1:C:2380:ILE:HG13	1:C:2469:ILE:HD13	2.03	0.41
1:C:3316:LEU:HD11	1:C:3346:VAL:HA	2.02	0.41
1:D:232:THR:HG21	1:D:252:VAL:HG12	2.03	0.41
1:D:2380:ILE:HG13	1:D:2469:ILE:HD13	2.03	0.41
1:D:2500:ALA:HB2	1:D:2553:TYR:HD1	1.86	0.41
1:D:2997:PHE:O	1:D:3001:ILE:HB	2.21	0.41
1:D:3132:THR:HG23	1:D:3136:LEU:HD23	2.02	0.41
1:D:3695:PRO:HB3	1:D:3699:HIS:CD2	2.56	0.41
1:A:2007:ASN:O	1:A:2011:HIS:HB2	2.21	0.41
1:A:2742:THR:HB	1:A:2814:LYS:HB3	2.03	0.41
1:A:2997:PHE:O	1:A:3001:ILE:HB	2.21	0.41
1:A:3316:LEU:HD11	1:A:3346:VAL:HA	2.02	0.41
1:A:3592:ILE:HA	1:A:3595:ARG:HG2	2.02	0.41
1:B:687:ALA:HA	1:B:713:SER:HA	2.03	0.41
1:B:2961:GLN:O	1:B:2965:ARG:HG3	2.21	0.41
1:C:27:THR:OG1	1:C:32:GLN:OE1	2.30	0.41
1:C:1575:LEU:HD23	1:C:1575:LEU:HA	1.95	0.41
1:C:3891:LEU:HB3	1:C:3899:PHE:CE2	2.56	0.41
1:C:4219:PHE:O	1:C:4223:ASN:HB2	2.21	0.41
1:D:700:GLU:N	1:D:705:ASN:OD1	2.54	0.41
1:D:897:ARG:HH21	1:D:901:LYS:HD2	1.86	0.41
1:D:1249:PRO:HA	1:D:1250:PRO:HD3	1.95	0.41
1:D:2007:ASN:O	1:D:2011:HIS:HB2	2.21	0.41
1:D:2961:GLN:O	1:D:2965:ARG:HG3	2.21	0.41
1:D:3249:LEU:HD23	1:D:3277:LEU:HD21	2.02	0.41
1:D:3705:PHE:HA	1:D:3708:THR:HG22	2.03	0.41
2:E:16:PRO:HG2	2:E:64:ALA:HA	2.03	0.41
2:H:16:PRO:HG2	2:H:64:ALA:HA	2.03	0.41
1:A:838:HIS:CE1	1:A:1201:HIS:HB2	2.56	0.40
1:A:897:ARG:HH21	1:A:901:LYS:HD2	1.86	0.40
1:A:2656:CYS:HA	1:A:2711:PRO:HG3	2.02	0.40
1:A:2902:HIS:CE1	1:A:2904:LEU:HB2	2.56	0.40
1:A:3938:SER:HA	1:A:4002:LYS:HZ1	1.86	0.40
1:B:2007:ASN:O	1:B:2011:HIS:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2714:TYR:O	1:B:2955:PHE:N	2.54	0.40
1:B:3523:ASN:O	1:B:3582:ARG:NH2	2.55	0.40
1:C:2792:ARG:HB2	1:C:2797:PHE:HD1	1.86	0.40
1:D:39:ALA:HB2	1:D:47:CYS:HA	2.02	0.40
1:D:234:SER:HB2	1:D:242:ARG:HA	2.03	0.40
1:D:829:TYR:HB3	1:D:1073:ARG:HH11	1.85	0.40
1:D:1739:THR:O	1:D:1743[B]:ARG:HG3	2.21	0.40
1:D:2196:ASN:OD1	1:D:2199:ARG:NH2	2.47	0.40
1:D:3256:LEU:HB3	1:D:3266:MET:HE1	2.02	0.40
1:D:4548:ARG:HE	1:D:4548:ARG:HB3	1.74	0.40
1:D:5006:GLN:H	1:D:5006:GLN:HG2	1.64	0.40
2:H:4:ILE:HD11	2:H:66:MET:HB3	2.02	0.40
1:A:2859:PRO:HA	1:A:2860:PRO:HD3	1.99	0.40
1:A:3249:LEU:HD23	1:A:3277:LEU:HD21	2.02	0.40
1:B:3695:PRO:HB3	1:B:3699:HIS:CD2	2.56	0.40
1:B:4649:LEU:HD12	1:B:4649:LEU:HA	1.95	0.40
1:C:838:HIS:CE1	1:C:1201:HIS:HB2	2.56	0.40
1:C:2924:GLN:O	1:C:2928:LYS:HG2	2.21	0.40
1:D:869:ARG:CZ	1:D:870:ILE:HB	2.51	0.40
1:D:2004:GLU:HA	1:D:2007:ASN:HB2	2.03	0.40
1:D:4155:PRO:HG3	1:D:5036:LEU:HD23	2.02	0.40
1:A:759:ILE:HG22	1:A:764:VAL:HG22	2.03	0.40
1:A:4090:LYS:HE2	1:A:4090:LYS:HB3	1.89	0.40
1:A:4649:LEU:HD12	1:A:4649:LEU:HA	1.95	0.40
1:B:3891:LEU:HB3	1:B:3899:PHE:CE2	2.56	0.40
1:C:234:SER:HB2	1:C:242:ARG:HA	2.03	0.40
1:C:2500:ALA:HB2	1:C:2553:TYR:HD1	1.86	0.40
1:C:4943:LEU:O	1:C:4947:GLN:HG2	2.21	0.40
1:D:1842:LEU:HD23	1:D:1842:LEU:HA	1.96	0.40
1:D:4219:PHE:O	1:D:4223:ASN:HB2	2.21	0.40
1:D:5029:ARG:HE	1:D:5029:ARG:HB3	1.68	0.40
1:A:234:SER:HB2	1:A:242:ARG:HA	2.03	0.40
1:A:277:GLY:N	1:A:316:PHE:O	2.43	0.40
1:A:2023:LEU:HD23	1:A:2023:LEU:HA	1.93	0.40
1:A:2682:ILE:HD13	1:A:2682:ILE:HA	1.90	0.40
1:A:4722:ARG:HE	1:A:4722:ARG:HB3	1.43	0.40
1:D:3891:LEU:HB3	1:D:3899:PHE:CE2	2.56	0.40
1:D:4569:LEU:HD12	1:D:4569:LEU:HA	1.95	0.40
1:A:687:ALA:HA	1:A:713:SER:HA	2.02	0.40
1:A:1110:ARG:HE	1:A:1110:ARG:HB3	1.78	0.40
1:A:2419:GLY:O	1:A:2423:MET:HG3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2792:ARG:HB2	1:A:2797:PHE:HD1	1.86	0.40
1:A:2978:GLU:OE2	1:A:3053:ARG:NH1	2.43	0.40
1:A:3705:PHE:HA	1:A:3708:THR:HG22	2.03	0.40
1:A:4083:ASP:OD2	1:A:4085:ARG:NH2	2.47	0.40
1:A:4219:PHE:O	1:A:4223:ASN:HB2	2.21	0.40
1:B:531:ARG:NH2	1:B:562:GLU:OE2	2.40	0.40
1:B:2182:ILE:O	1:B:2186:MET:HG2	2.22	0.40
1:D:838:HIS:CE1	1:D:1201:HIS:HB2	2.56	0.40
1:D:2309:SER:OG	1:D:2321:ILE:O	2.34	0.40
1:D:2902:HIS:CE1	1:D:2904:LEU:HB2	2.56	0.40
2:E:4:ILE:HD11	2:E:66:MET:HB3	2.02	0.40
2:F:16:PRO:HG2	2:F:64:ALA:HA	2.03	0.40
2:G:16:PRO:HG2	2:G:64:ALA:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	4355/5037 (86%)	4230 (97%)	120 (3%)	5 (0%)	51	84
1	B	4355/5037 (86%)	4230 (97%)	120 (3%)	5 (0%)	51	84
1	C	4355/5037 (86%)	4230 (97%)	120 (3%)	5 (0%)	51	84
1	D	4355/5037 (86%)	4230 (97%)	120 (3%)	5 (0%)	51	84
2	E	105/350 (30%)	103 (98%)	2 (2%)	0	100	100
2	F	105/350 (30%)	103 (98%)	2 (2%)	0	100	100
2	G	105/350 (30%)	103 (98%)	2 (2%)	0	100	100
2	H	105/350 (30%)	103 (98%)	2 (2%)	0	100	100
All	All	17840/21548 (83%)	17332 (97%)	488 (3%)	20 (0%)	54	84

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3615	SER
1	B	3615	SER
1	C	3615	SER
1	D	3615	SER
1	A	3616	LYS
1	B	3616	LYS
1	C	3616	LYS
1	D	3616	LYS
1	A	4691	GLN
1	A	4712	PRO
1	B	4691	GLN
1	B	4712	PRO
1	C	4691	GLN
1	C	4712	PRO
1	D	4691	GLN
1	D	4712	PRO
1	A	4872	PRO
1	B	4872	PRO
1	C	4872	PRO
1	D	4872	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	3807/4276 (89%)	3695 (97%)	112 (3%)	42 71
1	B	3807/4276 (89%)	3695 (97%)	112 (3%)	42 71
1	C	3807/4276 (89%)	3695 (97%)	112 (3%)	42 71
1	D	3807/4276 (89%)	3695 (97%)	112 (3%)	42 71
2	E	88/304 (29%)	88 (100%)	0	100 100
2	F	88/304 (29%)	88 (100%)	0	100 100
2	G	88/304 (29%)	88 (100%)	0	100 100
2	H	88/304 (29%)	88 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	15580/18320 (85%)	15132 (97%)	448 (3%)	46 71

All (448) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	373	LYS
1	A	830	ARG
1	A	846	LEU
1	A	1128	ARG
1	A	1508	ARG
1	A	1534	LYS
1	A	1743[A]	ARG
1	A	1743[B]	ARG
1	A	1752	ARG
1	A	2100[A]	HIS
1	A	2100[B]	HIS
1	A	2369[A]	ARG
1	A	2369[B]	ARG
1	A	2531	ARG
1	A	2738	ARG
1	A	2786	LYS
1	A	2806	ARG
1	A	2827	ARG
1	A	2914	LYS
1	A	3053	ARG
1	A	3225	ARG
1	A	3614	LYS
1	A	3622	LYS
1	A	4180	ARG
1	A	4181	ILE
1	A	4192	ARG
1	A	4198	SER
1	A	4199	GLU
1	A	4200	THR
1	A	4202	ARG
1	A	4211	LYS
1	A	4213	SER
1	A	4221	VAL
1	A	4223	ASN
1	A	4227	GLU
1	A	4231	MET
1	A	4540	PHE

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Mol	Chain	Res	Type
1	A	4543	GLU
1	A	4544	LEU
1	A	4548	ARG
1	A	4549	VAL
1	A	4550	LYS
1	A	4555	LEU
1	A	4557	ARG
1	A	4569	LEU
1	A	4580	TYR
1	A	4581	LYS
1	A	4584	ASP
1	A	4585	SER
1	A	4627	MET
1	A	4628	VAL
1	A	4634	GLU
1	A	4635	SER
1	A	4641	PRO
1	A	4647	SER
1	A	4651	THR
1	A	4658	ILE
1	A	4662	ASN
1	A	4665	LYS
1	A	4666	VAL
1	A	4676	GLU
1	A	4681	LEU
1	A	4684	ASP
1	A	4694	ASP
1	A	4695	ASP
1	A	4697	VAL
1	A	4707	ASN
1	A	4708	THR
1	A	4710	SER
1	A	4717	ASP
1	A	4720	VAL
1	A	4722	ARG
1	A	4725	LEU
1	A	4731	ILE
1	A	4734	ARG
1	A	4736	ARG
1	A	4737	ILE
1	A	4743	MET
1	A	4747	SER

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Mol	Chain	Res	Type
1	A	4772	ASP
1	A	4773	VAL
1	A	4813	LEU
1	A	4818	MET
1	A	4820	VAL
1	A	4821	LYS
1	A	4822	THR
1	A	4823	LEU
1	A	4829	SER
1	A	4839	MET
1	A	4844	LEU
1	A	4861	LYS
1	A	4866	SER
1	A	4871	GLU
1	A	4879	MET
1	A	4880	MET
1	A	4882	CYS
1	A	4889	VAL
1	A	4953	ASP
1	A	4957	LYS
1	A	4965	SER
1	A	4966	ASP
1	A	4980	LEU
1	A	4989	MET
1	A	4992	LEU
1	A	4997	ASN
1	A	4999	ASP
1	A	5000	GLU
1	A	5001	THR
1	A	5013	MET
1	A	5027	CYS
1	A	5034	ASP
1	A	5035	GLN
1	B	373	LYS
1	B	830	ARG
1	B	846	LEU
1	B	1128	ARG
1	B	1508	ARG
1	B	1534	LYS
1	B	1743[A]	ARG
1	B	1743[B]	ARG
1	B	1752	ARG

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Mol	Chain	Res	Type
1	B	2100[A]	HIS
1	B	2100[B]	HIS
1	B	2369[A]	ARG
1	B	2369[B]	ARG
1	B	2531	ARG
1	B	2738	ARG
1	B	2786	LYS
1	B	2806	ARG
1	B	2827	ARG
1	B	2914	LYS
1	B	3053	ARG
1	B	3225	ARG
1	B	3614	LYS
1	B	3622	LYS
1	B	4180	ARG
1	B	4181	ILE
1	B	4192	ARG
1	B	4198	SER
1	B	4199	GLU
1	B	4200	THR
1	B	4202	ARG
1	B	4211	LYS
1	B	4213	SER
1	B	4221	VAL
1	B	4223	ASN
1	B	4227	GLU
1	B	4231	MET
1	B	4540	PHE
1	B	4543	GLU
1	B	4544	LEU
1	B	4548	ARG
1	B	4549	VAL
1	B	4550	LYS
1	B	4555	LEU
1	B	4557	ARG
1	B	4569	LEU
1	B	4580	TYR
1	B	4581	LYS
1	B	4584	ASP
1	B	4585	SER
1	B	4627	MET
1	B	4628	VAL

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Mol	Chain	Res	Type
1	B	4634	GLU
1	B	4635	SER
1	B	4641	PRO
1	B	4647	SER
1	B	4651	THR
1	B	4658	ILE
1	B	4662	ASN
1	B	4665	LYS
1	B	4666	VAL
1	B	4676	GLU
1	B	4681	LEU
1	B	4684	ASP
1	B	4694	ASP
1	B	4695	ASP
1	B	4697	VAL
1	B	4707	ASN
1	B	4708	THR
1	B	4710	SER
1	B	4717	ASP
1	B	4720	VAL
1	B	4722	ARG
1	B	4725	LEU
1	B	4731	ILE
1	B	4734	ARG
1	B	4736	ARG
1	B	4737	ILE
1	B	4743	MET
1	B	4747	SER
1	B	4772	ASP
1	B	4773	VAL
1	B	4813	LEU
1	B	4818	MET
1	B	4820	VAL
1	B	4821	LYS
1	B	4822	THR
1	B	4823	LEU
1	B	4829	SER
1	B	4839	MET
1	B	4844	LEU
1	B	4861	LYS
1	B	4866	SER
1	B	4871	GLU

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Mol	Chain	Res	Type
1	B	4879	MET
1	B	4880	MET
1	B	4882	CYS
1	B	4889	VAL
1	B	4953	ASP
1	B	4957	LYS
1	B	4965	SER
1	B	4966	ASP
1	B	4980	LEU
1	B	4989	MET
1	B	4992	LEU
1	B	4997	ASN
1	B	4999	ASP
1	B	5000	GLU
1	B	5001	THR
1	B	5013	MET
1	B	5027	CYS
1	B	5034	ASP
1	B	5035	GLN
1	C	373	LYS
1	C	830	ARG
1	C	846	LEU
1	C	1128	ARG
1	C	1508	ARG
1	C	1534	LYS
1	C	1743[A]	ARG
1	C	1743[B]	ARG
1	C	1752	ARG
1	C	2100[A]	HIS
1	C	2100[B]	HIS
1	C	2369[A]	ARG
1	C	2369[B]	ARG
1	C	2531	ARG
1	C	2738	ARG
1	C	2786	LYS
1	C	2806	ARG
1	C	2827	ARG
1	C	2914	LYS
1	C	3053	ARG
1	C	3225	ARG
1	C	3614	LYS
1	C	3622	LYS

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Mol	Chain	Res	Type
1	C	4180	ARG
1	C	4181	ILE
1	C	4192	ARG
1	C	4198	SER
1	C	4199	GLU
1	C	4200	THR
1	C	4202	ARG
1	C	4211	LYS
1	C	4213	SER
1	C	4221	VAL
1	C	4223	ASN
1	C	4227	GLU
1	C	4231	MET
1	C	4540	PHE
1	C	4543	GLU
1	C	4544	LEU
1	C	4548	ARG
1	C	4549	VAL
1	C	4550	LYS
1	C	4555	LEU
1	C	4557	ARG
1	C	4569	LEU
1	C	4580	TYR
1	C	4581	LYS
1	C	4584	ASP
1	C	4585	SER
1	C	4627	MET
1	C	4628	VAL
1	C	4634	GLU
1	C	4635	SER
1	C	4641	PRO
1	C	4647	SER
1	C	4651	THR
1	C	4658	ILE
1	C	4662	ASN
1	C	4665	LYS
1	C	4666	VAL
1	C	4676	GLU
1	C	4681	LEU
1	C	4684	ASP
1	C	4694	ASP
1	C	4695	ASP

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Mol	Chain	Res	Type
1	C	4697	VAL
1	C	4707	ASN
1	C	4708	THR
1	C	4710	SER
1	C	4717	ASP
1	C	4720	VAL
1	C	4722	ARG
1	C	4725	LEU
1	C	4731	ILE
1	C	4734	ARG
1	C	4736	ARG
1	C	4737	ILE
1	C	4743	MET
1	C	4747	SER
1	C	4772	ASP
1	C	4773	VAL
1	C	4813	LEU
1	C	4818	MET
1	C	4820	VAL
1	C	4821	LYS
1	C	4822	THR
1	C	4823	LEU
1	C	4829	SER
1	C	4839	MET
1	C	4844	LEU
1	C	4861	LYS
1	C	4866	SER
1	C	4871	GLU
1	C	4879	MET
1	C	4880	MET
1	C	4882	CYS
1	C	4889	VAL
1	C	4953	ASP
1	C	4957	LYS
1	C	4965	SER
1	C	4966	ASP
1	C	4980	LEU
1	C	4989	MET
1	C	4992	LEU
1	C	4997	ASN
1	C	4999	ASP
1	C	5000	GLU

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Mol	Chain	Res	Type
1	C	5001	THR
1	C	5013	MET
1	C	5027	CYS
1	C	5034	ASP
1	C	5035	GLN
1	D	373	LYS
1	D	830	ARG
1	D	846	LEU
1	D	1128	ARG
1	D	1508	ARG
1	D	1534	LYS
1	D	1743[A]	ARG
1	D	1743[B]	ARG
1	D	1752	ARG
1	D	2100[A]	HIS
1	D	2100[B]	HIS
1	D	2369[A]	ARG
1	D	2369[B]	ARG
1	D	2531	ARG
1	D	2738	ARG
1	D	2786	LYS
1	D	2806	ARG
1	D	2827	ARG
1	D	2914	LYS
1	D	3053	ARG
1	D	3225	ARG
1	D	3614	LYS
1	D	3622	LYS
1	D	4180	ARG
1	D	4181	ILE
1	D	4192	ARG
1	D	4198	SER
1	D	4199	GLU
1	D	4200	THR
1	D	4202	ARG
1	D	4211	LYS
1	D	4213	SER
1	D	4221	VAL
1	D	4223	ASN
1	D	4227	GLU
1	D	4231	MET
1	D	4540	PHE

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Mol	Chain	Res	Type
1	D	4543	GLU
1	D	4544	LEU
1	D	4548	ARG
1	D	4549	VAL
1	D	4550	LYS
1	D	4555	LEU
1	D	4557	ARG
1	D	4569	LEU
1	D	4580	TYR
1	D	4581	LYS
1	D	4584	ASP
1	D	4585	SER
1	D	4627	MET
1	D	4628	VAL
1	D	4634	GLU
1	D	4635	SER
1	D	4641	PRO
1	D	4647	SER
1	D	4651	THR
1	D	4658	ILE
1	D	4662	ASN
1	D	4665	LYS
1	D	4666	VAL
1	D	4676	GLU
1	D	4681	LEU
1	D	4684	ASP
1	D	4694	ASP
1	D	4695	ASP
1	D	4697	VAL
1	D	4707	ASN
1	D	4708	THR
1	D	4710	SER
1	D	4717	ASP
1	D	4720	VAL
1	D	4722	ARG
1	D	4725	LEU
1	D	4731	ILE
1	D	4734	ARG
1	D	4736	ARG
1	D	4737	ILE
1	D	4743	MET
1	D	4747	SER

Continued on next page...

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Mol	Chain	Res	Type
1	D	4772	ASP
1	D	4773	VAL
1	D	4813	LEU
1	D	4818	MET
1	D	4820	VAL
1	D	4821	LYS
1	D	4822	THR
1	D	4823	LEU
1	D	4829	SER
1	D	4839	MET
1	D	4844	LEU
1	D	4861	LYS
1	D	4866	SER
1	D	4871	GLU
1	D	4879	MET
1	D	4880	MET
1	D	4882	CYS
1	D	4889	VAL
1	D	4953	ASP
1	D	4957	LYS
1	D	4965	SER
1	D	4966	ASP
1	D	4980	LEU
1	D	4989	MET
1	D	4992	LEU
1	D	4997	ASN
1	D	4999	ASP
1	D	5000	GLU
1	D	5001	THR
1	D	5013	MET
1	D	5027	CYS
1	D	5034	ASP
1	D	5035	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	203	ASN
1	A	838	HIS
1	A	877	ASN
1	A	1463	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1563	GLN
1	A	1586	ASN
1	A	1590	GLN
1	A	2003	GLN
1	A	2877	GLN
1	A	2971	GLN
1	A	3378	GLN
1	A	3683	GLN
1	A	3895	HIS
1	A	4216	GLN
1	A	5035	GLN
1	B	23	GLN
1	B	203	ASN
1	B	838	HIS
1	B	877	ASN
1	B	1563	GLN
1	B	1586	ASN
1	B	1590	GLN
1	B	2003	GLN
1	B	2877	GLN
1	B	2971	GLN
1	B	3378	GLN
1	B	3683	GLN
1	B	3766	GLN
1	B	3895	HIS
1	B	4216	GLN
1	B	5035	GLN
1	C	23	GLN
1	C	203	ASN
1	C	838	HIS
1	C	877	ASN
1	C	1586	ASN
1	C	1590	GLN
1	C	2003	GLN
1	C	2877	GLN
1	C	2971	GLN
1	C	3378	GLN
1	C	3683	GLN
1	C	3766	GLN
1	C	3895	HIS
1	C	4216	GLN
1	C	5035	GLN

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Mol	Chain	Res	Type
1	D	23	GLN
1	D	203	ASN
1	D	838	HIS
1	D	877	ASN
1	D	1463	ASN
1	D	1563	GLN
1	D	1586	ASN
1	D	1590	GLN
1	D	2003	GLN
1	D	2877	GLN
1	D	2971	GLN
1	D	3378	GLN
1	D	3683	GLN
1	D	3895	HIS
1	D	4216	GLN
1	D	5035	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

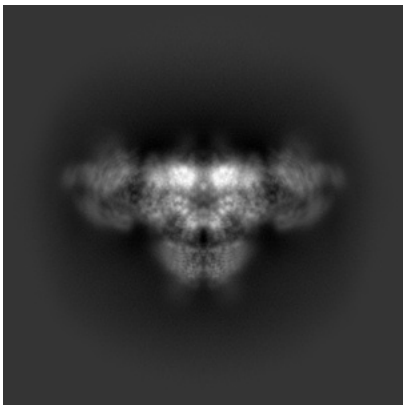
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-40422. These allow visual inspection of the internal detail of the map and identification of artifacts.

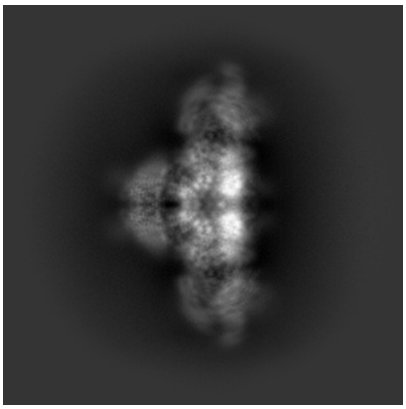
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

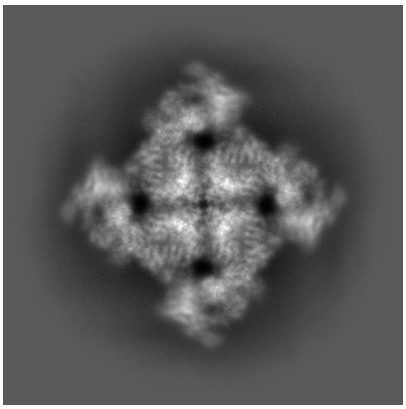
6.1.1 Primary map



X

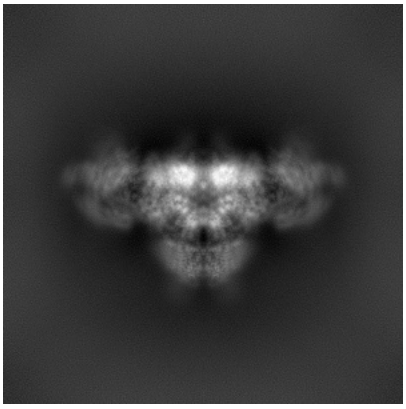


Y

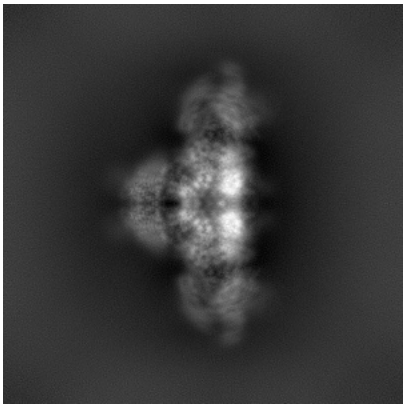


Z

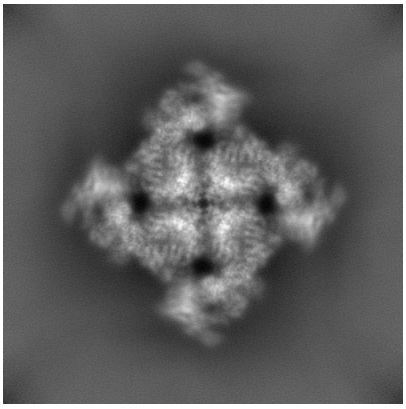
6.1.2 Raw map



X



Y

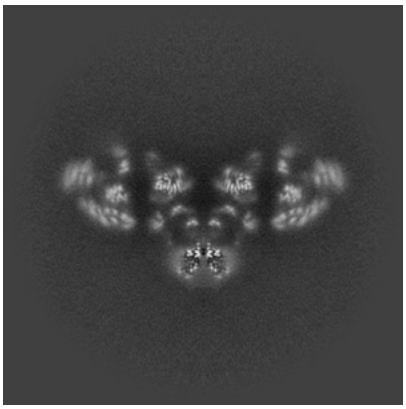


Z

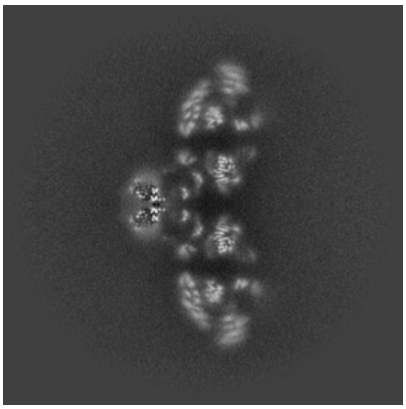
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

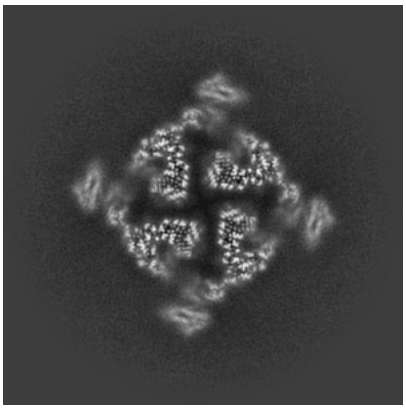
6.2.1 Primary map



X Index: 200

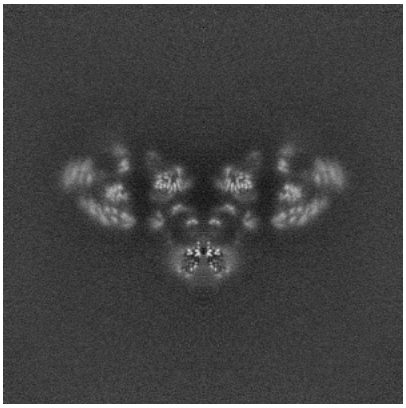


Y Index: 200

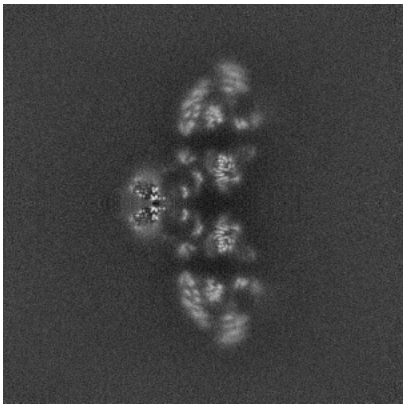


Z Index: 200

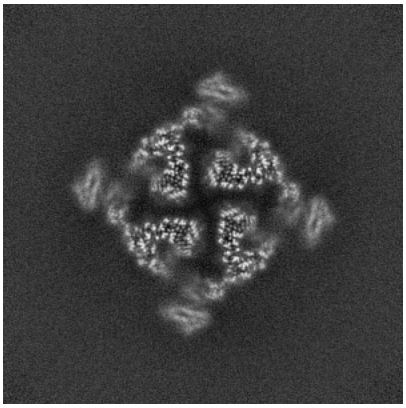
6.2.2 Raw map



X Index: 200



Y Index: 200

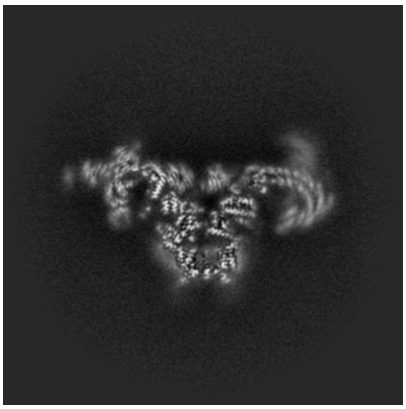


Z Index: 200

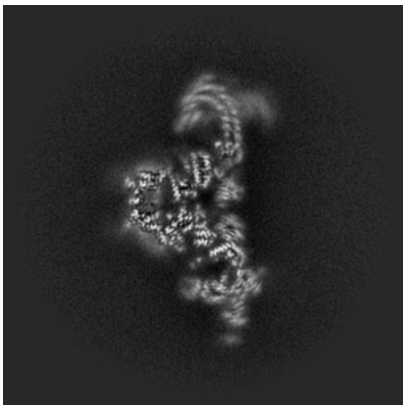
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

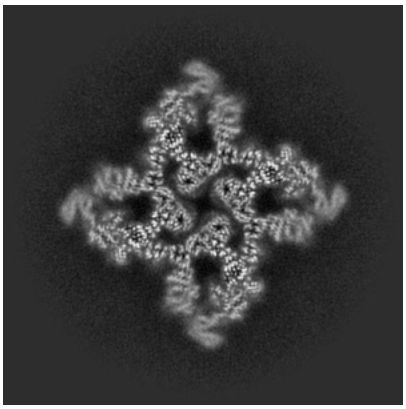
6.3.1 Primary map



X Index: 218

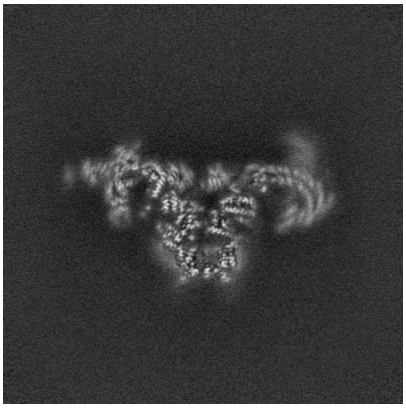


Y Index: 182

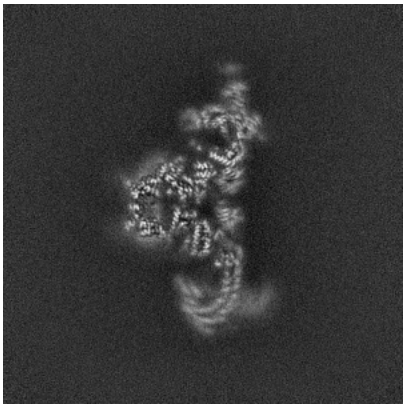


Z Index: 225

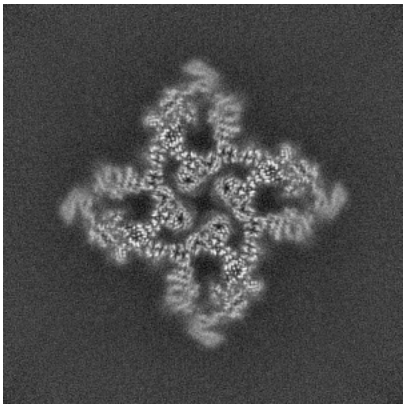
6.3.2 Raw map



X Index: 218



Y Index: 218



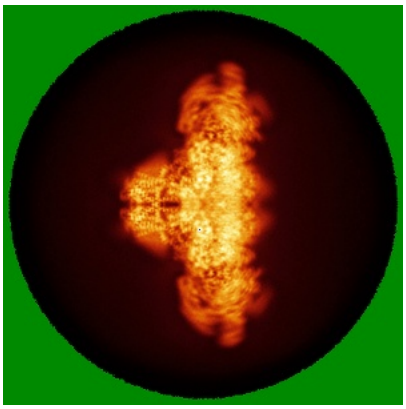
Z Index: 225

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

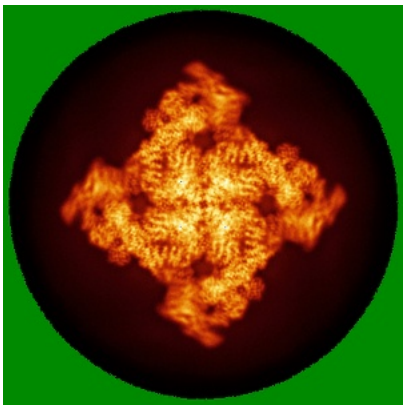
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map

X



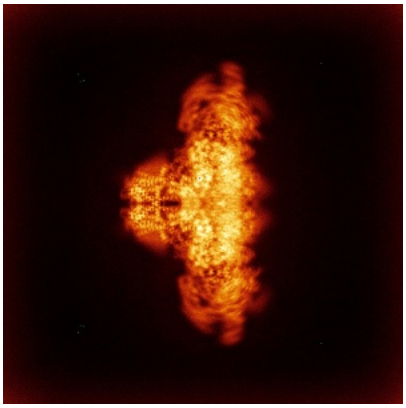
Y



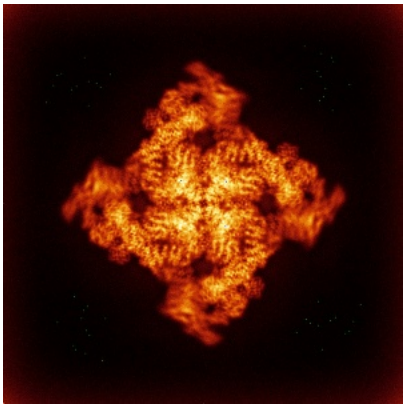
Z

6.4.2 Raw map

X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

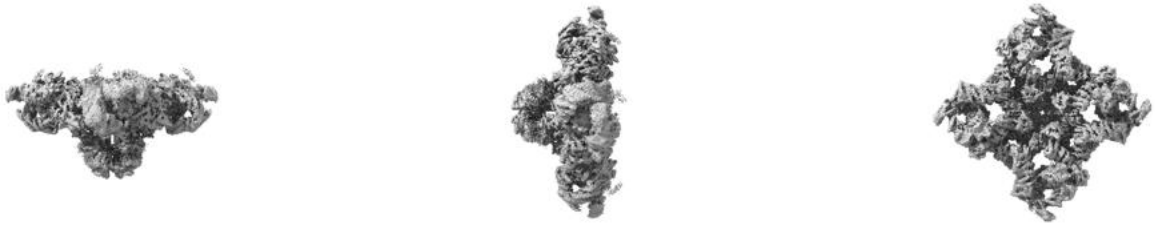
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.428. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

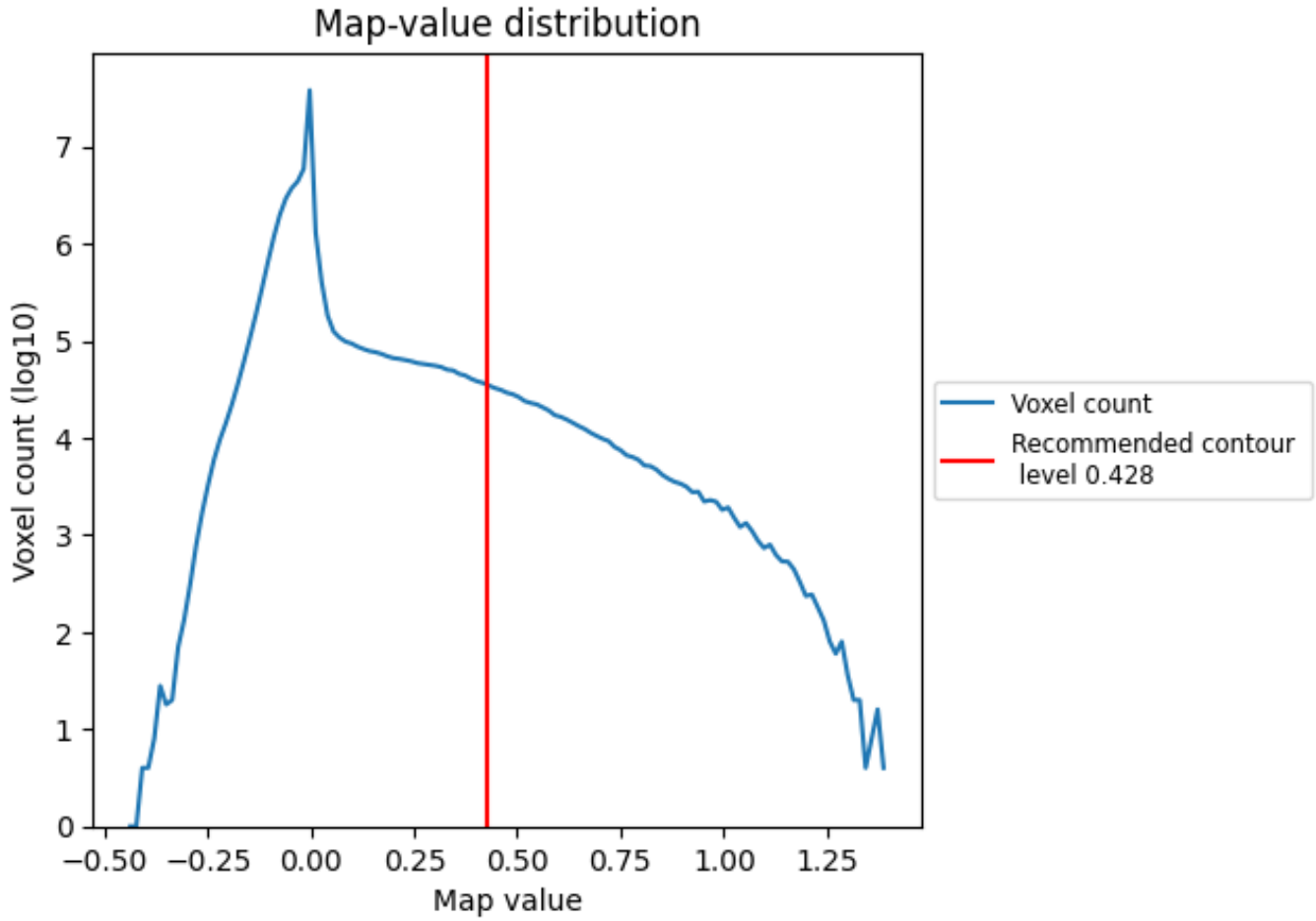
6.6 Mask visualisation (i)

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

7 Map analysis

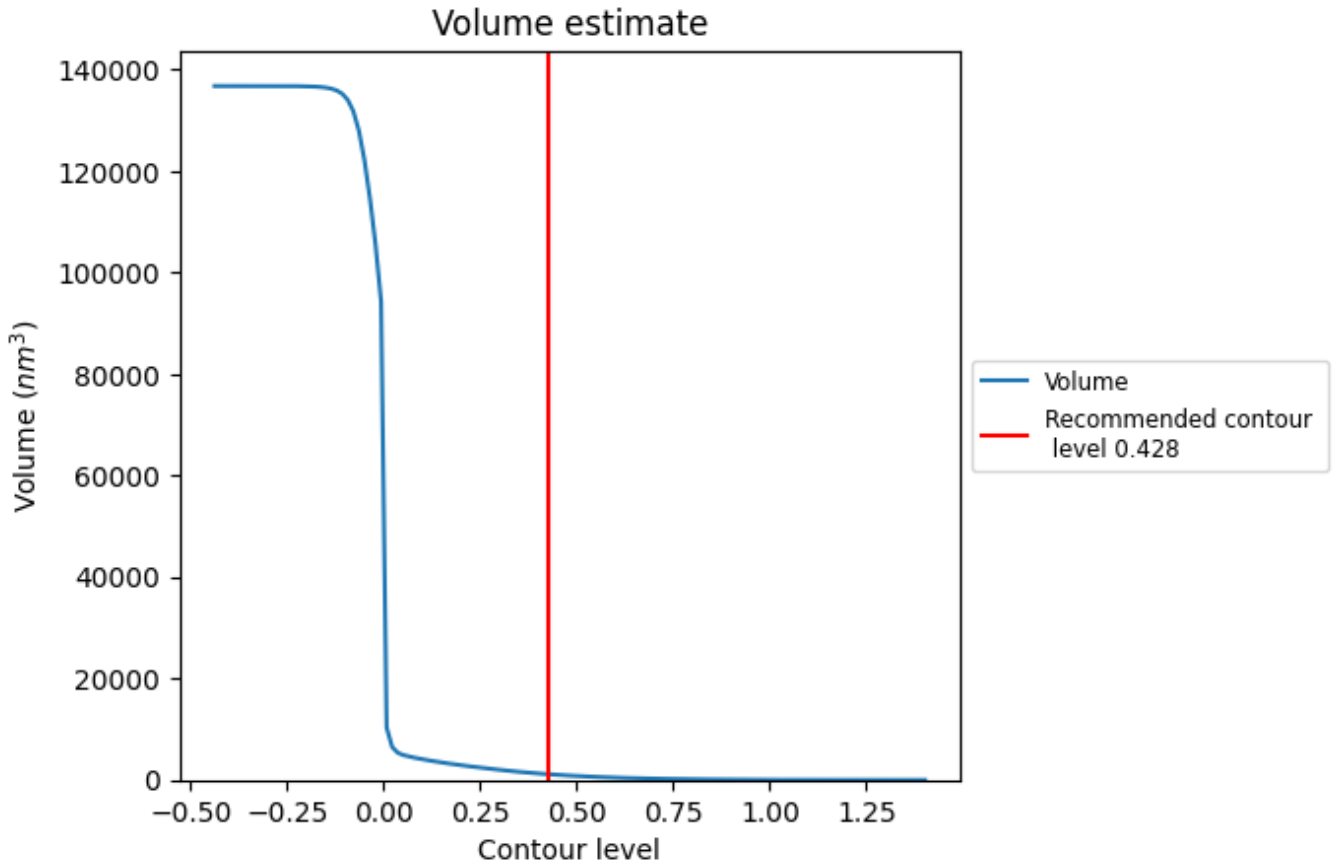
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

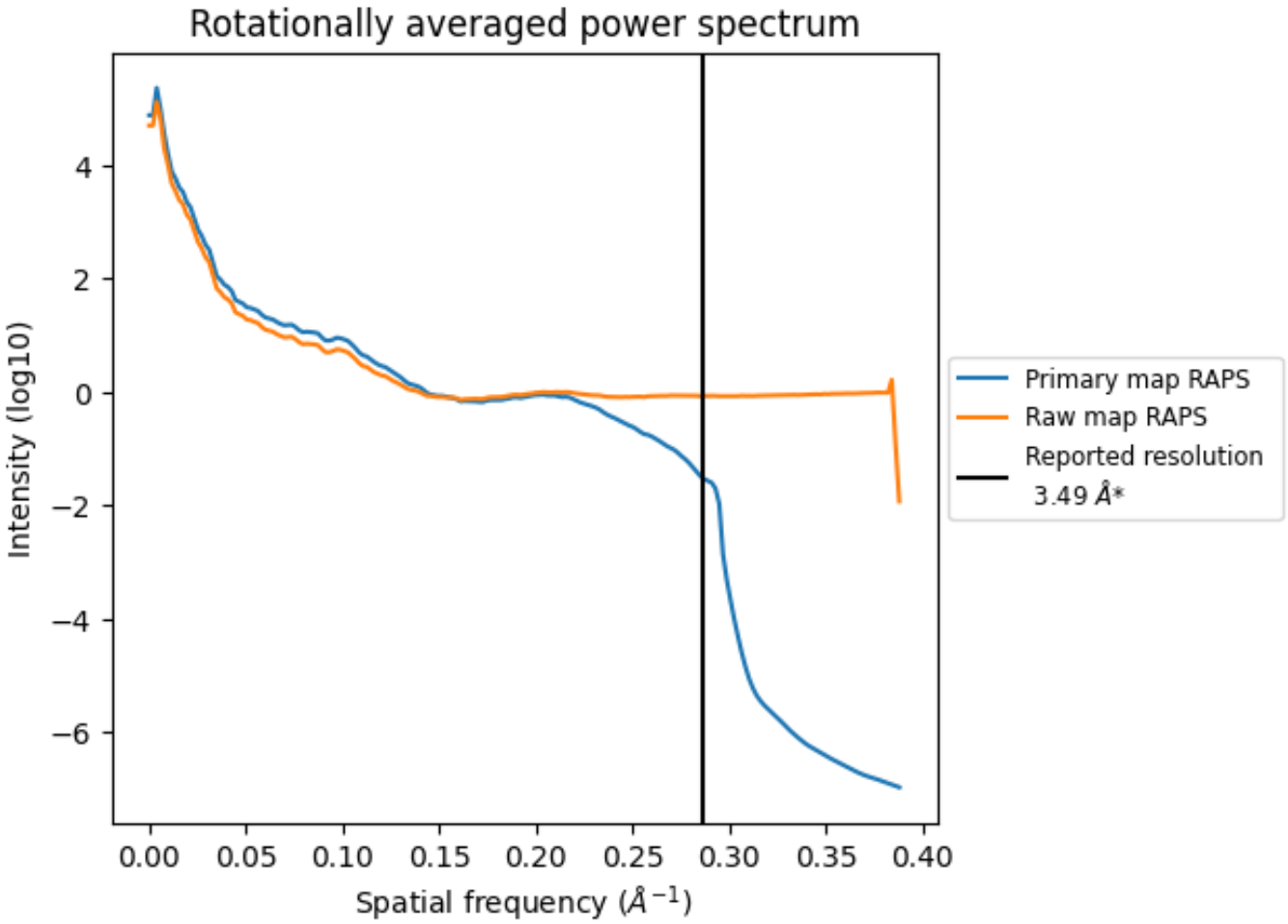
7.2 Volume estimate



The volume at the recommended contour level is 1121 nm^3; this corresponds to an approximate mass of 1013 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)

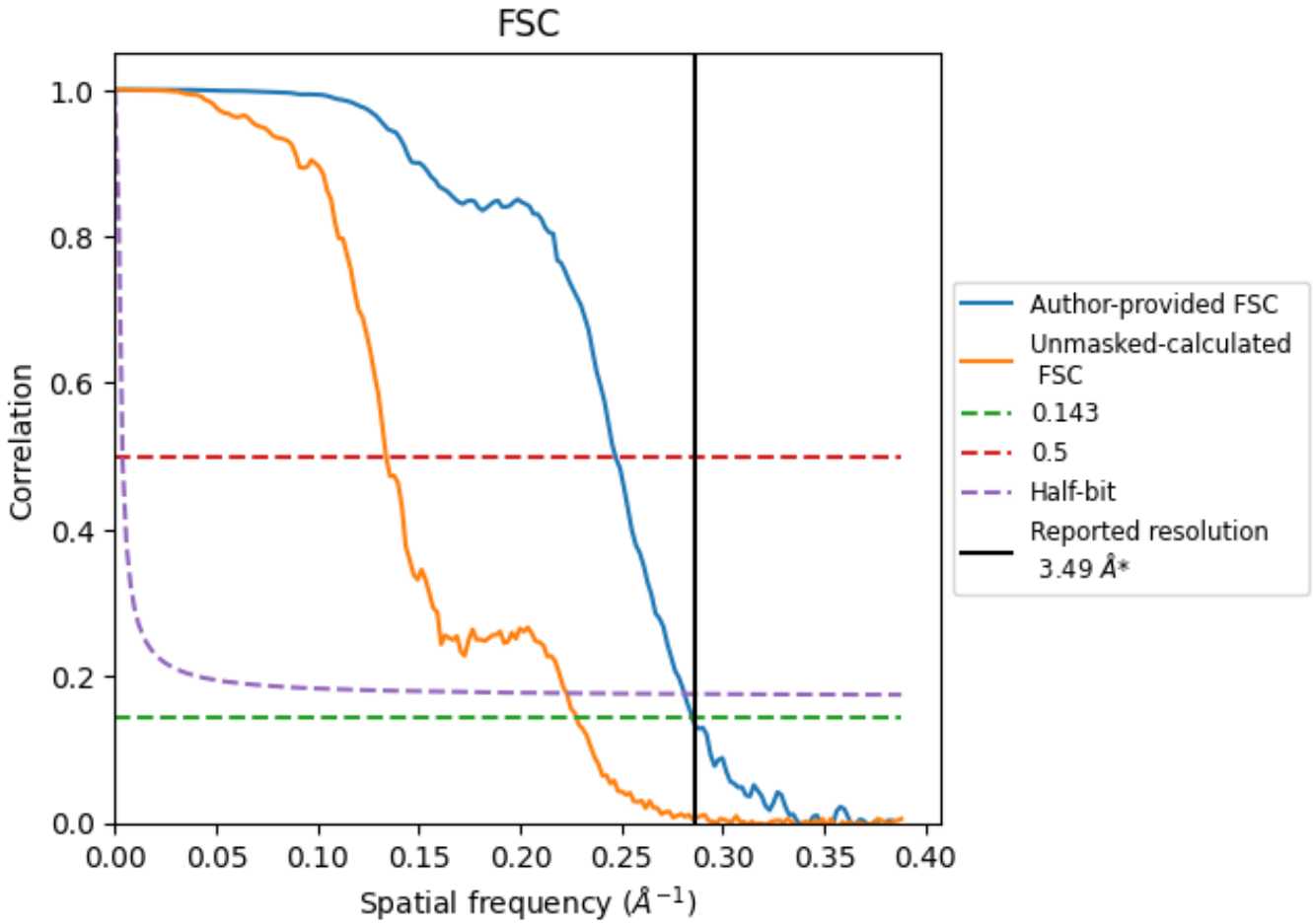


*Reported resolution corresponds to spatial frequency of 0.287 Å^{-1}

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 0.287 Å^{-1}

8.2 Resolution estimates (i)

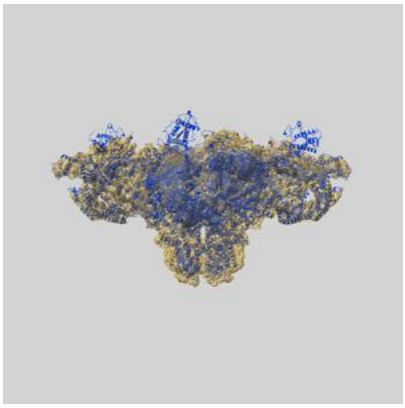
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.49	-	-
Author-provided FSC curve	3.51	4.05	3.56
Unmasked-calculated*	4.39	7.47	4.48

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.39 differs from the reported value 3.49 by more than 10 %

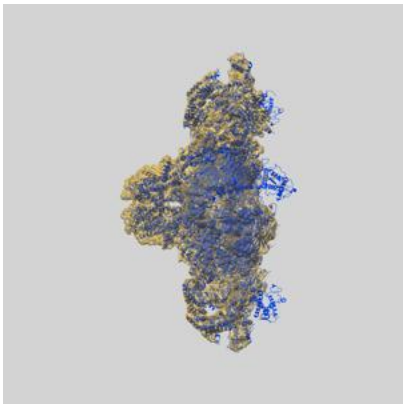
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-40422 and PDB model 8SEN. Per-residue inclusion information can be found in section 3 on page 7.

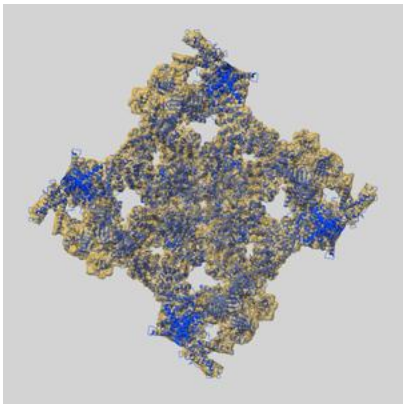
9.1 Map-model overlay



X



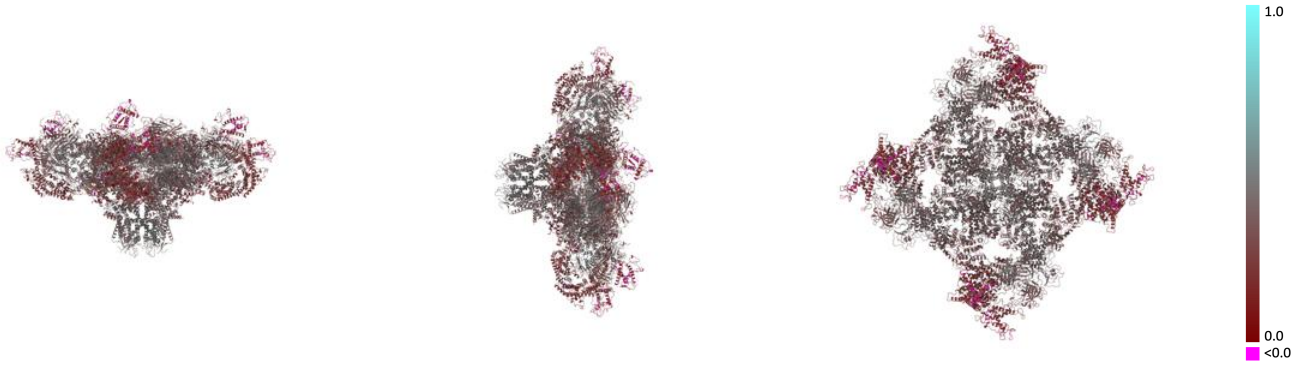
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.428 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.

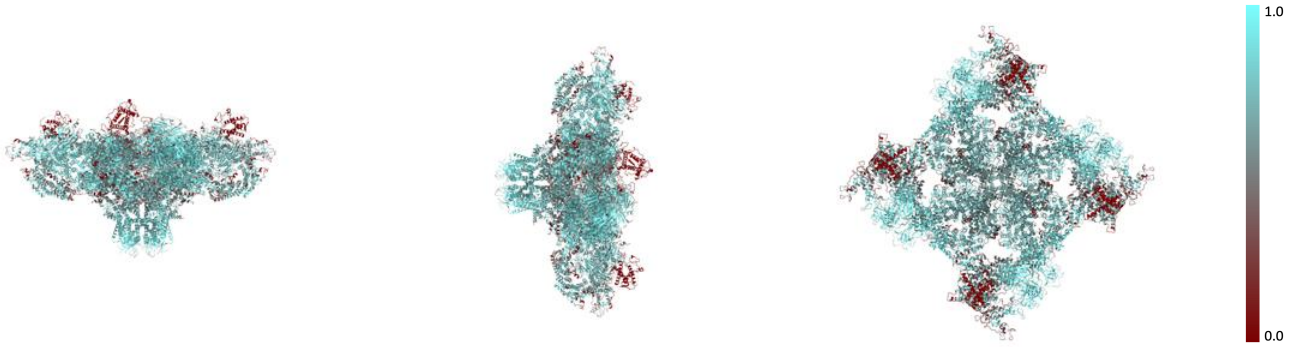
9.2 Q-score mapped to coordinate model (i)



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.

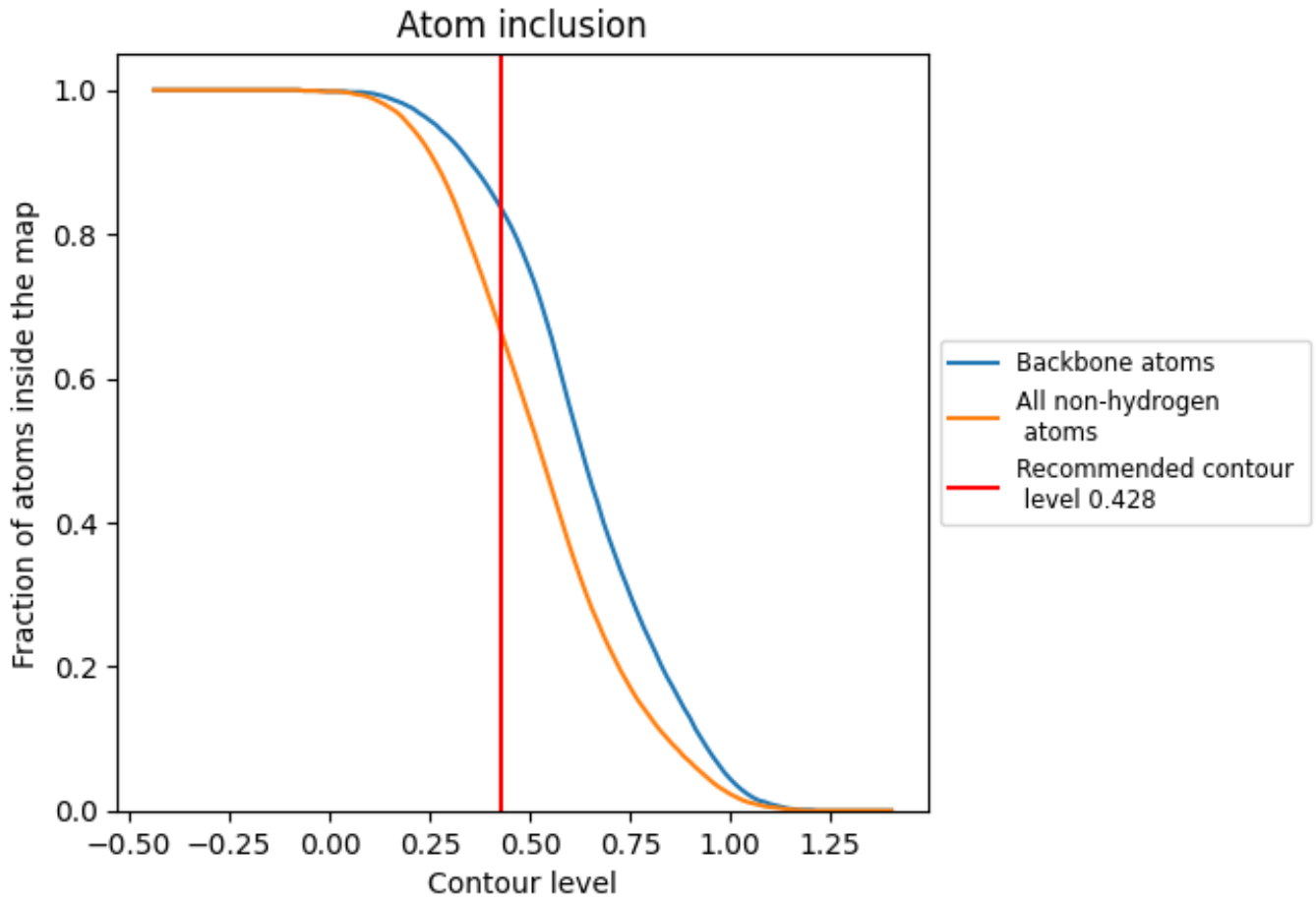
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.428).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 66% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.428) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6640	0.3380
A	0.6600	0.3370
B	0.6600	0.3360
C	0.6600	0.3360
D	0.6600	0.3370
E	0.8210	0.4140
F	0.8210	0.4130
G	0.8210	0.4130
H	0.8210	0.4160