Full wwPDB/EMDataBank EM Map/Model Validation Report (i)

Mar 2, 2017 – 12:38 pm GMT

PDB ID	:	5GKZ
EMDB ID:	:	EMD-9519
Title	:	Structure of RyR1 in a closed state (C3 conformer)
Authors	:	Bai, X.C.; Yan, Z.; Wu, J.P.; Yan, N.
Deposited on	:	2016-07-07
Resolution	:	4.00 Å(reported)

This is a Full wwPDB/EMDataBank EM Map/Model Validation Report for a publicly released PDB/EMDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

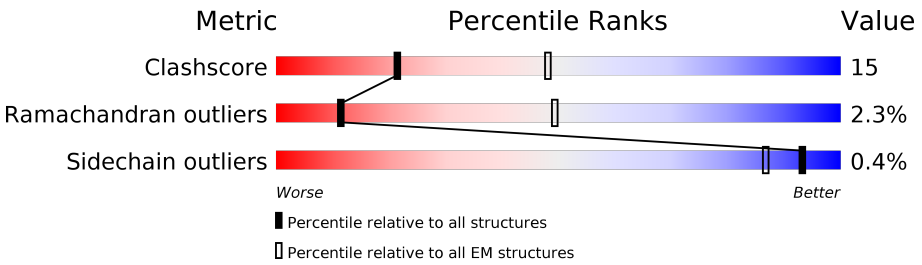
MolProbity	:	4.02b-467
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc29047

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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%

Mol	Chain	Length	Quality of chain
1	A	5037	49% 22% • 27%
1	C	5037	48% 23% • 27%
1	E	5037	48% 23% • 27%
1	G	5037	49% 22% • 27%
2	B	108	67% 32% •
2	D	108	65% 34% •
2	F	108	68% 31% •
2	H	108	69% 30% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 111000 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
			Total	C	N	O	S		
1	A	3660	26917	17107	4682	4971	157	0	0
1	C	3660	26917	17107	4682	4971	157	0	0
1	E	3660	26917	17107	4682	4971	157	0	0
1	G	3660	26917	17107	4682	4971	157	0	0

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	107	832	527	146	155	4	0	0
2	D	107	832	527	146	155	4	0	0
2	F	107	832	527	146	155	4	0	0
2	H	107	832	527	146	155	4	0	0

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

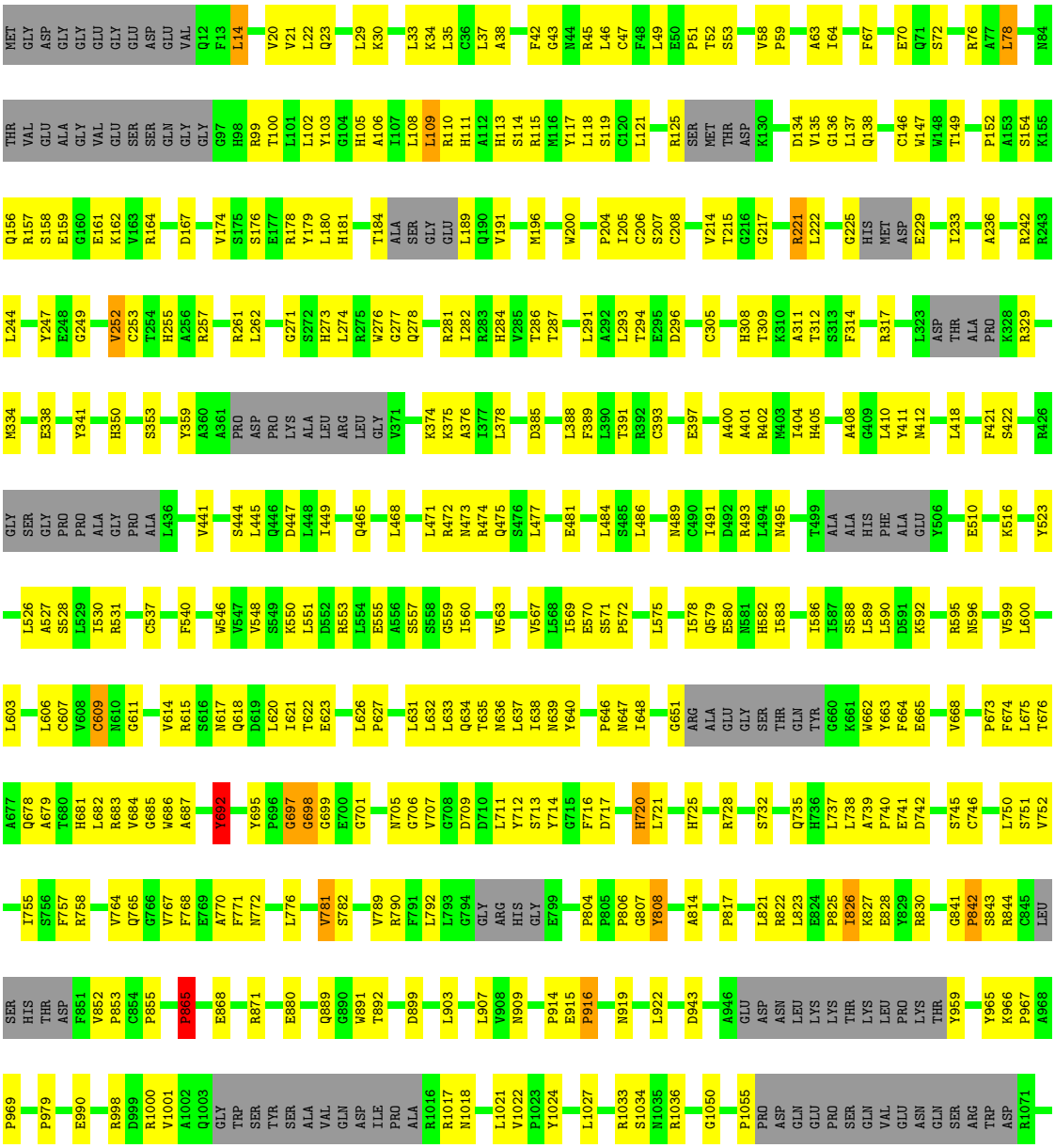
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
3	G	1	1	1	0
3	A	1	1	1	0
3	C	1	1	1	0
3	E	1	1	1	0

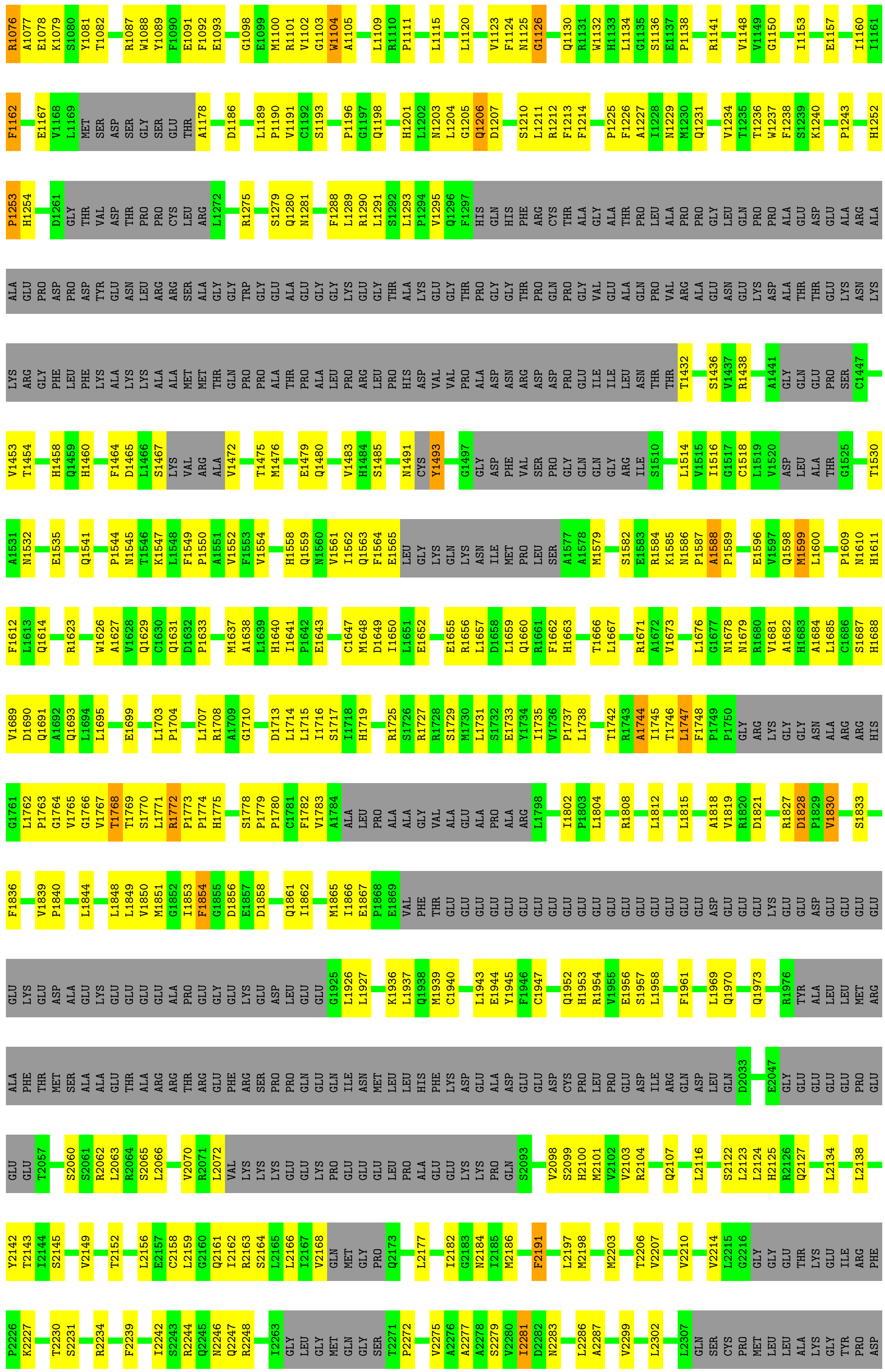
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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. 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. 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: 49% 22% • 27%

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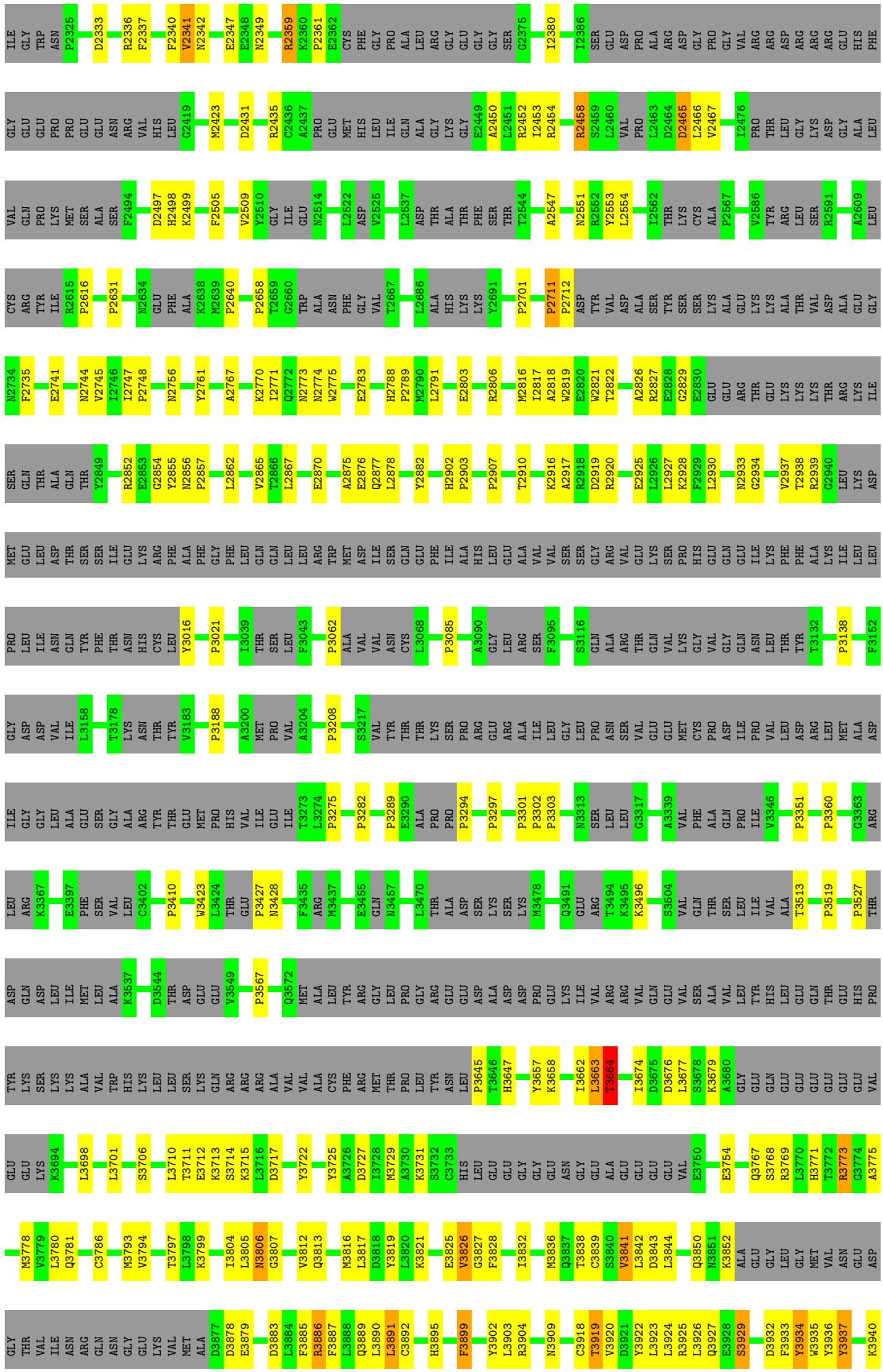
F1162 E1167 V1168 L1169 MET SER ASP SER GLY SER GLU THR A1178 D1186 L1189 P1190 V1191 C1192 S1193 P1196 G1197 Q1198 H1201 L1202 N1203 L1204 G1205 Q1206 D1207 S1210 L1211 R1212 F1213 F1214 P1225 F1226 A1227 I1228 N1229 M1230 Q1231 V1234 T1235 T1236 W1237 F1238 S1239 K1240 P1243 H1252
P1253 H1254 D1261 GLY THR VAL ASP THR PRO PRO CYS LEU ARG L1272 R1275 S1279 Q1280 N1281 F1288 L1289 R1290 L1291 S1292 L1293 P1294 V1295 Q1296 F1297 HIS GLN HIS PHE ARG CYS THR ALA GLY ALA THR PRO LEU ALA PRO PRO GLY LEU GLN PRO PRO ALA GLU ASP GLU ALA ARG ALA
ALA GLU PRO ASP PRO ASP TYR GLU ASN LEU ARG ARG SER ALA GLY GLY TRP GLY GLU ALA GLU GLY GLY LYS GLU GLY THR ALA LYS GLU GLY THR PRO GLY GLY THR PRO GLN PRO GLY VAL GLU ALA GLN PRO VAL ARG ALA GLU ASN GLU LYS ASP ALA THR THR GLU LYS ASN LYS
LYS ARG GLY PHE LEU PHE LYS ALA LYS LYS ALA ALA MET MET THR GLN PRO PRO ALA THR PRO ALA LEU PRO ARG LEU PRO HIS ASP VAL VAL PRO ALA ASP ASN ARG ASP ASP PRO GLU ILE ILE LEU ASN THR THR T1432 S1436 V1437 R1438 A1441 GLY GLN GLU PRO SER C1447
V1453 T1454 H1458 Q1459 H1460 F1464 D1465 L1466 S1467 LYS VAL ARG ALA V1472 T1475 M1476 E1479 Q1480 V1483 H1484 S1485 N1491 CYS Y1493 G1497 GLY ASP PHE VAL SER PRO GLY GLN GLN GLY ARG ILE S1510 L1514 V1515 I1516 G1517 C1518 L1519 V1520 ASP LEU ALA THR G1525 T1530
A1531 N1532 E1535 Q1541 P1544 N1545 T1546 K1547 L1548 F1549 P1550 A1551 V1552 F1553 V1554 H1558 Q1559 N1560 V1561 I1562 Q1563 F1564 E1565 LEU GLY LYS GLN LYS ASN ILE MET PRO LEU SER A1577 A1578 M1579 S1582 E1583 R1584 K1585 N1586 P1587 A1588 P1589 E1596 V1597 Q1598 M1599 L1600 P1609 N1610 H1611
F1612 L1613 Q1614 R1623 W1626 A1627 V1628 Q1629 C1630 Q1631 D1632 P1633 M1637 A1638 L1639 H1640 I1641 P1642 E1643 C1647 M1648 D1649 I1650 L1651 E1652 E1655 R1656 L1657 D1658 L1659 Q1660 R1661 F1662 H1663 T1666 L1667 R1671 A1672 V1673 L1676 G1677 N1678 N1679 R1680 V1681 A1682 H1683 A1684 L1685 C1686 S1687 H1688
V1689 D1690 Q1691 A1692 Q1693 L1694 L1695 E1699 L1703 P1704 L1707 R1708 A1709 G1710 D1713 L1714 L1715 I1716 S1717 I1718 H1719 R1725 S1726 R1727 R1728 S1729 M1730 L1731 S1732 E1733 Y1734 I1735 V1736 P1737 L1738 T1742 R1743 A1744 I1745 T1746 L1747 F1748 P1749 P1750 GLY ARG LYS GLY GLY ASN ALA ARG ARG HIS
G1761 L1762 P1763 G1764 V1765 G1766 V1767 T1768 T1769 S1770 L1771 R1772 P1773 P1774 H1775 S1778 P1779 P1780 C1781 F1782 V1783 A1784 ALA LEU PRO ALA ALA GLY VAL ALA GLU ALA PRO ALA ARG L1798 I1802 P1803 L1804 R1808 L1812 L1815 A1818 V1819 R1820 D1821 R1827 D1828 P1829 V1830 S1833
F1836 V1839 P1840 L1844 L1848 L1849 V1850 M1851 G1852 I1853 F1854 G1855 D1856 E1857 D1858 Q1861 I1862 M1865 I1866 E1867 P1868 E1869 VAL PHE THR GLU GLU GLU 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 LYS GLU ASP ALA GLU LYS GLU GLU GLU GLU ALA PRO GLU GLY GLU LYS GLU ASP LEU GLU GLU G1925 L1926 L1927 K1936 L1937 Q1938 M1939 C1940 L1943 E1944 Y1945 F1946 C1947 Q1952 H1953 R1954 V1955 E1956 S1957 L1958 F1961 L1969 Q1970 Q1973 R1976 TYR ALA LEU LEU MET ARG
ALA PHE THR MET SER ALA ALA GLU THR ALA ARG ARG THR ARG GLU PHE ARG SER PRO PRO GLN GLU GLN ILE ASN MET LEU LEU HIS PHE LYS ASP GLU ALA ASP GLU GLU ASP CYS PRO LEU PRO GLU ASP ILE ARG GLN ASP LEU GLN D2033 E2047 GLY GLU GLU GLU GLU PRO GLU
GLU GLU T2057 S2060 S2061 R2062 L2063 R2064 S2065 L2066 V2070 R2071 L2072 VAL LYS LYS LYS GLU GLU LYS PRO GLU GLU GLU LEU PRO ALA GLU GLU LYS LYS PRO GLN S2093 V2098 S2099 H2100 M2101 V2102 V2103 R2104 Q2107 L2116 S2122 L2123 L2124 H2125 R2126 Q2127 L2134 L2138
Y2142 T2143 I2144 S2145 V2149 T2152 L2156 E2157 C2158 L2159 G2160 Q2161 I2162 R2163 S2164 L2165 L2166 I2167 V2168 GLN MET GLY PRO Q2173 L2177 I2182 G2183 N2184 I2185 M2186 F2191 L2197 M2198 M2203 T2206 V2207 V2210 V2214 L2215 G2216 GLY GLY GLU THR LYS GLU ILE ARG PHE
P2226 K2227 T2230 S2231 R2234 F2239 I2242 S2243 R2244 Q2245 N2246 Q2247 R2248 I2263 GLY LEU GLY MET GLN GLY SER T2271 P2272 V2275 A2276 A2277 A2278 S2279 V2280 I2281 D2282 N2283 L2286 A2287 V2299 L2302 L2307 GLN SER CYS PRO MET LEU LEU ALA LYS GLY TYR PRO ASP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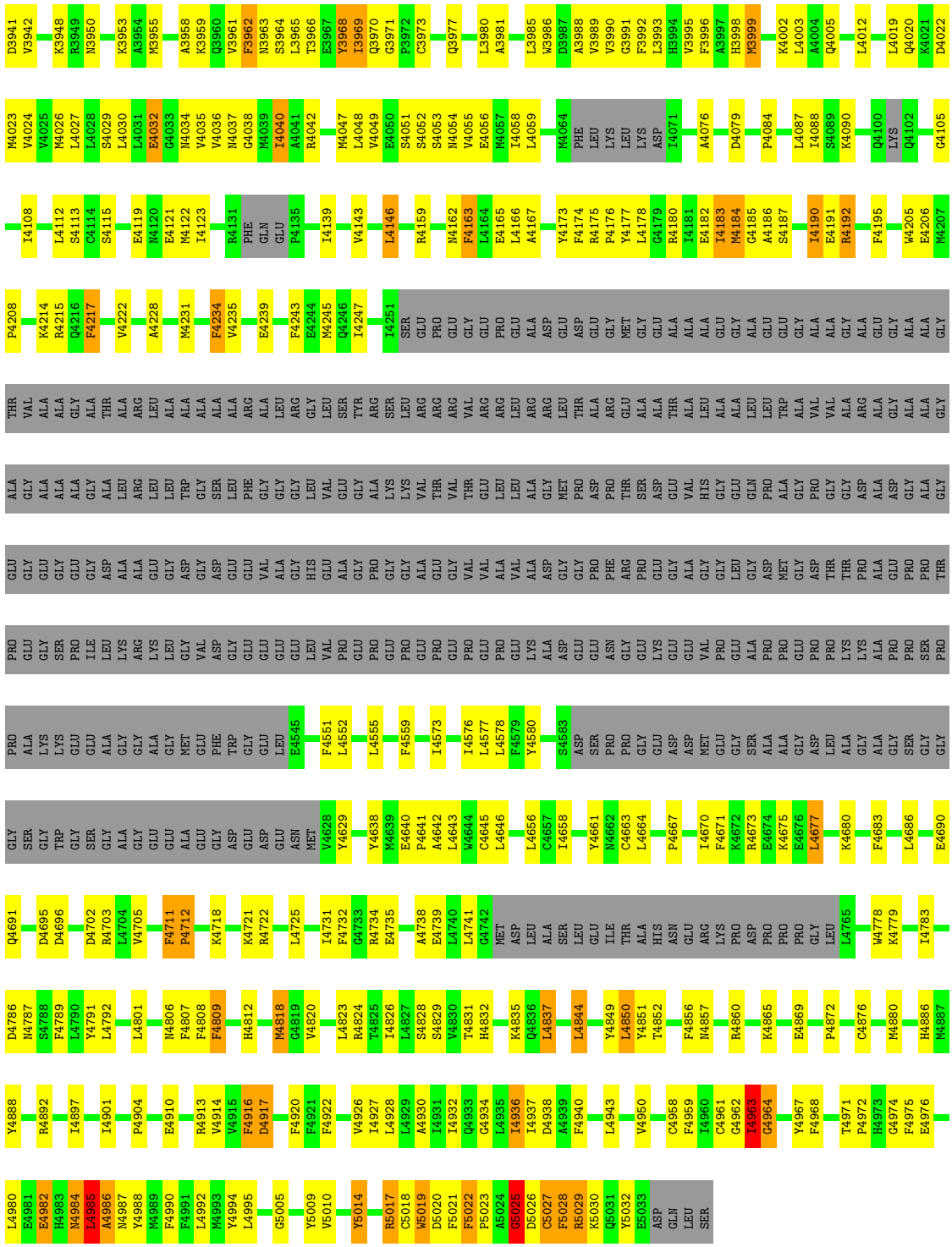
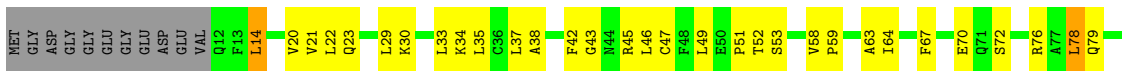
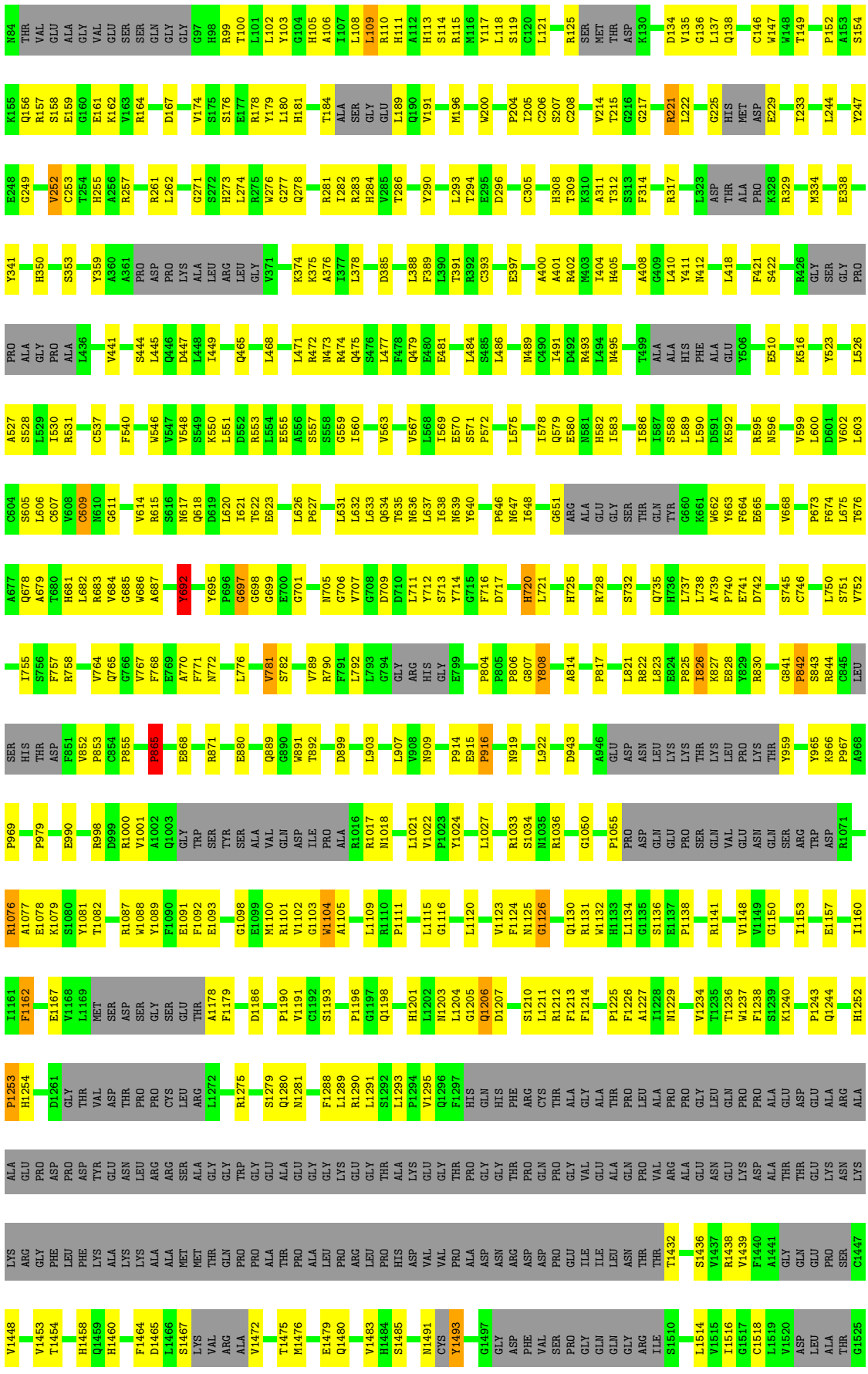
GLU GLU LYS K3694 L3698 L3701 S3706 L3710 T3711 E3712 K3713 S3714 K3715 L3716 D3717 Y3722 Y3725 A3726 D3727 I3728 M3729 A3730 K3731 S3732 C3733
TYR LYS SER LYS LYS ALA VAL TRP HIS LYS LEU LEU SER LYS GLN ARG ARG ARG ALA VAL VAL ALA LEU CYS PHE ARG MET THR PRO LEU TYR ASN LEU P3645 T3646 H3647 Y3657 K3658 I3662 L3663 T3664 I3674 D3675 D3676 L3677 S3678 K3679 A3680
ASP GLN ASP LEU ILE MET LEU ALA K3537 D3544 THR ASP GLU GLU V3549 P3567 Q3572 MET ALA LEU TYR ARG GLY LEU PRO GLY ARG GLU GLU ASP ALA ASP ASP PRO GLU LYS ILE VAL ARG ARG VAL GLN GLU GLU VAL LEU TYR HIS LEU GLU GLU THR GLU HIS PRO
LEU ARG K3367 E3397 PHE SER VAL LEU C3402 P3410 W3423 L3424 THR GLU P3427 N3428 F3435 ARG M3437 E3455 GLN N3457 L3470 THR ALA ASP SER LYS SER LYS M3478 Q3491 GLU ARG T3494 K3495 K3496 S3504 VAL GLN THR SER LEU ILE VAL ALA T3513 P3519 P3527 THR
ILE GLY GLY LEU ALA GLU SER GLY ALA ARG TYR THR GLU MET PRO HIS VAL ILE GLU ILE T3273 L3274 P3275 P3282 P3289 E3290 ALA PRO PRO P3294 P3297 P3301 P3302 P3303 N3313 SER LEU LEU G3317 A3339 VAL PHE ALA GLN PRO ILE V3346 P3351 P3360 G3363 ARG
GLY ASP ASP VAL ILE L3158 T3178 LYS ASN THR TYR V3183 P3188 A3200 MET PRO VAL A3204 P3208 S3217 VAL VAL TYR THR THR LYS SER PRO ARG GLU ARG ALA ILE LEU GLY LEU PRO ASN SER VAL GLU GLU MET CYS PRO ASP ILE PRO VAL LEU LEU ASP ARG LEU MET ALA ASP
PRO LEU ILE ASN GLN TYR PHE THR ASN HIS CYS LEU Y3016 P3021 I3039 THR SER LEU F3043 P3062 ALA VAL VAL ASN CYS L3068 P3085 A3090 GLY LEU ARG SER F3095 S3116 GLN ALA ARG THR GLN VAL LYS GLY VAL GLY GLN GLN ASN LEU THR TYR T3132 P3138 F3152
MET GLU LEU ASP THR SER SER ILE GLU LYS ARG PHE ALA PHE GLY PHE LEU GLN GLN LEU LEU ARG TRP MET ASP ILE SER GLN GLU PHE ILE ALA HIS LEU GLU ALA VAL VAL SER SER GLY ARG VAL GLU LYS SER PRO HIS GLU GLN GLU ILE LYS PHE PHE ALA LYS ILE LEU LEU
SER GLN THR ALA GLN THR Y2849 R2852 E2853 G2854 Y2855 N2856 P2857 L2862 V2865 T2866 L2867 E2870 A2875 E2876 Q2877 L2878 Y2882 H2902 P2903 P2907 T2910 K2916 A2917 R2918 D2919 R2920 E2925 L2926 L2927 K2928 F2929 L2930 N2933 G2934 V2937 T2938 R2939 G2940 LEU LYS ASP
N2734 F2735 E2741 N2744 V2745 I2746 I2747 P2748 N2756 Y2761 A2767 K2770 I2771 Q2772 N2773 N2774 W2775 E2783 H2788 P2789 M2790 L2791 E2803 R2806 M2816 I2817 A2818 W2819 E2820 W2821 T2822 A2826 R2827 E2828 G2829 E2830 GLU GLU ARG THR GLU LYS LYS LYS THR ARG LYS ILE
CYS ARG TYR ILE R2615 P2616 P2631 N2634 GLU PHE ALA K2638 M2639 P2640 P2658 T2659 G2660 TRP ALA ASN PHE GLY VAL T2667 L2686 ALA HIS LYS LYS Y2691 P2701 P2711 P2712 ASP TYR VAL ASP ALA SER TYR SER SER LYS ALA GLU LYS LYS ALA THR VAL ASP ALA GLU GLY
VAL GLN PRO LYS MET SER ALA SER F2494 D2497 H2498 K2499 F2505 V2509 Y2510 GLY ILE GLU N2514 L2522 ASP V2525 L2537 ASP THR ALA THR PHE SER THR T2544 A2547 N2551 R2552 Y2553 L2554 I2562 THR LYS CYS ALA P2567 V2586 TYR ARG LEU SER R2591 A2609 LEU
GLY GLU GLU PRO PRO GLU GLU ASN ARG VAL HIS LEU G2419 M2423 D2431 R2435 C2436 A2437 PRU GLU MET HIS LEU ILE GLN ALA GLY LYS GLY E2449 A2450 L2451 R2452 I2453 R2454 R2458 S2459 L2460 VAL PRO L2463 D2464 D2465 L2466 V2467 I2476 PRO THR LEU GLY LYS ASP GLY ALA LEU
ILE GLY TRP ASN P2325 D2333 R2336 F2337 F2340 V2341 N2342 E2347 E2348 N2349 R2359 K2360 P2361 E2362 CYS PHE GLY PRO ALA ARG ASP GLY PRO GLY VAL ARG ASP ARG ARG ARG GLU HIS PHE



- Molecule 1: Ryanodine receptor 1

Chain C:

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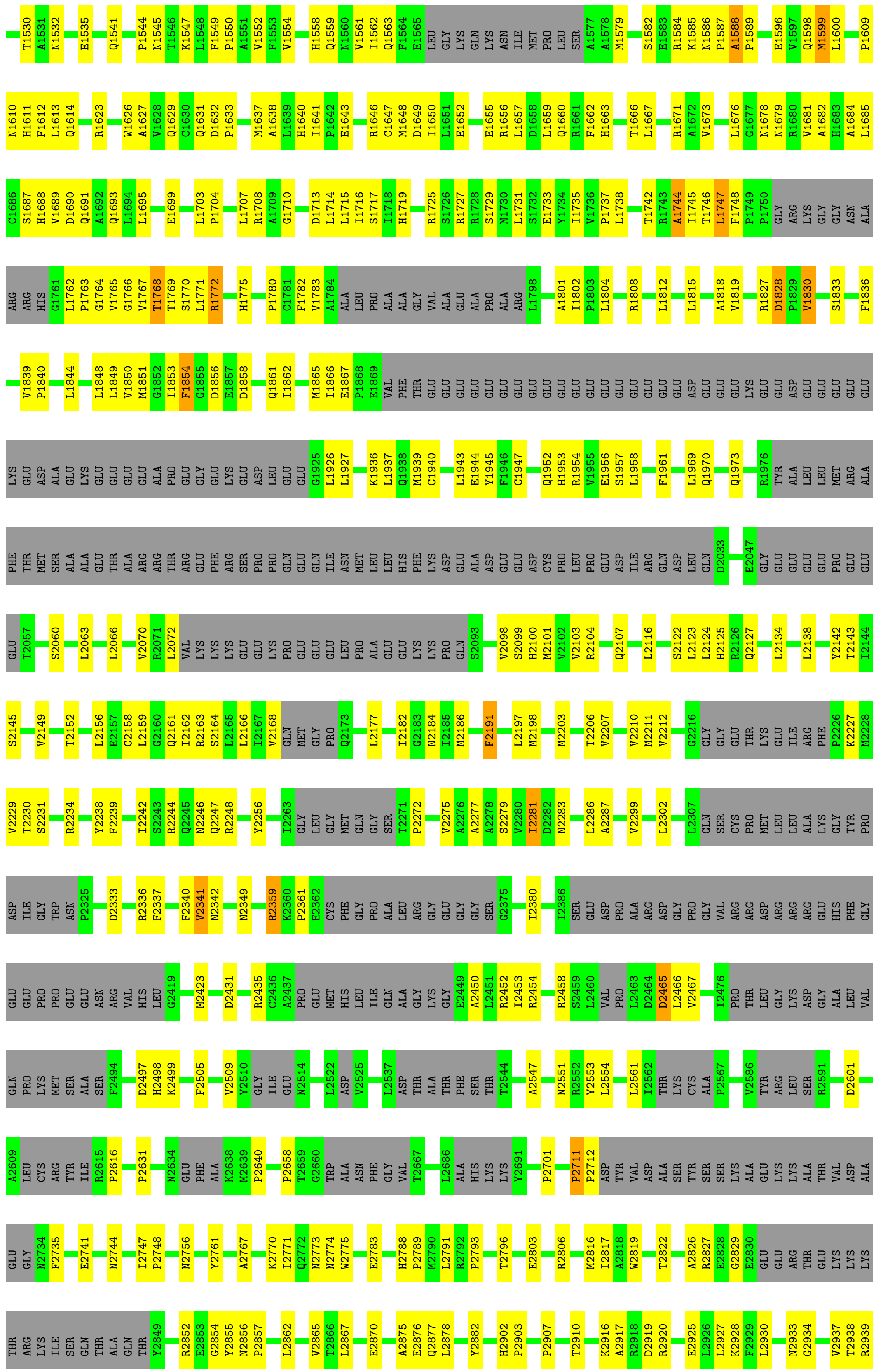
K155 Q156 R157 S158 E159 G160 E161 K162 V163 R164 D167 V174 S175 S176 E177 R178 Y179 L180 H181 T184 ALA SER GLY GLU L189 Q190 V191 M196 W200 P204 I205 C206 S207 C208 V214 T215 G216 G217 R221 L222 G225 HIS MET ASP E229 I233 L244 Y247
E248 G249 V252 C253 T254 H255 A256 R257 R261 L262 G271 S272 H273 L274 R275 W276 G277 Q278 R281 I282 R283 H284 V285 T286 Y290 L293 T294 E295 D296 C305 H308 T309 K310 A311 T312 S313 F314 R317 L323 ASP THR ALA PRO K328 R329 M334 E338
Y341 H350 S353 Y359 A360 A361 PRO ASP PRO LYS ALA LEU ARG LEU GLY V371 K374 K375 A376 I377 L378 D385 L388 F389 L390 T391 R392 C393 E397 A400 A401 R402 M403 I404 H405 A408 G409 L410 Y411 N412 L418 F421 S422 R426 GLY SER GLY PRO
PRO ALA GLY PRO ALA L436 V441 S444 L445 Q446 D447 L448 I449 Q465 L468 L471 R472 N473 R474 Q475 S476 L477 F478 Q479 E480 E481 L484 S485 L486 N489 C490 I491 D492 R493 L494 N495 T499 ALA ALA HIS PHE ALA GLU Y506 E510 K516 Y523 L526
A527 S528 L529 I530 R531 C537 F540 W546 V547 V548 S549 K550 L551 D552 R553 L554 E555 A556 S557 S558 C559 I560 V563 V567 L568 I569 E570 S571 P572 L575 I578 Q579 E580 N581 H582 I583 I586 I587 S588 L589 L590 D591 K592 R595 N596 V599 L600 D601 V602 L603
C604 S605 L606 C607 V608 C609 N610 G611 V614 R615 S616 N617 Q618 D619 L620 I621 T622 E623 L626 P627 L631 L632 L633 Q634 T635 N636 L637 I638 N639 Y640 P646 N647 I648 G651 ARG ALA GLU GLY SER THR GLN TYR G660 K661 W662 Y663 F664 E665 V668 P673 F674 L675 T676
A677 Q678 A679 T680 H681 L682 R683 V684 G685 W686 A687 Y692 Y695 P696 G697 G698 G699 E700 G701 N705 G706 V707 G708 D709 D710 L711 Y712 S713 Y714 G715 F716 D717 H720 L721 H725 R728 S732 Q735 H736 L737 L738 A739 P740 E741 D742 S745 C746 L750 S751 V752
I755 S756 F757 R758 V764 Q765 G766 V767 F768 E769 A770 F771 N772 L776 V781 S782 V789 R790 F791 L792 L793 G794 GLY ARG HIS GLY E799 P804 P805 P806 G807 Y808 A814 P817 L821 R822 L823 E824 P825 I826 K827 E828 Y829 R830 G841 P842 S843 R844 C845 LEU
SER HIS THR ASP F851 V852 P853 C854 P855 P865 E868 R871 E880 Q889 G890 W891 T892 D899 L903 L907 V908 N909 P914 E915 P916 N919 L922 D943 A946 GLU ASP ASN LEU LYS LYS THR LYS LEU PRO LYS THR Y959 Y965 K966 P967 A968
P969 P979 E990 R998 D999 R1000 V1001 A1002 Q1003 GLY TRP SER TYR SER ALA VAL GLN ASP ILE PRO ALA R1016 R1017 N1018 L1021 V1022 P1023 Y1024 L1027 R1033 S1034 N1035 R1036 G1050 P1055 PRO ASP GLN GLU PRO SER GLN VAL GLU ASN GLN SER ARG TRP ASP R1071
R1076 A1077 E1078 K1079 S1080 Y1081 T1082 R1087 W1088 Y1089 F1090 E1091 F1092 E1093 G1098 E1099 M1100 R1101 V1102 G1103 W1104 A1105 L1109 R1110 P1111 L1115 G1116 L1120 V1123 F1124 N1125 G1126 Q1130 R1131 W1132 H1133 L1134 G1135 S1136 E1137 P1138 R1141 V1148 V1149 G1150 I1153 E1157 I1160
I1161 F1162 E1167 V1168 L1169 MET SER ASP SER GLY SER GLU THR A1178 F1179 D1186 P1190 V1191 C1192 S1193 P1196 G1197 Q1198 H1201 L1202 N1203 L1204 G1205 Q1206 D1207 S1210 L1211 R1212 F1213 F1214 P1225 F1226 A1227 I1228 N1229 V1234 T1235 T1236 W1237 F1238 S1239 K1240 P1243 Q1244 H1252
P1253 H1254 D1261 GLY THR VAL ASP THR PRO PRO CYS LEU ARG L1272 R1275 S1279 Q1280 N1281 F1288 L1289 R1290 L1291 S1292 L1293 P1294 V1295 Q1296 F1297 HIS GLN HIS PHE ARG CYS THR 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 ALA THR 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 MET MET THR GLN PRO PRO ALA THR PRO ALA LEU PRO ARG LEU PRO HIS ASP VAL VAL PRO ALA ASP ARG ASP PRO GLU ILE ILE LEU ASN THR THR T1432 S1436 V1437 R1438 V1439 F1440 A1441 GLY GLN GLU PRO SER C1447
V1448 V1453 T1454 H1458 Q1459 H1460 F1464 D1465 L1466 S1467 LYS VAL ARG ALA V1472 T1475 M1476 E1479 Q1480 V1483 H1484 S1485 N1491 CYS Y1493 G1497 GLY ASP PHE VAL SER PRO GLY GLN GLN GLY ARG ILE S1510 L1514 V1515 I1516 G1517 C1518 L1519 V1520 ASP LEU ALA THR G1525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ARG ARG HIS G1761 L1762 P1763 G1764 V1765 G1766 V1767 T1768 T1769 S1770 L1771 R1772 H1775 P1780 C1781 F1782 V1783 A1784 ALA LEU PRO ALA ALA GLY VAL ALA GLU ALA PRO ALA ARG L1798 A1801 I1802 P1803 L1804 R1808 L1812 L1815 A1818 V1819 R1827 D1828 P1829 V1830 S1833 F1836
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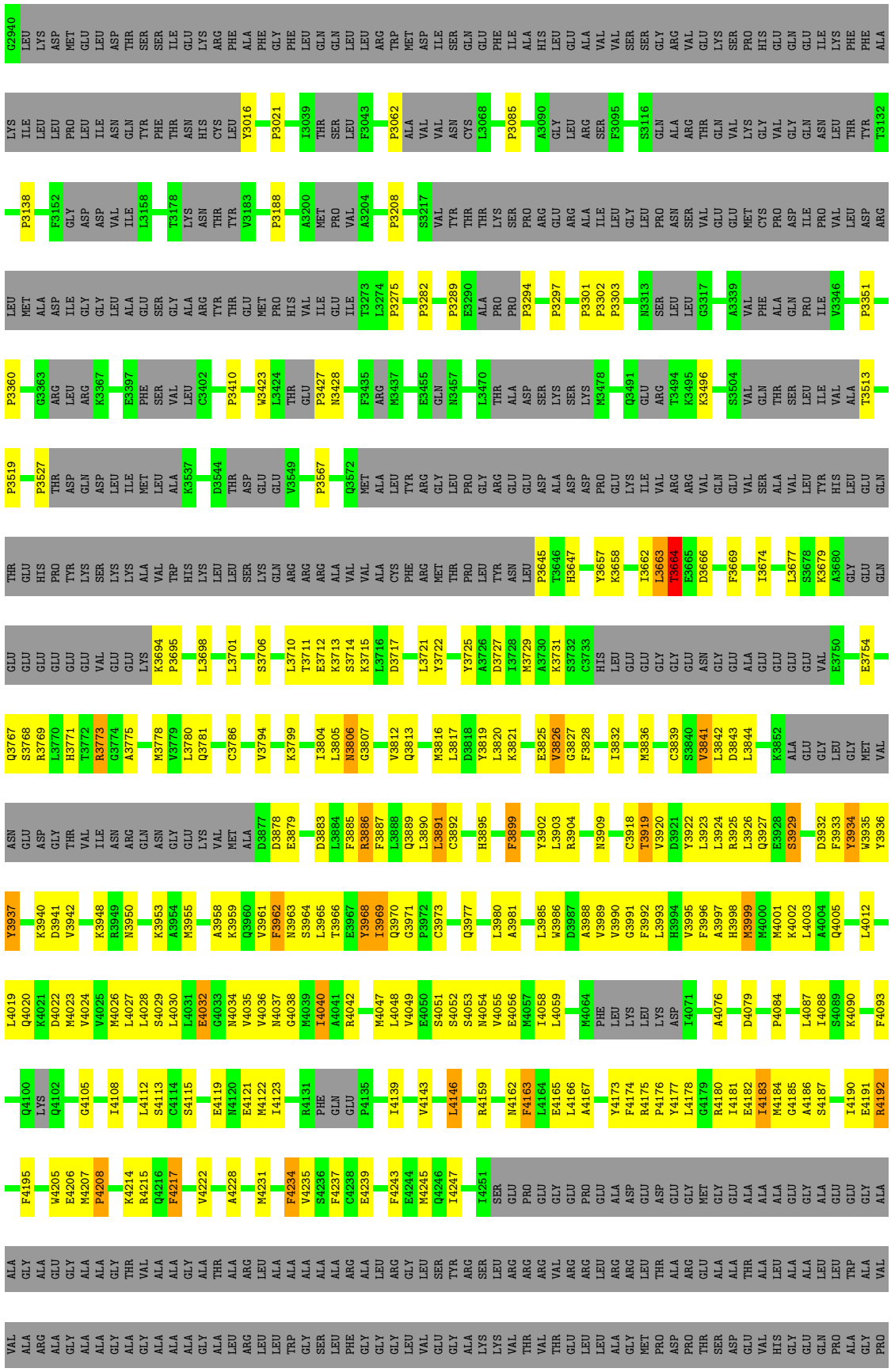
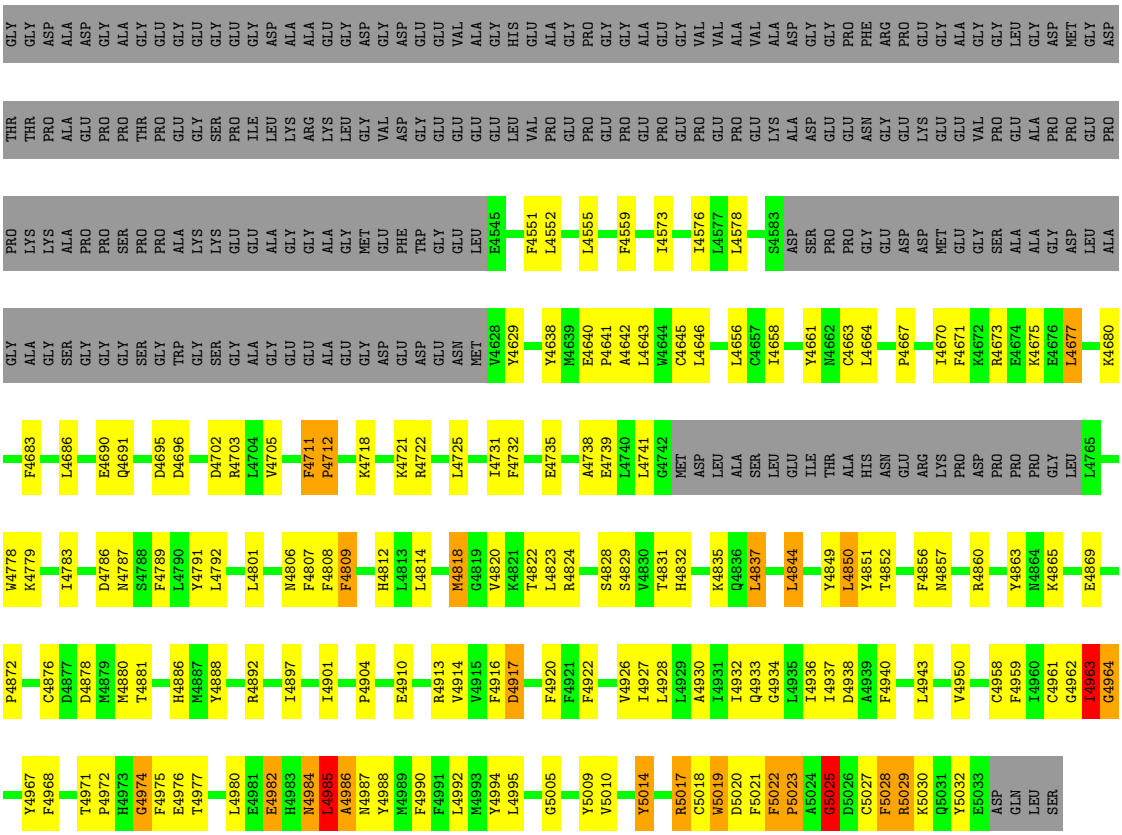
LYS GLU ASP ALA GLU LYS GLU GLU GLU GLU ALA PRO GLU GLY GLU LYS GLU ASP LEU GLU GLU G1925 L1926 L1927 K1936 L1937 Q1938 M1939 C1940 L1943 E1944 Y1945 F1946 C1947 Q1952 H1953 R1954 V1955 E1956 S1957 L1958 F1961 L1969 Q1970 Q1973 R1976 TYR ALA LEU LEU MET ARG ALA
PHE THR MET SER ALA ALA GLU THR ALA ARG ARG THR ARG GLU PHE ARG SER PRO PRO GLN GLU GLN ILE ASN MET LEU LEU HIS PHE LYS ASP GLU ALA ASP GLU GLU ASP CYS PRO LEU PRO GLU ASP ILE ARG GLN ASP LEU GLN D2033 E2047 GLY GLU GLU GLU GLU PRO GLU GLU
GLU T2057 S2060 L2063 L2066 V2070 R2071 L2072 VAL LYS LYS LYS GLU GLU LYS PRO GLU GLU GLU LEU PRO ALA GLU GLU LYS LYS PRO GLN S2093 V2098 S2099 H2100 M2101 V2102 V2103 R2104 Q2107 L2116 S2122 L2123 L2124 H2125 R2126 Q2127 L2134 L2138 Y2142 T2143 I2144
S2145 V2149 T2152 L2156 E2157 C2158 L2159 G2160 Q2161 I2162 R2163 S2164 L2165 L2166 I2167 V2168 GLN MET GLY PRO Q2173 L2177 I2182 G2183 N2184 I2185 M2186 F2191 L2197 M2198 M2203 T2206 V2207 V2210 M2211 V2212 G2216 GLY GLY GLU THR LYS GLU ILE ARG PHE P2226 K2227 M2228
V2229 T2230 S2231 R2234 Y2238 F2239 I2242 S2243 R2244 Q2245 N2246 Q2247 R2248 Y2256 I2263 GLY LEU GLY MET GLN GLY SER T2271 P2272 V2275 A2276 A2277 A2278 S2279 V2280 I2281 D2282 N2283 L2286 A2287 V2299 L2302 L2307 GLN SER CYS PRO MET LEU LEU ALA LYS GLY TYR PRO
ASP ILE GLY TRP ASN P2325 D2333 R2336 F2337 F2340 V2341 N2342 N2349 R2359 K2360 P2361 E2362 CYS PHE GLY PRO ALA LEU ARG GLY GLU GLY GLY SER G2375 I2380 I2386 SER GLU ASP PRO ALA ARG ASP GLY PRO GLY VAL ARG ARG ASP ARG ARG ARG GLU HIS PHE GLY
GLU GLU PRO PRO GLU GLU ASN ARG VAL HIS LEU G2419 M2423 D2431 R2435 C2436 A2437 PRO GLU MET HIS LEU ILE GLN ALA GLY LYS GLY E2449 A2450 L2451 R2452 I2453 R2454 R2458 S2459 L2460 VAL PRO L2463 D2464 D2465 L2466 V2467 I2476 PRO THR LEU GLY LYS ASP GLY ALA LEU VAL
GLN PRO LYS MET SER ALA SER F2494 D2497 H2498 K2499 F2505 V2509 Y2510 GLY ILE GLU N2514 L2522 ASP V2525 L2537 ASP THR ALA THR PHE SER THR T2544 A2547 N2551 R2552 Y2553 L2554 L2561 I2562 THR LYS CYS ALA P2567 V2586 TYR ARG LEU SER R2591 D2601
A2609 LEU CYS ARG TYR ILE R2615 P2616 P2631 N2634 GLU PHE ALA K2638 M2639 P2640 P2658 T2659 G2660 TRP ALA ASN PHE GLY VAL T2667 L2686 ALA HIS LYS LYS Y2691 P2701 P2711 P2712 ASP TYR VAL ASP ALA SER TYR SER SER LYS ALA GLU LYS LYS ALA THR VAL ASP ALA
GLU GLY N2734 F2735 E2741 N2744 I2747 P2748 N2756 Y2761 A2767 K2770 I2771 Q2772 N2773 N2774 W2775 E2783 H2788 P2789 M2790 L2791 R2792 P2793 T2796 E2803 R2806 M2816 I2817 A2818 W2819 T2822 A2826 R2827 E2828 G2829 E2830 GLU GLU ARG THR GLU LYS LYS LYS
THR ARG LYS ILE SER GLN THR ALA GLN THR Y2849 R2852 E2853 G2854 Y2855 N2856 P2857 L2862 V2865 T2866 L2867 E2870 A2875 E2876 Q2877 L2878 Y2882 H2902 P2903 P2907 T2910 K2916 A2917 R2918 D2919 R2920 E2925 L2926 L2927 K2928 F2929 L2930 N2933 G2934 V2937 T2938 R2939

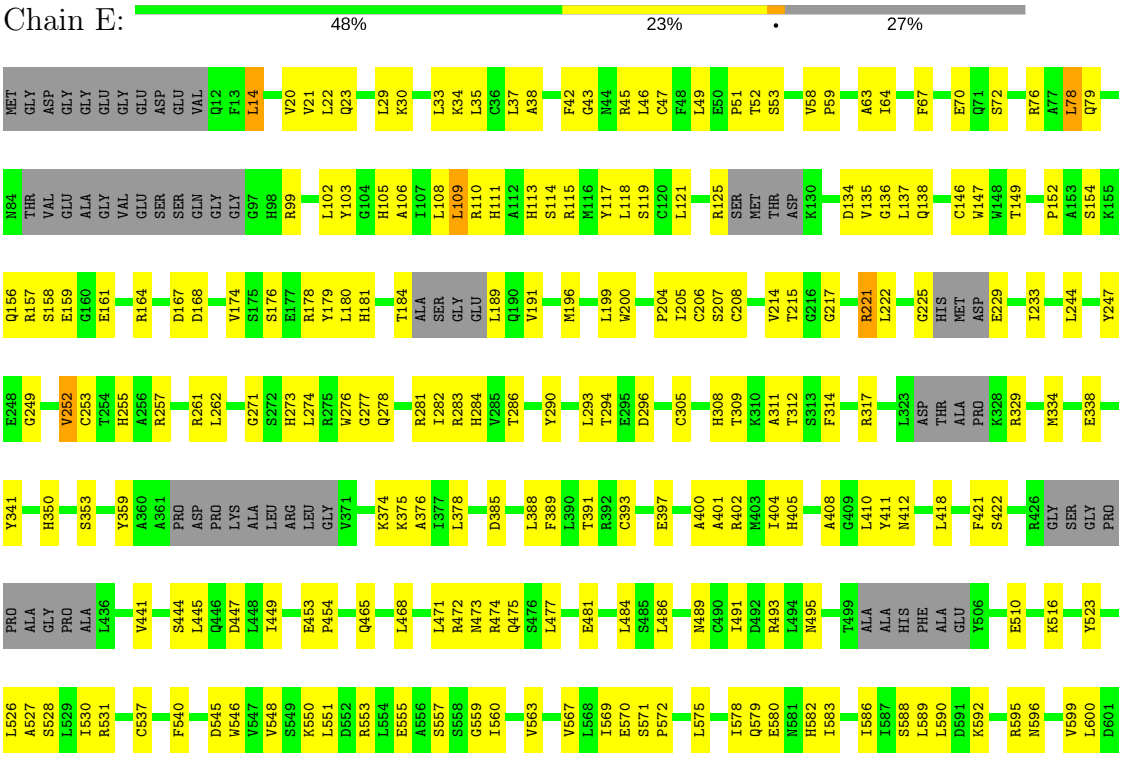


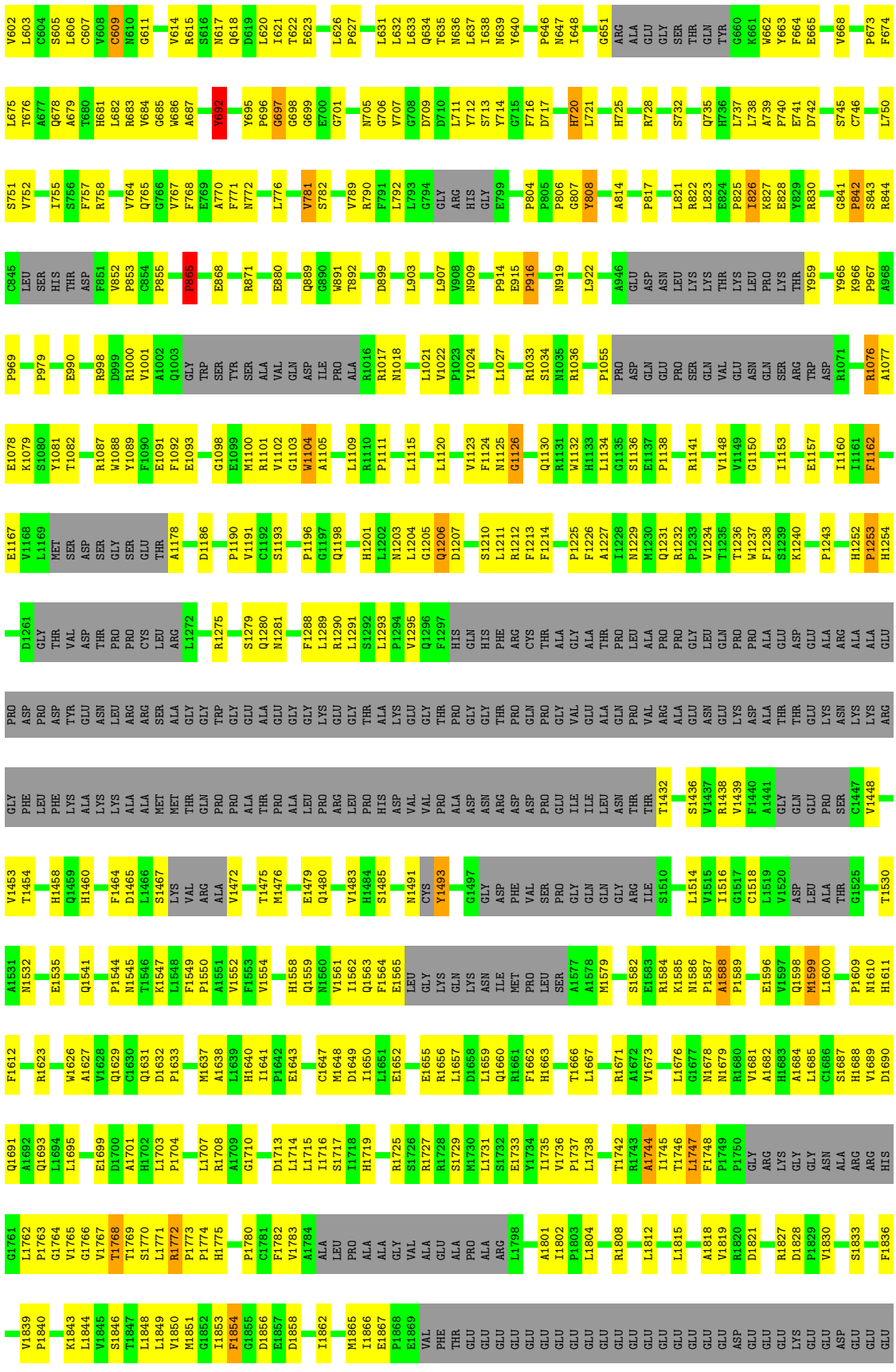
WORLDWIDE PDB PROTEIN DATA BANK
EMDataBank Unified Data Resource for 3DEM



• Molecule 1: Ryanodine receptor 1

Chain E:

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L675 T676 A677 Q678 A679 T680 H681 L682 R683 V684 G685 W686 A687 Y692 Y695 P696 G697 G698 G699 E700 G701 N705 G706 V707 G708 D709 D710 L711 Y712 S713 Y714 G715 F716 D717 H720 L721 H725 R728 S732 Q735 H736 L737 L738 A739 P740 E741 D742 S745 C746 L750
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P969 P979 E990 R998 D999 R1000 V1001 A1002 Q1003 GLY TRP SER TYR SER ALA VAL GLN ASP ILE PRO ALA R1016 R1017 N1018 L1021 V1022 P1023 Y1024 L1027 R1033 S1034 N1035 R1036 P1055 PRO ASP GLN GLU PRO SER GLN VAL GLU ASN GLN SER ARG TRP ASP R1071 R1076 A1077
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E1167 V1168 L1169 MET SER ASP SER GLY SER GLU THR A1178 D1186 P1190 V1191 G1192 S1193 P1196 G1197 Q1198 H1201 L1202 N1203 L1204 G1205 Q1206 D1207 S1210 L1211 R1212 F1213 F1214 P1225 F1226 A1227 I1228 N1229 M1230 Q1231 R1232 P1233 V1234 T1235 T1236 W1237 F1238 S1239 K1240 P1243 H1252 P1253 H1254
D1261 GLY THR VAL ASP THR PRO PRO CYS LEU ARG L1272 R1275 S1279 Q1280 N1281 F1288 L1289 R1290 L1291 S1292 L1293 P1294 V1295 Q1296 F1297 HIS GLN HIS PHE ARG CYS THR ALA GLY ALA THR PRO LEU ALA PRO PRO GLY LEU GLN PRO PRO ALA ARG 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 GLY THR PRO ASP PRO GLN PRO GLY VAL GLU ALA GLN PRO VAL ARG ALA GLU ASN GLU LYS ASP ALA ALA THR THR LYS LYS ARG
GLY PHE LEU PHE LYS ALA LYS LYS ALA ALA MET MET THR GLN PRO PRO ALA THR PRO ALA LEU PRO ARG LEU PRO HIS ASP VAL VAL PRO ALA ASP ASN ARG ASP PRO GLU ILE ILE LEU ASN THR THR T1432 S1436 V1437 R1438 V1439 F1440 A1441 GLY GLN GLU PRO SER C1447 V1448
V1453 T1454 H1458 Q1459 H1460 F1464 D1465 L1466 S1467 LYS VAL ARG ALA V1472 T1475 M1476 E1479 Q1480 V1483 H1484 S1485 N1491 CYS Y1493 G1497 GLY ASP PHE VAL SER PRO GLY GLN GLN GLY ARG ILE S1510 L1514 V1515 I1516 G1517 C1518 L1519 V1520 ASP LEU ALA THR C1525 T1530
A1531 N1532 E1535 Q1541 P1544 N1545 T1546 K1547 L1548 F1549 P1550 A1551 V1552 F1553 V1554 H1558 Q1559 N1560 V1561 I1562 Q1563 F1564 E1565 LEU GLY LYS GLN LYS ASN ILE MET PRO LEU SER A1577 A1578 M1579 S1582 E1583 R1584 K1585 N1586 P1587 A1588 P1589 E1596 V1597 Q1598 M1599 L1600 P1609 N1610 H1611
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G1761 L1762 P1763 G1764 V1765 G1766 V1767 T1768 T1769 S1770 L1771 R1772 P1773 P1774 H1775 P1780 C1781 F1782 V1783 A1784 ALA LEU PRO ALA ALA GLY VAL ALA GLU ALA PRO ALA ARG L1798 A1801 I1802 P1803 L1804 R1808 L1812 L1815 A1818 V1819 R1820 D1821 R1827 D1828 P1829 V1830 S1833 F1836
V1839 P1840 K1843 L1844 V1845 S1846 T1847 L1848 L1849 V1850 M1851 G1852 I1853 F1854 G1855 D1856 E1857 D1858 I1862 M1865 I1866 E1867 P1868 E1869 VAL PHE THR GLU GLU GLU

GLU GLU LYS GLU ASP ALA GLU LYS GLU GLU GLU ALA PRO GLU GLY GLU LYS GLU ASP LEU GLU GLU G1925 L1926 L1927 K1936 L1937 Q1938 M1939 C1940 L1943 E1944 Y1945 F1946 C1947 Q1952 H1953 R1954 V1955 E1956 S1957 L1958 F1961 L1969 Q1970 Q1973 R1976 TYR ALA LEU LEU MET
ARG ALA PHE THR MET SER ALA ALA GLU THR ALA ARG ARG THR ARG GLU PHE ARG SER PRO PRO GLN GLU GLU GLN ILE ASN MET LEU LEU HIS PHE LYS ASP GLU ALA ASP GLU GLU ASP CYS PRO LEU PRO GLU ASP ILE ARG GLN ASP LEU GLN D2033 E2047 GLY GLU GLU GLU GLU PRO
GLU GLU GLU T2057 S2060 L2063 L2066 V2070 R2071 L2072 VAL LYS LYS LYS GLU GLU LYS PRO GLU GLU LEU PRO ALA GLU GLU LYS LYS PRO GLN S2093 V2098 S2099 H2100 M2101 V2102 V2103 R2104 Q2107 L2116 S2122 L2123 L2124 H2125 R2126 Q2127 L2134 L2138 Y2142
T2143 I2144 S2145 V2149 T2152 L2156 E2157 C2158 L2159 G2160 Q2161 I2162 R2163 S2164 L2165 L2166 I2167 V2168 GLN MET GLY PRO Q2173 L2177 I2182 G2183 N2184 I2185 M2186 F2191 L2197 M2198 M2203 T2206 V2207 V2210 M2211 V2212 N2213 V2214 L2215 G2216 GLY GLY GLU THR LYS GLU ILE ARG
PHE P2226 K2227 M2228 V2229 T2230 S2231 R2234 F2239 I2242 S2243 R2244 Q2245 N2246 Q2247 R2248 Y2256 I2263 GLY LEU GLY MET GLN GLY SER T2271 P2272 V2275 A2276 A2277 A2278 S2279 V2280 I2281 D2282 N2283 L2286 A2287 V2299 L2302 L2307 GLN SER CYS PRO MET LEU LEU ALA LYS
GLY TYR PRO ASP ILE GLY TRP ASN P2325 D2333 R2336 F2337 F2340 V2341 N2342 N2349 R2359 K2360 P2361 E2362 CYS PHE GLY PRO ALA LEU ARG GLY GLU GLY GLY SER G2375 I2380 I2386 SER GLU ASP PRO ALA ARG ASP GLY PRO GLY VAL ARG ARG ASP ARG ARG ARG GLU
HIS PHE GLY GLU GLU PRO PRO GLU GLU ASN ARG VAL HIS LEU G2419 M2423 D2431 R2435 C2436 A2437 PRO GLU MET HIS LEU ILE GLN ALA GLY LYS GLY E2449 A2450 L2451 R2452 I2453 R2454 R2458 S2459 L2460 VAL PRO L2463 D2464 D2465 L2466 V2467 I2476 PRO THR LEU GLY LYS ASP GLY
ALA LEU VAL GLN PRO LYS MET SER ALA SER F2494 D2497 H2498 K2499 F2505 V2509 Y2510 GLY ILE GLU N2514 L2522 ASP V2525 L2537 ASP THR ALA THR PHE SER THR T2544 A2547 N2551 R2552 Y2553 L2554 L2561 I2562 THR LYS CYS ALA P2567 V2586 TYR ARG LEU SER R2591
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VAL ASP ALA GLU GLY N2734 F2735 E2741 N2744 V2745 I2746 I2747 P2748 N2756 Y2761 A2767 K2770 I2771 Q2772 N2773 N2774 W2775 E2783 H2788 P2789 M2790 L2791 E2803 R2806 K2810 M2816 I2817 A2818 W2819 E2820 W2821 T2822 A2826 R2827 E2828 G2829 E2830 GLU GLU ARG THR GLU
LYS LYS LYS THR ARG LYS ILE SER GLN THR ALA GLN THR Y2849 R2852 E2853 G2854 Y2855 N2856 P2857 L2862 V2865 T2866 L2867 E2870 A2875 E2876 Q2877 L2878 Y2882 H2902 P2903 P2907 T2910 K2916 A2917 R2918 D2919 R2920 E2925 L2926 L2927 K2928 F2929 L2930 N2933 G2934
V2937 T2938 R2939 G2940 LEU LYS ASP MET GLU LEU ASP THR SER SER ILE GLU LYS ARG PHE ALA PHE GLY PHE LEU GLN GLN LEU LEU ARG TRP MET ASP ILE SER GLN GLU PHE PHE ILE ALA HIS LEU LEU GLU ALA VAL VAL SER SER GLY ARG VAL GLU LYS SER VAL LYS GLY VAL GLY GLN GLU GLN ILE LYS
PHE PHE ALA LYS ILE LEU LEU PRO LEU ILE ASN GLN TYR PHE THR ASN HIS CYS LEU Y3016 P3021 I3039 THR SER LEU F3043 P3062 ALA VAL VAL ASN CYS L3068 P3085 A3090 GLY LEU ARG SER F3095 S3116 GLN ALA ARG THR GLN VAL LYS GLY VAL GLY GLN ASN LEU
THR TYR T3132 P3138 F3152 GLY ASP ASP VAL ILE L3158 T3178 LYS ASN THR TYR V3183 P3188 A3200 MET PRO VAL A3204 P3208 S3217 VAL TYR THR THR LYS SER PRO ARG GLU ARG ALA ILE LEU GLY LEU PRO ASN SER VAL GLU GLU GLU MET CYS PRO ASP ILE PRO VAL
LEU ASP ARG LEU MET ALA ASP ILE GLY GLY LEU ALA GLU SER GLY ALA ARG TYR THR GLU MET PRO HIS VAL ILE GLU ILE T3273 L3274 P3275 P3282 P3289 E3290 ALA PRO PRO P3294 P3297 P3301 P3302 P3303 N3313 SER LEU LEU G3317 A3339 VAL PHE ALA GLN PRO ILE V3346
P3351 P3360 G3363 ARG LEU ARG K3367 E3397 PHE SER VAL LEU C3402 P3410 W3423 L3424 THR GLU P3427 N3428 F3435 ARG M3437 E3455 GLN N3457 L3470 THR ALA ASP SER LYS SER LYS M3478 Q3491 GLU ARG T3494 K3495 K3496 S3504 VAL GLN THR SER LEU ILE VAL

ALA T3513 P3519 P3527 THR ASP GLN ASP LEU ILE MET LEU ALA K3537 D3544 THR ASP GLU GLU V3549 P3567 Q3572 MET ALA LEU TYR ARG GLY LEU PRO GLY ARG GLU GLU ASP ALA ASP ASP PRO GLU LYS ILE VAL ARG ARG VAL GLN GLU VAL SER ALA VAL LEU TYR HIS
LEU GLU GLN THR GLU HIS PRO TYR LYS SER LYS LYS ALA VAL TRP HIS LYS LEU LEU SER LYS GLN ARG ARG ARG ALA VAL VAL ALA CYS PHE ARG MET THR PRO LEU TYR ASN LEU P3645 T3646 H3647 Y3657 K3658 I3662 L3663 T3664 I3674 L3677 S3678 K3679 A3680 GLY GLU GLN GLU
GLU GLU GLU GLU GLU VAL GLU GLU LYS K3694 L3698 L3701 S3706 L3710 T3711 E3712 K3713 S3714 K3715 L3716 D3717 Y3722 Y3725 A3726 D3727 I3728 M3729 A3730 K3731 S3732 C3733 HIS LEU GLU GLU GLY GLY GLU ASN GLY GLU ALA GLU GLU GLU GLU VAL E3750 E3754 Q3767 S3768 R3769
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ASN GLU ASP GLY THR VAL ILE ASN ARG GLN ASN GLY GLU LYS VAL MET ALA D3877 D3878 E3879 D3883 L3884 L3965 F3885 R3886 F3887 L3888 Q3889 L3890 L3891 C3892 H3895 F3899 Y3902 L3903 R3904 N3909 C3918 T3919 V3920 D3921 Y3922 L3923 L3924 R3925 L3926 Q3927 E3928 S3929 D3932 F3933 Y3934 W3935 Y3936
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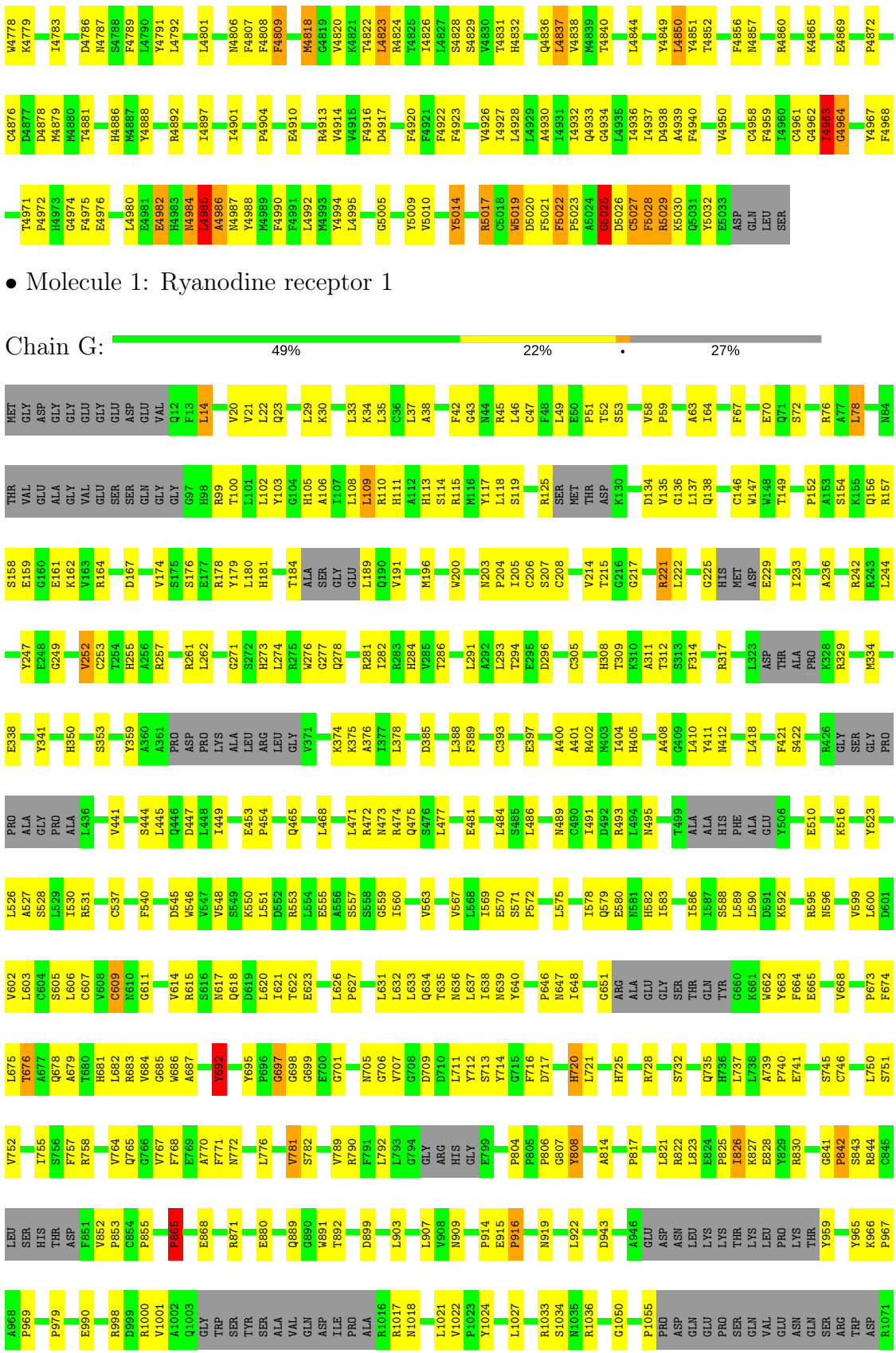
GLU GLY GLY ALA ALA GLY THR VAL ALA ALA GLY ALA THR ALA ALA ARG ALA LEU ARG GLY LEU SER TYR ARG SER LEU ARG ARG ARG ARG VAL ARG ARG LEU ARG ARG LEU THR ALA ARG GLU ALA ALA THR ALA LEU ALA LEU ALA ALA ARG
ALA GLY ALA ALA GLY ALA ALA ALA ALA GLY ALA ALA LEU ALA ALA GLY GLY LEU SER LEU LYS LYS VAL THR VAL THR GLU LEU LEU ALA GLY MET PRO ASP PRO THR SER ASP GLU VAL HIS GLY GLU GLN PRO ALA ALA GLY PRO GLY ASP
ALA ASP GLY ALA GLY GLU GLU GLY GLU GLU ASP ALA GLU GLY GLY ALA GLU GLY VAL ALA ALA ASP GLY GLY PRO PHE ARG PRO GLU GLY ALA ALA GLY ASP PRO GLU GLU GLY LEU LEU GLY ALA GLU GLU GLY ALA ALA GLY PRO THR PRO
ALA GLU PRO PRO THR PRO GLU GLY SER PRO GLU ILE LEU LYS ARG LYS LEU GLY VAL ASP GLY GLU GLU GLU VAL LEU PRO GLU PRO GLU PRO GLU PRO GLU GLU LYS LYS LEU GLU LYS LYS LYS



- Molecule 1: Ryanodine receptor 1

Chain G: 49% 22% • 27%

R1076 A1077 E1078 K1079 S1080 Y1081 T1082 R1087 W1088 Y1089 F1090 E1091 F1092 E1093 G1098 E1099 M1100 R1101 V1102 G1103 W1104 A1105 L1109 R1110 P1111 L1115 G1116 L1120 V1123 F1124 N1125 G1126 Q1130 R1131 W1132 H1133 L1134 G1135 S1136 E1137 P1138 R1141 V1148 V1149 G1150 I1153 E1157

I1160 I1161 F1162 E1167 V1168 L1169 MET SER ASP SER GLY SER GLU THR A1178 D1186 L1189 P1190 V1191 C1192 S1193 P1196 G1197 Q1198 H1201 L1202 N1203 L1204 G1205 Q1206 D1207 S1210 L1211 R1212 F1213 F1214 P1225 F1226 A1227 I1228 N1229 R1232 P1233 V1234 T1235 T1236 W1237 F1238 S1239 K1240 P1243

Q1244 H1252 P1253 H1254 D1261 GLY THR VAL ASP THR PRO PRO CYS LEU ARG L1272 R1275 S1279 Q1280 N1281 F1288 L1289 R1290 L1291 S1292 L1293 P1294 V1295 Q1296 F1297 HIS GLN HIS PHE ARG CYS THR ALA GLY ALA THR PRO LEU ALA PRO PRO GLY LEU GLN PRO PRO ALA ALA GLU ASP GLU

ALA ARG ALA ALA GLU PRO ASP PRO ASP TYR GLU ASN LEU ARG ARG SER ALA GLY GLY TRP GLY GLU ALA GLU GLY GLY LYS GLU GLY THR ALA LYS GLU GLY THR PRO GLY GLY THR PRO GLN PRO GLY VAL GLU ALA GLN PRO VAL ARG ALA GLU ASN GLU LYS ASP ALA THR THR GLU

LYS ASN LYS LYS ARG GLY PHE LEU PHE LYS ALA LYS LYS ALA ALA MET MET THR GLN PRO PRO ALA THR PRO ALA LEU PRO ARG LEU PRO HIS ASP VAL VAL PRO ALA ASP ASN ARG ASP ASP PRO GLU ILE ILE LEU ASN THR THR T1432 S1436 V1437 R1438 V1439 F1440 A1441 GLY GLN GLU

PRO SER C1447 V1448 V1453 T1454 P1455 H1458 Q1459 H1460 F1464 D1465 L1466 S1467 LYS VAL ARG ALA V1472 T1475 M1476 E1479 Q1480 V1483 H1484 S1485 N1491 CYS Y1493 G1497 GLY ASP PHE VAL SER PRO GLY GLN GLN GLY ARG ILE S1510 L1514 V1515 I1516 G1517 C1518 L1519 V1520 ASP

LEU ALA THR G1525 T1530 A1531 N1532 E1535 Q1541 P1544 N1545 T1546 K1547 L1548 F1549 P1550 A1551 V1552 F1553 V1554 H1558 Q1559 N1560 V1561 I1562 Q1563 F1564 E1565 LEU GLY LYS GLN LYS ASN ILE MET PRO LEU SER A1577 A1578 M1579 S1582 E1583 R1584 K1585 N1586 P1587 A1588 P1589 E1596 V1597 Q1598

M1599 L1600 P1609 N1610 H1611 F1612 R1623 W1626 A1627 V1628 Q1629 C1630 Q1631 D1632 P1633 M1637 A1638 L1639 L1640 I1641 P1642 E1643 R1646 C1647 M1648 D1649 I1650 L1651 E1652 E1655 R1656 L1657 D1658 L1659 Q1660 R1661 F1662 H1663 T1666 L1667 R1671 A1672 V1673 C1674 A1675 L1676 G1677 N1678 N1679 R1680 V1681 A1682

H1683 A1684 L1685 C1686 S1687 H1688 V1689 D1690 Q1691 A1692 Q1693 L1694 L1695 E1699 D1700 A1701 H1702 L1703 P1704 L1707 R1708 A1709 G1710 D1713 L1714 L1715 I1716 S1717 I1718 H1719 R1725 S1726 R1727 R1728 S1729 M1730 L1731 S1732 E1733 Y1734 I1735 V1736 P1737 L1738 T1742 R1743 A1744 I1745 T1746 L1747 F1748 P1749 P1750 GLY ARG

LYS GLY GLY ASN ALA ARG HIS G1761 L1762 P1763 G1764 V1765 G1766 V1767 T1768 T1769 S1770 L1771 R1772 H1775 P1780 C1781 F1782 V1783 A1784 ALA LEU PRO ALA ALA GLY VAL ALA GLU ALA PRO ALA ARG L1798 A1801 I1802 P1803 L1804 R1808 L1812 L1815 A1818 V1819 R1827 D1828 P1829

V1830 S1833 F1836 V1839 P1840 L1844 L1848 L1849 V1850 M1851 G1852 I1853 F1854 G1855 D1856 E1857 D1858 Q1861 I1862 M1865 I1866 E1867 P1868 E1869 VAL PHE THR GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU ASP GLU GLU GLU LYS GLU GLU ASP

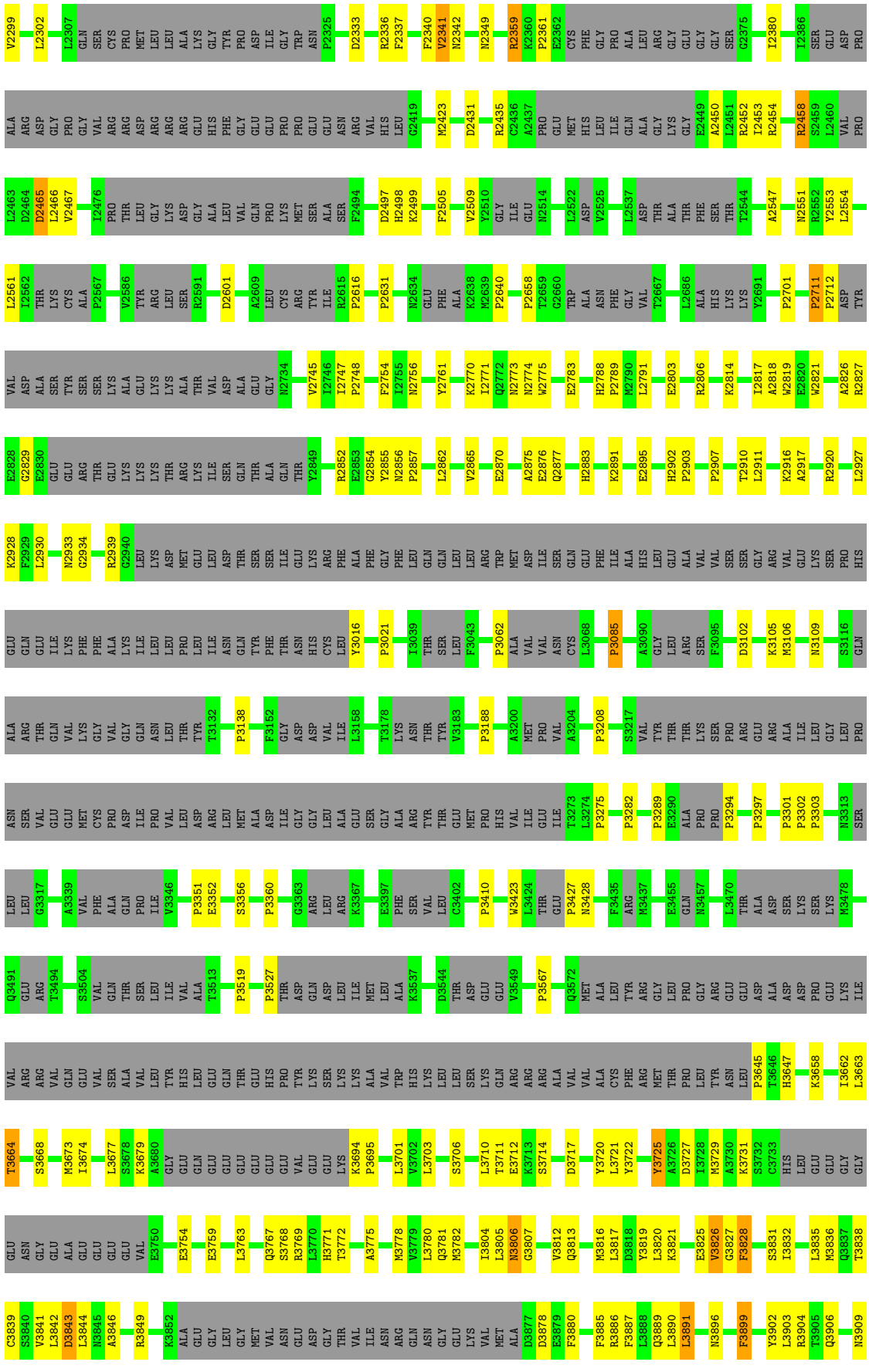
GLU GLU GLU GLU GLU LYS GLU ASP ALA GLU LYS GLU GLU GLU GLU ALA PRO GLU GLY GLU LYS GLU ASP LEU GLU GLU G1925 L1926 L1927 K1936 L1937 Q1938 M1939 C1940 L1943 E1944 Y1945 F1946 C1947 Q1952 H1953 R1954 V1955 E1956 S1957 L1958 F1961 L1969 Q1970 Q1973 R1976 TYR ALA

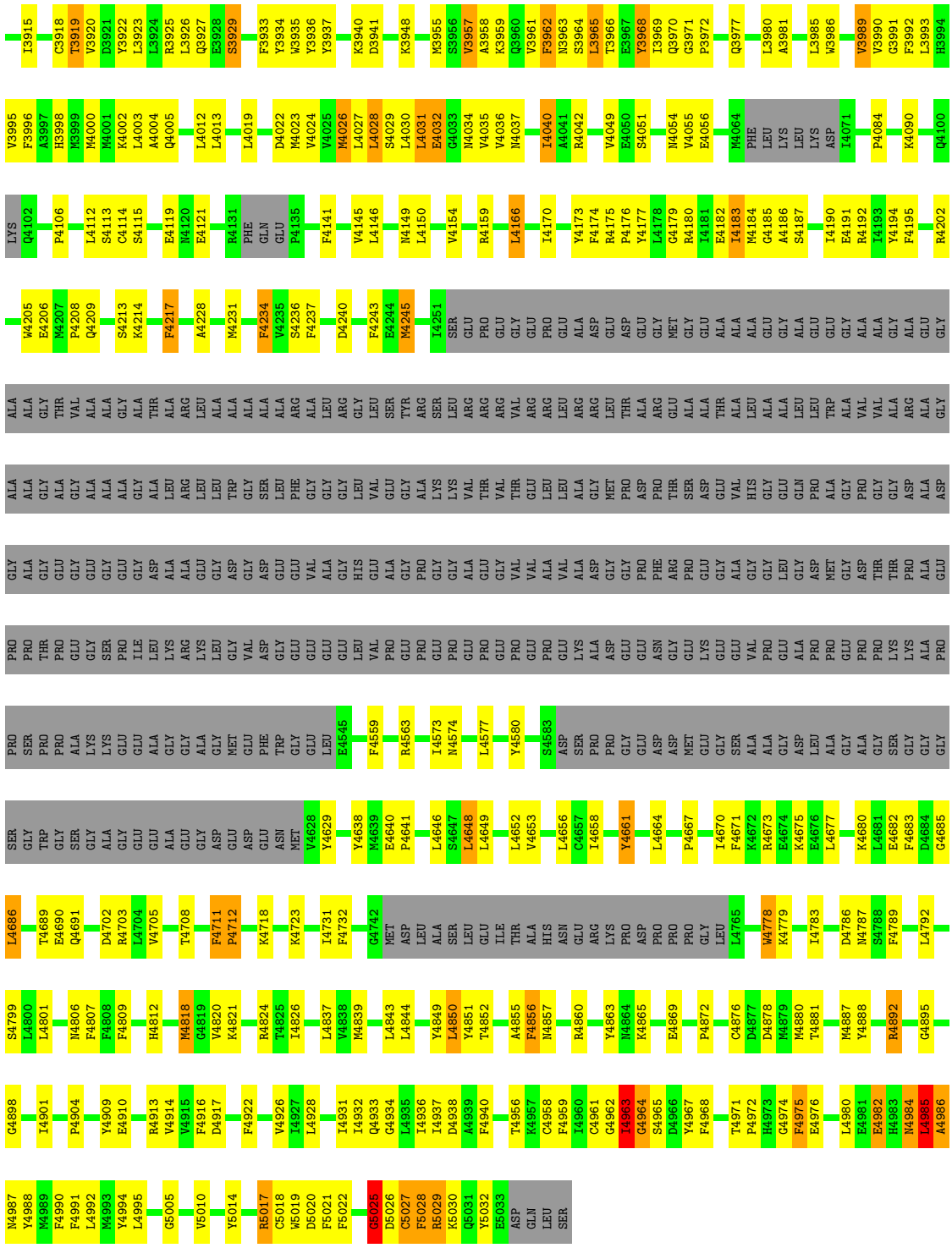
LEU LEU MET ARG ALA PHE THR MET SER ALA ALA GLU THR ALA ARG ARG THR ARG GLU PHE ARG SER PRO PRO GLN GLU GLN ILE ASN MET LEU LEU HIS PHE LYS ASP GLU ALA ASP GLU GLU ASP CYS PRO LEU PRO GLU ASP ILE ARG GLN ASP LEU GLN D2033 I2044 E2047 GLY

GLU GLU GLU GLU PRO GLU GLU GLU T2057 S2060 S2061 R2062 L2063 R2064 S2065 L2066 V2070 R2071 L2072 VAL LYS LYS LYS GLU GLU LYS PRO GLU GLU GLU LEU PRO ALA GLU GLU LYS LYS PRO GLN S2093 V2098 S2099 H2100 M2101 V2102 V2103 R2104 Q2107 L2116 F2121 S2122 L2123 L2124 H2125

R2126 Q2127 L2131 G2132 E2133 L2134 L2135 R2136 A2137 L2138 P2139 Y2142 T2143 I2144 S2145 V2149 T2152 L2156 E2157 C2158 L2159 G2160 Q2161 I2162 R2163 S2164 L2165 L2166 I2167 V2168 GLN MET GLY PRO Q2173 L2177 I2182 G2183 N2184 I2185 M2186 F2191 L2197 M2198 M2203 T2206 V2207 V2210

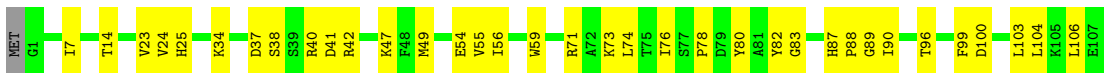
M2211 V2212 N2213 V2214 L2215 G2216 GLY GLY GLU THR LYS GLU ILE ARG PHE P2226 K2227 T2230 S2231 R2234 F2239 I2242 S2243 R2244 Q2245 N2246 Q2247 R2248 Y2256 I2263 GLY LEU GLY MET GLN GLY SER T2271 P2272 V2275 A2276 A2277 A2278 S2279 V2280 I2281 D2282 N2283 L2286 A2287 L2288


V2299 L2302 L2307 GLN SER CYS PRO MET LEU LEU ALA ALA LYS GLY TYR PRO ASP ILE GLY TRP ASN P2325 D2333 R2336 F2337 F2340 V2341 N2342 N2349 R2359 K2360 P2361 E2362 CYS PHE GLY PRO ALA LEU ARG GLY GLU GLY GLY SER G2375 I2380 I2386 SER GLU ASP PRO
ALA ARG ASP GLY PRO GLY VAL ARG ARG ASP ARG ARG GLU HIS PHE GLY GLU GLU PRO PRO GLU GLU ASN ARG VAL HIS LEU G2419 M2423 D2431 R2435 C2436 A2437 PRO GLU MET HIS LEU ILE GLN ALA GLY LYS GLY E2449 A2450 L2451 R2452 I2453 R2454 R2458 S2459 L2460 VAL PRO
L2463 D2464 D2465 L2466 V2467 I2476 PRO THR LEU GLY LYS ASP GLY ALA LEU VAL GLN PRO LYS MET SER ALA SER F2494 D2497 H2498 K2499 F2505 V2509 Y2510 GLY ILE GLU N2514 L2522 ASP V2525 L2537 ASP THR ALA THR PHE SER THR T2544 A2547 N2551 R2552 Y2553 L2554
L2561 I2562 THR LYS CYS ALA P2567 V2586 TYR ARG LEU SER R2591 D2601 A2609 LEU CYS ARG TYR ILE R2615 P2616 P2631 N2634 GLU PHE ALA K2638 M2639 P2640 P2658 T2659 G2660 TRP ALA ASN PHE GLY VAL T2667 L2686 ALA HIS LYS LYS Y2691 P2701 P2711 P2712 ASP TYR
VAL ASP ALA SER TYR SER SER LYS ALA GLU LYS LYS ALA THR VAL ASP ALA GLU GLY N2734 V2745 I2746 I2747 P2748 F2754 I2755 N2756 Y2761 K2770 I2771 Q2772 N2773 N2774 W2775 E2783 H2788 P2789 M2790 L2791 E2803 R2806 K2814 I2817 A2818 W2819 E2820 W2821 A2826 R2827
E2828 G2829 E2830 GLU GLU ARG THR GLU LYS LYS LYS THR ARG LYS ILE SER GLN THR ALA GLN THR Y2849 R2852 E2853 G2854 Y2855 N2856 P2857 L2862 V2865 E2870 A2875 E2876 Q2877 H2883 K2891 E2895 H2902 P2903 P2907 T2910 L2911 K2916 A2917 R2920 L2927
K2928 F2929 L2930 N2933 G2934 R2939 G2940 LEU LYS ASP MET GLU LEU ASP THR SER SER ILE GLU LYS ARG PHE ALA PHE PHE GLY PHE LEU GLN GLN LEU LEU ARG TRP MET ASP ILE SER GLN GLU PHE ILE ALA HIS LEU GLU ALA VAL VAL SER SER GLY GLY ARG VAL GLU LYS SER PRO HIS
GLU GLN GLU ILE LYS PHE PHE ALA LYS ILE LEU LEU PRO LEU ILE ASN GLN TYR PHE THR ASN HIS CYS LEU Y3016 P3021 I3039 THR SER LEU F3043 P3062 ALA VAL VAL ASN CYS L3068 P3085 A3090 GLY LEU ARG SER F3095 D3102 K3105 M3106 N3109 S3116 GLN
ALA ARG THR GLN VAL LYS GLY VAL GLY GLN ASN LEU THR TYR T3132 P3138 F3152 GLY ASP ASP VAL ILE L3158 T3178 LYS ASN THR TYR V3183 P3188 A3200 MET PRO VAL A3204 P3208 S3217 VAL TYR THR THR LYS SER PRO ARG GLU ARG ALA ILE LEU GLY LEU PRO
ASN SER VAL GLU GLU MET CYS PRO ASP ILE PRO VAL LEU ASP ARG LEU MET ALA ASP ILE GLY GLY LEU ALA GLU SER GLY ALA ARG TYR THR GLU MET PRO HIS VAL ILE GLU ILE T3273 L3274 P3275 P3282 P3289 E3290 ALA PRO PRO P3294 P3297 P3301 P3302 P3303 N3313 SER
LEU LEU G3317 A3339 VAL PHE ALA GLN PRO ILE V3346 P3351 E3352 S3356 P3360 G3363 ARG LEU ARG K3367 E3397 PHE SER VAL LEU C3402 P3410 W3423 L3424 THR GLU F3435 ARG M3437 E3455 GLN N3457 L3470 THR ALA ASP SER LYS SER LYS M3478
Q3491 GLU ARG T3494 S3504 VAL GLN THR SER LEU ILE VAL ALA T3513 P3519 P3527 THR ASP GLN ASP LEU ILE MET LEU ALA K3537 D3544 THR ASP GLU GLU V3549 P3567 Q3572 MET ALA LEU TYR ARG GLY LEU PRO GLY ARG GLU GLU ASP ASP ALA ASP ASP PRO GLU LYS ILE
VAL ARG ARG VAL GLN GLU VAL SER ALA VAL LEU TYR HIS LEU GLU GLN THR GLU HIS PRO TYR LYS SER LYS LYS ALA VAL TRP HIS LYS LEU LEU SER LYS GLN ARG ARG ARG ALA VAL VAL ALA CYS PHE ARG MET THR PRO LEU TYR ASN LEU P3645 T3646 H3647 K3658 I3662 L3663
T3664 S3668 M3673 I3674 L3677 S3678 K3679 A3680 GLY GLU GLN GLU GLU GLU GLU GLU VAL GLU GLU LYS K3694 P3695 L3701 V3702 L3703 S3706 L3710 T3711 E3712 K3713 S3714 D3717 Y3720 L3721 Y3722 Y3725 A3726 D3727 I3728 M3729 A3730 K3731 S3732 C3733 HIS LEU GLU GLU GLY GLY
GLU ASN GLY GLU ALA GLU GLU GLU VAL E3750 E3754 E3759 L3763 Q3767 S3768 R3769 L3770 H3771 T3772 A3775 M3778 V3779 L3780 Q3781 M3782 I3804 L3805 N3806 G3807 V3812 Q3813 M3816 L3817 D3818 Y3819 L3820 K3821 E3825 V3826 G3827 F3828 S3831 I3832 L3835 M3836 Q3837 T3838
C3839 S3840 V3841 L3842 D3843 L3844 N3845 A3846 R3849 K3852 ALA GLU GLY LEU GLY MET VAL ASN GLU ASP GLY THR VAL ILE ASN ARG GLN ASN GLY GLU LYS VAL MET ALA D3877 D3878 E3879 F3880 F3885 R3886 F3887 L3888 Q3889 L3890 L3891 N3896 F3899 Y3902 L3903 R3904 T3905 Q3906 N3909



- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain B: 67% 32%



- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain D: 65% 34%

MET G1 T6 I7 T14 V23 V24 H25 K34 D37 S38 S39 R40 D41 R42 K47 F48 M49 E54 V55 I56 W59 Q70 R71 A72 K73 L74 T75 I76 S77 P78 D79 Y80 A81 Y82 G83 H87 P88 G89 I90 T96 F99 D100 L103 L104 K105 L106

E107

• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain F: 68% 31%

MET G1 I7 T14 V23 V24 H25 K34 D37 S38 S39 R40 D41 R42 K47 E54 V55 I56 W59 R71 A72 K73 L74 T75 I76 S77 P78 D79 Y80 A81 Y82 G83 H87 P88 G89 I90 T96 F99 D100 L103 L104 K105 L106 E107

• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain H: 69% 30%

MET G1 V2 D11 T14 V23 V24 H25 D37 S38 S39 R40 D41 R42 F46 K47 V55 I56 W59 S67 V68 G69 Q70 R71 I76 Y82 H87 P88 G89 I90 F99 D100 V101 E102 L103 L104 K105 L106 E107

4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	64000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	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	#$\|Z\|$ >2	RMSZ	#$\|Z\|$ >2
1	A	0.98	87/27385 (0.3%)	0.88	108/37104 (0.3%)
1	C	0.98	89/27385 (0.3%)	0.88	114/37104 (0.3%)
1	E	0.98	87/27385 (0.3%)	0.88	108/37104 (0.3%)
1	G	0.99	94/27385 (0.3%)	0.88	112/37104 (0.3%)
2	B	0.63	0/851	0.63	0/1146
2	D	0.63	0/851	0.63	0/1146
2	F	0.63	0/851	0.63	0/1146
2	H	0.63	0/851	0.62	0/1146
All	All	0.98	357/112944 (0.3%)	0.88	442/153000 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	20
1	C	0	20
1	E	0	20
1	G	0	20
All	All	0	80

All (357) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	4988	TYR	CG-CD2	-20.55	1.12	1.39
1	E	4988	TYR	CG-CD2	-19.42	1.14	1.39
1	C	4988	TYR	CG-CD2	-19.41	1.14	1.39
1	A	4988	TYR	CG-CD2	-19.37	1.14	1.39
1	G	4988	TYR	CE1-CZ	-17.94	1.15	1.38
1	E	4988	TYR	CE1-CZ	-14.63	1.19	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	4988	TYR	CE1-CZ	-14.61	1.19	1.38
1	A	4988	TYR	CE1-CZ	-14.58	1.19	1.38
1	G	4988	TYR	CG-CD1	-13.87	1.21	1.39
1	G	4988	TYR	CE2-CZ	-12.60	1.22	1.38
1	C	4988	TYR	CG-CD1	-11.96	1.23	1.39
1	A	4988	TYR	CG-CD1	-11.95	1.23	1.39
1	E	4988	TYR	CG-CD1	-11.94	1.23	1.39
1	A	5021	PHE	CG-CD2	-11.06	1.22	1.38
1	C	5021	PHE	CG-CD2	-10.94	1.22	1.38
1	E	5021	PHE	CG-CD2	-10.91	1.22	1.38
1	G	5021	PHE	CG-CD2	-10.77	1.22	1.38
1	A	4988	TYR	CE2-CZ	-10.50	1.25	1.38
1	C	4988	TYR	CE2-CZ	-10.47	1.25	1.38
1	E	4988	TYR	CE2-CZ	-10.39	1.25	1.38
1	C	3922	TYR	CG-CD2	-10.29	1.25	1.39
1	A	3922	TYR	CG-CD2	-10.22	1.25	1.39
1	E	3922	TYR	CG-CD2	-10.22	1.25	1.39
1	G	4851	TYR	CE1-CZ	-10.01	1.25	1.38
1	C	3922	TYR	CE2-CZ	-9.93	1.25	1.38
1	A	3922	TYR	CE2-CZ	-9.90	1.25	1.38
1	A	5014	TYR	CG-CD1	-9.86	1.26	1.39
1	E	3922	TYR	CE2-CZ	-9.86	1.25	1.38
1	G	3922	TYR	CG-CD2	-9.78	1.26	1.39
1	G	4234	PHE	CG-CD1	-9.67	1.24	1.38
1	G	3922	TYR	CE2-CZ	-9.64	1.26	1.38
1	A	5022	PHE	CG-CD1	-9.62	1.24	1.38
1	E	5022	PHE	CG-CD1	-9.62	1.24	1.38
1	C	5022	PHE	CG-CD1	-9.56	1.24	1.38
1	C	5014	TYR	CG-CD1	-9.50	1.26	1.39
1	E	3886	ARG	CZ-NH1	9.48	1.45	1.33
1	A	3886	ARG	CZ-NH1	9.38	1.45	1.33
1	C	3886	ARG	CZ-NH1	9.34	1.45	1.33
1	E	5014	TYR	CG-CD1	-9.29	1.27	1.39
1	G	3922	TYR	CE1-CZ	-9.11	1.26	1.38
1	G	5022	PHE	CG-CD1	-9.08	1.25	1.38
1	E	4234	PHE	CG-CD1	-8.71	1.25	1.38
1	C	4234	PHE	CG-CD1	-8.50	1.26	1.38
1	C	4234	PHE	CG-CD2	-8.49	1.26	1.38
1	A	4234	PHE	CG-CD1	-8.48	1.26	1.38
1	A	4234	PHE	CG-CD2	-8.47	1.26	1.38
1	E	4234	PHE	CG-CD2	-8.47	1.26	1.38
1	G	5014	TYR	CG-CD1	-8.39	1.28	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	3937	TYR	CG-CD1	-8.37	1.28	1.39
1	G	3922	TYR	CG-CD1	-8.25	1.28	1.39
1	E	5019	TRP	CE3-CZ3	-8.21	1.24	1.38
1	A	4177	TYR	CB-CG	-8.19	1.39	1.51
1	E	4177	TYR	CB-CG	-8.19	1.39	1.51
1	A	5019	TRP	CE3-CZ3	-8.12	1.24	1.38
1	C	4177	TYR	CB-CG	-8.08	1.39	1.51
1	A	3919	THR	CB-CG2	-8.02	1.25	1.52
1	E	3919	THR	CB-CG2	-7.99	1.25	1.52
1	C	3919	THR	CB-CG2	-7.88	1.26	1.52
1	A	4671	PHE	CG-CD1	-7.87	1.26	1.38
1	C	4671	PHE	CG-CD1	-7.86	1.26	1.38
1	C	5019	TRP	CE3-CZ3	-7.86	1.25	1.38
1	G	4671	PHE	CG-CD1	-7.75	1.27	1.38
1	G	3722	TYR	CE1-CZ	-7.73	1.28	1.38
1	E	4671	PHE	CG-CD1	-7.72	1.27	1.38
1	G	4177	TYR	CB-CG	-7.72	1.40	1.51
1	G	4234	PHE	CG-CD2	-7.67	1.27	1.38
1	A	5014	TYR	CE2-CZ	-7.65	1.28	1.38
1	G	4982	GLU	C-O	-7.58	1.08	1.23
1	E	5014	TYR	CE2-CZ	-7.55	1.28	1.38
1	C	5014	TYR	CE2-CZ	-7.55	1.28	1.38
1	G	4958	CYS	CB-SG	-7.46	1.69	1.82
1	E	4195	PHE	CG-CD2	-7.46	1.27	1.38
1	G	5019	TRP	CE3-CZ3	-7.42	1.25	1.38
1	G	3885	PHE	CG-CD2	-7.41	1.27	1.38
1	C	4559	PHE	CG-CD1	-7.40	1.27	1.38
1	A	4195	PHE	CG-CD2	-7.38	1.27	1.38
1	C	4195	PHE	CG-CD2	-7.37	1.27	1.38
1	A	4559	PHE	CG-CD1	-7.34	1.27	1.38
1	E	4559	PHE	CG-CD1	-7.34	1.27	1.38
1	A	3922	TYR	CG-CD1	-7.26	1.29	1.39
1	E	3922	TYR	CG-CD1	-7.26	1.29	1.39
1	C	3922	TYR	CG-CD1	-7.17	1.29	1.39
1	G	3968	TYR	CE1-CZ	-7.14	1.29	1.38
1	E	3968	TYR	CE2-CZ	-7.13	1.29	1.38
1	C	4174	PHE	CG-CD2	-7.12	1.28	1.38
1	A	4174	PHE	CG-CD2	-7.08	1.28	1.38
1	G	4195	PHE	CG-CD2	-7.05	1.28	1.38
1	G	4174	PHE	CG-CD2	-7.03	1.28	1.38
1	E	4174	PHE	CG-CD2	-7.03	1.28	1.38
1	C	3968	TYR	CE2-CZ	-7.00	1.29	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3968	TYR	CE2-CZ	-6.99	1.29	1.38
1	E	4217	PHE	CG-CD1	-6.97	1.28	1.38
1	A	5019	TRP	CB-CG	-6.95	1.37	1.50
1	E	5019	TRP	CB-CG	-6.94	1.37	1.50
1	G	4032	GLU	CD-OE1	-6.93	1.18	1.25
1	G	4968	PHE	CG-CD2	-6.92	1.28	1.38
1	C	5019	TRP	CB-CG	-6.90	1.37	1.50
1	C	4180	ARG	CZ-NH2	-6.89	1.24	1.33
1	E	4180	ARG	CZ-NH2	-6.87	1.24	1.33
1	G	5014	TYR	CE2-CZ	-6.87	1.29	1.38
1	A	4968	PHE	CG-CD2	-6.83	1.28	1.38
1	A	4217	PHE	CG-CD1	-6.82	1.28	1.38
1	G	3725	TYR	CG-CD2	-6.82	1.30	1.39
1	C	4217	PHE	CG-CD1	-6.82	1.28	1.38
1	G	5019	TRP	CB-CG	-6.80	1.38	1.50
1	C	4968	PHE	CG-CD2	-6.78	1.28	1.38
1	E	4968	PHE	CG-CD2	-6.74	1.28	1.38
1	A	4180	ARG	CZ-NH2	-6.70	1.24	1.33
1	E	4958	CYS	CB-SG	-6.66	1.71	1.82
1	G	3919	THR	CB-CG2	-6.65	1.30	1.52
1	A	4180	ARG	C-O	-6.63	1.10	1.23
1	A	4963	ILE	C-O	6.62	1.35	1.23
1	E	4963	ILE	C-O	6.61	1.35	1.23
1	C	3722	TYR	CE1-CZ	-6.57	1.30	1.38
1	C	4778	TRP	CE3-CZ3	-6.56	1.27	1.38
1	E	4778	TRP	CE3-CZ3	-6.56	1.27	1.38
1	E	5032	TYR	CE1-CZ	-6.55	1.30	1.38
1	G	4851	TYR	CG-CD2	-6.55	1.30	1.39
1	G	4559	PHE	CG-CD1	-6.54	1.28	1.38
1	A	3968	TYR	CG-CD1	-6.51	1.30	1.39
1	C	3968	TYR	CG-CD1	-6.51	1.30	1.39
1	C	3929	SER	CA-CB	-6.51	1.43	1.52
1	A	3722	TYR	CE1-CZ	-6.51	1.30	1.38
1	A	5032	TYR	CE1-CZ	-6.51	1.30	1.38
1	E	3722	TYR	CE1-CZ	-6.50	1.30	1.38
1	A	3929	SER	CA-CB	-6.50	1.43	1.52
1	C	4963	ILE	C-O	6.50	1.35	1.23
1	C	4974	GLY	CA-C	-6.48	1.41	1.51
1	C	4180	ARG	C-O	-6.48	1.11	1.23
1	A	4778	TRP	CE3-CZ3	-6.46	1.27	1.38
1	E	3929	SER	CA-CB	-6.46	1.43	1.52
1	E	3968	TYR	CG-CD1	-6.45	1.30	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	4958	CYS	CB-SG	-6.45	1.71	1.82
1	E	4180	ARG	C-O	-6.44	1.11	1.23
1	A	3885	PHE	CG-CD2	-6.42	1.29	1.38
1	A	4982	GLU	C-O	-6.42	1.11	1.23
1	C	3885	PHE	CG-CD2	-6.42	1.29	1.38
1	E	4974	GLY	CA-C	-6.39	1.41	1.51
1	C	5032	TYR	CE1-CZ	-6.38	1.30	1.38
1	G	3929	SER	CA-CB	-6.38	1.43	1.52
1	A	4958	CYS	CB-SG	-6.33	1.71	1.82
1	E	3885	PHE	CG-CD2	-6.29	1.29	1.38
1	C	4982	GLU	C-O	-6.27	1.11	1.23
1	A	4974	GLY	CA-C	-6.27	1.41	1.51
1	G	4963	ILE	C-O	6.27	1.35	1.23
1	G	3935	TRP	CG-CD1	-6.24	1.28	1.36
1	E	4982	GLU	C-O	-6.23	1.11	1.23
1	A	3899	PHE	CG-CD2	-6.22	1.29	1.38
1	E	3899	PHE	CG-CD2	-6.21	1.29	1.38
1	G	3968	TYR	CD2-CE2	-6.18	1.30	1.39
1	G	5032	TYR	CE1-CZ	-6.17	1.30	1.38
1	G	4988	TYR	CB-CG	-6.17	1.42	1.51
1	C	3899	PHE	CG-CD2	-6.16	1.29	1.38
1	G	3887	PHE	CD2-CE2	-6.14	1.26	1.39
1	G	3922	TYR	CA-CB	-6.11	1.40	1.53
1	C	4975	PHE	CG-CD2	-6.09	1.29	1.38
1	E	4975	PHE	CG-CD2	-6.09	1.29	1.38
1	G	5028	PHE	CG-CD2	-6.08	1.29	1.38
1	C	4173	TYR	CG-CD1	-6.07	1.31	1.39
1	C	4851	TYR	CE2-CZ	-6.07	1.30	1.38
1	G	4964	GLY	C-O	-6.07	1.14	1.23
1	A	4975	PHE	CG-CD2	-6.05	1.29	1.38
1	E	4851	TYR	CE2-CZ	-6.04	1.30	1.38
1	G	3964	SER	CA-CB	-6.04	1.43	1.52
1	G	4974	GLY	CA-C	-6.04	1.42	1.51
1	A	4851	TYR	CE2-CZ	-6.03	1.30	1.38
1	C	4032	GLU	CD-OE1	-6.02	1.19	1.25
1	A	4173	TYR	CG-CD1	-6.01	1.31	1.39
1	E	4173	TYR	CG-CD1	-6.01	1.31	1.39
1	A	3968	TYR	CE1-CZ	-6.00	1.30	1.38
1	G	3968	TYR	CE2-CZ	-6.00	1.30	1.38
1	G	4243	PHE	CG-CD2	-5.99	1.29	1.38
1	A	4032	GLU	CD-OE1	-5.97	1.19	1.25
1	A	5028	PHE	CG-CD2	-5.97	1.29	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	3968	TYR	CE1-CZ	-5.97	1.30	1.38
1	C	5028	PHE	CG-CD2	-5.95	1.29	1.38
1	C	4986	ALA	CA-CB	-5.92	1.40	1.52
1	G	3722	TYR	CG-CD1	-5.88	1.31	1.39
1	E	4190	ILE	C-O	-5.85	1.12	1.23
1	A	4190	ILE	C-O	-5.84	1.12	1.23
1	G	4217	PHE	CG-CD1	-5.84	1.29	1.38
1	A	3887	PHE	CD2-CE2	-5.83	1.27	1.39
1	G	4994	TYR	CG-CD1	-5.83	1.31	1.39
1	E	5028	PHE	CG-CD2	-5.82	1.30	1.38
1	E	4986	ALA	CA-CB	-5.81	1.40	1.52
1	E	5025	GLY	C-O	-5.81	1.14	1.23
1	A	4986	ALA	CA-CB	-5.80	1.40	1.52
1	E	3937	TYR	CG-CD2	-5.80	1.31	1.39
1	E	3887	PHE	CD2-CE2	-5.79	1.27	1.39
1	C	3887	PHE	CD2-CE2	-5.78	1.27	1.39
1	E	3968	TYR	CE1-CZ	-5.78	1.31	1.38
1	E	4032	GLU	CD-OE1	-5.78	1.19	1.25
1	G	4990	PHE	CB-CG	-5.77	1.41	1.51
1	A	3937	TYR	CG-CD2	-5.75	1.31	1.39
1	E	4936	ILE	C-O	5.74	1.34	1.23
1	G	5025	GLY	C-O	-5.74	1.14	1.23
1	C	3885	PHE	CD1-CE1	-5.73	1.27	1.39
1	E	1104	TRP	CG-CD1	-5.73	1.28	1.36
1	A	3922	TYR	CA-CB	-5.73	1.41	1.53
1	E	3922	TYR	CA-CB	-5.73	1.41	1.53
1	A	1104	TRP	CG-CD1	-5.72	1.28	1.36
1	C	4180	ARG	CA-C	-5.72	1.38	1.52
1	C	3922	TYR	CA-CB	-5.72	1.41	1.53
1	E	3885	PHE	CD1-CE1	-5.72	1.27	1.39
1	G	3722	TYR	CG-CD2	-5.72	1.31	1.39
1	C	3892	CYS	C-O	-5.71	1.12	1.23
1	G	5018	CYS	CB-SG	-5.71	1.72	1.81
1	A	4936	ILE	C-O	5.70	1.34	1.23
1	A	3892	CYS	C-O	-5.70	1.12	1.23
1	G	3957	VAL	CB-CG1	-5.70	1.40	1.52
1	E	3892	CYS	C-O	-5.70	1.12	1.23
1	A	3885	PHE	CD1-CE1	-5.70	1.27	1.39
1	C	3937	TYR	CG-CD2	-5.70	1.31	1.39
1	A	3935	TRP	CB-CG	-5.70	1.40	1.50
1	C	4190	ILE	C-O	-5.68	1.12	1.23
1	C	4936	ILE	C-O	5.67	1.34	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	3935	TRP	CB-CG	-5.65	1.40	1.50
1	E	4959	PHE	CG-CD2	-5.64	1.30	1.38
1	E	3935	TRP	CB-CG	-5.64	1.40	1.50
1	G	4173	TYR	CG-CD1	-5.63	1.31	1.39
1	G	4975	PHE	CG-CD2	-5.61	1.30	1.38
1	C	1104	TRP	CG-CD1	-5.61	1.28	1.36
1	C	3968	TYR	CD2-CE2	-5.59	1.30	1.39
1	E	4195	PHE	CG-CD1	-5.58	1.30	1.38
1	E	4192	ARG	CZ-NH1	-5.58	1.25	1.33
1	C	4994	TYR	CG-CD1	-5.57	1.31	1.39
1	G	4180	ARG	CA-C	-5.57	1.38	1.52
1	G	4190	ILE	C-O	-5.56	1.12	1.23
1	C	3922	TYR	CE1-CZ	-5.56	1.31	1.38
1	G	3885	PHE	CD1-CE1	-5.56	1.28	1.39
1	A	4195	PHE	CG-CD1	-5.55	1.30	1.38
1	A	4180	ARG	CA-C	-5.54	1.38	1.52
1	C	4959	PHE	CG-CD2	-5.54	1.30	1.38
1	A	4711	PHE	CG-CD2	-5.54	1.30	1.38
1	E	4711	PHE	CG-CD2	-5.54	1.30	1.38
1	G	4778	TRP	CE3-CZ3	-5.53	1.29	1.38
1	A	5029	ARG	CZ-NH2	-5.52	1.25	1.33
1	A	4994	TYR	CG-CD1	-5.52	1.31	1.39
1	G	3922	TYR	CB-CG	-5.52	1.43	1.51
1	A	4192	ARG	CZ-NH1	-5.51	1.25	1.33
1	A	5025	GLY	C-O	-5.51	1.14	1.23
1	E	3968	TYR	CD2-CE2	-5.51	1.31	1.39
1	C	4711	PHE	CG-CD2	-5.50	1.30	1.38
1	A	3968	TYR	CD2-CE2	-5.50	1.31	1.39
1	E	4180	ARG	CA-C	-5.50	1.38	1.52
1	G	4195	PHE	CG-CD1	-5.50	1.30	1.38
1	C	4195	PHE	CG-CD1	-5.50	1.30	1.38
1	E	3922	TYR	CE1-CZ	-5.49	1.31	1.38
1	G	1104	TRP	CG-CD1	-5.49	1.29	1.36
1	A	3922	TYR	CE1-CZ	-5.49	1.31	1.38
1	E	4182	GLU	CA-C	-5.48	1.38	1.52
1	C	5025	GLY	C-O	-5.47	1.14	1.23
1	C	117	TYR	CE1-CZ	-5.47	1.31	1.38
1	C	4192	ARG	CZ-NH1	-5.46	1.25	1.33
1	E	117	TYR	CE1-CZ	-5.46	1.31	1.38
1	G	4936	ILE	C-O	5.43	1.33	1.23
1	E	5029	ARG	CZ-NH2	-5.43	1.25	1.33
1	C	3968	TYR	CD1-CE1	-5.42	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	5019	TRP	CG-CD1	-5.41	1.29	1.36
1	C	5029	ARG	CZ-NH2	-5.41	1.26	1.33
1	C	4964	GLY	C-O	-5.41	1.15	1.23
1	A	3902	TYR	CG-CD2	-5.40	1.32	1.39
1	A	3968	TYR	CD1-CE1	-5.39	1.31	1.39
1	G	4177	TYR	CG-CD1	-5.39	1.32	1.39
1	A	4959	PHE	CG-CD2	-5.39	1.30	1.38
1	G	3937	TYR	CE2-CZ	-5.38	1.31	1.38
1	G	117	TYR	CE1-CZ	-5.38	1.31	1.38
1	G	3828	PHE	CG-CD2	-5.37	1.30	1.38
1	C	4182	GLU	C-O	-5.36	1.13	1.23
1	A	117	TYR	CE1-CZ	-5.35	1.31	1.38
1	E	3968	TYR	CD1-CE1	-5.35	1.31	1.39
1	E	4964	GLY	C-O	-5.35	1.15	1.23
1	A	4182	GLU	CA-C	-5.34	1.39	1.52
1	G	4191	GLU	CG-CD	5.33	1.59	1.51
1	C	4182	GLU	CA-C	-5.33	1.39	1.52
1	E	4243	PHE	CG-CD2	-5.33	1.30	1.38
1	A	4243	PHE	CG-CD2	-5.33	1.30	1.38
1	E	4661	TYR	CG-CD1	-5.33	1.32	1.39
1	C	4243	PHE	CG-CD2	-5.33	1.30	1.38
1	E	1076	ARG	CZ-NH2	-5.32	1.26	1.33
1	A	5018	CYS	CB-SG	-5.31	1.73	1.81
1	C	4661	TYR	CG-CD1	-5.31	1.32	1.39
1	E	1162	PHE	CG-CD1	-5.31	1.30	1.38
1	G	3899	PHE	CG-CD2	-5.31	1.30	1.38
1	E	4994	TYR	CG-CD1	-5.29	1.32	1.39
1	A	1162	PHE	CG-CD1	-5.28	1.30	1.38
1	G	4179	GLY	CA-C	-5.28	1.43	1.51
1	G	4182	GLU	C-O	-5.28	1.13	1.23
1	G	4988	TYR	N-CA	-5.27	1.35	1.46
1	G	4180	ARG	CZ-NH2	-5.27	1.26	1.33
1	A	692	TYR	CE1-CZ	-5.27	1.31	1.38
1	E	692	TYR	CE1-CZ	-5.27	1.31	1.38
1	A	4038	GLY	C-O	-5.25	1.15	1.23
1	C	692	TYR	CE1-CZ	-5.25	1.31	1.38
1	G	3902	TYR	CG-CD2	-5.25	1.32	1.39
1	C	3902	TYR	CG-CD2	-5.24	1.32	1.39
1	G	4975	PHE	CG-CD1	-5.24	1.30	1.38
1	G	5029	ARG	CZ-NH2	-5.23	1.26	1.33
1	C	3964	SER	CA-CB	-5.23	1.45	1.52
1	G	4991	PHE	CG-CD2	-5.23	1.30	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	5021	PHE	CE1-CZ	-5.23	1.27	1.37
1	C	4038	GLY	C-O	-5.22	1.15	1.23
1	E	5009	TYR	CG-CD1	-5.22	1.32	1.39
1	A	4661	TYR	CG-CD1	-5.22	1.32	1.39
1	G	3816	MET	CG-SD	-5.22	1.67	1.81
1	G	692	TYR	CE1-CZ	-5.21	1.31	1.38
1	C	5018	CYS	CB-SG	-5.20	1.73	1.81
1	E	3964	SER	CA-CB	-5.20	1.45	1.52
1	G	1162	PHE	CG-CD1	-5.20	1.30	1.38
1	A	4964	GLY	C-O	-5.19	1.15	1.23
1	A	4990	PHE	CB-CG	-5.19	1.42	1.51
1	E	4988	TYR	CB-CG	-5.18	1.43	1.51
1	E	4990	PHE	CB-CG	-5.18	1.42	1.51
1	C	1162	PHE	CG-CD1	-5.18	1.30	1.38
1	C	5009	TYR	CG-CD1	-5.18	1.32	1.39
1	E	4975	PHE	CG-CD1	-5.18	1.30	1.38
1	A	5022	PHE	CE2-CZ	-5.17	1.27	1.37
1	A	4975	PHE	CG-CD1	-5.16	1.31	1.38
1	C	4990	PHE	CB-CG	-5.16	1.42	1.51
1	G	5020	ASP	CB-CG	5.16	1.62	1.51
1	A	5009	TYR	CG-CD1	-5.15	1.32	1.39
1	E	4182	GLU	C-O	-5.15	1.13	1.23
1	A	4182	GLU	C-O	-5.15	1.13	1.23
1	G	4202	ARG	CZ-NH2	5.15	1.39	1.33
1	A	3964	SER	CA-CB	-5.14	1.45	1.52
1	E	4038	GLY	C-O	-5.14	1.15	1.23
1	E	3902	TYR	CG-CD2	-5.13	1.32	1.39
1	A	4988	TYR	CB-CG	-5.13	1.44	1.51
1	E	4191	GLU	CD-OE1	-5.12	1.20	1.25
1	C	4988	TYR	CB-CG	-5.12	1.44	1.51
1	A	4191	GLU	CD-OE1	-5.12	1.20	1.25
1	E	5020	ASP	CB-CG	5.11	1.62	1.51
1	C	5020	ASP	CB-CG	5.11	1.62	1.51
1	C	5022	PHE	CE2-CZ	-5.11	1.27	1.37
1	C	4975	PHE	CG-CD1	-5.10	1.31	1.38
1	G	4711	PHE	CG-CD2	-5.10	1.31	1.38
1	E	4851	TYR	CG-CD1	-5.10	1.32	1.39
1	G	1275	ARG	CZ-NH1	-5.10	1.26	1.33
1	G	4179	GLY	C-O	5.10	1.31	1.23
1	E	4232	GLU	CD-OE1	5.10	1.31	1.25
1	G	4661	TYR	CG-CD1	-5.09	1.32	1.39
1	G	4194	TYR	CB-CG	-5.09	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	4959	PHE	CG-CD2	-5.09	1.31	1.38
1	E	4177	TYR	CG-CD1	-5.08	1.32	1.39
1	E	1275	ARG	CZ-NH1	-5.07	1.26	1.33
1	A	5020	ASP	CB-CG	5.06	1.62	1.51
1	G	4968	PHE	CE1-CZ	-5.05	1.27	1.37
1	A	1275	ARG	CZ-NH1	-5.04	1.26	1.33
1	C	4177	TYR	CG-CD1	-5.04	1.32	1.39
1	A	5019	TRP	CG-CD1	-5.03	1.29	1.36
1	C	1275	ARG	CZ-NH1	-5.03	1.26	1.33
1	C	4863	TYR	CE1-CZ	-5.03	1.32	1.38
1	G	4967	TYR	CG-CD1	-5.02	1.32	1.39
1	C	4191	GLU	CD-OE1	-5.02	1.20	1.25
1	C	5023	PRO	C-O	5.01	1.33	1.23
1	C	4093	PHE	CB-CG	5.00	1.59	1.51
1	A	4851	TYR	CE1-CZ	-5.00	1.32	1.38

All (442) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	5029	ARG	NE-CZ-NH1	10.79	125.69	120.30
1	E	5029	ARG	NE-CZ-NH1	10.60	125.60	120.30
1	E	4988	TYR	CB-CG-CD1	10.56	127.34	121.00
1	A	4988	TYR	CB-CG-CD1	10.55	127.33	121.00
1	C	4988	TYR	CB-CG-CD1	10.53	127.32	121.00
1	C	5029	ARG	NE-CZ-NH1	10.31	125.46	120.30
1	E	5017	ARG	NE-CZ-NH2	-10.20	115.20	120.30
1	C	5017	ARG	NE-CZ-NH2	-10.19	115.20	120.30
1	A	5017	ARG	NE-CZ-NH2	-10.19	115.21	120.30
1	A	1076	ARG	NE-CZ-NH1	10.16	125.38	120.30
1	G	1076	ARG	NE-CZ-NH1	10.13	125.36	120.30
1	A	5029	ARG	NE-CZ-NH1	10.12	125.36	120.30
1	E	1076	ARG	NE-CZ-NH1	10.07	125.34	120.30
1	G	4231	MET	CG-SD-CE	9.87	116.00	100.20
1	C	1076	ARG	NE-CZ-NH1	9.60	125.10	120.30
1	G	4988	TYR	CB-CG-CD1	9.33	126.60	121.00
1	G	5010	VAL	CG1-CB-CG2	-9.18	96.21	110.90
1	G	3729	MET	CG-SD-CE	-8.96	85.86	100.20
1	A	4231	MET	CG-SD-CE	8.91	114.46	100.20
1	C	4231	MET	CG-SD-CE	8.78	114.25	100.20
1	C	4146	LEU	CB-CG-CD1	-8.71	96.19	111.00
1	E	4231	MET	CG-SD-CE	8.69	114.10	100.20
1	E	5029	ARG	NE-CZ-NH2	-8.65	115.97	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	4146	LEU	CB-CG-CD1	-8.63	96.33	111.00
1	G	4850	LEU	CB-CG-CD1	8.62	125.65	111.00
1	A	4146	LEU	CB-CG-CD1	-8.55	96.47	111.00
1	C	3729	MET	CG-SD-CE	-8.42	86.72	100.20
1	E	3729	MET	CG-SD-CE	-8.39	86.77	100.20
1	G	4985	LEU	CB-CG-CD1	-8.39	96.73	111.00
1	A	3729	MET	CG-SD-CE	-8.36	86.83	100.20
1	A	5029	ARG	NE-CZ-NH2	-8.27	116.17	120.30
1	E	3886	ARG	NE-CZ-NH2	-8.20	116.20	120.30
1	C	5029	ARG	NE-CZ-NH2	-8.09	116.25	120.30
1	G	5029	ARG	NE-CZ-NH2	-8.00	116.30	120.30
1	A	3886	ARG	NE-CZ-NH2	-7.97	116.32	120.30
1	C	3886	ARG	NE-CZ-NH2	-7.94	116.33	120.30
1	C	1275	ARG	NE-CZ-NH2	7.90	124.25	120.30
1	G	1275	ARG	NE-CZ-NH2	7.88	124.24	120.30
1	A	1275	ARG	NE-CZ-NH2	7.86	124.23	120.30
1	G	4013	LEU	CB-CG-CD1	7.86	124.35	111.00
1	E	1275	ARG	NE-CZ-NH2	7.85	124.22	120.30
1	E	3841	VAL	CA-CB-CG1	7.81	122.62	110.90
1	C	3841	VAL	CA-CB-CG1	7.79	122.59	110.90
1	C	5010	VAL	CG1-CB-CG2	-7.79	98.44	110.90
1	A	3841	VAL	CA-CB-CG1	7.76	122.54	110.90
1	C	4184	MET	CB-CG-SD	-7.75	89.14	112.40
1	E	5010	VAL	CG1-CB-CG2	-7.72	98.55	110.90
1	A	5010	VAL	CG1-CB-CG2	-7.69	98.59	110.90
1	A	4184	MET	CB-CG-SD	-7.68	89.37	112.40
1	C	5021	PHE	CB-CG-CD2	-7.65	115.45	120.80
1	G	4184	MET	CB-CG-SD	-7.64	89.48	112.40
1	A	4850	LEU	CB-CG-CD1	7.59	123.91	111.00
1	G	4563	ARG	NE-CZ-NH1	-7.52	116.54	120.30
1	A	5021	PHE	CB-CG-CD2	-7.46	115.58	120.80
1	E	3891	LEU	CB-CG-CD2	-7.44	98.36	111.00
1	A	3891	LEU	CB-CG-CD2	-7.42	98.38	111.00
1	A	2168	VAL	CG1-CB-CG2	7.42	122.77	110.90
1	G	3841	VAL	CA-CB-CG1	7.42	122.03	110.90
1	G	2168	VAL	CG1-CB-CG2	7.39	122.73	110.90
1	E	4850	LEU	CB-CG-CD1	7.39	123.56	111.00
1	C	4850	LEU	CB-CG-CD1	7.38	123.54	111.00
1	E	5021	PHE	CB-CG-CD2	-7.38	115.64	120.80
1	E	2168	VAL	CG1-CB-CG2	7.34	122.65	110.90
1	C	2168	VAL	CG1-CB-CG2	7.34	122.64	110.90
1	A	4985	LEU	CB-CG-CD1	-7.31	98.57	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	4184	MET	CB-CG-SD	-7.30	90.50	112.40
1	A	808	TYR	N-CA-CB	7.29	123.72	110.60
1	E	808	TYR	N-CA-CB	7.28	123.71	110.60
1	G	808	TYR	N-CA-CB	7.26	123.66	110.60
1	C	808	TYR	N-CA-CB	7.25	123.65	110.60
1	C	3891	LEU	CB-CG-CD2	-7.23	98.70	111.00
1	G	4988	TYR	CB-CG-CD2	-7.21	116.67	121.00
1	G	4856	PHE	CB-CG-CD2	-7.20	115.76	120.80
1	A	4995	LEU	CB-CG-CD1	-7.18	98.79	111.00
1	E	4995	LEU	CB-CG-CD1	-7.13	98.88	111.00
1	C	4995	LEU	CB-CG-CD1	-7.09	98.94	111.00
1	C	4985	LEU	CB-CG-CD1	-7.06	99.00	111.00
1	A	4578	LEU	CB-CG-CD1	-7.04	99.03	111.00
1	C	3903	LEU	CB-CG-CD1	7.04	122.96	111.00
1	G	3782	MET	CG-SD-CE	7.02	111.43	100.20
1	E	4985	LEU	CB-CG-CD1	-6.92	99.23	111.00
1	A	3903	LEU	CB-CG-CD1	6.92	122.76	111.00
1	C	3567	PRO	N-CA-CB	6.88	111.56	103.30
1	A	3567	PRO	N-CA-CB	6.88	111.56	103.30
1	G	4183	ILE	CG1-CB-CG2	-6.88	96.27	111.40
1	C	4916	PHE	CB-CG-CD1	-6.87	115.99	120.80
1	E	3138	PRO	N-CA-CB	6.86	111.53	103.30
1	E	3567	PRO	N-CA-CB	6.85	111.53	103.30
1	A	3138	PRO	N-CA-CB	6.85	111.52	103.30
1	C	3138	PRO	N-CA-CB	6.84	111.51	103.30
1	G	4217	PHE	CB-CG-CD1	-6.81	116.03	120.80
1	E	3664	THR	N-CA-CB	6.81	123.24	110.30
1	G	4995	LEU	CB-CG-CD1	-6.80	99.44	111.00
1	E	3903	LEU	CB-CG-CD1	6.79	122.55	111.00
1	E	1493	TYR	N-CA-CB	6.79	122.81	110.60
1	A	4916	PHE	CB-CG-CD1	-6.78	116.06	120.80
1	A	3664	THR	N-CA-CB	6.76	123.14	110.30
1	G	3567	PRO	N-CA-CB	6.72	111.37	103.30
1	A	1493	TYR	N-CA-CB	6.71	122.68	110.60
1	C	3664	THR	N-CA-CB	6.71	123.05	110.30
1	E	3903	LEU	CD1-CG-CD2	-6.71	90.38	110.50
1	G	1493	TYR	N-CA-CB	6.70	122.66	110.60
1	C	1493	TYR	N-CA-CB	6.69	122.64	110.60
1	E	4916	PHE	CB-CG-CD1	-6.66	116.14	120.80
1	A	3903	LEU	CD1-CG-CD2	-6.66	90.53	110.50
1	G	3062	PRO	N-CA-CB	6.65	111.28	103.30
1	C	3903	LEU	CD1-CG-CD2	-6.63	90.60	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	5021	PHE	CB-CG-CD1	6.57	125.40	120.80
1	E	3773	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	C	3773	ARG	NE-CZ-NH2	-6.52	117.04	120.30
1	A	4183	ILE	CG1-CB-CG2	-6.52	97.05	111.40
1	C	4578	LEU	CB-CG-CD1	-6.50	99.95	111.00
1	E	4578	LEU	CB-CG-CD1	-6.48	99.98	111.00
1	A	4818	MET	CG-SD-CE	6.48	110.56	100.20
1	A	4844	LEU	CB-CG-CD2	-6.47	100.00	111.00
1	A	5021	PHE	CB-CG-CD1	6.46	125.32	120.80
1	C	5019	TRP	CB-CA-C	-6.43	97.54	110.40
1	E	3297	PRO	N-CA-CB	6.42	111.00	103.30
1	A	3297	PRO	N-CA-CB	6.42	111.00	103.30
1	C	4844	LEU	CB-CG-CD2	-6.41	100.10	111.00
1	E	5019	TRP	CB-CA-C	-6.41	97.58	110.40
1	C	3297	PRO	N-CA-CB	6.40	110.98	103.30
1	C	4818	MET	CG-SD-CE	6.39	110.43	100.20
1	C	4183	ILE	CG1-CB-CG2	-6.39	97.35	111.40
1	E	4183	ILE	CG1-CB-CG2	-6.38	97.36	111.40
1	E	5021	PHE	CB-CG-CD1	6.38	125.27	120.80
1	A	3773	ARG	NE-CZ-NH2	-6.37	117.11	120.30
1	E	3519	PRO	N-CA-CB	6.37	110.94	103.30
1	A	5019	TRP	CB-CA-C	-6.36	97.68	110.40
1	A	3519	PRO	N-CA-CB	6.35	110.92	103.30
1	C	3519	PRO	N-CA-CB	6.35	110.92	103.30
1	G	3926	LEU	CB-CG-CD2	-6.33	100.23	111.00
1	C	3021	PRO	N-CA-CB	6.32	110.88	103.30
1	A	3275	PRO	N-CA-CB	6.31	110.87	103.30
1	A	3021	PRO	N-CA-CB	6.29	110.85	103.30
1	E	2631	PRO	N-CA-CB	6.29	110.85	103.30
1	E	4818	MET	CG-SD-CE	6.29	110.27	100.20
1	E	3021	PRO	N-CA-CB	6.28	110.84	103.30
1	G	3965	LEU	CB-CG-CD1	-6.28	100.32	111.00
1	E	3289	PRO	N-CA-CB	6.26	110.81	103.30
1	G	2631	PRO	N-CA-CB	6.26	110.81	103.30
1	A	2712	PRO	N-CA-CB	6.25	110.80	103.30
1	E	3275	PRO	N-CA-CB	6.25	110.80	103.30
1	A	2631	PRO	N-CA-CB	6.25	110.80	103.30
1	C	2631	PRO	N-CA-CB	6.23	110.78	103.30
1	C	3275	PRO	N-CA-CB	6.23	110.78	103.30
1	A	3289	PRO	N-CA-CB	6.22	110.77	103.30
1	C	3289	PRO	N-CA-CB	6.22	110.77	103.30
1	C	2712	PRO	N-CA-CB	6.22	110.77	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	4173	TYR	CB-CG-CD1	-6.21	117.27	121.00
1	G	2640	PRO	N-CA-CB	6.21	110.76	103.30
1	E	2712	PRO	N-CA-CB	6.21	110.75	103.30
1	C	2640	PRO	N-CA-CB	6.21	110.75	103.30
1	G	2712	PRO	N-CA-CB	6.21	110.75	103.30
1	A	2640	PRO	N-CA-CB	6.20	110.74	103.30
1	G	3904	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	A	3188	PRO	N-CA-CB	6.19	110.72	103.30
1	E	3188	PRO	N-CA-CB	6.18	110.72	103.30
1	C	3188	PRO	N-CA-CB	6.17	110.70	103.30
1	E	2640	PRO	N-CA-CB	6.17	110.70	103.30
1	E	4173	TYR	CB-CG-CD1	-6.16	117.31	121.00
1	G	3519	PRO	N-CA-CB	6.16	110.69	103.30
1	G	3275	PRO	N-CA-CB	6.14	110.67	103.30
1	A	3360	PRO	N-CA-CB	6.12	110.64	103.30
1	A	4809	PHE	CB-CG-CD2	-6.12	116.52	120.80
1	A	4988	TYR	CB-CG-CD2	-6.11	117.33	121.00
1	E	3360	PRO	N-CA-CB	6.11	110.63	103.30
1	G	3297	PRO	N-CA-CB	6.11	110.63	103.30
1	C	3360	PRO	N-CA-CB	6.10	110.62	103.30
1	G	3903	LEU	CB-CG-CD2	6.10	121.36	111.00
1	E	3903	LEU	CB-CG-CD2	6.09	121.36	111.00
1	G	3903	LEU	CD1-CG-CD2	-6.08	92.25	110.50
1	C	1076	ARG	NE-CZ-NH2	-6.07	117.26	120.30
1	G	4648	LEU	CB-CG-CD2	6.06	121.30	111.00
1	A	3698	LEU	CB-CG-CD2	-6.05	100.71	111.00
1	C	3903	LEU	CB-CG-CD2	6.05	121.29	111.00
1	G	3282	PRO	N-CA-CB	6.05	110.56	103.30
1	E	3698	LEU	CB-CG-CD2	-6.05	100.72	111.00
1	A	4173	TYR	CB-CG-CD1	-6.04	117.37	121.00
1	E	4988	TYR	CB-CG-CD2	-6.04	117.38	121.00
1	G	2701	PRO	N-CA-CB	6.04	110.55	103.30
1	G	3289	PRO	N-CA-CB	6.04	110.55	103.30
1	E	2701	PRO	N-CA-CB	6.04	110.54	103.30
1	C	2701	PRO	N-CA-CB	6.04	110.54	103.30
1	E	3410	PRO	N-CA-CB	6.04	110.54	103.30
1	G	3138	PRO	N-CA-CB	6.03	110.54	103.30
1	E	3301	PRO	N-CA-CB	6.03	110.54	103.30
1	E	3282	PRO	N-CA-CB	6.03	110.54	103.30
1	C	3282	PRO	N-CA-CB	6.03	110.53	103.30
1	G	3303	PRO	N-CA-CB	6.02	110.53	103.30
1	A	2701	PRO	N-CA-CB	6.02	110.53	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	3832	ILE	CG1-CB-CG2	-6.02	98.16	111.40
1	A	3282	PRO	N-CA-CB	6.01	110.52	103.30
1	G	4028	LEU	CB-CG-CD1	-6.01	100.78	111.00
1	G	3410	PRO	N-CA-CB	6.01	110.52	103.30
1	C	3698	LEU	CB-CG-CD2	-6.01	100.78	111.00
1	E	3351	PRO	N-CA-CB	6.01	110.51	103.30
1	G	3957	VAL	CG1-CB-CG2	-6.01	101.28	110.90
1	C	2711	PRO	N-CA-CB	6.00	110.50	103.30
1	A	3410	PRO	N-CA-CB	6.00	110.50	103.30
1	G	3021	PRO	N-CA-CB	6.00	110.50	103.30
1	C	221	ARG	NE-CZ-NH2	-5.99	117.30	120.30
1	A	2711	PRO	N-CA-CB	5.98	110.48	103.30
1	C	4988	TYR	CB-CG-CD2	-5.98	117.41	121.00
1	E	2711	PRO	N-CA-CB	5.98	110.47	103.30
1	C	3301	PRO	N-CA-CB	5.97	110.46	103.30
1	E	221	ARG	NE-CZ-NH2	-5.97	117.32	120.30
1	C	3410	PRO	N-CA-CB	5.96	110.45	103.30
1	G	4880	MET	CG-SD-CE	5.96	109.74	100.20
1	G	3891	LEU	CB-CG-CD2	-5.96	100.88	111.00
1	C	3527	PRO	N-CA-CB	5.95	110.44	103.30
1	G	4703	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	A	3527	PRO	N-CA-CB	5.94	110.43	103.30
1	E	3527	PRO	N-CA-CB	5.93	110.42	103.30
1	G	3527	PRO	N-CA-CB	5.93	110.42	103.30
1	A	3301	PRO	N-CA-CB	5.93	110.42	103.30
1	A	3351	PRO	N-CA-CB	5.93	110.41	103.30
1	G	2711	PRO	N-CA-CB	5.92	110.41	103.30
1	C	3351	PRO	N-CA-CB	5.92	110.40	103.30
1	C	3302	PRO	N-CA-CB	5.91	110.39	103.30
1	E	3302	PRO	N-CA-CB	5.91	110.39	103.30
1	E	4844	LEU	CB-CG-CD2	-5.91	100.96	111.00
1	G	3188	PRO	N-CA-CB	5.91	110.39	103.30
1	G	3933	PHE	CB-CG-CD1	-5.90	116.67	120.80
1	A	3302	PRO	N-CA-CB	5.89	110.37	103.30
1	G	3301	PRO	N-CA-CB	5.89	110.37	103.30
1	G	221	ARG	NE-CZ-NH2	-5.87	117.36	120.30
1	C	109	LEU	CB-CG-CD2	-5.86	101.04	111.00
1	G	1659	LEU	CB-CG-CD1	-5.85	101.05	111.00
1	A	3903	LEU	CB-CG-CD2	5.84	120.94	111.00
1	G	3302	PRO	N-CA-CB	5.84	110.31	103.30
1	E	3933	PHE	CB-CG-CD1	-5.84	116.71	120.80
1	G	4801	LEU	CB-CG-CD2	5.84	120.92	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	4818	MET	CG-SD-CE	5.83	109.53	100.20
1	A	1659	LEU	CB-CG-CD1	-5.82	101.10	111.00
1	A	3303	PRO	N-CA-CB	5.82	110.29	103.30
1	A	4988	TYR	CE1-CZ-OH	5.82	135.81	120.10
1	E	3303	PRO	N-CA-CB	5.82	110.28	103.30
1	G	3360	PRO	N-CA-CB	5.82	110.28	103.30
1	E	3995	VAL	CA-CB-CG2	-5.81	102.18	110.90
1	G	4967	TYR	CB-CG-CD1	-5.81	117.51	121.00
1	E	4180	ARG	NE-CZ-NH2	-5.81	117.40	120.30
1	G	5017	ARG	NE-CZ-NH2	-5.81	117.40	120.30
1	A	3990	VAL	CG1-CB-CG2	-5.80	101.62	110.90
1	C	3995	VAL	CA-CB-CG2	-5.80	102.20	110.90
1	E	1659	LEU	CB-CG-CD1	-5.80	101.14	111.00
1	A	3995	VAL	CA-CB-CG2	-5.79	102.21	110.90
1	C	4988	TYR	CE1-CZ-OH	5.79	135.74	120.10
1	E	4988	TYR	CE1-CZ-OH	5.79	135.74	120.10
1	G	3351	PRO	N-CA-CB	5.79	110.24	103.30
1	C	3303	PRO	N-CA-CB	5.79	110.24	103.30
1	C	1659	LEU	CB-CG-CD1	-5.78	101.17	111.00
1	G	3427	PRO	N-CA-CB	5.78	110.23	103.30
1	G	1076	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	A	3933	PHE	CB-CG-CD1	-5.74	116.78	120.80
1	G	4986	ALA	CB-CA-C	-5.74	101.49	110.10
1	G	109	LEU	CB-CG-CD2	-5.74	101.25	111.00
1	A	221	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	A	3427	PRO	N-CA-CB	5.72	110.17	103.30
1	G	4629	TYR	CB-CG-CD2	-5.72	117.57	121.00
1	G	4990	PHE	CB-CG-CD1	-5.71	116.80	120.80
1	A	3085	PRO	N-CA-CB	5.71	110.15	103.30
1	A	4703	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	G	3294	PRO	N-CA-CB	5.70	110.14	103.30
1	C	3933	PHE	CB-CG-CD1	-5.70	116.81	120.80
1	E	3990	VAL	CG1-CB-CG2	-5.69	101.79	110.90
1	G	5021	PHE	CB-CG-CD2	-5.69	116.81	120.80
1	G	5017	ARG	CG-CD-NE	-5.69	99.85	111.80
1	E	3085	PRO	N-CA-CB	5.69	110.13	103.30
1	C	3085	PRO	N-CA-CB	5.68	110.12	103.30
1	A	45	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	C	3294	PRO	N-CA-CB	5.68	110.12	103.30
1	G	5028	PHE	CB-CG-CD1	5.68	124.78	120.80
1	A	3294	PRO	N-CA-CB	5.68	110.12	103.30
1	C	3427	PRO	N-CA-CB	5.68	110.11	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	3926	LEU	CB-CG-CD2	-5.68	101.35	111.00
1	C	3990	VAL	CG1-CB-CG2	-5.67	101.82	110.90
1	E	3427	PRO	N-CA-CB	5.67	110.11	103.30
1	A	109	LEU	CB-CG-CD2	-5.67	101.36	111.00
1	G	4851	TYR	CB-CG-CD1	5.67	124.40	121.00
1	C	4629	TYR	CB-CG-CD1	5.67	124.40	121.00
1	G	3880	PHE	CB-CG-CD1	-5.66	116.83	120.80
1	E	3887	PHE	CB-CG-CD2	-5.65	116.84	120.80
1	A	4217	PHE	CB-CG-CD1	-5.65	116.85	120.80
1	E	3294	PRO	N-CA-CB	5.64	110.07	103.30
1	A	4673	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	E	4703	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	E	109	LEU	CB-CG-CD2	-5.63	101.42	111.00
1	C	3962	PHE	CB-CG-CD2	-5.63	116.86	120.80
1	G	4629	TYR	CB-CG-CD1	5.63	124.38	121.00
1	C	45	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	C	4673	ARG	NE-CZ-NH2	-5.61	117.49	120.30
1	G	3208	PRO	N-CA-CB	5.61	110.03	103.30
1	E	45	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	E	14	LEU	CB-CG-CD1	-5.60	101.47	111.00
1	E	3962	PHE	CB-CG-CD2	-5.60	116.88	120.80
1	A	14	LEU	CB-CG-CD1	-5.59	101.49	111.00
1	G	3989	VAL	CG1-CB-CG2	-5.58	101.96	110.90
1	A	5028	PHE	CB-CG-CD1	5.58	124.71	120.80
1	A	3962	PHE	CB-CG-CD2	-5.58	116.90	120.80
1	C	14	LEU	CB-CG-CD1	-5.57	101.52	111.00
1	G	3962	PHE	CB-CG-CD2	-5.56	116.91	120.80
1	A	3887	PHE	CB-CG-CD2	-5.56	116.91	120.80
1	A	4837	LEU	CB-CG-CD2	-5.56	101.55	111.00
1	G	45	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	E	5017	ARG	NH1-CZ-NH2	5.54	125.49	119.40
1	G	3721	LEU	CB-CG-CD1	5.54	120.41	111.00
1	G	4892	ARG	NE-CZ-NH1	-5.54	117.53	120.30
1	A	4215	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	A	2616	PRO	N-CA-CB	5.53	109.94	103.30
1	C	4703	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	E	4217	PHE	CB-CG-CD1	-5.53	116.93	120.80
1	G	14	LEU	CB-CG-CD1	-5.53	101.61	111.00
1	C	4629	TYR	CB-CG-CD2	-5.52	117.69	121.00
1	C	4112	LEU	CB-CG-CD1	-5.52	101.62	111.00
1	A	2658	PRO	N-CA-CB	5.51	109.92	103.30
1	A	4112	LEU	CB-CG-CD1	-5.51	101.62	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	4217	PHE	CB-CG-CD1	-5.51	116.94	120.80
1	G	2658	PRO	N-CA-CB	5.51	109.91	103.30
1	E	4112	LEU	CB-CG-CD1	-5.51	101.64	111.00
1	A	3926	LEU	CB-CG-CD2	-5.50	101.64	111.00
1	E	2658	PRO	N-CA-CB	5.50	109.90	103.30
1	A	4943	LEU	CB-CG-CD1	5.50	120.34	111.00
1	E	3832	ILE	CG1-CB-CG2	-5.49	99.32	111.40
1	E	4673	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	E	4629	TYR	CB-CG-CD1	5.49	124.29	121.00
1	G	2616	PRO	N-CA-CB	5.49	109.88	103.30
1	C	4180	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	E	2616	PRO	N-CA-CB	5.48	109.88	103.30
1	C	2658	PRO	N-CA-CB	5.48	109.87	103.30
1	C	3832	ILE	CG1-CB-CG2	-5.47	99.38	111.40
1	C	2616	PRO	N-CA-CB	5.46	109.86	103.30
1	E	3926	LEU	CB-CG-CD2	-5.46	101.72	111.00
1	G	78	LEU	CB-CG-CD2	-5.46	101.72	111.00
1	A	3832	ILE	CG1-CB-CG2	-5.46	99.40	111.40
1	C	78	LEU	CB-CG-CD2	-5.46	101.73	111.00
1	E	4215	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	G	3918	CYS	CA-CB-SG	-5.45	104.19	114.00
1	C	3887	PHE	CB-CG-CD2	-5.45	116.98	120.80
1	G	5019	TRP	CB-CA-C	-5.45	99.51	110.40
1	C	3208	PRO	N-CA-CB	5.44	109.83	103.30
1	E	3208	PRO	N-CA-CB	5.44	109.83	103.30
1	E	3999	MET	CG-SD-CE	5.44	108.91	100.20
1	C	5028	PHE	CB-CG-CD1	5.44	124.61	120.80
1	A	3999	MET	CG-SD-CE	5.43	108.89	100.20
1	C	3999	MET	CG-SD-CE	5.43	108.89	100.20
1	A	3208	PRO	N-CA-CB	5.43	109.81	103.30
1	A	4178	LEU	CB-CG-CD2	5.42	120.22	111.00
1	G	3995	VAL	CA-CB-CG2	-5.42	102.77	110.90
1	E	4809	PHE	CB-CG-CD2	-5.40	117.02	120.80
1	G	4992	LEU	CB-CG-CD1	-5.39	101.84	111.00
1	G	5021	PHE	CB-CG-CD1	5.38	124.56	120.80
1	C	5017	ARG	NH1-CZ-NH2	5.38	125.31	119.40
1	G	4217	PHE	CB-CG-CD2	5.37	124.56	120.80
1	G	3085	PRO	N-CA-CB	5.37	109.74	103.30
1	A	5017	ARG	NH1-CZ-NH2	5.36	125.30	119.40
1	C	4992	LEU	CB-CG-CD1	-5.36	101.89	111.00
1	C	4215	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	G	4237	PHE	CB-CG-CD1	-5.36	117.05	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	4677	LEU	CB-CG-CD1	-5.35	101.90	111.00
1	E	4629	TYR	CB-CG-CD2	-5.35	117.79	121.00
1	E	4838	VAL	CG1-CB-CG2	5.34	119.45	110.90
1	E	5028	PHE	CB-CG-CD1	5.34	124.54	120.80
1	E	4920	PHE	CB-CG-CD2	-5.34	117.06	120.80
1	C	4880	MET	CG-SD-CE	5.32	108.71	100.20
1	C	5017	ARG	CG-CD-NE	-5.32	100.63	111.80
1	E	4992	LEU	CB-CG-CD1	-5.31	101.97	111.00
1	A	4992	LEU	CB-CG-CD1	-5.31	101.98	111.00
1	E	5017	ARG	CG-CD-NE	-5.31	100.66	111.80
1	C	4809	PHE	CB-CG-CD2	-5.30	117.09	120.80
1	A	4677	LEU	CB-CG-CD1	-5.30	102.00	111.00
1	E	78	LEU	CB-CG-CD2	-5.27	102.05	111.00
1	E	4178	LEU	CB-CG-CD2	5.27	119.95	111.00
1	A	3816	MET	CG-SD-CE	5.26	108.62	100.20
1	A	4180	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	G	4180	ARG	CD-NE-CZ	-5.25	116.25	123.60
1	C	4173	TYR	CB-CG-CD2	5.25	124.15	121.00
1	A	78	LEU	CB-CG-CD2	-5.24	102.09	111.00
1	E	4677	LEU	CB-CG-CD1	-5.23	102.11	111.00
1	E	4180	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	E	3816	MET	CG-SD-CE	5.22	108.55	100.20
1	C	4163	PHE	CB-CG-CD1	-5.22	117.15	120.80
1	E	4173	TYR	CB-CG-CD2	5.21	124.13	121.00
1	C	4943	LEU	CB-CG-CD1	5.20	119.84	111.00
1	A	4173	TYR	CB-CG-CD2	5.20	124.12	121.00
1	G	3915	ILE	CG1-CB-CG2	-5.20	99.96	111.40
1	C	3062	PRO	N-CA-CB	5.20	109.53	103.30
1	C	3918	CYS	CA-CB-SG	-5.20	104.65	114.00
1	A	4163	PHE	CB-CG-CD1	-5.19	117.17	120.80
1	C	4178	LEU	CB-CG-CD2	5.19	119.83	111.00
1	C	3816	MET	CG-SD-CE	5.19	108.50	100.20
1	E	3062	PRO	N-CA-CB	5.18	109.52	103.30
1	G	4170	ILE	CG1-CB-CG2	-5.18	100.00	111.40
1	G	4245	MET	CG-SD-CE	-5.18	91.91	100.20
1	C	3934	TYR	CB-CG-CD1	-5.18	117.89	121.00
1	E	4837	LEU	CB-CG-CD2	-5.18	102.20	111.00
1	E	3969	ILE	CG1-CB-CG2	-5.16	100.04	111.40
1	A	3062	PRO	N-CA-CB	5.16	109.49	103.30
1	C	3904	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	G	4686	LEU	CB-CG-CD2	-5.16	102.23	111.00
1	G	4844	LEU	CB-CG-CD2	-5.15	102.24	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	3918	CYS	CA-CB-SG	-5.15	104.74	114.00
1	E	3918	CYS	CA-CB-SG	-5.15	104.74	114.00
1	A	4967	TYR	CB-CG-CD1	-5.14	117.92	121.00
1	A	5017	ARG	CG-CD-NE	-5.14	101.01	111.80
1	G	4673	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	C	4823	LEU	CB-CG-CD1	-5.13	102.27	111.00
1	G	4112	LEU	CB-CG-CD1	-5.13	102.27	111.00
1	C	4917	ASP	CB-CG-OD2	5.13	122.91	118.30
1	A	3904	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	C	3969	ILE	CG1-CB-CG2	-5.12	100.13	111.40
1	A	4180	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	G	4711	PHE	CB-CG-CD2	-5.11	117.22	120.80
1	A	3934	TYR	CB-CG-CD1	-5.11	117.93	121.00
1	G	4887	MET	CG-SD-CE	5.11	108.38	100.20
1	A	4917	ASP	CB-CG-OD2	5.11	122.90	118.30
1	A	3969	ILE	CG1-CB-CG2	-5.11	100.16	111.40
1	G	2458	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	C	4837	LEU	CB-CG-CD2	-5.09	102.35	111.00
1	E	4163	PHE	CB-CG-CD1	-5.08	117.24	120.80
1	C	4920	PHE	CB-CG-CD2	-5.08	117.24	120.80
1	G	3885	PHE	CB-CG-CD2	-5.08	117.24	120.80
1	C	4180	ARG	NE-CZ-NH1	5.07	122.84	120.30
1	G	4173	TYR	CB-CG-CD1	-5.07	117.96	121.00
1	C	4181	ILE	CG1-CB-CG2	-5.07	100.25	111.40
1	E	4823	LEU	CB-CG-CD1	-5.07	102.39	111.00
1	G	3664	THR	N-CA-C	5.07	124.67	111.00
1	C	4237	PHE	CB-CG-CD1	-5.05	117.26	120.80
1	G	4026	MET	CG-SD-CE	-5.05	92.12	100.20
1	E	4181	ILE	CG1-CB-CG2	-5.04	100.30	111.40
1	C	4967	TYR	CB-CG-CD1	-5.04	117.97	121.00
1	E	2458	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	A	4880	MET	CG-SD-CE	5.03	108.25	100.20
1	A	4920	PHE	CB-CG-CD2	-5.03	117.28	120.80
1	E	4967	TYR	CB-CG-CD1	-5.03	117.98	121.00
1	G	4653	VAL	CG1-CB-CG2	-5.02	102.86	110.90
1	E	3904	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	G	5019	TRP	N-CA-C	5.01	124.53	111.00
1	C	4177	TYR	N-CA-C	5.01	124.52	111.00
1	A	2458	ARG	NE-CZ-NH2	-5.01	117.80	120.30
1	C	3721	LEU	CB-CG-CD2	-5.00	102.50	111.00
1	A	4629	TYR	CB-CG-CD1	5.00	124.00	121.00

There are no chirality outliers.

All (80) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1464	PHE	Mainchain,Peptide
1	A	1465	ASP	Peptide
1	A	1588	ALA	Mainchain,Peptide
1	A	1744	ALA	Mainchain,Peptide
1	A	1828	ASP	Mainchain,Peptide
1	A	1867	GLU	Peptide
1	A	2361	PRO	Mainchain,Peptide
1	A	3663	LEU	Mainchain,Peptide
1	A	697	GLY	Mainchain,Peptide
1	A	807	GLY	Mainchain,Peptide
1	A	841	GLY	Mainchain,Peptide
1	C	1464	PHE	Mainchain,Peptide
1	C	1465	ASP	Peptide
1	C	1588	ALA	Mainchain,Peptide
1	C	1744	ALA	Mainchain,Peptide
1	C	1828	ASP	Mainchain,Peptide
1	C	1867	GLU	Peptide
1	C	2361	PRO	Mainchain,Peptide
1	C	3663	LEU	Mainchain,Peptide
1	C	697	GLY	Mainchain,Peptide
1	C	807	GLY	Mainchain,Peptide
1	C	841	GLY	Mainchain,Peptide
1	E	1464	PHE	Mainchain,Peptide
1	E	1465	ASP	Peptide
1	E	1588	ALA	Mainchain,Peptide
1	E	1744	ALA	Mainchain,Peptide
1	E	1828	ASP	Mainchain,Peptide
1	E	1867	GLU	Peptide
1	E	2361	PRO	Mainchain,Peptide
1	E	3663	LEU	Mainchain,Peptide
1	E	697	GLY	Mainchain,Peptide
1	E	807	GLY	Mainchain,Peptide
1	E	841	GLY	Mainchain,Peptide
1	G	1464	PHE	Mainchain,Peptide
1	G	1465	ASP	Peptide
1	G	1588	ALA	Mainchain,Peptide
1	G	1744	ALA	Mainchain,Peptide
1	G	1828	ASP	Mainchain,Peptide
1	G	1867	GLU	Peptide
1	G	2361	PRO	Mainchain,Peptide
1	G	3663	LEU	Mainchain,Peptide
1	G	697	GLY	Mainchain,Peptide

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Mol	Chain	Res	Type	Group
1	G	807	GLY	Mainchain,Peptide
1	G	841	GLY	Mainchain,Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	26917	0	24461	801	0
1	C	26917	0	24461	789	0
1	E	26917	0	24461	787	0
1	G	26917	0	24461	770	0
2	B	832	0	831	34	0
2	D	832	0	831	35	0
2	F	832	0	831	33	0
2	H	832	0	831	28	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
All	All	111000	0	101168	3132	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 15.

All (3132) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1782:PHE:O	2:H:82:TYR:OH	1.75	1.03
1:A:1782:PHE:O	2:B:82:TYR:OH	1.76	1.03
1:A:4888:TYR:CD1	1:G:4914:VAL:HG23	1.95	1.02
1:C:1782:PHE:O	2:D:82:TYR:OH	1.78	1.01
1:E:1782:PHE:O	2:F:82:TYR:OH	1.77	1.00
1:E:4934:GLY:HA3	1:G:4937:ILE:HG12	1.44	1.00
1:G:3936:TYR:O	1:G:3940:LYS:NZ	1.99	0.95
1:A:4914:VAL:HG23	1:C:4888:TYR:CD1	2.02	0.95
1:C:4914:VAL:HG23	1:E:4888:TYR:CD1	2.03	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3936:TYR:O	1:A:3940:LYS:NZ	2.03	0.92
1:C:3936:TYR:O	1:C:3940:LYS:NZ	2.03	0.92
1:C:4865:LYS:NZ	1:C:4876:CYS:SG	2.44	0.91
1:E:3936:TYR:O	1:E:3940:LYS:NZ	2.03	0.91
1:A:4865:LYS:NZ	1:A:4876:CYS:SG	2.45	0.90
1:E:4914:VAL:HG23	1:G:4888:TYR:CD1	2.07	0.89
1:A:2452:ARG:NH1	1:G:174:VAL:O	2.05	0.89
1:E:174:VAL:O	1:G:2452:ARG:NH1	2.06	0.88
1:E:4865:LYS:NZ	1:E:4876:CYS:SG	2.45	0.88
1:A:174:VAL:O	1:C:2452:ARG:NH1	2.07	0.87
1:C:174:VAL:O	1:E:2452:ARG:NH1	2.07	0.87
1:A:1708:ARG:NH1	1:A:1836:PHE:O	2.08	0.87
1:G:1708:ARG:NH1	1:G:1836:PHE:O	2.08	0.87
1:A:2347:GLU:OE2	1:A:3852:LYS:HE3	1.74	0.87
1:E:1243:PRO:HD2	1:E:1458:HIS:HB3	1.56	0.87
1:E:1708:ARG:NH1	1:E:1836:PHE:O	2.07	0.86
1:C:1708:ARG:NH1	1:C:1836:PHE:O	2.08	0.86
1:C:683:ARG:NH1	1:C:705:ASN:O	2.09	0.86
1:A:4938:ASP:OD2	1:C:4940:PHE:HB3	1.76	0.86
1:A:277:GLY:HA2	1:A:317:ARG:HH12	1.40	0.85
1:A:683:ARG:NH1	1:A:705:ASN:O	2.10	0.85
1:C:277:GLY:HA2	1:C:317:ARG:HH12	1.40	0.85
1:E:277:GLY:HA2	1:E:317:ARG:HH12	1.40	0.85
1:E:683:ARG:NH1	1:E:705:ASN:O	2.09	0.85
1:C:4938:ASP:OD2	1:E:4940:PHE:HB3	1.76	0.85
1:A:2347:GLU:OE2	1:A:3852:LYS:CE	2.25	0.85
1:G:1610:ASN:ND2	1:G:1652:GLU:OE2	2.09	0.85
1:G:277:GLY:HA2	1:G:317:ARG:HH12	1.40	0.84
1:G:683:ARG:NH1	1:G:705:ASN:O	2.09	0.84
1:E:1727:ARG:NH1	1:E:1851:MET:O	2.11	0.84
1:C:1610:ASN:ND2	1:C:1652:GLU:OE2	2.09	0.84
1:G:1727:ARG:NH1	1:G:1851:MET:O	2.10	0.84
1:A:1727:ARG:NH1	1:A:1851:MET:O	2.11	0.84
1:E:1610:ASN:ND2	1:E:1652:GLU:OE2	2.11	0.83
1:E:495:ASN:HB3	1:E:553:ARG:HH22	1.43	0.83
1:G:4865:LYS:NZ	1:G:4876:CYS:SG	2.52	0.83
1:G:495:ASN:HB3	1:G:553:ARG:HH22	1.43	0.83
1:C:1727:ARG:NH1	1:C:1851:MET:O	2.11	0.83
1:E:4049:VAL:HG21	1:E:4159:ARG:HD3	1.61	0.83
1:A:4934:GLY:HA3	1:C:4937:ILE:HG12	1.58	0.82
1:A:2341:VAL:HG13	1:A:2342:ASN:H	1.45	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2341:VAL:HG13	1:C:2342:ASN:H	1.45	0.82
1:A:1610:ASN:ND2	1:A:1652:GLU:OE2	2.12	0.82
1:A:4049:VAL:HG21	1:A:4159:ARG:HD3	1.62	0.82
1:A:3969:ILE:HD11	1:A:3980:LEU:HD13	1.62	0.82
1:A:495:ASN:HB3	1:A:553:ARG:HH22	1.43	0.82
1:C:4049:VAL:HG21	1:C:4159:ARG:HD3	1.61	0.82
1:C:3969:ILE:HD11	1:C:3980:LEU:HD13	1.63	0.81
1:C:495:ASN:HB3	1:C:553:ARG:HH22	1.43	0.81
1:C:622:THR:HG23	1:C:626:LEU:HD12	1.61	0.81
1:A:622:THR:HG23	1:A:626:LEU:HD12	1.61	0.81
1:C:1243:PRO:HD2	1:C:1458:HIS:HB3	1.62	0.80
1:E:2341:VAL:HG13	1:E:2342:ASN:H	1.45	0.80
1:C:595:ARG:NE	1:C:1643:GLU:OE2	2.14	0.80
1:E:3969:ILE:HD11	1:E:3980:LEU:HD13	1.63	0.80
1:G:595:ARG:NE	1:G:1643:GLU:OE2	2.14	0.80
1:G:2341:VAL:HG13	1:G:2342:ASN:H	1.46	0.80
1:C:1206:GLN:H	1:C:1227:ALA:HB3	1.47	0.80
1:E:622:THR:HG23	1:E:626:LEU:HD12	1.61	0.80
1:E:4938:ASP:OD2	1:G:4940:PHE:HB3	1.81	0.80
1:G:622:THR:HG23	1:G:626:LEU:HD12	1.62	0.80
1:G:35:LEU:HD13	1:G:49:LEU:HD22	1.65	0.79
1:A:2770:LYS:HB3	1:A:2775:TRP:HB2	1.65	0.79
1:E:595:ARG:NE	1:E:1643:GLU:OE2	2.14	0.79
1:E:35:LEU:HD13	1:E:49:LEU:HD22	1.65	0.79
1:A:595:ARG:NE	1:A:1643:GLU:OE2	2.14	0.79
1:C:2770:LYS:HB3	1:C:2775:TRP:HB2	1.65	0.79
1:E:2770:LYS:HB3	1:E:2775:TRP:HB2	1.65	0.79
1:C:35:LEU:HD13	1:C:49:LEU:HD22	1.65	0.78
1:E:1125:ASN:HD22	1:E:1130:GLN:HG3	1.47	0.78
1:G:1206:GLN:H	1:G:1227:ALA:HB3	1.47	0.78
1:A:1125:ASN:HD22	1:A:1130:GLN:HG3	1.47	0.78
1:A:1206:GLN:H	1:A:1227:ALA:HB3	1.47	0.78
1:G:3927:GLN:HE21	1:G:3991:GLY:HA3	1.47	0.78
1:A:4658:ILE:HG22	1:A:4792:LEU:HB3	1.66	0.78
1:C:4658:ILE:HG22	1:C:4792:LEU:HB3	1.66	0.78
1:A:157:ARG:NH1	1:A:167:ASP:OD2	2.17	0.78
1:E:72:SER:O	1:E:99:ARG:NH1	2.17	0.78
1:E:157:ARG:NH1	1:E:167:ASP:OD2	2.17	0.78
1:G:2124:LEU:HD21	1:G:3677:LEU:HD21	1.66	0.78
1:G:2770:LYS:HB3	1:G:2775:TRP:HB2	1.64	0.77
1:A:35:LEU:HD13	1:A:49:LEU:HD22	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4934:GLY:HA3	1:E:4937:ILE:HG12	1.67	0.77
1:A:1623:ARG:HH11	1:A:1626:TRP:HE1	1.33	0.77
1:C:157:ARG:NH1	1:C:167:ASP:OD2	2.18	0.77
1:G:157:ARG:NH1	1:G:167:ASP:OD2	2.17	0.77
1:C:579:GLN:H	1:C:582:HIS:HD2	1.33	0.76
1:E:4658:ILE:HG22	1:E:4792:LEU:HB3	1.66	0.76
2:H:24:VAL:HG12	2:H:103:LEU:HA	1.66	0.76
1:A:3927:GLN:HE21	1:A:3991:GLY:HA3	1.50	0.76
1:A:674:PHE:HB3	2:B:40:ARG:HH12	1.51	0.76
1:C:674:PHE:HB3	2:D:40:ARG:HH12	1.50	0.76
1:C:76:ARG:HE	1:E:3844:LEU:HD21	1.51	0.76
1:E:674:PHE:HB3	2:F:40:ARG:HH12	1.50	0.76
1:A:579:GLN:H	1:A:582:HIS:HD2	1.33	0.75
1:A:72:SER:O	1:A:99:ARG:NH1	2.20	0.75
1:E:138:GLN:NE2	1:E:146:CYS:SG	2.58	0.75
1:G:3948:LYS:HG3	1:G:4012:LEU:HD12	1.66	0.75
1:C:138:GLN:NE2	1:C:146:CYS:SG	2.59	0.75
1:E:3927:GLN:HE21	1:E:3991:GLY:HA3	1.50	0.75
1:C:1623:ARG:HH11	1:C:1626:TRP:HE1	1.33	0.75
1:E:1206:GLN:H	1:E:1227:ALA:HB3	1.51	0.75
1:E:1623:ARG:HH11	1:E:1626:TRP:HE1	1.33	0.75
1:C:72:SER:O	1:C:99:ARG:NH1	2.20	0.75
1:A:138:GLN:NE2	1:A:146:CYS:SG	2.59	0.74
1:G:4984:ASN:O	1:G:4986:ALA:N	2.20	0.74
1:C:3927:GLN:HE21	1:C:3991:GLY:HA3	1.50	0.74
1:E:579:GLN:H	1:E:582:HIS:HD2	1.33	0.74
1:A:732:SER:HB3	1:A:764:VAL:HG13	1.70	0.74
1:A:76:ARG:HE	1:C:3844:LEU:HD21	1.51	0.74
1:E:674:PHE:HB3	2:F:40:ARG:NH1	2.02	0.74
1:G:1623:ARG:HH11	1:G:1626:TRP:HE1	1.32	0.74
1:C:408:ALA:O	1:C:412:ASN:ND2	2.21	0.74
1:A:408:ALA:O	1:A:412:ASN:ND2	2.21	0.74
1:C:2124:LEU:HD21	1:C:3677:LEU:HD21	1.70	0.74
1:G:72:SER:O	1:G:99:ARG:NH1	2.20	0.74
1:C:674:PHE:HB3	2:D:40:ARG:NH1	2.02	0.74
1:E:408:ALA:O	1:E:412:ASN:ND2	2.21	0.74
1:E:732:SER:HB3	1:E:764:VAL:HG13	1.70	0.74
1:E:2124:LEU:HD21	1:E:3677:LEU:HD21	1.70	0.73
1:A:674:PHE:HB3	2:B:40:ARG:NH1	2.02	0.73
1:G:579:GLN:H	1:G:582:HIS:HD2	1.33	0.73
1:G:138:GLN:NE2	1:G:146:CYS:SG	2.59	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4192:ARG:NH1	1:C:4982:GLU:OE1	2.22	0.73
1:E:663:TYR:OH	1:E:665:GLU:OE2	2.04	0.73
1:A:3844:LEU:HD21	1:G:76:ARG:HE	1.52	0.73
1:A:2124:LEU:HD21	1:A:3677:LEU:HD21	1.70	0.73
1:C:732:SER:HB3	1:C:764:VAL:HG13	1.70	0.73
1:E:1731:LEU:HA	1:E:1772:ARG:HE	1.53	0.73
1:E:3836:MET:HA	1:E:3839:CYS:SG	2.28	0.73
1:G:1731:LEU:HA	1:G:1772:ARG:HE	1.53	0.73
1:E:4192:ARG:NH1	1:E:4982:GLU:OE1	2.21	0.73
1:A:4192:ARG:NH1	1:A:4982:GLU:OE1	2.22	0.73
1:G:1703:LEU:HD12	1:G:1704:PRO:HD2	1.70	0.73
1:G:2198:MET:HE3	1:G:2203:MET:SD	2.28	0.73
1:G:732:SER:HB3	1:G:764:VAL:HG13	1.70	0.73
1:A:1105:ALA:HB3	1:A:1191:VAL:HG21	1.71	0.73
1:C:1703:LEU:HD12	1:C:1704:PRO:HD2	1.70	0.73
1:C:1731:LEU:HA	1:C:1772:ARG:HE	1.53	0.73
1:E:2198:MET:HE3	1:E:2203:MET:SD	2.28	0.73
1:C:663:TYR:OH	1:C:665:GLU:OE2	2.04	0.72
1:A:1731:LEU:HA	1:A:1772:ARG:HE	1.53	0.72
1:A:3836:MET:HA	1:A:3839:CYS:SG	2.29	0.72
1:A:215:THR:HG22	1:A:273:HIS:HA	1.72	0.72
1:E:1105:ALA:HB3	1:E:1191:VAL:HG21	1.70	0.72
1:E:1676:LEU:HD12	1:E:1725:ARG:HD3	1.72	0.72
1:A:3781:GLN:NE2	1:A:3819:TYR:OH	2.23	0.72
1:E:1766:GLY:HA2	1:E:1856:ASP:OD2	1.90	0.72
1:E:1703:LEU:HD12	1:E:1704:PRO:HD2	1.70	0.72
1:C:1676:LEU:HD12	1:C:1725:ARG:HD3	1.72	0.72
1:A:1703:LEU:HD12	1:A:1704:PRO:HD2	1.70	0.72
1:C:1766:GLY:HA2	1:C:1856:ASP:OD2	1.90	0.72
1:C:3836:MET:HA	1:C:3839:CYS:SG	2.29	0.72
1:G:215:THR:HG22	1:G:273:HIS:HA	1.72	0.72
1:A:1766:GLY:HA2	1:A:1856:ASP:OD2	1.90	0.71
1:C:215:THR:HG22	1:C:273:HIS:HA	1.71	0.71
1:E:706:GLY:H	1:E:711:LEU:HD13	1.55	0.71
1:A:706:GLY:H	1:A:711:LEU:HD13	1.55	0.71
1:G:1076:ARG:HD3	1:G:1109:LEU:HD11	1.72	0.71
1:C:1105:ALA:HB3	1:C:1191:VAL:HG21	1.72	0.71
1:G:1766:GLY:HA2	1:G:1856:ASP:OD2	1.90	0.71
1:A:745:SER:HB3	1:A:758:ARG:HB2	1.72	0.71
1:C:706:GLY:H	1:C:711:LEU:HD13	1.56	0.71
1:G:1676:LEU:HD12	1:G:1725:ARG:HD3	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:745:SER:HB3	1:G:758:ARG:HB2	1.72	0.71
1:A:1676:LEU:HD12	1:A:1725:ARG:HD3	1.71	0.71
2:B:24:VAL:HG12	2:B:103:LEU:HA	1.72	0.71
1:A:2198:MET:HE3	1:A:2203:MET:SD	2.29	0.71
1:G:408:ALA:O	1:G:412:ASN:ND2	2.21	0.71
1:G:674:PHE:HB3	2:H:40:ARG:NH1	2.06	0.71
1:C:1253:PRO:O	1:C:1281:ASN:ND2	2.24	0.70
1:E:3767:GLN:NE2	1:E:3805:LEU:O	2.25	0.70
1:G:706:GLY:H	1:G:711:LEU:HD13	1.56	0.70
1:A:1253:PRO:O	1:A:1281:ASN:ND2	2.24	0.70
1:E:215:THR:HG22	1:E:273:HIS:HA	1.72	0.70
1:C:3767:GLN:NE2	1:C:3805:LEU:O	2.25	0.70
2:D:24:VAL:HG12	2:D:103:LEU:HA	1.72	0.70
1:G:1808:ARG:NH1	1:G:1858:ASP:OD2	2.25	0.70
1:E:745:SER:HB3	1:E:758:ARG:HB2	1.73	0.70
1:A:1076:ARG:HD3	1:A:1109:LEU:HD11	1.73	0.70
1:E:3781:GLN:NE2	1:E:3819:TYR:OH	2.24	0.70
1:G:1105:ALA:HB3	1:G:1191:VAL:HG21	1.72	0.70
1:C:2198:MET:HE3	1:C:2203:MET:SD	2.30	0.70
1:C:745:SER:HB3	1:C:758:ARG:HB2	1.72	0.70
1:C:3842:LEU:HB3	1:C:3929:SER:OG	1.92	0.70
1:G:3836:MET:HA	1:G:3839:CYS:SG	2.32	0.70
1:A:1808:ARG:NH1	1:A:1858:ASP:OD2	2.25	0.70
1:A:3842:LEU:HB3	1:A:3929:SER:OG	1.92	0.70
1:G:4005:GLN:OE1	1:G:4113:SER:OG	2.09	0.70
1:C:1808:ARG:NH1	1:C:1858:ASP:OD2	2.24	0.70
1:C:3948:LYS:HG3	1:C:4012:LEU:HD12	1.73	0.70
1:G:4027:LEU:HA	1:G:4030:LEU:HB3	1.72	0.70
1:A:3920:VAL:HG22	1:A:3985:LEU:HD12	1.75	0.69
1:G:1253:PRO:O	1:G:1281:ASN:ND2	2.24	0.69
1:A:3948:LYS:HG3	1:A:4012:LEU:HD12	1.74	0.69
2:F:24:VAL:HG12	2:F:103:LEU:HA	1.72	0.69
1:G:1243:PRO:HD2	1:G:1458:HIS:HB3	1.72	0.69
1:C:76:ARG:NE	1:E:3844:LEU:HD21	2.07	0.69
1:E:1253:PRO:O	1:E:1281:ASN:ND2	2.24	0.69
1:C:1780:PRO:HG2	2:D:42:ARG:HE	1.58	0.69
1:E:1808:ARG:NH1	1:E:1858:ASP:OD2	2.25	0.69
1:C:1690:ASP:OD1	1:C:1691:GLN:N	2.26	0.69
1:E:3948:LYS:HG3	1:E:4012:LEU:HD12	1.74	0.69
1:G:1762:LEU:HD12	1:G:1763:PRO:HD2	1.73	0.69
1:A:2870:GLU:OE2	1:A:2939:ARG:NE	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3844:LEU:HD21	1:G:76:ARG:NE	2.07	0.69
1:C:1719:HIS:HB3	1:C:1802:ILE:HD11	1.75	0.69
1:C:607:CYS:SG	1:C:618:GLN:NE2	2.66	0.69
1:A:1719:HIS:HB3	1:A:1802:ILE:HD11	1.75	0.69
1:C:3781:GLN:NE2	1:C:3819:TYR:OH	2.24	0.69
1:E:3842:LEU:HB3	1:E:3929:SER:OG	1.92	0.69
1:G:1690:ASP:OD1	1:G:1691:GLN:N	2.26	0.69
1:A:3767:GLN:NE2	1:A:3805:LEU:O	2.25	0.69
1:E:110:ARG:HH21	1:E:115:ARG:HD2	1.59	0.69
1:A:475:GLN:NE2	1:A:528:SER:O	2.27	0.68
1:E:607:CYS:SG	1:E:618:GLN:NE2	2.66	0.68
1:G:475:GLN:NE2	1:G:528:SER:O	2.27	0.68
1:E:1719:HIS:HB3	1:E:1802:ILE:HD11	1.74	0.68
1:A:1690:ASP:OD1	1:A:1691:GLN:N	2.26	0.68
1:A:1762:LEU:HD12	1:A:1763:PRO:HD2	1.74	0.68
1:E:2870:GLU:OE2	1:E:2939:ARG:NE	2.26	0.68
1:A:607:CYS:SG	1:A:618:GLN:NE2	2.66	0.68
1:E:1762:LEU:HD12	1:E:1763:PRO:HD2	1.74	0.68
1:E:475:GLN:NE2	1:E:528:SER:O	2.27	0.68
2:B:23:VAL:HG22	2:B:47:LYS:HG2	1.75	0.68
1:C:1076:ARG:HD3	1:C:1109:LEU:HD11	1.73	0.68
1:C:1596:GLU:HB2	1:C:1599:MET:HG3	1.76	0.68
1:C:1762:LEU:HD12	1:C:1763:PRO:HD2	1.75	0.68
1:C:3920:VAL:HG22	1:C:3985:LEU:HD12	1.75	0.68
1:G:4573:ILE:HG21	1:G:4809:PHE:HE2	1.58	0.68
1:A:569:ILE:HG23	1:A:570:GLU:HG3	1.75	0.68
1:E:3920:VAL:HG22	1:E:3985:LEU:HD12	1.75	0.68
1:E:4030:LEU:HG	1:E:4040:ILE:HD11	1.76	0.68
1:G:1596:GLU:HB2	1:G:1599:MET:HG3	1.76	0.68
1:E:3780:LEU:HD12	1:E:3828:PHE:CE1	2.29	0.68
2:F:23:VAL:HG22	2:F:47:LYS:HG2	1.75	0.68
1:G:4236:SER:O	1:G:4675:LYS:NZ	2.26	0.68
1:C:475:GLN:NE2	1:C:528:SER:O	2.27	0.68
1:C:2876:GLU:OE2	1:C:2916:LYS:HD3	1.94	0.68
1:E:1076:ARG:HD3	1:E:1109:LEU:HD11	1.75	0.68
1:E:1596:GLU:HB2	1:E:1599:MET:HG3	1.76	0.68
1:G:607:CYS:SG	1:G:618:GLN:NE2	2.66	0.68
1:G:755:ILE:HB	1:G:768:PHE:HB2	1.76	0.68
1:A:76:ARG:NE	1:C:3844:LEU:HD21	2.07	0.68
1:E:1780:PRO:HG2	2:F:42:ARG:HE	1.59	0.67
1:A:1596:GLU:HB2	1:A:1599:MET:HG3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:755:ILE:HB	1:A:768:PHE:HB2	1.77	0.67
1:C:1432:THR:N	1:C:1518:CYS:SG	2.68	0.67
1:E:1432:THR:N	1:E:1518:CYS:SG	2.68	0.67
1:E:569:ILE:HG23	1:E:570:GLU:HG3	1.75	0.67
1:A:4030:LEU:HG	1:A:4040:ILE:HD11	1.76	0.67
1:C:2870:GLU:OE2	1:C:2939:ARG:NE	2.26	0.67
1:E:4971:THR:OG1	1:E:5029:ARG:NH2	2.27	0.67
1:G:1719:HIS:HB3	1:G:1802:ILE:HD11	1.75	0.67
1:G:569:ILE:HG23	1:G:570:GLU:HG3	1.75	0.67
1:A:1780:PRO:HG2	2:B:42:ARG:HE	1.57	0.67
1:C:4971:THR:OG1	1:C:5029:ARG:NH2	2.28	0.67
1:A:23:GLN:HE21	1:A:34:LYS:HB3	1.60	0.67
1:A:4934:GLY:CA	1:C:4937:ILE:HG12	2.23	0.67
1:C:3780:LEU:HD12	1:C:3828:PHE:CE1	2.29	0.67
1:A:1432:THR:N	1:A:1518:CYS:SG	2.68	0.67
1:A:1667:LEU:HG	1:A:1714:LEU:HD11	1.77	0.67
1:A:2876:GLU:OE2	1:A:2916:LYS:HD3	1.94	0.67
1:A:2917:ALA:HA	1:A:2920:ARG:HB3	1.77	0.67
1:C:569:ILE:HG23	1:C:570:GLU:HG3	1.75	0.67
1:E:1690:ASP:OD1	1:E:1691:GLN:N	2.27	0.67
1:C:1667:LEU:HG	1:C:1714:LEU:HD11	1.77	0.67
1:C:3966:THR:HG22	1:C:4026:MET:HA	1.77	0.67
1:E:3966:THR:HG22	1:E:4026:MET:HA	1.77	0.67
1:E:755:ILE:HB	1:E:768:PHE:HB2	1.76	0.67
1:G:2876:GLU:OE2	1:G:2916:LYS:HD3	1.93	0.67
1:C:2917:ALA:HA	1:C:2920:ARG:HB3	1.77	0.67
1:E:2917:ALA:HA	1:E:2920:ARG:HB3	1.77	0.67
1:C:110:ARG:HH21	1:C:115:ARG:HD2	1.59	0.67
1:C:3817:LEU:HD11	1:C:3821:LYS:HE2	1.77	0.67
2:D:23:VAL:HG22	2:D:47:LYS:HG2	1.75	0.67
1:G:1432:THR:N	1:G:1518:CYS:SG	2.68	0.67
1:A:110:ARG:HH21	1:A:115:ARG:HD2	1.59	0.67
1:C:755:ILE:HB	1:C:768:PHE:HB2	1.77	0.67
1:E:2876:GLU:OE2	1:E:2916:LYS:HD3	1.95	0.67
1:E:4934:GLY:CA	1:G:4937:ILE:HG12	2.21	0.67
1:A:3780:LEU:HD12	1:A:3828:PHE:CE1	2.29	0.66
1:A:3817:LEU:HD11	1:A:3821:LYS:HE2	1.78	0.66
1:G:110:ARG:HH21	1:G:115:ARG:HD2	1.60	0.66
1:G:2865:VAL:O	1:G:2928:LYS:NZ	2.28	0.66
1:A:4940:PHE:HB3	1:G:4938:ASP:OD2	1.95	0.66
1:C:35:LEU:HD22	1:C:49:LEU:HD13	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:35:LEU:HD22	1:E:49:LEU:HD13	1.77	0.66
1:E:1667:LEU:HG	1:E:1714:LEU:HD11	1.77	0.66
1:G:1735:ILE:HD11	1:G:2156:LEU:HD11	1.77	0.66
1:G:35:LEU:HD22	1:G:49:LEU:HD13	1.77	0.66
1:A:4971:THR:OG1	1:A:5029:ARG:NH2	2.29	0.66
1:G:3948:LYS:HE3	1:G:4012:LEU:HB2	1.77	0.66
1:A:4937:ILE:HG12	1:G:4934:GLY:HA3	1.78	0.66
1:A:2547:ALA:O	1:A:2551:ASN:ND2	2.28	0.66
1:C:665:GLU:HB2	1:C:792:LEU:HB2	1.78	0.66
1:E:176:SER:HB2	1:E:178:ARG:HH21	1.60	0.66
1:E:2547:ALA:O	1:E:2551:ASN:ND2	2.28	0.66
1:E:34:LYS:O	1:E:52:THR:OG1	2.14	0.66
1:E:3958:ALA:HA	1:E:3961:VAL:HG12	1.78	0.66
1:G:176:SER:HB2	1:G:178:ARG:HH21	1.60	0.66
1:G:618:GLN:OE1	1:G:1678:ASN:ND2	2.29	0.66
1:A:34:LYS:O	1:A:52:THR:OG1	2.14	0.66
1:A:3966:THR:HG22	1:A:4026:MET:HA	1.77	0.66
1:C:176:SER:HB2	1:C:178:ARG:HH21	1.60	0.66
1:E:23:GLN:HE21	1:E:34:LYS:HB3	1.60	0.66
1:C:2547:ALA:O	1:C:2551:ASN:ND2	2.28	0.66
1:A:3958:ALA:HA	1:A:3961:VAL:HG12	1.78	0.66
1:A:4917:ASP:OD2	1:C:4892:ARG:CZ	2.43	0.66
1:C:4027:LEU:HD11	1:C:4146:LEU:HD11	1.77	0.66
1:G:2547:ALA:O	1:G:2551:ASN:ND2	2.28	0.66
1:C:3958:ALA:HA	1:C:3961:VAL:HG12	1.78	0.66
1:E:4573:ILE:HD11	1:E:4646:LEU:HB3	1.78	0.66
1:E:1783:VAL:O	2:F:56:ILE:HG23	1.96	0.66
1:C:23:GLN:HE21	1:C:34:LYS:HB3	1.60	0.65
1:E:4037:ASN:HB3	1:E:4042:ARG:HH21	1.61	0.65
1:C:4030:LEU:HG	1:C:4040:ILE:HD11	1.76	0.65
1:E:3817:LEU:HD11	1:E:3821:LYS:HE2	1.78	0.65
1:G:34:LYS:O	1:G:52:THR:OG1	2.14	0.65
1:A:2822:THR:HG1	1:A:2938:THR:HG1	1.42	0.65
1:C:4901:ILE:HG21	1:C:4913:ARG:HH21	1.60	0.65
1:C:4917:ASP:OD2	1:E:4892:ARG:CZ	2.44	0.65
1:C:404:ILE:HD13	1:C:481:GLU:HG3	1.78	0.65
1:E:3754:GLU:OE2	1:E:4718:LYS:HE3	1.97	0.65
1:G:665:GLU:HB2	1:G:792:LEU:HB2	1.78	0.65
1:A:176:SER:HB2	1:A:178:ARG:HH21	1.60	0.65
1:A:2227:LYS:O	1:A:2230:THR:OG1	2.13	0.65
1:E:404:ILE:HD13	1:E:481:GLU:HG3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:78:LEU:HD11	1:G:147:TRP:CG	2.32	0.65
1:G:1667:LEU:HG	1:G:1714:LEU:HD11	1.77	0.65
1:G:1783:VAL:O	2:H:56:ILE:HG23	1.96	0.65
1:G:23:GLN:HE21	1:G:34:LYS:HB3	1.60	0.65
1:A:206:CYS:HB3	1:A:271:GLY:HA3	1.78	0.65
1:A:4901:ILE:HG21	1:A:4913:ARG:HH21	1.61	0.65
1:E:2227:LYS:O	1:E:2230:THR:OG1	2.13	0.65
1:E:627:PRO:HG3	2:F:89:GLY:HA2	1.79	0.65
1:G:1438:ARG:HB3	1:G:1563:GLN:HB3	1.79	0.65
1:G:206:CYS:HB3	1:G:271:GLY:HA3	1.77	0.65
1:A:78:LEU:HD11	1:A:147:TRP:CG	2.32	0.65
1:E:4027:LEU:HD11	1:E:4146:LEU:HD11	1.78	0.65
1:G:404:ILE:HD13	1:G:481:GLU:HG3	1.78	0.65
1:C:34:LYS:O	1:C:52:THR:OG1	2.14	0.65
1:G:2227:LYS:O	1:G:2230:THR:OG1	2.13	0.65
1:A:4027:LEU:HD11	1:A:4146:LEU:HD11	1.78	0.64
1:A:4573:ILE:HD11	1:A:4646:LEU:HB3	1.79	0.64
1:A:663:TYR:OH	1:A:665:GLU:OE2	2.04	0.64
1:C:1735:ILE:HD11	1:C:2156:LEU:HD11	1.78	0.64
1:G:3966:THR:O	1:G:3970:GLN:N	2.29	0.64
1:A:1438:ARG:HB3	1:A:1563:GLN:HB3	1.79	0.64
1:A:665:GLU:HB2	1:A:792:LEU:HB2	1.78	0.64
1:G:865:PRO:HA	1:G:868:GLU:HB2	1.79	0.64
1:C:4037:ASN:HB3	1:C:4042:ARG:HH21	1.61	0.64
1:E:1611:HIS:HB2	1:E:1652:GLU:HB2	1.77	0.64
1:G:3754:GLU:OE2	1:G:4718:LYS:HE3	1.97	0.64
1:G:588:SER:O	1:G:592:LYS:HG2	1.98	0.64
1:G:674:PHE:O	2:H:40:ARG:NH1	2.29	0.64
1:A:1735:ILE:HD11	1:A:2156:LEU:HD11	1.77	0.64
1:A:35:LEU:HD22	1:A:49:LEU:HD13	1.78	0.64
1:C:277:GLY:HA2	1:C:317:ARG:NH1	2.13	0.64
1:C:4573:ILE:HD11	1:C:4646:LEU:HB3	1.78	0.64
1:C:865:PRO:HA	1:C:868:GLU:HB2	1.79	0.64
1:E:4185:GLY:O	1:E:4187:SER:N	2.30	0.64
1:G:1744:ALA:HB3	1:G:1745:ILE:HA	1.80	0.64
1:G:4185:GLY:O	1:G:4187:SER:N	2.31	0.64
1:A:4185:GLY:O	1:A:4187:SER:N	2.31	0.64
1:A:491:ILE:O	1:A:495:ASN:ND2	2.31	0.64
1:C:1115:LEU:HD13	1:C:1193:SER:HB2	1.80	0.64
1:E:618:GLN:OE1	1:E:1678:ASN:ND2	2.31	0.64
1:A:683:ARG:HD2	1:A:705:ASN:HB3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1438:ARG:HB3	1:C:1563:GLN:HB3	1.80	0.64
1:C:3754:GLU:OE2	1:C:4718:LYS:HE3	1.96	0.64
1:E:206:CYS:HB3	1:E:271:GLY:HA3	1.79	0.64
1:E:665:GLU:HB2	1:E:792:LEU:HB2	1.78	0.64
1:E:683:ARG:HD2	1:E:705:ASN:HB3	1.80	0.64
1:A:1611:HIS:HB2	1:A:1652:GLU:HB2	1.79	0.64
1:C:1611:HIS:HB2	1:C:1652:GLU:HB2	1.80	0.64
1:C:1716:ILE:HD11	1:C:1844:LEU:HA	1.80	0.64
1:C:206:CYS:HB3	1:C:271:GLY:HA3	1.78	0.64
1:C:588:SER:O	1:C:592:LYS:HG2	1.98	0.64
2:D:14:THR:HG22	2:D:106:LEU:HD12	1.80	0.64
1:E:1438:ARG:HB3	1:E:1563:GLN:HB3	1.79	0.64
1:A:1744:ALA:HB3	1:A:1745:ILE:HA	1.80	0.64
1:A:4037:ASN:HB3	1:A:4042:ARG:HH21	1.61	0.64
1:A:3754:GLU:OE2	1:A:4718:LYS:HE3	1.97	0.64
1:A:865:PRO:HA	1:A:868:GLU:HB2	1.79	0.64
1:C:618:GLN:OE1	1:C:1678:ASN:ND2	2.31	0.64
1:C:78:LEU:HD11	1:C:147:TRP:CG	2.32	0.64
1:E:1716:ILE:HD11	1:E:1844:LEU:HA	1.80	0.64
1:G:683:ARG:HD2	1:G:705:ASN:HB3	1.80	0.64
1:C:491:ILE:O	1:C:495:ASN:ND2	2.31	0.64
1:E:1744:ALA:HB3	1:E:1745:ILE:HA	1.80	0.64
1:C:1744:ALA:HB3	1:C:1745:ILE:HA	1.80	0.64
1:E:1735:ILE:HD11	1:E:2156:LEU:HD11	1.78	0.64
1:G:1737:PRO:HG2	1:G:1742:THR:HG21	1.80	0.64
1:G:674:PHE:HB3	2:H:40:ARG:HH12	1.61	0.64
1:A:588:SER:O	1:A:592:LYS:HG2	1.98	0.63
1:G:1611:HIS:HB2	1:G:1652:GLU:HB2	1.79	0.63
1:A:627:PRO:HG3	2:B:89:GLY:HA2	1.80	0.63
1:A:1783:VAL:O	2:B:56:ILE:HG23	1.98	0.63
1:E:4914:VAL:CG2	1:G:4888:TYR:HB2	2.28	0.63
2:F:14:THR:HG22	2:F:106:LEU:HD12	1.80	0.63
1:A:1716:ILE:HD11	1:A:1844:LEU:HA	1.80	0.63
1:A:4034:ASN:OD1	1:A:4035:VAL:N	2.32	0.63
1:C:1783:VAL:O	2:D:56:ILE:HG23	1.97	0.63
1:C:627:PRO:HG3	2:D:89:GLY:HA2	1.79	0.63
1:E:546:TRP:HE1	1:E:550:LYS:HZ1	1.47	0.63
1:G:1716:ILE:HD11	1:G:1844:LEU:HA	1.80	0.63
1:G:2166:LEU:HD12	1:G:2206:THR:HG23	1.80	0.63
1:A:404:ILE:HD13	1:A:481:GLU:HG3	1.78	0.63
1:E:1115:LEU:HD13	1:E:1193:SER:HB2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:491:ILE:O	1:G:495:ASN:ND2	2.31	0.63
1:A:1115:LEU:HD13	1:A:1193:SER:HB2	1.81	0.63
1:A:2166:LEU:HD12	1:A:2206:THR:HG23	1.80	0.63
2:B:71:ARG:NH2	2:B:100:ASP:OD2	2.32	0.63
1:E:491:ILE:O	1:E:495:ASN:ND2	2.31	0.63
1:E:588:SER:O	1:E:592:LYS:HG2	1.98	0.63
1:C:683:ARG:HD2	1:C:705:ASN:HB3	1.79	0.63
1:E:4917:ASP:OD2	1:G:4892:ARG:CZ	2.46	0.63
1:A:618:GLN:OE1	1:A:1678:ASN:ND2	2.31	0.63
2:B:14:THR:HG22	2:B:106:LEU:HD12	1.80	0.63
1:C:4984:ASN:O	1:C:4986:ALA:N	2.31	0.63
1:E:4034:ASN:OD1	1:E:4035:VAL:N	2.32	0.63
1:E:4984:ASN:O	1:E:4986:ALA:N	2.32	0.63
1:G:623:GLU:OE2	2:H:89:GLY:N	2.32	0.63
1:C:3813:GLN:NE2	1:C:3890:LEU:O	2.32	0.63
1:C:4034:ASN:OD1	1:C:4035:VAL:N	2.32	0.63
1:E:3958:ALA:HB3	1:E:4019:LEU:HD11	1.81	0.63
2:F:74:LEU:HB2	2:F:99:PHE:HB2	1.81	0.63
1:C:3958:ALA:HB3	1:C:4019:LEU:HD11	1.81	0.63
1:E:2166:LEU:HD12	1:E:2206:THR:HG23	1.81	0.63
1:G:1115:LEU:HD13	1:G:1193:SER:HB2	1.81	0.63
1:A:2149:VAL:O	1:A:2152:THR:OG1	2.15	0.62
1:C:1115:LEU:HD21	1:C:1123:VAL:HG11	1.81	0.62
1:C:687:ALA:HB2	1:C:711:LEU:HD23	1.81	0.62
1:E:3786:CYS:SG	1:E:3794:VAL:HG22	2.39	0.62
1:G:4962:GLY:O	1:G:4964:GLY:N	2.32	0.62
1:G:707:VAL:HA	1:G:725:HIS:HB2	1.82	0.62
1:A:1243:PRO:HD2	1:A:1458:HIS:HB3	1.82	0.62
1:C:3786:CYS:SG	1:C:3794:VAL:HG22	2.38	0.62
1:E:687:ALA:HB2	1:E:711:LEU:HD23	1.81	0.62
1:G:4049:VAL:HG21	1:G:4159:ARG:HD3	1.81	0.62
1:A:4962:GLY:O	1:A:4964:GLY:N	2.32	0.62
1:C:4934:GLY:CA	1:E:4937:ILE:HG12	2.30	0.62
1:G:4034:ASN:OD1	1:G:4035:VAL:N	2.32	0.62
1:C:4185:GLY:O	1:C:4187:SER:N	2.31	0.62
1:A:1115:LEU:HD21	1:A:1123:VAL:HG11	1.81	0.62
1:A:3813:GLN:NE2	1:A:3890:LEU:O	2.33	0.62
1:G:1115:LEU:HD21	1:G:1123:VAL:HG11	1.81	0.62
1:G:3781:GLN:NE2	1:G:3819:TYR:OH	2.28	0.62
1:A:276:TRP:NE1	1:A:338:GLU:OE2	2.28	0.62
1:A:3958:ALA:HB3	1:A:4019:LEU:HD11	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:790:ARG:HA	1:C:1627:ALA:HA	1.82	0.62
1:C:38:ALA:HB1	1:C:64:ILE:HD12	1.81	0.62
1:E:1737:PRO:HG2	1:E:1742:THR:HG21	1.81	0.62
1:G:4037:ASN:HB3	1:G:4042:ARG:HH21	1.63	0.62
1:C:1098:GLY:HA3	1:C:1198:GLN:HE21	1.65	0.62
1:C:3843:ASP:OD1	1:C:3844:LEU:N	2.32	0.62
1:C:4962:GLY:O	1:C:4964:GLY:N	2.32	0.62
1:E:78:LEU:HD11	1:E:147:TRP:CG	2.35	0.62
1:E:3992:PHE:O	1:E:3996:PHE:N	2.29	0.62
1:E:707:VAL:HA	1:E:725:HIS:HB2	1.82	0.62
1:E:739:ALA:O	1:E:741:GLU:N	2.30	0.62
1:E:76:ARG:NH1	1:E:79:GLN:OE1	2.32	0.62
1:A:1125:ASN:ND2	1:A:1130:GLN:O	2.33	0.62
1:A:707:VAL:HA	1:A:725:HIS:HB2	1.82	0.62
2:D:74:LEU:HB2	2:D:99:PHE:HB2	1.80	0.62
1:E:3919:THR:HG21	1:E:3968:TYR:HE2	1.65	0.62
1:A:4888:TYR:HD1	1:G:4914:VAL:HG23	1.57	0.62
1:C:2166:LEU:HD12	1:C:2206:THR:HG23	1.81	0.62
1:E:4962:GLY:O	1:E:4964:GLY:N	2.32	0.62
1:E:865:PRO:HA	1:E:868:GLU:HB2	1.80	0.62
1:G:3969:ILE:HG23	1:G:3977:GLN:HG2	1.80	0.62
1:C:2227:LYS:O	1:C:2230:THR:OG1	2.14	0.61
1:C:276:TRP:NE1	1:C:338:GLU:OE2	2.28	0.61
1:E:3813:GLN:NE2	1:E:3890:LEU:O	2.33	0.61
1:G:276:TRP:NE1	1:G:338:GLU:OE2	2.28	0.61
1:C:707:VAL:HA	1:C:725:HIS:HB2	1.82	0.61
1:E:1125:ASN:ND2	1:E:1130:GLN:O	2.33	0.61
1:G:627:PRO:HG3	2:H:89:GLY:HA2	1.81	0.61
1:A:2107:GLN:NE2	1:A:3679:LYS:O	2.33	0.61
1:A:38:ALA:HB1	1:A:64:ILE:HD12	1.81	0.61
1:A:4984:ASN:O	1:A:4986:ALA:N	2.32	0.61
1:A:687:ALA:HB2	1:A:711:LEU:HD23	1.81	0.61
2:B:74:LEU:HB2	2:B:99:PHE:HB2	1.81	0.61
1:A:76:ARG:HH21	1:C:3844:LEU:HD21	1.65	0.61
1:C:34:LYS:N	1:C:53:SER:OG	2.33	0.61
1:E:465:GLN:NE2	1:E:3712:GLU:OE1	2.33	0.61
1:G:38:ALA:HB1	1:G:64:ILE:HD12	1.81	0.61
1:C:2107:GLN:NE2	1:C:3679:LYS:O	2.33	0.61
1:E:3843:ASP:OD1	1:E:3844:LEU:N	2.32	0.61
1:G:3813:GLN:NE2	1:G:3890:LEU:O	2.33	0.61
1:A:465:GLN:NE2	1:A:3712:GLU:OE1	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:LEU:HD11	1:A:51:PRO:HB3	1.82	0.61
1:A:790:ARG:HA	1:A:1627:ALA:HA	1.82	0.61
1:C:4027:LEU:HD11	1:C:4146:LEU:CD1	2.31	0.61
1:C:465:GLN:NE2	1:C:3712:GLU:OE1	2.34	0.61
1:C:4828:SER:HA	1:C:4831:THR:HG22	1.83	0.61
1:E:2107:GLN:NE2	1:E:3679:LYS:O	2.33	0.61
1:G:3423:TRP:O	1:G:3428:ASN:N	2.32	0.61
1:G:687:ALA:HB2	1:G:711:LEU:HD23	1.81	0.61
1:A:4005:GLN:OE1	1:A:4113:SER:OG	2.19	0.61
1:C:1737:PRO:HG2	1:C:1742:THR:HG21	1.81	0.61
1:C:3919:THR:HG21	1:C:3968:TYR:HE2	1.65	0.61
1:E:38:ALA:HB1	1:E:64:ILE:HD12	1.82	0.61
1:E:4828:SER:HA	1:E:4831:THR:HG22	1.82	0.61
1:G:4837:LEU:HD11	1:G:4932:ILE:HG23	1.81	0.61
1:A:3844:LEU:HD21	1:G:76:ARG:HH21	1.65	0.61
1:C:1970:GLN:NE2	1:C:3645:PRO:O	2.29	0.61
1:A:1098:GLY:HA3	1:A:1198:GLN:HE21	1.65	0.61
1:E:276:TRP:NE1	1:E:338:GLU:OE2	2.28	0.61
1:E:34:LYS:N	1:E:53:SER:OG	2.33	0.61
2:F:71:ARG:NH2	2:F:100:ASP:OD2	2.32	0.61
1:G:2149:VAL:O	1:G:2152:THR:OG1	2.14	0.61
1:G:2917:ALA:HA	1:G:2920:ARG:HB3	1.83	0.61
1:A:34:LYS:N	1:A:53:SER:OG	2.33	0.61
1:C:76:ARG:HH21	1:E:3844:LEU:HD21	1.66	0.61
2:D:71:ARG:NH2	2:D:100:ASP:OD2	2.31	0.61
1:E:4901:ILE:HG21	1:E:4913:ARG:HH21	1.65	0.61
1:G:790:ARG:HA	1:G:1627:ALA:HA	1.82	0.61
1:G:4573:ILE:HG21	1:G:4809:PHE:CE2	2.36	0.61
1:A:277:GLY:HA2	1:A:317:ARG:NH1	2.13	0.60
1:A:2865:VAL:O	1:A:2928:LYS:NZ	2.33	0.60
1:A:3919:THR:HG21	1:A:3968:TYR:HE2	1.65	0.60
1:A:4828:SER:HA	1:A:4831:THR:HG22	1.81	0.60
1:A:489:ASN:HB3	1:A:493:ARG:NH1	2.16	0.60
1:C:3805:LEU:O	1:C:3807:GLY:N	2.34	0.60
1:G:3969:ILE:HD11	1:G:3980:LEU:HD13	1.83	0.60
1:A:1737:PRO:HG2	1:A:1742:THR:HG21	1.82	0.60
1:E:4027:LEU:HD11	1:E:4146:LEU:CD1	2.31	0.60
1:G:3969:ILE:HD13	1:G:4030:LEU:HD13	1.83	0.60
1:A:4963:ILE:HD12	1:A:5030:LYS:NZ	2.16	0.60
1:C:1252:HIS:C	1:C:1254:HIS:H	2.05	0.60
1:G:33:LEU:HD11	1:G:51:PRO:HB3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1252:HIS:C	1:A:1254:HIS:H	2.05	0.60
1:A:699:GLY:O	1:A:1647:CYS:N	2.35	0.60
1:E:790:ARG:HA	1:E:1627:ALA:HA	1.82	0.60
1:E:2822:THR:OG1	1:E:2938:THR:OG1	2.19	0.60
1:A:3844:LEU:HD21	1:G:76:ARG:NH2	2.16	0.60
1:E:1115:LEU:HD21	1:E:1123:VAL:HG11	1.81	0.60
1:C:1125:ASN:HD22	1:C:1130:GLN:HG3	1.66	0.60
1:G:1098:GLY:HA3	1:G:1198:GLN:HE21	1.65	0.60
1:G:489:ASN:HB3	1:G:493:ARG:NH1	2.16	0.60
1:C:4963:ILE:HD12	1:C:5030:LYS:NZ	2.16	0.60
1:C:681:HIS:HA	1:C:716:PHE:CD1	2.37	0.60
1:E:3805:LEU:O	1:E:3807:GLY:N	2.33	0.60
1:C:33:LEU:HD11	1:C:51:PRO:HB3	1.83	0.60
1:E:1252:HIS:C	1:E:1254:HIS:H	2.05	0.60
1:G:681:HIS:HA	1:G:716:PHE:CD1	2.37	0.60
1:A:4027:LEU:HD11	1:A:4146:LEU:CD1	2.31	0.60
1:C:714:TYR:HB3	1:C:757:PHE:HD2	1.66	0.60
1:G:34:LYS:N	1:G:53:SER:OG	2.33	0.60
1:G:3920:VAL:HG22	1:G:3985:LEU:HD12	1.84	0.60
1:G:739:ALA:O	1:G:741:GLU:N	2.31	0.60
1:A:714:TYR:HB3	1:A:757:PHE:HD2	1.66	0.60
1:C:2149:VAL:O	1:C:2152:THR:OG1	2.15	0.60
1:C:489:ASN:HB3	1:C:493:ARG:NH1	2.16	0.60
1:E:1098:GLY:HA3	1:E:1198:GLN:HE21	1.65	0.60
1:E:2149:VAL:O	1:E:2152:THR:OG1	2.15	0.60
1:A:1927:LEU:HD21	1:A:2101:MET:HG2	1.83	0.59
1:A:4228:ALA:HB2	1:C:4976:GLU:OE1	2.01	0.59
1:E:4836:GLN:HB3	1:G:4826:ILE:HD11	1.83	0.59
1:E:674:PHE:O	2:F:40:ARG:NH1	2.35	0.59
1:A:1237:TRP:HD1	1:A:1611:HIS:HA	1.68	0.59
1:C:4005:GLN:OE1	1:C:4113:SER:OG	2.19	0.59
1:E:3891:LEU:HB3	1:E:3899:PHE:CE2	2.37	0.59
1:E:714:TYR:HB3	1:E:757:PHE:HD2	1.66	0.59
1:G:714:TYR:HB3	1:G:757:PHE:HD2	1.67	0.59
1:E:106:ALA:HA	1:E:149:THR:HA	1.83	0.59
1:E:4005:GLN:OE1	1:E:4113:SER:OG	2.18	0.59
1:G:1780:PRO:HG2	2:H:42:ARG:HE	1.67	0.59
1:A:2336:ARG:HG3	1:A:2435:ARG:HG3	1.85	0.59
1:C:2159:LEU:O	1:C:2162:ILE:HG22	2.02	0.59
1:C:4228:ALA:HB2	1:E:4976:GLU:OE1	2.02	0.59
1:E:1552:VAL:HG12	1:E:1554:VAL:HG23	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1927:LEU:HD21	1:E:2101:MET:HG2	1.84	0.59
1:E:4963:ILE:HD12	1:E:5030:LYS:NZ	2.17	0.59
1:G:2333:ASP:OD1	1:G:2336:ARG:NH2	2.36	0.59
1:A:1552:VAL:HG12	1:A:1554:VAL:HG23	1.84	0.59
1:A:2159:LEU:O	1:A:2162:ILE:HG22	2.02	0.59
1:C:1101:ARG:HG3	1:C:1193:SER:HB3	1.85	0.59
1:C:2336:ARG:HG3	1:C:2435:ARG:HG3	1.85	0.59
1:E:1243:PRO:HD2	1:E:1458:HIS:CB	2.29	0.59
1:E:3878:ASP:OD2	1:E:3953:LYS:HG3	2.03	0.59
1:C:106:ALA:HA	1:C:149:THR:HA	1.83	0.59
1:C:3878:ASP:OD2	1:C:3953:LYS:HG3	2.03	0.59
1:C:402:ARG:NH1	1:C:405:HIS:HD2	2.01	0.59
1:C:76:ARG:NH2	1:E:3844:LEU:HD21	2.17	0.59
1:E:2159:LEU:O	1:E:2162:ILE:HG22	2.02	0.59
1:G:1252:HIS:C	1:G:1254:HIS:H	2.05	0.59
1:G:1288:PHE:HE2	1:G:1460:HIS:HA	1.68	0.59
1:G:1552:VAL:HG12	1:G:1554:VAL:HG23	1.85	0.59
1:G:1648:MET:SD	1:G:1656:ARG:NH2	2.76	0.59
1:G:277:GLY:HA2	1:G:317:ARG:NH1	2.13	0.59
1:A:4928:LEU:O	1:A:4932:ILE:HD12	2.03	0.59
1:C:1637:MET:HG3	1:C:1650:ILE:HD13	1.85	0.59
1:C:3891:LEU:HB3	1:C:3899:PHE:CE2	2.37	0.59
1:C:4928:LEU:O	1:C:4932:ILE:HD12	2.03	0.59
1:E:699:GLY:O	1:E:1647:CYS:N	2.36	0.59
1:G:1637:MET:HG3	1:G:1650:ILE:HD13	1.84	0.59
1:A:3805:LEU:O	1:A:3807:GLY:N	2.33	0.59
1:A:3878:ASP:OD2	1:A:3953:LYS:HG3	2.03	0.59
1:C:674:PHE:O	2:D:40:ARG:NH1	2.36	0.59
1:G:1101:ARG:HG3	1:G:1193:SER:HB3	1.84	0.59
1:G:2336:ARG:HG3	1:G:2435:ARG:HG3	1.85	0.59
1:G:2756:ASN:OD1	1:G:2806:ARG:NH2	2.35	0.59
1:G:2875:ALA:HB2	1:G:2927:LEU:HD12	1.84	0.59
1:G:3891:LEU:HB3	1:G:3899:PHE:CE2	2.37	0.59
1:A:106:ALA:HA	1:A:149:THR:HA	1.83	0.59
1:A:1637:MET:HG3	1:A:1650:ILE:HD13	1.85	0.59
1:A:674:PHE:O	2:B:40:ARG:NH1	2.35	0.59
1:C:1648:MET:SD	1:C:1656:ARG:NH2	2.76	0.59
1:E:2333:ASP:OD1	1:E:2336:ARG:NH2	2.36	0.59
1:E:33:LEU:HD11	1:E:51:PRO:HB3	1.83	0.59
1:G:2107:GLN:NE2	1:G:3679:LYS:O	2.35	0.59
1:A:2333:ASP:OD1	1:A:2336:ARG:NH2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4059:LEU:HD13	1:A:4167:ALA:HB2	1.85	0.59
1:A:4963:ILE:HD11	1:A:5025:GLY:O	2.03	0.59
1:C:2248:ARG:HG2	1:C:2286:LEU:HD11	1.85	0.59
1:C:530:ILE:HG23	1:C:537:CYS:HB3	1.85	0.59
1:E:489:ASN:HB3	1:E:493:ARG:NH1	2.16	0.59
1:G:106:ALA:HA	1:G:149:THR:HA	1.83	0.59
1:G:3805:LEU:O	1:G:3807:GLY:N	2.32	0.59
1:G:4963:ILE:HD11	1:G:5025:GLY:O	2.03	0.59
1:G:4971:THR:OG1	1:G:5029:ARG:NH2	2.36	0.59
1:A:822:ARG:HA	1:A:1623:ARG:HH12	1.68	0.58
1:A:402:ARG:NH1	1:A:405:HIS:HD2	2.01	0.58
1:C:1927:LEU:HD21	1:C:2101:MET:HG2	1.84	0.58
1:A:76:ARG:NH2	1:C:3844:LEU:HD21	2.16	0.58
1:C:3879:GLU:OE2	1:C:3883:ASP:OD2	2.21	0.58
1:E:1648:MET:SD	1:E:1656:ARG:NH2	2.76	0.58
1:E:2248:ARG:HG2	1:E:2286:LEU:HD11	1.85	0.58
1:G:530:ILE:HG23	1:G:537:CYS:HB3	1.85	0.58
1:C:4963:ILE:HD11	1:C:5025:GLY:O	2.03	0.58
1:E:1091:GLU:HB2	1:E:1203:ASN:HB2	1.86	0.58
1:E:1970:GLN:NE2	1:E:3645:PRO:O	2.29	0.58
1:E:880:GLU:HG2	1:E:967:PRO:HG2	1.85	0.58
1:C:1079:LYS:HA	1:C:1082:THR:HG23	1.85	0.58
1:E:1637:MET:HG3	1:E:1650:ILE:HD13	1.84	0.58
1:E:3727:ASP:HB3	1:E:3731:LYS:NZ	2.18	0.58
1:G:1657:LEU:HA	1:G:1660:GLN:HG2	1.85	0.58
1:G:402:ARG:NH1	1:G:405:HIS:HD2	2.01	0.58
1:A:3843:ASP:OD1	1:A:3844:LEU:N	2.31	0.58
1:A:3992:PHE:O	1:A:3996:PHE:N	2.29	0.58
1:A:681:HIS:HA	1:A:716:PHE:CD1	2.37	0.58
1:C:1552:VAL:HG12	1:C:1554:VAL:HG23	1.85	0.58
1:C:880:GLU:HG2	1:C:967:PRO:HG2	1.85	0.58
1:E:4214:LYS:HD2	1:E:4985:LEU:HD23	1.84	0.58
1:A:1648:MET:SD	1:A:1656:ARG:NH2	2.76	0.58
1:A:3879:GLU:OE2	1:A:3883:ASP:OD2	2.21	0.58
1:C:3992:PHE:O	1:C:3996:PHE:N	2.29	0.58
1:E:2336:ARG:HG3	1:E:2435:ARG:HG3	1.86	0.58
1:G:2159:LEU:O	1:G:2162:ILE:HG22	2.02	0.58
1:G:4818:MET:HA	1:G:4824:ARG:HG2	1.84	0.58
1:A:1091:GLU:HB2	1:A:1203:ASN:HB2	1.86	0.58
1:A:3891:LEU:HB3	1:A:3899:PHE:CE2	2.38	0.58
1:A:489:ASN:HB3	1:A:493:ARG:HH12	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2865:VAL:O	1:C:2928:LYS:NZ	2.34	0.58
1:C:739:ALA:O	1:C:741:GLU:N	2.31	0.58
1:G:1125:ASN:HD22	1:G:1130:GLN:HG3	1.67	0.58
1:G:717:ASP:O	1:G:720:HIS:NE2	2.35	0.58
1:A:2248:ARG:HG2	1:A:2286:LEU:HD11	1.85	0.58
1:A:2875:ALA:HB2	1:A:2927:LEU:HD12	1.86	0.58
1:A:1970:GLN:NE2	1:A:3645:PRO:O	2.29	0.58
1:A:3727:ASP:HB3	1:A:3731:LYS:NZ	2.18	0.58
1:C:990:GLU:HG3	1:C:1024:TYR:HB3	1.86	0.58
1:E:277:GLY:HA2	1:E:317:ARG:NH1	2.13	0.58
1:G:1091:GLU:HB2	1:G:1203:ASN:HB2	1.86	0.58
1:G:465:GLN:HE21	1:G:3711:THR:HA	1.68	0.58
1:G:537:CYS:HB2	1:G:567:VAL:HG13	1.86	0.58
1:A:1101:ARG:HG3	1:A:1193:SER:HB3	1.86	0.58
1:A:1657:LEU:HA	1:A:1660:GLN:HG2	1.85	0.58
1:C:822:ARG:HA	1:C:1623:ARG:HH12	1.69	0.58
1:C:37:LEU:HD13	1:C:191:VAL:HG21	1.86	0.58
1:C:537:CYS:HB2	1:C:567:VAL:HG13	1.85	0.58
1:E:1944:GLU:HG3	1:E:2123:LEU:HD21	1.86	0.58
1:E:465:GLN:HE21	1:E:3711:THR:HA	1.69	0.58
1:E:530:ILE:HG23	1:E:537:CYS:HB3	1.85	0.58
1:G:3813:GLN:OE1	1:G:3896:ASN:ND2	2.37	0.58
1:G:3817:LEU:HD11	1:G:3821:LYS:HE2	1.84	0.58
1:G:489:ASN:HB3	1:G:493:ARG:HH12	1.69	0.58
1:A:3701:LEU:HD11	1:A:3725:TYR:CD1	2.39	0.58
1:C:1091:GLU:HB2	1:C:1203:ASN:HB2	1.86	0.58
1:C:699:GLY:O	1:C:1647:CYS:N	2.36	0.58
1:C:1657:LEU:HA	1:C:1660:GLN:HG2	1.85	0.58
1:C:465:GLN:HE21	1:C:3711:THR:HA	1.69	0.58
1:G:603:LEU:HA	1:G:606:LEU:HD12	1.86	0.58
1:G:699:GLY:O	1:G:1647:CYS:N	2.36	0.58
1:A:2347:GLU:OE2	1:A:3852:LYS:CD	2.52	0.58
1:A:2347:GLU:OE2	1:A:3852:LYS:HD3	2.04	0.58
1:C:1802:ILE:HB	1:C:1804:LEU:HD12	1.86	0.58
1:C:2875:ALA:HB2	1:C:2927:LEU:HD12	1.86	0.58
1:C:4054:ASN:OD1	1:C:4055:VAL:N	2.37	0.58
1:C:546:TRP:HE1	1:C:550:LYS:HZ1	1.52	0.58
1:E:1657:LEU:HA	1:E:1660:GLN:HG2	1.85	0.58
1:E:402:ARG:NH1	1:E:405:HIS:HD2	2.01	0.58
1:E:537:CYS:HB2	1:E:567:VAL:HG13	1.85	0.58
1:E:681:HIS:HA	1:E:716:PHE:CD1	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1079:LYS:HA	1:G:1082:THR:HG23	1.86	0.58
1:G:822:ARG:HA	1:G:1623:ARG:HH12	1.68	0.58
1:G:1927:LEU:HD21	1:G:2101:MET:HG2	1.84	0.58
1:G:880:GLU:HG2	1:G:967:PRO:HG2	1.85	0.58
1:A:465:GLN:HE21	1:A:3711:THR:HA	1.69	0.57
1:A:37:LEU:HD13	1:A:191:VAL:HG21	1.86	0.57
1:A:603:LEU:HA	1:A:606:LEU:HD12	1.86	0.57
1:A:880:GLU:HG2	1:A:967:PRO:HG2	1.85	0.57
1:E:1101:ARG:HG3	1:E:1193:SER:HB3	1.86	0.57
1:G:2870:GLU:OE2	1:G:2939:ARG:NE	2.37	0.57
1:C:1944:GLU:HG3	1:C:2123:LEU:HD21	1.86	0.57
1:C:3701:LEU:HD11	1:C:3725:TYR:CD1	2.39	0.57
1:E:1288:PHE:HE2	1:E:1460:HIS:HA	1.68	0.57
1:A:1079:LYS:HA	1:A:1082:THR:HG23	1.85	0.57
1:A:546:TRP:HE1	1:A:550:LYS:HZ1	1.51	0.57
1:C:3727:ASP:HB3	1:C:3731:LYS:NZ	2.18	0.57
1:E:1077:ALA:HA	1:E:1236:THR:HG22	1.87	0.57
1:E:2875:ALA:HB2	1:E:2927:LEU:HD12	1.86	0.57
1:G:1093:GLU:HB2	1:G:1201:HIS:HB3	1.87	0.57
1:G:1819:VAL:HG22	1:G:1926:LEU:HD13	1.87	0.57
1:A:990:GLU:HG3	1:A:1024:TYR:HB3	1.86	0.57
1:C:1819:VAL:HG22	1:C:1926:LEU:HD13	1.87	0.57
1:C:4059:LEU:HD13	1:C:4167:ALA:HB2	1.86	0.57
1:E:37:LEU:HD11	1:E:47:CYS:HB3	1.87	0.57
1:E:3879:GLU:OE2	1:E:3883:ASP:OD2	2.22	0.57
2:H:14:THR:HG22	2:H:106:LEU:HD12	1.86	0.57
1:C:489:ASN:HB3	1:C:493:ARG:HH12	1.69	0.57
1:E:1078:GLU:HA	1:E:1237:TRP:CZ3	2.40	0.57
1:E:37:LEU:HD13	1:E:191:VAL:HG21	1.86	0.57
1:E:4059:LEU:HD13	1:E:4167:ALA:HB2	1.85	0.57
1:E:4934:GLY:HA3	1:G:4937:ILE:CG1	2.29	0.57
1:G:1078:GLU:HA	1:G:1237:TRP:CZ3	2.40	0.57
1:A:1671:ARG:HD2	1:A:1713:ASP:HB3	1.87	0.57
1:C:1638:ALA:HA	1:C:1649:ASP:HA	1.87	0.57
1:E:990:GLU:HG3	1:E:1024:TYR:HB3	1.86	0.57
1:E:1638:ALA:HA	1:E:1649:ASP:HA	1.87	0.57
1:E:4054:ASN:OD1	1:E:4055:VAL:N	2.37	0.57
1:E:4849:TYR:O	1:E:4852:THR:HG22	2.05	0.57
1:G:990:GLU:HG3	1:G:1024:TYR:HB3	1.86	0.57
1:A:3937:TYR:HA	1:A:3940:LYS:HZ3	1.70	0.57
1:A:4054:ASN:OD1	1:A:4055:VAL:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:530:ILE:HG23	1:A:537:CYS:HB3	1.85	0.57
1:A:551:LEU:HG	1:A:589:LEU:HD22	1.87	0.57
1:E:1093:GLU:HB2	1:E:1201:HIS:HB3	1.87	0.57
1:E:489:ASN:HB3	1:E:493:ARG:HH12	1.69	0.57
1:E:4963:ILE:HD11	1:E:5025:GLY:O	2.04	0.57
1:E:603:LEU:HA	1:E:606:LEU:HD12	1.86	0.57
1:E:717:ASP:O	1:E:720:HIS:NE2	2.38	0.57
1:A:1802:ILE:HB	1:A:1804:LEU:HD12	1.86	0.57
1:A:4214:LYS:HD2	1:A:4985:LEU:HD23	1.86	0.57
1:A:717:ASP:O	1:A:720:HIS:NE2	2.38	0.57
1:C:110:ARG:HH21	1:C:115:ARG:HH21	1.53	0.57
1:A:1638:ALA:HA	1:A:1649:ASP:HA	1.87	0.57
1:C:2333:ASP:OD1	1:C:2336:ARG:NH2	2.36	0.57
1:C:603:LEU:HA	1:C:606:LEU:HD12	1.86	0.57
1:C:717:ASP:O	1:C:720:HIS:NE2	2.38	0.57
1:G:1237:TRP:HD1	1:G:1611:HIS:HA	1.69	0.57
1:G:37:LEU:HD13	1:G:191:VAL:HG21	1.86	0.57
1:G:37:LEU:HD11	1:G:47:CYS:HB3	1.86	0.57
1:A:108:LEU:HB2	1:A:147:TRP:CZ3	2.40	0.57
1:A:1093:GLU:HB2	1:A:1201:HIS:HB3	1.86	0.57
1:A:1819:VAL:HG22	1:A:1926:LEU:HD13	1.87	0.57
1:C:1078:GLU:HA	1:C:1237:TRP:CZ3	2.40	0.57
1:E:110:ARG:HH21	1:E:115:ARG:HH21	1.53	0.57
1:E:1819:VAL:HG22	1:E:1926:LEU:HD13	1.87	0.57
1:G:108:LEU:HB2	1:G:147:TRP:CZ3	2.40	0.57
1:G:3780:LEU:HD12	1:G:3828:PHE:CE1	2.39	0.57
1:C:1514:LEU:O	1:C:1532:ASN:N	2.36	0.56
1:C:2829:GLY:HA3	1:C:2933:ASN:HA	1.86	0.56
1:C:37:LEU:HD11	1:C:47:CYS:HB3	1.86	0.56
1:E:3701:LEU:HD11	1:E:3725:TYR:CD1	2.39	0.56
1:G:2248:ARG:HG2	1:G:2286:LEU:HD11	1.87	0.56
1:C:1237:TRP:HD1	1:C:1611:HIS:HA	1.70	0.56
1:C:1671:ARG:HD2	1:C:1713:ASP:HB3	1.87	0.56
1:E:822:ARG:HA	1:E:1623:ARG:HH12	1.69	0.56
1:G:1944:GLU:HG3	1:G:2123:LEU:HD21	1.86	0.56
1:G:4000:MET:HA	1:G:4003:LEU:HB2	1.85	0.56
1:A:110:ARG:HH21	1:A:115:ARG:HH21	1.53	0.56
1:A:37:LEU:HD11	1:A:47:CYS:HB3	1.86	0.56
1:A:537:CYS:HB2	1:A:567:VAL:HG13	1.86	0.56
1:C:1093:GLU:HB2	1:C:1201:HIS:HB3	1.86	0.56
1:E:4917:ASP:OD2	1:G:4892:ARG:NH2	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:110:ARG:HH21	1:G:115:ARG:HH21	1.52	0.56
1:G:1638:ALA:HA	1:G:1649:ASP:HA	1.87	0.56
1:G:1970:GLN:NE2	1:G:3645:PRO:O	2.33	0.56
1:C:4214:LYS:HD2	1:C:4985:LEU:HD23	1.85	0.56
1:C:551:LEU:HG	1:C:589:LEU:HD22	1.87	0.56
1:C:705:ASN:OD1	1:C:706:GLY:N	2.39	0.56
1:E:1237:TRP:HD1	1:E:1611:HIS:HA	1.69	0.56
1:C:4721:LYS:HG3	1:C:4741:LEU:HB3	1.88	0.56
1:E:1211:LEU:HG	1:E:1212:ARG:H	1.70	0.56
1:E:4928:LEU:O	1:E:4932:ILE:HD12	2.04	0.56
1:G:1211:LEU:HG	1:G:1212:ARG:H	1.71	0.56
1:G:46:LEU:HD22	1:G:134:ASP:OD2	2.06	0.56
1:G:2829:GLY:HA3	1:G:2933:ASN:HA	1.87	0.56
1:A:739:ALA:O	1:A:741:GLU:N	2.30	0.56
1:C:684:VAL:HG22	1:C:781:VAL:HA	1.87	0.56
1:E:1802:ILE:HB	1:E:1804:LEU:HD12	1.86	0.56
1:E:551:LEU:HG	1:E:589:LEU:HD22	1.87	0.56
1:G:4214:LYS:HD2	1:G:4985:LEU:HD23	1.86	0.56
1:A:1944:GLU:HG3	1:A:2123:LEU:HD21	1.86	0.56
1:A:3786:CYS:SG	1:A:3794:VAL:HG22	2.46	0.56
1:A:3993:LEU:HD13	1:A:4055:VAL:HG22	1.88	0.56
2:D:25:HIS:CG	2:D:40:ARG:HE	2.24	0.56
1:E:1561:VAL:HG13	1:E:1562:ILE:HG22	1.88	0.56
1:G:1802:ILE:HB	1:G:1804:LEU:HD12	1.86	0.56
1:G:3989:VAL:HG13	1:G:4023:MET:SD	2.45	0.56
1:G:548:VAL:HG11	1:G:582:HIS:HA	1.88	0.56
1:G:705:ASN:OD1	1:G:706:GLY:N	2.39	0.56
1:A:1211:LEU:HG	1:A:1212:ARG:H	1.70	0.56
1:A:46:LEU:HD22	1:A:134:ASP:OD2	2.05	0.56
1:A:768:PHE:HB3	1:A:771:PHE:HE2	1.71	0.56
1:C:3993:LEU:HD13	1:C:4055:VAL:HG22	1.88	0.56
1:C:4849:TYR:O	1:C:4852:THR:HG22	2.06	0.56
1:E:3993:LEU:HD13	1:E:4055:VAL:HG22	1.87	0.56
1:G:1104:TRP:HH2	1:G:1226:PHE:HZ	1.54	0.56
1:G:3886:ARG:O	1:G:3890:LEU:HD13	2.06	0.56
1:A:2829:GLY:HA3	1:A:2933:ASN:HA	1.87	0.56
1:A:3841:VAL:HG12	1:A:3843:ASP:H	1.71	0.56
1:C:1211:LEU:HG	1:C:1212:ARG:H	1.71	0.56
1:E:548:VAL:HG11	1:E:582:HIS:HA	1.88	0.56
1:G:1109:LEU:HA	1:G:1120:LEU:HD13	1.87	0.56
1:G:551:LEU:HG	1:G:589:LEU:HD22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:705:ASN:OD1	1:A:706:GLY:N	2.39	0.56
1:A:684:VAL:HG22	1:A:781:VAL:HA	1.87	0.56
1:C:4664:LEU:O	1:C:4667:PRO:HD2	2.06	0.56
1:E:2756:ASN:OD1	1:E:2806:ARG:NH2	2.39	0.56
1:E:4721:LYS:HG3	1:E:4741:LEU:HB3	1.88	0.56
1:G:1077:ALA:HA	1:G:1236:THR:HG22	1.88	0.56
1:A:1078:GLU:HA	1:A:1237:TRP:CZ3	2.40	0.56
1:A:2756:ASN:OD1	1:A:2806:ARG:NH2	2.39	0.56
1:C:768:PHE:HB3	1:C:771:PHE:HE2	1.71	0.56
1:E:46:LEU:HD22	1:E:134:ASP:OD2	2.06	0.56
1:E:2854:GLY:O	1:E:2856:ASN:ND2	2.39	0.56
1:E:684:VAL:HG22	1:E:781:VAL:HA	1.87	0.56
2:F:25:HIS:CG	2:F:40:ARG:HE	2.24	0.56
1:A:1077:ALA:HA	1:A:1236:THR:HG22	1.87	0.55
1:A:1561:VAL:HG13	1:A:1562:ILE:HG22	1.88	0.55
1:C:108:LEU:HB2	1:C:147:TRP:CZ3	2.40	0.55
1:C:46:LEU:HD22	1:C:134:ASP:OD2	2.05	0.55
1:E:705:ASN:OD1	1:E:706:GLY:N	2.39	0.55
1:G:3990:VAL:HG13	1:G:4051:SER:HB2	1.88	0.55
1:A:3923:LEU:HD12	1:A:3961:VAL:HG13	1.89	0.55
1:A:3965:LEU:HD23	1:A:3968:TYR:HD2	1.71	0.55
1:A:4721:LYS:HG3	1:A:4741:LEU:HB3	1.88	0.55
1:C:2756:ASN:OD1	1:C:2806:ARG:NH2	2.39	0.55
1:E:636:ASN:OD1	1:E:637:LEU:N	2.39	0.55
1:G:1207:ASP:O	1:G:1210:SER:OG	2.19	0.55
1:G:2927:LEU:HD23	1:G:2930:LEU:HD12	1.87	0.55
1:A:2854:GLY:O	1:A:2856:ASN:ND2	2.39	0.55
1:A:768:PHE:HB3	1:A:771:PHE:CE2	2.41	0.55
1:C:113:HIS:CE1	1:C:402:ARG:HB3	2.42	0.55
1:C:2277:ALA:O	1:C:2281:ILE:HG13	2.07	0.55
1:E:4228:ALA:HB2	1:G:4976:GLU:OE1	2.06	0.55
1:G:636:ASN:OD1	1:G:637:LEU:N	2.39	0.55
1:G:768:PHE:HB3	1:G:771:PHE:HE2	1.71	0.55
1:C:1561:VAL:HG13	1:C:1562:ILE:HG22	1.89	0.55
1:C:2287:ALA:O	1:C:2349:ASN:ND2	2.31	0.55
1:C:2465:ASP:O	1:C:2467:VAL:N	2.40	0.55
1:C:3841:VAL:HG12	1:C:3843:ASP:H	1.71	0.55
1:C:3923:LEU:HD12	1:C:3961:VAL:HG13	1.89	0.55
1:C:636:ASN:OD1	1:C:637:LEU:N	2.39	0.55
1:C:768:PHE:HB3	1:C:771:PHE:CE2	2.41	0.55
1:E:1079:LYS:HA	1:E:1082:THR:HG23	1.86	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1671:ARG:HD2	1:E:1713:ASP:HB3	1.87	0.55
1:E:42:PHE:HA	1:E:447:ASP:OD2	2.07	0.55
1:E:768:PHE:HB3	1:E:771:PHE:CE2	2.41	0.55
1:G:3767:GLN:NE2	1:G:3805:LEU:O	2.37	0.55
1:G:42:PHE:HA	1:G:447:ASP:OD2	2.06	0.55
1:A:4807:PHE:CZ	1:G:4856:PHE:CE2	2.94	0.55
1:A:627:PRO:HG3	2:B:89:GLY:CA	2.37	0.55
1:C:627:PRO:HG3	2:D:89:GLY:CA	2.36	0.55
1:E:2277:ALA:O	1:E:2281:ILE:HG13	2.07	0.55
1:E:627:PRO:HG3	2:F:89:GLY:CA	2.36	0.55
1:G:2907:PRO:O	1:G:2910:THR:OG1	2.19	0.55
2:H:23:VAL:HG12	2:H:104:LEU:HD12	1.88	0.55
1:A:2287:ALA:O	1:A:2349:ASN:ND2	2.31	0.55
1:A:2465:ASP:O	1:A:2467:VAL:N	2.40	0.55
1:A:636:ASN:OD1	1:A:637:LEU:N	2.39	0.55
2:B:25:HIS:CG	2:B:40:ARG:HE	2.24	0.55
1:C:274:LEU:HD12	1:C:278:GLN:HE21	1.71	0.55
1:G:3825:GLU:O	1:G:3827:GLY:N	2.37	0.55
1:A:4892:ARG:CZ	1:G:4917:ASP:OD2	2.55	0.55
1:A:42:PHE:HA	1:A:447:ASP:OD2	2.07	0.55
1:A:4664:LEU:O	1:A:4667:PRO:HD2	2.07	0.55
1:E:108:LEU:HB2	1:E:147:TRP:CZ3	2.42	0.55
1:E:1684:ALA:O	1:E:1687:SER:HB3	2.06	0.55
1:E:2865:VAL:O	1:E:2928:LYS:NZ	2.34	0.55
1:E:572:PRO:HB3	1:E:609:CYS:HB3	1.89	0.55
1:E:768:PHE:HB3	1:E:771:PHE:HE2	1.71	0.55
1:G:4712:PRO:O	1:G:4718:LYS:NZ	2.29	0.55
1:G:684:VAL:HG22	1:G:781:VAL:HA	1.87	0.55
1:A:606:LEU:O	1:A:617:ASN:ND2	2.40	0.55
1:C:1745:ILE:O	1:C:1746:THR:OG1	2.25	0.55
1:C:2854:GLY:O	1:C:2856:ASN:ND2	2.39	0.55
1:E:113:HIS:CE1	1:E:402:ARG:HB3	2.42	0.55
1:E:2287:ALA:O	1:E:2349:ASN:ND2	2.31	0.55
1:E:2465:ASP:O	1:E:2467:VAL:N	2.40	0.55
1:E:3825:GLU:O	1:E:3827:GLY:N	2.34	0.55
1:E:3841:VAL:HG12	1:E:3843:ASP:H	1.72	0.55
1:G:103:TYR:CD1	1:G:152:PRO:HG3	2.41	0.55
1:G:1684:ALA:O	1:G:1687:SER:HB3	2.06	0.55
1:G:2431:ASP:O	1:G:2435:ARG:HG2	2.07	0.55
1:G:2854:GLY:O	1:G:2856:ASN:ND2	2.39	0.55
1:A:2277:ALA:O	1:A:2281:ILE:HG13	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4849:TYR:O	1:A:4852:THR:HG22	2.06	0.55
1:A:548:VAL:HG11	1:A:582:HIS:HA	1.88	0.55
1:C:1077:ALA:HA	1:C:1236:THR:HG22	1.88	0.55
1:C:606:LEU:O	1:C:617:ASN:ND2	2.40	0.55
1:E:3965:LEU:HD23	1:E:3968:TYR:HD2	1.71	0.55
1:E:590:LEU:HB2	1:E:599:VAL:HG11	1.89	0.55
1:A:1109:LEU:HA	1:A:1120:LEU:HD13	1.89	0.55
1:A:4051:SER:OG	1:A:4054:ASN:OD1	2.25	0.55
1:A:572:PRO:HB3	1:A:609:CYS:HB3	1.89	0.55
1:C:1684:ALA:O	1:C:1687:SER:HB3	2.07	0.55
1:C:548:VAL:HG11	1:C:582:HIS:HA	1.88	0.55
1:G:606:LEU:O	1:G:617:ASN:ND2	2.40	0.55
1:A:76:ARG:CZ	1:C:3844:LEU:HD21	2.37	0.54
1:C:1243:PRO:HD2	1:C:1458:HIS:CB	2.34	0.54
1:C:42:PHE:HA	1:C:447:ASP:OD2	2.07	0.54
1:G:2465:ASP:O	1:G:2467:VAL:N	2.40	0.54
1:G:4029:SER:HA	1:G:4032:GLU:HG3	1.89	0.54
1:A:274:LEU:HD12	1:A:278:GLN:HE21	1.71	0.54
1:C:590:LEU:HB2	1:C:599:VAL:HG11	1.89	0.54
1:C:572:PRO:HB3	1:C:609:CYS:HB3	1.90	0.54
1:E:3937:TYR:HA	1:E:3940:LYS:NZ	2.22	0.54
1:E:3999:MET:O	1:E:4003:LEU:N	2.37	0.54
1:E:919:ASN:HA	1:E:922:LEU:HB2	1.88	0.54
1:G:1671:ARG:HD2	1:G:1713:ASP:HB3	1.87	0.54
1:E:274:LEU:HD12	1:E:278:GLN:HE21	1.71	0.54
1:E:4664:LEU:O	1:E:4667:PRO:HD2	2.07	0.54
1:E:606:LEU:O	1:E:617:ASN:ND2	2.39	0.54
1:G:1514:LEU:O	1:G:1532:ASN:N	2.36	0.54
1:G:3889:GLN:HE22	1:G:3963:ASN:HB3	1.71	0.54
1:G:590:LEU:HB2	1:G:599:VAL:HG11	1.89	0.54
1:G:768:PHE:HB3	1:G:771:PHE:CE2	2.41	0.54
1:A:4055:VAL:HA	1:A:4058:ILE:HG12	1.89	0.54
1:C:2431:ASP:O	1:C:2435:ARG:HG2	2.07	0.54
1:C:4051:SER:OG	1:C:4054:ASN:OD1	2.25	0.54
1:C:4917:ASP:OD2	1:E:4892:ARG:NH2	2.41	0.54
1:E:2829:GLY:HA3	1:E:2933:ASN:HA	1.87	0.54
1:E:3989:VAL:HG13	1:E:4023:MET:SD	2.48	0.54
1:G:1561:VAL:HG13	1:G:1562:ILE:HG22	1.89	0.54
1:C:4055:VAL:HA	1:C:4058:ILE:HG12	1.89	0.54
1:G:33:LEU:HD12	1:G:53:SER:HB2	1.89	0.54
1:A:103:TYR:CD1	1:A:152:PRO:HG3	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1684:ALA:O	1:A:1687:SER:HB3	2.06	0.54
1:A:2431:ASP:O	1:A:2435:ARG:HG2	2.07	0.54
1:E:103:TYR:CD1	1:E:152:PRO:HG3	2.43	0.54
1:G:111:HIS:HD2	1:G:114:SER:H	1.55	0.54
1:G:2277:ALA:O	1:G:2281:ILE:HG13	2.07	0.54
1:G:4677:LEU:HD22	1:G:4711:PHE:CE1	2.42	0.54
1:G:4980:LEU:HA	1:G:4984:ASN:HB3	1.89	0.54
1:G:572:PRO:HB3	1:G:609:CYS:HB3	1.90	0.54
1:A:3932:ASP:OD1	1:G:76:ARG:HG2	2.08	0.54
2:H:11:ASP:OD2	2:H:68:VAL:HB	2.06	0.54
2:H:71:ARG:NH2	2:H:100:ASP:OD2	2.40	0.54
1:G:627:PRO:HG3	2:H:89:GLY:CA	2.38	0.54
1:A:157:ARG:HH22	1:A:164:ARG:HD2	1.73	0.54
1:A:1663:HIS:O	1:A:1666:THR:OG1	2.19	0.54
1:A:3999:MET:O	1:A:4003:LEU:N	2.37	0.54
1:C:103:TYR:CD1	1:C:152:PRO:HG3	2.42	0.54
1:C:3423:TRP:O	1:C:3428:ASN:N	2.41	0.54
1:A:4917:ASP:OD2	1:C:4892:ARG:NH2	2.41	0.54
1:E:157:ARG:HH22	1:E:164:ARG:HD2	1.73	0.54
1:E:4901:ILE:HG21	1:E:4913:ARG:NH2	2.23	0.54
1:E:33:LEU:HD12	1:E:53:SER:HB2	1.89	0.54
1:G:4030:LEU:HG	1:G:4040:ILE:HD11	1.89	0.54
1:A:113:HIS:CE1	1:A:402:ARG:HB3	2.42	0.54
1:A:4683:PHE:HE2	1:A:5017:ARG:HD2	1.73	0.54
1:C:2827:ARG:HB2	1:C:2934:GLY:HA3	1.90	0.54
1:C:76:ARG:CZ	1:E:3844:LEU:HD21	2.38	0.54
1:G:1243:PRO:HD2	1:G:1458:HIS:CB	2.38	0.54
1:G:274:LEU:HD12	1:G:278:GLN:HE21	1.71	0.54
1:A:2902:HIS:CG	1:A:2903:PRO:HD2	2.43	0.54
1:A:3423:TRP:O	1:A:3428:ASN:N	2.41	0.54
1:C:3965:LEU:HD23	1:C:3968:TYR:HD2	1.72	0.54
1:E:4051:SER:OG	1:E:4054:ASN:OD1	2.25	0.54
1:G:113:HIS:CE1	1:G:402:ARG:HB3	2.42	0.54
1:G:4240:ASP:CG	1:G:4675:LYS:HZ3	2.10	0.54
1:A:33:LEU:HD12	1:A:53:SER:HB2	1.90	0.54
1:C:157:ARG:HH22	1:C:164:ARG:HD2	1.73	0.54
1:C:2822:THR:OG1	1:C:2938:THR:OG1	2.19	0.54
1:C:4735:GLU:HA	1:C:4738:ALA:HB3	1.90	0.54
1:E:1104:TRP:HH2	1:E:1226:PHE:HZ	1.54	0.54
1:E:2431:ASP:O	1:E:2435:ARG:HG2	2.07	0.54
1:E:3923:LEU:HD12	1:E:3961:VAL:HG13	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:537:CYS:SG	1:E:571:SER:HB3	2.48	0.54
1:G:965:TYR:CZ	1:G:967:PRO:HG3	2.43	0.54
1:A:965:TYR:CZ	1:A:967:PRO:HG3	2.43	0.53
1:E:111:HIS:HD2	1:E:114:SER:H	1.56	0.53
1:G:3826:VAL:HA	1:G:3906:GLN:HE22	1.72	0.53
1:G:4901:ILE:HG21	1:G:4913:ARG:NH2	2.22	0.53
1:G:699:GLY:H	1:G:1647:CYS:HB3	1.72	0.53
1:A:634:GLN:HB3	1:A:1640:HIS:CE1	2.44	0.53
1:A:4026:MET:O	1:A:4029:SER:OG	2.21	0.53
1:C:2927:LEU:HD23	1:C:2930:LEU:HD12	1.90	0.53
1:E:1109:LEU:HA	1:E:1120:LEU:HD13	1.89	0.53
1:G:2244:ARG:HB2	1:G:2283:ASN:HD21	1.72	0.53
1:A:1104:TRP:HH2	1:A:1226:PHE:HZ	1.56	0.53
1:A:3989:VAL:HG13	1:A:4023:MET:SD	2.48	0.53
1:A:590:LEU:HB2	1:A:599:VAL:HG11	1.89	0.53
1:C:965:TYR:CZ	1:C:967:PRO:HG3	2.43	0.53
1:E:2244:ARG:HB2	1:E:2283:ASN:HD21	1.73	0.53
1:E:2902:HIS:CG	1:E:2903:PRO:HD2	2.43	0.53
1:G:294:THR:HG22	1:G:296:ASP:H	1.74	0.53
1:A:3937:TYR:HA	1:A:3940:LYS:NZ	2.22	0.53
1:A:3969:ILE:HD13	1:A:4030:LEU:HD13	1.90	0.53
1:A:4712:PRO:O	1:A:4718:LYS:NZ	2.32	0.53
1:C:634:GLN:HB3	1:C:1640:HIS:CE1	2.43	0.53
1:C:3969:ILE:HD13	1:C:4030:LEU:HD13	1.91	0.53
1:G:4677:LEU:HD22	1:G:4711:PHE:CZ	2.43	0.53
1:A:76:ARG:HG2	1:C:3932:ASP:OD1	2.08	0.53
1:C:537:CYS:SG	1:C:571:SER:HB3	2.48	0.53
1:C:699:GLY:H	1:C:1647:CYS:HB3	1.73	0.53
1:G:1237:TRP:CD1	1:G:1611:HIS:HA	2.44	0.53
1:G:2902:HIS:CG	1:G:2903:PRO:HD2	2.44	0.53
1:C:1104:TRP:HH2	1:C:1226:PHE:HZ	1.56	0.53
1:E:1745:ILE:O	1:E:1746:THR:OG1	2.25	0.53
1:E:3423:TRP:O	1:E:3428:ASN:N	2.41	0.53
1:E:3969:ILE:HD13	1:E:4030:LEU:HD13	1.91	0.53
1:E:4712:PRO:O	1:E:4718:LYS:NZ	2.32	0.53
1:G:1947:CYS:SG	1:G:2127:GLN:NE2	2.82	0.53
1:A:3844:LEU:HD21	1:G:76:ARG:CZ	2.38	0.53
1:A:2907:PRO:O	1:A:2910:THR:OG1	2.18	0.53
1:A:2927:LEU:HD23	1:A:2930:LEU:HD12	1.90	0.53
1:A:294:THR:HG22	1:A:296:ASP:H	1.74	0.53
1:C:1109:LEU:HA	1:C:1120:LEU:HD13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3825:GLU:O	1:C:3827:GLY:N	2.34	0.53
1:E:2827:ARG:HB2	1:E:2934:GLY:HA3	1.90	0.53
1:E:3937:TYR:HA	1:E:3940:LYS:HZ3	1.73	0.53
1:A:1100:MET:O	1:A:1126:GLY:N	2.38	0.53
1:A:111:HIS:HD2	1:A:114:SER:H	1.56	0.53
1:A:3955:MET:SD	1:A:4019:LEU:HD13	2.49	0.53
1:A:537:CYS:SG	1:A:571:SER:HB3	2.48	0.53
1:C:76:ARG:HG2	1:E:3932:ASP:OD1	2.08	0.53
1:E:3959:LYS:HG3	1:E:4022:ASP:OD2	2.09	0.53
1:G:102:LEU:HB2	1:G:105:HIS:CE1	2.44	0.53
1:G:634:GLN:HB3	1:G:1640:HIS:CE1	2.44	0.53
1:G:537:CYS:SG	1:G:571:SER:HB3	2.49	0.53
1:A:495:ASN:HA	1:A:553:ARG:HH12	1.74	0.53
1:C:3937:TYR:HA	1:C:3940:LYS:NZ	2.23	0.53
1:C:3989:VAL:HG13	1:C:4023:MET:SD	2.48	0.53
1:C:70:GLU:HB2	1:C:108:LEU:HD23	1.91	0.53
1:E:1240:LYS:HD3	1:E:1610:ASN:OD1	2.08	0.53
1:E:2927:LEU:HD23	1:E:2930:LEU:HD12	1.90	0.53
1:E:3962:PHE:O	1:E:3966:THR:HG23	2.09	0.53
1:G:663:TYR:OH	1:G:665:GLU:OE2	2.04	0.53
1:A:4731:ILE:HG23	1:A:4732:PHE:CD2	2.44	0.53
1:C:3955:MET:SD	1:C:4019:LEU:HD13	2.49	0.53
1:C:445:LEU:O	1:C:449:ILE:HG13	2.09	0.53
1:E:965:TYR:CZ	1:E:967:PRO:HG3	2.44	0.53
1:G:157:ARG:HH22	1:G:164:ARG:HD2	1.73	0.53
1:A:445:LEU:O	1:A:449:ILE:HG13	2.09	0.52
1:A:622:THR:O	1:A:627:PRO:HD3	2.09	0.52
1:C:33:LEU:HD12	1:C:53:SER:HB2	1.90	0.52
1:C:3959:LYS:HG3	1:C:4022:ASP:OD2	2.09	0.52
1:C:3962:PHE:O	1:C:3966:THR:HG23	2.09	0.52
1:E:1610:ASN:HA	1:E:1652:GLU:OE2	2.09	0.52
1:E:699:GLY:H	1:E:1647:CYS:HB3	1.74	0.52
1:A:1229:ASN:HB3	1:A:1827:ARG:HH11	1.74	0.52
1:A:1514:LEU:O	1:A:1532:ASN:N	2.36	0.52
1:A:1237:TRP:CD1	1:A:1611:HIS:HA	2.44	0.52
1:C:1229:ASN:HB3	1:C:1827:ARG:HH11	1.74	0.52
1:C:2855:TYR:CD2	1:C:2857:PRO:HD3	2.44	0.52
1:C:4026:MET:O	1:C:4029:SER:OG	2.21	0.52
1:E:284:HIS:HE2	1:E:286:THR:HG1	1.56	0.52
1:E:4055:VAL:HA	1:E:4058:ILE:HG12	1.89	0.52
1:E:4779:LYS:O	1:E:4783:ILE:HG12	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:LEU:HB2	1:A:105:HIS:CE1	2.45	0.52
1:C:102:LEU:HB2	1:C:105:HIS:CE1	2.45	0.52
1:C:111:HIS:HD2	1:C:114:SER:H	1.55	0.52
1:C:2902:HIS:CG	1:C:2903:PRO:HD2	2.43	0.52
1:E:445:LEU:O	1:E:449:ILE:HG13	2.09	0.52
1:G:4658:ILE:HG22	1:G:4792:LEU:HB3	1.91	0.52
1:G:4856:PHE:O	1:G:4860:ARG:NH1	2.42	0.52
1:A:2827:ARG:HB2	1:A:2934:GLY:HA3	1.90	0.52
1:C:4731:ILE:HG23	1:C:4732:PHE:CD2	2.44	0.52
1:C:750:LEU:O	1:C:752:VAL:N	2.43	0.52
1:E:705:ASN:ND2	1:E:782:SER:OG	2.43	0.52
1:G:1101:ARG:NH1	1:G:1115:LEU:O	2.43	0.52
1:G:647:ASN:HB2	1:G:822:ARG:O	2.10	0.52
1:A:600:LEU:HD21	1:A:1666:THR:HG22	1.92	0.52
1:A:623:GLU:OE2	2:B:89:GLY:N	2.42	0.52
1:C:2244:ARG:HB2	1:C:2283:ASN:HD21	1.74	0.52
1:E:1101:ARG:NH1	1:E:1115:LEU:O	2.42	0.52
1:E:1237:TRP:CD1	1:E:1611:HIS:HA	2.45	0.52
1:E:3955:MET:SD	1:E:4019:LEU:HD13	2.49	0.52
1:E:4934:GLY:HA2	1:E:4937:ILE:HD12	1.90	0.52
1:E:4683:PHE:HE2	1:E:5017:ARG:HD2	1.73	0.52
1:E:495:ASN:HA	1:E:553:ARG:HH12	1.74	0.52
1:E:70:GLU:HB2	1:E:108:LEU:HD23	1.91	0.52
1:C:1237:TRP:CD1	1:C:1611:HIS:HA	2.44	0.52
1:C:622:THR:O	1:C:627:PRO:HD3	2.09	0.52
1:C:705:ASN:ND2	1:C:782:SER:OG	2.43	0.52
1:E:1961:PHE:CE2	1:E:2066:LEU:HD22	2.45	0.52
1:E:4961:CYS:HB3	1:E:4963:ILE:HG12	1.92	0.52
1:G:445:LEU:O	1:G:449:ILE:HG13	2.09	0.52
1:E:4937:ILE:HD12	1:G:4937:ILE:HD13	1.91	0.52
1:A:1101:ARG:NH1	1:A:1115:LEU:O	2.42	0.52
1:A:1240:LYS:HD3	1:A:1610:ASN:OD1	2.10	0.52
1:A:3962:PHE:O	1:A:3966:THR:HG23	2.09	0.52
1:C:3836:MET:O	1:C:3925:ARG:NH2	2.43	0.52
1:C:4683:PHE:HE2	1:C:5017:ARG:HD2	1.73	0.52
1:E:623:GLU:OE2	2:F:89:GLY:N	2.43	0.52
1:G:465:GLN:NE2	1:G:3712:GLU:OE1	2.43	0.52
1:E:4914:VAL:HG23	1:G:4888:TYR:CG	2.42	0.52
1:G:70:GLU:HB2	1:G:108:LEU:HD23	1.91	0.52
1:A:3496:LYS:O	1:A:3513:THR:N	2.43	0.52
1:A:35:LEU:HA	1:A:51:PRO:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:750:LEU:O	1:A:752:VAL:N	2.43	0.52
1:C:1130:GLN:HA	1:C:1138:PRO:HA	1.92	0.52
1:C:623:GLU:OE2	2:D:89:GLY:N	2.43	0.52
1:E:634:GLN:HB3	1:E:1640:HIS:CE1	2.44	0.52
1:G:695:TYR:CD2	1:G:1240:LYS:HE3	2.45	0.52
1:G:2855:TYR:CD2	1:G:2857:PRO:HD3	2.45	0.52
1:G:3966:THR:HG22	1:G:4026:MET:HA	1.92	0.52
1:G:750:LEU:O	1:G:752:VAL:N	2.43	0.52
1:A:647:ASN:HB2	1:A:822:ARG:O	2.09	0.52
1:E:294:THR:HG22	1:E:296:ASP:H	1.75	0.52
1:E:4731:ILE:HG23	1:E:4732:PHE:CD2	2.44	0.52
1:E:4735:GLU:HA	1:E:4738:ALA:HB3	1.92	0.52
1:E:750:LEU:O	1:E:752:VAL:N	2.43	0.52
1:G:2745:VAL:HG21	1:G:2818:ALA:HB2	1.92	0.52
1:G:3804:ILE:HG22	1:G:3812:VAL:HG11	1.92	0.52
1:G:4731:ILE:HG23	1:G:4732:PHE:CD2	2.44	0.52
1:A:2855:TYR:CD2	1:A:2857:PRO:HD3	2.45	0.52
1:A:3825:GLU:O	1:A:3827:GLY:N	2.35	0.52
1:C:3496:LYS:O	1:C:3513:THR:N	2.43	0.52
1:C:495:ASN:HA	1:C:553:ARG:HH12	1.74	0.52
1:G:1100:MET:O	1:G:1126:GLY:N	2.39	0.52
1:G:495:ASN:HA	1:G:553:ARG:HH12	1.74	0.52
1:A:1207:ASP:O	1:A:1210:SER:OG	2.19	0.51
1:A:1961:PHE:CE2	1:A:2066:LEU:HD22	2.45	0.51
1:A:284:HIS:HE2	1:A:286:THR:HG1	1.53	0.51
1:A:3959:LYS:HG3	1:A:4022:ASP:OD2	2.09	0.51
1:A:76:ARG:HE	1:C:3844:LEU:CD2	2.23	0.51
1:C:1291:LEU:HB3	1:C:1550:PRO:HG2	1.92	0.51
1:C:35:LEU:HA	1:C:51:PRO:HA	1.93	0.51
1:E:1623:ARG:NH1	1:E:1626:TRP:HE1	2.06	0.51
1:G:4909:TYR:O	1:G:4913:ARG:N	2.43	0.51
1:A:699:GLY:H	1:A:1647:CYS:HB3	1.74	0.51
1:A:3836:MET:O	1:A:3925:ARG:NH2	2.43	0.51
1:C:600:LEU:HD21	1:C:1666:THR:HG22	1.92	0.51
1:E:1491:ASN:H	1:E:1493:TYR:HA	1.76	0.51
1:E:3496:LYS:O	1:E:3513:THR:N	2.43	0.51
1:G:2158:CYS:SG	1:G:2184:ASN:ND2	2.80	0.51
1:A:1598:GLN:O	1:A:1600:LEU:N	2.44	0.51
1:A:2341:VAL:HG13	1:A:2342:ASN:N	2.22	0.51
2:B:23:VAL:HG12	2:B:104:LEU:HD12	1.93	0.51
1:C:1663:HIS:O	1:C:1666:THR:OG1	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:294:THR:HG22	1:C:296:ASP:H	1.75	0.51
1:G:158:SER:H	1:G:161:GLU:HG3	1.75	0.51
1:G:3971:GLY:HA2	1:G:5005:GLY:HA3	1.92	0.51
1:G:4928:LEU:O	1:G:4932:ILE:HD12	2.08	0.51
1:G:583:ILE:HD12	1:G:620:LEU:HD22	1.92	0.51
1:G:622:THR:O	1:G:627:PRO:HD3	2.09	0.51
1:A:70:GLU:HB2	1:A:108:LEU:HD23	1.91	0.51
1:A:4239:GLU:OE2	1:A:5014:TYR:OH	2.18	0.51
1:A:4779:LYS:O	1:A:4783:ILE:HG12	2.10	0.51
1:C:647:ASN:HB2	1:C:822:ARG:O	2.10	0.51
1:E:1100:MET:O	1:E:1126:GLY:N	2.39	0.51
1:E:33:LEU:HD23	1:E:35:LEU:HD23	1.93	0.51
1:E:35:LEU:HA	1:E:51:PRO:HA	1.92	0.51
1:E:622:THR:O	1:E:627:PRO:HD3	2.09	0.51
1:E:647:ASN:HB2	1:E:822:ARG:O	2.10	0.51
1:A:1291:LEU:HB3	1:A:1550:PRO:HG2	1.92	0.51
1:A:1453:VAL:HG12	1:A:1454:THR:O	2.11	0.51
1:A:583:ILE:HD12	1:A:620:LEU:HD22	1.92	0.51
1:C:78:LEU:HD11	1:C:147:TRP:CD2	2.45	0.51
1:E:1111:PRO:HG3	1:E:1609:PRO:HD3	1.92	0.51
1:E:2158:CYS:SG	1:E:2184:ASN:ND2	2.80	0.51
1:G:3826:VAL:HA	1:G:3906:GLN:NE2	2.25	0.51
1:G:3980:LEU:HD21	1:G:3985:LEU:HD13	1.91	0.51
1:A:1808:ARG:HA	1:A:1848:LEU:HD21	1.93	0.51
1:A:4217:PHE:CZ	1:A:4234:PHE:HA	2.46	0.51
1:A:4888:TYR:HB2	1:G:4914:VAL:CG2	2.41	0.51
1:C:1132:TRP:CD1	1:C:1136:SER:HA	2.46	0.51
1:C:1598:GLN:O	1:C:1600:LEU:N	2.44	0.51
1:C:33:LEU:HD23	1:C:35:LEU:HD23	1.93	0.51
1:C:3999:MET:O	1:C:4003:LEU:N	2.37	0.51
1:E:583:ILE:HD12	1:E:620:LEU:HD22	1.93	0.51
1:E:668:VAL:HA	1:E:789:VAL:HG12	1.93	0.51
2:F:23:VAL:HG12	2:F:104:LEU:HD12	1.93	0.51
1:G:1293:LEU:HD23	1:G:1584:ARG:HG2	1.93	0.51
1:G:1291:LEU:HB3	1:G:1550:PRO:HG2	1.92	0.51
1:G:233:ILE:O	1:G:257:ARG:NH1	2.44	0.51
1:G:721:LEU:HD11	1:G:728:ARG:HB2	1.93	0.51
1:G:705:ASN:ND2	1:G:782:SER:OG	2.42	0.51
2:H:25:HIS:CD2	2:H:104:LEU:HD11	2.46	0.51
1:A:1937:LEU:HD12	1:A:2116:LEU:HB2	1.93	0.51
1:A:4222:VAL:HG11	1:A:4950:VAL:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:705:ASN:ND2	1:A:782:SER:OG	2.43	0.51
1:C:1111:PRO:HG3	1:C:1609:PRO:HD3	1.93	0.51
1:C:4712:PRO:O	1:C:4718:LYS:NZ	2.31	0.51
1:C:919:ASN:HA	1:C:922:LEU:HB2	1.93	0.51
1:E:1204:LEU:HD22	1:E:1226:PHE:CD2	2.46	0.51
1:E:3836:MET:O	1:E:3925:ARG:NH2	2.44	0.51
1:G:1132:TRP:CD1	1:G:1136:SER:HA	2.45	0.51
1:G:1229:ASN:HB3	1:G:1827:ARG:HH11	1.74	0.51
1:G:2883:HIS:CE1	1:G:2911:LEU:HD11	2.45	0.51
1:A:4735:GLU:HA	1:A:4738:ALA:HB3	1.92	0.51
1:C:20:VAL:O	1:C:67:PHE:N	2.42	0.51
1:C:695:TYR:CD2	1:C:1240:LYS:HE3	2.45	0.51
1:E:1207:ASP:O	1:E:1210:SER:OG	2.18	0.51
1:E:1293:LEU:HD23	1:E:1584:ARG:HG2	1.93	0.51
1:E:3769:ARG:O	1:E:3773:ARG:NH1	2.41	0.51
1:E:4222:VAL:HG11	1:E:4950:VAL:HA	1.92	0.51
1:G:14:LEU:HD21	1:G:204:PRO:HG3	1.92	0.51
1:G:2142:TYR:CD2	1:G:2197:LEU:HD12	2.46	0.51
1:G:3919:THR:HG21	1:G:3968:TYR:HE2	1.76	0.51
1:G:4956:THR:O	1:G:4965:SER:N	2.41	0.51
1:G:668:VAL:HA	1:G:789:VAL:HG12	1.92	0.51
1:A:158:SER:H	1:A:161:GLU:HG3	1.76	0.51
1:A:78:LEU:HD11	1:A:147:TRP:CD2	2.46	0.51
1:C:1101:ARG:NH1	1:C:1115:LEU:O	2.43	0.51
1:C:1579:MET:O	1:C:1582:SER:OG	2.17	0.51
1:C:1937:LEU:HD12	1:C:2116:LEU:HB2	1.93	0.51
1:C:400:ALA:O	1:C:404:ILE:HG13	2.11	0.51
1:C:4222:VAL:HG11	1:C:4950:VAL:HA	1.93	0.51
1:C:4779:LYS:O	1:C:4783:ILE:HG12	2.09	0.51
1:C:4961:CYS:HB3	1:C:4963:ILE:HG12	1.92	0.51
1:E:600:LEU:HD21	1:E:1666:THR:HG22	1.92	0.51
1:E:2855:TYR:CD2	1:E:2857:PRO:HD3	2.45	0.51
1:G:2287:ALA:O	1:G:2349:ASN:ND2	2.30	0.51
1:A:2244:ARG:HB2	1:A:2283:ASN:HD21	1.74	0.51
1:A:4934:GLY:HA3	1:C:4937:ILE:CG1	2.34	0.51
2:B:74:LEU:HD23	2:B:76:ILE:HD11	1.93	0.51
1:C:1100:MET:O	1:C:1126:GLY:N	2.39	0.51
1:C:1961:PHE:CE2	1:C:2066:LEU:HD22	2.46	0.51
1:C:4217:PHE:CZ	1:C:4234:PHE:HA	2.46	0.51
1:E:1033:ARG:HA	1:E:1036:ARG:HG2	1.94	0.51
1:E:1078:GLU:HG3	1:E:1237:TRP:CH2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1141:ARG:NH2	1:E:1167:GLU:OE1	2.44	0.51
1:E:1291:LEU:HB3	1:E:1550:PRO:HG2	1.92	0.51
1:E:1514:LEU:O	1:E:1532:ASN:N	2.36	0.51
1:E:1663:HIS:O	1:E:1666:THR:OG1	2.19	0.51
1:E:1961:PHE:CD2	1:E:2066:LEU:HD22	2.46	0.51
1:E:4217:PHE:CZ	1:E:4234:PHE:HA	2.47	0.51
1:G:1453:VAL:HG12	1:G:1454:THR:O	2.11	0.51
1:G:1775:HIS:O	1:G:1775:HIS:ND1	2.44	0.51
1:G:1866:ILE:HG23	1:G:1927:LEU:HB2	1.93	0.51
1:G:78:LEU:HD11	1:G:147:TRP:CD2	2.46	0.51
1:A:1033:ARG:HA	1:A:1036:ARG:HG2	1.93	0.50
1:A:2340:PHE:HB2	1:A:2435:ARG:HB3	1.94	0.50
1:A:4055:VAL:HG11	1:A:4163:PHE:HZ	1.77	0.50
1:A:4914:VAL:CG2	1:C:4888:TYR:HB2	2.41	0.50
1:C:1190:PRO:HG2	1:C:1226:PHE:HE2	1.76	0.50
1:C:1853:ILE:O	1:C:1854:PHE:HB2	2.11	0.50
1:C:3674:ILE:HD13	1:C:3677:LEU:HD12	1.94	0.50
1:C:4735:GLU:O	1:C:4739:GLU:N	2.42	0.50
1:E:1775:HIS:ND1	1:E:1775:HIS:O	2.44	0.50
1:E:1853:ILE:O	1:E:1854:PHE:HB2	2.12	0.50
1:E:3992:PHE:HB3	1:E:3996:PHE:CE2	2.47	0.50
1:G:1130:GLN:HA	1:G:1138:PRO:HA	1.93	0.50
1:G:4963:ILE:HD12	1:G:5030:LYS:NZ	2.26	0.50
1:G:35:LEU:HA	1:G:51:PRO:HA	1.93	0.50
1:A:4961:CYS:HB3	1:A:4963:ILE:HG12	1.92	0.50
1:E:1453:VAL:HG12	1:E:1454:THR:O	2.11	0.50
1:E:1937:LEU:HD12	1:E:2116:LEU:HB2	1.93	0.50
1:E:721:LEU:HD11	1:E:728:ARG:HB2	1.92	0.50
1:G:1033:ARG:HA	1:G:1036:ARG:HG2	1.93	0.50
1:G:600:LEU:HD21	1:G:1666:THR:HG22	1.92	0.50
1:G:4683:PHE:HE2	1:G:5017:ARG:HD2	1.76	0.50
1:A:3850:GLN:O	1:A:3850:GLN:HG3	2.10	0.50
1:A:646:PRO:HA	1:A:823:LEU:HA	1.94	0.50
1:C:2191:PHE:HD1	1:C:2198:MET:HE1	1.76	0.50
1:C:4055:VAL:HG11	1:C:4163:PHE:HZ	1.76	0.50
1:C:668:VAL:HA	1:C:789:VAL:HG12	1.93	0.50
2:D:23:VAL:HG12	2:D:104:LEU:HD12	1.93	0.50
1:E:400:ALA:O	1:E:404:ILE:HG13	2.11	0.50
1:E:4055:VAL:HG11	1:E:4163:PHE:HZ	1.76	0.50
1:G:1623:ARG:NH1	1:G:1626:TRP:HE1	2.07	0.50
1:G:1808:ARG:HA	1:G:1848:LEU:HD21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:580:GLU:HB3	1:G:620:LEU:HD11	1.94	0.50
1:A:1078:GLU:HG3	1:A:1237:TRP:CH2	2.46	0.50
1:A:1436:SER:HA	1:A:1516:ILE:HA	1.93	0.50
1:A:2158:CYS:SG	1:A:2184:ASN:ND2	2.80	0.50
1:A:4677:LEU:HD22	1:A:4711:PHE:CE1	2.46	0.50
1:A:721:LEU:HD11	1:A:728:ARG:HB2	1.93	0.50
1:C:1288:PHE:HE2	1:C:1460:HIS:HA	1.77	0.50
1:A:4930:ALA:HB2	1:C:4933:GLN:HG2	1.93	0.50
1:E:2803:GLU:HA	1:E:2806:ARG:HB2	1.94	0.50
1:E:3674:ILE:HD13	1:E:3677:LEU:HD12	1.93	0.50
1:G:1141:ARG:NH2	1:G:1167:GLU:OE1	2.44	0.50
1:G:1111:PRO:HG3	1:G:1609:PRO:HD3	1.92	0.50
1:G:3806:ASN:H	1:G:3890:LEU:HD23	1.76	0.50
1:G:516:LYS:HG3	1:G:555:GLU:OE2	2.11	0.50
1:A:1141:ARG:NH2	1:A:1167:GLU:OE1	2.45	0.50
1:A:1961:PHE:CD2	1:A:2066:LEU:HD22	2.46	0.50
1:A:4837:LEU:HD11	1:A:4932:ILE:HG23	1.93	0.50
1:C:1207:ASP:O	1:C:1210:SER:OG	2.19	0.50
1:C:1453:VAL:HG12	1:C:1454:THR:O	2.11	0.50
1:C:1623:ARG:NH1	1:C:1626:TRP:HE1	2.06	0.50
1:C:3992:PHE:HB3	1:C:3996:PHE:CE2	2.47	0.50
1:C:4806:ASN:O	1:C:4809:PHE:HB3	2.12	0.50
1:C:4914:VAL:CG2	1:E:4888:TYR:HB2	2.42	0.50
1:E:1744:ALA:CB	1:E:1745:ILE:HA	2.41	0.50
1:E:4677:LEU:HD22	1:E:4711:PHE:CE1	2.47	0.50
1:E:516:LYS:HG3	1:E:555:GLU:OE2	2.11	0.50
1:E:638:ILE:HD12	1:E:678:GLN:NE2	2.27	0.50
1:G:1598:GLN:O	1:G:1600:LEU:N	2.44	0.50
1:G:401:ALA:HA	1:G:404:ILE:HD12	1.93	0.50
1:G:716:PHE:O	1:G:737:LEU:HG	2.12	0.50
1:A:1491:ASN:H	1:A:1493:TYR:HA	1.76	0.50
1:C:1240:LYS:HD3	1:C:1610:ASN:OD1	2.12	0.50
1:C:1491:ASN:H	1:C:1493:TYR:HA	1.77	0.50
1:C:1808:ARG:HA	1:C:1848:LEU:HD21	1.93	0.50
1:A:179:TYR:OH	1:C:2359:ARG:NE	2.45	0.50
1:C:516:LYS:HG3	1:C:555:GLU:OE2	2.11	0.50
1:C:583:ILE:HD12	1:C:620:LEU:HD22	1.93	0.50
1:C:646:PRO:HA	1:C:823:LEU:HA	1.94	0.50
1:E:14:LEU:HD21	1:E:204:PRO:HG3	1.92	0.50
1:E:4002:LYS:HA	1:E:4005:GLN:HG2	1.93	0.50
1:E:4806:ASN:O	1:E:4809:PHE:HB3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4857:ASN:HD21	1:G:4807:PHE:HD2	1.60	0.50
1:G:1579:MET:O	1:G:1582:SER:OG	2.17	0.50
1:G:214:VAL:HG22	1:G:341:TYR:CE1	2.47	0.50
1:G:2299:VAL:HA	1:G:2302:LEU:HD12	1.94	0.50
1:G:4680:LYS:O	1:G:4685:GLY:N	2.37	0.50
1:A:1853:ILE:O	1:A:1854:PHE:HB2	2.11	0.50
1:A:595:ARG:HH12	1:A:632:LEU:HA	1.77	0.50
1:A:891:TRP:CH2	1:A:899:ASP:HA	2.47	0.50
1:C:1141:ARG:NH2	1:C:1167:GLU:OE1	2.45	0.50
1:C:1866:ILE:HG23	1:C:1927:LEU:HB2	1.93	0.50
1:C:473:ASN:O	1:C:477:LEU:HG	2.12	0.50
1:E:580:GLU:HB3	1:E:620:LEU:HD11	1.94	0.50
1:E:891:TRP:CH2	1:E:899:ASP:HA	2.47	0.50
1:G:1853:ILE:O	1:G:1854:PHE:HB2	2.11	0.50
1:G:2124:LEU:HG	1:G:3673:MET:HE3	1.94	0.50
1:G:4961:CYS:HB3	1:G:4963:ILE:HG12	1.93	0.50
1:G:732:SER:N	1:G:735:GLN:OE1	2.45	0.50
1:A:3674:ILE:HD13	1:A:3677:LEU:HD12	1.93	0.50
1:A:2347:GLU:CD	1:A:3852:LYS:HE3	2.32	0.50
1:A:3992:PHE:HB3	1:A:3996:PHE:CE2	2.47	0.50
1:C:1033:ARG:HA	1:C:1036:ARG:HG2	1.93	0.50
1:C:1436:SER:HA	1:C:1516:ILE:HA	1.93	0.50
1:C:2340:PHE:HB2	1:C:2435:ARG:HB3	1.94	0.50
1:C:233:ILE:O	1:C:257:ARG:NH1	2.45	0.50
1:C:4934:GLY:HA3	1:E:4937:ILE:CG1	2.40	0.50
1:E:20:VAL:O	1:E:67:PHE:N	2.42	0.50
1:E:214:VAL:HG22	1:E:341:TYR:CE1	2.47	0.50
1:E:401:ALA:HA	1:E:404:ILE:HD12	1.93	0.50
1:A:2359:ARG:NE	1:G:179:TYR:OH	2.45	0.50
1:A:4937:ILE:HG12	1:G:4934:GLY:CA	2.40	0.50
1:C:1000:ARG:HB3	1:C:1021:LEU:HD21	1.94	0.50
1:C:1293:LEU:HD23	1:C:1584:ARG:HG2	1.93	0.50
2:D:74:LEU:HD23	2:D:76:ILE:HD11	1.93	0.50
1:E:1436:SER:HA	1:E:1516:ILE:HA	1.93	0.50
1:E:1866:ILE:HG23	1:E:1927:LEU:HB2	1.93	0.50
1:E:2907:PRO:O	1:E:2910:THR:OG1	2.18	0.50
1:E:473:ASN:O	1:E:477:LEU:HG	2.12	0.50
1:E:4837:LEU:HD11	1:E:4932:ILE:HG23	1.94	0.50
1:G:1744:ALA:CB	1:G:1745:ILE:HA	2.41	0.50
1:G:400:ALA:O	1:G:404:ILE:HG13	2.11	0.50
1:G:473:ASN:O	1:G:477:LEU:HG	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:919:ASN:HA	1:G:922:LEU:HB2	1.93	0.50
1:A:1111:PRO:HG3	1:A:1609:PRO:HD3	1.94	0.49
1:A:1775:HIS:O	1:A:1775:HIS:ND1	2.45	0.49
1:A:2299:VAL:HA	1:A:2302:LEU:HD12	1.94	0.49
1:A:3769:ARG:O	1:A:3773:ARG:NH1	2.41	0.49
1:A:3965:LEU:HD13	1:A:4026:MET:HE1	1.94	0.49
1:C:2158:CYS:SG	1:C:2184:ASN:ND2	2.80	0.49
1:C:2803:GLU:HA	1:C:2806:ARG:HB2	1.94	0.49
1:C:4002:LYS:HA	1:C:4005:GLN:HG2	1.93	0.49
1:C:721:LEU:HD11	1:C:728:ARG:HB2	1.93	0.49
1:E:1808:ARG:HA	1:E:1848:LEU:HD21	1.93	0.49
1:E:2340:PHE:HB2	1:E:2435:ARG:HB3	1.93	0.49
2:F:74:LEU:HD23	2:F:76:ILE:HD11	1.93	0.49
1:G:1190:PRO:HG2	1:G:1226:PHE:HE2	1.77	0.49
1:G:2340:PHE:HB2	1:G:2435:ARG:HB3	1.94	0.49
1:G:3891:LEU:HD23	1:G:3899:PHE:CZ	2.47	0.49
1:G:646:PRO:HA	1:G:823:LEU:HA	1.94	0.49
1:A:1293:LEU:HD23	1:A:1584:ARG:HG2	1.93	0.49
1:A:214:VAL:HG22	1:A:341:TYR:CE1	2.47	0.49
1:A:2242:ILE:HD11	1:A:2246:ASN:ND2	2.27	0.49
1:A:4677:LEU:HD22	1:A:4711:PHE:CZ	2.47	0.49
1:C:1738:LEU:HD11	1:C:2143:THR:HB	1.94	0.49
1:C:1762:LEU:HG	1:C:1764:GLY:H	1.76	0.49
1:C:3769:ARG:O	1:C:3773:ARG:NH1	2.40	0.49
1:C:401:ALA:HA	1:C:404:ILE:HD12	1.93	0.49
1:C:580:GLU:HB3	1:C:620:LEU:HD11	1.94	0.49
1:E:1671:ARG:NH1	1:E:1713:ASP:OD2	2.46	0.49
1:E:233:ILE:O	1:E:257:ARG:NH1	2.45	0.49
1:E:526:LEU:HD11	1:E:540:PHE:HZ	1.77	0.49
1:E:595:ARG:HH12	1:E:632:LEU:HA	1.78	0.49
1:G:4799:SER:OG	1:G:4812:HIS:NE2	2.36	0.49
1:G:891:TRP:CH2	1:G:899:ASP:HA	2.47	0.49
1:A:244:LEU:HD22	1:A:375:LYS:NZ	2.27	0.49
1:A:233:ILE:O	1:A:257:ARG:NH1	2.45	0.49
1:A:291:LEU:O	1:A:312:THR:OG1	2.23	0.49
1:A:516:LYS:HG3	1:A:555:GLU:OE2	2.11	0.49
1:A:668:VAL:HA	1:A:789:VAL:HG12	1.93	0.49
1:A:716:PHE:O	1:A:737:LEU:HG	2.13	0.49
1:A:919:ASN:HA	1:A:922:LEU:HB2	1.93	0.49
1:C:2907:PRO:O	1:C:2910:THR:OG1	2.18	0.49
1:C:4239:GLU:OE2	1:C:5014:TYR:OH	2.18	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:732:SER:N	1:C:735:GLN:OE1	2.46	0.49
1:E:1103:GLY:HA3	1:E:1123:VAL:HA	1.94	0.49
1:E:1190:PRO:HG2	1:E:1226:PHE:HE2	1.77	0.49
1:E:1738:LEU:HD11	1:E:2143:THR:HB	1.94	0.49
1:E:3965:LEU:HD13	1:E:4026:MET:HE1	1.94	0.49
1:E:695:TYR:O	1:E:697:GLY:N	2.42	0.49
1:E:732:SER:N	1:E:735:GLN:OE1	2.45	0.49
1:G:1609:PRO:O	1:G:1610:ASN:ND2	2.45	0.49
1:G:1240:LYS:HD3	1:G:1610:ASN:OD1	2.12	0.49
1:G:4024:VAL:O	1:G:4028:LEU:N	2.41	0.49
1:G:559:GLY:O	1:G:563:VAL:HG23	2.12	0.49
1:A:1103:GLY:HA3	1:A:1123:VAL:HA	1.94	0.49
1:A:14:LEU:HD21	1:A:204:PRO:HG3	1.93	0.49
1:A:2142:TYR:CD2	1:A:2197:LEU:HD12	2.47	0.49
1:A:559:GLY:O	1:A:563:VAL:HG23	2.12	0.49
1:A:575:LEU:HD12	1:A:609:CYS:SG	2.53	0.49
1:C:1775:HIS:O	1:C:1775:HIS:ND1	2.45	0.49
1:C:4677:LEU:HD22	1:C:4711:PHE:CE1	2.46	0.49
1:C:4677:LEU:HD22	1:C:4711:PHE:CZ	2.47	0.49
1:E:1076:ARG:HH22	1:E:1609:PRO:HB3	1.77	0.49
1:E:4217:PHE:HZ	1:E:4234:PHE:HA	1.78	0.49
1:G:1436:SER:HA	1:G:1516:ILE:HA	1.93	0.49
1:G:1491:ASN:H	1:G:1493:TYR:HA	1.76	0.49
1:G:20:VAL:O	1:G:67:PHE:N	2.42	0.49
1:G:2499:LYS:HB3	1:G:2553:TYR:OH	2.13	0.49
1:G:33:LEU:HD23	1:G:35:LEU:HD23	1.93	0.49
1:G:42:PHE:HD1	1:G:447:ASP:OD2	1.95	0.49
1:G:526:LEU:HD11	1:G:540:PHE:HZ	1.78	0.49
1:A:1762:LEU:HG	1:A:1764:GLY:H	1.77	0.49
1:A:1952:GLN:NE2	1:A:1956:GLU:OE2	2.45	0.49
1:C:158:SER:H	1:C:161:GLU:HG3	1.76	0.49
1:C:2142:TYR:CD2	1:C:2197:LEU:HD12	2.47	0.49
1:C:221:ARG:NE	1:C:253:CYS:O	2.45	0.49
1:C:244:LEU:HD22	1:C:375:LYS:NZ	2.27	0.49
1:C:575:LEU:HD12	1:C:609:CYS:SG	2.53	0.49
1:E:2142:TYR:CD2	1:E:2197:LEU:HD12	2.47	0.49
1:E:3889:GLN:HE22	1:E:3963:ASN:HB3	1.78	0.49
1:E:42:PHE:HD1	1:E:447:ASP:OD2	1.95	0.49
1:E:575:LEU:HD12	1:E:609:CYS:SG	2.53	0.49
1:E:826:ILE:O	1:E:828:GLU:N	2.46	0.49
1:G:1937:LEU:HD12	1:G:2116:LEU:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3934:TYR:OH	1:G:3998:HIS:HB3	2.11	0.49
1:G:638:ILE:HD12	1:G:678:GLN:NE2	2.27	0.49
1:A:2499:LYS:HB3	1:A:2553:TYR:OH	2.12	0.49
1:A:3799:LYS:HE3	1:A:3879:GLU:OE2	2.12	0.49
1:A:400:ALA:O	1:A:404:ILE:HG13	2.11	0.49
1:A:473:ASN:O	1:A:477:LEU:HG	2.12	0.49
1:A:826:ILE:O	1:A:828:GLU:N	2.46	0.49
1:C:2299:VAL:HA	1:C:2302:LEU:HD12	1.94	0.49
1:C:3727:ASP:O	1:C:3731:LYS:NZ	2.42	0.49
1:C:3937:TYR:HA	1:C:3940:LYS:HZ3	1.77	0.49
1:C:825:PRO:HG2	1:C:828:GLU:HG3	1.95	0.49
1:C:891:TRP:CH2	1:C:899:ASP:HA	2.47	0.49
1:E:1952:GLN:NE2	1:E:1956:GLU:OE2	2.45	0.49
1:E:2161:GLN:HE21	1:E:2177:LEU:HB3	1.77	0.49
1:E:716:PHE:O	1:E:737:LEU:HG	2.13	0.49
1:G:615:ARG:NH1	1:G:1678:ASN:OD1	2.46	0.49
1:G:2242:ILE:HD11	1:G:2246:ASN:ND2	2.27	0.49
1:G:3825:GLU:C	1:G:3827:GLY:H	2.16	0.49
1:A:3844:LEU:CD2	1:G:76:ARG:HE	2.23	0.49
1:A:1671:ARG:NH1	1:A:1713:ASP:OD2	2.46	0.49
1:A:1738:LEU:HD11	1:A:2143:THR:HB	1.95	0.49
1:A:33:LEU:HD23	1:A:35:LEU:HD23	1.93	0.49
1:C:1078:GLU:HG3	1:C:1237:TRP:CH2	2.47	0.49
1:C:1671:ARG:NH1	1:C:1713:ASP:OD2	2.46	0.49
1:C:4217:PHE:HZ	1:C:4234:PHE:HA	1.78	0.49
1:C:4702:ASP:O	1:C:4705:VAL:HG12	2.13	0.49
1:C:595:ARG:HH12	1:C:632:LEU:HA	1.78	0.49
1:E:4702:ASP:O	1:E:4705:VAL:HG12	2.12	0.49
1:G:1078:GLU:HG3	1:G:1237:TRP:CH2	2.48	0.49
1:G:4205:TRP:HB2	1:G:4245:MET:HE1	1.95	0.49
1:A:20:VAL:O	1:A:67:PHE:N	2.42	0.49
1:A:732:SER:N	1:A:735:GLN:OE1	2.46	0.49
1:A:825:PRO:HG2	1:A:828:GLU:HG3	1.95	0.49
1:C:14:LEU:HD21	1:C:204:PRO:HG3	1.93	0.49
1:C:1952:GLN:NE2	1:C:1956:GLU:OE2	2.45	0.49
1:C:2242:ILE:HD11	1:C:2246:ASN:ND2	2.28	0.49
1:C:4139:ILE:O	1:C:4143:VAL:HG23	2.13	0.49
1:C:767:VAL:O	1:C:1475:THR:OG1	2.23	0.49
1:C:826:ILE:O	1:C:828:GLU:N	2.46	0.49
1:E:2299:VAL:HA	1:E:2302:LEU:HD12	1.95	0.49
1:E:244:LEU:HD22	1:E:375:LYS:NZ	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:646:PRO:HA	1:E:823:LEU:HA	1.94	0.49
1:G:1000:ARG:HB3	1:G:1021:LEU:HD21	1.94	0.49
1:G:244:LEU:HD22	1:G:375:LYS:NZ	2.27	0.49
1:G:4183:ILE:HD12	1:G:4185:GLY:H	1.78	0.49
1:G:4820:VAL:O	1:G:4824:ARG:HG3	2.12	0.49
1:G:583:ILE:HD11	1:G:617:ASN:OD1	2.13	0.49
1:A:2505:PHE:CE1	1:A:2509:VAL:HG21	2.48	0.49
1:A:3727:ASP:HB3	1:A:3731:LYS:HZ1	1.76	0.49
1:A:4002:LYS:HA	1:A:4005:GLN:HG2	1.94	0.49
1:A:526:LEU:HD11	1:A:540:PHE:HZ	1.77	0.49
1:A:692:TYR:CE1	1:A:711:LEU:HD21	2.48	0.49
1:C:2142:TYR:HD2	1:C:2197:LEU:HD12	1.78	0.49
1:C:214:VAL:HG22	1:C:341:TYR:CE1	2.47	0.49
1:E:158:SER:OG	1:E:159:GLU:N	2.45	0.49
1:E:350:HIS:HD2	1:E:353:SER:H	1.61	0.49
1:A:1091:GLU:HA	1:A:1150:GLY:HA2	1.95	0.49
1:A:109:LEU:HB2	1:A:118:LEU:HB3	1.95	0.49
1:A:1744:ALA:CB	1:A:1745:ILE:HA	2.41	0.49
1:A:2142:TYR:HD2	1:A:2197:LEU:HD12	1.78	0.49
1:A:2803:GLU:HA	1:A:2806:ARG:HB2	1.95	0.49
1:A:4247:ILE:HD11	1:A:4667:PRO:HB2	1.95	0.49
1:A:4976:GLU:OE1	1:G:4228:ALA:HB2	2.13	0.49
1:C:1744:ALA:CB	1:C:1745:ILE:HA	2.41	0.49
1:C:526:LEU:HD11	1:C:540:PHE:HZ	1.77	0.49
1:E:4677:LEU:HD22	1:E:4711:PHE:CZ	2.48	0.49
1:G:1762:LEU:HG	1:G:1764:GLY:H	1.78	0.49
1:G:3842:LEU:HB3	1:G:3929:SER:OG	2.13	0.49
1:A:1000:ARG:HB3	1:A:1021:LEU:HD21	1.94	0.48
1:A:1190:PRO:HG2	1:A:1226:PHE:HE2	1.77	0.48
1:A:1623:ARG:NH1	1:A:1626:TRP:HE1	2.06	0.48
1:A:1866:ILE:HG23	1:A:1927:LEU:HB2	1.93	0.48
1:A:2450:ALA:O	1:A:2453:ILE:HG12	2.13	0.48
1:A:402:ARG:NH1	1:A:405:HIS:CD2	2.81	0.48
1:A:401:ALA:HA	1:A:404:ILE:HD12	1.94	0.48
1:A:583:ILE:HD11	1:A:617:ASN:OD1	2.13	0.48
1:C:1961:PHE:CD2	1:C:2066:LEU:HD22	2.47	0.48
1:C:2867:LEU:HG	1:C:2928:LYS:HZ3	1.77	0.48
1:C:3727:ASP:HB3	1:C:3731:LYS:HZ1	1.77	0.48
1:C:638:ILE:HD12	1:C:678:GLN:NE2	2.27	0.48
1:C:695:TYR:O	1:C:697:GLY:N	2.42	0.48
1:E:2242:ILE:HD11	1:E:2246:ASN:ND2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1663:HIS:O	1:G:1666:THR:OG1	2.19	0.48
1:G:1671:ARG:NH1	1:G:1713:ASP:OD2	2.46	0.48
1:G:1961:PHE:CE2	1:G:2066:LEU:HD22	2.48	0.48
1:G:484:LEU:HD11	1:G:530:ILE:HD11	1.95	0.48
1:A:4192:ARG:NH1	1:A:5028:PHE:CD2	2.81	0.48
1:A:42:PHE:HD1	1:A:447:ASP:OD2	1.95	0.48
1:C:1091:GLU:HA	1:C:1150:GLY:HA2	1.95	0.48
1:C:2161:GLN:HE21	1:C:2177:LEU:HB3	1.77	0.48
1:C:2505:PHE:CE1	1:C:2509:VAL:HG21	2.48	0.48
1:C:2499:LYS:HB3	1:C:2553:TYR:OH	2.13	0.48
1:C:3965:LEU:HD13	1:C:4026:MET:HE1	1.94	0.48
1:E:2499:LYS:HB3	1:E:2553:TYR:OH	2.13	0.48
1:E:4162:ASN:HA	1:E:4165:GLU:HG2	1.95	0.48
1:E:4923:PHE:O	1:E:4928:LEU:HD13	2.13	0.48
1:G:4664:LEU:O	1:G:4667:PRO:HD2	2.13	0.48
1:A:4162:ASN:HA	1:A:4165:GLU:HG2	1.95	0.48
1:A:4702:ASP:O	1:A:4705:VAL:HG12	2.12	0.48
1:A:4735:GLU:O	1:A:4739:GLU:N	2.44	0.48
1:A:580:GLU:HB3	1:A:620:LEU:HD11	1.94	0.48
1:C:158:SER:OG	1:C:159:GLU:N	2.46	0.48
1:E:4856:PHE:O	1:E:4860:ARG:NH1	2.46	0.48
1:E:583:ILE:HD11	1:E:617:ASN:OD1	2.13	0.48
1:E:692:TYR:CE1	1:E:711:LEU:HD21	2.48	0.48
1:G:1077:ALA:HB3	1:G:1190:PRO:HD2	1.96	0.48
1:G:2505:PHE:CE1	1:G:2509:VAL:HG21	2.48	0.48
1:G:2775:TRP:HH2	1:G:2783:GLU:HA	1.78	0.48
1:G:2803:GLU:HA	1:G:2806:ARG:HB2	1.95	0.48
1:G:825:PRO:HG2	1:G:828:GLU:HG3	1.95	0.48
1:G:826:ILE:O	1:G:828:GLU:N	2.46	0.48
1:A:1579:MET:O	1:A:1582:SER:OG	2.17	0.48
1:A:2191:PHE:HD1	1:A:2198:MET:HE1	1.78	0.48
1:A:2775:TRP:HH2	1:A:2783:GLU:HA	1.79	0.48
1:C:1609:PRO:O	1:C:1610:ASN:ND2	2.46	0.48
1:C:1815:LEU:HB3	1:C:1865:MET:HE3	1.94	0.48
1:C:3799:LYS:HE3	1:C:3879:GLU:OE2	2.12	0.48
1:C:42:PHE:HD1	1:C:447:ASP:OD2	1.96	0.48
1:C:559:GLY:O	1:C:563:VAL:HG23	2.12	0.48
1:E:1000:ARG:HB3	1:E:1021:LEU:HD21	1.94	0.48
1:E:102:LEU:HB2	1:E:105:HIS:CE1	2.47	0.48
1:E:1598:GLN:O	1:E:1600:LEU:N	2.43	0.48
1:E:1849:LEU:HG	1:E:1945:TYR:CE2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2341:VAL:HG13	1:E:2342:ASN:N	2.22	0.48
1:E:3799:LYS:HE3	1:E:3879:GLU:OE2	2.12	0.48
1:E:4139:ILE:O	1:E:4143:VAL:HG23	2.13	0.48
1:E:825:PRO:HG2	1:E:828:GLU:HG3	1.95	0.48
1:G:350:HIS:HD2	1:G:353:SER:H	1.61	0.48
1:G:603:LEU:HD22	1:G:621:ILE:HD12	1.96	0.48
1:G:63:ALA:HA	1:G:261:ARG:NH2	2.29	0.48
1:A:4806:ASN:O	1:A:4809:PHE:HB3	2.13	0.48
1:A:590:LEU:HD23	1:A:631:LEU:HD21	1.95	0.48
1:E:1077:ALA:HB3	1:E:1190:PRO:HD2	1.96	0.48
1:E:4192:ARG:NH1	1:E:5028:PHE:CD2	2.82	0.48
1:E:484:LEU:HD11	1:E:530:ILE:HD11	1.96	0.48
1:E:559:GLY:O	1:E:563:VAL:HG23	2.12	0.48
1:G:1091:GLU:HA	1:G:1150:GLY:HA2	1.96	0.48
1:G:1849:LEU:HG	1:G:1945:TYR:CE2	2.48	0.48
1:G:3959:LYS:HG3	1:G:4022:ASP:OD2	2.14	0.48
1:G:3993:LEU:HD13	1:G:4055:VAL:HG22	1.96	0.48
1:G:4175:ARG:N	1:G:4176:PRO:HD2	2.29	0.48
1:A:158:SER:OG	1:A:159:GLU:N	2.46	0.48
1:A:2161:GLN:HE21	1:A:2177:LEU:HB3	1.78	0.48
1:A:4901:ILE:HG21	1:A:4913:ARG:NH2	2.27	0.48
1:A:683:ARG:HB3	1:A:713:SER:HB2	1.96	0.48
1:C:1077:ALA:HB3	1:C:1190:PRO:HD2	1.95	0.48
1:C:2341:VAL:HG13	1:C:2342:ASN:N	2.22	0.48
1:C:484:LEU:HD11	1:C:530:ILE:HD11	1.96	0.48
1:C:4835:LYS:HG2	1:E:4822:THR:HG21	1.94	0.48
1:G:109:LEU:HB2	1:G:118:LEU:HB3	1.95	0.48
1:G:2161:GLN:HE21	1:G:2177:LEU:HB3	1.78	0.48
1:G:2450:ALA:O	1:G:2453:ILE:HG12	2.14	0.48
1:G:4002:LYS:HA	1:G:4005:GLN:HG2	1.96	0.48
1:G:4031:LEU:HD12	1:G:4034:ASN:HD22	1.79	0.48
1:G:4677:LEU:CD1	1:G:4702:ASP:HB3	2.44	0.48
1:A:4807:PHE:CE2	1:G:4856:PHE:CD2	3.01	0.48
1:G:692:TYR:CE1	1:G:711:LEU:HD21	2.48	0.48
1:A:1088:TRP:HB2	1:A:1153:ILE:CG2	2.44	0.48
1:A:1849:LEU:HG	1:A:1945:TYR:CE2	2.48	0.48
1:C:1849:LEU:HG	1:C:1945:TYR:CE2	2.48	0.48
1:C:2450:ALA:O	1:C:2453:ILE:HG12	2.13	0.48
1:C:2793:PRO:O	1:C:2796:THR:OG1	2.24	0.48
1:C:4162:ASN:HA	1:C:4165:GLU:HG2	1.95	0.48
1:C:583:ILE:HD11	1:C:617:ASN:OD1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:109:LEU:HB2	1:E:118:LEU:HB3	1.95	0.48
1:E:1205:GLY:HA2	1:E:1225:PRO:HB3	1.96	0.48
1:E:603:LEU:HD22	1:E:621:ILE:HD12	1.95	0.48
1:E:4914:VAL:HG21	1:G:4888:TYR:HB2	1.94	0.48
1:C:1088:TRP:HB2	1:C:1153:ILE:CG2	2.44	0.48
1:C:4192:ARG:NH1	1:C:5028:PHE:CD2	2.82	0.48
1:E:22:LEU:HB3	1:E:200:TRP:CZ3	2.49	0.48
1:E:3727:ASP:HB3	1:E:3731:LYS:HZ1	1.77	0.48
1:E:4984:ASN:OD1	1:E:4987:ASN:ND2	2.47	0.48
1:G:3836:MET:O	1:G:3925:ARG:NH2	2.47	0.48
1:A:2142:TYR:CD2	1:A:2197:LEU:HB2	2.49	0.48
1:A:4139:ILE:O	1:A:4143:VAL:HG23	2.13	0.48
1:A:4984:ASN:OD1	1:A:4987:ASN:ND2	2.47	0.48
1:C:615:ARG:NH1	1:C:1678:ASN:OD1	2.47	0.48
1:C:350:HIS:HD2	1:C:353:SER:H	1.61	0.48
1:C:4552:LEU:HD11	1:C:4663:CYS:SG	2.54	0.48
1:C:692:TYR:CE1	1:C:711:LEU:HD21	2.48	0.48
1:E:1088:TRP:HB2	1:E:1153:ILE:CG2	2.44	0.48
1:E:2505:PHE:CE1	1:E:2509:VAL:HG21	2.48	0.48
1:E:709:ASP:OD2	1:E:1491:ASN:HA	2.14	0.48
1:G:1961:PHE:CD2	1:G:2066:LEU:HD22	2.49	0.48
1:G:3962:PHE:O	1:G:3966:THR:HG23	2.13	0.48
1:A:1687:SER:HB2	1:A:1782:PHE:CZ	2.49	0.48
1:A:2454:ARG:O	1:A:2458:ARG:HG3	2.14	0.48
1:C:2066:LEU:O	1:C:2070:VAL:HG23	2.14	0.48
1:C:4901:ILE:HG21	1:C:4913:ARG:NH2	2.27	0.48
1:C:4904:PRO:HB2	1:C:4910:GLU:HG3	1.96	0.48
1:C:590:LEU:HD23	1:C:631:LEU:HD21	1.95	0.48
1:C:602:VAL:O	1:C:605:SER:OG	2.22	0.48
1:E:3804:ILE:HG22	1:E:3812:VAL:HG11	1.96	0.48
1:G:1018:ASN:H	1:G:1021:LEU:HD12	1.79	0.48
1:G:2454:ARG:O	1:G:2458:ARG:HG3	2.14	0.48
1:A:615:ARG:NH1	1:A:1678:ASN:OD1	2.46	0.47
1:A:229:GLU:HA	1:A:249:GLY:HA2	1.96	0.47
1:A:3805:LEU:HB2	1:A:3890:LEU:HD23	1.95	0.47
1:A:3889:GLN:HE22	1:A:3963:ASN:HB3	1.78	0.47
1:A:4076:ALA:HA	1:A:4079:ASP:HB3	1.96	0.47
1:A:4914:VAL:HG23	1:C:4888:TYR:CG	2.48	0.47
1:A:638:ILE:HD12	1:A:678:GLN:NE2	2.27	0.47
1:E:2142:TYR:HD2	1:E:2197:LEU:HD12	1.78	0.47
1:E:2771:ILE:HD11	1:E:2857:PRO:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3768:SER:HA	1:E:3771:HIS:CE1	2.49	0.47
1:E:3980:LEU:HD21	1:E:3985:LEU:HD13	1.96	0.47
1:E:646:PRO:O	1:E:648:ILE:N	2.41	0.47
1:E:855:PRO:HG2	1:E:998:ARG:HD2	1.96	0.47
2:F:37:ASP:OD1	2:F:38:SER:N	2.47	0.47
2:F:76:ILE:O	2:F:96:THR:HG23	2.14	0.47
1:G:546:TRP:HE1	1:G:550:LYS:HZ1	1.61	0.47
1:G:595:ARG:HH12	1:G:632:LEU:HA	1.79	0.47
1:A:1077:ALA:HB3	1:A:1190:PRO:HD2	1.96	0.47
1:C:3768:SER:HA	1:C:3771:HIS:CE1	2.49	0.47
1:C:4984:ASN:OD1	1:C:4987:ASN:ND2	2.47	0.47
1:E:158:SER:H	1:E:161:GLU:HG3	1.79	0.47
1:E:2142:TYR:CD2	1:E:2197:LEU:HB2	2.48	0.47
1:E:2450:ALA:O	1:E:2453:ILE:HG12	2.14	0.47
1:E:683:ARG:HB3	1:E:713:SER:HB2	1.96	0.47
1:G:1676:LEU:O	1:G:1676:LEU:HD23	2.15	0.47
1:G:1952:GLN:NE2	1:G:1956:GLU:OE2	2.47	0.47
1:G:575:LEU:HD12	1:G:609:CYS:SG	2.53	0.47
1:A:4552:LEU:HD11	1:A:4663:CYS:SG	2.54	0.47
1:A:484:LEU:HD11	1:A:530:ILE:HD11	1.96	0.47
1:A:63:ALA:HA	1:A:261:ARG:NH2	2.30	0.47
1:C:2775:TRP:HH2	1:C:2783:GLU:HA	1.79	0.47
2:D:37:ASP:OD1	2:D:38:SER:N	2.47	0.47
1:E:615:ARG:NH1	1:E:1678:ASN:OD1	2.46	0.47
1:E:4247:ILE:HD11	1:E:4667:PRO:HB2	1.95	0.47
1:E:590:LEU:HD23	1:E:631:LEU:HD21	1.95	0.47
1:G:1746:THR:O	1:G:1748:PHE:N	2.48	0.47
1:G:2827:ARG:HB2	1:G:2934:GLY:HA3	1.96	0.47
1:G:402:ARG:NH1	1:G:405:HIS:CD2	2.81	0.47
1:A:2066:LEU:O	1:A:2070:VAL:HG23	2.15	0.47
1:A:4217:PHE:HZ	1:A:4234:PHE:HA	1.78	0.47
1:C:830:ARG:HD3	1:C:1612:PHE:CZ	2.50	0.47
1:C:2142:TYR:CD2	1:C:2197:LEU:HB2	2.49	0.47
1:E:1687:SER:HB2	1:E:1782:PHE:CZ	2.49	0.47
1:E:2775:TRP:HH2	1:E:2783:GLU:HA	1.79	0.47
1:E:402:ARG:NH1	1:E:405:HIS:CD2	2.81	0.47
1:G:1088:TRP:HB2	1:G:1153:ILE:CG2	2.44	0.47
1:G:1081:TYR:CD2	1:G:1234:VAL:HG13	2.49	0.47
1:G:1662:PHE:O	1:G:1666:THR:HG23	2.15	0.47
1:G:3826:VAL:HG23	1:G:3909:ASN:HB3	1.96	0.47
1:G:4573:ILE:HD11	1:G:4646:LEU:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:LEU:HB3	1:A:200:TRP:CZ3	2.50	0.47
1:A:350:HIS:HD2	1:A:353:SER:H	1.61	0.47
1:A:4963:ILE:HD12	1:A:5030:LYS:HZ1	1.78	0.47
1:A:603:LEU:HD22	1:A:621:ILE:HD12	1.96	0.47
1:C:1729:SER:O	1:C:1733:GLU:HG2	2.15	0.47
1:C:2454:ARG:O	1:C:2458:ARG:HG3	2.14	0.47
1:E:1132:TRP:CD1	1:E:1136:SER:HA	2.50	0.47
1:E:1662:PHE:O	1:E:1666:THR:HG23	2.15	0.47
1:E:1746:THR:O	1:E:1748:PHE:N	2.47	0.47
1:E:4175:ARG:N	1:E:4176:PRO:HD2	2.30	0.47
1:E:4552:LEU:HD11	1:E:4663:CYS:SG	2.54	0.47
1:G:2136:ARG:HH11	1:G:3720:TYR:HE2	1.62	0.47
2:H:38:SER:HB3	2:H:41:ASP:OD2	2.15	0.47
2:B:76:ILE:O	2:B:96:THR:HG23	2.15	0.47
1:C:109:LEU:HB2	1:C:118:LEU:HB3	1.96	0.47
1:C:3805:LEU:HB2	1:C:3890:LEU:HD23	1.96	0.47
1:C:4205:TRP:HB2	1:C:4245:MET:HE1	1.95	0.47
1:C:709:ASP:OD2	1:C:1491:ASN:HA	2.14	0.47
1:C:716:PHE:O	1:C:737:LEU:HG	2.13	0.47
1:E:1815:LEU:HB3	1:E:1865:MET:HE3	1.96	0.47
1:E:221:ARG:NE	1:E:253:CYS:O	2.44	0.47
1:E:4221:VAL:HG11	1:E:4230:LYS:HG3	1.96	0.47
1:E:4818:MET:HA	1:E:4824:ARG:HG2	1.96	0.47
1:E:4904:PRO:HB2	1:E:4910:GLU:HG3	1.97	0.47
1:E:695:TYR:CD2	1:E:1240:LYS:HE3	2.50	0.47
1:G:1091:GLU:HG2	1:G:1213:PHE:CD1	2.50	0.47
1:G:675:LEU:CD2	1:G:1633:PRO:HG3	2.45	0.47
1:G:3780:LEU:HD23	1:G:3819:TYR:CD2	2.49	0.47
1:A:1018:ASN:H	1:A:1021:LEU:HD12	1.80	0.47
1:A:4030:LEU:CG	1:A:4040:ILE:HD11	2.44	0.47
1:A:714:TYR:CB	1:A:757:PHE:HD2	2.28	0.47
1:C:1018:ASN:H	1:C:1021:LEU:HD12	1.80	0.47
1:C:111:HIS:CD2	1:C:113:HIS:HB3	2.50	0.47
1:C:1091:GLU:HG2	1:C:1213:PHE:CD1	2.49	0.47
1:C:1662:PHE:O	1:C:1666:THR:HG23	2.15	0.47
1:C:402:ARG:NH1	1:C:405:HIS:CD2	2.81	0.47
1:C:4791:TYR:HD2	1:C:4792:LEU:HD12	1.80	0.47
1:E:1091:GLU:HG2	1:E:1213:PHE:CD1	2.50	0.47
1:E:1748:PHE:HZ	1:E:2072:LEU:HB2	1.79	0.47
1:E:4677:LEU:HD11	1:E:4702:ASP:HB3	1.97	0.47
1:E:4791:TYR:HD2	1:E:4792:LEU:HD12	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1676:LEU:HD21	1:G:2164:SER:O	2.15	0.47
1:G:1940:CYS:SG	1:G:2123:LEU:HD12	2.55	0.47
1:G:2771:ILE:HD11	1:G:2857:PRO:HD2	1.96	0.47
1:G:3889:GLN:NE2	1:G:3963:ASN:HB3	2.29	0.47
1:G:4646:LEU:HA	1:G:4649:LEU:HB3	1.97	0.47
1:A:4892:ARG:NH2	1:G:4917:ASP:OD2	2.48	0.47
1:G:4984:ASN:OD1	1:G:4987:ASN:ND2	2.48	0.47
1:A:1130:GLN:HA	1:A:1138:PRO:HA	1.97	0.47
1:A:1662:PHE:O	1:A:1666:THR:HG23	2.15	0.47
1:A:4205:TRP:HB2	1:A:4245:MET:HE1	1.97	0.47
1:A:4818:MET:HA	1:A:4824:ARG:HG2	1.95	0.47
1:A:843:SER:OG	1:A:844:ARG:N	2.48	0.47
2:B:37:ASP:OD1	2:B:38:SER:N	2.47	0.47
1:C:1687:SER:HB2	1:C:1782:PHE:CZ	2.49	0.47
1:C:3889:GLN:HE22	1:C:3963:ASN:HB3	1.78	0.47
1:C:4247:ILE:HD11	1:C:4667:PRO:HB2	1.96	0.47
1:E:1609:PRO:O	1:E:1610:ASN:ND2	2.48	0.47
1:E:3805:LEU:HB2	1:E:3890:LEU:HD23	1.96	0.47
1:E:3962:PHE:HD1	1:E:4026:MET:SD	2.38	0.47
1:G:2066:LEU:O	1:G:2070:VAL:HG23	2.14	0.47
1:G:4855:ALA:HB1	1:G:4863:TYR:HE2	1.80	0.47
1:G:709:ASP:OD2	1:G:1491:ASN:HA	2.14	0.47
2:H:25:HIS:CG	2:H:40:ARG:HE	2.33	0.47
1:A:1132:TRP:CD1	1:A:1136:SER:HA	2.50	0.47
1:A:3768:SER:HA	1:A:3771:HIS:CE1	2.49	0.47
1:A:4183:ILE:HD12	1:A:4185:GLY:H	1.80	0.47
1:A:4791:TYR:HD2	1:A:4792:LEU:HD12	1.80	0.47
1:C:22:LEU:HB3	1:C:200:TRP:CZ3	2.49	0.47
1:C:2206:THR:O	1:C:2210:VAL:HG23	2.15	0.47
1:C:4030:LEU:CG	1:C:4040:ILE:HD11	2.44	0.47
1:C:4837:LEU:HD11	1:C:4932:ILE:HG23	1.97	0.47
1:C:603:LEU:HD22	1:C:621:ILE:HD12	1.96	0.47
1:E:2454:ARG:O	1:E:2458:ARG:HG3	2.14	0.47
1:G:2819:TRP:CZ3	1:G:2877:GLN:HG2	2.50	0.47
1:G:3981:ALA:HA	1:G:3986:TRP:HE1	1.80	0.47
1:G:4141:PHE:O	1:G:4145:VAL:HG23	2.15	0.47
2:H:37:ASP:OD1	2:H:38:SER:N	2.48	0.47
1:A:1476:MET:H	1:A:1485:SER:HA	1.80	0.47
1:A:1610:ASN:HA	1:A:1652:GLU:OE2	2.15	0.47
1:A:1850:VAL:HA	1:A:1945:TYR:CE1	2.50	0.47
1:A:3980:LEU:HD21	1:A:3985:LEU:HD13	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4087:LEU:HD23	1:A:4122:MET:HB3	1.97	0.47
1:A:4904:PRO:HB2	1:A:4910:GLU:HG3	1.97	0.47
1:A:646:PRO:O	1:A:648:ILE:N	2.41	0.47
1:C:3980:LEU:HD21	1:C:3985:LEU:HD13	1.96	0.47
1:C:411:TYR:HB2	1:C:486:LEU:HD21	1.97	0.47
1:C:4175:ARG:N	1:C:4176:PRO:HD2	2.29	0.47
1:E:2206:THR:O	1:E:2210:VAL:HG23	2.15	0.47
1:E:4087:LEU:HD23	1:E:4122:MET:HB3	1.97	0.47
1:E:495:ASN:CA	1:E:553:ARG:HH12	2.28	0.47
1:G:1679:ASN:HA	1:G:1682:ALA:HB3	1.97	0.47
1:G:1850:VAL:HA	1:G:1945:TYR:CE1	2.50	0.47
1:G:843:SER:OG	1:G:844:ARG:N	2.48	0.47
1:A:3962:PHE:HD1	1:A:4026:MET:SD	2.38	0.47
1:A:695:TYR:CD2	1:A:1240:LYS:HE3	2.50	0.47
2:D:76:ILE:O	2:D:96:THR:HG23	2.15	0.47
1:E:1812:LEU:HA	1:E:1815:LEU:HD12	1.97	0.47
1:E:418:LEU:HA	1:E:421:PHE:CE2	2.50	0.47
1:G:22:LEU:HB3	1:G:200:TRP:CZ3	2.50	0.47
1:G:2100:HIS:O	1:G:2104:ARG:HG2	2.15	0.47
1:G:683:ARG:HB3	1:G:713:SER:HB2	1.96	0.47
2:H:23:VAL:HG22	2:H:47:LYS:HG2	1.96	0.47
1:A:2100:HIS:O	1:A:2104:ARG:HG2	2.16	0.46
1:A:2206:THR:O	1:A:2210:VAL:HG23	2.15	0.46
1:A:2771:ILE:HD11	1:A:2857:PRO:HD2	1.96	0.46
1:A:495:ASN:CA	1:A:553:ARG:HH12	2.28	0.46
1:A:709:ASP:OD2	1:A:1491:ASN:HA	2.14	0.46
1:C:1676:LEU:HD23	1:C:1676:LEU:O	2.15	0.46
1:C:229:GLU:HA	1:C:249:GLY:HA2	1.97	0.46
1:C:663:TYR:OH	1:C:804:PRO:HD2	2.16	0.46
2:F:55:VAL:HG21	2:F:59:TRP:HD1	1.81	0.46
1:G:158:SER:OG	1:G:159:GLU:N	2.46	0.46
1:G:1685:LEU:O	1:G:1689:VAL:HG12	2.15	0.46
1:G:3955:MET:SD	1:G:4019:LEU:HD13	2.55	0.46
1:G:495:ASN:CA	1:G:553:ARG:HH12	2.28	0.46
1:G:590:LEU:HD23	1:G:631:LEU:HD21	1.95	0.46
1:G:855:PRO:HG2	1:G:998:ARG:HD2	1.96	0.46
1:A:221:ARG:NE	1:A:253:CYS:O	2.45	0.46
1:A:284:HIS:NE2	1:A:286:THR:OG1	2.47	0.46
1:A:4175:ARG:N	1:A:4176:PRO:HD2	2.30	0.46
2:B:87:HIS:HD2	2:B:88:PRO:HD2	1.81	0.46
1:C:1746:THR:O	1:C:1748:PHE:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2771:ILE:HD11	1:C:2857:PRO:HD2	1.96	0.46
1:C:2927:LEU:HD22	1:C:2937:VAL:HG11	1.97	0.46
1:C:4076:ALA:HA	1:C:4079:ASP:HB3	1.96	0.46
1:C:63:ALA:HA	1:C:261:ARG:NH2	2.29	0.46
2:D:55:VAL:HG21	2:D:59:TRP:HD1	1.81	0.46
1:E:1018:ASN:H	1:E:1021:LEU:HD12	1.80	0.46
1:E:1091:GLU:HA	1:E:1150:GLY:HA2	1.97	0.46
1:E:1762:LEU:HG	1:E:1764:GLY:H	1.79	0.46
1:E:411:TYR:HB2	1:E:486:LEU:HD21	1.97	0.46
1:E:843:SER:OG	1:E:844:ARG:N	2.48	0.46
1:G:229:GLU:HA	1:G:249:GLY:HA2	1.97	0.46
1:A:1091:GLU:HG2	1:A:1213:PHE:CD1	2.49	0.46
1:A:1204:LEU:HD22	1:A:1226:PHE:CD2	2.51	0.46
1:A:1748:PHE:HZ	1:A:2072:LEU:HB2	1.80	0.46
1:A:418:LEU:HA	1:A:421:PHE:CE2	2.50	0.46
1:A:663:TYR:OH	1:A:804:PRO:HD2	2.16	0.46
1:C:1093:GLU:HG2	1:C:1148:VAL:HG22	1.97	0.46
1:C:1476:MET:H	1:C:1485:SER:HA	1.80	0.46
1:C:1676:LEU:HD21	1:C:2164:SER:O	2.16	0.46
1:A:4835:LYS:HG2	1:C:4822:THR:HG21	1.96	0.46
1:C:909:ASN:HA	1:C:965:TYR:CE1	2.51	0.46
1:E:229:GLU:HA	1:E:249:GLY:HA2	1.96	0.46
2:F:87:HIS:HD2	2:F:88:PRO:HD2	1.80	0.46
1:G:1204:LEU:HD22	1:G:1226:PHE:CD2	2.51	0.46
1:G:1476:MET:H	1:G:1485:SER:HA	1.81	0.46
1:G:714:TYR:CB	1:G:757:PHE:HD2	2.28	0.46
1:A:110:ARG:NH2	1:A:115:ARG:HD2	2.29	0.46
1:A:1746:THR:O	1:A:1748:PHE:N	2.48	0.46
1:A:4677:LEU:HD11	1:A:4702:ASP:HB3	1.97	0.46
1:A:651:GLY:HA2	1:A:776:LEU:HG	1.98	0.46
2:B:73:LYS:HA	2:B:99:PHE:O	2.16	0.46
1:C:3934:TYR:OH	1:C:3998:HIS:HB3	2.15	0.46
1:C:4053:SER:O	1:C:4056:GLU:HB3	2.15	0.46
1:C:4183:ILE:HD12	1:C:4185:GLY:H	1.80	0.46
1:C:843:SER:OG	1:C:844:ARG:N	2.48	0.46
1:E:1081:TYR:CD2	1:E:1234:VAL:HG13	2.51	0.46
1:E:1476:MET:H	1:E:1485:SER:HA	1.80	0.46
1:E:4053:SER:O	1:E:4056:GLU:HB3	2.15	0.46
1:E:63:ALA:HA	1:E:261:ARG:NH2	2.29	0.46
1:G:2341:VAL:HG13	1:G:2342:ASN:N	2.22	0.46
1:G:3703:LEU:HD23	1:G:3703:LEU:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3727:ASP:HB3	1:G:3731:LYS:NZ	2.31	0.46
1:G:3927:GLN:HE21	1:G:3991:GLY:CA	2.22	0.46
1:G:418:LEU:HA	1:G:421:PHE:CE2	2.50	0.46
1:A:4053:SER:O	1:A:4056:GLU:HB3	2.15	0.46
1:C:3962:PHE:HD1	1:C:4026:MET:SD	2.38	0.46
1:C:418:LEU:HA	1:C:421:PHE:CE2	2.50	0.46
1:C:855:PRO:HG2	1:C:998:ARG:HD2	1.96	0.46
1:E:1130:GLN:HA	1:E:1138:PRO:HA	1.97	0.46
1:E:111:HIS:CD2	1:E:113:HIS:HB3	2.50	0.46
1:E:1685:LEU:O	1:E:1689:VAL:HG12	2.15	0.46
1:E:2066:LEU:O	1:E:2070:VAL:HG23	2.15	0.46
1:E:4076:ALA:HA	1:E:4079:ASP:HB3	1.97	0.46
1:G:221:ARG:NE	1:G:253:CYS:O	2.44	0.46
1:G:4904:PRO:HB2	1:G:4910:GLU:HG3	1.97	0.46
1:A:1093:GLU:HG2	1:A:1148:VAL:HG22	1.97	0.46
1:A:1685:LEU:O	1:A:1689:VAL:HG12	2.15	0.46
1:A:3804:ILE:HG22	1:A:3812:VAL:HG11	1.96	0.46
1:A:4807:PHE:HZ	1:G:4856:PHE:CE2	2.32	0.46
1:C:1204:LEU:HD22	1:C:1226:PHE:CD2	2.51	0.46
1:C:1685:LEU:O	1:C:1689:VAL:HG12	2.15	0.46
1:C:4677:LEU:HD11	1:C:4702:ASP:HB3	1.97	0.46
1:C:4914:VAL:HG23	1:E:4888:TYR:CG	2.49	0.46
1:E:1076:ARG:HH22	1:E:1609:PRO:CB	2.29	0.46
1:E:1729:SER:O	1:E:1733:GLU:HG2	2.15	0.46
1:E:1770:SER:OG	1:E:1771:LEU:N	2.49	0.46
1:E:3934:TYR:OH	1:E:3998:HIS:HB3	2.16	0.46
1:G:1748:PHE:HZ	1:G:2072:LEU:HB2	1.80	0.46
1:G:284:HIS:NE2	1:G:286:THR:OG1	2.48	0.46
1:G:3352:GLU:O	1:G:3356:SER:N	2.46	0.46
1:G:646:PRO:O	1:G:648:ILE:N	2.40	0.46
1:A:111:HIS:CD2	1:A:113:HIS:HB3	2.50	0.46
1:A:1676:LEU:HD21	1:A:2164:SER:O	2.15	0.46
1:A:1679:ASN:HA	1:A:1682:ALA:HB3	1.98	0.46
1:A:1812:LEU:HA	1:A:1815:LEU:HD12	1.97	0.46
2:B:55:VAL:HG21	2:B:59:TRP:HD1	1.81	0.46
1:C:1081:TYR:CD2	1:C:1234:VAL:HG13	2.50	0.46
1:C:1586:ASN:O	1:C:1588:ALA:N	2.47	0.46
1:C:282:ILE:HD12	1:C:314:PHE:HD2	1.81	0.46
1:C:4783:ILE:HG22	1:C:4789:PHE:CD2	2.51	0.46
1:C:651:GLY:HA2	1:C:776:LEU:HG	1.98	0.46
1:E:1679:ASN:HA	1:E:1682:ALA:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1229:ASN:CG	1:E:1827:ARG:HH11	2.19	0.46
1:E:207:SER:HB3	1:E:334:MET:SD	2.56	0.46
1:E:4205:TRP:HB2	1:E:4245:MET:HE1	1.96	0.46
1:E:404:ILE:HG21	1:E:481:GLU:HG3	1.97	0.46
1:E:651:GLY:HA2	1:E:776:LEU:HG	1.98	0.46
1:G:111:HIS:CD2	1:G:113:HIS:HB3	2.50	0.46
1:G:1943:LEU:HD11	1:G:2098:VAL:HG22	1.98	0.46
1:E:179:TYR:OH	1:G:2359:ARG:NE	2.49	0.46
1:G:3658:LYS:HA	1:G:3662:ILE:HG13	1.97	0.46
1:G:3768:SER:HA	1:G:3771:HIS:CE1	2.51	0.46
1:A:1586:ASN:O	1:A:1588:ALA:N	2.47	0.46
1:A:1676:LEU:O	1:A:1676:LEU:HD23	2.16	0.46
1:A:207:SER:HB3	1:A:334:MET:SD	2.56	0.46
1:A:350:HIS:HD2	1:A:353:SER:N	2.14	0.46
1:A:4783:ILE:HG22	1:A:4789:PHE:CD2	2.51	0.46
1:C:1238:PHE:HE2	1:C:1612:PHE:HA	1.81	0.46
1:C:3804:ILE:HG22	1:C:3812:VAL:HG11	1.96	0.46
1:C:76:ARG:HE	1:E:3844:LEU:CD2	2.22	0.46
1:C:76:ARG:HH21	1:E:3844:LEU:CD2	2.29	0.46
1:E:118:LEU:HA	1:E:137:LEU:HD23	1.98	0.46
1:E:2100:HIS:O	1:E:2104:ARG:HG2	2.15	0.46
1:E:1676:LEU:HD21	1:E:2164:SER:O	2.15	0.46
1:G:4192:ARG:NH1	1:G:4982:GLU:OE1	2.48	0.46
1:A:1609:PRO:O	1:A:1610:ASN:ND2	2.49	0.46
1:C:4818:MET:HA	1:C:4824:ARG:HG2	1.96	0.46
1:E:1087:ARG:HH12	1:E:1157:GLU:HB3	1.81	0.46
1:E:119:SER:HB3	1:E:146:CYS:HA	1.98	0.46
1:E:891:TRP:HB3	1:E:907:LEU:HD11	1.98	0.46
2:F:25:HIS:CD2	2:F:104:LEU:HD11	2.51	0.46
1:G:2206:THR:O	1:G:2210:VAL:HG23	2.15	0.46
1:G:4577:LEU:HG	1:G:4580:TYR:HE1	1.80	0.46
1:A:1081:TYR:CD2	1:A:1234:VAL:HG13	2.50	0.46
1:A:1729:SER:O	1:A:1733:GLU:HG2	2.15	0.46
1:A:411:TYR:HB2	1:A:486:LEU:HD21	1.97	0.46
1:A:909:ASN:HA	1:A:965:TYR:CE1	2.51	0.46
1:C:118:LEU:HA	1:C:137:LEU:HD23	1.98	0.46
1:C:1850:VAL:HA	1:C:1945:TYR:CE1	2.50	0.46
1:C:350:HIS:HD2	1:C:353:SER:N	2.14	0.46
1:C:739:ALA:C	1:C:741:GLU:H	2.18	0.46
2:D:73:LYS:HA	2:D:99:PHE:O	2.16	0.46
1:E:1676:LEU:O	1:E:1676:LEU:HD23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3658:LYS:HA	1:E:3662:ILE:HG13	1.98	0.46
1:E:4783:ILE:HG22	1:E:4789:PHE:CD2	2.51	0.46
1:E:4801:LEU:HB3	1:E:4808:PHE:HD2	1.81	0.46
1:E:4829:SER:HA	1:E:4832:HIS:CD2	2.51	0.46
1:E:909:ASN:HA	1:E:965:TYR:CE1	2.51	0.46
1:G:118:LEU:HA	1:G:137:LEU:HD23	1.98	0.46
1:A:3844:LEU:CD2	1:G:76:ARG:HH21	2.29	0.46
1:G:1688:HIS:HE1	2:H:89:GLY:O	1.99	0.46
1:A:3658:LYS:HA	1:A:3662:ILE:HG13	1.98	0.45
1:C:1087:ARG:HH12	1:C:1157:GLU:HB3	1.81	0.45
1:C:1679:ASN:HA	1:C:1682:ALA:HB3	1.98	0.45
1:C:3919:THR:HG21	1:C:3968:TYR:CE2	2.50	0.45
1:C:4856:PHE:O	1:C:4860:ARG:NH1	2.49	0.45
1:C:683:ARG:HB3	1:C:713:SER:HB2	1.97	0.45
1:E:111:HIS:NE2	1:E:113:HIS:HB3	2.31	0.45
1:E:1862:ILE:O	1:E:1865:MET:HB3	2.16	0.45
1:E:3727:ASP:O	1:E:3731:LYS:NZ	2.42	0.45
1:E:3826:VAL:HG23	1:E:3909:ASN:HB3	1.98	0.45
1:E:4105:GLY:HA2	1:E:4108:ILE:HD12	1.98	0.45
1:E:675:LEU:CD2	1:E:1633:PRO:HG3	2.46	0.45
2:F:38:SER:HB3	2:F:41:ASP:OD2	2.16	0.45
1:G:1687:SER:HB2	1:G:1782:PHE:CZ	2.51	0.45
1:G:767:VAL:O	1:G:1475:THR:OG1	2.24	0.45
1:A:3826:VAL:HG23	1:A:3909:ASN:HB3	1.98	0.45
1:A:830:ARG:HD3	1:A:1612:PHE:CZ	2.51	0.45
1:A:891:TRP:HB3	1:A:907:LEU:HD11	1.98	0.45
1:C:2099:SER:O	1:C:2103:VAL:HG23	2.17	0.45
1:C:2761:TYR:HE2	1:C:2925:GLU:OE2	2.00	0.45
1:C:3826:VAL:HG23	1:C:3909:ASN:HB3	1.98	0.45
1:C:4087:LEU:HD23	1:C:4122:MET:HB3	1.98	0.45
2:D:38:SER:HB3	2:D:41:ASP:OD2	2.16	0.45
1:E:2867:LEU:HG	1:E:2928:LYS:HZ3	1.82	0.45
1:G:110:ARG:NH2	1:G:115:ARG:HD2	2.28	0.45
1:G:1812:LEU:HA	1:G:1815:LEU:HD12	1.97	0.45
1:G:3102:ASP:O	1:G:3106:MET:N	2.49	0.45
1:G:207:SER:HB3	1:G:334:MET:SD	2.56	0.45
1:A:4888:TYR:HB2	1:G:4914:VAL:HG21	1.98	0.45
1:G:651:GLY:HA2	1:G:776:LEU:HG	1.98	0.45
1:A:111:HIS:NE2	1:A:113:HIS:HB3	2.32	0.45
1:A:3663:LEU:HA	1:A:3664:THR:O	2.17	0.45
1:A:4856:PHE:O	1:A:4860:ARG:NH1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:739:ALA:C	1:A:741:GLU:H	2.18	0.45
1:A:855:PRO:HG2	1:A:998:ARG:HD2	1.96	0.45
1:C:46:LEU:HD13	1:C:125:ARG:NH1	2.32	0.45
1:C:1812:LEU:HA	1:C:1815:LEU:HD12	1.97	0.45
1:E:110:ARG:NH2	1:E:115:ARG:HD2	2.28	0.45
1:E:2122:SER:O	1:E:2125:HIS:HB3	2.17	0.45
1:E:767:VAL:O	1:E:1475:THR:OG1	2.24	0.45
1:G:111:HIS:NE2	1:G:113:HIS:HB3	2.31	0.45
1:G:1205:GLY:HA2	1:G:1225:PRO:HB3	1.99	0.45
1:G:1611:HIS:HB2	1:G:1652:GLU:CB	2.45	0.45
1:G:1862:ILE:O	1:G:1865:MET:HB3	2.16	0.45
1:G:350:HIS:HD2	1:G:353:SER:N	2.14	0.45
1:G:3838:THR:OG1	1:G:3839:CYS:N	2.49	0.45
1:G:4192:ARG:NH1	1:G:5028:PHE:CD2	2.84	0.45
1:G:4640:GLU:HB3	1:G:4641:PRO:HD3	1.98	0.45
1:G:663:TYR:OH	1:G:804:PRO:HD2	2.16	0.45
1:G:830:ARG:HD3	1:G:1612:PHE:CZ	2.50	0.45
1:A:1862:ILE:O	1:A:1865:MET:HB3	2.16	0.45
1:C:1688:HIS:HE1	2:D:89:GLY:O	2.00	0.45
1:C:2711:PRO:HA	1:C:3016:TYR:HA	1.98	0.45
1:C:3971:GLY:HA2	1:C:5005:GLY:HA3	1.98	0.45
1:C:4047:MET:HG3	1:C:4048:LEU:N	2.32	0.45
1:G:842:PRO:HD2	1:G:1196:PRO:HA	1.99	0.45
1:G:1238:PHE:HE2	1:G:1612:PHE:HA	1.81	0.45
1:G:1954:ARG:HG2	1:G:2134:LEU:HD12	1.98	0.45
1:G:4686:LEU:HA	1:G:4690:GLU:HB2	1.98	0.45
1:G:909:ASN:HA	1:G:965:TYR:CE1	2.50	0.45
1:A:1087:ARG:HH12	1:A:1157:GLU:HB3	1.81	0.45
1:A:1940:CYS:SG	1:A:2123:LEU:HD12	2.57	0.45
1:A:1947:CYS:SG	1:A:2127:GLN:NE2	2.89	0.45
1:A:3934:TYR:OH	1:A:3998:HIS:HB3	2.16	0.45
1:A:76:ARG:HH21	1:C:3844:LEU:CD2	2.29	0.45
1:C:2100:HIS:O	1:C:2104:ARG:HG2	2.15	0.45
1:C:1940:CYS:SG	1:C:2123:LEU:HD12	2.57	0.45
1:C:207:SER:HB3	1:C:334:MET:SD	2.56	0.45
1:C:5022:PHE:HA	1:C:5023:PRO:HD3	1.71	0.45
1:C:891:TRP:HB3	1:C:907:LEU:HD11	1.98	0.45
1:E:1767:VAL:O	1:E:1769:THR:N	2.50	0.45
1:E:2761:TYR:HE2	1:E:2925:GLU:OE2	1.99	0.45
1:G:772:ASN:HD21	1:G:1467:SER:HA	1.82	0.45
1:A:1745:ILE:O	1:A:1746:THR:OG1	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1770:SER:OG	1:A:1771:LEU:N	2.49	0.45
1:A:282:ILE:HD12	1:A:314:PHE:HD2	1.81	0.45
1:C:111:HIS:NE2	1:C:113:HIS:HB3	2.32	0.45
1:C:1770:SER:OG	1:C:1771:LEU:N	2.49	0.45
1:C:1862:ILE:O	1:C:1865:MET:HB3	2.16	0.45
1:C:1748:PHE:HZ	1:C:2072:LEU:HB2	1.81	0.45
1:C:3663:LEU:HA	1:C:3664:THR:O	2.16	0.45
1:E:1093:GLU:HG2	1:E:1148:VAL:HG22	1.97	0.45
1:E:1940:CYS:SG	1:E:2123:LEU:HD12	2.57	0.45
1:E:2283:ASN:HB2	1:E:2286:LEU:HB2	1.99	0.45
1:E:739:ALA:C	1:E:741:GLU:H	2.18	0.45
1:G:2142:TYR:CD2	1:G:2197:LEU:HB2	2.52	0.45
1:G:2247:GLN:HE21	1:G:2279:SER:C	2.20	0.45
1:G:282:ILE:HD12	1:G:314:PHE:HD2	1.81	0.45
1:G:411:TYR:HB2	1:G:486:LEU:HD21	1.98	0.45
1:G:633:LEU:HB2	1:G:1663:HIS:HD2	1.82	0.45
2:H:67:SER:N	2:H:70:GLN:OE1	2.38	0.45
1:A:1954:ARG:HG2	1:A:2134:LEU:HD12	1.99	0.45
1:A:527:ALA:O	1:A:531:ARG:HG3	2.17	0.45
1:A:635:THR:HG23	1:A:1693:GLN:HE22	1.82	0.45
1:C:262:LEU:HD23	1:C:282:ILE:HG12	1.99	0.45
1:C:4105:GLY:HA2	1:C:4108:ILE:HD12	1.98	0.45
1:E:772:ASN:HD21	1:E:1467:SER:HA	1.82	0.45
1:E:154:SER:HB3	1:E:156:GLN:OE1	2.17	0.45
1:E:830:ARG:HD3	1:E:1612:PHE:CZ	2.52	0.45
1:E:633:LEU:HB2	1:E:1663:HIS:HD2	1.82	0.45
1:E:1850:VAL:HA	1:E:1945:TYR:CE1	2.51	0.45
1:E:2060:SER:HA	1:E:2063:LEU:HD12	1.99	0.45
1:E:2247:GLN:HE21	1:E:2279:SER:C	2.20	0.45
1:E:262:LEU:HD23	1:E:282:ILE:HG12	1.99	0.45
1:E:491:ILE:HG22	1:E:495:ASN:HD21	1.82	0.45
1:G:1729:SER:O	1:G:1733:GLU:HG2	2.16	0.45
1:G:2122:SER:O	1:G:2125:HIS:HB3	2.17	0.45
1:G:2191:PHE:HD1	1:G:2198:MET:HE1	1.81	0.45
1:G:2283:ASN:HB2	1:G:2286:LEU:HB2	1.99	0.45
1:G:2497:ASP:OD1	1:G:2498:HIS:N	2.50	0.45
1:G:3768:SER:O	1:G:3772:THR:OG1	2.22	0.45
1:A:3838:THR:OG1	1:A:3839:CYS:N	2.50	0.45
1:C:1767:VAL:O	1:C:1769:THR:N	2.50	0.45
1:C:2819:TRP:CZ3	1:C:2877:GLN:HG2	2.52	0.45
1:C:404:ILE:HG21	1:C:481:GLU:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:491:ILE:HG22	1:C:495:ASN:HD21	1.82	0.45
2:D:25:HIS:CD2	2:D:104:LEU:HD11	2.51	0.45
1:E:1690:ASP:OD1	2:F:41:ASP:HB3	2.17	0.45
1:E:2497:ASP:OD1	1:E:2498:HIS:N	2.50	0.45
1:E:2773:ASN:HB3	1:E:2775:TRP:CD1	2.52	0.45
1:E:282:ILE:HD12	1:E:314:PHE:HD2	1.81	0.45
1:E:4047:MET:HG3	1:E:4048:LEU:N	2.32	0.45
1:C:4930:ALA:HB2	1:E:4933:GLN:HG2	1.98	0.45
1:E:663:TYR:OH	1:E:804:PRO:HD2	2.15	0.45
1:G:1229:ASN:CB	1:G:1827:ARG:HH11	2.30	0.45
1:G:1770:SER:OG	1:G:1771:LEU:N	2.49	0.45
1:G:1815:LEU:HB3	1:G:1865:MET:HE3	1.98	0.45
1:A:4807:PHE:HD2	1:G:4857:ASN:HD21	1.60	0.45
1:A:1943:LEU:HD11	1:A:2098:VAL:HG22	1.99	0.45
1:A:2099:SER:O	1:A:2103:VAL:HG23	2.17	0.45
1:A:2423:MET:HG3	1:A:2498:HIS:CE1	2.52	0.45
1:A:2773:ASN:HB3	1:A:2775:TRP:CD1	2.52	0.45
1:A:3891:LEU:HB3	1:A:3899:PHE:HE2	1.82	0.45
1:A:401:ALA:O	1:A:404:ILE:HB	2.17	0.45
2:B:25:HIS:CD2	2:B:104:LEU:HD11	2.51	0.45
1:C:1229:ASN:CB	1:C:1827:ARG:HH11	2.30	0.45
1:C:1947:CYS:SG	1:C:2127:GLN:NE2	2.89	0.45
1:C:4555:LEU:HD11	1:C:4656:LEU:HG	1.98	0.45
1:C:4801:LEU:HB3	1:C:4808:PHE:HD2	1.81	0.45
1:E:2819:TRP:CZ3	1:E:2877:GLN:HG2	2.52	0.45
1:E:3663:LEU:HA	1:E:3664:THR:O	2.16	0.45
1:E:3971:GLY:HA2	1:E:5005:GLY:HA3	1.98	0.45
2:F:73:LYS:HA	2:F:99:PHE:O	2.16	0.45
1:G:1087:ARG:HH12	1:G:1157:GLU:HB3	1.81	0.45
1:G:1198:GLN:N	1:G:1198:GLN:OE1	2.49	0.45
1:G:1289:LEU:HD12	1:G:1562:ILE:HD13	1.99	0.45
1:G:2773:ASN:HB3	1:G:2775:TRP:CD1	2.52	0.45
1:G:4056:GLU:OE2	1:G:4166:LEU:HD11	2.17	0.45
1:G:527:ALA:O	1:G:531:ARG:HG3	2.17	0.45
1:A:118:LEU:HA	1:A:137:LEU:HD23	1.98	0.45
1:A:1076:ARG:HH22	1:A:1609:PRO:CB	2.30	0.45
1:A:247:TYR:CE2	1:A:359:TYR:HB3	2.52	0.45
1:A:2711:PRO:HA	1:A:3016:TYR:HA	1.98	0.45
1:C:1205:GLY:HA2	1:C:1225:PRO:HB3	1.99	0.45
1:C:2122:SER:O	1:C:2125:HIS:HB3	2.17	0.45
1:C:284:HIS:NE2	1:C:286:THR:OG1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4963:ILE:HD12	1:C:5030:LYS:HZ1	1.80	0.45
1:E:2927:LEU:HD22	1:E:2937:VAL:HG11	1.98	0.45
1:E:3842:LEU:HD11	1:E:3950:ASN:O	2.17	0.45
1:E:4030:LEU:CG	1:E:4040:ILE:HD11	2.44	0.45
1:E:401:ALA:O	1:E:404:ILE:HB	2.17	0.45
1:E:4183:ILE:HD12	1:E:4185:GLY:H	1.81	0.45
1:E:4555:LEU:HD11	1:E:4656:LEU:HG	1.98	0.45
1:E:4735:GLU:O	1:E:4739:GLU:N	2.45	0.45
1:G:1104:TRP:CD1	1:G:1153:ILE:HB	2.52	0.45
1:G:3105:LYS:O	1:G:3109:ASN:N	2.49	0.45
1:A:1288:PHE:HE2	1:A:1460:HIS:HA	1.82	0.44
1:A:1280:GLN:NE2	1:A:1559:GLN:OE1	2.51	0.44
1:A:2497:ASP:OD1	1:A:2498:HIS:N	2.50	0.44
1:A:2761:TYR:HE2	1:A:2925:GLU:OE2	1.99	0.44
1:A:2927:LEU:HD22	1:A:2937:VAL:HG11	1.98	0.44
1:A:4849:TYR:HA	1:A:4852:THR:HG22	1.98	0.44
1:C:119:SER:HB3	1:C:146:CYS:HA	2.00	0.44
1:C:1954:ARG:HG2	1:C:2134:LEU:HD12	1.99	0.44
1:C:247:TYR:CE2	1:C:359:TYR:HB3	2.52	0.44
1:C:3658:LYS:HA	1:C:3662:ILE:HG13	1.98	0.44
1:C:3842:LEU:HD11	1:C:3950:ASN:O	2.17	0.44
1:E:1947:CYS:SG	1:E:2127:GLN:NE2	2.89	0.44
1:E:3919:THR:HG21	1:E:3968:TYR:CE2	2.49	0.44
1:E:4023:MET:O	1:E:4026:MET:HB3	2.17	0.44
1:E:4677:LEU:CD1	1:E:4702:ASP:HB3	2.47	0.44
1:G:293:LEU:HD13	1:G:378:LEU:HD12	1.99	0.44
1:G:3965:LEU:HD13	1:G:4026:MET:HE1	1.98	0.44
1:G:401:ALA:O	1:G:404:ILE:HB	2.17	0.44
1:G:491:ILE:HG22	1:G:495:ASN:HD21	1.82	0.44
1:A:842:PRO:HD2	1:A:1196:PRO:HA	1.99	0.44
1:A:1243:PRO:HD2	1:A:1458:HIS:CB	2.47	0.44
1:A:100:THR:HG21	1:A:162:LYS:NZ	2.33	0.44
1:A:675:LEU:CD2	1:A:1633:PRO:HG3	2.46	0.44
1:A:2060:SER:HA	1:A:2063:LEU:HD12	1.98	0.44
1:A:2247:GLN:HE21	1:A:2279:SER:C	2.20	0.44
1:A:3842:LEU:HD11	1:A:3950:ASN:O	2.17	0.44
1:A:4801:LEU:HB3	1:A:4808:PHE:HD2	1.83	0.44
1:A:4573:ILE:HG21	1:A:4809:PHE:CE2	2.53	0.44
2:B:25:HIS:NE2	2:B:104:LEU:HD11	2.33	0.44
1:C:2497:ASP:OD1	1:C:2498:HIS:N	2.50	0.44
1:C:4638:TYR:O	1:C:4641:PRO:HD2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:495:ASN:CA	1:C:553:ARG:HH12	2.28	0.44
1:C:635:THR:HG23	1:C:1693:GLN:HE22	1.83	0.44
2:D:25:HIS:NE2	2:D:104:LEU:HD11	2.33	0.44
1:E:2099:SER:O	1:E:2103:VAL:HG23	2.17	0.44
1:E:2816:MET:HG2	1:E:2878:LEU:HD21	1.99	0.44
1:E:284:HIS:NE2	1:E:286:THR:OG1	2.49	0.44
1:G:247:TYR:CE2	1:G:359:TYR:HB3	2.53	0.44
1:G:3658:LYS:HA	1:G:3662:ILE:CG1	2.47	0.44
1:G:404:ILE:HG21	1:G:481:GLU:HG3	1.98	0.44
1:A:46:LEU:HD13	1:A:125:ARG:NH1	2.32	0.44
1:A:1727:ARG:HG2	1:A:1727:ARG:O	2.17	0.44
1:A:1773:PRO:HA	1:A:1774:PRO:HD3	1.90	0.44
1:A:2242:ILE:HD11	1:A:2246:ASN:HD22	1.83	0.44
1:A:58:VAL:HG22	1:A:305:CYS:HA	1.99	0.44
1:A:3886:ARG:O	1:A:3890:LEU:HD13	2.17	0.44
1:A:3940:LYS:O	1:A:3942:VAL:N	2.50	0.44
1:A:4047:MET:HG3	1:A:4048:LEU:N	2.32	0.44
1:A:771:PHE:HE1	1:A:1472:VAL:HG13	1.82	0.44
2:B:38:SER:HB3	2:B:41:ASP:OD2	2.16	0.44
1:C:134:ASP:OD1	1:C:135:VAL:N	2.51	0.44
1:C:1969:LEU:O	1:C:1973:GLN:HG3	2.18	0.44
1:C:3706:SER:O	1:C:3710:LEU:HG	2.17	0.44
1:C:4680:LYS:HE2	1:C:4686:LEU:HD21	2.00	0.44
1:E:842:PRO:HD2	1:E:1196:PRO:HA	1.99	0.44
1:E:1280:GLN:NE2	1:E:1559:GLN:OE1	2.51	0.44
1:E:1579:MET:O	1:E:1582:SER:OG	2.17	0.44
1:E:350:HIS:HD2	1:E:353:SER:N	2.15	0.44
1:E:4922:PHE:HA	1:E:4926:VAL:HB	1.97	0.44
1:G:3674:ILE:HG22	1:G:3769:ARG:HD3	2.00	0.44
1:G:673:PRO:O	1:G:679:ALA:HA	2.17	0.44
1:A:119:SER:HB3	1:A:146:CYS:HA	2.00	0.44
1:A:1205:GLY:HA2	1:A:1225:PRO:HB3	1.99	0.44
1:A:1767:VAL:O	1:A:1769:THR:N	2.50	0.44
1:A:4640:GLU:HB3	1:A:4641:PRO:HD3	2.00	0.44
1:A:495:ASN:HB3	1:A:553:ARG:NH2	2.23	0.44
1:A:1690:ASP:OD1	2:B:41:ASP:HB3	2.17	0.44
1:C:1629:GLN:HE21	1:C:1631:GLN:HE21	1.65	0.44
1:C:1704:PRO:HG2	1:C:1707:LEU:HD12	1.99	0.44
1:C:527:ALA:O	1:C:531:ARG:HG3	2.17	0.44
1:E:1727:ARG:HG2	1:E:1727:ARG:O	2.17	0.44
1:E:1765:VAL:HG21	1:E:1953:HIS:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1936:LYS:HA	1:E:1939:MET:HB3	2.00	0.44
1:E:402:ARG:CZ	1:E:405:HIS:HD2	2.31	0.44
1:E:4239:GLU:OE2	1:E:5014:TYR:OH	2.18	0.44
1:G:1093:GLU:HG2	1:G:1148:VAL:HG22	1.98	0.44
1:G:771:PHE:HE1	1:G:1472:VAL:HG13	1.82	0.44
1:G:1765:VAL:HG21	1:G:1953:HIS:CE1	2.52	0.44
1:G:2060:SER:HA	1:G:2063:LEU:HD12	1.98	0.44
1:G:2336:ARG:HD2	1:G:2435:ARG:NH1	2.33	0.44
1:G:2754:PHE:CZ	1:G:2930:LEU:HD23	2.53	0.44
1:G:3992:PHE:O	1:G:3996:PHE:N	2.37	0.44
1:A:1238:PHE:HE1	1:A:1612:PHE:HA	1.82	0.44
1:A:1765:VAL:HG21	1:A:1953:HIS:CE1	2.52	0.44
1:A:2283:ASN:HB2	1:A:2286:LEU:HB2	1.99	0.44
1:A:2819:TRP:CZ3	1:A:2877:GLN:HG2	2.52	0.44
1:A:3971:GLY:HA2	1:A:5005:GLY:HA3	1.98	0.44
1:A:404:ILE:HG21	1:A:481:GLU:HG3	1.98	0.44
1:A:4105:GLY:HA2	1:A:4108:ILE:HD12	1.98	0.44
1:A:4555:LEU:HD11	1:A:4656:LEU:HG	1.98	0.44
1:A:4577:LEU:HG	1:A:4580:TYR:HE1	1.82	0.44
1:C:100:THR:HG21	1:C:162:LYS:NZ	2.33	0.44
1:C:1690:ASP:OD1	2:D:41:ASP:HB3	2.17	0.44
1:C:1833:SER:HB3	1:C:1836:PHE:HD2	1.83	0.44
1:C:2060:SER:HA	1:C:2063:LEU:HD12	1.98	0.44
1:C:2423:MET:HG3	1:C:2498:HIS:CE1	2.53	0.44
1:C:359:TYR:CD1	1:C:374:LYS:HD3	2.53	0.44
1:E:4088:ILE:O	1:E:4123:ILE:N	2.51	0.44
1:E:4642:ALA:HA	1:E:4645:CYS:SG	2.58	0.44
1:E:4786:ASP:OD1	1:E:4787:ASN:N	2.51	0.44
2:F:25:HIS:NE2	2:F:104:LEU:HD11	2.33	0.44
1:G:1745:ILE:O	1:G:1746:THR:OG1	2.25	0.44
1:G:1833:SER:HB3	1:G:1836:PHE:HD2	1.82	0.44
1:G:2747:ILE:HG12	1:G:2817:ILE:HD12	1.98	0.44
1:G:402:ARG:CZ	1:G:405:HIS:HD2	2.31	0.44
1:A:1629:GLN:HE21	1:A:1631:GLN:HE21	1.66	0.44
1:A:4638:TYR:O	1:A:4641:PRO:HD2	2.18	0.44
1:A:959:TYR:HE2	1:A:966:LYS:HB2	1.83	0.44
1:A:1688:HIS:HE1	2:B:89:GLY:O	2.00	0.44
1:C:2283:ASN:HB2	1:C:2286:LEU:HB2	1.99	0.44
1:C:402:ARG:CZ	1:C:405:HIS:HD2	2.30	0.44
1:C:4677:LEU:CD1	1:C:4702:ASP:HB3	2.48	0.44
1:C:4849:TYR:HA	1:C:4852:THR:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1198:GLN:OE1	1:E:1198:GLN:N	2.49	0.44
1:E:1289:LEU:HD12	1:E:1562:ILE:HD13	1.99	0.44
1:E:134:ASP:OD1	1:E:135:VAL:N	2.51	0.44
1:E:247:TYR:CE2	1:E:359:TYR:HB3	2.53	0.44
1:E:3706:SER:O	1:E:3710:LEU:HG	2.17	0.44
1:E:4026:MET:O	1:E:4029:SER:OG	2.21	0.44
1:E:527:ALA:O	1:E:531:ARG:HG3	2.17	0.44
2:F:78:PRO:O	2:F:83:GLY:N	2.51	0.44
1:G:1610:ASN:HA	1:G:1652:GLU:OE2	2.18	0.44
1:G:1704:PRO:HG2	1:G:1707:LEU:HD12	1.99	0.44
1:G:2891:LYS:O	1:G:2895:GLU:HG3	2.18	0.44
1:G:3701:LEU:HD11	1:G:3725:TYR:CD1	2.52	0.44
1:G:4004:ALA:O	1:G:4114:CYS:HA	2.18	0.44
1:E:4879:MET:HG2	1:G:4577:LEU:O	2.18	0.44
1:G:746:CYS:HA	1:G:757:PHE:CD1	2.53	0.44
1:A:180:LEU:O	1:A:200:TRP:NE1	2.51	0.44
1:A:1229:ASN:CB	1:A:1827:ARG:HH11	2.30	0.44
1:A:1833:SER:HB3	1:A:1836:PHE:HD2	1.83	0.44
1:A:2336:ARG:HD2	1:A:2435:ARG:NH1	2.33	0.44
1:A:3706:SER:O	1:A:3710:LEU:HG	2.18	0.44
1:A:3727:ASP:O	1:A:3731:LYS:NZ	2.42	0.44
1:A:4642:ALA:HA	1:A:4645:CYS:SG	2.58	0.44
1:A:746:CYS:HA	1:A:757:PHE:CD1	2.53	0.44
1:C:772:ASN:HD21	1:C:1467:SER:HA	1.82	0.44
1:C:1289:LEU:HD12	1:C:1562:ILE:HD13	1.98	0.44
1:C:2242:ILE:HD11	1:C:2246:ASN:HD22	1.83	0.44
1:C:4023:MET:O	1:C:4026:MET:HB3	2.17	0.44
1:C:4974:GLY:O	1:C:4977:THR:OG1	2.25	0.44
1:E:1238:PHE:HE1	1:E:1612:PHE:HA	1.83	0.44
1:E:3940:LYS:O	1:E:3942:VAL:N	2.50	0.44
1:E:4680:LYS:HE2	1:E:4686:LEU:HD21	1.99	0.44
1:E:771:PHE:HE1	1:E:1472:VAL:HG13	1.82	0.44
1:G:119:SER:HB3	1:G:146:CYS:HA	2.00	0.44
1:G:1244:GLN:HE22	1:G:1646:ARG:HH21	1.66	0.44
1:G:635:THR:HG23	1:G:1693:GLN:HE22	1.83	0.44
1:G:1767:VAL:O	1:G:1769:THR:N	2.50	0.44
1:G:1936:LYS:HA	1:G:1939:MET:HB3	2.00	0.44
1:G:1969:LEU:O	1:G:1973:GLN:HG3	2.18	0.44
2:H:88:PRO:O	2:H:90:ILE:HD12	2.16	0.44
1:A:2336:ARG:HD2	1:A:2435:ARG:CZ	2.48	0.44
1:A:4677:LEU:CD1	1:A:4702:ASP:HB3	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1280:GLN:NE2	1:C:1559:GLN:OE1	2.51	0.44
1:C:675:LEU:CD2	1:C:1633:PRO:HG3	2.47	0.44
1:C:2380:ILE:HG23	1:C:2423:MET:SD	2.58	0.44
1:C:2773:ASN:HB3	1:C:2775:TRP:CD1	2.52	0.44
1:C:401:ALA:O	1:C:404:ILE:HB	2.17	0.44
1:E:1089:TYR:CE2	1:E:1214:PHE:HD1	2.36	0.44
1:E:21:VAL:HG13	1:E:205:ILE:HD11	2.00	0.44
1:E:2244:ARG:O	1:E:2247:GLN:HB3	2.18	0.44
1:E:293:LEU:HD13	1:E:378:LEU:HD12	2.00	0.44
1:E:4640:GLU:HB3	1:E:4641:PRO:HD3	2.00	0.44
1:G:1727:ARG:HG2	1:G:1727:ARG:O	2.18	0.44
1:A:4807:PHE:CZ	1:G:4856:PHE:CD2	3.06	0.44
1:A:1839:VAL:HB	1:A:1840:PRO:HD3	2.00	0.44
1:A:2122:SER:O	1:A:2125:HIS:HB3	2.17	0.44
1:A:2142:TYR:CE2	1:A:2197:LEU:HB2	2.53	0.44
1:A:3895:HIS:HE1	1:A:3970:GLN:HG3	1.83	0.44
1:A:402:ARG:CZ	1:A:405:HIS:HD2	2.30	0.44
1:A:633:LEU:HB2	1:A:1663:HIS:HD2	1.82	0.44
1:C:1244:GLN:HE22	1:C:1646:ARG:HH21	1.66	0.44
1:C:3940:LYS:O	1:C:3942:VAL:N	2.50	0.44
1:E:2336:ARG:HD2	1:E:2435:ARG:NH1	2.33	0.44
1:E:3886:ARG:O	1:E:3890:LEU:HD13	2.17	0.44
1:G:1254:HIS:HD2	1:G:1280:GLN:HB2	1.83	0.44
1:G:1629:GLN:HE21	1:G:1631:GLN:HE21	1.66	0.44
1:G:1738:LEU:HD11	1:G:2143:THR:HB	2.00	0.44
1:G:2242:ILE:HD11	1:G:2246:ASN:HD22	1.82	0.44
1:G:2423:MET:HG3	1:G:2498:HIS:CE1	2.52	0.44
1:G:2551:ASN:HA	1:G:2554:LEU:HG	2.00	0.44
1:G:3878:ASP:HB2	1:G:3957:VAL:HG21	2.00	0.44
1:E:4926:VAL:HG12	1:G:4932:ILE:HG21	2.00	0.44
1:G:484:LEU:HD21	1:G:540:PHE:CE1	2.53	0.44
1:G:602:VAL:O	1:G:605:SER:OG	2.23	0.44
1:A:1293:LEU:HD21	1:A:1585:LYS:NZ	2.33	0.43
1:A:293:LEU:HD13	1:A:378:LEU:HD12	1.99	0.43
1:A:468:LEU:O	1:A:472:ARG:HG2	2.18	0.43
1:A:491:ILE:HG22	1:A:495:ASN:HD21	1.82	0.43
2:B:7:ILE:HD11	2:B:73:LYS:HB2	1.99	0.43
1:C:1198:GLN:OE1	1:C:1198:GLN:N	2.49	0.43
1:C:1727:ARG:HG2	1:C:1727:ARG:O	2.17	0.43
1:C:1765:VAL:HG21	1:C:1953:HIS:CE1	2.53	0.43
1:C:2247:GLN:HE21	1:C:2279:SER:C	2.20	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2336:ARG:HD2	1:C:2435:ARG:CZ	2.48	0.43
1:C:3657:TYR:O	1:C:3662:ILE:HG12	2.18	0.43
1:C:484:LEU:HD21	1:C:540:PHE:CE1	2.53	0.43
1:E:2134:LEU:O	1:E:2138:LEU:HG	2.18	0.43
1:E:2380:ILE:HG23	1:E:2423:MET:SD	2.58	0.43
1:E:359:TYR:CD1	1:E:374:LYS:HD3	2.53	0.43
1:E:764:VAL:O	1:E:764:VAL:HG12	2.18	0.43
1:E:1688:HIS:HE1	2:F:89:GLY:O	2.00	0.43
1:G:1293:LEU:HD21	1:G:1585:LYS:NZ	2.33	0.43
1:G:222:LEU:HB3	1:G:388:LEU:HD13	2.00	0.43
1:G:4209:GLN:O	1:G:4213:SER:N	2.47	0.43
1:G:4849:TYR:HA	1:G:4852:THR:HG22	2.00	0.43
1:G:891:TRP:HB3	1:G:907:LEU:HD11	1.99	0.43
1:A:1104:TRP:CD1	1:A:1153:ILE:HB	2.53	0.43
1:A:1254:HIS:HD2	1:A:1280:GLN:HB2	1.83	0.43
1:A:772:ASN:HD21	1:A:1467:SER:HA	1.82	0.43
1:A:1611:HIS:HB2	1:A:1652:GLU:CB	2.47	0.43
1:A:1828:ASP:HB3	1:A:1830:VAL:H	1.83	0.43
1:A:1936:LYS:HA	1:A:1939:MET:HB3	2.01	0.43
1:A:2340:PHE:CD1	1:A:2435:ARG:HD2	2.54	0.43
1:A:2380:ILE:HG23	1:A:2423:MET:SD	2.58	0.43
1:A:2551:ASN:HA	1:A:2554:LEU:HG	2.00	0.43
1:A:359:TYR:CD1	1:A:374:LYS:HD3	2.53	0.43
1:A:4023:MET:O	1:A:4026:MET:HB3	2.17	0.43
1:A:764:VAL:O	1:A:764:VAL:HG12	2.18	0.43
1:C:1710:GLY:O	1:C:1714:LEU:HG	2.19	0.43
1:C:2163:ARG:O	1:C:2166:LEU:HB3	2.18	0.43
1:C:2770:LYS:HB3	1:C:2775:TRP:CB	2.44	0.43
1:C:4640:GLU:HB3	1:C:4641:PRO:HD3	2.00	0.43
1:C:633:LEU:HB2	1:C:1663:HIS:HD2	1.82	0.43
1:C:673:PRO:O	1:C:679:ALA:HA	2.18	0.43
1:C:771:PHE:HE1	1:C:1472:VAL:HG13	1.82	0.43
1:E:1954:ARG:HG2	1:E:2134:LEU:HD12	1.99	0.43
1:E:2191:PHE:HD1	1:E:2198:MET:HE1	1.83	0.43
1:E:2747:ILE:HG22	1:E:2748:PRO:O	2.18	0.43
1:E:4980:LEU:HA	1:E:4984:ASN:HB3	2.01	0.43
1:E:892:THR:O	1:E:903:LEU:HA	2.19	0.43
1:E:959:TYR:HE2	1:E:966:LYS:HB2	1.83	0.43
1:G:46:LEU:HD13	1:G:125:ARG:NH1	2.32	0.43
1:G:359:TYR:CD1	1:G:374:LYS:HD3	2.53	0.43
1:G:2145:SER:HB3	1:G:3647:HIS:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3923:LEU:HD12	1:G:3961:VAL:HG13	2.00	0.43
1:A:4576:ILE:HG22	1:A:4643:LEU:HD12	2.01	0.43
1:A:4680:LYS:HE2	1:A:4686:LEU:HD21	2.00	0.43
1:A:664:PHE:HE2	1:A:686:TRP:CZ2	2.36	0.43
1:C:1828:ASP:HB3	1:C:1830:VAL:H	1.83	0.43
1:C:2134:LEU:O	1:C:2138:LEU:HG	2.18	0.43
1:C:2551:ASN:HA	1:C:2554:LEU:HG	2.00	0.43
1:C:746:CYS:HA	1:C:757:PHE:CD1	2.53	0.43
1:C:714:TYR:CB	1:C:757:PHE:HD2	2.28	0.43
1:C:892:THR:O	1:C:903:LEU:HA	2.19	0.43
1:E:1232:ARG:HE	1:E:1701:ALA:HB3	1.83	0.43
1:E:1293:LEU:HD21	1:E:1585:LYS:NZ	2.33	0.43
1:E:635:THR:HG23	1:E:1693:GLN:HE22	1.82	0.43
1:E:180:LEU:O	1:E:200:TRP:NE1	2.51	0.43
1:E:2142:TYR:CE2	1:E:2197:LEU:HB2	2.54	0.43
1:E:2423:MET:HG3	1:E:2498:HIS:CE1	2.52	0.43
2:F:7:ILE:HD11	2:F:73:LYS:HB2	2.00	0.43
1:G:4661:TYR:HE2	1:G:4789:PHE:HB2	1.83	0.43
2:H:2:VAL:HG23	2:H:76:ILE:HA	1.99	0.43
1:A:1289:LEU:HD12	1:A:1562:ILE:HD13	1.99	0.43
1:A:1969:LEU:O	1:A:1973:GLN:HG3	2.18	0.43
1:A:222:LEU:HB3	1:A:388:LEU:HD13	2.01	0.43
1:A:2244:ARG:O	1:A:2247:GLN:HB3	2.18	0.43
1:A:2816:MET:HG2	1:A:2878:LEU:HD21	1.99	0.43
1:A:4922:PHE:HA	1:A:4926:VAL:HB	2.00	0.43
1:A:484:LEU:HD21	1:A:540:PHE:CE1	2.54	0.43
1:C:217:GLY:O	1:C:261:ARG:NH1	2.52	0.43
1:C:4829:SER:HA	1:C:4832:HIS:CD2	2.54	0.43
1:C:4980:LEU:HA	1:C:4984:ASN:HB3	2.00	0.43
1:E:1969:LEU:O	1:E:1973:GLN:HG3	2.17	0.43
1:E:2242:ILE:HD11	1:E:2246:ASN:HD22	1.82	0.43
1:E:2336:ARG:HD2	1:E:2435:ARG:CZ	2.48	0.43
1:E:3657:TYR:O	1:E:3662:ILE:HG12	2.18	0.43
1:E:3985:LEU:HA	1:E:3988:ALA:HB3	2.00	0.43
1:E:46:LEU:HD13	1:E:125:ARG:NH1	2.33	0.43
1:E:468:LEU:O	1:E:472:ARG:HG2	2.18	0.43
1:E:746:CYS:HA	1:E:757:PHE:CD1	2.53	0.43
1:G:1828:ASP:HB3	1:G:1830:VAL:H	1.83	0.43
1:G:764:VAL:HG12	1:G:764:VAL:O	2.18	0.43
1:A:1252:HIS:C	1:A:1254:HIS:N	2.72	0.43
1:A:765:GLN:HE21	1:A:1479:GLU:H	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1704:PRO:HG2	1:A:1707:LEU:HD12	1.99	0.43
1:A:4980:LEU:HA	1:A:4984:ASN:HB3	2.00	0.43
1:C:1293:LEU:HD21	1:C:1585:LYS:NZ	2.33	0.43
1:C:1936:LYS:HA	1:C:1939:MET:HB3	2.00	0.43
1:C:1958:LEU:HD23	1:C:2138:LEU:HD21	2.01	0.43
1:C:2142:TYR:CE2	1:C:2197:LEU:HB2	2.54	0.43
1:C:58:VAL:HG22	1:C:305:CYS:HA	2.01	0.43
1:C:308:HIS:CE1	1:C:311:ALA:HB2	2.54	0.43
1:C:4239:GLU:OE1	1:C:4675:LYS:HD2	2.18	0.43
1:C:4786:ASP:OD1	1:C:4787:ASN:N	2.51	0.43
1:C:4922:PHE:HA	1:C:4926:VAL:HB	2.00	0.43
1:C:764:VAL:O	1:C:764:VAL:HG12	2.19	0.43
1:C:959:TYR:HE2	1:C:966:LYS:HB2	1.83	0.43
1:E:1018:ASN:HB3	1:E:1021:LEU:HG	2.00	0.43
1:E:1254:HIS:HD2	1:E:1280:GLN:HB2	1.83	0.43
1:E:2340:PHE:CD1	1:E:2435:ARG:HD2	2.53	0.43
1:E:2711:PRO:HA	1:E:3016:TYR:HA	1.98	0.43
1:E:484:LEU:HD21	1:E:540:PHE:CE1	2.54	0.43
1:E:673:PRO:O	1:E:679:ALA:HA	2.18	0.43
1:G:1280:GLN:NE2	1:G:1559:GLN:OE1	2.51	0.43
1:G:4855:ALA:HB1	1:G:4863:TYR:CE2	2.54	0.43
2:H:99:PHE:HB3	2:H:101:VAL:HG23	2.00	0.43
1:A:134:ASP:OD1	1:A:135:VAL:N	2.51	0.43
1:A:2747:ILE:HG22	1:A:2748:PRO:O	2.19	0.43
1:A:4786:ASP:OD1	1:A:4787:ASN:N	2.51	0.43
1:C:110:ARG:NH2	1:C:115:ARG:HD2	2.29	0.43
1:C:842:PRO:HD2	1:C:1196:PRO:HA	2.00	0.43
1:C:20:VAL:HG12	1:C:204:PRO:HA	2.00	0.43
1:C:4088:ILE:O	1:C:4123:ILE:N	2.51	0.43
1:C:4235:VAL:HG21	1:C:5019:TRP:CZ3	2.53	0.43
2:D:87:HIS:HD2	2:D:88:PRO:HD2	1.84	0.43
2:D:88:PRO:O	2:D:90:ILE:HD12	2.18	0.43
1:E:1629:GLN:HE21	1:E:1631:GLN:HE21	1.66	0.43
1:E:1839:VAL:HB	1:E:1840:PRO:HD3	2.00	0.43
1:E:1943:LEU:HD11	1:E:2098:VAL:HG22	1.99	0.43
1:E:2551:ASN:HA	1:E:2554:LEU:HG	2.01	0.43
1:G:1189:LEU:HA	1:G:1190:PRO:HD3	1.87	0.43
1:G:100:THR:HG21	1:G:162:LYS:NZ	2.33	0.43
1:G:1710:GLY:O	1:G:1714:LEU:HG	2.18	0.43
1:G:176:SER:HB2	1:G:178:ARG:NH2	2.32	0.43
1:G:20:VAL:HG12	1:G:204:PRO:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:2134:LEU:O	1:G:2138:LEU:HG	2.18	0.43
1:G:2163:ARG:O	1:G:2166:LEU:HB3	2.19	0.43
1:G:2380:ILE:HG23	1:G:2423:MET:SD	2.58	0.43
1:G:262:LEU:HD23	1:G:282:ILE:HG12	1.99	0.43
1:G:4682:GLU:OE2	1:G:4723:LYS:HD2	2.18	0.43
1:E:4840:THR:OG1	1:G:4826:ILE:HD13	2.19	0.43
1:A:1695:LEU:O	1:A:1699:GLU:HG3	2.19	0.43
1:A:262:LEU:HD23	1:A:282:ILE:HG12	1.99	0.43
1:A:308:HIS:CE1	1:A:311:ALA:HB2	2.54	0.43
1:A:3924:LEU:O	1:A:3927:GLN:HB3	2.19	0.43
1:A:892:THR:O	1:A:903:LEU:HA	2.19	0.43
1:C:1101:ARG:CG	1:C:1193:SER:HB3	2.47	0.43
1:C:21:VAL:HG13	1:C:205:ILE:HD11	2.01	0.43
1:C:2747:ILE:HG22	1:C:2748:PRO:O	2.18	0.43
1:C:2816:MET:HG2	1:C:2878:LEU:HD21	1.99	0.43
1:C:293:LEU:HD13	1:C:378:LEU:HD12	2.00	0.43
1:C:3886:ARG:O	1:C:3890:LEU:HD13	2.17	0.43
1:C:3895:HIS:HE1	1:C:3970:GLN:HG3	1.83	0.43
1:C:4814:LEU:HD23	1:C:4814:LEU:HA	1.91	0.43
1:C:637:LEU:O	1:C:638:ILE:HD13	2.19	0.43
1:E:4239:GLU:OE1	1:E:4675:LYS:HD2	2.19	0.43
1:E:4849:TYR:HA	1:E:4852:THR:HG22	2.01	0.43
1:G:1022:VAL:HG23	1:G:1027:LEU:HB3	2.00	0.43
1:G:1252:HIS:C	1:G:1254:HIS:N	2.72	0.43
1:G:1586:ASN:O	1:G:1588:ALA:N	2.47	0.43
1:G:1715:LEU:HD13	1:G:1844:LEU:HD11	2.01	0.43
1:G:1958:LEU:HD22	1:G:2134:LEU:HD11	2.01	0.43
1:G:4705:VAL:HB	1:G:4778:TRP:CD2	2.54	0.43
1:G:892:THR:O	1:G:903:LEU:HA	2.18	0.43
1:A:21:VAL:HG13	1:A:205:ILE:HD11	2.01	0.43
1:A:3985:LEU:HA	1:A:3988:ALA:HB3	2.01	0.43
1:A:889:GLN:HB3	1:A:891:TRP:HD1	1.84	0.43
2:B:88:PRO:O	2:B:90:ILE:HD12	2.18	0.43
1:C:2336:ARG:HD2	1:C:2435:ARG:NH1	2.33	0.43
1:C:4642:ALA:HA	1:C:4645:CYS:SG	2.58	0.43
1:A:4856:PHE:CE2	1:C:4807:PHE:CZ	3.07	0.43
1:C:664:PHE:HE2	1:C:686:TRP:CZ2	2.36	0.43
1:C:889:GLN:HB3	1:C:891:TRP:HD1	1.84	0.43
1:E:1022:VAL:HG23	1:E:1027:LEU:HB3	2.00	0.43
1:E:214:VAL:HG22	1:E:341:TYR:CZ	2.54	0.43
1:E:3891:LEU:HB3	1:E:3899:PHE:HE2	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4235:VAL:HG21	1:E:5019:TRP:CZ3	2.54	0.43
1:E:889:GLN:HB3	1:E:891:TRP:HD1	1.84	0.43
1:G:1018:ASN:HB3	1:G:1021:LEU:HG	2.01	0.43
1:G:2711:PRO:HA	1:G:3016:TYR:HA	2.00	0.43
1:G:2774:ASN:OD1	1:G:2852:ARG:NE	2.52	0.43
1:G:959:TYR:HE2	1:G:966:LYS:HB2	1.83	0.43
1:A:1124:PHE:HB2	1:A:1162:PHE:CE2	2.54	0.43
1:A:20:VAL:HG12	1:A:204:PRO:HA	2.00	0.43
1:A:2063:LEU:O	1:A:2066:LEU:HB3	2.19	0.43
1:A:2163:ARG:O	1:A:2166:LEU:HB3	2.19	0.43
1:A:214:VAL:HG22	1:A:341:TYR:CZ	2.54	0.43
1:A:4235:VAL:HG21	1:A:5019:TRP:CZ3	2.53	0.43
1:A:673:PRO:O	1:A:679:ALA:HA	2.18	0.43
1:C:1076:ARG:HH22	1:C:1609:PRO:CB	2.32	0.43
1:C:1695:LEU:O	1:C:1699:GLU:HG3	2.19	0.43
1:C:1812:LEU:HD21	1:C:1861:GLN:HG2	2.01	0.43
1:C:1943:LEU:HD11	1:C:2098:VAL:HG22	1.99	0.43
1:C:252:VAL:HA	1:C:255:HIS:CE1	2.54	0.43
1:E:2063:LEU:O	1:E:2066:LEU:HB3	2.19	0.43
1:E:222:LEU:HB3	1:E:388:LEU:HD13	2.00	0.43
1:E:252:VAL:HA	1:E:255:HIS:CE1	2.54	0.43
1:E:308:HIS:CE1	1:E:311:ALA:HB2	2.54	0.43
1:E:4638:TYR:O	1:E:4641:PRO:HD2	2.18	0.43
1:E:602:VAL:O	1:E:605:SER:OG	2.22	0.43
2:F:82:TYR:CE1	2:F:87:HIS:HB2	2.54	0.43
1:G:134:ASP:OD1	1:G:135:VAL:N	2.51	0.43
1:G:1780:PRO:HD3	1:G:1801:ALA:H	1.84	0.43
1:G:180:LEU:O	1:G:200:TRP:NE1	2.51	0.43
1:G:1958:LEU:HD23	1:G:2138:LEU:HD21	2.01	0.43
1:G:217:GLY:O	1:G:261:ARG:NH1	2.52	0.43
1:G:2244:ARG:O	1:G:2247:GLN:HB3	2.18	0.43
1:G:4806:ASN:O	1:G:4809:PHE:HB3	2.18	0.43
2:H:55:VAL:HG21	2:H:59:TRP:HD1	1.84	0.43
1:A:2770:LYS:HG3	1:A:2791:LEU:HD21	2.01	0.43
1:A:4888:TYR:O	1:A:4892:ARG:HD3	2.19	0.43
1:C:1715:LEU:HD13	1:C:1844:LEU:HD11	2.01	0.43
1:C:3971:GLY:O	1:C:3973:CYS:N	2.51	0.43
1:E:1089:TYR:HE2	1:E:1214:PHE:HD1	1.67	0.43
1:E:1715:LEU:HD13	1:E:1844:LEU:HD11	2.01	0.43
1:E:20:VAL:HG12	1:E:204:PRO:HA	2.00	0.43
1:E:217:GLY:O	1:E:261:ARG:NH1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4856:PHE:CE2	1:E:4807:PHE:CZ	3.06	0.43
1:E:495:ASN:HB3	1:E:553:ARG:NH2	2.23	0.43
1:E:664:PHE:HE2	1:E:686:TRP:CZ2	2.36	0.43
2:F:88:PRO:O	2:F:90:ILE:HD12	2.18	0.43
1:G:821:LEU:HD23	1:G:1626:TRP:CZ2	2.54	0.43
1:G:1839:VAL:HB	1:G:1840:PRO:HD3	2.00	0.43
1:G:203:ASN:HA	1:G:204:PRO:HD3	1.89	0.43
1:G:21:VAL:HG13	1:G:205:ILE:HD11	2.01	0.43
1:G:291:LEU:O	1:G:312:THR:OG1	2.24	0.43
1:G:393:CYS:SG	1:G:397:GLU:HB2	2.59	0.43
1:G:4145:VAL:O	1:G:4149:ASN:N	2.49	0.43
1:G:664:PHE:HE2	1:G:686:TRP:CZ2	2.36	0.43
1:A:181:HIS:CD2	1:A:196:MET:HB2	2.54	0.42
1:A:3717:ASP:N	1:A:3717:ASP:OD1	2.52	0.42
1:A:4239:GLU:OE1	1:A:4675:LYS:HD2	2.19	0.42
1:A:4667:PRO:HA	1:A:4670:ILE:HG22	2.02	0.42
1:A:614:VAL:HG13	1:A:617:ASN:HB3	2.01	0.42
1:A:771:PHE:CE1	1:A:1472:VAL:HG13	2.54	0.42
2:B:78:PRO:O	2:B:83:GLY:N	2.51	0.42
1:C:222:LEU:HB3	1:C:388:LEU:HD13	2.00	0.42
1:C:2340:PHE:CD1	1:C:2435:ARG:HD2	2.53	0.42
1:C:3981:ALA:O	1:C:3986:TRP:NE1	2.46	0.42
1:C:821:LEU:HD23	1:C:1626:TRP:CZ2	2.54	0.42
1:E:1124:PHE:HB2	1:E:1162:PHE:CE2	2.54	0.42
1:E:1773:PRO:HA	1:E:1774:PRO:HD3	1.90	0.42
1:E:1833:SER:HB3	1:E:1836:PHE:HD2	1.84	0.42
1:E:181:HIS:CD2	1:E:196:MET:HB2	2.54	0.42
1:E:2163:ARG:O	1:E:2166:LEU:HB3	2.19	0.42
1:E:637:LEU:O	1:E:638:ILE:HD13	2.19	0.42
1:G:1101:ARG:CG	1:G:1193:SER:HB3	2.48	0.42
1:G:765:GLN:HE21	1:G:1479:GLU:H	1.67	0.42
1:G:2336:ARG:HD2	1:G:2435:ARG:CZ	2.49	0.42
1:G:2340:PHE:CD1	1:G:2435:ARG:HD2	2.54	0.42
1:G:2747:ILE:HG22	1:G:2748:PRO:O	2.19	0.42
1:G:43:GLY:HA2	1:G:444:SER:HA	2.01	0.42
1:G:637:LEU:O	1:G:638:ILE:HD13	2.19	0.42
1:A:1652:GLU:O	1:A:1655:GLU:HG2	2.19	0.42
1:A:2134:LEU:O	1:A:2138:LEU:HG	2.18	0.42
1:A:2741:GLU:HB3	1:A:2744:ASN:HD22	1.84	0.42
1:C:1103:GLY:HA3	1:C:1123:VAL:HA	2.00	0.42
1:C:1124:PHE:HB2	1:C:1162:PHE:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1611:HIS:HB2	1:C:1652:GLU:CB	2.46	0.42
1:C:1767:VAL:C	1:C:1768:THR:HG1	2.23	0.42
1:C:2244:ARG:O	1:C:2247:GLN:HB3	2.18	0.42
1:C:59:PRO:HB3	1:C:281:ARG:CZ	2.49	0.42
1:C:468:LEU:O	1:C:472:ARG:HG2	2.18	0.42
1:C:771:PHE:CE1	1:C:1472:VAL:HG13	2.54	0.42
1:E:1279:SER:HB3	1:E:1558:HIS:HA	2.02	0.42
1:E:771:PHE:CE1	1:E:1472:VAL:HG13	2.54	0.42
1:E:1586:ASN:O	1:E:1588:ALA:N	2.48	0.42
1:E:1652:GLU:O	1:E:1655:GLU:HG2	2.19	0.42
1:E:1958:LEU:HD23	1:E:2138:LEU:HD21	2.01	0.42
1:E:3924:LEU:O	1:E:3927:GLN:HB3	2.19	0.42
1:E:43:GLY:HA2	1:E:444:SER:HA	2.01	0.42
1:G:154:SER:HB3	1:G:156:GLN:OE1	2.19	0.42
1:G:468:LEU:O	1:G:472:ARG:HG2	2.19	0.42
1:G:580:GLU:HA	1:G:620:LEU:HD21	2.01	0.42
1:A:1160:ILE:O	1:A:1178:ALA:N	2.53	0.42
1:A:1189:LEU:HA	1:A:1190:PRO:HD3	1.87	0.42
1:A:1198:GLN:N	1:A:1198:GLN:OE1	2.50	0.42
1:A:1649:ASP:N	1:A:1649:ASP:OD1	2.53	0.42
1:A:1958:LEU:HD23	1:A:2138:LEU:HD21	2.02	0.42
1:A:252:VAL:HA	1:A:255:HIS:CE1	2.54	0.42
1:A:2761:TYR:CE2	1:A:2862:LEU:HD22	2.53	0.42
1:A:2774:ASN:OD1	1:A:2852:ARG:NE	2.52	0.42
1:A:2788:HIS:CG	1:A:2789:PRO:HD2	2.54	0.42
1:C:1290:ARG:HH21	1:C:1549:PHE:HE2	1.66	0.42
1:C:1229:ASN:CG	1:C:1827:ARG:HH11	2.23	0.42
1:C:2788:HIS:CG	1:C:2789:PRO:HD2	2.54	0.42
1:C:685:GLY:HA3	1:C:712:TYR:O	2.20	0.42
1:C:765:GLN:HE21	1:C:1479:GLU:H	1.66	0.42
1:C:868:GLU:O	1:C:871:ARG:HB2	2.20	0.42
2:D:7:ILE:HD11	2:D:73:LYS:HB2	2.00	0.42
1:E:1586:ASN:N	1:E:1587:PRO:HD2	2.35	0.42
1:E:1695:LEU:O	1:E:1699:GLU:HG3	2.19	0.42
1:E:176:SER:HB2	1:E:178:ARG:NH2	2.32	0.42
1:E:1231:GLN:OE1	1:E:1821:ASP:HB2	2.20	0.42
1:E:4667:PRO:HA	1:E:4670:ILE:HG22	2.01	0.42
1:E:586:ILE:O	1:E:589:LEU:HB3	2.19	0.42
1:E:852:VAL:HG22	1:E:853:PRO:HD2	2.01	0.42
1:G:2182:ILE:O	1:G:2186:MET:HG2	2.20	0.42
1:G:58:VAL:HG22	1:G:305:CYS:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:214:VAL:HG22	1:G:341:TYR:CZ	2.54	0.42
1:G:4965:SER:HA	1:G:4975:PHE:CD1	2.54	0.42
1:A:1101:ARG:CG	1:A:1193:SER:HB3	2.48	0.42
1:A:1710:GLY:O	1:A:1714:LEU:HG	2.19	0.42
1:A:1767:VAL:C	1:A:1768:THR:HG1	2.23	0.42
1:A:1747:LEU:HB2	1:A:1957:SER:OG	2.19	0.42
1:A:2145:SER:HB3	1:A:3647:HIS:CD2	2.54	0.42
1:A:2767:ALA:HB3	1:A:2857:PRO:HG3	2.01	0.42
1:A:3657:TYR:O	1:A:3662:ILE:HG12	2.18	0.42
1:A:821:LEU:HD23	1:A:1626:TRP:CZ2	2.54	0.42
1:A:868:GLU:O	1:A:871:ARG:HB2	2.19	0.42
1:C:1279:SER:HB3	1:C:1558:HIS:HA	2.02	0.42
1:C:180:LEU:O	1:C:200:TRP:NE1	2.51	0.42
1:C:4667:PRO:HA	1:C:4670:ILE:HG22	2.01	0.42
2:D:78:PRO:O	2:D:83:GLY:N	2.52	0.42
1:E:2182:ILE:O	1:E:2186:MET:HG2	2.20	0.42
1:E:2761:TYR:CE2	1:E:2862:LEU:HD22	2.54	0.42
1:E:393:CYS:SG	1:E:397:GLU:HB2	2.60	0.42
1:E:3895:HIS:HE1	1:E:3970:GLN:HG3	1.83	0.42
1:G:59:PRO:HB3	1:G:281:ARG:CZ	2.50	0.42
1:G:23:GLN:NE2	1:G:34:LYS:HB3	2.32	0.42
1:G:3958:ALA:HA	1:G:3961:VAL:HG12	2.02	0.42
1:G:4090:LYS:N	1:G:4121:GLU:O	2.53	0.42
1:G:495:ASN:HB3	1:G:553:ARG:NH2	2.23	0.42
1:G:586:ILE:O	1:G:589:LEU:HB3	2.20	0.42
1:G:638:ILE:HG23	1:G:678:GLN:HE22	1.84	0.42
1:G:889:GLN:HB3	1:G:891:TRP:HD1	1.85	0.42
1:A:1022:VAL:HG23	1:A:1027:LEU:HB3	2.00	0.42
1:A:1673:VAL:HG11	1:A:1681:VAL:HG11	2.02	0.42
1:A:43:GLY:HA2	1:A:444:SER:HA	2.01	0.42
1:A:4809:PHE:O	1:A:4812:HIS:ND1	2.48	0.42
1:A:685:GLY:HA3	1:A:712:TYR:O	2.19	0.42
2:B:56:ILE:HB	2:B:80:TYR:O	2.19	0.42
1:C:1254:HIS:HD2	1:C:1280:GLN:HB2	1.83	0.42
1:C:1610:ASN:HA	1:C:1652:GLU:OE2	2.18	0.42
1:C:2182:ILE:O	1:C:2186:MET:HG2	2.20	0.42
1:E:1673:VAL:HG11	1:E:1681:VAL:HG11	2.01	0.42
1:E:1704:PRO:HG2	1:E:1707:LEU:HD12	1.99	0.42
1:E:1710:GLY:O	1:E:1714:LEU:HG	2.19	0.42
1:E:1747:LEU:HB2	1:E:1957:SER:OG	2.19	0.42
1:E:184:THR:HA	1:E:189:LEU:HD23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2741:GLU:HB3	1:E:2744:ASN:HD22	1.84	0.42
1:E:4963:ILE:HD12	1:E:5030:LYS:HZ1	1.83	0.42
1:E:685:GLY:HA3	1:E:712:TYR:O	2.19	0.42
1:E:714:TYR:CB	1:E:757:PHE:HD2	2.28	0.42
1:G:1747:LEU:HB2	1:G:1957:SER:OG	2.19	0.42
1:G:2063:LEU:O	1:G:2066:LEU:HB3	2.18	0.42
1:G:2142:TYR:CE2	1:G:2197:LEU:HB2	2.54	0.42
1:G:3694:LYS:HA	1:G:3695:PRO:HD3	1.80	0.42
1:G:4028:LEU:HD23	1:G:4146:LEU:HD12	2.02	0.42
1:G:4786:ASP:OD1	1:G:4787:ASN:N	2.52	0.42
1:G:695:TYR:O	1:G:697:GLY:N	2.42	0.42
1:A:2867:LEU:HG	1:A:2928:LYS:HZ3	1.84	0.42
1:A:3958:ALA:CB	1:A:4019:LEU:HD11	2.47	0.42
1:A:4829:SER:HA	1:A:4832:HIS:CD2	2.54	0.42
1:A:4934:GLY:HA2	1:A:4937:ILE:HD12	2.02	0.42
1:A:5022:PHE:HA	1:A:5023:PRO:HD3	1.72	0.42
1:A:767:VAL:O	1:A:1475:THR:OG1	2.24	0.42
2:B:82:TYR:CE1	2:B:87:HIS:HB2	2.55	0.42
1:C:2063:LEU:O	1:C:2066:LEU:HB3	2.19	0.42
1:C:2145:SER:HB3	1:C:3647:HIS:CD2	2.54	0.42
1:C:2770:LYS:HG3	1:C:2791:LEU:HD21	2.01	0.42
1:C:3713:LYS:O	1:C:3715:LYS:N	2.53	0.42
1:C:3985:LEU:HA	1:C:3988:ALA:HB3	2.02	0.42
1:C:4576:ILE:HG22	1:C:4643:LEU:HD12	2.02	0.42
1:C:580:GLU:HA	1:C:620:LEU:HD21	2.02	0.42
1:E:3775:ALA:O	1:E:3778:MET:HG2	2.20	0.42
1:E:4576:ILE:HG22	1:E:4643:LEU:HD12	2.01	0.42
1:E:5026:ASP:O	1:E:5027:CYS:SG	2.75	0.42
1:E:588:SER:HB3	1:E:592:LYS:NZ	2.35	0.42
1:E:614:VAL:HG13	1:E:617:ASN:HB3	2.01	0.42
1:G:118:LEU:HD12	1:G:136:GLY:O	2.20	0.42
1:G:1695:LEU:O	1:G:1699:GLU:HG3	2.19	0.42
1:G:2770:LYS:HB3	1:G:2775:TRP:CB	2.43	0.42
1:G:2747:ILE:HD11	1:G:2814:LYS:HG3	2.02	0.42
1:E:4938:ASP:CG	1:G:4940:PHE:HB3	2.39	0.42
1:G:739:ALA:C	1:G:741:GLU:H	2.18	0.42
1:A:1279:SER:HB3	1:A:1558:HIS:HA	2.02	0.42
1:A:1715:LEU:HD13	1:A:1844:LEU:HD11	2.01	0.42
1:A:548:VAL:HG21	1:A:582:HIS:HB3	2.02	0.42
1:C:1530:THR:HG22	1:C:1535:GLU:HA	2.01	0.42
1:C:1839:VAL:HB	1:C:1840:PRO:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2761:TYR:CE2	1:C:2862:LEU:HD22	2.54	0.42
1:C:393:CYS:SG	1:C:397:GLU:HB2	2.60	0.42
1:C:4963:ILE:HD12	1:C:4963:ILE:HG23	1.86	0.42
1:C:548:VAL:HG21	1:C:582:HIS:HB3	2.02	0.42
1:E:1530:THR:HG22	1:E:1535:GLU:HA	2.02	0.42
1:E:1564:PHE:HB3	1:E:1565:GLU:H	1.70	0.42
1:E:821:LEU:HD23	1:E:1626:TRP:CZ2	2.54	0.42
1:E:2788:HIS:CG	1:E:2789:PRO:HD2	2.54	0.42
1:G:1652:GLU:O	1:G:1655:GLU:HG2	2.20	0.42
1:G:2121:PHE:CD1	1:G:3701:LEU:HD12	2.55	0.42
1:G:2161:GLN:NE2	1:G:2177:LEU:HB3	2.35	0.42
1:G:3825:GLU:O	1:G:3826:VAL:HG12	2.20	0.42
1:G:4054:ASN:OD1	1:G:4055:VAL:N	2.53	0.42
1:G:4217:PHE:CZ	1:G:4234:PHE:HA	2.55	0.42
1:G:4898:GLY:HA2	1:G:4901:ILE:HG22	2.02	0.42
1:G:639:ASN:OD1	1:G:640:TYR:N	2.53	0.42
1:A:2272:PRO:O	1:A:2275:VAL:HB	2.20	0.42
1:A:3825:GLU:C	1:A:3827:GLY:H	2.22	0.42
1:A:3919:THR:HG21	1:A:3968:TYR:CE2	2.49	0.42
1:A:3971:GLY:O	1:A:3973:CYS:N	2.51	0.42
1:A:410:LEU:HD21	1:A:441:VAL:HG22	2.02	0.42
1:A:586:ILE:O	1:A:589:LEU:HB3	2.19	0.42
1:A:580:GLU:HA	1:A:620:LEU:HD21	2.02	0.42
1:C:1089:TYR:CE2	1:C:1214:PHE:HD1	2.38	0.42
1:C:633:LEU:HD22	1:C:1641:ILE:HG22	2.02	0.42
1:C:221:ARG:N	1:C:391:THR:O	2.44	0.42
1:C:3924:LEU:O	1:C:3927:GLN:HB3	2.19	0.42
1:C:4573:ILE:HG21	1:C:4809:PHE:CE2	2.54	0.42
1:C:588:SER:HB3	1:C:592:LYS:NZ	2.35	0.42
1:E:118:LEU:HD12	1:E:136:GLY:O	2.20	0.42
1:E:2203:MET:O	1:E:2207:VAL:HG23	2.20	0.42
1:E:2145:SER:HB3	1:E:3647:HIS:CD2	2.55	0.42
1:E:410:LEU:HD21	1:E:441:VAL:HG22	2.02	0.42
1:E:580:GLU:HA	1:E:620:LEU:HD21	2.02	0.42
1:E:765:GLN:HE21	1:E:1479:GLU:H	1.66	0.42
2:F:56:ILE:HB	2:F:80:TYR:O	2.19	0.42
1:G:1279:SER:HB3	1:G:1558:HIS:HA	2.02	0.42
1:G:2770:LYS:HG3	1:G:2791:LEU:HD21	2.01	0.42
1:G:3775:ALA:O	1:G:3778:MET:HG2	2.19	0.42
1:G:4922:PHE:HA	1:G:4926:VAL:HB	2.01	0.42
1:A:4088:ILE:O	1:A:4123:ILE:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4886:HIS:CE1	1:A:4897:ILE:HD12	2.55	0.42
1:A:4930:ALA:HB1	1:C:4933:GLN:HA	2.02	0.42
1:A:738:LEU:HA	1:A:742:ASP:OD2	2.20	0.42
1:C:118:LEU:HD12	1:C:136:GLY:O	2.20	0.42
1:C:154:SER:HB3	1:C:156:GLN:OE1	2.19	0.42
1:C:1747:LEU:HB2	1:C:1957:SER:OG	2.19	0.42
1:C:214:VAL:HG22	1:C:341:TYR:CZ	2.54	0.42
1:C:2203:MET:O	1:C:2207:VAL:HG23	2.20	0.42
1:C:2882:TYR:HD2	1:C:2919:ASP:HB3	1.85	0.42
1:C:3694:LYS:HA	1:C:3695:PRO:HD3	1.79	0.42
1:C:410:LEU:HD21	1:C:441:VAL:HG22	2.02	0.42
1:C:43:GLY:HA2	1:C:444:SER:HA	2.00	0.42
1:C:646:PRO:O	1:C:648:ILE:N	2.41	0.42
1:E:1160:ILE:O	1:E:1178:ALA:N	2.53	0.42
1:E:2770:LYS:HG3	1:E:2791:LEU:HD21	2.01	0.42
1:E:471:LEU:HA	1:E:474:ARG:HE	1.85	0.42
1:G:252:VAL:HA	1:G:255:HIS:CE1	2.54	0.42
1:G:2561:LEU:HD11	1:G:2601:ASP:HA	2.02	0.42
1:G:4652:LEU:O	1:G:4656:LEU:N	2.51	0.42
1:G:548:VAL:HG21	1:G:582:HIS:HB3	2.01	0.42
1:G:771:PHE:CE1	1:G:1472:VAL:HG13	2.54	0.42
1:A:1018:ASN:HB3	1:A:1021:LEU:HG	2.01	0.42
1:A:154:SER:HB3	1:A:156:GLN:OE1	2.19	0.42
1:A:1655:GLU:HG3	1:A:1656:ARG:HG3	2.02	0.42
1:A:1229:ASN:CG	1:A:1827:ARG:HH11	2.23	0.42
1:A:3713:LYS:O	1:A:3715:LYS:N	2.53	0.42
1:C:181:HIS:CD2	1:C:196:MET:HB2	2.55	0.42
1:C:3806:ASN:H	1:C:3890:LEU:HD23	1.85	0.42
1:C:76:ARG:NH1	1:C:79:GLN:OE1	2.53	0.42
1:E:2272:PRO:O	1:E:2275:VAL:HB	2.20	0.42
1:E:4020:GLN:O	1:E:4024:VAL:HG22	2.20	0.42
1:E:868:GLU:O	1:E:871:ARG:HB2	2.20	0.42
1:G:1767:VAL:C	1:G:1768:THR:HG1	2.23	0.42
1:G:685:GLY:HA3	1:G:712:TYR:O	2.19	0.42
1:A:3806:ASN:H	1:A:3890:LEU:HD23	1.85	0.41
2:B:54:GLU:HG3	2:B:55:VAL:HG13	2.02	0.41
1:C:184:THR:HA	1:C:189:LEU:HD23	2.01	0.41
1:C:2161:GLN:NE2	1:C:2177:LEU:HB3	2.35	0.41
1:C:2741:GLU:HB3	1:C:2744:ASN:HD22	1.84	0.41
1:C:4047:MET:O	1:C:4051:SER:N	2.51	0.41
1:C:586:ILE:O	1:C:589:LEU:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:662:TRP:CZ3	1:C:814:ALA:HB2	2.56	0.41
1:E:1101:ARG:CG	1:E:1193:SER:HB3	2.48	0.41
1:E:2774:ASN:OD1	1:E:2852:ARG:NE	2.52	0.41
1:E:3713:LYS:O	1:E:3715:LYS:N	2.53	0.41
1:G:1290:ARG:HH21	1:G:1549:PHE:HE2	1.67	0.41
1:G:1673:VAL:HG11	1:G:1681:VAL:HG11	2.02	0.41
1:G:2131:LEU:HD21	1:G:3662:ILE:O	2.20	0.41
1:G:2788:HIS:CG	1:G:2789:PRO:HD2	2.54	0.41
1:G:3780:LEU:HD21	1:G:3820:LEU:HG	2.01	0.41
1:G:4677:LEU:HD11	1:G:4702:ASP:HB3	2.01	0.41
1:G:4913:ARG:O	1:G:4916:PHE:HB3	2.20	0.41
1:G:686:TRP:HD1	1:G:757:PHE:HZ	1.68	0.41
1:A:1081:TYR:HD2	1:A:1234:VAL:HG13	1.85	0.41
1:A:2231:SER:HA	1:A:2234:ARG:HH11	1.85	0.41
1:A:4963:ILE:HD12	1:A:4963:ILE:HG23	1.85	0.41
1:A:637:LEU:O	1:A:638:ILE:HD13	2.19	0.41
1:A:662:TRP:CZ3	1:A:814:ALA:HB2	2.56	0.41
1:C:1295:VAL:O	1:C:1547:LYS:HA	2.21	0.41
1:C:1652:GLU:O	1:C:1655:GLU:HG2	2.20	0.41
1:C:1685:LEU:HA	1:C:1685:LEU:HD23	1.92	0.41
1:C:3969:ILE:HG22	1:C:3969:ILE:O	2.20	0.41
1:C:471:LEU:HA	1:C:474:ARG:HE	1.85	0.41
1:C:852:VAL:HG22	1:C:853:PRO:HD2	2.01	0.41
1:E:111:HIS:CD2	1:E:113:HIS:H	2.38	0.41
1:E:633:LEU:HD22	1:E:1641:ILE:HG22	2.03	0.41
1:E:168:ASP:HB3	1:E:199:LEU:HD22	2.03	0.41
1:E:2767:ALA:HB3	1:E:2857:PRO:HG3	2.01	0.41
1:E:4573:ILE:HG21	1:E:4809:PHE:CE2	2.54	0.41
1:E:58:VAL:HG22	1:E:305:CYS:HA	2.02	0.41
1:G:1081:TYR:HD2	1:G:1234:VAL:HG13	1.84	0.41
1:G:1295:VAL:O	1:G:1547:LYS:HA	2.20	0.41
1:G:1655:GLU:HG3	1:G:1656:ARG:HG3	2.02	0.41
1:G:2133:GLU:HA	1:G:2136:ARG:HE	1.85	0.41
1:G:2211:MET:HE1	1:G:2272:PRO:HB3	2.02	0.41
1:G:308:HIS:CE1	1:G:311:ALA:HB2	2.55	0.41
1:G:359:TYR:HA	1:G:376:ALA:HA	2.03	0.41
1:G:410:LEU:HD21	1:G:441:VAL:HG22	2.02	0.41
1:A:943:ASP:HB3	1:A:1050:GLY:HA3	2.02	0.41
1:A:1089:TYR:CE2	1:A:1214:PHE:HD1	2.38	0.41
1:A:1812:LEU:HD21	1:A:1861:GLN:HG2	2.02	0.41
1:A:3775:ALA:O	1:A:3778:MET:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:ARG:N	1:A:391:THR:O	2.44	0.41
1:A:682:LEU:O	1:A:684:VAL:HG23	2.21	0.41
1:A:852:VAL:HG22	1:A:853:PRO:HD2	2.01	0.41
1:C:1081:TYR:HD2	1:C:1234:VAL:HG13	1.85	0.41
1:C:1586:ASN:N	1:C:1587:PRO:HD2	2.35	0.41
1:E:2145:SER:HB3	1:E:3647:HIS:HD2	1.85	0.41
1:E:59:PRO:HB3	1:E:281:ARG:CZ	2.50	0.41
1:E:4028:LEU:HD21	1:E:4146:LEU:HA	2.03	0.41
1:G:943:ASP:HB3	1:G:1050:GLY:HA3	2.03	0.41
1:G:1530:THR:HG22	1:G:1535:GLU:HA	2.02	0.41
1:G:1586:ASN:N	1:G:1587:PRO:HD2	2.36	0.41
1:G:633:LEU:HD22	1:G:1641:ILE:HG22	2.02	0.41
1:G:2231:SER:HA	1:G:2234:ARG:HH11	1.85	0.41
1:G:2821:TRP:HH2	1:G:2877:GLN:HB3	1.85	0.41
1:A:64:ILE:O	1:A:111:HIS:HE1	2.04	0.41
1:A:217:GLY:O	1:A:261:ARG:NH1	2.53	0.41
1:A:393:CYS:SG	1:A:397:GLU:HB2	2.60	0.41
1:A:3965:LEU:HA	1:A:3968:TYR:CD2	2.55	0.41
1:A:588:SER:HB3	1:A:592:LYS:NZ	2.35	0.41
1:C:1116:GLY:O	1:C:1132:TRP:HB3	2.20	0.41
1:C:1673:VAL:HG11	1:C:1681:VAL:HG11	2.02	0.41
1:C:359:TYR:HA	1:C:376:ALA:HA	2.03	0.41
1:C:3717:ASP:OD1	1:C:3717:ASP:N	2.51	0.41
1:C:3775:ALA:O	1:C:3778:MET:HG2	2.20	0.41
1:C:4056:GLU:OE2	1:C:4166:LEU:HD11	2.20	0.41
1:C:257:ARG:HB3	1:C:481:GLU:OE2	2.20	0.41
1:C:614:VAL:HG13	1:C:617:ASN:HB3	2.01	0.41
1:C:179:TYR:OH	1:E:2359:ARG:NE	2.53	0.41
1:E:2745:VAL:HG21	1:E:2818:ALA:HB2	2.03	0.41
1:E:3717:ASP:OD1	1:E:3717:ASP:N	2.51	0.41
1:E:4930:ALA:HB1	1:G:4933:GLN:HA	2.01	0.41
1:E:548:VAL:HG21	1:E:582:HIS:HB3	2.02	0.41
2:F:54:GLU:HG3	2:F:55:VAL:HG13	2.02	0.41
1:G:1089:TYR:HE2	1:G:1214:PHE:HD1	1.69	0.41
1:G:184:THR:HA	1:G:189:LEU:HD23	2.01	0.41
1:G:2210:VAL:O	1:G:2214:VAL:HG23	2.21	0.41
1:G:2136:ARG:NH1	1:G:3720:TYR:HE2	2.19	0.41
1:G:4878:ASP:HB3	1:G:4881:THR:OG1	2.20	0.41
1:G:495:ASN:HB2	1:G:550:LYS:HZ3	1.85	0.41
1:G:662:TRP:CZ3	1:G:814:ALA:HB2	2.55	0.41
1:G:1783:VAL:HG11	2:H:46:PHE:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1564:PHE:HB3	1:A:1565:GLU:H	1.70	0.41
1:A:1815:LEU:HB3	1:A:1865:MET:HE3	2.01	0.41
1:A:2161:GLN:NE2	1:A:2177:LEU:HB3	2.35	0.41
1:A:2182:ILE:O	1:A:2186:MET:HG2	2.20	0.41
1:A:3817:LEU:HD13	1:A:3899:PHE:HD1	1.86	0.41
1:A:471:LEU:HA	1:A:474:ARG:HE	1.85	0.41
1:A:5026:ASP:O	1:A:5027:CYS:SG	2.76	0.41
1:A:639:ASN:OD1	1:A:640:TYR:N	2.54	0.41
1:C:1018:ASN:HB3	1:C:1021:LEU:HG	2.01	0.41
1:C:1022:VAL:HG23	1:C:1027:LEU:HB3	2.00	0.41
1:C:1089:TYR:HE2	1:C:1214:PHE:HD1	1.68	0.41
1:C:2145:SER:HB3	1:C:3647:HIS:HD2	1.85	0.41
1:C:639:ASN:OD1	1:C:640:TYR:N	2.54	0.41
1:E:1092:PHE:CD2	1:E:1102:VAL:HG21	2.56	0.41
1:E:1295:VAL:O	1:E:1547:LYS:HA	2.21	0.41
1:E:359:TYR:HA	1:E:376:ALA:HA	2.02	0.41
1:E:3981:ALA:O	1:E:3986:TRP:NE1	2.46	0.41
1:E:4820:VAL:O	1:E:4824:ARG:HG3	2.20	0.41
1:E:639:ASN:OD1	1:E:640:TYR:N	2.53	0.41
1:G:1116:GLY:O	1:G:1132:TRP:HB3	2.20	0.41
1:G:1160:ILE:O	1:G:1178:ALA:N	2.53	0.41
1:G:1783:VAL:O	2:H:56:ILE:N	2.54	0.41
1:G:181:HIS:CD2	1:G:196:MET:HB2	2.55	0.41
1:G:3972:PRO:HD3	1:G:5005:GLY:HA3	2.02	0.41
1:G:588:SER:HB3	1:G:592:LYS:NZ	2.35	0.41
1:A:1290:ARG:HH21	1:A:1549:PHE:HE2	1.67	0.41
1:A:1295:VAL:O	1:A:1547:LYS:HA	2.20	0.41
1:A:1586:ASN:N	1:A:1587:PRO:HD2	2.35	0.41
1:A:2882:TYR:HD2	1:A:2919:ASP:HB3	1.85	0.41
1:A:359:TYR:HA	1:A:376:ALA:HA	2.03	0.41
1:A:4857:ASN:HD21	1:C:4807:PHE:HD2	1.64	0.41
1:A:686:TRP:HD1	1:A:757:PHE:HZ	1.68	0.41
1:C:111:HIS:CD2	1:C:113:HIS:H	2.38	0.41
1:C:3965:LEU:HA	1:C:3968:TYR:CD2	2.55	0.41
1:C:4020:GLN:O	1:C:4024:VAL:HG22	2.20	0.41
2:D:56:ILE:HB	2:D:80:TYR:O	2.20	0.41
1:E:1104:TRP:CD1	1:E:1153:ILE:HB	2.56	0.41
1:E:1293:LEU:HB3	1:E:1584:ARG:HG2	2.03	0.41
1:E:1685:LEU:HD23	1:E:1685:LEU:HA	1.92	0.41
1:E:2161:GLN:NE2	1:E:2177:LEU:HB3	2.35	0.41
1:E:2281:ILE:HG12	1:E:2337:PHE:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2882:TYR:HD2	1:E:2919:ASP:HB3	1.85	0.41
1:G:1812:LEU:HD21	1:G:1861:GLN:HG2	2.01	0.41
1:G:2203:MET:O	1:G:2207:VAL:HG23	2.20	0.41
1:G:685:GLY:HA3	1:G:713:SER:HA	2.02	0.41
1:A:3969:ILE:O	1:A:3969:ILE:HG22	2.20	0.41
1:A:4020:GLN:O	1:A:4024:VAL:HG22	2.21	0.41
1:A:4695:ASP:OD1	1:A:4696:ASP:N	2.54	0.41
1:A:596:ASN:HB2	1:A:599:VAL:HG23	2.02	0.41
1:C:4090:LYS:N	1:C:4121:GLU:O	2.54	0.41
1:C:4695:ASP:OD1	1:C:4696:ASP:N	2.54	0.41
1:E:121:LEU:HD11	1:E:136:GLY:HA3	2.03	0.41
1:E:274:LEU:HD12	1:E:278:GLN:NE2	2.36	0.41
1:E:4927:ILE:HG22	1:E:4928:LEU:HD12	2.03	0.41
1:E:682:LEU:O	1:E:684:VAL:HG23	2.21	0.41
1:E:76:ARG:NE	1:G:3844:LEU:HD23	2.36	0.41
1:G:1076:ARG:HH22	1:G:1609:PRO:CB	2.33	0.41
1:G:111:HIS:CD2	1:G:113:HIS:H	2.38	0.41
1:G:1649:ASP:OD1	1:G:1649:ASP:N	2.53	0.41
1:G:3717:ASP:OD1	1:G:3717:ASP:N	2.52	0.41
1:G:4685:GLY:O	1:G:4689:THR:N	2.54	0.41
1:G:596:ASN:HB2	1:G:599:VAL:HG23	2.03	0.41
1:G:614:VAL:HG13	1:G:617:ASN:HB3	2.01	0.41
1:A:1089:TYR:HE2	1:A:1214:PHE:HD1	1.68	0.41
1:A:236:ALA:HA	1:A:242:ARG:NH1	2.36	0.41
1:A:257:ARG:O	1:A:284:HIS:HE1	2.03	0.41
1:A:3793:MET:O	1:A:3797:THR:HG23	2.21	0.41
1:A:4090:LYS:N	1:A:4121:GLU:O	2.54	0.41
1:C:121:LEU:HD11	1:C:136:GLY:HA3	2.02	0.41
1:C:1655:GLU:HG3	1:C:1656:ARG:HG3	2.02	0.41
1:C:4686:LEU:HA	1:C:4690:GLU:HB2	2.03	0.41
1:C:4820:VAL:O	1:C:4824:ARG:HG3	2.21	0.41
1:C:4930:ALA:HB1	1:E:4933:GLN:HA	2.03	0.41
1:C:575:LEU:O	1:C:578:ILE:HG22	2.21	0.41
1:C:596:ASN:HB2	1:C:599:VAL:HG23	2.02	0.41
1:C:682:LEU:O	1:C:684:VAL:HG23	2.21	0.41
1:E:1736:VAL:HA	1:E:1737:PRO:HD2	1.90	0.41
1:E:2210:VAL:O	1:E:2214:VAL:HG23	2.21	0.41
1:E:3997:ALA:O	1:E:4001:MET:HG2	2.21	0.41
1:E:4047:MET:O	1:E:4051:SER:N	2.51	0.41
1:E:4056:GLU:OE2	1:E:4166:LEU:HD11	2.20	0.41
1:E:257:ARG:HB3	1:E:481:GLU:OE2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:76:ARG:NE	1:G:3844:LEU:CD2	2.84	0.41
1:G:1124:PHE:HB2	1:G:1162:PHE:CE2	2.55	0.41
1:G:1229:ASN:CG	1:G:1827:ARG:HH11	2.23	0.41
1:G:2761:TYR:CE2	1:G:2862:LEU:HD22	2.55	0.41
1:G:3843:ASP:OD2	1:G:3846:ALA:HB2	2.21	0.41
1:A:4936:ILE:HG21	1:G:4931:ILE:HG12	2.03	0.41
1:G:5026:ASP:O	1:G:5027:CYS:SG	2.76	0.41
1:G:523:TYR:CD1	1:G:560:ILE:HG13	2.56	0.41
1:G:868:GLU:O	1:G:871:ARG:HB2	2.19	0.41
1:A:184:THR:HA	1:A:189:LEU:HD23	2.01	0.41
1:A:2239:PHE:O	1:A:2242:ILE:HG12	2.20	0.41
1:A:4056:GLU:OE2	1:A:4166:LEU:HD11	2.20	0.41
1:A:4807:PHE:CD2	1:G:4857:ASN:ND2	2.87	0.41
1:A:685:GLY:HA3	1:A:713:SER:HA	2.03	0.41
1:C:1104:TRP:CD1	1:C:1153:ILE:HB	2.55	0.41
1:C:1632:ASP:HA	1:C:1633:PRO:HD2	1.77	0.41
1:C:2231:SER:HA	1:C:2234:ARG:HH11	1.85	0.41
1:C:2272:PRO:O	1:C:2275:VAL:HB	2.21	0.41
1:C:4028:LEU:HD21	1:C:4146:LEU:HA	2.03	0.41
1:C:4722:ARG:HA	1:C:4725:LEU:HG	2.03	0.41
1:C:4886:HIS:CE1	1:C:4897:ILE:HD12	2.56	0.41
1:C:638:ILE:HG23	1:C:678:GLN:HE22	1.86	0.41
1:C:738:LEU:HA	1:C:742:ASP:OD2	2.21	0.41
1:E:1846:SER:O	1:E:1850:VAL:HG23	2.21	0.41
1:E:2231:SER:HA	1:E:2234:ARG:HH11	1.85	0.41
1:E:281:ARG:HG2	1:E:312:THR:HG23	2.03	0.41
1:E:3841:VAL:HG12	1:E:3843:ASP:N	2.36	0.41
1:E:4708:THR:HA	1:E:4709:PRO:HD3	1.91	0.41
1:E:5022:PHE:HA	1:E:5023:PRO:HD3	1.72	0.41
1:E:686:TRP:HD1	1:E:757:PHE:HZ	1.68	0.41
1:G:1238:PHE:CE2	1:G:1612:PHE:HA	2.55	0.41
1:G:149:THR:HG23	1:G:174:VAL:HG22	2.03	0.41
1:G:2239:PHE:O	1:G:2242:ILE:HG12	2.20	0.41
1:G:225:GLY:HA2	1:G:389:PHE:HE2	1.86	0.41
1:G:3759:GLU:O	1:G:3763:LEU:N	2.48	0.41
1:G:682:LEU:O	1:G:684:VAL:HG23	2.21	0.41
1:A:1530:THR:HG22	1:A:1535:GLU:HA	2.02	0.41
1:A:2203:MET:O	1:A:2207:VAL:HG23	2.20	0.41
1:A:59:PRO:HB3	1:A:281:ARG:CZ	2.50	0.41
1:A:2735:PHE:CD1	1:A:2907:PRO:HA	2.56	0.41
1:A:3969:ILE:HG23	1:A:3977:GLN:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4722:ARG:HA	1:A:4725:LEU:HG	2.03	0.41
1:A:695:TYR:O	1:A:697:GLY:N	2.42	0.41
1:A:697:GLY:HA2	1:A:698:GLY:HA2	1.86	0.41
1:C:1252:HIS:CG	1:C:1253:PRO:HD2	2.56	0.41
1:C:2212:VAL:HG21	1:C:2256:TYR:CE2	2.56	0.41
1:C:2774:ASN:OD1	1:C:2852:ARG:NE	2.52	0.41
1:C:281:ARG:HG2	1:C:312:THR:HG23	2.03	0.41
1:C:225:GLY:HA2	1:C:389:PHE:HE2	1.86	0.41
1:C:3969:ILE:HG23	1:C:3977:GLN:HG2	2.03	0.41
2:D:6:THR:HG23	2:D:70:GLN:HE21	1.85	0.41
1:E:1767:VAL:C	1:E:1768:THR:HG1	2.23	0.41
1:E:2561:LEU:HD11	1:E:2601:ASP:HA	2.03	0.41
1:E:221:ARG:N	1:E:391:THR:O	2.44	0.41
1:E:4722:ARG:HA	1:E:4725:LEU:HG	2.03	0.41
1:E:596:ASN:HB2	1:E:599:VAL:HG23	2.02	0.41
1:E:695:TYR:HA	1:E:696:PRO:HD3	1.84	0.41
1:G:1439:VAL:HG11	1:G:1448:VAL:HG21	2.03	0.41
1:G:236:ALA:HA	1:G:242:ARG:NH1	2.36	0.41
1:G:4648:LEU:O	1:G:4652:LEU:N	2.48	0.41
1:G:4667:PRO:O	1:G:4670:ILE:HG22	2.20	0.41
2:H:87:HIS:HD2	2:H:88:PRO:HD2	1.86	0.41
1:A:4184:MET:HG2	1:A:4190:ILE:HG12	2.03	0.41
1:A:523:TYR:CD1	1:A:560:ILE:HG13	2.56	0.41
2:B:49:MET:N	2:B:54:GLU:OE2	2.54	0.41
1:C:2767:ALA:HB3	1:C:2857:PRO:HG3	2.02	0.41
1:C:3666:ASP:O	1:C:3669:PHE:HD1	2.04	0.41
1:C:4037:ASN:HB3	1:C:4042:ARG:NH2	2.34	0.41
1:C:479:GLN:OE1	1:C:484:LEU:HD13	2.21	0.41
1:C:4809:PHE:HA	1:C:4812:HIS:CE1	2.56	0.41
1:E:1632:ASP:HA	1:E:1633:PRO:HD2	1.75	0.41
1:E:3965:LEU:HA	1:E:3968:TYR:CD2	2.56	0.41
1:E:3969:ILE:O	1:E:3969:ILE:HG22	2.20	0.41
1:E:4207:MET:N	1:E:4208:PRO:HD3	2.36	0.41
1:E:523:TYR:CD1	1:E:560:ILE:HG13	2.56	0.41
1:E:638:ILE:HG23	1:E:678:GLN:HE22	1.86	0.41
1:E:662:TRP:CZ3	1:E:814:ALA:HB2	2.56	0.41
1:E:738:LEU:HA	1:E:742:ASP:OD2	2.20	0.41
1:G:2138:LEU:N	1:G:2139:PRO:HD2	2.36	0.41
1:G:2212:VAL:HG21	1:G:2256:TYR:CE2	2.56	0.41
1:G:453:GLU:HA	1:G:454:PRO:HD3	1.91	0.41
1:G:4638:TYR:O	1:G:4641:PRO:HD2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:575:LEU:O	1:G:578:ILE:HG22	2.21	0.41
1:A:1231:GLN:OE1	1:A:1821:ASP:HB2	2.21	0.40
1:A:2210:VAL:O	1:A:2214:VAL:HG23	2.21	0.40
1:A:3969:ILE:HG21	1:A:4030:LEU:HA	2.03	0.40
1:A:4820:VAL:O	1:A:4824:ARG:HG3	2.21	0.40
1:A:4913:ARG:O	1:A:4916:PHE:HB3	2.22	0.40
1:A:4927:ILE:HG22	1:A:4928:LEU:HD12	2.01	0.40
1:C:1293:LEU:HB3	1:C:1584:ARG:HG2	2.04	0.40
1:C:283:ARG:HB2	1:C:290:TYR:CE2	2.57	0.40
1:C:3780:LEU:HD21	1:C:3820:LEU:HG	2.04	0.40
1:C:4927:ILE:HG22	1:C:4928:LEU:HD12	2.03	0.40
1:E:1290:ARG:HH21	1:E:1549:PHE:HE2	1.68	0.40
1:E:1780:PRO:HD3	1:E:1801:ALA:H	1.86	0.40
1:E:1843:LYS:O	1:E:1846:SER:OG	2.25	0.40
1:E:2212:VAL:HG21	1:E:2256:TYR:CE2	2.56	0.40
1:E:3943:ILE:HB	1:E:4009:GLN:NE2	2.36	0.40
1:E:4711:PHE:HB3	1:E:4712:PRO:HD3	2.03	0.40
1:G:1103:GLY:HA3	1:G:1123:VAL:HA	2.04	0.40
1:G:2272:PRO:O	1:G:2275:VAL:HB	2.21	0.40
1:G:2288:LEU:O	1:G:3849:ARG:HD3	2.21	0.40
1:G:4023:MET:O	1:G:4026:MET:HB3	2.21	0.40
1:G:257:ARG:HB3	1:G:481:GLU:OE2	2.21	0.40
1:A:111:HIS:CD2	1:A:113:HIS:H	2.38	0.40
1:A:1252:HIS:CG	1:A:1253:PRO:HD2	2.56	0.40
1:A:2062:ARG:O	1:A:2065:SER:OG	2.33	0.40
1:A:2145:SER:HB3	1:A:3647:HIS:HD2	1.85	0.40
1:A:2747:ILE:HG12	1:A:2817:ILE:HD12	2.03	0.40
1:A:274:LEU:HD12	1:A:278:GLN:NE2	2.36	0.40
1:A:2745:VAL:HG21	1:A:2818:ALA:HB2	2.02	0.40
1:A:2103:VAL:HG21	1:A:3676:ASP:OD2	2.21	0.40
1:A:3878:ASP:OD1	1:A:3879:GLU:N	2.55	0.40
1:A:4047:MET:O	1:A:4051:SER:N	2.51	0.40
1:A:4551:PHE:O	1:A:4555:LEU:HB2	2.21	0.40
1:A:4686:LEU:HA	1:A:4690:GLU:HB2	2.03	0.40
1:A:4823:LEU:HA	1:A:4826:ILE:HD12	2.03	0.40
1:A:575:LEU:O	1:A:578:ILE:HG22	2.21	0.40
1:C:64:ILE:O	1:C:111:HIS:HE1	2.04	0.40
1:C:1238:PHE:CE2	1:C:1612:PHE:HA	2.55	0.40
1:C:1780:PRO:HD3	1:C:1801:ALA:H	1.86	0.40
1:C:2561:LEU:HD11	1:C:2601:ASP:HA	2.03	0.40
1:C:2747:ILE:HG12	1:C:2817:ILE:HD12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4551:PHE:O	1:C:4555:LEU:HB2	2.21	0.40
1:C:4878:ASP:HB3	1:C:4881:THR:OG1	2.21	0.40
1:E:1439:VAL:HG11	1:E:1448:VAL:HG21	2.03	0.40
1:E:2211:MET:HG3	1:E:2229:VAL:HG13	2.03	0.40
1:E:4886:HIS:CE1	1:E:4897:ILE:HD12	2.56	0.40
1:E:4888:TYR:O	1:E:4892:ARG:HD3	2.21	0.40
1:E:545:ASP:HA	1:E:582:HIS:CE1	2.56	0.40
1:G:2142:TYR:HD2	1:G:2197:LEU:HD12	1.86	0.40
1:G:3831:SER:O	1:G:3835:LEU:HG	2.21	0.40
1:G:3919:THR:HG21	1:G:3968:TYR:CE2	2.54	0.40
1:G:471:LEU:HA	1:G:474:ARG:HE	1.85	0.40
1:G:852:VAL:HG22	1:G:853:PRO:HD2	2.02	0.40
1:A:1293:LEU:HB3	1:A:1584:ARG:HG2	2.03	0.40
1:A:1778:SER:HA	1:A:1779:PRO:HD3	1.89	0.40
1:A:2821:TRP:HH2	1:A:2877:GLN:HB3	1.87	0.40
1:A:23:GLN:NE2	1:A:34:LYS:HB3	2.32	0.40
1:A:3981:ALA:O	1:A:3986:TRP:NE1	2.46	0.40
1:C:1160:ILE:O	1:C:1178:ALA:N	2.55	0.40
1:C:1439:VAL:HG11	1:C:1448:VAL:HG21	2.03	0.40
1:C:149:THR:HG23	1:C:174:VAL:HG22	2.03	0.40
1:C:2239:PHE:O	1:C:2242:ILE:HG12	2.20	0.40
1:C:2281:ILE:HG12	1:C:2337:PHE:CD1	2.56	0.40
1:C:2735:PHE:CD1	1:C:2907:PRO:HA	2.56	0.40
1:C:3817:LEU:HD13	1:C:3899:PHE:HD1	1.86	0.40
1:C:3958:ALA:CB	1:C:4019:LEU:HD11	2.47	0.40
1:C:3969:ILE:HG21	1:C:4030:LEU:HA	2.03	0.40
1:C:4207:MET:N	1:C:4208:PRO:HD3	2.36	0.40
1:C:4809:PHE:O	1:C:4812:HIS:ND1	2.49	0.40
2:D:82:TYR:CE1	2:D:87:HIS:HB2	2.57	0.40
1:E:64:ILE:O	1:E:111:HIS:HE1	2.03	0.40
1:E:4695:ASP:OD1	1:E:4696:ASP:N	2.54	0.40
1:E:4878:ASP:HB3	1:E:4881:THR:OG1	2.21	0.40
1:E:575:LEU:O	1:E:578:ILE:HG22	2.21	0.40
1:G:1232:ARG:HE	1:G:1701:ALA:HB3	1.86	0.40
1:G:3706:SER:O	1:G:3710:LEU:HG	2.21	0.40
1:G:4002:LYS:HB3	1:G:4002:LYS:HE2	1.84	0.40
1:G:4150:LEU:O	1:G:4154:VAL:N	2.38	0.40
1:G:545:ASP:HA	1:G:582:HIS:CE1	2.57	0.40
1:A:121:LEU:HD11	1:A:136:GLY:HA3	2.03	0.40
1:A:225:GLY:HA2	1:A:389:PHE:HE2	1.86	0.40
1:A:2281:ILE:HG12	1:A:2337:PHE:CD1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:HIS:CD2	1:A:287:THR:H	2.39	0.40
1:A:4711:PHE:HB3	1:A:4712:PRO:HD3	2.04	0.40
1:A:633:LEU:HD22	1:A:1641:ILE:HG22	2.04	0.40
1:C:2238:TYR:O	1:C:2242:ILE:HG23	2.22	0.40
1:C:3844:LEU:HD22	1:C:3932:ASP:OD2	2.22	0.40
1:C:3997:ALA:O	1:C:4001:MET:HG2	2.21	0.40
1:C:523:TYR:CD1	1:C:560:ILE:HG13	2.56	0.40
2:D:54:GLU:HG3	2:D:55:VAL:HG13	2.03	0.40
2:D:49:MET:N	2:D:54:GLU:OE2	2.55	0.40
1:E:1076:ARG:HH11	1:E:1109:LEU:HD11	1.86	0.40
1:E:2239:PHE:O	1:E:2242:ILE:HG12	2.20	0.40
1:E:244:LEU:HD22	1:E:375:LYS:HZ3	1.86	0.40
1:E:283:ARG:HB2	1:E:290:TYR:CE2	2.56	0.40
1:E:2821:TRP:HH2	1:E:2877:GLN:HB3	1.87	0.40
1:E:3878:ASP:OD1	1:E:3879:GLU:N	2.55	0.40
1:E:3958:ALA:CB	1:E:4019:LEU:HD11	2.48	0.40
1:E:453:GLU:HA	1:E:454:PRO:HD3	1.91	0.40
1:E:4686:LEU:HA	1:E:4690:GLU:HB2	2.02	0.40
1:E:4829:SER:O	1:E:4939:ALA:HB1	2.21	0.40
1:G:1089:TYR:CE2	1:G:1214:PHE:HD1	2.38	0.40
1:G:2099:SER:O	1:G:2103:VAL:HG23	2.20	0.40
1:G:2281:ILE:HG12	1:G:2337:PHE:CD1	2.56	0.40
1:G:4839:MET:O	1:G:4843:LEU:N	2.52	0.40
1:G:675:LEU:HD23	1:G:676:THR:OG1	2.22	0.40
1:A:1092:PHE:CD2	1:A:1102:VAL:HG21	2.56	0.40
1:A:1238:PHE:CE1	1:A:1612:PHE:HA	2.57	0.40
1:A:281:ARG:HG2	1:A:312:THR:HG23	2.03	0.40
1:A:626:LEU:HB3	1:A:1688:HIS:CE1	2.56	0.40
1:C:943:ASP:HB3	1:C:1050:GLY:HA3	2.03	0.40
1:C:1092:PHE:CD2	1:C:1102:VAL:HG21	2.57	0.40
1:C:1131:ARG:NH1	1:C:1179:PHE:CD1	2.89	0.40
1:C:1612:PHE:O	1:C:1613:LEU:HB2	2.22	0.40
1:C:2211:MET:HG3	1:C:2229:VAL:HG13	2.04	0.40
1:C:4857:ASN:HD21	1:E:4807:PHE:HD2	1.64	0.40
1:E:2803:GLU:OE2	1:E:2810:LYS:NZ	2.54	0.40
1:E:2735:PHE:CD1	1:E:2907:PRO:HA	2.56	0.40
1:E:3793:MET:O	1:E:3797:THR:HG23	2.22	0.40
1:E:225:GLY:HA2	1:E:389:PHE:HE2	1.86	0.40
1:E:3971:GLY:O	1:E:3973:CYS:N	2.51	0.40
1:E:4823:LEU:HA	1:E:4826:ILE:HD12	2.03	0.40
1:G:1293:LEU:HB3	1:G:1584:ARG:HG2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1674:CYS:SG	1:G:1685:LEU:HD12	2.62	0.40
1:G:626:LEU:HB3	1:G:1688:HIS:CE1	2.56	0.40
1:G:2062:ARG:O	1:G:2065:SER:OG	2.30	0.40
1:G:281:ARG:HG2	1:G:312:THR:HG23	2.03	0.40
1:G:4574:ASN:HA	1:G:4577:LEU:HD13	2.03	0.40
1:G:4705:VAL:O	1:G:4708:THR:OG1	2.29	0.40
1:G:4779:LYS:O	1:G:4783:ILE:HG12	2.22	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	3496/5037 (69%)	3185 (91%)	227 (6%)	84 (2%)	7	45
1	C	3496/5037 (69%)	3185 (91%)	228 (6%)	83 (2%)	7	45
1	E	3496/5037 (69%)	3187 (91%)	226 (6%)	83 (2%)	7	45
1	G	3496/5037 (69%)	3192 (91%)	217 (6%)	87 (2%)	6	44
2	B	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
2	D	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
2	F	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
2	H	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
All	All	14404/20580 (70%)	13130 (91%)	937 (6%)	337 (2%)	11	46

All (337) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	701	GLY
1	A	915	GLU
1	A	916	PRO

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Mol	Chain	Res	Type
1	A	969	PRO
1	A	1589	PRO
1	A	2341	VAL
1	A	2466	LEU
1	A	3826	VAL
1	A	4084	PRO
1	A	4115	SER
1	A	4984	ASN
1	A	4985	LEU
1	C	701	GLY
1	C	808	TYR
1	C	915	GLU
1	C	916	PRO
1	C	969	PRO
1	C	1589	PRO
1	C	2341	VAL
1	C	2466	LEU
1	C	3826	VAL
1	C	4084	PRO
1	C	4115	SER
1	C	4984	ASN
1	C	4985	LEU
1	E	701	GLY
1	E	915	GLU
1	E	916	PRO
1	E	969	PRO
1	E	2341	VAL
1	E	2466	LEU
1	E	3826	VAL
1	E	4084	PRO
1	E	4115	SER
1	E	4984	ASN
1	E	4985	LEU
1	G	701	GLY
1	G	808	TYR
1	G	915	GLU
1	G	916	PRO
1	G	969	PRO
1	G	1589	PRO
1	G	2341	VAL
1	G	2466	LEU
1	G	3664	THR

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Mol	Chain	Res	Type
1	G	3826	VAL
1	G	4084	PRO
1	G	4115	SER
1	G	4984	ASN
1	G	4985	LEU
1	A	208	CYS
1	A	329	ARG
1	A	385	ASP
1	A	510	GLU
1	A	557	SER
1	A	609	CYS
1	A	808	TYR
1	A	865	PRO
1	A	1480	GLN
1	A	1768	THR
1	A	2281	ILE
1	A	2359	ARG
1	A	2465	ASP
1	A	3714	SER
1	A	3806	ASN
1	A	3941	ASP
1	A	4206	GLU
1	C	208	CYS
1	C	329	ARG
1	C	385	ASP
1	C	510	GLU
1	C	557	SER
1	C	609	CYS
1	C	865	PRO
1	C	1480	GLN
1	C	1768	THR
1	C	2281	ILE
1	C	2359	ARG
1	C	2465	ASP
1	C	3714	SER
1	C	3806	ASN
1	C	3941	ASP
1	C	4206	GLU
1	E	208	CYS
1	E	329	ARG
1	E	385	ASP
1	E	510	GLU

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Mol	Chain	Res	Type
1	E	557	SER
1	E	609	CYS
1	E	808	TYR
1	E	865	PRO
1	E	1480	GLN
1	E	1768	THR
1	E	2281	ILE
1	E	2359	ARG
1	E	2465	ASP
1	E	3714	SER
1	E	3806	ASN
1	E	3941	ASP
1	E	4206	GLU
1	G	208	CYS
1	G	329	ARG
1	G	385	ASP
1	G	510	GLU
1	G	557	SER
1	G	609	CYS
1	G	865	PRO
1	G	1480	GLN
1	G	1768	THR
1	G	2281	ILE
1	G	2359	ARG
1	G	2465	ASP
1	G	3714	SER
1	G	3806	ASN
1	G	3843	ASP
1	G	3941	ASP
1	G	4031	LEU
1	G	4036	VAL
1	A	692	TYR
1	A	698	GLY
1	A	720	HIS
1	A	770	ALA
1	A	817	PRO
1	A	827	LYS
1	A	1034	SER
1	A	1483	VAL
1	A	1545	ASN
1	A	1599	MET
1	A	1717	SER

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Mol	Chain	Res	Type
1	A	1747	LEU
1	A	1818	ALA
1	A	1854	PHE
1	A	2826	ALA
1	A	4036	VAL
1	A	4186	ALA
1	C	30	LYS
1	C	692	TYR
1	C	698	GLY
1	C	720	HIS
1	C	770	ALA
1	C	817	PRO
1	C	827	LYS
1	C	1034	SER
1	C	1483	VAL
1	C	1545	ASN
1	C	1599	MET
1	C	1717	SER
1	C	1747	LEU
1	C	1818	ALA
1	C	1854	PHE
1	C	2826	ALA
1	C	4036	VAL
1	C	4186	ALA
1	E	30	LYS
1	E	692	TYR
1	E	698	GLY
1	E	720	HIS
1	E	770	ALA
1	E	817	PRO
1	E	827	LYS
1	E	1034	SER
1	E	1483	VAL
1	E	1545	ASN
1	E	1599	MET
1	E	1717	SER
1	E	1747	LEU
1	E	1818	ALA
1	E	1854	PHE
1	E	2826	ALA
1	E	4186	ALA
1	G	692	TYR

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Mol	Chain	Res	Type
1	G	698	GLY
1	G	720	HIS
1	G	770	ALA
1	G	817	PRO
1	G	827	LYS
1	G	1034	SER
1	G	1483	VAL
1	G	1545	ASN
1	G	1599	MET
1	G	1717	SER
1	G	1747	LEU
1	G	1818	ALA
1	G	1854	PHE
1	G	4186	ALA
1	G	4691	GLN
1	G	5025	GLY
1	A	29	LEU
1	A	30	LYS
1	A	309	THR
1	A	676	THR
1	A	826	ILE
1	A	1134	LEU
1	A	1186	ASP
1	A	1206	GLN
1	A	1541	GLN
1	A	4032	GLU
1	A	4052	SER
1	A	4119	GLU
1	A	4691	GLN
1	A	4869	GLU
1	C	29	LEU
1	C	676	THR
1	C	826	ILE
1	C	1134	LEU
1	C	1186	ASP
1	C	1206	GLN
1	C	1541	GLN
1	C	1614	GLN
1	C	4032	GLU
1	C	4052	SER
1	C	4119	GLU
1	C	4691	GLN

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Mol	Chain	Res	Type
1	C	4869	GLU
1	E	29	LEU
1	E	676	THR
1	E	826	ILE
1	E	1134	LEU
1	E	1186	ASP
1	E	1206	GLN
1	E	1541	GLN
1	E	4032	GLU
1	E	4036	VAL
1	E	4052	SER
1	E	4119	GLU
1	E	4691	GLN
1	E	4869	GLU
1	E	5025	GLY
1	G	29	LEU
1	G	30	LYS
1	G	676	THR
1	G	826	ILE
1	G	1134	LEU
1	G	1186	ASP
1	G	1206	GLN
1	G	1541	GLN
1	G	2826	ALA
1	G	4119	GLU
1	G	4206	GLU
1	G	4869	GLU
1	G	5027	CYS
1	A	252	VAL
1	A	422	SER
1	A	751	SER
1	A	1017	ARG
1	A	1126	GLY
1	A	1614	GLN
1	A	1772	ARG
1	A	2191	PHE
1	A	3664	THR
1	A	4208	PRO
1	A	5025	GLY
1	A	5027	CYS
1	C	252	VAL
1	C	309	THR

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Mol	Chain	Res	Type
1	C	422	SER
1	C	751	SER
1	C	1017	ARG
1	C	1772	ARG
1	C	2191	PHE
1	C	3664	THR
1	C	4208	PRO
1	C	5025	GLY
1	C	5027	CYS
1	E	252	VAL
1	E	309	THR
1	E	422	SER
1	E	751	SER
1	E	1017	ARG
1	E	1126	GLY
1	E	1772	ARG
1	E	2191	PHE
1	E	3664	THR
1	E	4208	PRO
1	E	5027	CYS
1	G	252	VAL
1	G	309	THR
1	G	422	SER
1	G	751	SER
1	G	1017	ARG
1	G	1772	ARG
1	G	2191	PHE
1	G	3668	SER
1	G	4040	ILE
1	G	4208	PRO
1	G	4821	LYS
1	A	611	GLY
1	A	740	PRO
1	A	4712	PRO
1	A	4734	ARG
1	A	4872	PRO
1	C	611	GLY
1	C	740	PRO
1	C	1126	GLY
1	C	4712	PRO
1	C	4872	PRO
1	E	611	GLY

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Mol	Chain	Res	Type
1	E	740	PRO
1	E	4712	PRO
1	E	4734	ARG
1	E	4872	PRO
1	G	611	GLY
1	G	740	PRO
1	G	1126	GLY
1	G	4872	PRO
1	G	4963	ILE
1	A	781	VAL
1	A	1830	VAL
1	A	4040	ILE
1	A	4963	ILE
1	C	781	VAL
1	C	1830	VAL
1	C	4040	ILE
1	C	4963	ILE
1	E	781	VAL
1	E	1830	VAL
1	E	4040	ILE
1	E	4963	ILE
1	G	781	VAL
1	G	1830	VAL
1	G	3085	PRO
1	G	4712	PRO
1	C	842	PRO
1	G	842	PRO
1	G	2044	ILE
1	A	842	PRO
1	A	1544	PRO
1	E	842	PRO
1	E	1544	PRO
1	E	1589	PRO
1	G	4895	GLY
1	C	1544	PRO
1	G	1544	PRO
1	A	1253	PRO
1	C	1253	PRO
1	E	1253	PRO
1	G	1253	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	2503/4276 (58%)	2493 (100%)	10 (0%)	93	96
1	C	2502/4276 (58%)	2492 (100%)	10 (0%)	93	96
1	E	2500/4276 (58%)	2491 (100%)	9 (0%)	93	96
1	G	2501/4276 (58%)	2489 (100%)	12 (0%)	91	96
2	B	89/90 (99%)	88 (99%)	1 (1%)	78	89
2	D	89/90 (99%)	88 (99%)	1 (1%)	78	89
2	F	89/90 (99%)	88 (99%)	1 (1%)	78	89
2	H	89/90 (99%)	89 (100%)	0	100	100
All	All	10362/17464 (59%)	10318 (100%)	44 (0%)	93	96

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	806	PRO
1	A	865	PRO
1	A	914	PRO
1	A	916	PRO
1	A	979	PRO
1	A	1001	VAL
1	A	1055	PRO
1	A	4844	LEU
1	A	4850	LEU
1	A	4972	PRO
2	B	34	LYS
1	C	806	PRO
1	C	865	PRO
1	C	914	PRO
1	C	916	PRO
1	C	979	PRO
1	C	1001	VAL
1	C	1055	PRO
1	C	4844	LEU

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Mol	Chain	Res	Type
1	C	4850	LEU
1	C	4972	PRO
2	D	34	LYS
1	E	806	PRO
1	E	865	PRO
1	E	914	PRO
1	E	916	PRO
1	E	979	PRO
1	E	1001	VAL
1	E	1055	PRO
1	E	4850	LEU
1	E	4972	PRO
2	F	34	LYS
1	G	806	PRO
1	G	865	PRO
1	G	914	PRO
1	G	916	PRO
1	G	979	PRO
1	G	1001	VAL
1	G	1055	PRO
1	G	1455	PRO
1	G	4106	PRO
1	G	4166	LEU
1	G	4850	LEU
1	G	4972	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (208) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	105	HIS
1	A	111	HIS
1	A	113	HIS
1	A	138	GLN
1	A	218	HIS
1	A	278	GLN
1	A	379	HIS
1	A	405	HIS
1	A	460	GLN
1	A	465	GLN
1	A	582	HIS
1	A	596	ASN

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Mol	Chain	Res	Type
1	A	610	ASN
1	A	618	GLN
1	A	678	GLN
1	A	765	GLN
1	A	772	ASN
1	A	838	HIS
1	A	1125	ASN
1	A	1201	HIS
1	A	1254	HIS
1	A	1631	GLN
1	A	1663	HIS
1	A	1665	HIS
1	A	1678	ASN
1	A	2107	GLN
1	A	2127	GLN
1	A	2161	GLN
1	A	2184	ASN
1	A	2194	HIS
1	A	2260	ASN
1	A	2420	HIS
1	A	2744	ASN
1	A	3647	HIS
1	A	3651	ASN
1	A	3781	GLN
1	A	3895	HIS
1	A	3906	GLN
1	A	3960	GLN
1	A	3970	GLN
1	A	3998	HIS
1	A	4009	GLN
1	A	4162	ASN
1	A	4223	ASN
1	A	4691	GLN
1	A	4803	HIS
1	A	4836	GLN
1	A	4857	ASN
1	A	4886	HIS
1	A	4987	ASN
1	A	5003	HIS
2	B	25	HIS
2	B	87	HIS
1	C	57	ASN

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Mol	Chain	Res	Type
1	C	105	HIS
1	C	111	HIS
1	C	113	HIS
1	C	138	GLN
1	C	218	HIS
1	C	278	GLN
1	C	379	HIS
1	C	405	HIS
1	C	460	GLN
1	C	465	GLN
1	C	582	HIS
1	C	596	ASN
1	C	678	GLN
1	C	765	GLN
1	C	772	ASN
1	C	838	HIS
1	C	1201	HIS
1	C	1254	HIS
1	C	1631	GLN
1	C	1663	HIS
1	C	1665	HIS
1	C	2107	GLN
1	C	2127	GLN
1	C	2161	GLN
1	C	2184	ASN
1	C	2194	HIS
1	C	2260	ASN
1	C	2420	HIS
1	C	2744	ASN
1	C	3647	HIS
1	C	3651	ASN
1	C	3781	GLN
1	C	3895	HIS
1	C	3906	GLN
1	C	3960	GLN
1	C	3970	GLN
1	C	3998	HIS
1	C	4009	GLN
1	C	4162	ASN
1	C	4223	ASN
1	C	4691	GLN
1	C	4803	HIS

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Mol	Chain	Res	Type
1	C	4836	GLN
1	C	4857	ASN
1	C	4886	HIS
1	C	4987	ASN
1	C	5003	HIS
2	D	25	HIS
2	D	87	HIS
1	E	57	ASN
1	E	105	HIS
1	E	111	HIS
1	E	113	HIS
1	E	138	GLN
1	E	218	HIS
1	E	278	GLN
1	E	379	HIS
1	E	405	HIS
1	E	460	GLN
1	E	465	GLN
1	E	582	HIS
1	E	596	ASN
1	E	618	GLN
1	E	678	GLN
1	E	765	GLN
1	E	772	ASN
1	E	838	HIS
1	E	1125	ASN
1	E	1201	HIS
1	E	1254	HIS
1	E	1280	GLN
1	E	1559	GLN
1	E	1631	GLN
1	E	1663	HIS
1	E	1665	HIS
1	E	1678	ASN
1	E	2107	GLN
1	E	2127	GLN
1	E	2161	GLN
1	E	2184	ASN
1	E	2194	HIS
1	E	2260	ASN
1	E	2420	HIS
1	E	2744	ASN

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Mol	Chain	Res	Type
1	E	3647	HIS
1	E	3651	ASN
1	E	3781	GLN
1	E	3895	HIS
1	E	3906	GLN
1	E	3960	GLN
1	E	3970	GLN
1	E	3998	HIS
1	E	4009	GLN
1	E	4162	ASN
1	E	4691	GLN
1	E	4803	HIS
1	E	4836	GLN
1	E	4857	ASN
1	E	4886	HIS
1	E	4987	ASN
1	E	5003	HIS
2	F	25	HIS
2	F	87	HIS
1	G	57	ASN
1	G	105	HIS
1	G	111	HIS
1	G	113	HIS
1	G	138	GLN
1	G	218	HIS
1	G	278	GLN
1	G	379	HIS
1	G	405	HIS
1	G	460	GLN
1	G	465	GLN
1	G	582	HIS
1	G	596	ASN
1	G	610	ASN
1	G	678	GLN
1	G	765	GLN
1	G	772	ASN
1	G	838	HIS
1	G	1201	HIS
1	G	1254	HIS
1	G	1631	GLN
1	G	1663	HIS
1	G	2107	GLN

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Mol	Chain	Res	Type
1	G	2127	GLN
1	G	2161	GLN
1	G	2184	ASN
1	G	2194	HIS
1	G	2260	ASN
1	G	2420	HIS
1	G	2744	ASN
1	G	3651	ASN
1	G	3781	GLN
1	G	3895	HIS
1	G	3896	ASN
1	G	3906	GLN
1	G	3960	GLN
1	G	3998	HIS
1	G	4009	GLN
1	G	4020	GLN
1	G	4153	HIS
1	G	4162	ASN
1	G	4223	ASN
1	G	4650	HIS
1	G	4691	GLN
1	G	4836	GLN
1	G	4857	ASN
1	G	4886	HIS
1	G	4987	ASN
2	H	25	HIS
2	H	87	HIS

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 carbohydrates 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.