Full wwPDB EM Validation Report ⓘ

Nov 23, 2022 – 07:38 AM EST

PDB ID	:	7UA9
EMDB ID	:	EMD-26416
Title	:	Structure of dephosphorylated human RyR2 in the open state
Authors	:	Miotto, M.C.; Marks, A.R.
Deposited on	:	2022-03-11
Resolution	:	3.59 Å(reported)
Based on initial model	:	7U9Q

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

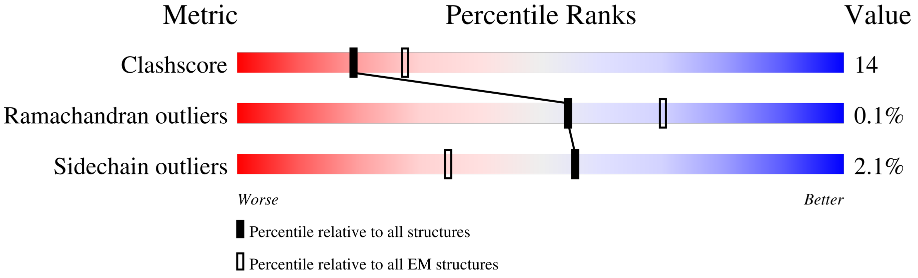
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance ⓘ

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

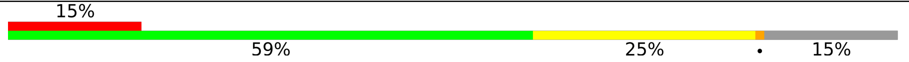
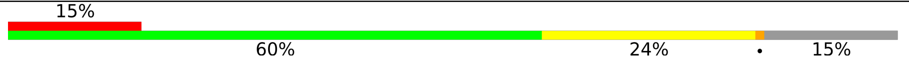
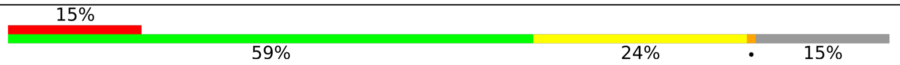
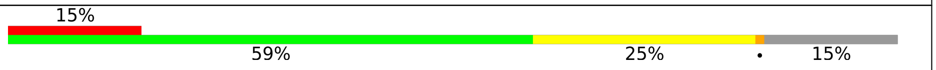
The reported resolution of this entry is 3.59 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	E	108	
1	F	108	
1	G	108	
1	H	108	
2	A	4967	
2	B	4967	
2	C	4967	
2	D	4967	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 138656 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

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

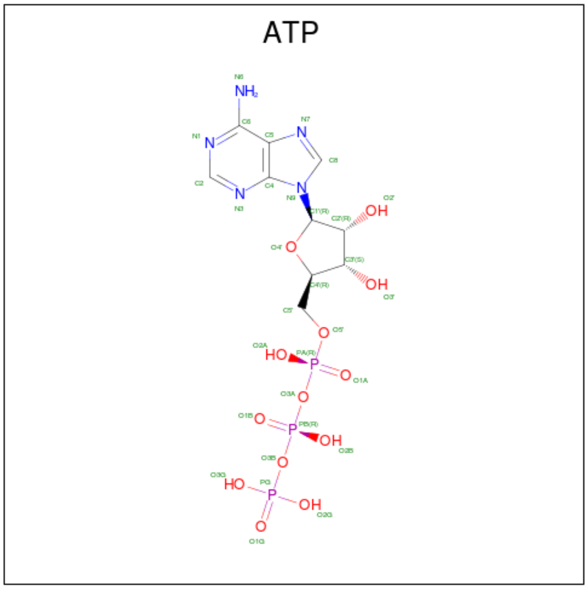
- Molecule 2 is a protein called Ryanodine receptor 2.

Mol	Chain	Residues	Atoms	AltConf	Trace
2	A	4224	Total C N O S 33771 21516 5745 6280 230	2	0
2	B	4224	Total C N O S 33771 21516 5745 6280 230	2	0
2	C	4224	Total C N O S 33771 21516 5745 6280 230	2	0
2	D	4224	Total C N O S 33771 21516 5745 6280 230	2	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
4	A	1	62	20	10	26	6	0
4	A	1	62	20	10	26	6	0
4	B	1	62	20	10	26	6	0
4	B	1	62	20	10	26	6	0
4	C	1	62	20	10	26	6	0
4	C	1	62	20	10	26	6	0
4	D	1	62	20	10	26	6	0
4	D	1	62	20	10	26	6	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
5	A	1	1	1	0
5	B	1	1	1	0

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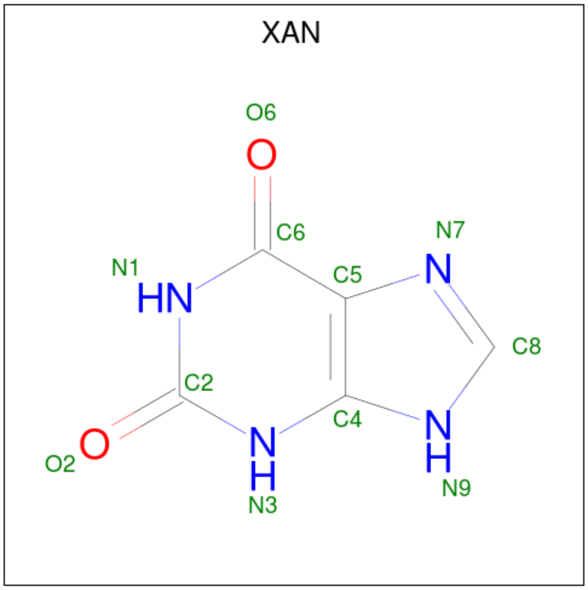
Mol	Chain	Residues	Atoms		AltConf
5	C	1	Total 1	Ca 1	0
5	D	1	Total 1	Ca 1	0

- Molecule 6 is XANTHINE (three-letter code: XAN) (formula: $C_5H_4N_4O_2$) (labeled as "Ligand of Interest" by depositor).

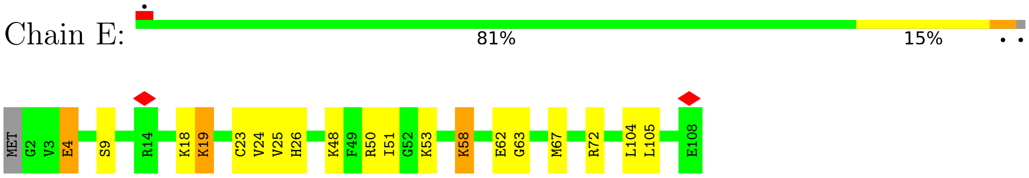


Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total 11	C 5	N 4	O 2	0
6	B	1	Total 11	C 5	N 4	O 2	0
6	C	1	Total 11	C 5	N 4	O 2	0
6	D	1	Total 11	C 5	N 4	O 2	0

3 Residue-property plots ⓘ

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

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



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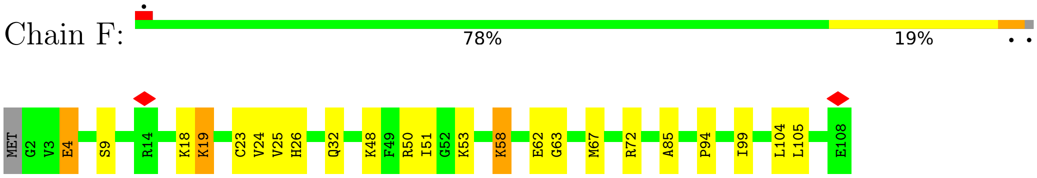

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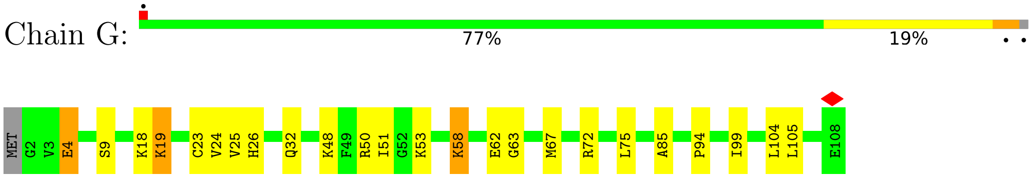
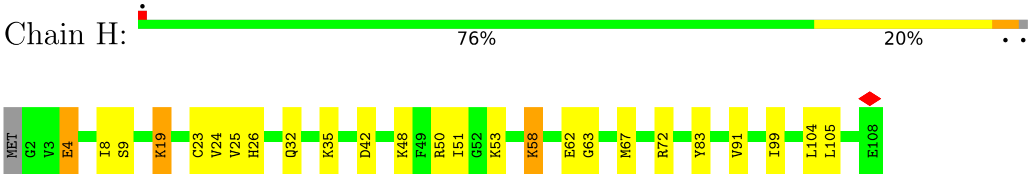
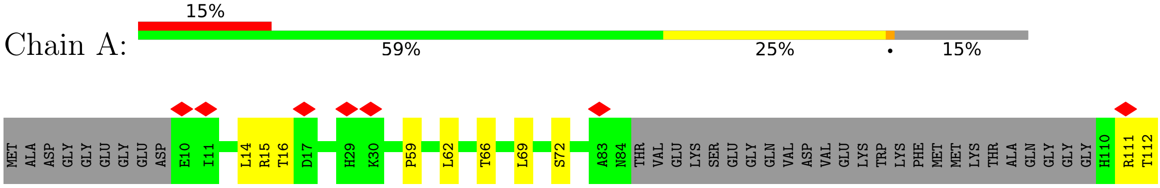
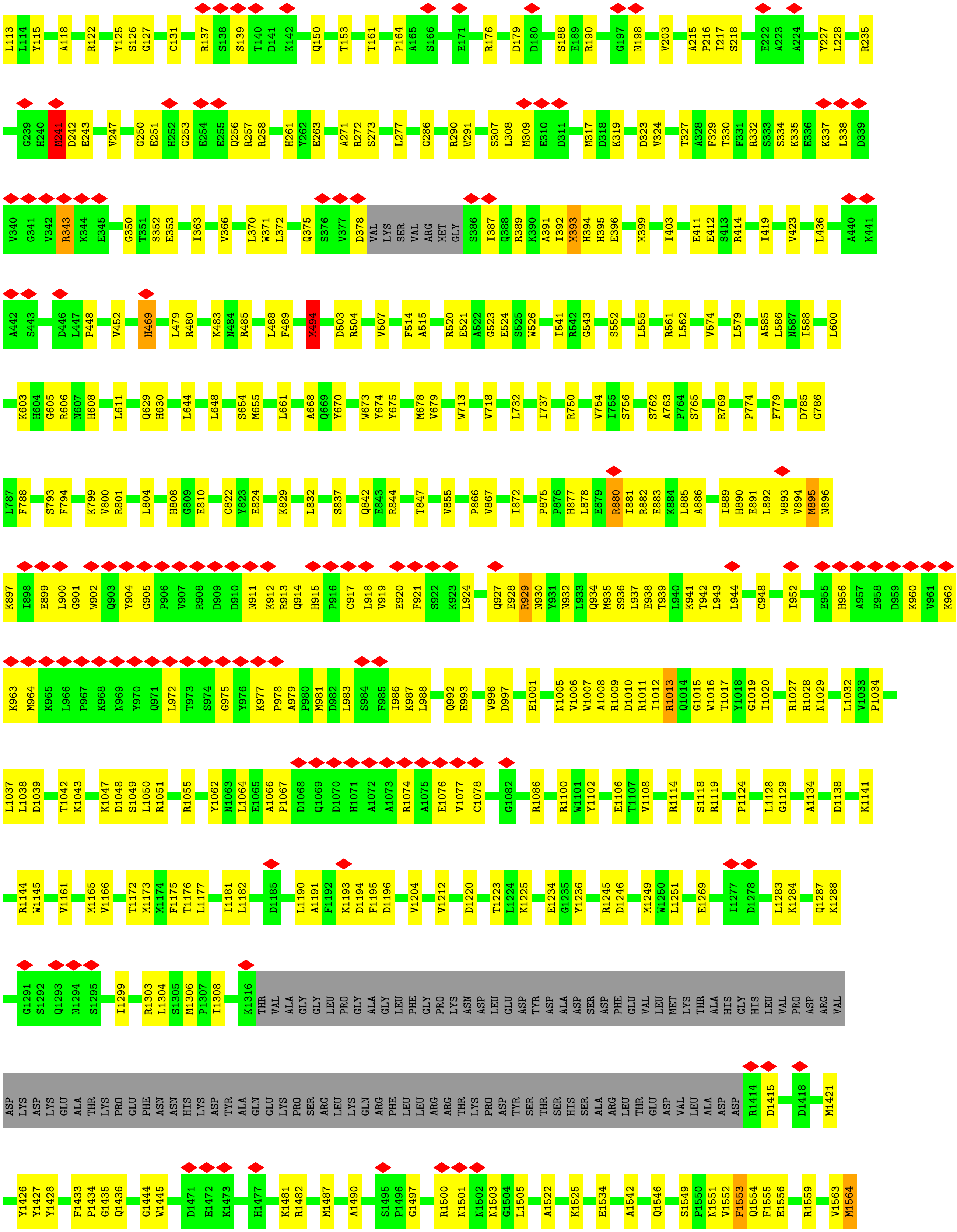


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



- Molecule 2: Ryanodine receptor 2

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G239 H240 M241 D242 E243 V247 G250 E251 H252 G253 E254 E255 Q256 R257 R258 H261 Y262 E263 A271 R272 S273 L277 G286 R290 W291 S307 L308 M309 E310 D311 M317 D318 K319 D323 V324 T327 A328 F329 T330 F331 R332 S333 S334 K335 E336 K337 L338 D339
V340 G341 V342 R343 K344 E345 G350 T351 S352 E353 I363 V366 L370 W371 L372 Q375 S376 V377 D378 VAL LYS SER VAL ARG MET GLY S386 I387 Q388 R389 K390 A391 I392 M393 H394 H395 E396 M399 I403 E411 E412 S413 R414 I419 V423 L436 A440 K441
A442 S443 D446 L447 P448 V452 H469 L479 R480 K483 N484 R485 L488 F489 M494 D503 R504 V507 F514 A515 R520 E521 A522 G523 E524 S525 W526 I541 R542 G543 S552 L555 R561 L562 V574 L579 A585 L586 N587 I588 L600
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K963 M964 K965 L966 P967 K968 N969 Y970 Q971 L972 T973 S974 G975 Y976 K977 P978 A979 P980 M981 D982 L983 S984 F985 I986 K987 L988 Q992 E993 V996 D997 E1001 N1005 V1006 W1007 A1008 R1009 D1010 R1011 I1012 R1013 Q1014 G1015 W1016 T1017 Y1018 G1019 I1020 R1027 R1028 N1029 L1032 V1033 P1034
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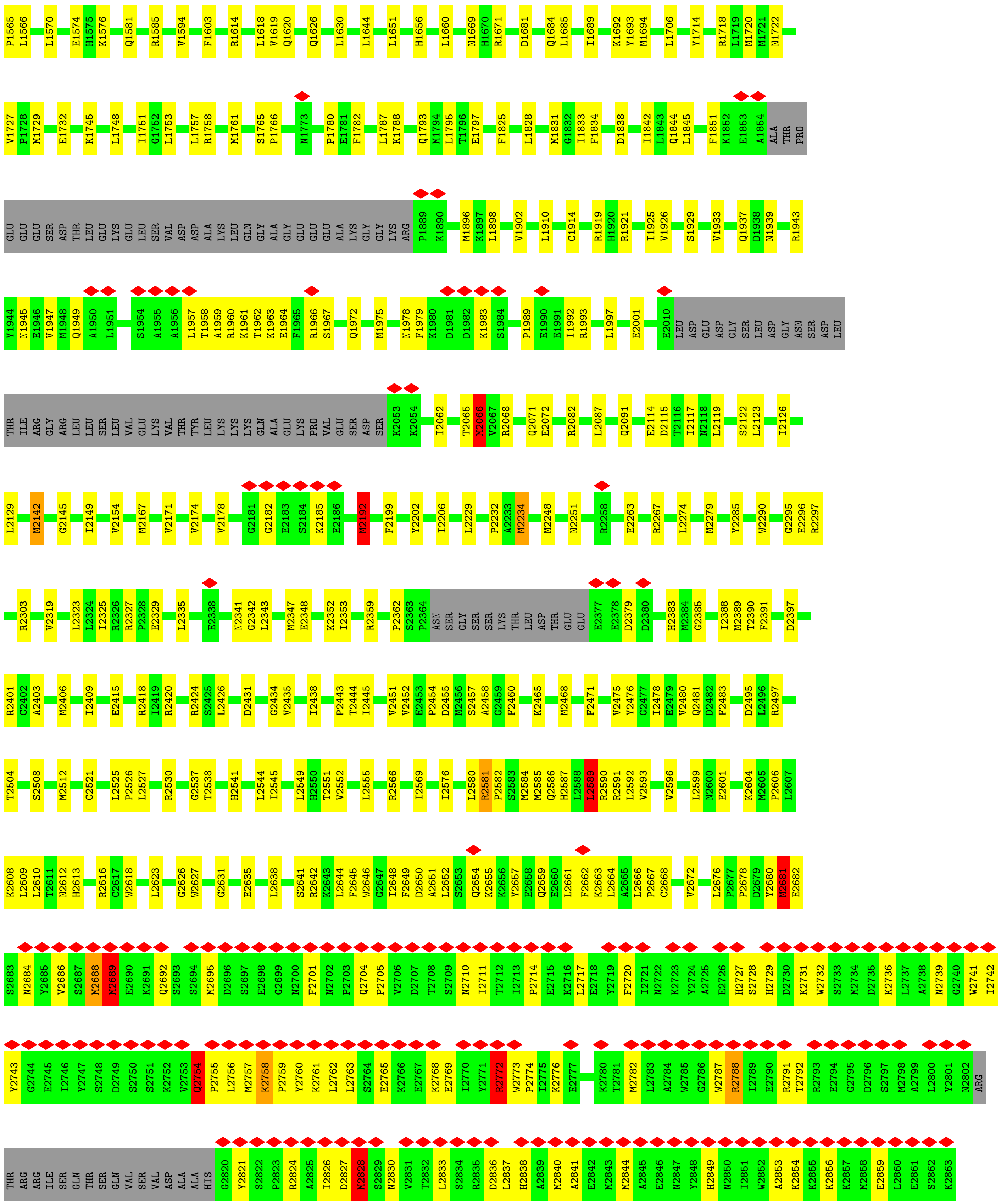
R1144 W1145 V1161 M1165 V1166 T1172 M1173 M1174 F1175 T1176 L1177 I1181 L1182 D1185 L1190 A1191 F1192 K1193 D1194 F1195 D1196 V1204 V1212 D1220 T1223 L1224 K1225 E1234 G1235 Y1236 R1245 D1246 M1249 W1250 L1251 E1269 I1277 D1278 L1283 K1284 Q1287 K1288
G1291 S1292 Q1293 N1294 S1295 I1299 R1303 L1304 S1305 M1306 P1307 I1308 K1316 THR VAL ALA GLY GLY LEU PRO GLY ALA GLY LEU PHE GLY PRO LYS ASN ASP LEU GLU GLU ASP TYR ASP ALA ASP SER ASP PHE GLU VAL LEU MET LYS THR ALA HIS GLY HIS LEU VAL PRO ASP ARG VAL
ASP LYS ASP LYS GLU ALA THR LYS PRO GLU PHE ASN ASN HIS LYS ASP TYR ALA GLN GLU LYS PRO SER ARG LEU LYS GLN ARG PHE LEU LEU ARG ARG THR LYS ASN PRO ASP TYR SER THR SER HIS SER ALA ARG LEU THR GLU ASP VAL LEU ALA ASP ASP R1414 D1415 D1418 M1421
Y1426 Y1427 Y1428 F1433 P1434 G1435 Q1436 G1444 W1445 D1471 E1472 K1473 H1477 K1481 R1482 M1487 A1490 S1495 P1496 G1497 R1500 N1501 N1502 N1503 G1504 L1505 A1522 K1525 E1534 A1542 Q1546 S1549 P1550 N1551 V1552 F1553 Q1554 F1555 E1556 R1559 V1563 M1564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GLU GLU GLU SER ASP THR LEU GLU LYS GLU LEU SER VAL ASP ASP ALA LYS LEU GLN GLY ALA GLY GLU GLU GLU ALA LYS GLY GLY LYS ARG P1889 K1890 M1896 K1897 L1898 V1902 L1910 C1914 R1919 H1920 R1921 I1925 V1926 S1929 V1933 Q1937 D1938 N1939 R1943
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THR ILE ARG GLY ARG LEU LEU SER LEU VAL GLU LYS VAL THR TYR LEU LYS LYS LYS GLN ALA GLU LYS PRO VAL GLU SER ASP SER K2053 K2054 I2062 T2065 M2066 V2067 R2068 Q2071 E2072 R2082 L2087 Q2091 E2114 D2115 T2116 I2117 N2118 L2119 S2122 L2123 I2126
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R2303 V2319 L2323 L2324 I2325 R2326 R2327 P2328 E2329 L2335 E2338 N2341 G2342 L2343 M2347 E2348 K2352 I2353 R2359 P2362 S2363 P2364 ASN SER GLY SER SER LYS THR LEU ASP THR GLU GLU E2377 E2378 D2379 D2380 H2383 M2384 G2385 I2388 M2389 T2390 F2391 D2397
R2401 C2402 A2403 M2406 I2409 E2415 R2418 I2419 R2420 R2424 S2425 L2426 D2431 G2434 V2435 I2438 P2443 T2444 I2445 V2451 V2452 E2453 P2454 D2455 M2456 S2457 A2458 G2459 F2460 K2465 M2468 F2471 V2475 Y2476 G2477 I2478 E2479 V2480 Q2481 D2482 F2483 D2495 L2496 R2497
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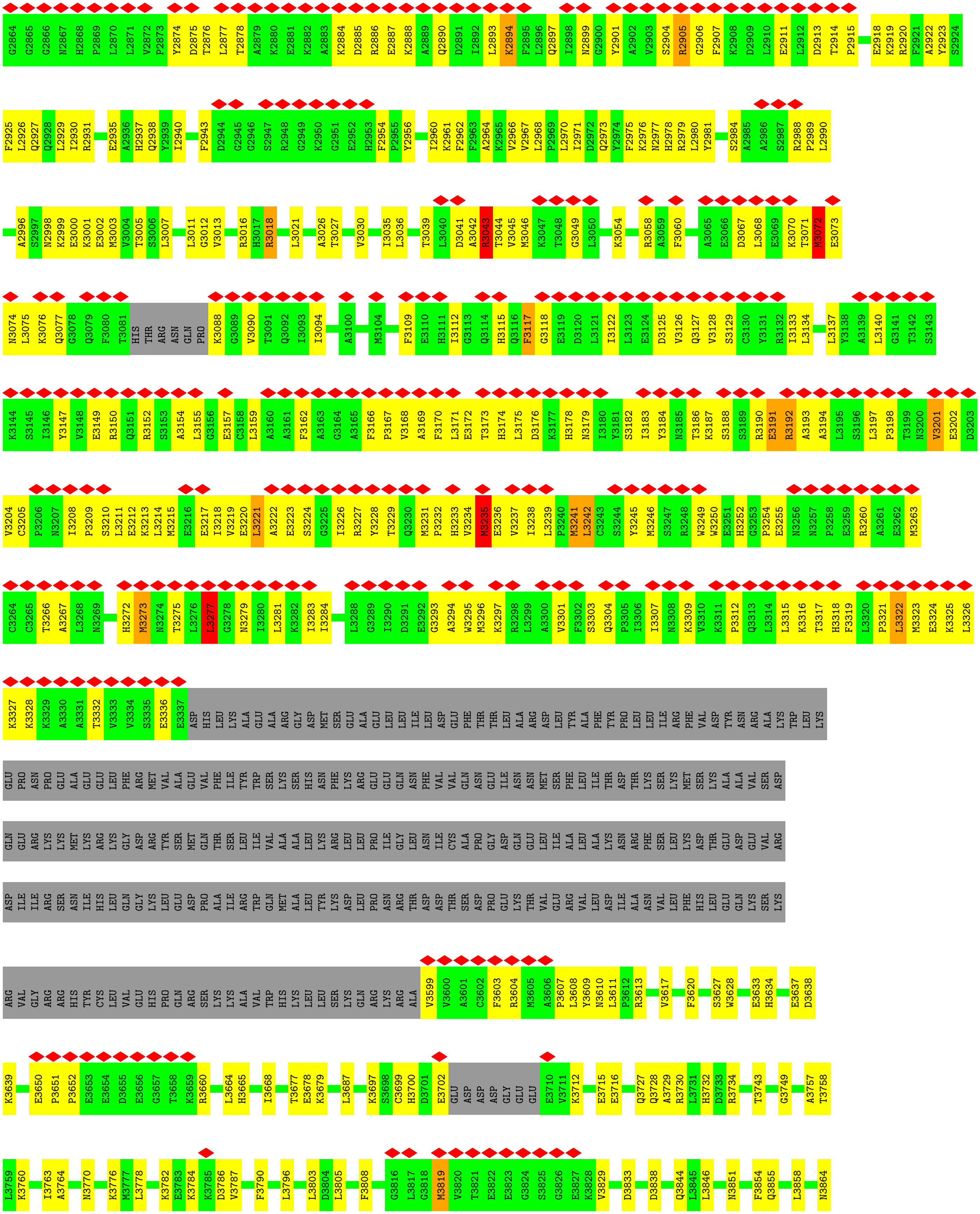
THR ARG ARG ILE SER GLN THR SER GLN VAL SER VAL ASP ALA ALA HIS G2820 Y2821 S2822 P2823 R2824 A2825 I2826 D2827 M2828 S2829 N2830 V2831 T2832 L2833 S2834 R2835 D2836 L2837 H2838 A2839 M2840 A2841 E2842 M2843 M2844 A2845 E2846 N2847 Y2848 H2849 N2850 I2851 W2852 A2853 K2854 K2855 K2856 K2857 M2858 E2859 L2860 E2861 S2862 K2863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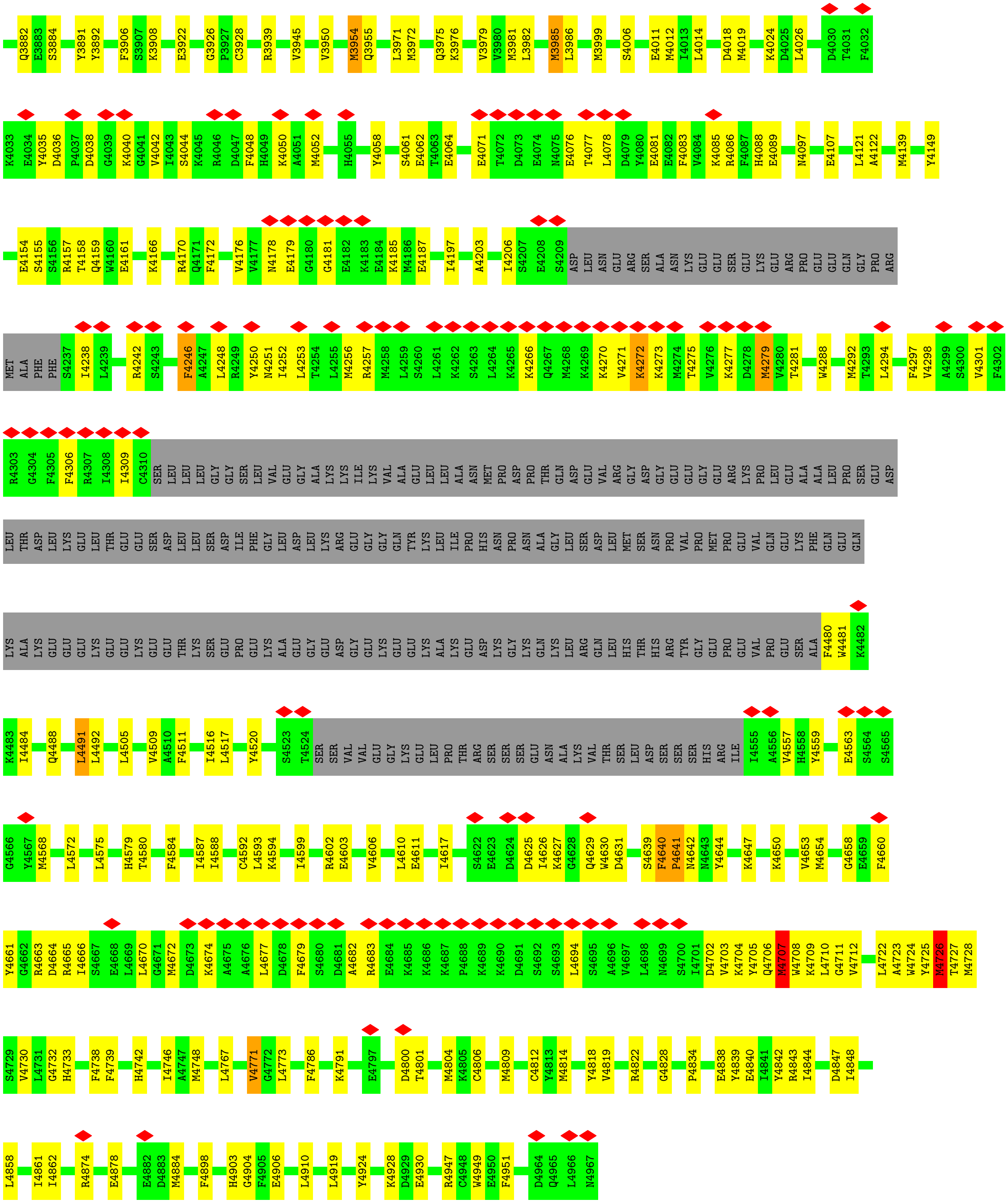
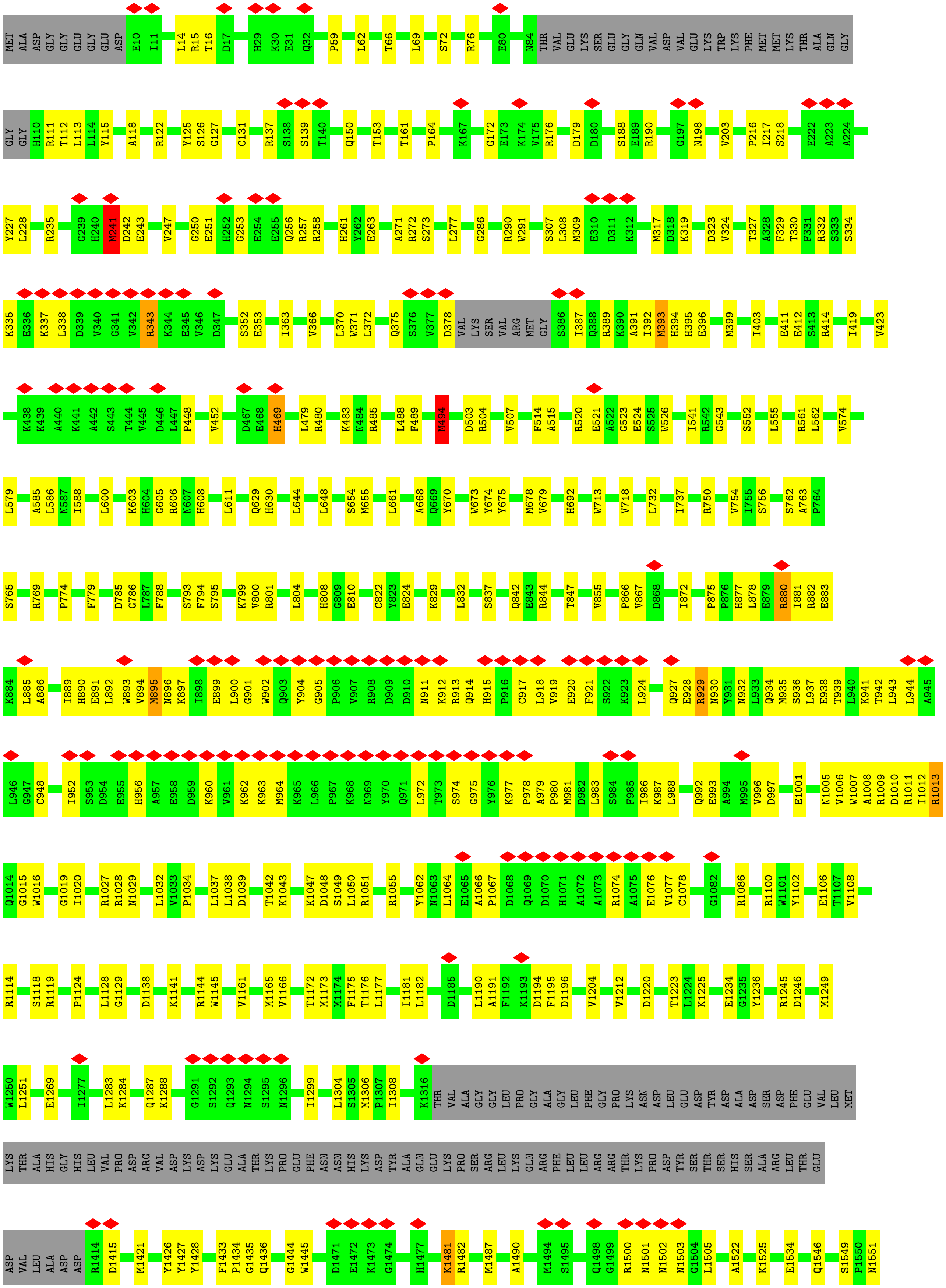
K3327 K3328 K3329 A3330 A3331 T3332 V3333 V3334 S3335 E3336 E3337 ASP HIS LEU LYS ALA GLU ALA ARG GLY ASP MET SER GLU ALA GLU LEU LEU ILE LEU ASP GLU PHE THR THR LEU ALA ARG ASP LEU TYR ALA PHE TYR PRO LEU LEU ILE ARG PHE VAL ASP TYR ASN ARG ALA LYS TRP LEU LYS
GLU PRO ASN PRO GLU ALA GLU GLU LEU PHE ARG MET VAL ALA GLU VAL PHE ILE TYR TRP SER LYS SER HIS ASN PHE LYS ARG GLU GLN ASN PHE VAL VAL GLN ASN GLU ILE ASN ASN MET SER PHE LEU ILE THR ASP THR LYS SER LYS MET SER LYS ALA ALA VAL SER ASP
GLN GLU ARG LYS LYS MET LYS ARG LYS GLY ASP ARG TYR SER MET GLN THR SER LEU ILE VAL ALA ALA LEU LYS ARG LEU LEU PRO ILE GLY LEU ASN ILE CYS ALA PRO GLY ASP GLN GLU LEU ILE ALA LEU ALA LYS ASN ARG PHE SER LEU LYS ASP THR GLU ASP GLU VAL ARG
ASP ILE ILE ARG SER ASN ILE HIS LEU GLN GLY LYS LEU GLU ASP PRO ALA ILE ARG TRP GLN MET ALA LEU TYR LYS ASP LEU PRO ASN ARG THR ASP ASP THR SER ASP PRO GLU LYS THR VAL GLU ARG VAL LEU ASP ILE ALA ASN VAL LEU PHE HIS LEU GLU GLN LYS SER LYS
ARG VAL GLY ARG ARG HIS TYR CYS LEU VAL GLU HIS PRO GLN ARG SER LYS LYS ALA VAL TRP HIS LYS LEU LEU SER LYS GLN ARG LYS ARG ALA V3599 V3600 A3601 C3602 F3603 R3604 M3605 A3606 P3607 L3608 Y3609 N3610 L3611 P3612 R3613 V3617 F3620 S3627 W3628 E3633 H3634 E3637 D3638
K3639 E3650 P3651 P3652 E3653 E3654 D3655 E3656 G3657 T3658 K3659 R3660 L3664 H3665 I3668 T3677 E3678 K3679 L3687 K3697 S3698 C3699 H3700 D3701 E3702 GLU ASP ASP ASP GLY GLU GLU E3710 V3711 K3712 E3715 E3716 Q3727 Q3728 A3729 R3730 L3731 H3732 D3733 R3734 T3743 G3749 A3757 T3758
L3759 K3760 I3763 A3764 N3770 K3776 M3777 L3778 K3782 E3783 K3784 K3785 D3786 V3787 F3790 L3796 L3803 D3804 L3805 F3808 G3816 L3817 G3818 M3819 V3820 T3821 E3822 E3823 G3824 S3825 G3826 E3827 K3828 V3829 D3833 D3838 Q3844 L3845 L3846 N3851 F3854 Q3855 L3858 N3864



- Molecule 2: Ryanodine receptor 2

Chain B: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GLY GLY H110 R111 T112 L113 L114 Y115 A118 R122 Y125 S126 G127 C131 R137 S138 S139 T140 Q150 T153 T161 P164 K167 G172 E173 K174 V175 R176 D179 D180 S188 E189 R190 G197 N198 V203 P216 I217 S218 E222 A223 A224
Y227 L228 R235 G239 H240 M241 D242 E243 V247 G250 E251 H252 G253 E254 E255 Q256 R257 R258 H261 Y262 E263 A271 R272 S273 L277 G286 R290 W291 S307 L308 M309 E310 D311 K312 M317 D318 K319 D323 V324 T327 A328 F329 T330 F331 R332 S333 S334
K335 E336 K337 L338 D339 V340 G341 V342 R343 K344 E345 V346 D347 S352 E353 I363 V366 L370 W371 L372 Q375 S376 V377 D378 VAL LYS SER VAL ARG MET GLY S386 I387 Q388 R389 K390 A391 I392 M393 H394 H395 E396 M399 I403 E411 E412 S413 R414 I419 V423
K438 K439 A440 K441 A442 S443 T444 V445 D446 L447 P448 V452 D467 E468 H469 L479 R480 K483 N484 R485 L488 F489 M494 D503 R504 V507 F514 A515 R520 E521 A522 G523 E524 S525 W526 I541 R542 G543 S552 L555 R561 L562 V574
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S765 R769 P774 F779 D785 G786 L787 F788 S793 F794 S795 K799 V800 R801 L804 H808 G809 E810 C822 Y823 E824 K829 L832 S837 Q842 E843 R844 T847 V855 P866 V867 D868 I872 P875 P876 H877 L878 E879 R880 I881 R882 E883
K884 L885 A886 I889 H890 E891 L892 W893 V894 M895 N896 K897 I898 E899 L900 G901 W902 Q903 Y904 G905 P906 V907 R908 D909 D910 N911 K912 R913 Q914 H915 P916 C917 L918 V919 E920 F921 S922 K923 L924 Q927 E928 R929 N930 Y931 N932 L933 Q934 M935 S936 L937 E938 T939 L940 K941 T942 L943 L944 A945
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Q1014 G1015 W1016 G1019 I1020 R1027 R1028 N1029 L1032 V1033 P1034 L1037 L1038 D1039 T1042 K1043 K1047 D1048 S1049 L1050 R1051 R1055 Y1062 N1063 L1064 E1065 A1066 P1067 D1068 Q1069 D1070 H1071 A1072 A1073 R1074 A1075 E1076 V1077 C1078 G1082 R1086 R1100 W1101 Y1102 E1106 T1107 V1108
R1114 S1118 R1119 P1124 L1128 G1129 D1138 K1141 R1144 W1145 V1161 M1165 V1166 T1172 M1173 M1174 F1175 T1176 L1177 I1181 L1182 D1185 L1190 A1191 F1192 K1193 D1194 F1195 D1196 V1204 V1212 D1220 T1223 L1224 K1225 E1234 G1235 Y1236 R1245 D1246 M1249
W1250 L1251 E1269 I1277 L1283 K1284 Q1287 K1288 G1291 S1292 Q1293 N1294 S1295 N1296 I1299 L1304 S1305 M1306 P1307 I1308 K1316 THR VAL ALA GLY GLY LEU PRO GLY ALA GLY LEU PHE GLY PRO LYS ASN ASP LEU GLU ASP TYR ASP ALA ASP SER ASP PHE GLU VAL LEU MET
LYS THR ALA HIS GLY HIS LEU VAL PRO ASP ARG VAL ASP LYS ASP LYS GLU ALA THR LYS PRO GLU PHE ASN ASN HIS LYS ASP TYR ALA GLN GLU LYS PRO SER ARG LEU LYS GLN ARG PHE LEU LEU ARG ARG THR LYS PRO ASP TYR SER THR SER HIS SER ALA ARG LEU THR GLU
ASP VAL LEU ALA ASP ASP R1414 D1415 M1421 Y1426 Y1427 Y1428 F1433 P1434 G1435 Q1436 G1444 W1445 D1471 E1472 K1473 G1474 H1477 K1481 R1482 M1487 A1490 M1494 S1495 Q1498 G1499 R1500 N1501 N1502 N1503 G1504 L1505 A1522 K1525 E1534 Q1546 S1549 P1550 N1551


V1552 F1553 Q1554 F1555 E1556 R1559 V1563 M1564 P1565 L1566 L1570 E1574 H1575 K1576 Q1581 R1585 V1594 P1600 F1603 R1614 L1618 V1619 Q1620 Q1626 L1630 H1656 L1660 N1669 H1670 R1671 D1681 Q1684 L1685 I1689 K1692 Y1693 M1694 L1697
L1706 Y1714 R1718 L1719 M1720 M1721 N1722 V1727 P1728 M1729 E1732 K1744 K1745 L1748 I1751 G1752 L1753 L1757 R1758 M1761 N1773 F1782 L1787 K1788 Q1793 M1794 L1795 T1796 E1797 K1800 F1825 L1828 M1831 G1832 I1833 F1834 D1838 I1842 L1843 Q1844 L1845
F1851 K1852 E1853 A1854 ALA THR PRO GLU GLU GLU SER ASP THR LEU GLU LYS GLU LEU SER VAL ASP ASP ALA LYS LEU GLN GLY ALA GLY GLU GLU GLU ALA LYS GLY GLY LYS ARG P1889 K1890 E1891 M1896 K1897 L1898 V1902 L1910 C1914 R1919 H1920 R1921 I1925 V1926
S1929 V1933 Q1937 D1938 N1939 R1943 Y1944 N1945 E1946 V1947 M1948 Q1949 A1950 L1951 S1954 A1955 A1956 L1957 T1958 A1959 R1960 K1961 T1962 K1963 E1964 F1965 R1966 S1967 Q1972 M1975 N1978 F1979 K1980 D1981 D1982 K1983 S1984 E1985 P1989 E1990 E1991 I1992 R1993 L1997 E2001 E2010 LEU ASP GLU
ASP GLY SER LEU ASP GLY ASN SER ASP LEU THR ILE ARG GLY ARG LEU LEU SER LEU VAL GLU LYS VAL THR TYR LEU LYS LYS LYS GLN ALA GLU LYS PRO VAL GLU SER ASP SER K2053 K2054 S2055 I2062 T2065 M2066 V2067 R2068 Q2071 E2072 R2082 L2087 Q2091 E2114
D2115 T2116 I2117 N2118 L2119 S2122 L2123 I2126 L2129 M2142 G2145 I2149 V2154 M2167 V2171 V2174 V2178 G2181 G2182 E2183 S2184 K2185 E2186 M2192 F2199 L2229 P2232 A2233 M2234 M2248 N2251 R2258 E2263 R2267 L2274 M2279
Y2285 W2290 G2295 E2296 R2297 R2303 V2319 L2323 L2324 I2325 R2326 R2327 P2328 E2329 L2335 E2338 N2341 G2342 L2343 M2347 E2348 K2352 I2353 R2359 P2362 S2363 P2364 ASN SER GLY SER SER LYS THR LEU ASP THR GLU GLU E2377 E2378 D2379 D2380 H2383 M2384 G2385
I2388 M2389 T2390 F2391 D2397 R2401 C2402 A2403 M2406 I2409 E2415 R2418 I2419 R2420 R2424 S2425 L2426 D2431 G2434 V2435 I2438 P2443 T2444 I2445 V2451 V2452 E2453 P2454 D2455 M2456 S2457 A2458 G2459 F2460 K2465 M2468 F2471 V2475 Y2476 G2477 I2478 E2479 V2480 Q2481
D2482 F2483 D2495 L2496 R2497 T2504 S2508 M2512 C2521 L2525 P2526 L2527 R2530 G2537 T2538 H2541 L2544 I2545 L2549 H2550 T2551 V2552 L2555 S2556 K2557 R2566 I2569 I2576 L2580 R2581 P2582 S2583 M2584 M2585 Q2586 H2587 L2588 L2589 R2590 R2591 L2592 V2593 V2596
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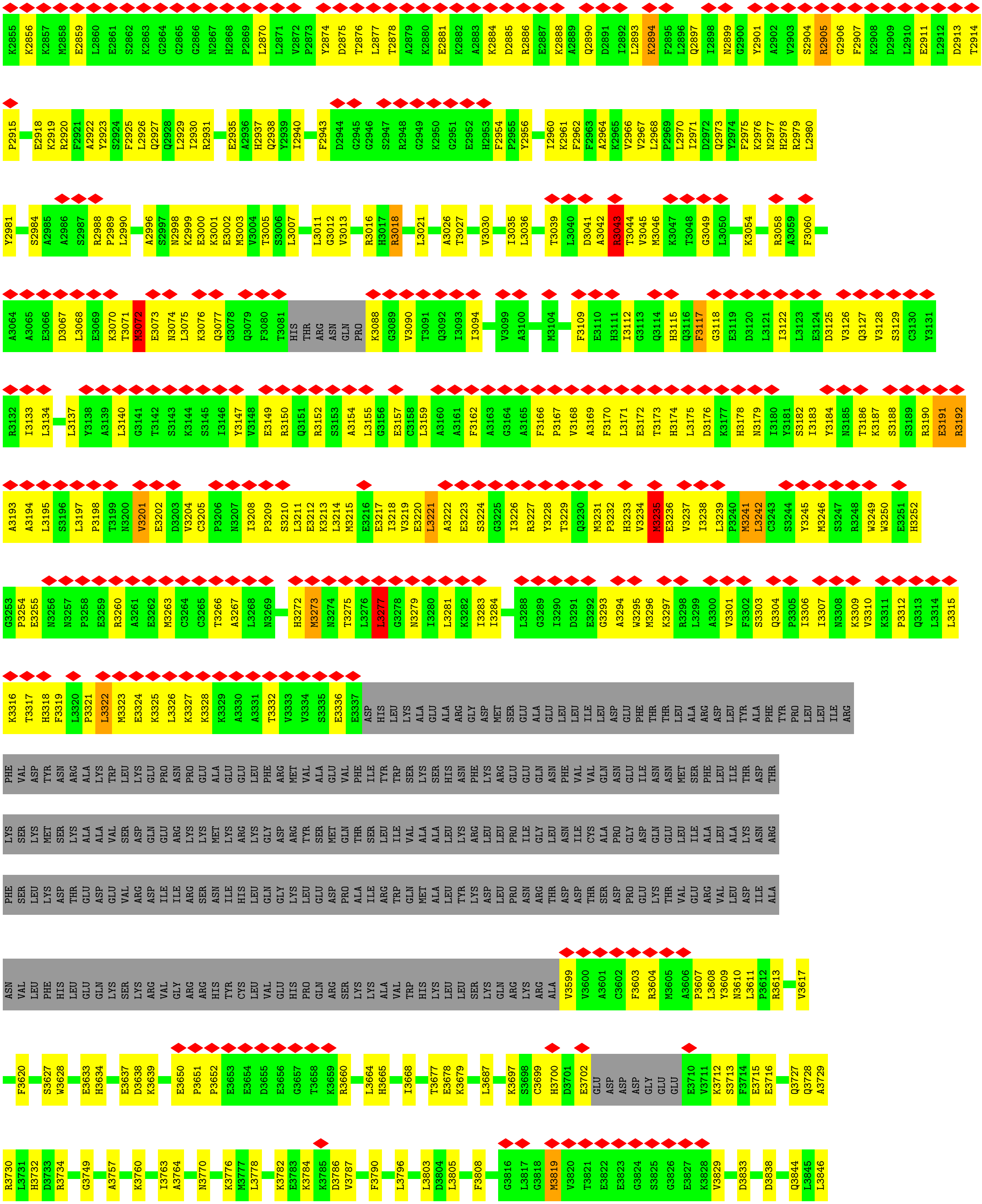
V2672 L2676 P2677 P2678 M2681 E2682 S2683 N2684 Y2685 V2686 S2687 M2688 M2689 E2690 K2691 Q2692 S2693 S2694 M2695 D2696 S2697 E2698 G2699 N2700 F2701 N2702 P2703 Q2704 P2705 V2706 D2707 T2708 S2709 N2710 I2711 T2712 I2713 P2714 E2715 K2716 L2717 E2718 Y2719 F2720 I2721 N2722 K2723 Y2724 A2725 E2726 H2727 S2728 H2729 D2730 K2731 W2732 S2733
M2734 D2735 K2736 L2737 A2738 N2739 G2740 W2741 I2742 Y2743 G2744 E2745 I2746 Y2747 S2748 D2749 S2750 S2751 K2752 V2753 Q2754 P2755 L2756 M2757 K2758 P2759 Y2760 K2761 L2762 L2763 S2764 E2765 K2766 E2767 K2768 E2769 I2770 Y2771 R2772 W2773 P2774 I2775 K2776 E2777 K2780 T2781 M2782 L2783 A2784 W2785 G2786 W2787 R2788 I2789 E2790 R2791 T2792 R2793 E2794
G2795 D2796 S2797 M2798 A2799 L2800 Y2801 N2802 ARG THR ARG ARG ILE SER GLN THR SER GLN VAL SER VAL ASP ALA ALA HIS G2820 Y2821 S2822 P2823 R2824 A2825 I2826 D2827 M2828 S2829 N2830 V2831 T2832 L2833 S2834 R2835 D2836 L2837 H2838 A2839 M2840 A2841 E2842 M2843 M2844 A2845 E2846 N2847 Y2848 H2849 N2850 I2851 W2852 A2853 K2854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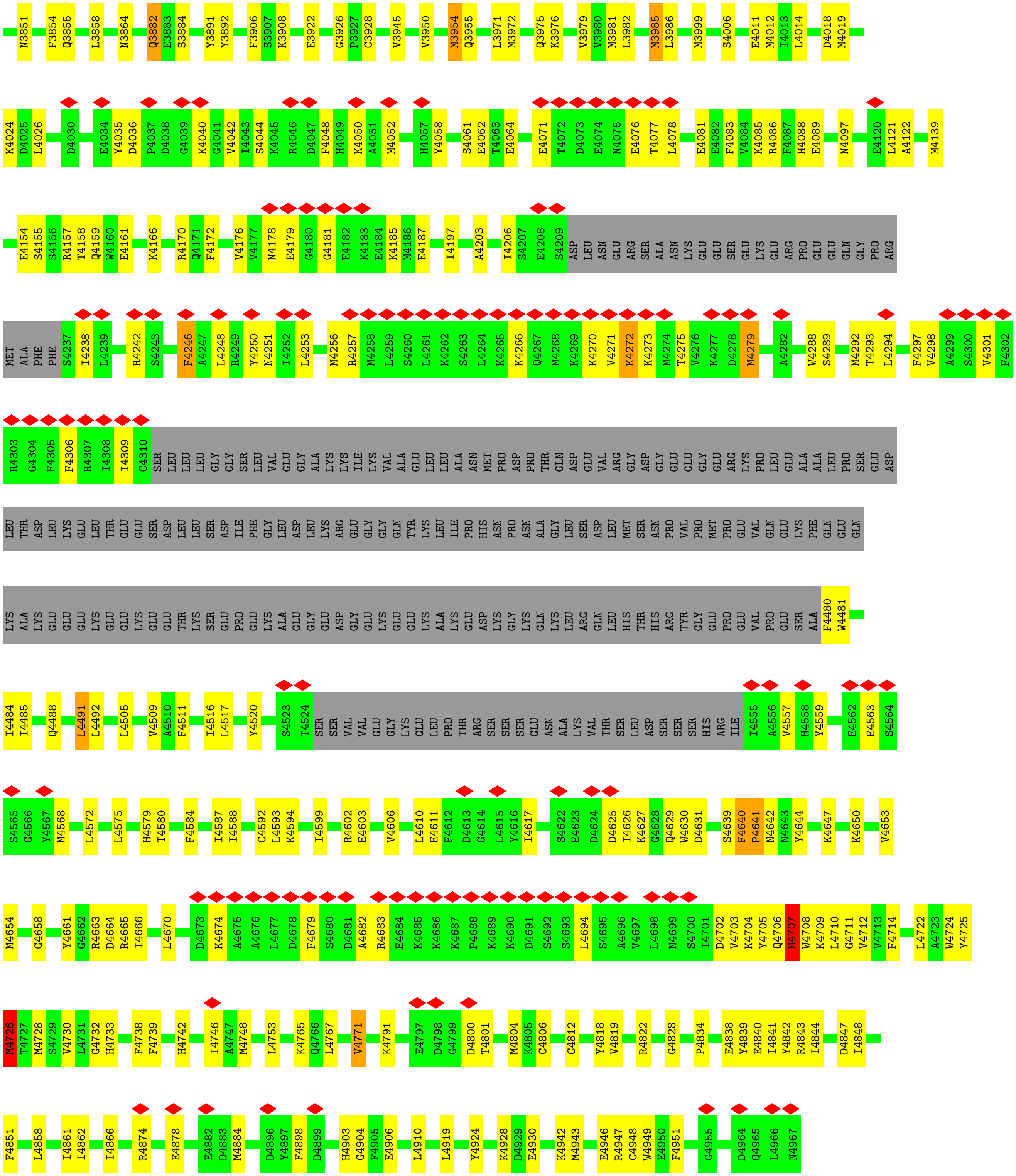
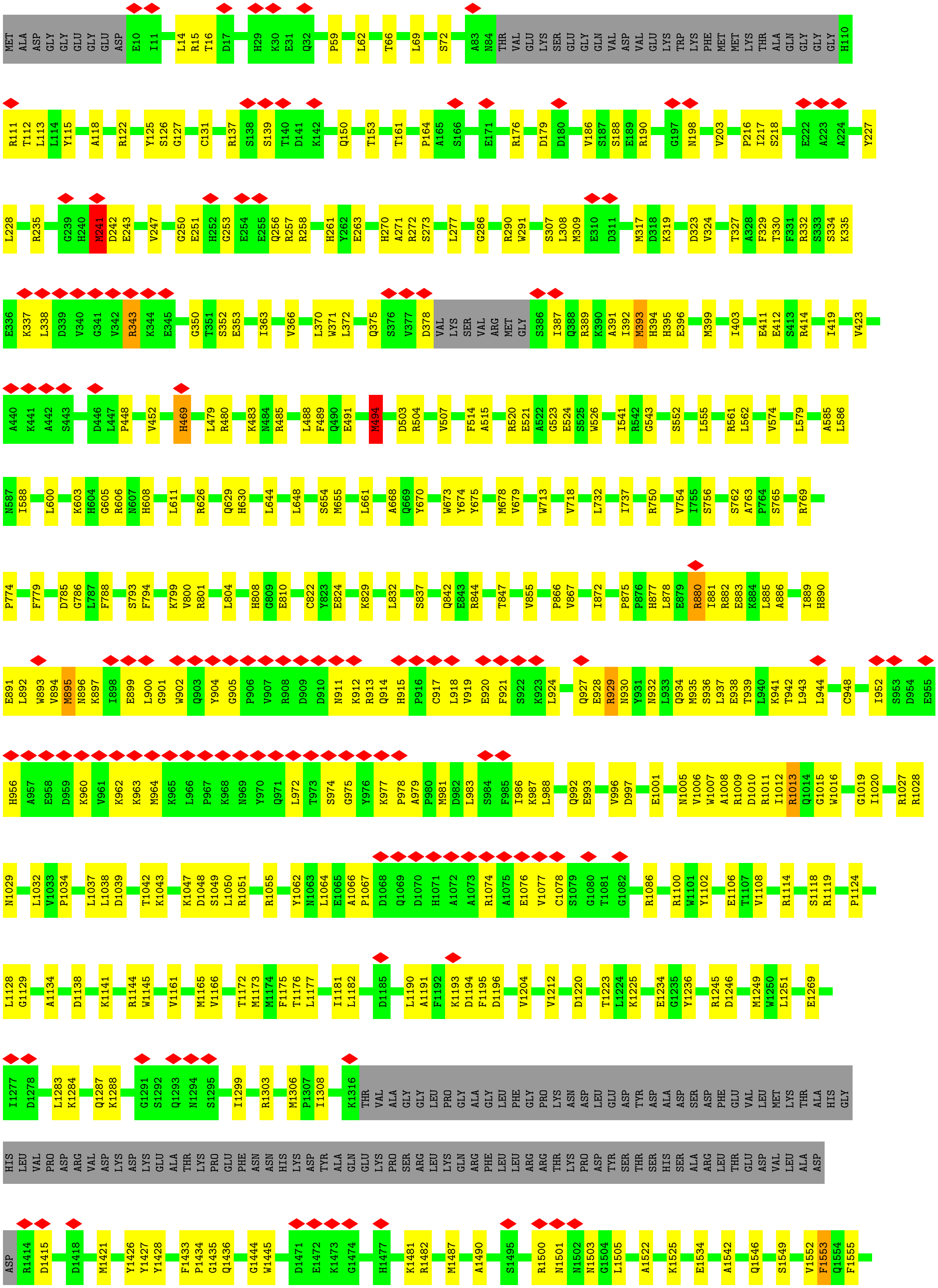
P2915 E2918 K2919 R2920 F2921 A2922 Y2923 S2924 F2925 L2926 Q2927 Q2928 L2929 I2930 R2931 E2935 A2936 H2937 Q2938 Y2939 I2940 F2943 D2944 G2945 G2946 S2947 R2948 G2949 K2950 G2951 E2952 H2953 F2954 P2955 Y2956 I2960 K2961 F2962 F2963 A2964 K2965 V2966 V2967 L2968 P2969 L2970 I2971 D2972 Q2973 Y2974 F2975 K2976 N2977 H2978 R2979 L2980
Y2981 S2984 A2985 A2986 S2987 R2988 P2989 L2990 A2996 S2997 N2998 K2999 E3000 K3001 E3002 M3003 V3004 T3005 S3006 L3007 L3011 G3012 V3013 R3016 H3017 R3018 L3021 A3026 T3027 V3030 I3035 L3036 T3039 L3040 D3041 A3042 R3043 T3044 V3045 M3046 K3047 T3048 G3049 L3050 K3054 R3058 A3059 F3060
A3064 A3065 E3066 D3067 L3068 E3069 K3070 T3071 M3072 E3073 N3074 L3075 K3076 Q3077 G3078 Q3079 F3080 T3081 HIS THR ARG ASN GLN PRO K3088 G3089 V3090 T3091 Q3092 I3093 I3094 V3099 A3100 M3104 F3109 E3110 H3111 I3112 G3113 Q3114 H3115 Q3116 F3117 G3118 E3119 D3120 L3121 I3122 L3123 E3124 D3125 V3126 Q3127 V3128 S3129 C3130 Y3131
R3132 I3133 L3134 L3137 Y3138 A3139 L3140 G3141 T3142 S3143 K3144 S3145 I3146 Y3147 V3148 E3149 R3150 Q3151 R3152 S3153 A3154 L3155 G3156 E3157 C3158 L3159 A3160 A3161 F3162 A3163 G3164 A3165 F3166 P3167 V3168 A3169 F3170 L3171 E3172 T3173 H3174 L3175 D3176 K3177 H3178 N3179 I3180 Y3181 S3182 I3183 Y3184 N3185 T3186 K3187 S3188 S3189 R3190 E3191 R3192
A3193 A3194 L3195 S3196 L3197 P3198 T3199 N3200 V3201 E3202 D3203 V3204 C3205 P3206 N3207 I3208 P3209 S3210 L3211 E3212 K3213 L3214 M3215 E3216 E3217 I3218 V3219 E3220 L3221 A3222 E3223 S3224 G3225 I3226 R3227 Y3228 T3229 Q3230 M3231 P3232 H3233 V3234 M3235 E3236 V3237 I3238 L3239 P3240 M3241 L3242 C3243 S3244 Y3245 M3246 S3247 R3248 W3249 W3250 E3251 H3252
G3253 P3254 E3255 N3256 N3257 P3258 E3259 R3260 A3261 E3262 M3263 C3264 C3265 T3266 A3267 L3268 N3269 H3272 M3273 N3274 T3275 L3276 L3277 G3278 N3279 I3280 L3281 K3282 I3283 I3284 L3288 G3289 I3290 D3291 E3292 G3293 A3294 W3295 M3296 K3297 R3298 L3299 A3300 V3301 F3302 S3303 Q3304 P3305 I3306 I3307 N3308 K3309 V3310 K3311 P3312 Q3313 L3314 L3315
K3316 T3317 H3318 F3319 L3320 P3321 L3322 M3323 E3324 K3325 L3326 K3327 K3328 K3329 A3330 A3331 T3332 V3333 V3334 S3335 E3336 E3337 ASP HIS LEU LYS ALA GLU ALA ARG GLY ASP MET SER GLU ALA GLU LEU ILE LEU ASP GLU PHE THR THR LEU ALA ARG ASP LEU TYR ALA PHE TYR PRO LEU LEU ILE ARG
PHE VAL ASP TYR ASN ARG ALA LYS TRP LEU LYS GLU PRO ASN PRO GLU ALA GLU GLU LEU PHE ARG MET VAL ALA GLU VAL PHE ILE TYR TRP SER LYS SER HIS ASN PHE LYS ARG GLU GLU GLN ASN PHE VAL VAL GLN ASN GLU ILE ASN ASN MET SER PHE LEU ILE THR ASP THR
LYS SER LYS MET SER LYS ALA ALA ALA VAL SER ASP GLN GLU ARG LYS LYS MET LYS ARG LYS GLY ASP ARG TYR SER MET GLN THR SER ILE ILE VAL ALA ALA LEU LYS ARG LEU LEU PRO ILE GLY LEU ASN ILE CYS ALA PRO GLY ASP GLN GLU LEU ILE ALA LEU ALA LYS ASN ARG
PHE SER LEU LYS ASP THR GLU ASP GLU VAL ARG ASP ILE ILE ARG SER ASN ILE HIS LEU GLN GLY LYS LEU GLU ASP PRO ALA ILE ARG TRP GLN MET ALA LEU TYR LYS ASP LEU PRO ASN ARG THR ASP ASP THR SER ASP PRO GLU LYS THR VAL GLU ARG VAL LEU ASP ILE ALA
ASN VAL LEU PHE HIS LEU GLU GLN LYS SER LYS ARG VAL GLY ARG ARG HIS TYR CYS LEU VAL GLU HIS PRO GLN ARG SER LYS LYS ALA VAL TRP HIS LYS LEU LEU SER LYS GLN ARG LYS ARG ALA V3599 V3600 A3601 C3602 F3603 R3604 M3605 A3606 P3607 L3608 Y3609 N3610 L3611 P3612 R3613 V3617
F3620 S3627 W3628 E3633 H3634 E3637 D3638 K3639 E3650 P3651 P3652 E3653 E3654 D3655 E3656 G3657 T3658 K3659 R3660 L3664 H3665 I3668 T3677 E3678 K3679 L3687 K3697 S3698 C3699 H3700 D3701 E3702 GLU ASP ASP ASP GLY GLU GLU E3710 V3711 K3712 S3713 F3714 E3715 E3716 Q3727 Q3728 A3729
R3730 L3731 H3732 D3733 R3734 G3749 A3757 K3760 I3763 A3764 N3770 K3776 M3777 L3778 K3782 E3783 K3784 K3785 D3786 V3787 F3790 L3796 L3803 D3804 L3805 F3808 G3816 L3817 G3818 M3819 V3820 T3821 E3822 E3823 G3824 S3825 G3826 E3827 K3828 V3829 D3833 D3838 Q3844 L3845 L3846



- Molecule 2: Ryanodine receptor 2

Chain C: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R111 T112 L113 L114 Y115 A118 R122 Y125 S126 G127 C131 R137 S138 S139 T140 D141 K142 Q150 T153 T161 P164 A165 S166 E171 R176 D179 D180 V186 S187 S188 E189 R190 G197 N198 V203 P216 I217 S218 E222 A223 A224 Y227
L228 R235 G239 H240 M241 D242 E243 V247 G250 E251 H252 G253 E254 E255 Q256 R257 R258 H261 Y262 E263 H270 A271 R272 S273 L277 G286 R290 W291 S307 L308 M309 E310 D311 M317 D318 K319 D323 V324 T327 A328 F329 T330 F331 R332 S333 S334 K335
E336 K337 L338 D339 V340 G341 V342 R343 K344 E345 G350 T351 S352 E353 I363 V366 L370 W371 L372 Q375 S376 V377 D378 VAL LYS SER VAL ARG MET GLY S386 I387 Q388 R389 K390 A391 I392 M393 H394 H395 E396 M399 I403 E411 E412 S413 R414 I419 V423
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N587 I588 L600 K603 H604 G605 R606 N607 H608 L611 R626 Q629 H630 L644 L648 S654 M655 L661 A668 Q669 Y670 W673 Y674 Y675 M678 V679 W713 V718 L732 I737 R750 V754 I755 S756 S762 A763 P764 S765 R769
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E891 L892 W893 V894 M895 N896 K897 I898 E899 L900 G901 W902 Q903 Y904 G905 P906 V907 R908 D909 D910 N911 K912 R913 Q914 H915 P916 C917 L918 V919 E920 F921 S922 K923 L924 Q927 E928 R929 N930 Y931 N932 L933 Q934 M935 S936 L937 E938 T939 L940 K941 T942 L943 L944 C948 I952 S953 D954 E955
H956 A957 E958 D959 K960 V961 K962 K963 M964 K965 L966 P967 K968 N969 Y970 Q971 L972 T973 S974 G975 Y976 K977 P978 A979 P980 M981 D982 L983 S984 F985 I986 K987 L988 Q992 E993 V996 D997 E1001 N1005 V1006 W1007 A1008 R1009 D1010 R1011 I1012 R1013 Q1014 G1015 W1016 G1019 I1020 R1027 R1028
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L1128 G1129 A1134 D1138 K1141 R1144 W1145 V1161 M1165 V1166 T1172 M1173 M1174 F1175 T1176 L1177 I1181 L1182 D1185 L1190 A1191 F1192 K1193 D1194 F1195 D1196 V1204 V1212 D1220 T1223 L1224 K1225 E1234 G1235 Y1236 R1245 D1246 M1249 W1250 L1251 E1269
I1277 D1278 L1283 K1284 Q1287 K1288 G1291 S1292 Q1293 N1294 S1295 I1299 R1303 M1306 P1307 I1308 K1316 THR VAL ALA GLY GLY LEU PRO GLY ALA GLY LEU PHE GLY PRO LYS ASN ASP LEU GLU ASP TYR ASP ALA ASP SER ASP PHE GLU VAL LEU MET LYS THR ALA HIS GLY
HIS LEU VAL PRO ASP ARG VAL ASP LYS ASP LYS GLU ALA THR LYS PRO GLU PHE ASN ASN HIS LYS ASP TYR ALA GLN GLU LYS PRO SER ARG LEU LYS GLN ARG PHE LEU LEU ARG ARG THR LYS PRO ASP TYR SER THR SER HIS SER ALA ARG LEU THR GLU ASP VAL LEU ALA ASP
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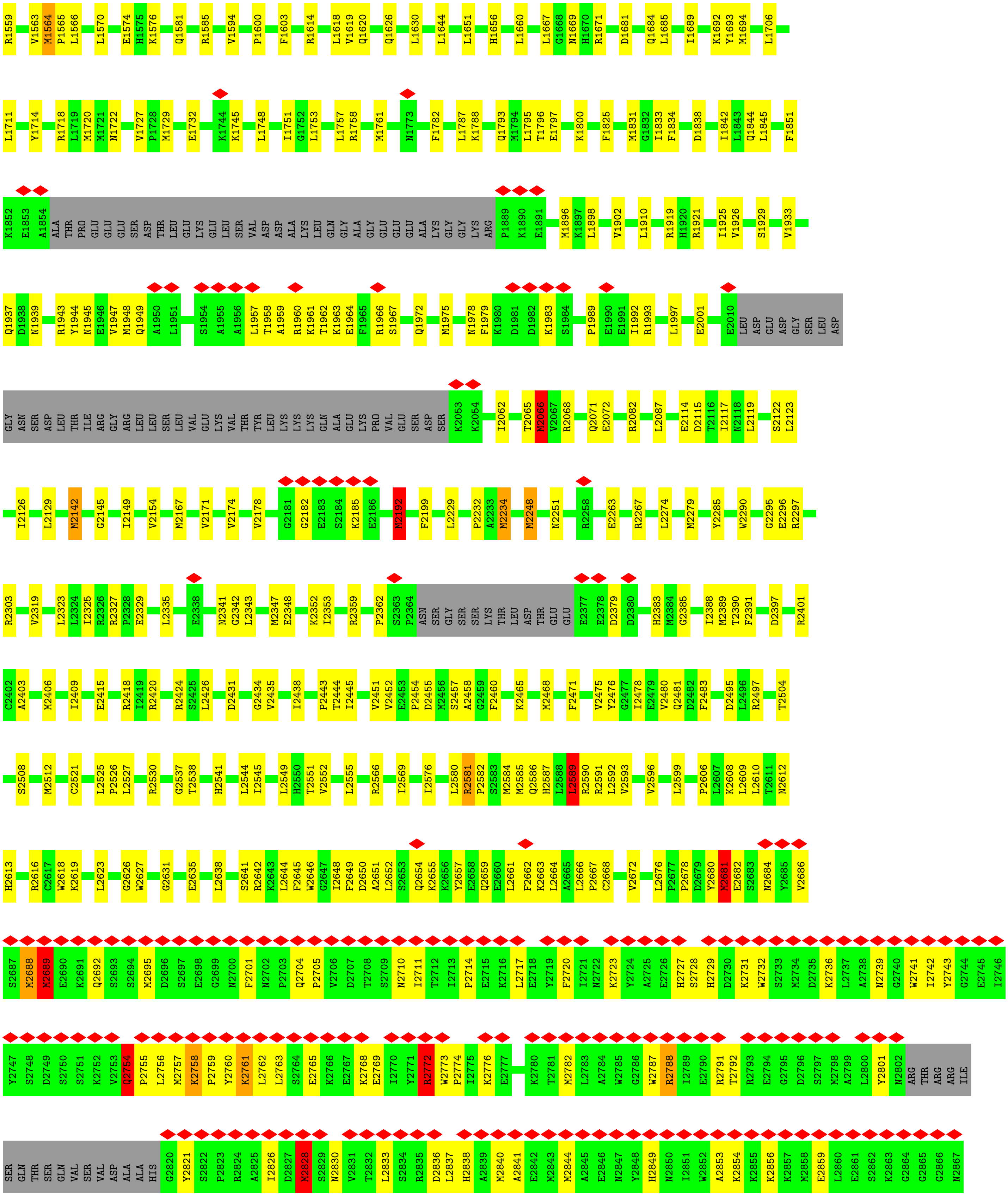
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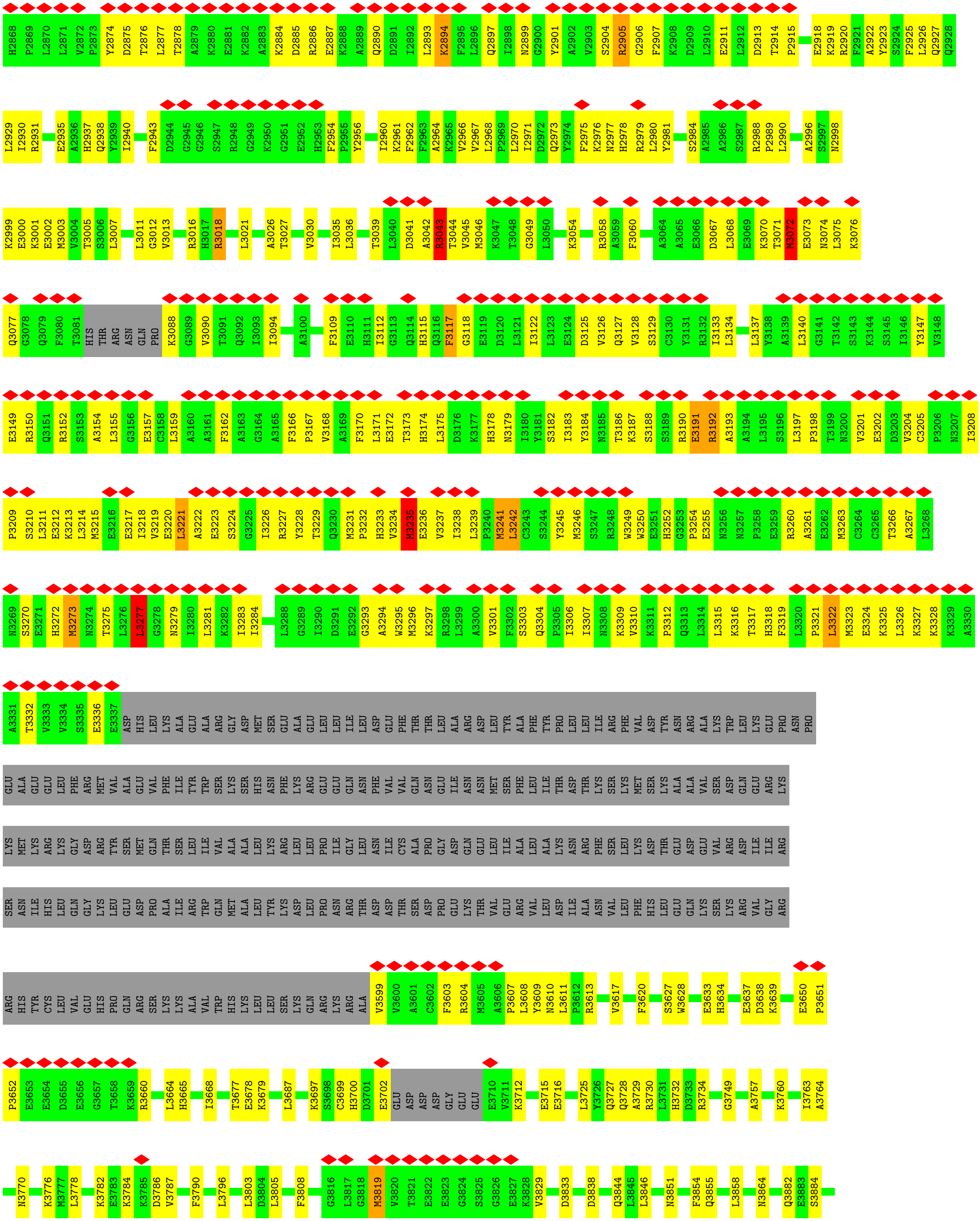
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GLU ALA GLU GLU LEU PHE ARG MET VAL ALA GLU VAL PHE ILE TYR TRP SER LYS SER HIS ASN PHE LYS ARG GLU GLU GLN ASN PHE VAL VAL GLN ASN GLU ILE ASN ASN MET SER PHE LEU ILE THR ASP THR LYS SER LYS MET SER LYS ALA ALA VAL SER ASP GLN GLU ARG LYS
LYS MET LYS ARG LYS GLY ASP ARG TYR SER MET GLN THR SER LEU ILE VAL ALA ALA LEU LYS ARG LEU LEU PRO ILE GLY LEU ASN ILE CYS ALA PRO GLY ASP GLN GLU LEU ILE ALA LEU ALA LYS ASN ARG PHE SER LEU LYS ASP THR GLU ASP GLU VAL ARG ASP ILE ARG
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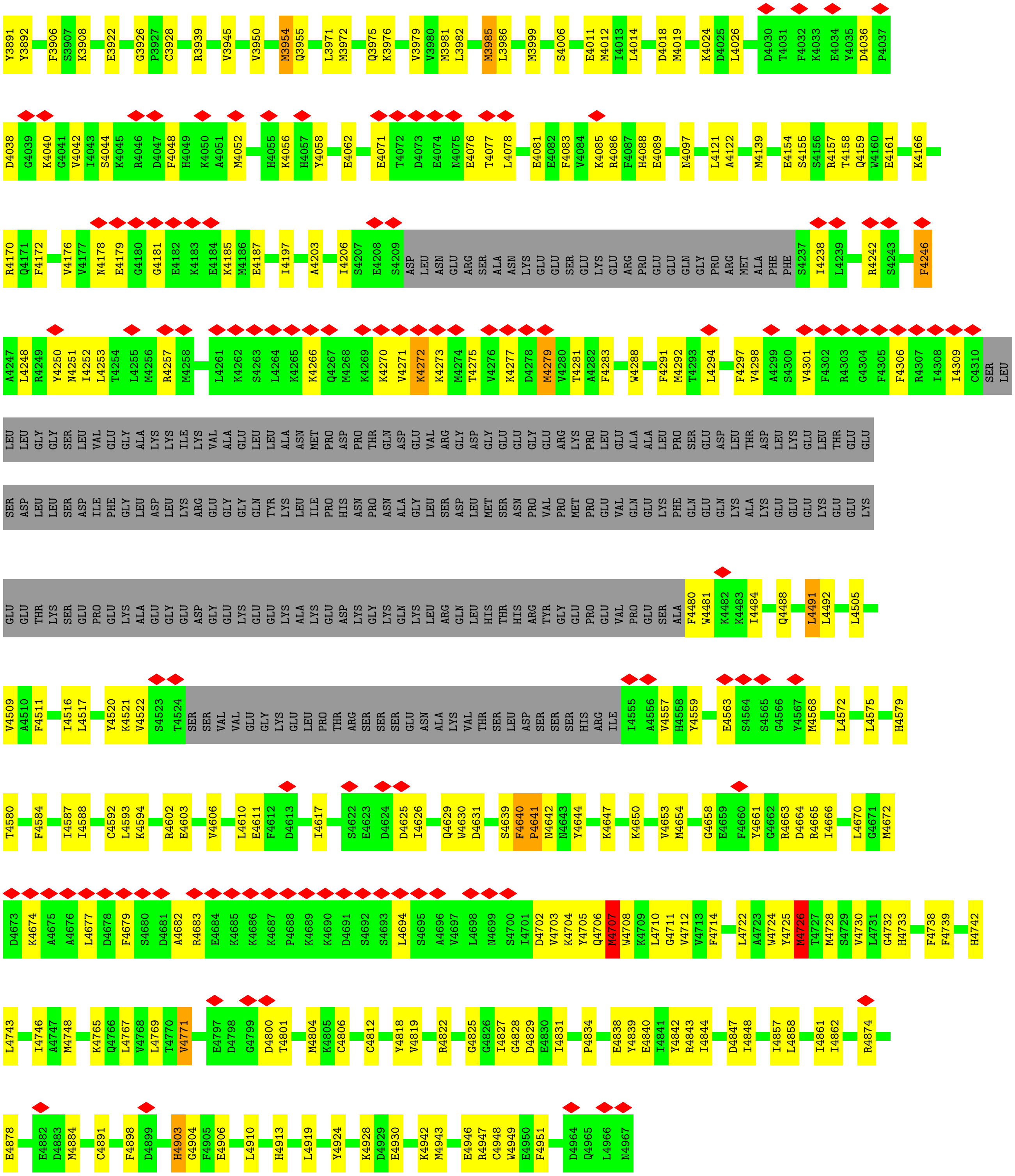
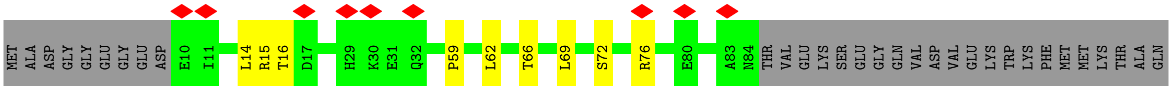
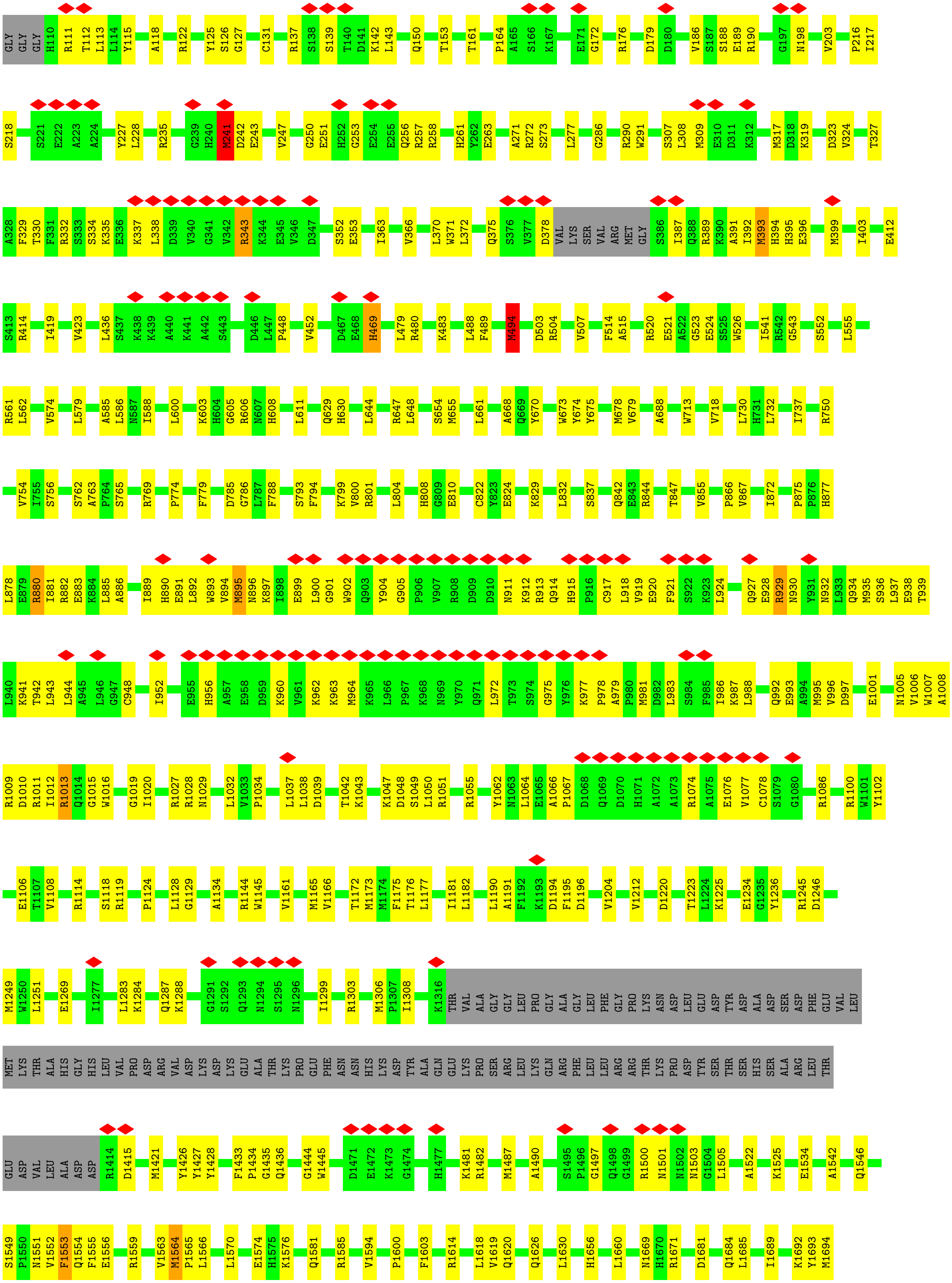


- Molecule 2: Ryanodine receptor 2

Chain D:

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MET LYS THR ALA HIS GLY HIS LEU VAL PRO ASP ARG VAL ASP LYS ASP LYS GLU ALA THR LYS PRO GLU PHE ASN ASN HIS LYS ASP TYR ALA GLN GLU LYS PRO SER ARG LEU LYS GLN ARG PHE LEU LEU ARG ARG THR LYS PRO ASP TYR SER THR SER HIS SER ALA ARG LEU THR
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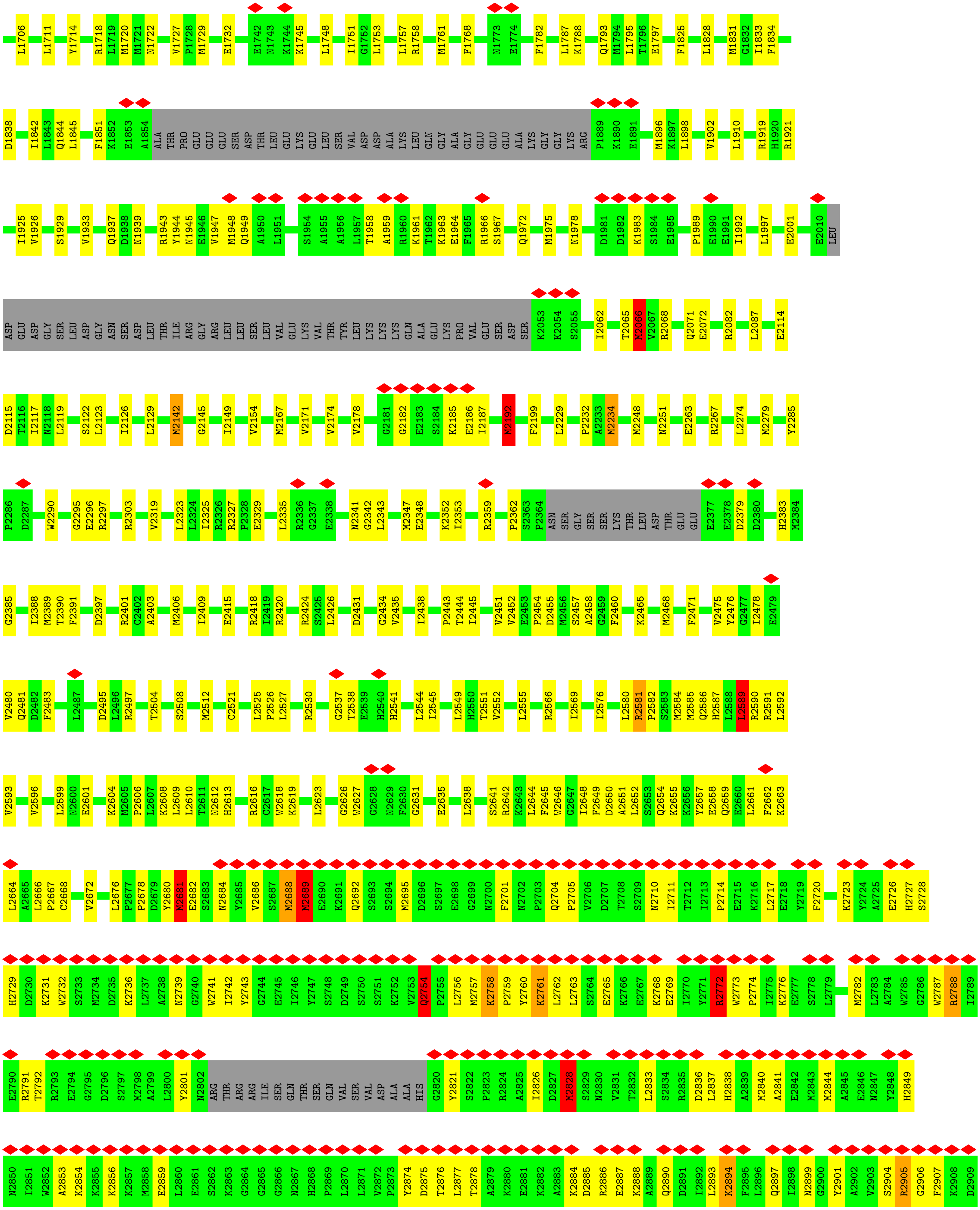
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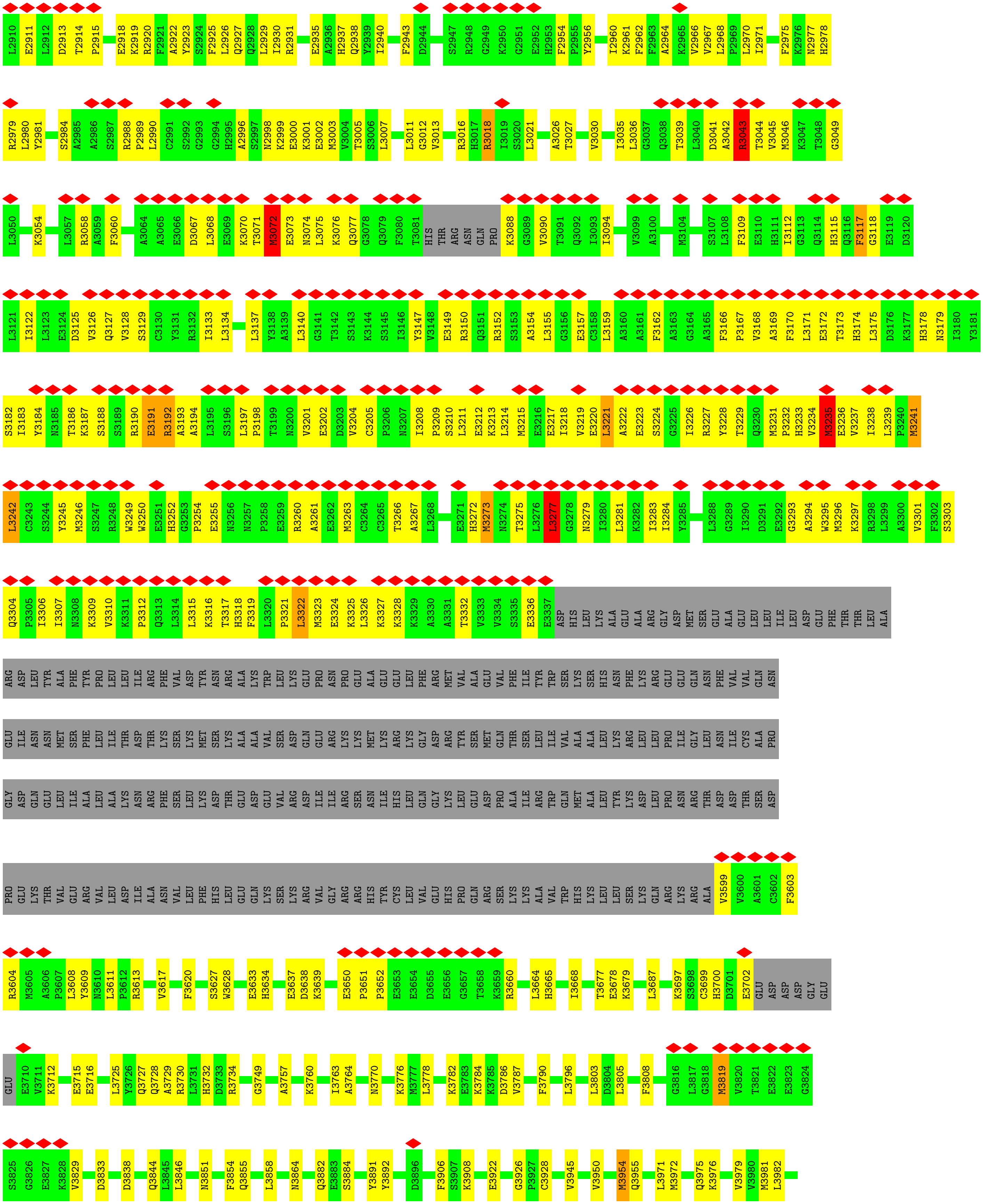
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R2979 L2980 Y2981 S2984 A2985 A2986 S2987 R2988 P2989 L2990 C2991 S2992 G2993 G2994 H2995 A2996 S2997 N2998 K2999 E3000 K3001 E3002 M3003 V3004 T3005 S3006 L3007 L3011 G3012 V3013 R3016 H3017 R3018 I3019 S3020 L3021 A3026 T3027 V3030 I3035 L3036 G3037 Q3038 T3039 L3040 D3041 A3042 R3043 T3044 V3045 M3046 K3047 T3048 G3049
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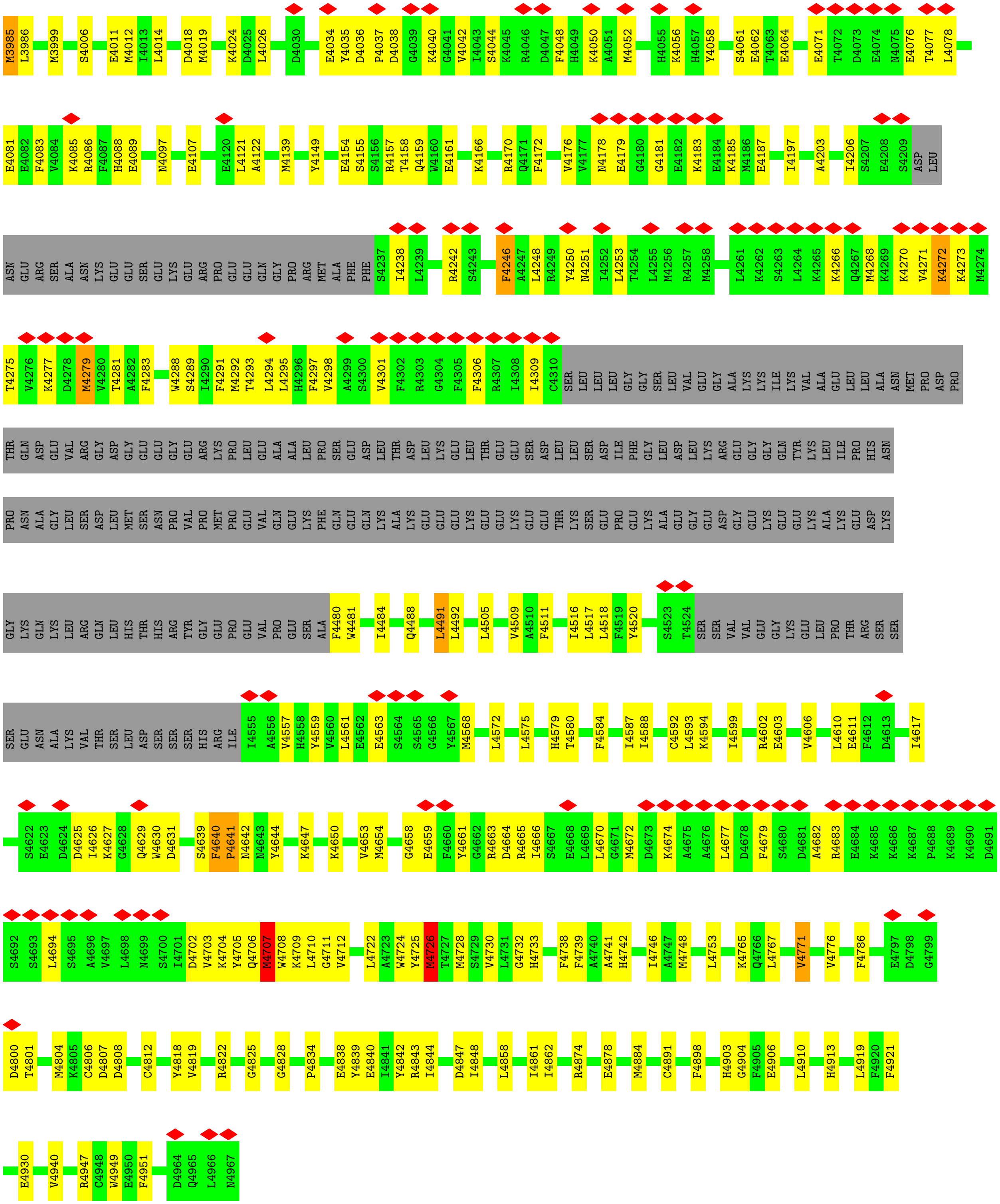
L3121 I3122 L3123 E3124 D3125 V3126 Q3127 V3128 S3129 C3130 Y3131 R3132 I3133 L3134 L3137 Y3138 A3139 L3140 G3141 T3142 S3143 K3144 S3145 I3146 Y3147 V3148 E3149 R3150 Q3151 R3152 S3153 A3154 L3155 G3156 E3157 C3158 L3159 A3160 A3161 F3162 A3163 G3164 A3165 F3166 P3167 V3168 A3169 F3170 L3171 E3172 T3173 H3174 L3175 D3176 K3177 H3178 N3179 I3180 Y3181
S3182 I3183 Y3184 N3185 T3186 K3187 S3188 S3189 R3190 E3191 R3192 A3193 A3194 L3195 S3196 L3197 P3198 T3199 N3200 V3201 E3202 D3203 V3204 C3205 P3206 N3207 I3208 P3209 S3210 L3211 E3212 K3213 L3214 M3215 E3216 E3217 I3218 V3219 E3220 L3221 A3222 E3223 S3224 G3225 I3226 R3227 Y3228 T3229 Q3230 M3231 P3232 H3233 V3234 M3235 E3236 V3237 I3238 L3239 P3240 M3241
L3242 C3243 S3244 Y3245 M3246 S3247 R3248 W3249 W3250 E3251 H3252 G3253 P3254 E3255 N3256 N3257 P3258 E3259 R3260 A3261 E3262 M3263 C3264 C3265 T3266 A3267 L3268 E3271 H3272 M3273 N3274 T3275 L3276 L3277 G3278 N3279 I3280 L3281 K3282 I3283 I3284 Y3285 L3288 G3289 I3290 D3291 E3292 G3293 A3294 W3295 M3296 K3297 R3298 L3299 A3300 V3301 F3302 S3303
Q3304 P3305 I3306 I3307 N3308 K3309 V3310 K3311 P3312 Q3313 L3314 L3315 K3316 T3317 H3318 F3319 L3320 P3321 L3322 M3323 E3324 K3325 L3326 K3327 K3328 K3329 A3330 A3331 T3332 V3333 V3334 S3335 E3336 E3337 ASP HIS LEU LYS ALA GLU ALA ARG GLY ASP MET SER GLU ALA GLU LEU LEU ILE LEU ASP GLU PHE THR THR LEU ALA
ARG ASP LEU TYR ALA PHE TYR PRO LEU LEU ILE ARG PHE VAL ASP TYR ASN ARG ALA LYS TRP LEU LYS GLU PRO ASN PRO GLU ALA GLU GLU LEU PHE ARG MET VAL ALA GLU VAL PHE ILE TYR SER LYS SER HIS ASN PHE LYS ARG GLU GLU GLN ASN PHE VAL VAL GLN ASN
GLU ILE ASN ASN MET SER PHE LEU ILE THR ASP THR LYS SER LYS MET SER LYS ALA ALA VAL SER ASP GLN GLU ARG LYS LYS MET LYS ARG LYS GLY ASP ARG TYR SER MET GLN THR SER LEU ILE VAL ALA ALA LEU LYS ARG LEU LEU PRO ILE GLY LEU ASN ILE CYS ALA PRO
GLY ASP GLN GLU LEU ILE ALA LEU ALA LYS ASN ARG PHE SER LEU LYS ASP THR GLU ASP GLU VAL ARG ASP ILE ILE ARG SER ASN ILE HIS LEU GLN GLY LYS LEU GLU ASP PRO ALA ILE ARG TRP GLN MET ALA LEU TYR LYS ASP LEU PRO ASN ARG THR ASP ASP THR SER ASP
PRO GLU LYS THR VAL GLU ARG VAL LEU ASP ILE ALA ASN VAL LEU PHE HIS LEU GLU GLN LYS SER LYS ARG VAL GLY ARG ARG HIS TYR CYS LEU VAL GLU HIS PRO GLN ARG SER LYS LYS ALA VAL TRP HIS LYS LEU LEU SER LYS GLN ARG LYS ARG ALA V3599 V3600 A3601 C3602 F3603
R3604 M3605 A3606 P3607 L3608 Y3609 N3610 L3611 P3612 R3613 V3617 F3620 S3627 W3628 E3633 H3634 E3637 D3638 K3639 E3650 P3651 P3652 E3653 E3654 D3655 E3656 G3657 T3658 K3659 R3660 L3664 H3665 I3668 T3677 E3678 K3679 L3687 K3697 S3698 C3699 H3700 D3701 E3702 GLU ASP ASP ASP GLY GLU
GLU E3710 V3711 K3712 E3715 E3716 L3725 Y3726 Q3727 Q3728 A3729 R3730 L3731 H3732 D3733 R3734 G3749 A3757 K3760 I3763 A3764 N3770 K3776 M3777 L3778 K3782 E3783 K3784 K3785 D3786 V3787 F3790 L3796 L3803 D3804 L3805 F3808 G3816 L3817 G3818 M3819 V3820 T3821 E3822 E3823 G3824
S3825 G3826 E3827 K3828 V3829 D3833 D3838 Q3844 L3845 L3846 N3851 F3854 Q3855 L3858 N3864 Q3882 E3883 S3884 Y3891 Y3892 D3896 F3906 S3907 K3908 E3922 G3926 P3927 C3928 V3945 V3950 M3954 Q3955 L3971 M3972 Q3975 K3976 V3979 V3980 M3981 L3982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E4081 E4082 F4083 V4084 K4085 R4086 F4087 H4088 E4089 N4097 E4107 E4120 L4121 A4122 M4139 Y4149 E4154 S4155 S4156 R4157 T4158 Q4159 W4160 E4161 K4166 R4170 Q4171 F4172 V4176 V4177 N4178 E4179 G4180 G4181 E4182 K4183 E4184 K4185 M4186 E4187 I4197 A4203 I4206 S4207 E4208 S4209 ASP LEU
ASN GLU ARG SER ALA ASN LYS GLU GLU SER GLU LYS GLU ARG PRO GLU GLN GLN GLY PRO ARG MET ALA PHE PHE S4237 I4238 L4239 R4242 S4243 F4246 A4247 L4248 R4249 Y4250 N4251 I4252 L4253 T4254 L4255 M4256 R4257 M4258 L4261 K4262 S4263 L4264 K4265 K4266 Q4267 M4268 K4269 K4270 V4271 K4272 K4273 M4274
T4275 V4276 K4277 D4278 M4279 V4280 T4281 A4282 F4283 W4288 S4289 I4290 F4291 M4292 T4293 L4294 L4295 H4296 F4297 V4298 A4299 S4300 V4301 F4302 R4303 G4304 F4305 F4306 R4307 I4308 I4309 C4310 SER LEU LEU LEU GLY GLY SER LEU VAL GLU GLY ALA LYS LYS ILE LYS VAL ALA GLU LEU LEU ALA ASN MET PRO ASP PRO
THR GLN ASP GLU VAL ARG GLY ASP GLY GLU GLU GLY GLU ARG LYS PRO LEU GLU ALA ALA LEU PRO SER GLU ASP LEU THR ASP LEU LYS GLU LEU THR GLU GLU SER ASP LEU LEU SER ASP ILE PHE GLY LEU ASP LEU LYS ARG GLU GLY GLY GLN TYR LYS LEU ILE PRO HIS ASN
PRO ASN ALA GLY LEU SER SER ASP LEU MET SER ASN PRO VAL PRO MET PRO GLU VAL GLN GLU LYS PHE GLN GLU GLN LYS ALA LYS GLU GLU LYS GLU GLU LYS GLU GLU THR LYS SER GLU PRO GLU LYS ALA GLU GLY GLU ASP GLY GLU LYS GLU GLU LYS ALA LYS GLU ASP LYS
GLY LYS GLN LYS LEU ARG GLN LEU HIS THR HIS ARG TYR GLY GLU PRO GLU VAL PRO GLU SER ALA F4480 W4481 I4484 Q4488 L4491 L4492 L4505 V4509 A4510 F4511 I4516 L4517 L4518 F4519 Y4520 S4523 T4524 SER SER VAL VAL GLU GLY LYS GLU LEU PRO THR ARG SER SER
SER GLU ASN ALA LYS VAL THR SER LEU ASP SER SER SER HIS ARG ILE I4555 A4556 V4557 H4558 Y4559 V4560 L4561 E4562 E4563 S4564 S4565 G4566 Y4567 M4568 L4572 L4575 H4579 T4580 F4584 I4587 I4588 C4592 L4593 K4594 I4599 R4602 E4603 V4606 L4610 E4611 F4612 D4613 I4617
S4622 E4623 D4624 D4625 I4626 K4627 G4628 Q4629 W4630 D4631 S4639 F4640 P4641 N4642 N4643 Y4644 K4647 K4650 V4653 M4654 G4658 E4659 F4660 Y4661 G4662 R4663 D4664 R4665 I4666 S4667 E4668 L4669 L4670 G4671 M4672 D4673 K4674 A4675 A4676 L4677 D4678 F4679 S4680 D4681 A4682 R4683 E4684 K4685 K4686 K4687 P4688 K4689 K4690 D4691
S4692 S4693 L4694 S4695 A4696 V4697 L4698 N4699 S4700 I4701 D4702 V4703 K4704 Y4705 Q4706 M4707 W4708 K4709 L4710 G4711 V4712 L4722 A4723 W4724 Y4725 M4726 T4727 M4728 S4729 V4730 L4731 G4732 H4733 F4738 F4739 A4740 A4741 H4742 I4746 A4747 M4748 L4753 K4765 Q4766 L4767 V4771 V4776 F4786 E4797 D4798 G4799
D4800 T4801 M4804 K4805 C4806 D4807 D4808 C4812 Y4818 V4819 R4822 G4825 G4828 P4834 E4838 Y4839 E4840 I4841 Y4842 R4843 I4844 D4847 I4848 L4858 I4861 I4862 R4874 E4878 M4884 C4891 F4898 H4903 G4904 F4905 E4906 L4910 H4913 L4919 F4920 F4921
E4930 V4940 R4947 C4948 W4949 E4950 F4951 D4964 Q4965 L4966 N4967

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	36491	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	58	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.549	Depositor
Minimum map value	-0.006	Depositor
Average map value	0.012	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.13	Depositor
Map size (Å)	428.544, 428.544, 428.544	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.837, 0.837, 0.837	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CA, ZN, XAN, ATP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	E	0.28	0/834	0.60	0/1123
1	F	0.27	0/834	0.60	0/1123
1	G	0.28	0/834	0.61	0/1123
1	H	0.27	0/834	0.61	0/1123
2	A	0.58	8/34511 (0.0%)	0.56	33/46614 (0.1%)
2	B	0.58	8/34511 (0.0%)	0.56	32/46614 (0.1%)
2	C	0.58	8/34511 (0.0%)	0.56	33/46614 (0.1%)
2	D	0.58	8/34511 (0.0%)	0.56	33/46614 (0.1%)
All	All	0.57	32/141380 (0.0%)	0.56	131/190948 (0.1%)

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
2	A	0	7
2	B	0	7
2	C	0	7
2	D	0	7
All	All	0	28

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3117	PHE	CD1-CE1	43.66	2.26	1.39
2	D	3117	PHE	CD1-CE1	43.66	2.26	1.39
2	A	3117	PHE	CD1-CE1	43.62	2.26	1.39
2	C	3117	PHE	CD1-CE1	43.59	2.26	1.39
2	A	3117	PHE	CE2-CZ	42.78	2.18	1.37
2	C	3117	PHE	CE2-CZ	42.73	2.18	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3117	PHE	CE2-CZ	42.73	2.18	1.37
2	D	3117	PHE	CE2-CZ	42.72	2.18	1.37
2	B	3117	PHE	CE1-CZ	42.39	2.17	1.37
2	C	3117	PHE	CE1-CZ	42.39	2.17	1.37
2	D	3117	PHE	CE1-CZ	42.39	2.17	1.37
2	A	3117	PHE	CE1-CZ	42.37	2.17	1.37
2	B	3117	PHE	CD2-CE2	41.22	2.21	1.39
2	C	3117	PHE	CD2-CE2	41.20	2.21	1.39
2	A	3117	PHE	CD2-CE2	41.19	2.21	1.39
2	D	3117	PHE	CD2-CE2	41.16	2.21	1.39
2	C	3117	PHE	CG-CD1	27.61	1.80	1.38
2	B	3117	PHE	CG-CD1	27.61	1.80	1.38
2	D	3117	PHE	CG-CD1	27.60	1.80	1.38
2	A	3117	PHE	CG-CD1	27.56	1.80	1.38
2	C	3117	PHE	CG-CD2	26.73	1.78	1.38
2	B	3117	PHE	CG-CD2	26.72	1.78	1.38
2	D	3117	PHE	CG-CD2	26.70	1.78	1.38
2	A	3117	PHE	CG-CD2	26.69	1.78	1.38
2	D	3043	ARG	CD-NE	14.06	1.70	1.46
2	C	3043	ARG	CD-NE	14.02	1.70	1.46
2	B	3043	ARG	CD-NE	14.01	1.70	1.46
2	A	3043	ARG	CD-NE	14.00	1.70	1.46
2	C	3043	ARG	NE-CZ	9.54	1.45	1.33
2	A	3043	ARG	NE-CZ	9.54	1.45	1.33
2	D	3043	ARG	NE-CZ	9.51	1.45	1.33
2	B	3043	ARG	NE-CZ	9.49	1.45	1.33

All (131) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	3043	ARG	CD-NE-CZ	22.54	155.15	123.60
2	B	3043	ARG	CD-NE-CZ	22.53	155.15	123.60
2	D	3043	ARG	CD-NE-CZ	22.52	155.13	123.60
2	C	3043	ARG	CD-NE-CZ	22.52	155.13	123.60
2	B	3043	ARG	CG-CD-NE	11.67	136.30	111.80
2	C	3043	ARG	CG-CD-NE	11.66	136.28	111.80
2	A	3043	ARG	CG-CD-NE	11.66	136.28	111.80
2	D	3043	ARG	CG-CD-NE	11.63	136.23	111.80
2	D	3043	ARG	NE-CZ-NH1	9.63	125.11	120.30
2	A	3043	ARG	NE-CZ-NH1	9.56	125.08	120.30
2	C	3043	ARG	NE-CZ-NH1	9.55	125.07	120.30
2	B	3043	ARG	NE-CZ-NH1	9.50	125.05	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	4707	MET	CA-CB-CG	8.76	128.20	113.30
2	A	4707	MET	CA-CB-CG	8.76	128.19	113.30
2	B	4707	MET	CA-CB-CG	8.75	128.18	113.30
2	D	4707	MET	CA-CB-CG	8.75	128.18	113.30
2	C	3235	MET	CA-CB-CG	8.34	127.48	113.30
2	B	3235	MET	CA-CB-CG	8.34	127.47	113.30
2	A	3235	MET	CA-CB-CG	8.33	127.46	113.30
2	D	3235	MET	CA-CB-CG	8.32	127.44	113.30
2	A	2589	LEU	CA-CB-CG	7.94	133.56	115.30
2	B	2589	LEU	CA-CB-CG	7.93	133.53	115.30
2	D	2589	LEU	CA-CB-CG	7.92	133.52	115.30
2	C	2589	LEU	CA-CB-CG	7.92	133.50	115.30
2	D	4726	MET	CB-CG-SD	7.56	135.09	112.40
2	B	4726	MET	CB-CG-SD	7.55	135.05	112.40
2	A	4726	MET	CB-CG-SD	7.54	135.03	112.40
2	C	4726	MET	CB-CG-SD	7.54	135.02	112.40
2	A	3072	MET	CB-CG-SD	7.25	134.16	112.40
2	B	3072	MET	CB-CG-SD	7.25	134.16	112.40
2	D	3072	MET	CB-CG-SD	7.25	134.16	112.40
2	D	4707	MET	CB-CG-SD	7.25	134.14	112.40
2	A	4707	MET	CB-CG-SD	7.25	134.14	112.40
2	B	4707	MET	CB-CG-SD	7.25	134.13	112.40
2	C	4707	MET	CB-CG-SD	7.24	134.12	112.40
2	C	3072	MET	CB-CG-SD	7.24	134.11	112.40
2	B	3235	MET	CB-CG-SD	6.94	133.23	112.40
2	A	3235	MET	CB-CG-SD	6.94	133.23	112.40
2	C	3235	MET	CB-CG-SD	6.94	133.22	112.40
2	D	3235	MET	CB-CG-SD	6.94	133.21	112.40
2	A	2689	MET	CA-CB-CG	6.80	124.85	113.30
2	C	2689	MET	CA-CB-CG	6.78	124.82	113.30
2	B	2689	MET	CA-CB-CG	6.77	124.82	113.30
2	D	2689	MET	CA-CB-CG	6.76	124.79	113.30
2	D	2066	MET	CB-CG-SD	6.75	132.65	112.40
2	A	2066	MET	CB-CG-SD	6.75	132.64	112.40
2	C	2066	MET	CB-CG-SD	6.74	132.62	112.40
2	B	2066	MET	CB-CG-SD	6.73	132.60	112.40
2	D	2681	MET	CB-CG-SD	6.62	132.28	112.40
2	D	2689	MET	CB-CG-SD	6.62	132.26	112.40
2	A	2681	MET	CB-CG-SD	6.62	132.25	112.40
2	C	2681	MET	CB-CG-SD	6.61	132.24	112.40
2	C	2689	MET	CB-CG-SD	6.61	132.24	112.40
2	B	2689	MET	CB-CG-SD	6.61	132.22	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2681	MET	CB-CG-SD	6.61	132.22	112.40
2	A	2689	MET	CB-CG-SD	6.60	132.21	112.40
2	D	3117	PHE	CB-CG-CD1	-6.11	116.52	120.80
2	A	3277	LEU	CA-CB-CG	6.06	129.24	115.30
2	B	3277	LEU	CA-CB-CG	6.05	129.22	115.30
2	C	3277	LEU	CA-CB-CG	6.05	129.22	115.30
2	A	3117	PHE	CB-CG-CD1	-6.05	116.57	120.80
2	D	3117	PHE	CD1-CG-CD2	6.05	126.16	118.30
2	D	3277	LEU	CA-CB-CG	6.04	129.20	115.30
2	B	3117	PHE	CB-CG-CD1	-6.04	116.57	120.80
2	C	3117	PHE	CB-CG-CD1	-6.04	116.57	120.80
2	A	3117	PHE	CD1-CG-CD2	6.04	126.15	118.30
2	B	3117	PHE	CD1-CG-CD2	6.03	126.14	118.30
2	C	3117	PHE	CD1-CG-CD2	6.03	126.14	118.30
2	C	241	MET	CB-CG-SD	5.92	130.17	112.40
2	B	241	MET	CB-CG-SD	5.92	130.16	112.40
2	A	241	MET	CB-CG-SD	5.91	130.12	112.40
2	D	241	MET	CB-CG-SD	5.91	130.12	112.40
2	B	3985	MET	CB-CG-SD	5.68	129.45	112.40
2	A	3985	MET	CB-CG-SD	5.68	129.44	112.40
2	D	3985	MET	CB-CG-SD	5.68	129.43	112.40
2	C	3985	MET	CB-CG-SD	5.67	129.40	112.40
2	C	3192	ARG	CA-CB-CG	5.59	125.70	113.40
2	D	3192	ARG	CA-CB-CG	5.59	125.69	113.40
2	B	3192	ARG	CA-CB-CG	5.59	125.69	113.40
2	A	3192	ARG	CA-CB-CG	5.57	125.64	113.40
2	B	3221	LEU	CA-CB-CG	5.56	128.09	115.30
2	A	3221	LEU	CA-CB-CG	5.55	128.07	115.30
2	C	3221	LEU	CA-CB-CG	5.55	128.06	115.30
2	D	3221	LEU	CA-CB-CG	5.52	128.00	115.30
2	C	3072	MET	CG-SD-CE	5.46	108.93	100.20
2	A	3072	MET	CG-SD-CE	5.45	108.93	100.20
2	D	3072	MET	CG-SD-CE	5.45	108.92	100.20
2	B	3072	MET	CG-SD-CE	5.45	108.92	100.20
2	B	494	MET	CB-CG-SD	5.45	128.73	112.40
2	D	494	MET	CB-CG-SD	5.44	128.72	112.40
2	C	4726	MET	CA-CB-CG	5.43	122.52	113.30
2	A	494	MET	CB-CG-SD	5.42	128.67	112.40
2	C	494	MET	CB-CG-SD	5.42	128.68	112.40
2	B	4726	MET	CA-CB-CG	5.42	122.51	113.30
2	A	4726	MET	CA-CB-CG	5.41	122.50	113.30
2	B	2681	MET	CA-CB-CG	5.40	122.48	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	2681	MET	CA-CB-CG	5.38	122.45	113.30
2	D	2681	MET	CA-CB-CG	5.38	122.45	113.30
2	A	4726	MET	CG-SD-CE	5.38	108.81	100.20
2	C	4726	MET	CG-SD-CE	5.38	108.80	100.20
2	D	4726	MET	CG-SD-CE	5.38	108.80	100.20
2	D	4726	MET	CA-CB-CG	5.37	122.43	113.30
2	A	2681	MET	CA-CB-CG	5.37	122.43	113.30
2	C	3192	ARG	CB-CG-CD	5.37	125.56	111.60
2	D	3192	ARG	CB-CG-CD	5.37	125.55	111.60
2	A	3192	ARG	CB-CG-CD	5.36	125.54	111.60
2	B	4726	MET	CG-SD-CE	5.36	108.78	100.20
2	B	3192	ARG	CB-CG-CD	5.35	125.51	111.60
2	B	2066	MET	CG-SD-CE	5.23	108.56	100.20
2	A	2066	MET	CG-SD-CE	5.21	108.53	100.20
2	C	2066	MET	CG-SD-CE	5.20	108.52	100.20
2	D	2066	MET	CG-SD-CE	5.19	108.50	100.20
2	B	3273	MET	CG-SD-CE	-5.11	92.03	100.20
2	C	3273	MET	CG-SD-CE	-5.11	92.03	100.20
2	A	3273	MET	CG-SD-CE	-5.10	92.04	100.20
2	A	2192	MET	CB-CG-SD	5.10	127.70	112.40
2	D	3273	MET	CG-SD-CE	-5.09	92.05	100.20
2	B	2192	MET	CB-CG-SD	5.09	127.67	112.40
2	C	2192	MET	CB-CG-SD	5.08	127.65	112.40
2	D	2192	MET	CB-CG-SD	5.08	127.64	112.40
2	A	3117	PHE	CB-CG-CD2	-5.06	117.26	120.80
2	D	2828	MET	CA-CB-CG	5.05	121.89	113.30
2	B	2828	MET	CA-CB-CG	5.05	121.88	113.30
2	C	2828	MET	CA-CB-CG	5.05	121.88	113.30
2	B	3117	PHE	CB-CG-CD2	-5.04	117.27	120.80
2	C	3117	PHE	CB-CG-CD2	-5.04	117.27	120.80
2	C	3985	MET	CA-CB-CG	5.04	121.87	113.30
2	A	2828	MET	CA-CB-CG	5.04	121.86	113.30
2	A	3985	MET	CA-CB-CG	5.03	121.85	113.30
2	D	3985	MET	CA-CB-CG	5.02	121.83	113.30
2	D	3117	PHE	CB-CG-CD2	-5.01	117.29	120.80

There are no chirality outliers.

All (28) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	2754	GLN	Peptide
2	A	2772	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	A	2828	MET	Peptide
2	A	3043	ARG	Sidechain
2	A	3191	GLU	Peptide
2	A	4640	PHE	Peptide
2	A	469	HIS	Peptide
2	B	2754	GLN	Peptide
2	B	2772	ARG	Sidechain
2	B	2828	MET	Peptide
2	B	3043	ARG	Sidechain
2	B	3191	GLU	Peptide
2	B	4640	PHE	Peptide
2	B	469	HIS	Peptide
2	C	2754	GLN	Peptide
2	C	2772	ARG	Sidechain
2	C	2828	MET	Peptide
2	C	3043	ARG	Sidechain
2	C	3191	GLU	Peptide
2	C	4640	PHE	Peptide
2	C	469	HIS	Peptide
2	D	2754	GLN	Peptide
2	D	2772	ARG	Sidechain
2	D	2828	MET	Peptide
2	D	3043	ARG	Sidechain
2	D	3191	GLU	Peptide
2	D	4640	PHE	Peptide
2	D	469	HIS	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	E	818	0	821	13	0
1	F	818	0	821	14	0
1	G	818	0	821	15	0
1	H	818	0	821	18	0
2	A	33771	0	33453	977	0
2	B	33771	0	33453	977	0
2	C	33771	0	33453	977	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	33771	0	33453	988	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	62	0	24	2	0
4	B	62	0	24	2	0
4	C	62	0	24	2	0
4	D	62	0	24	2	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	11	0	4	0	0
6	B	11	0	4	0	0
6	C	11	0	4	0	0
6	D	11	0	4	0	0
All	All	138656	0	137208	3905	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 14.

All (3905) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3117:PHE:CG	2:D:3117:PHE:CD1	1.80	1.67
2:B:3117:PHE:CD2	2:B:3117:PHE:CG	1.78	1.66
2:B:3117:PHE:CG	2:B:3117:PHE:CD1	1.80	1.66
2:D:3117:PHE:CG	2:D:3117:PHE:CD2	1.78	1.63
2:C:3117:PHE:CD2	2:C:3117:PHE:CG	1.78	1.62
2:A:3117:PHE:CD1	2:A:3117:PHE:CG	1.80	1.62
2:A:3117:PHE:CG	2:A:3117:PHE:CD2	1.78	1.62
2:C:3117:PHE:CG	2:C:3117:PHE:CD1	1.80	1.60
2:A:3043:ARG:NE	2:A:3043:ARG:CD	1.70	1.54
2:D:3043:ARG:NE	2:D:3043:ARG:CD	1.70	1.54
2:B:3043:ARG:CD	2:B:3043:ARG:NE	1.70	1.49
2:C:3043:ARG:NE	2:C:3043:ARG:CD	1.70	1.49
2:C:3043:ARG:NE	2:C:3117:PHE:CD2	1.94	1.36
2:A:3043:ARG:NE	2:A:3117:PHE:CD2	1.94	1.36
2:A:3117:PHE:CE1	2:A:3117:PHE:CZ	2.17	1.32
2:B:3043:ARG:NE	2:B:3117:PHE:CD2	1.94	1.32

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:3043:ARG:NE	2:C:3117:PHE:CE2	1.97	1.32
2:D:3043:ARG:NE	2:D:3117:PHE:CD2	1.93	1.32
2:D:3043:ARG:NE	2:D:3117:PHE:CE2	1.97	1.32
2:B:3117:PHE:CE1	2:B:3117:PHE:CZ	2.17	1.32
2:B:3117:PHE:CZ	2:B:3117:PHE:CE2	2.18	1.32
2:C:3117:PHE:CE2	2:C:3117:PHE:CZ	2.18	1.32
2:A:3117:PHE:CZ	2:A:3117:PHE:CE2	2.18	1.31
2:D:3117:PHE:CE1	2:D:3117:PHE:CZ	2.17	1.31
2:C:3117:PHE:CZ	2:C:3117:PHE:CE1	2.17	1.31
2:A:3043:ARG:NE	2:A:3117:PHE:CE2	1.97	1.30
2:B:3043:ARG:NE	2:B:3117:PHE:CE2	1.97	1.30
2:D:3117:PHE:CE2	2:D:3117:PHE:CZ	2.18	1.30
2:D:3117:PHE:CD2	2:D:3117:PHE:CE2	2.21	1.28
2:B:3117:PHE:CD2	2:B:3117:PHE:CE2	2.21	1.28
2:A:3117:PHE:CD2	2:A:3117:PHE:CE2	2.21	1.27
2:C:3117:PHE:CD2	2:C:3117:PHE:CE2	2.21	1.26
2:A:3117:PHE:CD1	2:A:3117:PHE:CE1	2.26	1.24
2:C:3117:PHE:CD1	2:C:3117:PHE:CE1	2.26	1.24
2:B:3117:PHE:CD1	2:B:3117:PHE:CE1	2.26	1.24
2:D:3043:ARG:NE	2:D:3117:PHE:CG	2.06	1.23
2:C:3043:ARG:NE	2:C:3117:PHE:CG	2.06	1.23
2:A:3043:ARG:NE	2:A:3117:PHE:CG	2.06	1.22
2:D:3117:PHE:CD1	2:D:3117:PHE:CE1	2.26	1.22
2:B:3043:ARG:NE	2:B:3117:PHE:CG	2.06	1.22
2:D:3043:ARG:NE	2:D:3117:PHE:CD1	2.12	1.17
2:A:3043:ARG:NE	2:A:3117:PHE:CD1	2.12	1.16
2:C:3043:ARG:NE	2:C:3117:PHE:CZ	2.14	1.16
2:A:3043:ARG:NE	2:A:3117:PHE:CZ	2.14	1.15
2:B:3043:ARG:NE	2:B:3117:PHE:CD1	2.12	1.15
2:D:3043:ARG:NE	2:D:3117:PHE:CZ	2.14	1.15
2:C:3043:ARG:NE	2:C:3117:PHE:CD1	2.12	1.15
2:B:3043:ARG:NE	2:B:3117:PHE:CZ	2.14	1.15
2:D:3043:ARG:NE	2:D:3117:PHE:CE1	2.21	1.09
2:C:3043:ARG:NE	2:C:3117:PHE:CE1	2.20	1.09
2:A:3043:ARG:NE	2:A:3117:PHE:CE1	2.20	1.09
2:B:3043:ARG:NE	2:B:3117:PHE:CE1	2.20	1.08
2:C:3043:ARG:CZ	2:C:3117:PHE:CE1	2.41	1.03
2:B:3043:ARG:CZ	2:B:3117:PHE:CE1	2.41	1.03
2:D:3043:ARG:CZ	2:D:3117:PHE:CE1	2.41	1.03
2:A:3043:ARG:CZ	2:A:3117:PHE:CE1	2.41	1.02
2:C:3043:ARG:CD	2:C:3117:PHE:CE1	2.42	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3043:ARG:CD	2:D:3117:PHE:CE1	2.43	1.02
2:A:3043:ARG:CZ	2:A:3117:PHE:CZ	2.43	1.01
2:C:3043:ARG:CZ	2:C:3117:PHE:CZ	2.43	1.01
2:B:3043:ARG:CD	2:B:3117:PHE:CE1	2.42	1.01
2:B:3043:ARG:CZ	2:B:3117:PHE:CZ	2.43	1.01
2:A:3043:ARG:CD	2:A:3117:PHE:CE1	2.43	1.01
2:D:3043:ARG:CZ	2:D:3117:PHE:CZ	2.43	1.01
2:D:4275:THR:O	2:D:4279:MET:HB2	1.64	0.98
2:A:4275:THR:O	2:A:4279:MET:HB2	1.64	0.97
2:C:4275:THR:O	2:C:4279:MET:HB2	1.64	0.97
2:C:3043:ARG:CD	2:C:3117:PHE:CD1	2.48	0.97
2:B:3043:ARG:CD	2:B:3117:PHE:CD1	2.48	0.96
2:D:3043:ARG:CD	2:D:3117:PHE:CD1	2.48	0.96
2:D:3172:GLU:HA	2:D:3211:LEU:HD22	1.49	0.95
2:A:3043:ARG:CD	2:A:3117:PHE:CD1	2.48	0.95
2:C:3043:ARG:HD2	2:C:3117:PHE:CE1	2.02	0.95
2:C:3172:GLU:HA	2:C:3211:LEU:HD22	1.49	0.95
2:B:4275:THR:O	2:B:4279:MET:HB2	1.64	0.94
2:D:3043:ARG:HD2	2:D:3117:PHE:CE1	2.02	0.94
2:A:3188:SER:O	2:A:3192:ARG:NH1	2.02	0.93
2:A:3043:ARG:HD2	2:A:3117:PHE:CD1	2.04	0.93
2:B:3188:SER:O	2:B:3192:ARG:NH1	2.02	0.93
2:C:3043:ARG:HD2	2:C:3117:PHE:CD1	2.04	0.93
2:B:3043:ARG:HD2	2:B:3117:PHE:CE1	2.02	0.93
2:B:3172:GLU:HA	2:B:3211:LEU:HD22	1.49	0.93
2:C:3188:SER:O	2:C:3192:ARG:NH1	2.02	0.92
2:D:3043:ARG:HD2	2:D:3117:PHE:CD1	2.04	0.92
2:A:3043:ARG:HD2	2:A:3117:PHE:CE1	2.02	0.92
2:A:3172:GLU:HA	2:A:3211:LEU:HD22	1.49	0.92
2:B:3043:ARG:HD2	2:B:3117:PHE:CD1	2.04	0.92
2:D:3188:SER:O	2:D:3192:ARG:NH1	2.02	0.91
2:C:3043:ARG:CZ	2:C:3117:PHE:CD1	2.56	0.88
2:D:3215:MET:SD	2:D:3272:HIS:NE2	2.47	0.88
2:A:3215:MET:SD	2:A:3272:HIS:NE2	2.47	0.88
2:B:3043:ARG:CZ	2:B:3117:PHE:CD1	2.56	0.88
2:B:3215:MET:SD	2:B:3272:HIS:NE2	2.47	0.88
2:C:3215:MET:SD	2:C:3272:HIS:NE2	2.47	0.88
2:D:3043:ARG:CZ	2:D:3117:PHE:CD1	2.56	0.87
2:A:3043:ARG:CZ	2:A:3117:PHE:CD1	2.56	0.87
2:B:3043:ARG:NH1	2:B:3117:PHE:CE1	2.43	0.87
2:A:1564:MET:HE3	2:A:1565:PRO:HD2	1.57	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:3043:ARG:NH1	2:C:3117:PHE:CE1	2.43	0.87
2:D:3043:ARG:NH1	2:D:3117:PHE:CE1	2.43	0.86
2:A:3043:ARG:NH1	2:A:3117:PHE:CE1	2.43	0.86
2:A:3043:ARG:CD	2:A:3117:PHE:CZ	2.59	0.86
2:C:15:ARG:HE	2:C:16:THR:H	1.21	0.86
2:B:1564:MET:HE3	2:B:1565:PRO:HD2	1.57	0.86
2:D:1500:ARG:HD2	2:D:1501:ASN:H	1.40	0.86
2:B:15:ARG:HE	2:B:16:THR:H	1.21	0.85
2:B:3043:ARG:CD	2:B:3117:PHE:CZ	2.59	0.85
2:A:1500:ARG:HD2	2:A:1501:ASN:H	1.40	0.85
2:C:3043:ARG:CD	2:C:3117:PHE:CZ	2.59	0.85
2:D:3043:ARG:CD	2:D:3117:PHE:CZ	2.59	0.85
2:D:2979:ARG:HH22	2:D:3035:ILE:HG23	1.41	0.85
2:D:2913:ASP:HB3	2:D:2919:LYS:HG3	1.59	0.85
2:C:1500:ARG:HD2	2:C:1501:ASN:H	1.40	0.84
2:D:1564:MET:HE3	2:D:1565:PRO:HD2	1.57	0.84
2:A:15:ARG:HE	2:A:16:THR:H	1.21	0.84
2:B:1500:ARG:HD2	2:B:1501:ASN:H	1.40	0.84
2:C:1564:MET:HE3	2:C:1565:PRO:HD2	1.58	0.84
2:C:2913:ASP:HB3	2:C:2919:LYS:HG3	1.59	0.84
2:C:3122:ILE:HG13	2:C:3127:GLN:HG2	1.60	0.84
2:B:2979:ARG:HH22	2:B:3035:ILE:HG23	1.41	0.84
2:A:2913:ASP:HB3	2:A:2919:LYS:HG3	1.59	0.83
2:B:3043:ARG:CZ	2:B:3117:PHE:CE2	2.61	0.83
2:A:3043:ARG:CZ	2:A:3117:PHE:CE2	2.61	0.83
2:C:2979:ARG:HH22	2:C:3035:ILE:HG23	1.41	0.83
2:B:2913:ASP:HB3	2:B:2919:LYS:HG3	1.59	0.82
2:B:3122:ILE:HG13	2:B:3127:GLN:HG2	1.60	0.82
2:D:3122:ILE:HG13	2:D:3127:GLN:HG2	1.60	0.82
2:D:2769:GLU:HA	2:D:2772:ARG:HG2	1.60	0.82
2:A:2979:ARG:HH22	2:A:3035:ILE:HG23	1.41	0.82
2:B:1086:ARG:HH21	2:B:1251:LEU:HD13	1.45	0.82
2:A:2841:ALA:HA	2:A:2844:MET:HG2	1.61	0.82
2:A:3043:ARG:NH1	2:A:3117:PHE:CD1	2.48	0.82
2:C:1086:ARG:HH21	2:C:1251:LEU:HD13	1.45	0.82
2:C:3043:ARG:CZ	2:C:3117:PHE:CE2	2.61	0.82
2:D:3043:ARG:CZ	2:D:3117:PHE:CE2	2.61	0.82
2:C:2736:LYS:HA	2:C:2741:TRP:HE3	1.45	0.82
2:D:15:ARG:HE	2:D:16:THR:H	1.21	0.82
2:C:3043:ARG:NH1	2:C:3117:PHE:CD1	2.48	0.81
2:B:2736:LYS:HA	2:B:2741:TRP:HE3	1.45	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2769:GLU:HA	2:B:2772:ARG:HG2	1.60	0.81
2:C:2841:ALA:HA	2:C:2844:MET:HG2	1.61	0.81
2:A:1086:ARG:HH21	2:A:1251:LEU:HD13	1.45	0.81
2:A:2830:ASN:ND2	2:B:1434:PRO:O	2.14	0.81
2:B:2841:ALA:HA	2:B:2844:MET:HG2	1.61	0.81
2:C:2769:GLU:HA	2:C:2772:ARG:HG2	1.60	0.81
2:D:3043:ARG:NH1	2:D:3117:PHE:CD1	2.48	0.81
2:A:2769:GLU:HA	2:A:2772:ARG:HG2	1.60	0.81
2:A:3043:ARG:CD	2:A:3117:PHE:CG	2.64	0.81
2:B:932:ASN:HA	2:B:935:MET:HG3	1.62	0.81
2:B:3043:ARG:NH1	2:B:3117:PHE:CD1	2.48	0.81
2:A:932:ASN:HA	2:A:935:MET:HG3	1.62	0.81
2:A:3122:ILE:HG13	2:A:3127:GLN:HG2	1.60	0.81
2:D:3043:ARG:CD	2:D:3117:PHE:CG	2.64	0.81
2:D:2841:ALA:HA	2:D:2844:MET:HG2	1.61	0.81
2:A:2736:LYS:HA	2:A:2741:TRP:HE3	1.45	0.81
2:A:2830:ASN:HD22	2:B:1435:GLY:HA3	1.43	0.81
2:C:3805:LEU:HD23	2:D:76:ARG:HH22	1.45	0.81
2:D:932:ASN:HA	2:D:935:MET:HG3	1.62	0.81
2:B:3043:ARG:CD	2:B:3117:PHE:CG	2.64	0.80
2:C:3043:ARG:CD	2:C:3117:PHE:CG	2.64	0.80
2:C:932:ASN:HA	2:C:935:MET:HG3	1.62	0.80
2:D:2736:LYS:HA	2:D:2741:TRP:HE3	1.45	0.80
2:B:332:ARG:HH21	2:B:338:LEU:HD23	1.47	0.80
2:D:1086:ARG:HH21	2:D:1251:LEU:HD13	1.45	0.80
2:D:332:ARG:HH21	2:D:338:LEU:HD23	1.47	0.78
2:B:948:CYS:HB3	2:B:1064:LEU:HD12	1.64	0.78
2:D:3950:VAL:O	2:D:3954:MET:HB2	1.84	0.78
2:D:1038:LEU:O	2:D:1043:LYS:NZ	2.17	0.78
2:A:3950:VAL:O	2:A:3954:MET:HB2	1.84	0.78
2:C:948:CYS:HB3	2:C:1064:LEU:HD12	1.64	0.78
2:A:332:ARG:HH21	2:A:338:LEU:HD23	1.47	0.78
2:C:3950:VAL:O	2:C:3954:MET:HB2	1.84	0.77
2:A:3945:VAL:HG23	2:A:4006:SER:HB3	1.67	0.77
2:A:1038:LEU:O	2:A:1043:LYS:NZ	2.17	0.77
2:B:897:LYS:O	2:B:902:TRP:HB2	1.85	0.77
2:C:332:ARG:HH21	2:C:338:LEU:HD23	1.47	0.77
2:D:897:LYS:O	2:D:902:TRP:HB2	1.85	0.77
2:A:897:LYS:O	2:A:902:TRP:HB2	1.85	0.77
2:A:948:CYS:HB3	2:A:1064:LEU:HD12	1.64	0.77
2:B:3950:VAL:O	2:B:3954:MET:HB2	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:948:CYS:HB3	2:D:1064:LEU:HD12	1.65	0.77
2:B:3945:VAL:HG23	2:B:4006:SER:HB3	1.67	0.77
2:A:4834:PRO:HB3	2:A:4843:ARG:HD3	1.67	0.77
2:C:3183:ILE:O	2:C:3187:LYS:HB2	1.85	0.77
2:C:3945:VAL:HG23	2:C:4006:SER:HB3	1.67	0.77
2:A:1732:GLU:HB2	2:A:1753:LEU:HD21	1.67	0.77
2:D:3183:ILE:O	2:D:3187:LYS:HB2	1.85	0.77
2:C:1038:LEU:O	2:C:1043:LYS:NZ	2.17	0.77
2:D:3945:VAL:HG23	2:D:4006:SER:HB3	1.67	0.77
2:B:1038:LEU:O	2:B:1043:LYS:NZ	2.17	0.77
2:C:126:SER:HA	2:C:414:ARG:HH12	1.50	0.76
2:D:188:SER:HB3	2:D:190:ARG:HD3	1.67	0.76
2:B:3183:ILE:O	2:B:3187:LYS:HB2	1.85	0.76
2:B:4834:PRO:HB3	2:B:4843:ARG:HD3	1.67	0.76
2:C:897:LYS:O	2:C:902:TRP:HB2	1.85	0.76
2:A:188:SER:HB3	2:A:190:ARG:HD3	1.67	0.76
2:B:1732:GLU:HB2	2:B:1753:LEU:HD21	1.67	0.76
2:D:1732:GLU:HB2	2:D:1753:LEU:HD21	1.67	0.76
2:B:126:SER:HA	2:B:414:ARG:HH12	1.50	0.76
2:C:3218:ILE:HG22	2:C:3279:ASN:ND2	2.01	0.76
2:B:188:SER:HB3	2:B:190:ARG:HD3	1.67	0.76
2:B:3043:ARG:HB2	2:B:3117:PHE:CE2	2.21	0.76
2:C:4834:PRO:HB3	2:C:4843:ARG:HD3	1.67	0.76
2:D:3218:ILE:HG22	2:D:3279:ASN:ND2	2.01	0.75
2:A:4641:PRO:HB3	2:A:4644:TYR:HB3	1.67	0.75
2:C:3043:ARG:HB2	2:C:3117:PHE:CE2	2.21	0.75
2:D:3844:GLN:HG3	2:D:3922:GLU:HG3	1.68	0.75
2:C:1732:GLU:HB2	2:C:1753:LEU:HD21	1.67	0.75
2:D:877:HIS:HA	2:D:880:ARG:NH1	2.02	0.75
2:D:4834:PRO:HB3	2:D:4843:ARG:HD3	1.67	0.75
2:B:4641:PRO:HB3	2:B:4644:TYR:HB3	1.67	0.75
2:C:3844:GLN:HG3	2:C:3922:GLU:HG3	1.68	0.75
2:A:241:MET:HA	2:A:241:MET:HE2	1.69	0.75
2:A:877:HIS:HA	2:A:880:ARG:NH1	2.02	0.75
2:B:2828:MET:HB3	2:B:2894:LYS:HE2	1.69	0.75
2:A:2828:MET:HB3	2:A:2894:LYS:HE2	1.69	0.74
2:A:3218:ILE:HG22	2:A:3279:ASN:ND2	2.01	0.74
2:C:188:SER:HB3	2:C:190:ARG:HD3	1.67	0.74
2:D:3043:ARG:HB2	2:D:3117:PHE:CE2	2.21	0.74
2:D:4641:PRO:HB3	2:D:4644:TYR:HB3	1.67	0.74
2:B:3218:ILE:HG22	2:B:3279:ASN:ND2	2.01	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3043:ARG:CD	2:D:3117:PHE:CE2	2.70	0.74
2:A:3043:ARG:HB2	2:A:3117:PHE:CE2	2.21	0.74
2:A:3183:ILE:O	2:A:3187:LYS:HB2	1.85	0.74
2:C:3043:ARG:CD	2:C:3117:PHE:CE2	2.70	0.74
2:C:4641:PRO:HB3	2:C:4644:TYR:HB3	1.67	0.74
2:A:126:SER:HA	2:A:414:ARG:HH12	1.50	0.74
2:A:3043:ARG:CD	2:A:3117:PHE:CE2	2.70	0.74
2:B:3043:ARG:CD	2:B:3117:PHE:CE2	2.70	0.74
2:D:2828:MET:HB3	2:D:2894:LYS:HE2	1.69	0.74
2:A:4818:TYR:CE1	2:B:4847:ASP:OD1	2.41	0.74
2:B:3043:ARG:CD	2:B:3117:PHE:CD2	2.71	0.74
2:D:126:SER:HA	2:D:414:ARG:HH12	1.50	0.73
2:B:4279:MET:CE	2:C:4484:ILE:HG22	2.18	0.73
2:A:3222:ALA:HB2	2:A:3279:ASN:OD1	1.88	0.73
2:A:3844:GLN:HG3	2:A:3922:GLU:HG3	1.68	0.73
2:C:877:HIS:HA	2:C:880:ARG:NH1	2.02	0.73
2:D:3222:ALA:HB2	2:D:3279:ASN:OD1	1.88	0.73
2:B:3844:GLN:HG3	2:B:3922:GLU:HG3	1.68	0.73
2:C:2426:LEU:O	2:D:142:LYS:NZ	2.19	0.73
2:A:3043:ARG:CD	2:A:3117:PHE:CD2	2.71	0.73
2:B:943:LEU:HB3	2:B:948:CYS:HB2	1.71	0.73
2:D:943:LEU:HB3	2:D:948:CYS:HB2	1.71	0.73
2:C:3013:VAL:O	2:C:3018:ARG:NH2	2.22	0.73
2:C:3043:ARG:CD	2:C:3117:PHE:CD2	2.71	0.73
2:C:943:LEU:HB3	2:C:948:CYS:HB2	1.71	0.73
2:C:2828:MET:HB3	2:C:2894:LYS:HE2	1.69	0.73
2:C:3018:ARG:HG3	2:C:3021:LEU:HD12	1.71	0.73
2:C:3222:ALA:HB2	2:C:3279:ASN:OD1	1.88	0.73
2:B:877:HIS:HA	2:B:880:ARG:NH1	2.02	0.73
2:B:3222:ALA:HB2	2:B:3279:ASN:OD1	1.88	0.73
2:A:943:LEU:HB3	2:A:948:CYS:HB2	1.71	0.73
2:A:3018:ARG:HG3	2:A:3021:LEU:HD12	1.71	0.73
2:D:3043:ARG:CD	2:D:3117:PHE:CD2	2.71	0.73
2:B:992:GLN:NE2	2:B:1064:LEU:O	2.22	0.72
2:B:3018:ARG:HG3	2:B:3021:LEU:HD12	1.71	0.72
2:A:992:GLN:NE2	2:A:1064:LEU:O	2.22	0.72
2:B:241:MET:HE2	2:B:241:MET:HA	1.70	0.72
2:C:992:GLN:NE2	2:C:1064:LEU:O	2.22	0.72
1:H:83:TYR:OH	2:D:1768:PHE:O	2.05	0.72
2:B:235:ARG:NH2	2:B:412:GLU:OE2	2.23	0.72
2:D:235:ARG:NH2	2:D:412:GLU:OE2	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:992:GLN:NE2	2:D:1064:LEU:O	2.22	0.72
2:B:3013:VAL:O	2:B:3018:ARG:NH2	2.22	0.72
2:D:3018:ARG:HG3	2:D:3021:LEU:HD12	1.71	0.72
1:F:58:LYS:NZ	1:F:62:GLU:OE2	2.23	0.72
2:D:608:HIS:HB2	2:D:1656:HIS:HD2	1.54	0.72
1:H:58:LYS:NZ	1:H:62:GLU:OE2	2.23	0.71
2:A:4818:TYR:HB2	2:B:4844:ILE:HG23	1.71	0.71
2:B:608:HIS:HB2	2:B:1656:HIS:HD2	1.55	0.71
2:D:241:MET:HA	2:D:241:MET:HE2	1.70	0.71
2:D:2657:TYR:HA	2:D:2662:PHE:HE2	1.56	0.71
2:A:235:ARG:NH2	2:A:412:GLU:OE2	2.23	0.71
2:C:608:HIS:HB2	2:C:1656:HIS:HD2	1.55	0.71
2:A:59:PRO:O	2:A:319:LYS:NZ	2.23	0.71
2:A:608:HIS:HB2	2:A:1656:HIS:HD2	1.55	0.71
2:A:3279:ASN:O	2:A:3283:ILE:HD12	1.91	0.71
2:C:1937:GLN:HG2	2:C:3609:TYR:HA	1.72	0.71
2:D:1937:GLN:HG2	2:D:3609:TYR:HA	1.72	0.71
2:B:59:PRO:O	2:B:319:LYS:NZ	2.23	0.71
2:B:3279:ASN:O	2:B:3283:ILE:HD12	1.91	0.71
2:C:235:ARG:NH2	2:C:412:GLU:OE2	2.23	0.71
1:E:58:LYS:NZ	1:E:62:GLU:OE2	2.23	0.71
1:G:58:LYS:NZ	1:G:62:GLU:OE2	2.23	0.71
2:B:3043:ARG:NH2	2:B:3117:PHE:CE2	2.59	0.71
2:B:4580:THR:OG1	2:B:4733:HIS:NE2	2.18	0.71
2:B:1937:GLN:HG2	2:B:3609:TYR:HA	1.72	0.70
2:C:59:PRO:O	2:C:319:LYS:NZ	2.23	0.70
2:C:2657:TYR:HA	2:C:2662:PHE:HE2	1.56	0.70
2:D:3013:VAL:O	2:D:3018:ARG:NH2	2.22	0.70
2:B:2657:TYR:HA	2:B:2662:PHE:HE2	1.56	0.70
2:D:3043:ARG:NH2	2:D:3117:PHE:CE2	2.59	0.70
2:C:1074:ARG:HH11	2:C:1076:GLU:HA	1.56	0.70
2:D:4563:GLU:HG2	2:D:4568:MET:HB2	1.73	0.70
2:A:1937:GLN:HG2	2:A:3609:TYR:HA	1.72	0.70
2:C:3043:ARG:NH2	2:C:3117:PHE:CE2	2.59	0.70
2:D:2890:GLN:O	2:D:2894:LYS:HG2	1.92	0.70
2:A:3043:ARG:NH2	2:A:3117:PHE:CE2	2.59	0.70
2:C:241:MET:HE2	2:C:241:MET:HA	1.72	0.70
2:D:3016:ARG:O	2:D:3018:ARG:NE	2.25	0.70
2:A:2657:TYR:HA	2:A:2662:PHE:HE2	1.56	0.70
2:B:905:GLY:HA3	2:B:914:GLN:HB3	1.74	0.70
2:D:1074:ARG:HH11	2:D:1076:GLU:HA	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:905:GLY:HA3	2:C:914:GLN:HB3	1.74	0.70
2:B:3016:ARG:O	2:B:3018:ARG:NE	2.25	0.70
2:D:59:PRO:O	2:D:319:LYS:NZ	2.23	0.70
2:A:1039:ASP:OD1	2:A:1042:THR:OG1	2.08	0.70
2:B:4563:GLU:HG2	2:B:4568:MET:HB2	1.73	0.70
2:C:4563:GLU:HG2	2:C:4568:MET:HB2	1.73	0.69
2:A:4580:THR:OG1	2:A:4733:HIS:NE2	2.18	0.69
2:C:3016:ARG:O	2:C:3018:ARG:NE	2.25	0.69
2:A:3013:VAL:O	2:A:3018:ARG:NH2	2.22	0.69
2:C:2890:GLN:O	2:C:2894:LYS:HG2	1.92	0.69
2:A:911:ASN:OD1	2:A:912:LYS:N	2.25	0.69
2:A:2736:LYS:HA	2:A:2741:TRP:CE3	2.27	0.69
2:A:2996:ALA:O	2:A:3001:LYS:NZ	2.25	0.69
2:B:911:ASN:OD1	2:B:912:LYS:N	2.25	0.69
2:C:2996:ALA:O	2:C:3001:LYS:NZ	2.25	0.69
2:D:3043:ARG:CZ	2:D:3117:PHE:CD2	2.76	0.69
2:B:875:PRO:HD2	2:B:878:LEU:HD12	1.75	0.69
2:D:2465:LYS:NZ	2:D:2495:ASP:OD2	2.25	0.69
2:D:2996:ALA:O	2:D:3001:LYS:NZ	2.25	0.69
2:D:3279:ASN:O	2:D:3283:ILE:HD12	1.91	0.69
2:A:905:GLY:HA3	2:A:914:GLN:HB3	1.74	0.69
2:A:4563:GLU:HG2	2:A:4568:MET:HB2	1.73	0.69
2:B:2996:ALA:O	2:B:3001:LYS:NZ	2.25	0.69
2:C:875:PRO:HD2	2:C:878:LEU:HD12	1.75	0.69
2:D:911:ASN:OD1	2:D:912:LYS:N	2.25	0.69
2:C:911:ASN:OD1	2:C:912:LYS:N	2.25	0.69
2:C:3279:ASN:O	2:C:3283:ILE:HD12	1.91	0.69
2:D:905:GLY:HA3	2:D:914:GLN:HB3	1.74	0.69
2:A:2465:LYS:NZ	2:A:2495:ASP:OD2	2.24	0.69
2:A:2890:GLN:O	2:A:2894:LYS:HG2	1.92	0.69
2:D:2736:LYS:HA	2:D:2741:TRP:CE3	2.27	0.69
2:A:4727:THR:OG1	2:D:4295:LEU:HD21	1.93	0.69
2:B:2736:LYS:HA	2:B:2741:TRP:CE3	2.27	0.68
2:A:3043:ARG:CZ	2:A:3117:PHE:CD2	2.76	0.68
2:D:3043:ARG:CZ	2:D:3117:PHE:CG	2.77	0.68
2:A:875:PRO:HD2	2:A:878:LEU:HD12	1.74	0.68
2:A:901:GLY:O	2:A:913:ARG:NH2	2.27	0.68
2:D:1039:ASP:OD1	2:D:1042:THR:OG1	2.07	0.68
2:C:2736:LYS:HA	2:C:2741:TRP:CE3	2.27	0.68
2:B:2890:GLN:O	2:B:2894:LYS:HG2	1.92	0.68
2:C:2905:ARG:HD3	2:C:2907:PHE:H	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1039:ASP:OD1	2:C:1042:THR:OG1	2.08	0.68
2:D:875:PRO:HD2	2:D:878:LEU:HD12	1.75	0.68
2:A:1074:ARG:HH11	2:A:1076:GLU:HA	1.57	0.68
2:A:3700:HIS:ND1	2:A:3702:GLU:OE1	2.27	0.68
2:D:2905:ARG:HD3	2:D:2907:PHE:H	1.59	0.68
2:A:2978:HIS:HB3	2:A:2981:TYR:HB3	1.76	0.67
2:A:3242:LEU:O	2:A:3246:MET:HG2	1.94	0.67
2:C:901:GLY:O	2:C:913:ARG:NH2	2.27	0.67
2:C:3043:ARG:CZ	2:C:3117:PHE:CD2	2.76	0.67
2:A:15:ARG:NE	2:A:16:THR:H	1.92	0.67
2:A:3016:ARG:O	2:A:3018:ARG:NE	2.25	0.67
2:B:901:GLY:O	2:B:913:ARG:NH2	2.27	0.67
2:B:3043:ARG:CZ	2:B:3117:PHE:CD2	2.76	0.67
2:D:2978:HIS:HB3	2:D:2981:TYR:HB3	1.76	0.67
2:A:1500:ARG:CD	2:A:1501:ASN:H	2.07	0.67
2:A:2481:GLN:NE2	2:A:2537:GLY:O	2.28	0.67
2:B:3242:LEU:O	2:B:3246:MET:HG2	1.94	0.67
2:B:3700:HIS:ND1	2:B:3702:GLU:OE1	2.27	0.67
2:D:901:GLY:O	2:D:913:ARG:NH2	2.27	0.67
2:D:2481:GLN:NE2	2:D:2537:GLY:O	2.28	0.67
2:A:3043:ARG:CZ	2:A:3117:PHE:CG	2.77	0.67
2:B:1074:ARG:HH11	2:B:1076:GLU:HA	1.56	0.67
2:B:3043:ARG:CZ	2:B:3117:PHE:CG	2.77	0.67
2:C:2978:HIS:HB3	2:C:2981:TYR:HB3	1.76	0.67
2:D:2650:ASP:O	2:D:2654:GLN:NE2	2.28	0.67
2:C:3043:ARG:CZ	2:C:3117:PHE:CG	2.77	0.67
2:D:1500:ARG:CD	2:D:1501:ASN:H	2.07	0.67
2:B:2481:GLN:NE2	2:B:2537:GLY:O	2.28	0.67
2:C:3242:LEU:O	2:C:3246:MET:HG2	1.94	0.67
2:D:2610:LEU:HA	2:D:2613:HIS:CE1	2.29	0.67
2:B:4822:ARG:NH2	2:C:4829:ASP:OD1	2.27	0.67
2:B:1039:ASP:OD1	2:B:1042:THR:OG1	2.07	0.67
2:D:3700:HIS:ND1	2:D:3702:GLU:OE1	2.27	0.67
2:C:2481:GLN:NE2	2:C:2537:GLY:O	2.28	0.67
2:C:2576:ILE:O	2:C:2580:LEU:HB2	1.95	0.67
2:B:2465:LYS:NZ	2:B:2495:ASP:OD2	2.25	0.67
2:A:2576:ILE:O	2:A:2580:LEU:HB2	1.95	0.66
2:B:1500:ARG:CD	2:B:1501:ASN:H	2.07	0.66
2:B:2905:ARG:HD3	2:B:2907:PHE:H	1.59	0.66
2:B:3174:HIS:CD2	2:B:3175:LEU:HG	2.30	0.66
2:C:3700:HIS:ND1	2:C:3702:GLU:OE1	2.27	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:882:ARG:NH2	2:A:883:GLU:OE1	2.28	0.66
2:A:2610:LEU:HA	2:A:2613:HIS:CE1	2.30	0.66
2:B:2650:ASP:O	2:B:2654:GLN:NE2	2.28	0.66
2:A:2943:PHE:HB2	2:A:2956:TYR:OH	1.96	0.66
2:B:882:ARG:NH2	2:B:883:GLU:OE1	2.28	0.66
2:B:2978:HIS:HB3	2:B:2981:TYR:HB3	1.77	0.66
2:C:2610:LEU:HA	2:C:2613:HIS:CE1	2.30	0.66
2:C:2688:MET:HB2	2:C:2689:MET:CE	2.25	0.66
2:D:2943:PHE:HB2	2:D:2956:TYR:OH	1.96	0.66
2:B:2791:ARG:NH2	2:B:2899:ASN:O	2.23	0.66
2:B:4822:ARG:NE	2:C:4825:GLY:O	2.28	0.66
2:C:15:ARG:NE	2:C:16:THR:H	1.92	0.66
2:D:882:ARG:NH2	2:D:883:GLU:OE1	2.29	0.66
2:D:4018:ASP:OD1	2:D:4019:MET:N	2.29	0.66
2:B:644:LEU:HD13	2:B:1630:LEU:HD21	1.78	0.66
2:B:983:LEU:HD12	2:B:1055:ARG:HB3	1.78	0.66
2:B:4018:ASP:OD1	2:B:4019:MET:N	2.29	0.66
2:C:882:ARG:NH2	2:C:883:GLU:OE1	2.28	0.66
2:C:983:LEU:HD12	2:C:1055:ARG:HB3	1.78	0.66
2:C:4018:ASP:OD1	2:C:4019:MET:N	2.29	0.66
2:C:4580:THR:OG1	2:C:4733:HIS:NE2	2.18	0.66
2:A:2650:ASP:O	2:A:2654:GLN:NE2	2.28	0.66
2:A:2688:MET:HB2	2:A:2689:MET:CE	2.25	0.66
2:B:2943:PHE:HB2	2:B:2956:TYR:OH	1.96	0.66
2:B:4279:MET:HE1	2:C:4484:ILE:HG22	1.76	0.66
2:C:2465:LYS:NZ	2:C:2495:ASP:OD2	2.24	0.66
2:C:2650:ASP:O	2:C:2654:GLN:NE2	2.28	0.66
2:C:3174:HIS:CD2	2:C:3175:LEU:HG	2.30	0.66
2:D:1029:ASN:ND2	4:D:5005:ATP:O1G	2.29	0.66
2:D:2591:ARG:NH2	2:D:2875:ASP:OD1	2.28	0.66
2:D:2688:MET:HB2	2:D:2689:MET:CE	2.25	0.66
2:D:3242:LEU:O	2:D:3246:MET:HG2	1.94	0.66
2:A:893:TRP:HB3	2:A:917:CYS:HB3	1.77	0.66
2:A:1029:ASN:ND2	4:A:5005:ATP:O1G	2.29	0.66
2:B:2576:ILE:O	2:B:2580:LEU:HB2	1.95	0.66
2:B:1842:ILE:HD12	2:B:1845:LEU:HD12	1.77	0.66
2:B:2263:GLU:OE2	2:B:2327:ARG:NH2	2.29	0.66
2:B:2651:ALA:O	2:B:2655:LYS:HG2	1.96	0.66
2:B:2688:MET:HB2	2:B:2689:MET:CE	2.25	0.66
2:C:1500:ARG:CD	2:C:1501:ASN:H	2.07	0.66
2:C:2856:LYS:HA	2:C:2859:GLU:HG2	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3174:HIS:CD2	2:D:3175:LEU:HG	2.30	0.66
2:A:2591:ARG:NH2	2:A:2875:ASP:OD1	2.28	0.66
2:B:2591:ARG:NH2	2:B:2875:ASP:OD1	2.28	0.66
2:C:2591:ARG:NH2	2:C:2875:ASP:OD1	2.28	0.66
2:C:2651:ALA:O	2:C:2655:LYS:HG2	1.96	0.66
2:C:4014:LEU:HD13	2:C:4122:ALA:HB2	1.78	0.66
2:D:3249:TRP:HA	2:D:3252:HIS:HB2	1.78	0.66
2:A:2856:LYS:HA	2:A:2859:GLU:HG2	1.78	0.66
2:A:2905:ARG:HD3	2:A:2907:PHE:H	1.59	0.66
2:B:2610:LEU:HA	2:B:2613:HIS:CE1	2.30	0.66
2:C:893:TRP:HB3	2:C:917:CYS:HB3	1.77	0.66
2:C:2263:GLU:OE2	2:C:2327:ARG:NH2	2.29	0.66
2:C:2714:PRO:HG2	2:C:2717:LEU:HD23	1.78	0.66
2:D:3043:ARG:HD3	2:D:3117:PHE:CG	2.31	0.66
1:H:19:LYS:HA	1:H:19:LYS:HE2	1.79	0.65
2:A:983:LEU:HD12	2:A:1055:ARG:HB3	1.78	0.65
2:B:2984:SER:HA	2:B:2989:PRO:HB2	1.78	0.65
2:D:2714:PRO:HG2	2:D:2717:LEU:HD23	1.78	0.65
2:D:2856:LYS:HA	2:D:2859:GLU:HG2	1.78	0.65
2:B:893:TRP:HB3	2:B:917:CYS:HB3	1.77	0.65
2:B:1029:ASN:ND2	4:B:5005:ATP:O1G	2.29	0.65
2:B:2684:ASN:HD22	2:B:2911:GLU:HB3	1.62	0.65
2:C:1842:ILE:HD12	2:C:1845:LEU:HD12	1.77	0.65
2:C:3198:PRO:HG2	2:C:3204:VAL:HA	1.79	0.65
2:D:2576:ILE:O	2:D:2580:LEU:HB2	1.95	0.65
2:D:2984:SER:HA	2:D:2989:PRO:HB2	1.78	0.65
2:A:3174:HIS:CD2	2:A:3175:LEU:HG	2.30	0.65
2:B:15:ARG:NE	2:B:16:THR:H	1.92	0.65
2:C:2684:ASN:HD22	2:C:2911:GLU:HB3	1.62	0.65
2:C:4036:ASP:OD1	2:C:4040:LYS:NZ	2.30	0.65
2:D:2263:GLU:OE2	2:D:2327:ARG:NH2	2.29	0.65
2:D:4036:ASP:OD1	2:D:4040:LYS:NZ	2.30	0.65
2:D:4250:TYR:HA	2:D:4253:LEU:HB2	1.78	0.65
2:C:392:ILE:HG13	2:C:393:MET:H	1.62	0.65
2:C:644:LEU:HD13	2:C:1630:LEU:HD21	1.78	0.65
2:C:1029:ASN:ND2	4:C:5005:ATP:O1G	2.29	0.65
2:C:2968:LEU:HD21	2:C:3011:LEU:HD21	1.79	0.65
2:D:3198:PRO:HG2	2:D:3204:VAL:HA	1.79	0.65
2:D:4014:LEU:HD13	2:D:4122:ALA:HB2	1.78	0.65
1:G:19:LYS:HE2	1:G:19:LYS:HA	1.78	0.65
2:B:2856:LYS:HA	2:B:2859:GLU:HG2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2968:LEU:HD21	2:B:3011:LEU:HD21	1.79	0.65
2:B:3803:LEU:HB2	2:B:3884:SER:HB2	1.79	0.65
2:C:2521:CYS:HA	2:C:2525:LEU:HD12	1.79	0.65
2:D:2791:ARG:NH2	2:D:2899:ASN:O	2.23	0.65
2:A:2263:GLU:OE2	2:A:2327:ARG:NH2	2.29	0.65
2:C:3249:TRP:HA	2:C:3252:HIS:HB2	1.77	0.65
2:D:983:LEU:HD12	2:D:1055:ARG:HB3	1.78	0.65
2:B:2714:PRO:HG2	2:B:2717:LEU:HD23	1.78	0.65
2:B:3198:PRO:HG2	2:B:3204:VAL:HA	1.79	0.65
2:B:4036:ASP:OD1	2:B:4040:LYS:NZ	2.30	0.65
2:C:2943:PHE:HB2	2:C:2956:TYR:OH	1.96	0.65
2:C:3043:ARG:HD3	2:C:3117:PHE:CG	2.31	0.65
2:A:392:ILE:HG13	2:A:393:MET:H	1.61	0.65
2:A:2684:ASN:HD22	2:A:2911:GLU:HB3	1.62	0.65
2:A:4018:ASP:OD1	2:A:4019:MET:N	2.29	0.65
2:B:890:HIS:HA	2:B:893:TRP:HE3	1.61	0.65
2:B:2652:LEU:HG	2:B:2662:PHE:CE1	2.32	0.65
2:C:890:HIS:HA	2:C:893:TRP:HE3	1.61	0.65
2:C:2929:LEU:HD21	2:C:2971:ILE:HG12	1.79	0.65
2:D:332:ARG:HH22	2:D:337:LYS:HA	1.62	0.65
2:D:3803:LEU:HB2	2:D:3884:SER:HB2	1.79	0.65
2:A:1842:ILE:HD12	2:A:1845:LEU:HD12	1.77	0.65
2:A:2984:SER:HA	2:A:2989:PRO:HB2	1.78	0.65
2:A:3198:PRO:HG2	2:A:3204:VAL:HA	1.79	0.65
2:B:4250:TYR:HA	2:B:4253:LEU:HB2	1.78	0.65
2:C:938:GLU:HA	2:C:941:LYS:HB3	1.79	0.65
2:C:2984:SER:HA	2:C:2989:PRO:HB2	1.78	0.65
2:D:644:LEU:HD13	2:D:1630:LEU:HD21	1.78	0.65
2:D:2929:LEU:HD21	2:D:2971:ILE:HG12	1.79	0.65
2:C:3803:LEU:HB2	2:C:3884:SER:HB2	1.79	0.65
2:D:890:HIS:HA	2:D:893:TRP:HE3	1.61	0.65
2:A:644:LEU:HD13	2:A:1630:LEU:HD21	1.78	0.64
2:A:890:HIS:HA	2:A:893:TRP:HE3	1.61	0.64
2:A:2929:LEU:HD21	2:A:2971:ILE:HG12	1.79	0.64
2:B:392:ILE:HG13	2:B:393:MET:H	1.62	0.64
2:B:1114:ARG:NH1	2:B:1128:LEU:O	2.29	0.64
2:C:3187:LYS:HE3	2:C:3197:LEU:HD11	1.79	0.64
2:D:2652:LEU:HG	2:D:2662:PHE:CE1	2.32	0.64
2:A:332:ARG:HH22	2:A:337:LYS:HA	1.62	0.64
2:A:2642:ARG:HH12	2:A:2682:GLU:HB2	1.62	0.64
2:A:2651:ALA:O	2:A:2655:LYS:HG2	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:3249:TRP:HA	2:A:3252:HIS:HB2	1.77	0.64
2:A:3803:LEU:HB2	2:A:3884:SER:HB2	1.79	0.64
2:A:4014:LEU:HD13	2:A:4122:ALA:HB2	1.78	0.64
2:B:3249:TRP:HA	2:B:3252:HIS:HB2	1.78	0.64
2:D:1842:ILE:HD12	2:D:1845:LEU:HD12	1.77	0.64
2:D:2968:LEU:HD21	2:D:3011:LEU:HD21	1.79	0.64
2:A:3805:LEU:HD23	2:B:76:ARG:HH22	1.62	0.64
2:B:2521:CYS:HA	2:B:2525:LEU:HD12	1.79	0.64
2:B:4014:LEU:HD13	2:B:4122:ALA:HB2	1.78	0.64
2:C:2642:ARG:HH12	2:C:2682:GLU:HB2	1.63	0.64
2:D:938:GLU:HA	2:D:941:LYS:HB3	1.79	0.64
2:A:3043:ARG:HD3	2:A:3117:PHE:CG	2.31	0.64
2:A:3187:LYS:HE3	2:A:3197:LEU:HD11	1.79	0.64
2:D:893:TRP:HB3	2:D:917:CYS:HB3	1.77	0.64
2:D:2684:ASN:HD22	2:D:2911:GLU:HB3	1.62	0.64
2:A:4511:PHE:HZ	2:A:4746:ILE:HD12	1.63	0.64
2:B:1100:ARG:NH1	2:B:1234:GLU:O	2.30	0.64
2:B:1144:ARG:NH1	2:B:1191:ALA:O	2.31	0.64
2:C:2652:LEU:HG	2:C:2662:PHE:CE1	2.32	0.64
2:A:2714:PRO:HG2	2:A:2717:LEU:HD23	1.78	0.64
2:A:4250:TYR:HA	2:A:4253:LEU:HB2	1.78	0.64
2:B:4511:PHE:HZ	2:B:4746:ILE:HD12	1.63	0.64
2:D:3187:LYS:HE3	2:D:3197:LEU:HD11	1.79	0.64
2:C:988:LEU:H	2:C:1055:ARG:HH21	1.46	0.64
2:D:392:ILE:HG13	2:D:393:MET:H	1.62	0.64
2:D:2642:ARG:HH12	2:D:2682:GLU:HB2	1.62	0.64
2:D:4580:THR:OG1	2:D:4733:HIS:NE2	2.18	0.64
2:B:3043:ARG:HD3	2:B:3117:PHE:CG	2.31	0.64
2:D:1144:ARG:NH1	2:D:1191:ALA:O	2.31	0.64
2:A:2968:LEU:HD21	2:A:3011:LEU:HD21	1.79	0.64
2:A:3152:ARG:NH2	2:A:3236:GLU:HB3	2.13	0.64
2:B:938:GLU:HA	2:B:941:LYS:HB3	1.79	0.64
2:B:2929:LEU:HD21	2:B:2971:ILE:HG12	1.79	0.64
2:C:503:ASP:HA	2:C:561:ARG:HH12	1.63	0.64
2:D:963:LYS:HE2	2:D:977:LYS:HE3	1.80	0.64
2:D:1100:ARG:NH1	2:D:1234:GLU:O	2.31	0.64
1:F:19:LYS:HE2	1:F:19:LYS:HA	1.78	0.64
2:A:2652:LEU:HG	2:A:2662:PHE:CE1	2.32	0.64
2:C:332:ARG:HH22	2:C:337:LYS:HA	1.62	0.64
2:C:1100:ARG:NH1	2:C:1234:GLU:O	2.30	0.64
2:C:3152:ARG:NH2	2:C:3236:GLU:HB3	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:4250:TYR:HA	2:C:4253:LEU:HB2	1.78	0.64
2:D:15:ARG:NE	2:D:16:THR:H	1.92	0.64
2:D:2651:ALA:O	2:D:2655:LYS:HG2	1.96	0.64
2:A:605:GLY:HA2	2:A:1585:ARG:HD2	1.80	0.63
2:D:2657:TYR:HA	2:D:2662:PHE:CE2	2.33	0.63
2:D:4511:PHE:HZ	2:D:4746:ILE:HD12	1.63	0.63
2:A:938:GLU:HA	2:A:941:LYS:HB3	1.79	0.63
2:B:3152:ARG:NH2	2:B:3236:GLU:HB3	2.13	0.63
2:C:605:GLY:HA2	2:C:1585:ARG:HD2	1.80	0.63
2:D:503:ASP:HA	2:D:561:ARG:HH12	1.63	0.63
2:D:988:LEU:H	2:D:1055:ARG:HH21	1.46	0.63
2:B:988:LEU:H	2:B:1055:ARG:HH21	1.46	0.63
2:C:1246:ASP:OD1	2:C:1693:TYR:OH	2.17	0.63
2:B:605:GLY:HA2	2:B:1585:ARG:HD2	1.80	0.63
2:B:963:LYS:HE2	2:B:977:LYS:HE3	1.80	0.63
2:B:2926:LEU:HA	2:B:2929:LEU:HB3	1.80	0.63
2:D:605:GLY:HA2	2:D:1585:ARG:HD2	1.80	0.63
2:A:2768:LYS:HE3	2:A:2772:ARG:HH12	1.64	0.63
2:A:4036:ASP:OD1	2:A:4040:LYS:NZ	2.30	0.63
2:C:4511:PHE:HZ	2:C:4746:ILE:HD12	1.63	0.63
2:D:3639:LYS:HD2	2:D:4683:ARG:HH12	1.64	0.63
2:A:2521:CYS:HA	2:A:2525:LEU:HD12	1.79	0.63
2:A:4773:LEU:HD22	2:D:4753:LEU:HD22	1.80	0.63
2:C:1114:ARG:NH1	2:C:1128:LEU:O	2.29	0.63
2:D:3152:ARG:NH2	2:D:3236:GLU:HB3	2.13	0.63
2:B:332:ARG:HH22	2:B:337:LYS:HA	1.62	0.63
2:B:503:ASP:HA	2:B:561:ARG:HH12	1.63	0.63
2:D:2926:LEU:HA	2:D:2929:LEU:HB3	1.80	0.63
2:A:4726:MET:HB3	2:D:4291:PHE:CZ	2.34	0.63
2:B:2768:LYS:HE3	2:B:2772:ARG:HH12	1.64	0.63
2:C:1844:GLN:NE2	2:C:1851:PHE:O	2.32	0.63
2:D:2521:CYS:HA	2:D:2525:LEU:HD12	1.79	0.63
2:A:1844:GLN:NE2	2:A:1851:PHE:O	2.32	0.62
2:A:3784:LYS:HG2	2:A:3786:ASP:HB2	1.81	0.62
2:B:2642:ARG:HH12	2:B:2682:GLU:HB2	1.63	0.62
2:B:3187:LYS:HE3	2:B:3197:LEU:HD11	1.79	0.62
2:D:3784:LYS:HG2	2:D:3786:ASP:HB2	1.81	0.62
1:E:19:LYS:HA	1:E:19:LYS:HE2	1.79	0.62
2:A:1100:ARG:NH1	2:A:1234:GLU:O	2.31	0.62
2:B:1246:ASP:OD1	2:B:1693:TYR:OH	2.17	0.62
2:B:3639:LYS:HD2	2:B:4683:ARG:HH12	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2497:ARG:NH2	2:C:2878:THR:OG1	2.32	0.62
2:A:14:LEU:HD21	2:A:216:PRO:HG3	1.81	0.62
2:A:963:LYS:HE2	2:A:977:LYS:HE3	1.80	0.62
2:B:2497:ARG:NH2	2:B:2878:THR:OG1	2.33	0.62
2:C:3639:LYS:HD2	2:C:4683:ARG:HH12	1.64	0.62
2:D:2741:TRP:HB3	2:D:2754:GLN:HB2	1.81	0.62
2:A:1114:ARG:NH1	2:A:1128:LEU:O	2.29	0.62
2:A:4818:TYR:CE1	2:B:4847:ASP:CG	2.72	0.62
2:B:1943:ARG:NH1	2:B:1964:GLU:OE2	2.32	0.62
2:B:2071:GLN:O	2:B:3660:ARG:NH2	2.33	0.62
2:C:3122:ILE:HD12	2:C:3126:VAL:HG13	1.81	0.62
2:D:1114:ARG:NH1	2:D:1128:LEU:O	2.29	0.62
2:B:235:ARG:NH1	2:B:273:SER:OG	2.33	0.62
2:C:2926:LEU:HA	2:C:2929:LEU:HB3	1.80	0.62
2:C:3187:LYS:NZ	2:C:3191:GLU:O	2.33	0.62
2:D:14:LEU:HD21	2:D:216:PRO:HG3	1.81	0.62
2:D:235:ARG:NH1	2:D:273:SER:OG	2.33	0.62
2:D:1246:ASP:OD1	2:D:1693:TYR:OH	2.17	0.62
2:D:2497:ARG:NH2	2:D:2878:THR:OG1	2.32	0.62
2:A:3122:ILE:HD12	2:A:3126:VAL:HG13	1.81	0.62
2:B:3173:THR:HG23	2:B:3202:GLU:HG3	1.82	0.62
2:A:503:ASP:OD1	2:A:561:ARG:NH2	2.33	0.62
2:A:988:LEU:H	2:A:1055:ARG:HH21	1.46	0.62
2:A:3173:THR:HG23	2:A:3202:GLU:HG3	1.81	0.62
2:A:4491:LEU:HD11	2:D:4283:PHE:CZ	2.34	0.62
2:B:15:ARG:HD3	2:B:111:ARG:O	2.00	0.62
2:B:4767:LEU:O	2:B:4771:VAL:HG13	2.00	0.62
2:C:2071:GLN:O	2:C:3660:ARG:NH2	2.33	0.62
2:C:2657:TYR:HA	2:C:2662:PHE:CE2	2.34	0.62
2:A:503:ASP:HA	2:A:561:ARG:HH12	1.63	0.62
2:A:801:ARG:HG2	2:A:1618:LEU:HA	1.82	0.62
2:B:801:ARG:HG2	2:B:1618:LEU:HA	1.82	0.62
2:C:1144:ARG:NH1	2:C:1191:ALA:O	2.31	0.62
2:D:801:ARG:HD3	2:D:1618:LEU:HD12	1.82	0.62
2:A:2071:GLN:O	2:A:3660:ARG:NH2	2.33	0.62
2:A:2926:LEU:HA	2:A:2929:LEU:HB3	1.80	0.62
2:B:713:TRP:HH2	2:B:1251:LEU:HD21	1.65	0.62
2:A:1246:ASP:OD1	2:A:1693:TYR:OH	2.17	0.62
2:A:2497:ARG:NH2	2:A:2878:THR:OG1	2.33	0.62
2:B:503:ASP:OD1	2:B:561:ARG:NH2	2.33	0.62
2:B:1844:GLN:NE2	2:B:1851:PHE:O	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2657:TYR:HA	2:B:2662:PHE:CE2	2.33	0.62
2:B:2979:ARG:HH21	2:B:3039:THR:HG23	1.64	0.62
2:B:3784:LYS:HG2	2:B:3786:ASP:HB2	1.81	0.62
2:C:2768:LYS:HE3	2:C:2772:ARG:HH12	1.64	0.62
2:D:2071:GLN:O	2:D:3660:ARG:NH2	2.33	0.62
2:A:235:ARG:NH1	2:A:273:SER:OG	2.33	0.61
2:A:912:LYS:HZ2	2:A:914:GLN:HB2	1.65	0.61
2:A:2742:ILE:O	2:A:2754:GLN:N	2.33	0.61
2:A:2830:ASN:ND2	2:B:1435:GLY:HA3	2.15	0.61
2:B:2742:ILE:O	2:B:2754:GLN:N	2.33	0.61
2:C:15:ARG:HD3	2:C:111:ARG:O	2.00	0.61
2:D:891:GLU:HA	2:D:894:VAL:HG22	1.82	0.61
2:D:2768:LYS:HE3	2:D:2772:ARG:HH12	1.64	0.61
2:D:3187:LYS:NZ	2:D:3191:GLU:O	2.33	0.61
2:D:4767:LEU:O	2:D:4771:VAL:HG13	2.00	0.61
2:A:15:ARG:HD3	2:A:111:ARG:O	2.00	0.61
2:A:1144:ARG:NH1	2:A:1191:ALA:O	2.31	0.61
2:B:3187:LYS:NZ	2:B:3191:GLU:O	2.33	0.61
2:C:235:ARG:NH1	2:C:273:SER:OG	2.33	0.61
2:C:2741:TRP:HB3	2:C:2754:GLN:HB2	1.81	0.61
2:C:3174:HIS:CE1	2:C:3211:LEU:HD21	2.35	0.61
2:C:4767:LEU:O	2:C:4771:VAL:HG13	2.00	0.61
2:D:1165:MET:HB3	2:D:1236:TYR:CE1	2.35	0.61
2:D:2979:ARG:HH21	2:D:3039:THR:HG23	1.64	0.61
2:C:3784:LYS:HG2	2:C:3786:ASP:HB2	1.81	0.61
2:D:503:ASP:OD1	2:D:561:ARG:NH2	2.33	0.61
2:D:1844:GLN:NE2	2:D:1851:PHE:O	2.32	0.61
2:A:713:TRP:HH2	2:A:1251:LEU:HD21	1.65	0.61
2:A:891:GLU:HA	2:A:894:VAL:HG22	1.82	0.61
2:A:2979:ARG:HH21	2:A:3039:THR:HG23	1.64	0.61
2:B:137:ARG:NH2	2:B:198:ASN:OD1	2.33	0.61
2:B:891:GLU:HA	2:B:894:VAL:HG22	1.82	0.61
2:B:2765:GLU:HA	2:B:2768:LYS:HB2	1.83	0.61
2:B:3174:HIS:CE1	2:B:3211:LEU:HD21	2.35	0.61
2:C:713:TRP:HH2	2:C:1251:LEU:HD21	1.65	0.61
2:C:4187:GLU:OE2	2:C:4947:ARG:NH2	2.34	0.61
2:D:713:TRP:HH2	2:D:1251:LEU:HD21	1.65	0.61
2:D:1010:ASP:OD1	2:D:1013:ARG:NH2	2.34	0.61
2:D:1943:ARG:NH1	2:D:1964:GLU:OE2	2.32	0.61
2:A:3639:LYS:HD2	2:A:4683:ARG:HH12	1.64	0.61
2:B:1165:MET:HB3	2:B:1236:TYR:CE1	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:963:LYS:HE2	2:C:977:LYS:HE3	1.80	0.61
2:C:2787:TRP:HD1	2:C:2904:SER:O	1.84	0.61
2:C:2979:ARG:HH21	2:C:3039:THR:HG23	1.64	0.61
2:D:801:ARG:HG2	2:D:1618:LEU:HA	1.82	0.61
2:A:2787:TRP:HD1	2:A:2904:SER:O	1.84	0.61
2:B:1010:ASP:OD1	2:B:1013:ARG:NH2	2.34	0.61
2:B:3122:ILE:HD12	2:B:3126:VAL:HG13	1.81	0.61
2:C:14:LEU:HD21	2:C:216:PRO:HG3	1.81	0.61
2:C:891:GLU:HA	2:C:894:VAL:HG22	1.83	0.61
2:C:1943:ARG:NH1	2:C:1964:GLU:OE2	2.32	0.61
2:D:2742:ILE:O	2:D:2754:GLN:N	2.33	0.61
2:D:3174:HIS:CE1	2:D:3211:LEU:HD21	2.35	0.61
2:A:801:ARG:HD3	2:A:1618:LEU:HD12	1.82	0.61
2:A:1010:ASP:OD1	2:A:1013:ARG:NH2	2.34	0.61
2:A:2657:TYR:HA	2:A:2662:PHE:CE2	2.34	0.61
2:B:2720:PHE:HD1	2:B:2899:ASN:HD22	1.49	0.61
2:C:1165:MET:HB3	2:C:1236:TYR:CE1	2.35	0.61
2:D:2787:TRP:HD1	2:D:2904:SER:O	1.84	0.61
2:A:4767:LEU:O	2:A:4771:VAL:HG13	2.00	0.61
2:B:2741:TRP:HB3	2:B:2754:GLN:HB2	1.81	0.61
2:B:3001:LYS:HE3	2:B:3044:THR:HG21	1.83	0.61
2:C:66:THR:HG22	2:C:217:ILE:HG13	1.82	0.61
2:D:3926:GLY:O	2:D:3928:CYS:N	2.34	0.61
2:A:2720:PHE:HD1	2:A:2899:ASN:HD22	1.49	0.61
2:B:3926:GLY:O	2:B:3928:CYS:N	2.34	0.61
2:D:1685:LEU:HD22	2:D:1706:LEU:HB2	1.82	0.61
2:D:2765:GLU:HA	2:D:2768:LYS:HB2	1.83	0.61
2:D:3173:THR:HG23	2:D:3202:GLU:HG3	1.81	0.61
2:A:2741:TRP:HB3	2:A:2754:GLN:HB2	1.81	0.60
2:A:3187:LYS:NZ	2:A:3191:GLU:O	2.33	0.60
2:B:14:LEU:HD21	2:B:216:PRO:HG3	1.81	0.60
2:B:801:ARG:HD3	2:B:1618:LEU:HD12	1.82	0.60
2:B:2415:GLU:OE1	2:B:2418:ARG:NH1	2.34	0.60
2:B:2787:TRP:HD1	2:B:2904:SER:O	1.84	0.60
2:C:801:ARG:HG2	2:C:1618:LEU:HA	1.82	0.60
2:D:1119:ARG:NH2	2:D:1196:ASP:OD1	2.34	0.60
2:D:4187:GLU:OE2	2:D:4947:ARG:NH2	2.34	0.60
2:D:4639:SER:HB3	2:D:4642:ASN:HD21	1.66	0.60
2:A:137:ARG:NH2	2:A:198:ASN:OD1	2.33	0.60
2:A:1574:GLU:OE2	2:A:1581:GLN:NE2	2.34	0.60
2:B:4139:MET:HB3	2:B:4951:PHE:HA	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:137:ARG:NH2	2:C:198:ASN:OD1	2.33	0.60
2:C:3173:THR:HG23	2:C:3202:GLU:HG3	1.81	0.60
2:C:4743:LEU:HD23	2:D:4776:VAL:HG13	1.83	0.60
2:D:15:ARG:HD3	2:D:111:ARG:O	2.00	0.60
2:D:1102:TYR:HD1	2:D:1165:MET:HG3	1.67	0.60
2:D:2736:LYS:HE2	2:D:2756:LEU:HB3	1.84	0.60
2:D:2833:LEU:HD23	2:D:2897:GLN:HE22	1.66	0.60
2:A:1898:LEU:HD13	2:A:1902:VAL:HG12	1.84	0.60
2:A:4639:SER:HB3	2:A:4642:ASN:HD21	1.66	0.60
2:C:801:ARG:HD3	2:C:1618:LEU:HD12	1.82	0.60
2:C:1119:ARG:NH2	2:C:1196:ASP:OD1	2.34	0.60
2:C:3926:GLY:O	2:C:3928:CYS:N	2.34	0.60
2:D:66:THR:HG22	2:D:217:ILE:HG13	1.82	0.60
2:D:912:LYS:HZ2	2:D:914:GLN:HB2	1.65	0.60
2:D:3122:ILE:HD12	2:D:3126:VAL:HG13	1.81	0.60
2:A:1421:MET:O	2:A:1576:LYS:NZ	2.35	0.60
2:B:1685:LEU:HD22	2:B:1706:LEU:HB2	1.82	0.60
2:C:2415:GLU:OE1	2:C:2418:ARG:NH1	2.34	0.60
2:C:4639:SER:HB3	2:C:4642:ASN:HD21	1.66	0.60
2:D:137:ARG:NH2	2:D:198:ASN:OD1	2.33	0.60
2:D:2841:ALA:HB1	2:D:2886:ARG:HH22	1.66	0.60
2:A:4187:GLU:OE2	2:A:4947:ARG:NH2	2.34	0.60
2:B:1574:GLU:OE2	2:B:1581:GLN:NE2	2.34	0.60
2:C:1102:TYR:HD1	2:C:1165:MET:HG3	1.67	0.60
2:C:4617:ILE:HD13	2:C:4666:ILE:HD11	1.84	0.60
2:D:1898:LEU:HD13	2:D:1902:VAL:HG12	1.83	0.60
2:D:2720:PHE:HD1	2:D:2899:ASN:HD22	1.49	0.60
2:A:1165:MET:HB3	2:A:1236:TYR:CE1	2.35	0.60
2:A:2765:GLU:HA	2:A:2768:LYS:HB2	1.83	0.60
2:A:4639:SER:O	2:A:4642:ASN:ND2	2.35	0.60
2:D:4617:ILE:HD13	2:D:4666:ILE:HD11	1.83	0.60
2:A:1685:LEU:HD22	2:A:1706:LEU:HB2	1.82	0.60
2:A:2415:GLU:OE1	2:A:2418:ARG:NH1	2.34	0.60
2:B:4187:GLU:OE2	2:B:4947:ARG:NH2	2.34	0.60
2:C:1010:ASP:OD1	2:C:1013:ARG:NH2	2.34	0.60
2:C:1685:LEU:HD22	2:C:1706:LEU:HB2	1.82	0.60
2:C:3001:LYS:HE3	2:C:3044:THR:HG21	1.83	0.60
2:C:4639:SER:O	2:C:4642:ASN:ND2	2.35	0.60
2:D:4639:SER:O	2:D:4642:ASN:ND2	2.35	0.60
2:A:2445:ILE:HA	2:A:2451:VAL:HA	1.84	0.60
2:A:3174:HIS:CE1	2:A:3211:LEU:HD21	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4639:SER:HB3	2:B:4642:ASN:HD21	1.66	0.60
2:C:2445:ILE:HA	2:C:2451:VAL:HA	1.84	0.60
2:C:2736:LYS:HE2	2:C:2756:LEU:HB3	1.84	0.60
2:D:2415:GLU:OE1	2:D:2418:ARG:NH1	2.34	0.60
2:D:2445:ILE:HA	2:D:2451:VAL:HA	1.84	0.60
2:A:1102:TYR:HD1	2:A:1165:MET:HG3	1.67	0.60
2:A:2833:LEU:HD23	2:A:2897:GLN:HE22	1.66	0.60
2:B:1102:TYR:HD1	2:B:1165:MET:HG3	1.67	0.60
2:B:2732:TRP:O	2:B:2732:TRP:HD1	1.85	0.60
2:B:3245:TYR:O	2:B:3249:TRP:HE3	1.85	0.60
2:C:2732:TRP:O	2:C:2732:TRP:HD1	1.85	0.60
2:A:2678:PRO:HB3	2:A:2922:ALA:HB2	1.84	0.60
2:B:2736:LYS:HE2	2:B:2756:LEU:HB3	1.84	0.60
2:B:2833:LEU:HD23	2:B:2897:GLN:HE22	1.66	0.60
2:C:1574:GLU:OE2	2:C:1581:GLN:NE2	2.34	0.60
2:D:1574:GLU:OE2	2:D:1581:GLN:NE2	2.34	0.60
2:D:4139:MET:HB3	2:D:4951:PHE:HA	1.84	0.60
2:A:3926:GLY:O	2:A:3928:CYS:N	2.34	0.59
2:A:4139:MET:HB3	2:A:4951:PHE:HA	1.84	0.59
2:B:1119:ARG:NH2	2:B:1196:ASP:OD1	2.34	0.59
2:B:2841:ALA:HB1	2:B:2886:ARG:HH22	1.66	0.59
2:C:1245:ARG:NH1	2:C:1692:LYS:O	2.35	0.59
2:C:2765:GLU:HA	2:C:2768:LYS:HB2	1.83	0.59
2:A:4617:ILE:HD13	2:A:4666:ILE:HD11	1.84	0.59
2:B:66:THR:HG22	2:B:217:ILE:HG13	1.82	0.59
2:B:1245:ARG:NH1	2:B:1692:LYS:O	2.35	0.59
2:B:2445:ILE:HA	2:B:2451:VAL:HA	1.84	0.59
2:B:2678:PRO:HB3	2:B:2922:ALA:HB2	1.84	0.59
2:B:3002:GLU:O	2:B:3005:THR:OG1	2.19	0.59
2:C:1016:TRP:HB3	2:C:1032:LEU:HD11	1.84	0.59
2:C:2720:PHE:HD1	2:C:2899:ASN:HD22	1.49	0.59
2:D:3001:LYS:HE3	2:D:3044:THR:HG21	1.83	0.59
2:D:3002:GLU:O	2:D:3005:THR:OG1	2.19	0.59
2:D:3245:TYR:O	2:D:3249:TRP:HE3	1.85	0.59
2:A:370:LEU:HD22	2:A:395:HIS:HA	1.84	0.59
2:A:2732:TRP:O	2:A:2732:TRP:HD1	1.85	0.59
2:A:2736:LYS:HE2	2:A:2756:LEU:HB3	1.84	0.59
2:B:1795:LEU:HD23	2:B:1842:ILE:HD11	1.85	0.59
2:B:4639:SER:O	2:B:4642:ASN:ND2	2.35	0.59
2:C:930:ASN:HB3	2:C:934:GLN:HE22	1.67	0.59
2:C:2833:LEU:HD23	2:C:2897:GLN:HE22	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:3846:LEU:HB3	2:C:3854:PHE:CE2	2.37	0.59
2:D:1795:LEU:HD23	2:D:1842:ILE:HD11	1.85	0.59
2:A:1119:ARG:NH2	2:A:1196:ASP:OD1	2.34	0.59
2:B:1898:LEU:HD13	2:B:1902:VAL:HG12	1.83	0.59
2:C:2426:LEU:HD12	2:D:143:LEU:HD11	1.84	0.59
2:C:3245:TYR:O	2:C:3249:TRP:HE3	1.85	0.59
2:D:555:LEU:HD22	2:D:585:ALA:HB1	1.85	0.59
2:D:1016:TRP:HB3	2:D:1032:LEU:HD11	1.84	0.59
2:D:894:VAL:HA	2:D:918:LEU:HD23	1.84	0.59
2:D:1245:ARG:NH1	2:D:1692:LYS:O	2.36	0.59
2:A:718:VAL:HG23	2:A:793:SER:HB3	1.85	0.59
2:A:1245:ARG:NH1	2:A:1692:LYS:O	2.35	0.59
2:A:2841:ALA:HB1	2:A:2886:ARG:HH22	1.66	0.59
2:A:3179:ASN:HA	2:A:3260:ARG:HH22	1.67	0.59
2:B:1421:MET:O	2:B:1576:LYS:NZ	2.35	0.59
2:B:3846:LEU:HB3	2:B:3854:PHE:CE2	2.37	0.59
2:C:2742:ILE:O	2:C:2754:GLN:N	2.33	0.59
2:C:2841:ALA:HB1	2:C:2886:ARG:HH22	1.67	0.59
2:C:3728:GLN:OE1	2:C:3770:ASN:ND2	2.33	0.59
2:D:4640:PHE:CD2	2:D:4641:PRO:HD3	2.38	0.59
2:A:66:THR:HG22	2:A:217:ILE:HG13	1.82	0.59
2:A:661:LEU:O	2:A:788:PHE:N	2.30	0.59
2:A:3001:LYS:HE3	2:A:3044:THR:HG21	1.83	0.59
2:A:3846:LEU:HB3	2:A:3854:PHE:CE2	2.37	0.59
2:C:503:ASP:OD1	2:C:561:ARG:NH2	2.33	0.59
2:C:661:LEU:O	2:C:788:PHE:N	2.30	0.59
2:C:1898:LEU:HD13	2:C:1902:VAL:HG12	1.83	0.59
2:D:930:ASN:HB3	2:D:934:GLN:HE22	1.67	0.59
2:A:962:LYS:HB3	2:A:981:MET:HA	1.85	0.59
2:A:3245:TYR:O	2:A:3249:TRP:HE3	1.85	0.59
2:B:555:LEU:HD22	2:B:585:ALA:HB1	1.85	0.59
2:B:4617:ILE:HD13	2:B:4666:ILE:HD11	1.84	0.59
2:D:962:LYS:HB3	2:D:981:MET:HA	1.85	0.59
2:D:1500:ARG:NH2	2:D:1505:LEU:HD22	2.18	0.59
2:D:2732:TRP:O	2:D:2732:TRP:HD1	1.85	0.59
2:A:1943:ARG:NH1	2:A:1964:GLU:OE2	2.32	0.59
2:B:247:VAL:O	2:B:272:ARG:NH1	2.36	0.59
2:C:247:VAL:O	2:C:272:ARG:NH1	2.36	0.59
2:D:247:VAL:O	2:D:272:ARG:NH1	2.36	0.59
2:D:4511:PHE:CZ	2:D:4746:ILE:HD12	2.38	0.59
2:A:1500:ARG:NH2	2:A:1505:LEU:HD22	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1016:TRP:HB3	2:B:1032:LEU:HD11	1.84	0.59
2:B:4818:TYR:CE2	2:B:4819:VAL:HG23	2.38	0.59
2:C:370:LEU:HD22	2:C:395:HIS:HA	1.84	0.59
2:C:894:VAL:HA	2:C:918:LEU:HD23	1.84	0.59
2:C:1500:ARG:NH2	2:C:1505:LEU:HD22	2.18	0.59
2:C:1795:LEU:HD23	2:C:1842:ILE:HD11	1.85	0.59
2:C:2791:ARG:NH2	2:C:2899:ASN:O	2.23	0.59
2:D:2599:LEU:HB2	2:D:2655:LYS:NZ	2.18	0.59
2:D:2678:PRO:HB3	2:D:2922:ALA:HB2	1.84	0.59
2:D:3846:LEU:HB3	2:D:3854:PHE:CE2	2.37	0.59
2:A:3043:ARG:HD3	2:A:3117:PHE:CD2	2.38	0.58
2:A:4818:TYR:CE2	2:A:4819:VAL:HG23	2.38	0.58
2:B:2593:VAL:HA	2:B:2644:LEU:HD21	1.85	0.58
2:C:2678:PRO:HB3	2:C:2922:ALA:HB2	1.84	0.58
2:C:4511:PHE:CZ	2:C:4746:ILE:HD12	2.38	0.58
2:C:4679:PHE:HA	2:C:4682:ALA:HB3	1.85	0.58
2:D:608:HIS:HB2	2:D:1656:HIS:CD2	2.38	0.58
2:D:3179:ASN:HA	2:D:3260:ARG:HH22	1.67	0.58
2:A:2659:GLN:HG3	2:A:2663:LYS:NZ	2.18	0.58
2:A:4640:PHE:CD2	2:A:4641:PRO:HD3	2.38	0.58
2:B:4511:PHE:CZ	2:B:4746:ILE:HD12	2.38	0.58
2:C:4139:MET:HB3	2:C:4951:PHE:HA	1.84	0.58
2:C:4818:TYR:CE2	2:C:4819:VAL:HG23	2.38	0.58
2:D:2635:GLU:HA	2:D:2638:LEU:HB2	1.85	0.58
2:D:2659:GLN:HG3	2:D:2663:LYS:NZ	2.18	0.58
2:D:3250:TRP:NE1	2:D:3255:GLU:OE2	2.33	0.58
2:B:930:ASN:HB3	2:B:934:GLN:HE22	1.68	0.58
2:B:2599:LEU:HB2	2:B:2655:LYS:NZ	2.18	0.58
2:C:718:VAL:HG23	2:C:793:SER:HB3	1.85	0.58
2:C:2593:VAL:HA	2:C:2644:LEU:HD21	1.85	0.58
2:D:1963:LYS:HB2	2:D:1966:ARG:HH21	1.69	0.58
2:D:3071:THR:HA	2:D:3074:ASN:ND2	2.19	0.58
2:D:4818:TYR:CE2	2:D:4819:VAL:HG23	2.38	0.58
2:A:1016:TRP:HB3	2:A:1032:LEU:HD11	1.84	0.58
2:A:2599:LEU:HB2	2:A:2655:LYS:NZ	2.18	0.58
2:B:912:LYS:HZ2	2:B:914:GLN:HB2	1.67	0.58
2:C:1421:MET:O	2:C:1576:LYS:NZ	2.35	0.58
2:C:2599:LEU:HB2	2:C:2655:LYS:NZ	2.18	0.58
2:C:2739:ASN:HB2	2:C:2741:TRP:CZ3	2.39	0.58
2:C:2849:HIS:CE1	2:C:2877:LEU:HD11	2.39	0.58
2:D:718:VAL:HG23	2:D:793:SER:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1795:LEU:HD23	2:A:1842:ILE:HD11	1.85	0.58
2:A:1963:LYS:HB2	2:A:1966:ARG:HH21	1.69	0.58
2:A:2833:LEU:HB2	2:A:2838[A]:HIS:NE2	2.19	0.58
2:B:894:VAL:HA	2:B:918:LEU:HD23	1.84	0.58
2:B:1500:ARG:NH2	2:B:1505:LEU:HD22	2.18	0.58
2:B:2943:PHE:CE1	2:B:2954:PHE:HE1	2.21	0.58
2:B:3179:ASN:HA	2:B:3260:ARG:HH22	1.67	0.58
2:C:3179:ASN:HA	2:C:3260:ARG:HH22	1.67	0.58
2:D:2739:ASN:HB2	2:D:2741:TRP:CZ3	2.39	0.58
2:D:2849:HIS:CE1	2:D:2877:LEU:HD11	2.39	0.58
2:A:608:HIS:HB2	2:A:1656:HIS:CD2	2.38	0.58
2:A:894:VAL:HA	2:A:918:LEU:HD23	1.84	0.58
2:A:4511:PHE:CZ	2:A:4746:ILE:HD12	2.38	0.58
2:C:2830:ASN:ND2	2:D:1434:PRO:O	2.37	0.58
2:D:2552:VAL:HG13	2:D:2569:ILE:HD11	1.85	0.58
2:A:247:VAL:O	2:A:272:ARG:NH1	2.36	0.58
2:A:930:ASN:HB3	2:A:934:GLN:HE22	1.67	0.58
2:A:3294:ALA:HA	2:A:3297:LYS:HE2	1.85	0.58
2:B:2772:ARG:O	2:B:2776:LYS:N	2.27	0.58
2:C:2943:PHE:CE1	2:C:2954:PHE:HE1	2.21	0.58
1:H:4:GLU:OE1	1:H:4:GLU:N	2.37	0.58
1:H:8:ILE:HA	2:D:730:LEU:HD11	1.85	0.58
2:A:2443:PRO:HD3	2:A:2512:MET:HG2	1.86	0.58
2:A:3072:MET:HB3	2:A:3076:LYS:NZ	2.19	0.58
2:B:370:LEU:HD22	2:B:395:HIS:HA	1.84	0.58
2:B:1963:LYS:HB2	2:B:1966:ARG:HH21	1.69	0.58
2:B:2552:VAL:HG13	2:B:2569:ILE:HD11	1.85	0.58
2:B:2589:LEU:O	2:B:2593:VAL:HG23	2.04	0.58
2:B:2849:HIS:CE1	2:B:2877:LEU:HD11	2.39	0.58
2:B:4593:LEU:HG	2:B:4594:LYS:HE3	1.86	0.58
2:C:3805:LEU:HD21	2:C:3891:TYR:HB2	1.85	0.58
2:C:4640:PHE:CD2	2:C:4641:PRO:HD3	2.38	0.58
2:D:370:LEU:HD22	2:D:395:HIS:HA	1.84	0.58
2:D:3072:MET:HB3	2:D:3076:LYS:NZ	2.19	0.58
2:A:555:LEU:HD22	2:A:585:ALA:HB1	1.85	0.58
2:A:2791:ARG:NH2	2:A:2899:ASN:O	2.23	0.58
2:A:2943:PHE:CE1	2:A:2954:PHE:HE1	2.21	0.58
2:B:115:TYR:HB3	2:B:164:PRO:HD3	1.86	0.58
2:B:3147:TYR:HD1	2:B:3150:ARG:HH22	1.52	0.58
2:D:115:TYR:HB3	2:D:164:PRO:HD3	1.86	0.58
2:D:3728:GLN:OE1	2:D:3770:ASN:ND2	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2296:GLU:HG3	2:A:2390:THR:HG22	1.86	0.58
2:A:2849:HIS:CE1	2:A:2877:LEU:HD11	2.39	0.58
2:A:4593:LEU:HG	2:A:4594:LYS:HE3	1.86	0.58
2:B:2443:PRO:HD3	2:B:2512:MET:HG2	1.86	0.58
2:B:3117:PHE:CD1	2:B:3117:PHE:CA	2.87	0.58
2:C:555:LEU:HD22	2:C:585:ALA:HB1	1.85	0.58
2:C:962:LYS:HB3	2:C:981:MET:HA	1.84	0.58
2:C:2635:GLU:HA	2:C:2638:LEU:HB2	1.85	0.58
2:C:2659:GLN:HG3	2:C:2663:LYS:NZ	2.18	0.58
2:C:3071:THR:HA	2:C:3074:ASN:ND2	2.19	0.58
2:D:4679:PHE:HA	2:D:4682:ALA:HB3	1.85	0.58
2:A:1959:ALA:O	2:A:1966:ARG:NH2	2.37	0.57
2:A:3071:THR:HA	2:A:3074:ASN:ND2	2.19	0.57
2:B:3043:ARG:HD3	2:B:3117:PHE:CD2	2.38	0.57
2:B:3294:ALA:HA	2:B:3297:LYS:HE2	1.85	0.57
2:C:1963:LYS:HB2	2:C:1966:ARG:HH21	1.69	0.57
2:C:4083:PHE:HD1	2:C:4086:ARG:HH21	1.52	0.57
2:D:1421:MET:O	2:D:1576:LYS:NZ	2.35	0.57
2:D:1959:ALA:O	2:D:1966:ARG:NH2	2.37	0.57
2:D:2943:PHE:CE1	2:D:2954:PHE:HE1	2.21	0.57
1:E:4:GLU:N	1:E:4:GLU:OE1	2.37	0.57
2:A:2833:LEU:HB2	2:A:2838[B]:HIS:NE2	2.19	0.57
2:A:3117:PHE:CD1	2:A:3117:PHE:CA	2.87	0.57
2:A:3147:TYR:HD1	2:A:3150:ARG:HH22	1.52	0.57
2:B:962:LYS:HB3	2:B:981:MET:HA	1.85	0.57
2:C:2589:LEU:O	2:C:2593:VAL:HG23	2.04	0.57
2:C:2772:ARG:O	2:C:2776:LYS:N	2.27	0.57
2:C:3072:MET:HB3	2:C:3076:LYS:NZ	2.19	0.57
2:A:2589:LEU:O	2:A:2593:VAL:HG23	2.04	0.57
2:B:2296:GLU:HG3	2:B:2390:THR:HG22	1.86	0.57
2:B:4640:PHE:CD2	2:B:4641:PRO:HD3	2.38	0.57
2:B:4703:VAL:O	2:B:4707:MET:HB2	2.05	0.57
2:C:1975:MET:HA	2:C:1978:ASN:OD1	2.04	0.57
2:D:4083:PHE:HD1	2:D:4086:ARG:HH21	1.52	0.57
2:D:4593:LEU:HG	2:D:4594:LYS:HE3	1.86	0.57
2:A:3013:VAL:HA	2:A:3016:ARG:HD3	1.87	0.57
2:B:2659:GLN:HG3	2:B:2663:LYS:NZ	2.18	0.57
2:B:3072:MET:HB3	2:B:3076:LYS:NZ	2.19	0.57
2:C:115:TYR:HB3	2:C:164:PRO:HD3	1.86	0.57
2:C:608:HIS:HB2	2:C:1656:HIS:CD2	2.38	0.57
2:C:3043:ARG:HD3	2:C:3117:PHE:CD2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2443:PRO:HD3	2:D:2512:MET:HG2	1.86	0.57
2:D:3043:ARG:HD3	2:D:3117:PHE:CD2	2.38	0.57
2:A:2635:GLU:HA	2:A:2638:LEU:HB2	1.85	0.57
2:A:3805:LEU:HD21	2:A:3891:TYR:HB2	1.85	0.57
2:B:718:VAL:HG23	2:B:793:SER:HB3	1.84	0.57
2:B:2739:ASN:HB2	2:B:2741:TRP:CZ3	2.39	0.57
2:B:3608:LEU:HA	2:B:3611:LEU:HD12	1.86	0.57
2:C:2552:VAL:HG13	2:C:2569:ILE:HD11	1.85	0.57
2:C:3117:PHE:CD1	2:C:3117:PHE:CA	2.87	0.57
2:C:3117:PHE:CD1	2:C:3117:PHE:CB	2.79	0.57
2:C:3608:LEU:HA	2:C:3611:LEU:HD12	1.86	0.57
2:C:4703:VAL:O	2:C:4707:MET:HB2	2.05	0.57
2:D:2296:GLU:HG3	2:D:2390:THR:HG22	1.86	0.57
2:D:3294:ALA:HA	2:D:3297:LYS:HE2	1.86	0.57
2:A:4083:PHE:HD1	2:A:4086:ARG:HH21	1.52	0.57
2:C:3002:GLU:O	2:C:3005:THR:OG1	2.19	0.57
2:D:1963:LYS:HA	2:D:1966:ARG:HE	1.70	0.57
2:D:2593:VAL:HA	2:D:2644:LEU:HD21	1.85	0.57
2:D:3013:VAL:HA	2:D:3016:ARG:HD3	1.87	0.57
2:A:996:VAL:HG11	2:A:1051:ARG:HG2	1.87	0.57
2:A:2552:VAL:HG13	2:A:2569:ILE:HD11	1.85	0.57
2:A:3002:GLU:O	2:A:3005:THR:OG1	2.19	0.57
2:B:608:HIS:HB2	2:B:1656:HIS:CD2	2.38	0.57
2:B:3805:LEU:HD21	2:B:3891:TYR:HB2	1.85	0.57
2:B:4679:PHE:HA	2:B:4682:ALA:HB3	1.85	0.57
2:C:2296:GLU:HG3	2:C:2390:THR:HG22	1.86	0.57
2:C:3294:ALA:HA	2:C:3297:LYS:HE2	1.86	0.57
2:D:2232:PRO:HG2	2:D:2379:ASP:HA	1.87	0.57
2:D:2589:LEU:O	2:D:2593:VAL:HG23	2.04	0.57
2:A:2739:ASN:HB2	2:A:2741:TRP:CZ3	2.39	0.57
2:A:3000:GLU:HA	2:A:3003:MET:HG2	1.87	0.57
2:A:4703:VAL:O	2:A:4707:MET:HB2	2.05	0.57
2:B:2704:GLN:HA	2:B:2854:LYS:HZ2	1.70	0.57
2:D:655:MET:HG2	2:D:794:PHE:HE1	1.70	0.57
2:D:3805:LEU:HD21	2:D:3891:TYR:HB2	1.85	0.57
2:A:842:GLN:HB2	2:A:1603:PHE:HB2	1.87	0.57
2:A:2251:ASN:HB2	2:A:3819:MET:HE1	1.85	0.57
2:A:2593:VAL:HA	2:A:2644:LEU:HD21	1.85	0.57
2:A:3117:PHE:CD1	2:A:3117:PHE:CB	2.79	0.57
2:A:4520:TYR:HE2	2:A:4559:TYR:HB3	1.70	0.57
2:B:1959:ALA:O	2:B:1966:ARG:NH2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4083:PHE:HD1	2:B:4086:ARG:HH21	1.52	0.57
2:C:4187:GLU:OE1	2:C:4949:TRP:NE1	2.38	0.57
2:D:1975:MET:HA	2:D:1978:ASN:OD1	2.04	0.57
2:D:3117:PHE:CD1	2:D:3117:PHE:CA	2.87	0.57
2:D:4520:TYR:HE2	2:D:4559:TYR:HB3	1.70	0.57
1:F:4:GLU:OE1	1:F:4:GLU:N	2.37	0.56
2:A:115:TYR:HB3	2:A:164:PRO:HD3	1.86	0.56
2:A:992:GLN:HG3	2:A:1066:ALA:HB2	1.87	0.56
2:A:1129:GLY:HA3	2:A:1145:TRP:HB3	1.87	0.56
2:A:4048:PHE:O	2:A:4052:MET:HG3	2.05	0.56
2:B:878:LEU:HD23	2:B:881:ILE:HD11	1.87	0.56
2:B:3000:GLU:HA	2:B:3003:MET:HG2	1.87	0.56
2:C:996:VAL:HG11	2:C:1051:ARG:HG2	1.87	0.56
2:C:1959:ALA:O	2:C:1966:ARG:NH2	2.37	0.56
2:C:2443:PRO:HD3	2:C:2512:MET:HG2	1.86	0.56
2:C:3013:VAL:HA	2:C:3016:ARG:HD3	1.87	0.56
2:C:3147:TYR:HD1	2:C:3150:ARG:HH22	1.52	0.56
2:D:1129:GLY:HA3	2:D:1145:TRP:HB3	1.87	0.56
2:D:2704:GLN:HA	2:D:2854:LYS:HZ2	1.70	0.56
1:G:4:GLU:OE1	1:G:4:GLU:N	2.37	0.56
2:B:996:VAL:HG11	2:B:1051:ARG:HG2	1.87	0.56
2:B:1975:MET:HA	2:B:1978:ASN:OD1	2.04	0.56
2:B:3728:GLN:OE1	2:B:3770:ASN:ND2	2.33	0.56
2:C:2232:PRO:HG2	2:C:2379:ASP:HA	1.87	0.56
2:A:655:MET:HG2	2:A:794:PHE:HE1	1.70	0.56
2:A:1975:MET:HA	2:A:1978:ASN:OD1	2.04	0.56
2:A:1978:ASN:HB3	2:A:1983:LYS:HE3	1.87	0.56
2:A:4256:MET:SD	2:B:4703:VAL:HG23	2.45	0.56
2:B:2635:GLU:HA	2:B:2638:LEU:HB2	1.85	0.56
2:B:3071:THR:HA	2:B:3074:ASN:ND2	2.19	0.56
2:B:3117:PHE:CD2	2:B:3117:PHE:CB	2.79	0.56
2:B:4048:PHE:O	2:B:4052:MET:HG3	2.05	0.56
2:C:878:LEU:HD23	2:C:881:ILE:HD11	1.87	0.56
2:C:902:TRP:HZ3	2:C:913:ARG:HA	1.71	0.56
2:D:2772:ARG:O	2:D:2776:LYS:N	2.27	0.56
2:D:4610:LEU:HD21	2:D:4670:LEU:HD11	1.88	0.56
2:A:387:ILE:HG21	2:A:389:ARG:HE	1.71	0.56
2:A:3218:ILE:HD13	2:A:3221:LEU:HD21	1.88	0.56
2:A:4187:GLU:OE1	2:A:4949:TRP:NE1	2.38	0.56
2:A:4679:PHE:HA	2:A:4682:ALA:HB3	1.85	0.56
2:B:387:ILE:HG21	2:B:389:ARG:HE	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3013:VAL:HA	2:B:3016:ARG:HD3	1.87	0.56
2:B:3072:MET:SD	2:B:3140:LEU:HG	2.46	0.56
2:C:4520:TYR:HE2	2:C:4559:TYR:HB3	1.70	0.56
2:D:603:LYS:NZ	2:D:1574:GLU:OE2	2.39	0.56
2:D:3072:MET:SD	2:D:3140:LEU:HG	2.46	0.56
2:A:878:LEU:HD23	2:A:881:ILE:HD11	1.87	0.56
2:A:3072:MET:SD	2:A:3140:LEU:HG	2.46	0.56
2:A:4610:LEU:HD21	2:A:4670:LEU:HD11	1.88	0.56
2:B:118:ALA:HA	2:B:161:THR:HA	1.87	0.56
2:B:4610:LEU:HD21	2:B:4670:LEU:HD11	1.88	0.56
2:C:4048:PHE:O	2:C:4052:MET:HG3	2.06	0.56
2:C:4593:LEU:HG	2:C:4594:LYS:HE3	1.86	0.56
2:D:902:TRP:HZ3	2:D:913:ARG:HA	1.71	0.56
2:D:3147:TYR:HD1	2:D:3150:ARG:HH22	1.52	0.56
2:D:3218:ILE:HD13	2:D:3221:LEU:HD21	1.88	0.56
2:D:4664:ASP:HA	2:D:4674:LYS:HZ1	1.70	0.56
2:D:4703:VAL:O	2:D:4707:MET:HB2	2.05	0.56
2:B:137:ARG:NE	2:B:139:SER:OG	2.39	0.56
2:B:992:GLN:HG3	2:B:1066:ALA:HB2	1.88	0.56
2:C:3218:ILE:HD13	2:C:3221:LEU:HD21	1.88	0.56
2:D:996:VAL:HG13	2:D:1050:LEU:HD22	1.88	0.56
2:D:3000:GLU:HA	2:D:3003:MET:HG2	1.87	0.56
2:D:3608:LEU:HA	2:D:3611:LEU:HD12	1.86	0.56
2:A:654:SER:OG	2:A:837:SER:OG	2.15	0.56
2:A:964:MET:H	2:A:979:ALA:HB1	1.71	0.56
2:A:2232:PRO:HG2	2:A:2379:ASP:HA	1.86	0.56
2:A:3608:LEU:HA	2:A:3611:LEU:HD12	1.86	0.56
2:B:661:LEU:O	2:B:788:PHE:N	2.30	0.56
2:B:899:GLU:HG3	2:B:900:LEU:HD12	1.88	0.56
2:B:902:TRP:HZ3	2:B:913:ARG:HA	1.71	0.56
2:B:964:MET:H	2:B:979:ALA:HB1	1.71	0.56
2:B:4661:TYR:HB3	2:B:4665:ARG:NH2	2.21	0.56
2:C:3000:GLU:HA	2:C:3003:MET:HG2	1.87	0.56
2:C:4610:LEU:HD21	2:C:4670:LEU:HD11	1.88	0.56
2:D:1490:ALA:HB1	2:D:1505:LEU:HD21	1.88	0.56
2:A:2772:ARG:O	2:A:2776:LYS:N	2.27	0.56
2:A:3729:ALA:HA	2:A:3732:HIS:CE1	2.41	0.56
2:A:3939:ARG:NH2	2:B:172:GLY:O	2.39	0.56
2:A:4661:TYR:HB3	2:A:4665:ARG:NH2	2.21	0.56
2:B:882:ARG:HH12	2:B:886:ALA:HB2	1.71	0.56
2:B:2759:PRO:HG2	2:B:2762:LEU:HD13	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2787:TRP:NE1	2:B:2840:MET:SD	2.75	0.56
2:B:4520:TYR:HE2	2:B:4559:TYR:HB3	1.70	0.56
2:C:964:MET:H	2:C:979:ALA:HB1	1.71	0.56
2:C:996:VAL:HG13	2:C:1050:LEU:HD22	1.88	0.56
2:C:1963:LYS:HA	2:C:1966:ARG:HE	1.70	0.56
2:D:118:ALA:HA	2:D:161:THR:HA	1.87	0.56
2:D:2763:LEU:O	2:D:2768:LYS:HD2	2.06	0.56
2:A:375:GLN:OE1	2:A:392:ILE:HB	2.06	0.56
2:B:842:GLN:HB2	2:B:1603:PHE:HB2	1.87	0.56
2:B:1978:ASN:HB3	2:B:1983:LYS:HE3	1.87	0.56
2:B:3218:ILE:HD13	2:B:3221:LEU:HD21	1.88	0.56
2:C:899:GLU:HG3	2:C:900:LEU:HD12	1.88	0.56
2:C:1564:MET:CE	2:C:1565:PRO:HD2	2.35	0.56
2:C:2704:GLN:HA	2:C:2854:LYS:HZ2	1.71	0.56
2:C:3072:MET:SD	2:C:3140:LEU:HG	2.46	0.56
2:D:4048:PHE:O	2:D:4052:MET:HG3	2.05	0.56
2:A:882:ARG:HH12	2:A:886:ALA:HB2	1.71	0.56
2:A:902:TRP:HZ3	2:A:913:ARG:HA	1.71	0.56
2:A:3190:ARG:HH21	2:A:3193:ALA:HB3	1.71	0.56
2:B:2232:PRO:HG2	2:B:2379:ASP:HA	1.87	0.56
2:C:603:LYS:NZ	2:C:1574:GLU:OE2	2.39	0.56
2:C:842:GLN:HB2	2:C:1603:PHE:HB2	1.87	0.56
2:C:3318:HIS:C	2:C:3321:PRO:HD2	2.26	0.56
2:D:1685:LEU:O	2:D:1689:ILE:HG12	2.06	0.56
2:D:1718:ARG:NH2	2:D:1758:ARG:HH11	2.04	0.56
2:A:118:ALA:HA	2:A:161:THR:HA	1.88	0.55
2:A:603:LYS:NZ	2:A:1574:GLU:OE2	2.39	0.55
2:A:2763:LEU:O	2:A:2768:LYS:HD2	2.06	0.55
2:B:1718:ARG:NH2	2:B:1758:ARG:HH11	2.04	0.55
2:B:3729:ALA:HA	2:B:3732:HIS:CE1	2.41	0.55
2:C:2443:PRO:HG3	2:C:2454:PRO:HD2	1.87	0.55
2:D:882:ARG:HH12	2:D:886:ALA:HB2	1.71	0.55
2:D:921:PHE:HB2	2:D:929:ARG:HG3	1.88	0.55
2:D:1978:ASN:HB3	2:D:1983:LYS:HE3	1.87	0.55
2:A:1963:LYS:HA	2:A:1966:ARG:HE	1.70	0.55
2:B:655:MET:HG2	2:B:794:PHE:HE1	1.70	0.55
2:B:996:VAL:HG13	2:B:1050:LEU:HD22	1.88	0.55
2:B:2763:LEU:O	2:B:2768:LYS:HD2	2.06	0.55
2:C:655:MET:HG2	2:C:794:PHE:HE1	1.70	0.55
2:C:1685:LEU:O	2:C:1689:ILE:HG12	2.06	0.55
2:C:2763:LEU:O	2:C:2768:LYS:HD2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4661:TYR:HB3	2:D:4665:ARG:NH2	2.21	0.55
2:A:1929:SER:HG	2:A:3620:PHE:HD2	1.54	0.55
2:A:2443:PRO:HG3	2:A:2454:PRO:HD2	1.88	0.55
2:B:603:LYS:NZ	2:B:1574:GLU:OE2	2.39	0.55
2:B:1685:LEU:O	2:B:1689:ILE:HG12	2.06	0.55
2:B:4520:TYR:CE2	2:B:4559:TYR:HB3	2.42	0.55
2:C:3190:ARG:HH21	2:C:3193:ALA:HB3	1.71	0.55
2:C:3729:ALA:HA	2:C:3732:HIS:CE1	2.41	0.55
2:D:992:GLN:HG3	2:D:1066:ALA:HB2	1.87	0.55
2:D:996:VAL:HG11	2:D:1051:ARG:HG2	1.87	0.55
2:A:2759:PRO:HG2	2:A:2762:LEU:HD13	1.88	0.55
2:A:3325:LYS:HA	2:A:3328:LYS:HE2	1.88	0.55
2:B:375:GLN:OE1	2:B:392:ILE:HB	2.06	0.55
2:C:387:ILE:HG21	2:C:389:ARG:HE	1.71	0.55
2:C:654:SER:OG	2:C:837:SER:OG	2.15	0.55
2:C:1978:ASN:HB3	2:C:1983:LYS:HE3	1.87	0.55
2:D:899:GLU:HG3	2:D:900:LEU:HD12	1.88	0.55
2:D:3325:LYS:HA	2:D:3328:LYS:HE2	1.88	0.55
2:A:921:PHE:HB2	2:A:929:ARG:HG3	1.88	0.55
2:B:1129:GLY:HA3	2:B:1145:TRP:HB3	1.87	0.55
2:B:4187:GLU:OE1	2:B:4949:TRP:NE1	2.38	0.55
2:C:3697:LYS:HA	2:C:3700:HIS:CD2	2.42	0.55
2:D:964:MET:H	2:D:979:ALA:HB1	1.71	0.55
2:D:2918:GLU:HA	2:D:2923:TYR:CD2	2.41	0.55
2:A:1552:VAL:HG22	2:A:1553:PHE:HD2	1.72	0.55
2:A:1685:LEU:O	2:A:1689:ILE:HG12	2.06	0.55
2:A:2918:GLU:HA	2:A:2923:TYR:CD2	2.41	0.55
2:A:3312:PRO:HA	2:A:3315:LEU:HD13	1.89	0.55
2:A:3697:LYS:HA	2:A:3700:HIS:CD2	2.42	0.55
2:B:1490:ALA:HB1	2:B:1505:LEU:HD21	1.88	0.55
2:B:1963:LYS:HA	2:B:1966:ARG:HE	1.70	0.55
2:B:2251:ASN:HB2	2:B:3819:MET:HE1	1.88	0.55
2:B:2599:LEU:HB2	2:B:2655:LYS:HZ2	1.71	0.55
2:B:2918:GLU:HA	2:B:2923:TYR:CD2	2.41	0.55
2:C:118:ALA:HA	2:C:161:THR:HA	1.87	0.55
2:C:882:ARG:HH12	2:C:886:ALA:HB2	1.71	0.55
2:C:3312:PRO:HA	2:C:3315:LEU:HD13	1.89	0.55
2:D:842:GLN:HB2	2:D:1603:PHE:HB2	1.87	0.55
2:D:878:LEU:HD23	2:D:881:ILE:HD11	1.87	0.55
2:D:2541:HIS:HB3	2:D:2544:LEU:HB3	1.88	0.55
2:D:2836:ASP:OD2	2:D:2837:LEU:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:996:VAL:HG13	2:A:1050:LEU:HD22	1.88	0.55
2:A:2787:TRP:NE1	2:A:2840:MET:SD	2.75	0.55
2:A:2836:ASP:OD2	2:A:2837:LEU:N	2.40	0.55
2:A:3318:HIS:C	2:A:3321:PRO:HD2	2.27	0.55
2:A:4294:LEU:HD12	2:B:4714:PHE:CD1	2.42	0.55
2:B:890:HIS:HA	2:B:893:TRP:CE3	2.42	0.55
2:B:2443:PRO:HG3	2:B:2454:PRO:HD2	1.87	0.55
2:B:2541:HIS:HB3	2:B:2544:LEU:HB3	1.88	0.55
2:C:912:LYS:HZ2	2:C:914:GLN:HB2	1.71	0.55
2:C:1008:ALA:O	2:C:1012:ILE:HG12	2.07	0.55
2:C:1129:GLY:HA3	2:C:1145:TRP:HB3	1.87	0.55
2:C:2918:GLU:HA	2:C:2923:TYR:CD2	2.41	0.55
2:C:4520:TYR:CE2	2:C:4559:TYR:HB3	2.42	0.55
2:D:3190:ARG:HH21	2:D:3193:ALA:HB3	1.71	0.55
2:D:3318:HIS:C	2:D:3321:PRO:HD2	2.27	0.55
2:A:4520:TYR:CE2	2:A:4559:TYR:HB3	2.42	0.55
2:B:1552:VAL:HG22	2:B:1553:PHE:HD2	1.72	0.55
2:B:1929:SER:HG	2:B:3620:PHE:HD2	1.55	0.55
2:B:3190:ARG:HH21	2:B:3193:ALA:HB3	1.71	0.55
2:D:15:ARG:HH21	2:D:16:THR:HB	1.72	0.55
2:D:2710:ASN:OD1	2:D:2711:ILE:N	2.40	0.55
2:D:3697:LYS:HA	2:D:3700:HIS:CD2	2.42	0.55
2:B:16:THR:OG1	2:B:69:LEU:O	2.22	0.55
2:B:2478:ILE:HD12	2:B:2527:LEU:HD11	1.88	0.55
2:C:992:GLN:HG3	2:C:1066:ALA:HB2	1.88	0.55
2:C:1490:ALA:HB1	2:C:1505:LEU:HD21	1.88	0.55
2:C:2759:PRO:HG2	2:C:2762:LEU:HD13	1.88	0.55
2:C:3325:LYS:HA	2:C:3328:LYS:HE2	1.88	0.55
2:C:4661:TYR:HB3	2:C:4665:ARG:NH2	2.21	0.55
2:D:3729:ALA:HA	2:D:3732:HIS:CE1	2.41	0.55
2:A:3728:GLN:OE1	2:A:3770:ASN:ND2	2.33	0.55
2:D:137:ARG:NE	2:D:139:SER:OG	2.39	0.55
2:D:2759:PRO:HG2	2:D:2762:LEU:HD13	1.88	0.55
2:D:3125:ASP:HA	2:D:3128:VAL:HG12	1.89	0.55
2:A:137:ARG:NE	2:A:139:SER:OG	2.39	0.54
2:A:899:GLU:HG3	2:A:900:LEU:HD12	1.88	0.54
2:A:1008:ALA:O	2:A:1012:ILE:HG12	2.07	0.54
2:A:2704:GLN:HA	2:A:2854:LYS:HZ2	1.72	0.54
2:A:3315:LEU:HA	2:A:3319:PHE:HB3	1.89	0.54
2:B:2710:ASN:OD1	2:B:2711:ILE:N	2.40	0.54
2:B:3312:PRO:HA	2:B:3315:LEU:HD13	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4294:LEU:HD12	2:C:4714:PHE:CD1	2.42	0.54
2:C:2149:ILE:HD13	2:C:2167:MET:HE1	1.89	0.54
2:C:4071:GLU:OE1	2:C:4086:ARG:NH2	2.30	0.54
2:D:375:GLN:OE1	2:D:392:ILE:HB	2.06	0.54
2:D:387:ILE:HG21	2:D:389:ARG:HE	1.71	0.54
2:D:668:ALA:HB2	2:D:1012:ILE:HD11	1.89	0.54
2:D:1220:ASP:O	2:D:1223:THR:OG1	2.26	0.54
2:D:3315:LEU:HA	2:D:3319:PHE:HB3	1.89	0.54
2:D:4520:TYR:CE2	2:D:4559:TYR:HB3	2.42	0.54
2:B:921:PHE:HB2	2:B:929:ARG:HG3	1.88	0.54
2:B:1001:GLU:OE2	2:B:1005:ASN:ND2	2.36	0.54
2:B:2608:LYS:O	2:B:2612:ASN:ND2	2.40	0.54
2:C:375:GLN:OE1	2:C:392:ILE:HB	2.06	0.54
2:C:2608:LYS:O	2:C:2612:ASN:ND2	2.40	0.54
2:D:514:PHE:HD2	2:D:526:TRP:HB2	1.72	0.54
2:D:1552:VAL:HG22	2:D:1553:PHE:HD2	1.72	0.54
2:D:2478:ILE:HD12	2:D:2527:LEU:HD11	1.88	0.54
2:D:3312:PRO:HA	2:D:3315:LEU:HD13	1.89	0.54
2:D:3637:GLU:HG2	2:D:3697:LYS:HE2	1.90	0.54
2:A:15:ARG:HH21	2:A:16:THR:HB	1.72	0.54
2:A:1490:ALA:HB1	2:A:1505:LEU:HD21	1.88	0.54
2:A:3125:ASP:HA	2:A:3128:VAL:HG12	1.89	0.54
2:B:1176:THR:HG22	2:B:1181:ILE:HD13	1.89	0.54
2:C:1718:ARG:NH2	2:C:1758:ARG:HH11	2.04	0.54
2:C:2787:TRP:NE1	2:C:2840:MET:SD	2.75	0.54
2:D:2720:PHE:HB2	2:D:2901:TYR:HE2	1.73	0.54
2:A:2149:ILE:HD13	2:A:2167:MET:HE1	1.88	0.54
2:A:2478:ILE:HD12	2:A:2527:LEU:HD11	1.88	0.54
2:A:3250:TRP:NE1	2:A:3255:GLU:OE2	2.33	0.54
2:B:3325:LYS:HA	2:B:3328:LYS:HE2	1.88	0.54
2:B:3697:LYS:HA	2:B:3700:HIS:CD2	2.42	0.54
2:C:1176:THR:HG22	2:C:1181:ILE:HD13	1.89	0.54
2:A:1001:GLU:OE2	2:A:1005:ASN:ND2	2.36	0.54
2:A:2541:HIS:HB3	2:A:2544:LEU:HB3	1.88	0.54
2:A:3637:GLU:HG2	2:A:3697:LYS:HE2	1.90	0.54
2:B:514:PHE:HD2	2:B:526:TRP:HB2	1.72	0.54
2:B:1008:ALA:O	2:B:1012:ILE:HG12	2.07	0.54
2:B:2642:ARG:NH1	2:B:2682:GLU:HB2	2.23	0.54
2:B:2720:PHE:HB2	2:B:2901:TYR:HE2	1.73	0.54
2:B:3318:HIS:C	2:B:3321:PRO:HD2	2.27	0.54
2:C:921:PHE:HB2	2:C:929:ARG:HG3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2418:ARG:HD3	2:D:189:GLU:OE1	2.08	0.54
2:C:2836:ASP:OD2	2:C:2837:LEU:N	2.40	0.54
2:D:2443:PRO:HG3	2:D:2454:PRO:HD2	1.88	0.54
2:A:2608:LYS:O	2:A:2612:ASN:ND2	2.40	0.54
2:A:4723:ALA:HB1	2:D:4294:LEU:HD22	1.90	0.54
2:C:917:CYS:HA	2:C:924:LEU:HD12	1.90	0.54
2:C:2710:ASN:OD1	2:C:2711:ILE:N	2.40	0.54
2:D:1008:ALA:O	2:D:1012:ILE:HG12	2.07	0.54
2:A:1718:ARG:NH2	2:A:1758:ARG:HH11	2.04	0.54
2:A:2943:PHE:HE2	2:A:3021:LEU:HD22	1.73	0.54
2:D:1564:MET:CE	2:D:1565:PRO:HD2	2.35	0.54
2:A:514:PHE:HD2	2:A:526:TRP:HB2	1.72	0.54
2:A:1793:GLN:NE2	2:A:1797:GLU:OE2	2.41	0.54
2:A:2325:ILE:HD13	2:A:2426:LEU:HD11	1.90	0.54
2:A:2710:ASN:OD1	2:A:2711:ILE:N	2.40	0.54
2:A:2830:ASN:HB2	2:B:1435:GLY:HA3	1.89	0.54
2:B:15:ARG:HH21	2:B:16:THR:HB	1.72	0.54
2:B:2998:ASN:OD1	2:B:2999:LYS:N	2.41	0.54
2:B:3122:ILE:HG23	2:B:3122:ILE:O	2.08	0.54
2:C:307:SER:HB2	2:C:327:THR:HG22	1.90	0.54
2:C:737:ILE:HD12	2:C:1482:ARG:HD3	1.90	0.54
2:C:2642:ARG:NH1	2:C:2682:GLU:HB2	2.23	0.54
2:D:1176:THR:HG22	2:D:1181:ILE:HD13	1.89	0.54
2:D:1958:THR:HA	2:D:1961:LYS:HG2	1.90	0.54
2:D:2608:LYS:O	2:D:2612:ASN:ND2	2.40	0.54
2:A:737:ILE:HD12	2:A:1482:ARG:HD3	1.90	0.54
2:A:2720:PHE:HB2	2:A:2901:TYR:HE2	1.73	0.54
2:A:3122:ILE:O	2:A:3122:ILE:HG23	2.08	0.54
2:B:2325:ILE:HD13	2:B:2426:LEU:HD11	1.90	0.54
2:B:3188:SER:OG	2:B:3191:GLU:HG3	2.08	0.54
2:C:514:PHE:HD2	2:C:526:TRP:HB2	1.72	0.54
2:C:2541:HIS:HB3	2:C:2544:LEU:HB3	1.88	0.54
2:D:2943:PHE:HE2	2:D:3021:LEU:HD22	1.73	0.54
2:D:2998:ASN:OD1	2:D:2999:LYS:N	2.41	0.54
2:D:3122:ILE:HG23	2:D:3122:ILE:O	2.08	0.54
2:D:3250:TRP:HE3	2:D:3309:LYS:HZ3	1.55	0.54
2:A:131:CYS:SG	2:A:150:GLN:HB2	2.48	0.54
2:A:4625:ASP:O	2:A:4629:GLN:NE2	2.41	0.54
2:A:4664:ASP:HA	2:A:4674:LYS:HZ1	1.72	0.54
2:A:4858:LEU:HA	2:A:4861:ILE:HB	1.90	0.54
2:B:737:ILE:HD12	2:B:1482:ARG:HD3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:882:ARG:HG3	2:B:937:LEU:HD21	1.90	0.54
2:B:917:CYS:HA	2:B:924:LEU:HD12	1.90	0.54
2:B:2149:ILE:HD13	2:B:2167:MET:HE1	1.89	0.54
2:B:3637:GLU:HG2	2:B:3697:LYS:HE2	1.90	0.54
2:C:882:ARG:HG3	2:C:937:LEU:HD21	1.90	0.54
2:C:2478:ILE:HD12	2:C:2527:LEU:HD11	1.88	0.54
2:C:3315:LEU:HA	2:C:3319:PHE:HB3	1.89	0.54
2:D:2325:ILE:HD13	2:D:2426:LEU:HD11	1.90	0.54
2:D:4187:GLU:OE1	2:D:4949:TRP:NE1	2.38	0.54
2:A:1161:VAL:HG21	2:A:1225:LYS:HE3	1.90	0.53
2:A:3174:HIS:HE1	2:A:3211:LEU:HD21	1.73	0.53
2:B:2943:PHE:HE2	2:B:3021:LEU:HD22	1.73	0.53
2:B:3012:GLY:O	2:B:3016:ARG:HD2	2.09	0.53
2:B:3117:PHE:CD1	2:B:3117:PHE:CB	2.79	0.53
2:B:3174:HIS:HE1	2:B:3211:LEU:HD21	1.73	0.53
2:C:668:ALA:HB2	2:C:1012:ILE:HD11	1.89	0.53
2:C:2325:ILE:HD13	2:C:2426:LEU:HD11	1.90	0.53
2:C:3637:GLU:HG2	2:C:3697:LYS:HE2	1.90	0.53
2:C:4625:ASP:O	2:C:4629:GLN:NE2	2.41	0.53
2:C:4903:HIS:HE1	2:D:4183:LYS:HG2	1.73	0.53
2:D:1793:GLN:NE2	2:D:1797:GLU:OE2	2.41	0.53
2:D:2688:MET:HB2	2:D:2689:MET:HE2	1.90	0.53
2:D:4625:ASP:O	2:D:4629:GLN:NE2	2.41	0.53
2:D:4858:LEU:HA	2:D:4861:ILE:HB	1.90	0.53
2:A:4480:PHE:CE2	2:D:4268:MET:HG3	2.43	0.53
2:B:2765:GLU:HA	2:B:2768:LYS:HD3	1.89	0.53
2:B:2836:ASP:OD2	2:B:2837:LEU:N	2.40	0.53
2:C:2765:GLU:HA	2:C:2768:LYS:HD3	1.89	0.53
2:C:3122:ILE:HG23	2:C:3122:ILE:O	2.08	0.53
2:C:4903:HIS:CE1	2:D:4183:LYS:HG2	2.44	0.53
1:H:24:VAL:HG22	1:H:48:LYS:HG2	1.90	0.53
2:A:1564:MET:CE	2:A:1565:PRO:HD2	2.35	0.53
2:A:1958:THR:HA	2:A:1961:LYS:HG2	1.90	0.53
2:A:2998:ASN:OD1	2:A:2999:LYS:N	2.41	0.53
2:C:1552:VAL:HG22	2:C:1553:PHE:HD2	1.72	0.53
2:C:3125:ASP:HA	2:C:3128:VAL:HG12	1.90	0.53
2:D:890:HIS:HA	2:D:893:TRP:CE3	2.42	0.53
2:D:1034:PRO:HG2	2:D:1037:LEU:HD13	1.91	0.53
2:D:3012:GLY:O	2:D:3016:ARG:HD2	2.08	0.53
2:A:882:ARG:HG3	2:A:937:LEU:HD21	1.90	0.53
2:A:1176:THR:HG22	2:A:1181:ILE:HD13	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2642:ARG:NH1	2:A:2682:GLU:HB2	2.22	0.53
2:A:2765:GLU:HA	2:A:2768:LYS:HD3	1.89	0.53
2:B:1793:GLN:NE2	2:B:1797:GLU:OE2	2.41	0.53
2:C:2943:PHE:HE2	2:C:3021:LEU:HD22	1.73	0.53
2:D:917:CYS:HA	2:D:924:LEU:HD12	1.90	0.53
2:D:920:GLU:OE2	2:D:975:GLY:N	2.38	0.53
2:D:1006:VAL:HA	2:D:1009:ARG:NH1	2.24	0.53
2:D:2642:ARG:NH1	2:D:2682:GLU:HB2	2.23	0.53
2:B:668:ALA:HB2	2:B:1012:ILE:HD11	1.89	0.53
2:B:3315:LEU:HA	2:B:3319:PHE:HB3	1.89	0.53
2:C:1006:VAL:HA	2:C:1009:ARG:NH1	2.24	0.53
2:C:2720:PHE:HB2	2:C:2901:TYR:HE2	1.73	0.53
2:D:3188:SER:OG	2:D:3191:GLU:HG3	2.08	0.53
2:A:668:ALA:HB2	2:A:1012:ILE:HD11	1.89	0.53
2:A:2999:LYS:NZ	2:A:3003:MET:HB3	2.24	0.53
2:B:131:CYS:SG	2:B:150:GLN:HB2	2.48	0.53
2:B:2999:LYS:NZ	2:B:3003:MET:HB3	2.24	0.53
2:B:3125:ASP:HA	2:B:3128:VAL:HG12	1.89	0.53
2:B:3272:HIS:O	2:B:3275:THR:OG1	2.25	0.53
2:D:131:CYS:SG	2:D:150:GLN:HB2	2.48	0.53
2:D:2599:LEU:HB2	2:D:2655:LYS:HZ1	1.74	0.53
2:D:3238:ILE:HG22	2:D:3242:LEU:HD23	1.89	0.53
2:A:16:THR:HA	2:A:69:LEU:HB2	1.91	0.53
2:A:2659:GLN:HG3	2:A:2663:LYS:HZ1	1.74	0.53
2:A:3188:SER:OG	2:A:3191:GLU:HG3	2.08	0.53
2:B:902:TRP:CZ3	2:B:913:ARG:HA	2.44	0.53
2:B:3238:ILE:HG22	2:B:3242:LEU:HD23	1.89	0.53
2:B:4664:ASP:HA	2:B:4674:LYS:HZ1	1.73	0.53
2:C:15:ARG:HH21	2:C:16:THR:HB	1.72	0.53
2:D:2999:LYS:NZ	2:D:3003:MET:HB3	2.24	0.53
2:A:1964:GLU:HG3	2:A:1975:MET:HE3	1.91	0.53
2:A:2642:ARG:HG2	2:A:2676:LEU:HD13	1.91	0.53
2:C:131:CYS:SG	2:C:150:GLN:HB2	2.48	0.53
2:C:1161:VAL:HG21	2:C:1225:LYS:HE3	1.90	0.53
2:C:2998:ASN:OD1	2:C:2999:LYS:N	2.41	0.53
2:C:3012:GLY:O	2:C:3016:ARG:HD2	2.09	0.53
2:D:737:ILE:HD12	2:D:1482:ARG:HD3	1.90	0.53
1:F:24:VAL:HG22	1:F:48:LYS:HG2	1.90	0.53
2:A:804:LEU:HD13	2:A:832:LEU:HD21	1.91	0.53
2:A:902:TRP:CZ3	2:A:913:ARG:HA	2.44	0.53
2:A:917:CYS:HA	2:A:924:LEU:HD12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:4155:SER:O	2:A:4159:GLN:HG2	2.09	0.53
2:A:4818:TYR:CD1	2:B:4847:ASP:OD1	2.62	0.53
2:B:15:ARG:HA	2:B:113:LEU:HD13	1.90	0.53
2:B:769:ARG:HG2	2:B:774:PRO:HA	1.91	0.53
2:C:15:ARG:HA	2:C:113:LEU:HD13	1.90	0.53
2:C:804:LEU:HD13	2:C:832:LEU:HD21	1.91	0.53
2:D:606:ARG:HH11	2:D:644:LEU:HD21	1.74	0.53
2:A:1220:ASP:O	2:A:1223:THR:OG1	2.26	0.53
2:A:3043:ARG:CG	2:A:3117:PHE:CZ	2.92	0.53
2:B:307:SER:HB2	2:B:327:THR:HG22	1.90	0.53
2:B:423:VAL:HG22	2:B:494:MET:HE1	1.91	0.53
2:B:606:ARG:HH11	2:B:644:LEU:HD21	1.74	0.53
2:B:2290:TRP:CZ2	2:B:2388:ILE:HG12	2.44	0.53
2:B:2642:ARG:HG2	2:B:2676:LEU:HD13	1.90	0.53
2:B:3043:ARG:CG	2:B:3117:PHE:CZ	2.92	0.53
2:B:3152:ARG:NH2	2:B:3233:HIS:HA	2.24	0.53
2:C:15:ARG:NH1	2:C:111:ARG:HG3	2.24	0.53
2:C:137:ARG:NE	2:C:139:SER:OG	2.39	0.53
2:C:1034:PRO:HG2	2:C:1037:LEU:HD13	1.91	0.53
2:C:1945:ASN:O	2:C:1949:GLN:HG2	2.09	0.53
2:D:2642:ARG:HG2	2:D:2676:LEU:HD13	1.91	0.53
2:D:3043:ARG:CG	2:D:3117:PHE:CZ	2.92	0.53
2:D:3152:ARG:NH2	2:D:3233:HIS:HA	2.24	0.53
2:D:3293:GLY:H	2:D:3296:MET:HE1	1.74	0.53
1:H:91:VAL:HG21	2:D:1768:PHE:CE1	2.44	0.52
2:A:423:VAL:HG22	2:A:494:MET:HE1	1.91	0.52
2:A:606:ARG:HH11	2:A:644:LEU:HD21	1.74	0.52
2:A:1006:VAL:HA	2:A:1009:ARG:NH1	2.24	0.52
2:A:3012:GLY:O	2:A:3016:ARG:HD2	2.09	0.52
2:A:4038:ASP:HB3	2:A:4040:LYS:HZ2	1.73	0.52
2:B:1006:VAL:HA	2:B:1009:ARG:NH1	2.24	0.52
2:B:3322:LEU:HB3	2:B:3323:MET:HE2	1.90	0.52
2:B:4858:LEU:HA	2:B:4861:ILE:HB	1.90	0.52
2:C:2599:LEU:HD12	2:C:2661:LEU:HD11	1.92	0.52
2:D:804:LEU:HD13	2:D:832:LEU:HD21	1.91	0.52
2:D:1161:VAL:HG21	2:D:1225:LYS:HE3	1.90	0.52
2:D:2251:ASN:HB2	2:D:3819:MET:HE1	1.91	0.52
2:D:2290:TRP:CZ2	2:D:2388:ILE:HG12	2.44	0.52
2:A:15:ARG:NH1	2:A:111:ARG:HG3	2.24	0.52
2:A:241:MET:HE2	2:A:241:MET:CA	2.39	0.52
2:A:1034:PRO:HG2	2:A:1037:LEU:HD13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2833:LEU:CD2	2:A:2897:GLN:HE22	2.23	0.52
2:A:3293:GLY:H	2:A:3296:MET:HE1	1.74	0.52
2:B:15:ARG:NH1	2:B:111:ARG:HG3	2.24	0.52
2:B:804:LEU:HD13	2:B:832:LEU:HD21	1.91	0.52
2:B:920:GLU:OE2	2:B:975:GLY:N	2.38	0.52
2:B:2618:TRP:HD1	2:B:2619:LYS:HZ2	1.56	0.52
2:B:2646:TRP:HH2	2:B:2925:PHE:HA	1.74	0.52
2:C:2274:LEU:HG	2:C:2329:GLU:HG3	1.92	0.52
2:D:1287:GLN:NE2	2:D:1549:SER:O	2.43	0.52
2:D:1929:SER:HG	2:D:3620:PHE:HD2	1.55	0.52
2:A:307:SER:HB2	2:A:327:THR:HG22	1.90	0.52
2:A:2274:LEU:HG	2:A:2329:GLU:HG3	1.92	0.52
2:B:1220:ASP:O	2:B:1223:THR:OG1	2.26	0.52
2:B:4625:ASP:O	2:B:4629:GLN:NE2	2.41	0.52
2:C:122:ARG:HD3	2:C:127:GLY:HA2	1.91	0.52
2:C:679:VAL:HA	2:C:800:VAL:HG12	1.91	0.52
2:C:2642:ARG:HG2	2:C:2676:LEU:HD13	1.90	0.52
2:D:2765:GLU:HA	2:D:2768:LYS:HD3	1.89	0.52
2:D:4155:SER:O	2:D:4159:GLN:HG2	2.09	0.52
2:D:4181:GLY:O	2:D:4185:LYS:N	2.41	0.52
2:B:1161:VAL:HG21	2:B:1225:LYS:HE3	1.90	0.52
2:B:1958:THR:HA	2:B:1961:LYS:HG2	1.90	0.52
2:B:2646:TRP:CH2	2:B:2925:PHE:HA	2.45	0.52
2:B:4704:LYS:O	2:B:4707:MET:HB3	2.09	0.52
2:C:1001:GLU:OE2	2:C:1005:ASN:ND2	2.36	0.52
2:C:3238:ILE:HG22	2:C:3242:LEU:HD23	1.89	0.52
2:C:4858:LEU:HA	2:C:4861:ILE:HB	1.90	0.52
2:D:15:ARG:NH1	2:D:111:ARG:HG3	2.24	0.52
2:D:679:VAL:HA	2:D:800:VAL:HG12	1.91	0.52
2:D:882:ARG:HG3	2:D:937:LEU:HD21	1.90	0.52
2:D:2787:TRP:NE1	2:D:2840:MET:SD	2.75	0.52
2:D:4672:MET:HE1	2:D:4677:LEU:HD21	1.91	0.52
1:G:24:VAL:HG22	1:G:48:LYS:HG2	1.90	0.52
2:B:16:THR:HA	2:B:69:LEU:HB2	1.91	0.52
2:B:122:ARG:HD3	2:B:127:GLY:HA2	1.91	0.52
2:B:2791:ARG:HE	2:B:2792:THR:H	1.58	0.52
2:B:2833:LEU:CD2	2:B:2897:GLN:HE22	2.23	0.52
2:B:3250:TRP:NE1	2:B:3255:GLU:OE2	2.33	0.52
2:B:4579:HIS:HD1	2:B:4739:PHE:HE1	1.57	0.52
2:C:769:ARG:HG2	2:C:774:PRO:HA	1.91	0.52
2:C:1958:THR:HA	2:C:1961:LYS:HG2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2833:LEU:HB2	2:C:2838[A]:HIS:NE2	2.24	0.52
2:C:2999:LYS:NZ	2:C:3003:MET:HB3	2.24	0.52
2:C:3322:LEU:HB3	2:C:3323:MET:HE2	1.91	0.52
2:C:4704:LYS:O	2:C:4707:MET:HB3	2.09	0.52
2:D:2791:ARG:HE	2:D:2792:THR:H	1.58	0.52
2:D:4704:LYS:O	2:D:4707:MET:HB3	2.09	0.52
2:A:122:ARG:HD3	2:A:127:GLY:HA2	1.91	0.52
2:A:1306:MET:HE2	2:A:1570:LEU:HB3	1.92	0.52
2:A:3214:LEU:O	2:A:3218:ILE:HG12	2.10	0.52
2:A:3238:ILE:HG22	2:A:3242:LEU:HD23	1.89	0.52
2:B:1048:ASP:OD1	2:B:1049:SER:N	2.43	0.52
2:B:2123:LEU:HD13	2:B:2167:MET:HG2	1.92	0.52
2:C:867:VAL:HG11	2:C:942:THR:HG23	1.91	0.52
2:C:3188:SER:OG	2:C:3191:GLU:HG3	2.08	0.52
2:D:2692:GLN:HG2	2:D:2695:MET:HB2	1.92	0.52
2:D:3272:HIS:O	2:D:3275:THR:OG1	2.25	0.52
2:A:3072:MET:HB3	2:A:3076:LYS:HZ2	1.74	0.52
2:B:494:MET:HA	2:B:494:MET:CE	2.40	0.52
2:B:2599:LEU:HD12	2:B:2661:LEU:HD11	1.92	0.52
2:B:3012:GLY:HA3	2:B:3060:PHE:HE1	1.75	0.52
2:B:3152:ARG:HA	2:B:3155:LEU:HD12	1.92	0.52
2:C:890:HIS:HA	2:C:893:TRP:CE3	2.42	0.52
2:C:2123:LEU:HD13	2:C:2167:MET:HG2	1.92	0.52
2:C:2791:ARG:HE	2:C:2792:THR:H	1.58	0.52
2:C:4155:SER:O	2:C:4159:GLN:HG2	2.09	0.52
2:D:769:ARG:HG2	2:D:774:PRO:HA	1.91	0.52
2:D:2646:TRP:HH2	2:D:2925:PHE:HA	1.74	0.52
2:A:769:ARG:HG2	2:A:774:PRO:HA	1.90	0.52
2:A:1945:ASN:O	2:A:1949:GLN:HG2	2.09	0.52
2:A:2178:VAL:HG21	2:A:2192:MET:HG3	1.92	0.52
2:A:2290:TRP:CZ2	2:A:2388:ILE:HG12	2.45	0.52
2:B:2692:GLN:HG2	2:B:2695:MET:HB2	1.92	0.52
2:C:16:THR:HA	2:C:69:LEU:HB2	1.91	0.52
2:C:2290:TRP:CZ2	2:C:2388:ILE:HG12	2.44	0.52
2:C:2833:LEU:CD2	2:C:2897:GLN:HE22	2.23	0.52
2:C:3939:ARG:NH2	2:D:172:GLY:O	2.43	0.52
2:C:4181:GLY:O	2:C:4185:LYS:N	2.41	0.52
2:D:15:ARG:HA	2:D:113:LEU:HD13	1.90	0.52
2:D:307:SER:HB2	2:D:327:THR:HG22	1.90	0.52
2:D:3152:ARG:HA	2:D:3155:LEU:HD12	1.92	0.52
2:D:3728:GLN:O	2:D:3732:HIS:ND1	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:24:VAL:HG22	1:E:48:LYS:HG2	1.90	0.52
1:H:35:LYS:HA	2:D:647:ARG:NH2	2.24	0.52
2:A:2229:LEU:HD13	2:A:2297:ARG:HB2	1.92	0.52
2:B:1011:ARG:HB3	2:B:1016:TRP:HB2	1.91	0.52
2:C:902:TRP:CZ3	2:C:913:ARG:HA	2.44	0.52
2:C:1220:ASP:O	2:C:1223:THR:OG1	2.26	0.52
2:C:2251:ASN:HB2	2:C:3819:MET:HE1	1.91	0.52
2:C:3041:ASP:O	2:C:3045:VAL:HG23	2.10	0.52
2:C:3152:ARG:HA	2:C:3155:LEU:HD12	1.92	0.52
2:D:902:TRP:CZ3	2:D:913:ARG:HA	2.44	0.52
2:D:2229:LEU:HD13	2:D:2297:ARG:HB2	1.92	0.52
2:D:3155:LEU:O	2:D:3159:LEU:HG	2.10	0.52
2:D:3174:HIS:HE1	2:D:3211:LEU:HD21	1.73	0.52
2:D:3214:LEU:O	2:D:3218:ILE:HG12	2.10	0.52
2:A:494:MET:HA	2:A:494:MET:CE	2.40	0.52
2:A:890:HIS:HA	2:A:893:TRP:CE3	2.42	0.52
2:A:1048:ASP:OD1	2:A:1049:SER:N	2.43	0.52
2:A:3715:GLU:OE2	2:A:4647:LYS:HE2	2.10	0.52
2:B:867:VAL:HG11	2:B:942:THR:HG23	1.91	0.52
2:B:1945:ASN:O	2:B:1949:GLN:HG2	2.09	0.52
2:B:2178:VAL:HG21	2:B:2192:MET:HG3	1.92	0.52
2:B:4071:GLU:OE1	2:B:4086:ARG:NH2	2.30	0.52
2:B:4155:SER:O	2:B:4159:GLN:HG2	2.09	0.52
2:C:920:GLU:OE2	2:C:975:GLY:N	2.38	0.52
2:C:1929:SER:HG	2:C:3620:PHE:HD2	1.56	0.52
2:C:2538:THR:OG1	2:C:2584:MET:SD	2.68	0.52
2:D:1945:ASN:O	2:D:1949:GLN:HG2	2.09	0.52
2:D:2645:PHE:HZ	2:D:2970:LEU:HD21	1.75	0.52
2:A:1727:VAL:HG11	2:A:1926:VAL:HG21	1.93	0.51
2:A:2581:ARG:HG2	2:A:2582:PRO:HD2	1.92	0.51
2:A:2586:GLN:HA	2:A:2589:LEU:HG	1.93	0.51
2:A:2646:TRP:HH2	2:A:2925:PHE:HA	1.74	0.51
2:A:3322:LEU:HB3	2:A:3323:MET:HE2	1.91	0.51
2:A:4809:MET:SD	2:D:4518:LEU:HA	2.50	0.51
2:B:2581:ARG:HG2	2:B:2582:PRO:HD2	1.92	0.51
2:B:3715:GLU:OE2	2:B:4647:LYS:HE2	2.10	0.51
2:C:494:MET:HA	2:C:494:MET:CE	2.40	0.51
2:C:1007:TRP:NE1	4:C:5005:ATP:O1B	2.40	0.51
2:C:3043:ARG:CG	2:C:3117:PHE:CZ	2.92	0.51
2:C:3174:HIS:HE1	2:C:3211:LEU:HD21	1.73	0.51
2:D:16:THR:HA	2:D:69:LEU:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2149:ILE:HD13	2:D:2167:MET:HE1	1.90	0.51
2:A:1722:ASN:O	2:A:1919:ARG:NH2	2.44	0.51
2:A:2123:LEU:HD13	2:A:2167:MET:HG2	1.92	0.51
2:A:2538:THR:OG1	2:A:2584:MET:SD	2.68	0.51
2:A:3152:ARG:NH2	2:A:3233:HIS:HA	2.24	0.51
2:B:1034:PRO:HG2	2:B:1037:LEU:HD13	1.91	0.51
2:B:2610:LEU:HD23	2:B:2613:HIS:HE1	1.75	0.51
2:C:1011:ARG:HB3	2:C:1016:TRP:HB2	1.92	0.51
2:C:1048:ASP:OD1	2:C:1049:SER:N	2.43	0.51
2:C:2646:TRP:CH2	2:C:2925:PHE:HA	2.45	0.51
2:C:3152:ARG:NH2	2:C:3233:HIS:HA	2.24	0.51
2:C:3214:LEU:O	2:C:3218:ILE:HG12	2.10	0.51
2:D:1048:ASP:OD1	2:D:1049:SER:N	2.43	0.51
2:A:15:ARG:HA	2:A:113:LEU:HD13	1.90	0.51
2:A:679:VAL:HA	2:A:800:VAL:HG12	1.91	0.51
2:A:2646:TRP:CH2	2:A:2925:PHE:HA	2.45	0.51
2:A:4704:LYS:O	2:A:4707:MET:HB3	2.09	0.51
2:B:2586:GLN:HA	2:B:2589:LEU:HG	1.92	0.51
2:C:552:SER:HB2	2:C:588:ILE:HD12	1.93	0.51
2:C:1287:GLN:NE2	2:C:1549:SER:O	2.43	0.51
2:C:1964:GLU:HG3	2:C:1975:MET:HE3	1.91	0.51
2:C:3155:LEU:O	2:C:3159:LEU:HG	2.10	0.51
2:D:655:MET:HG3	2:D:1619:VAL:HG11	1.92	0.51
2:D:1306:MET:HE2	2:D:1570:LEU:HB3	1.91	0.51
2:D:2586:GLN:HA	2:D:2589:LEU:HG	1.92	0.51
2:D:2956:TYR:HD2	2:D:2960:ILE:HG12	1.75	0.51
2:D:3715:GLU:OE2	2:D:4647:LYS:HE2	2.10	0.51
2:A:2688:MET:HB2	2:A:2689:MET:HE3	1.91	0.51
2:B:679:VAL:HA	2:B:800:VAL:HG12	1.91	0.51
2:B:1722:ASN:O	2:B:1919:ARG:NH2	2.44	0.51
2:B:2274:LEU:HG	2:B:2329:GLU:HG3	1.92	0.51
2:B:2389:MET:CE	2:B:2460:PHE:HD1	2.24	0.51
2:B:3041:ASP:O	2:B:3045:VAL:HG23	2.10	0.51
2:B:3068:LEU:O	2:B:3072:MET:HE3	2.10	0.51
2:B:3214:LEU:O	2:B:3218:ILE:HG12	2.10	0.51
2:B:4181:GLY:O	2:B:4185:LYS:N	2.41	0.51
2:C:2610:LEU:HD23	2:C:2613:HIS:HE1	1.75	0.51
2:C:2692:GLN:HG2	2:C:2695:MET:HB2	1.92	0.51
2:C:2956:TYR:HD2	2:C:2960:ILE:HG12	1.75	0.51
2:C:3250:TRP:NE1	2:C:3255:GLU:OE2	2.33	0.51
2:C:4579:HIS:HD1	2:C:4739:PHE:HE1	1.57	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1001:GLU:OE2	2:D:1005:ASN:ND2	2.36	0.51
2:D:2833:LEU:CD2	2:D:2897:GLN:HE22	2.23	0.51
2:D:3012:GLY:HA3	2:D:3060:PHE:HE1	1.75	0.51
2:A:2681:MET:HA	2:A:2681:MET:CE	2.41	0.51
2:A:2927:GLN:HB3	2:A:2931:ARG:NH2	2.26	0.51
2:B:882:ARG:HG2	2:B:882:ARG:HH11	1.76	0.51
2:B:1306:MET:HE2	2:B:1570:LEU:HB3	1.91	0.51
2:B:3155:LEU:O	2:B:3159:LEU:HG	2.10	0.51
2:C:1306:MET:HE2	2:C:1570:LEU:HB3	1.91	0.51
2:C:2586:GLN:HA	2:C:2589:LEU:HG	1.92	0.51
2:D:552:SER:HB2	2:D:588:ILE:HD12	1.93	0.51
2:D:2599:LEU:HD12	2:D:2661:LEU:HD11	1.92	0.51
2:D:2610:LEU:HD23	2:D:2613:HIS:HE1	1.75	0.51
2:D:2927:GLN:HB3	2:D:2931:ARG:NH2	2.26	0.51
2:D:3072:MET:HE2	2:D:3072:MET:N	2.25	0.51
2:D:3322:LEU:HB3	2:D:3323:MET:HE2	1.92	0.51
2:A:2389:MET:CE	2:A:2460:PHE:HD1	2.24	0.51
2:A:2692:GLN:HG2	2:A:2695:MET:HB2	1.92	0.51
2:A:3041:ASP:O	2:A:3045:VAL:HG23	2.10	0.51
2:B:3149:GLU:OE1	2:B:3152:ARG:NH1	2.43	0.51
2:C:4056:LYS:NZ	2:D:4659:GLU:O	2.43	0.51
2:D:122:ARG:HD3	2:D:127:GLY:HA2	1.92	0.51
2:D:494:MET:HA	2:D:494:MET:CE	2.40	0.51
2:D:2646:TRP:CH2	2:D:2925:PHE:HA	2.45	0.51
2:D:3041:ASP:O	2:D:3045:VAL:HG23	2.10	0.51
2:D:3072:MET:HB3	2:D:3076:LYS:HZ2	1.76	0.51
2:D:3851:ASN:O	2:D:3855:GLN:HG3	2.11	0.51
2:A:2791:ARG:HE	2:A:2792:THR:H	1.58	0.51
2:A:3117:PHE:CD2	2:A:3117:PHE:CB	2.79	0.51
2:A:3155:LEU:O	2:A:3159:LEU:HG	2.10	0.51
2:B:655:MET:HG3	2:B:1619:VAL:HG11	1.92	0.51
2:B:3727:GLN:HG2	2:B:3730:ARG:NH2	2.26	0.51
2:B:4838:GLU:OE1	2:B:4838:GLU:N	2.36	0.51
2:C:606:ARG:HH11	2:C:644:LEU:HD21	1.74	0.51
2:C:655:MET:HG3	2:C:1619:VAL:HG11	1.92	0.51
2:C:2681:MET:HA	2:C:2681:MET:CE	2.41	0.51
2:D:394:HIS:CE1	2:D:396:GLU:HG3	2.46	0.51
2:D:2114:GLU:HG2	2:D:2115:ASP:N	2.26	0.51
2:D:2538:THR:OG1	2:D:2584:MET:SD	2.68	0.51
2:D:4203:ALA:HA	2:D:4206:ILE:HG12	1.92	0.51
2:A:480:ARG:NH2	2:A:3678:GLU:OE2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:882:ARG:HH11	2:A:882:ARG:HG2	1.76	0.51
2:A:2788:ARG:NH1	2:A:2905:ARG:O	2.44	0.51
2:A:3152:ARG:HA	2:A:3155:LEU:HD12	1.92	0.51
2:A:3851:ASN:O	2:A:3855:GLN:HG3	2.11	0.51
2:B:983:LEU:CD1	2:B:1055:ARG:HB3	2.41	0.51
2:B:1727:VAL:HG11	2:B:1926:VAL:HG21	1.93	0.51
2:B:2229:LEU:HD13	2:B:2297:ARG:HB2	1.92	0.51
2:B:2681:MET:HA	2:B:2681:MET:CE	2.41	0.51
2:B:2927:GLN:HB3	2:B:2931:ARG:NH2	2.26	0.51
2:C:1722:ASN:O	2:C:1919:ARG:NH2	2.44	0.51
2:C:1727:VAL:HG11	2:C:1926:VAL:HG21	1.92	0.51
2:C:1793:GLN:NE2	2:C:1797:GLU:OE2	2.41	0.51
2:C:2341:ASN:OD1	2:C:2342:GLY:N	2.44	0.51
2:C:3072:MET:N	2:C:3072:MET:HE2	2.25	0.51
2:D:1722:ASN:O	2:D:1919:ARG:NH2	2.44	0.51
2:D:2123:LEU:HD13	2:D:2167:MET:HG2	1.92	0.51
2:D:2178:VAL:HG21	2:D:2192:MET:HG3	1.92	0.51
2:D:2389:MET:CE	2:D:2460:PHE:HD1	2.24	0.51
2:A:2341:ASN:OD1	2:A:2342:GLY:N	2.44	0.51
2:A:3727:GLN:HG2	2:A:3730:ARG:NH2	2.26	0.51
2:B:2538:THR:OG1	2:B:2584:MET:SD	2.68	0.51
2:B:2741:TRP:CD1	2:B:2754:GLN:HG3	2.46	0.51
2:B:3122:ILE:HD11	2:B:3127:GLN:HA	1.93	0.51
2:B:4203:ALA:HA	2:B:4206:ILE:HG12	1.92	0.51
2:C:394:HIS:CE1	2:C:396:GLU:HG3	2.46	0.51
2:C:2581:ARG:HG2	2:C:2582:PRO:HD2	1.92	0.51
2:C:2645:PHE:HZ	2:C:2970:LEU:HD21	1.75	0.51
2:C:2741:TRP:CD1	2:C:2754:GLN:HG3	2.46	0.51
2:C:2927:GLN:HB3	2:C:2931:ARG:NH2	2.26	0.51
2:C:3149:GLU:OE1	2:C:3152:ARG:NH1	2.43	0.51
2:D:3118:GLY:O	2:D:3122:ILE:HG22	2.11	0.51
2:A:308:LEU:HD13	2:A:393:MET:HG2	1.93	0.51
2:A:983:LEU:HD13	2:A:986:ILE:HD12	1.93	0.51
2:A:1011:ARG:HB3	2:A:1016:TRP:HB2	1.92	0.51
2:A:2599:LEU:HD12	2:A:2661:LEU:HD11	1.91	0.51
2:A:3122:ILE:HD11	2:A:3127:GLN:HA	1.93	0.51
2:B:2341:ASN:OD1	2:B:2342:GLY:N	2.44	0.51
2:B:2758:LYS:HD3	2:B:2763:LEU:HA	1.93	0.51
2:B:2999:LYS:HZ1	2:B:3003:MET:HB3	1.75	0.51
2:C:2646:TRP:HH2	2:C:2925:PHE:HA	1.74	0.51
2:C:3851:ASN:O	2:C:3855:GLN:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:4203:ALA:HA	2:C:4206:ILE:HG12	1.92	0.51
2:D:867:VAL:HG11	2:D:942:THR:HG23	1.91	0.51
2:D:1047:LYS:O	2:D:1051:ARG:HG3	2.11	0.51
2:D:2788:ARG:NH1	2:D:2905:ARG:O	2.44	0.51
2:A:987:LYS:NZ	2:A:988:LEU:O	2.44	0.50
2:A:1681:ASP:HB2	2:A:1684:GLN:HG3	1.93	0.50
2:A:2956:TYR:HD2	2:A:2960:ILE:HG12	1.75	0.50
2:A:3012:GLY:HA3	2:A:3060:PHE:HE1	1.75	0.50
2:A:3149:GLU:OE1	2:A:3152:ARG:NH1	2.43	0.50
2:B:1681:ASP:HB2	2:B:1684:GLN:HG3	1.93	0.50
2:C:308:LEU:HD13	2:C:393:MET:HG2	1.93	0.50
2:C:3012:GLY:HA3	2:C:3060:PHE:HE1	1.74	0.50
2:C:3316:LYS:O	2:C:3317:THR:OG1	2.28	0.50
2:C:3715:GLU:OE2	2:C:4647:LYS:HE2	2.10	0.50
2:D:1681:ASP:HB2	2:D:1684:GLN:HG3	1.93	0.50
2:D:2274:LEU:HG	2:D:2329:GLU:HG3	1.91	0.50
2:A:2981:TYR:O	2:A:2984:SER:OG	2.21	0.50
2:B:2688:MET:HB2	2:B:2689:MET:HE2	1.92	0.50
2:B:3851:ASN:O	2:B:3855:GLN:HG3	2.11	0.50
2:C:1047:LYS:O	2:C:1051:ARG:HG3	2.12	0.50
2:C:3272:HIS:O	2:C:3275:THR:OG1	2.25	0.50
2:D:241:MET:HE2	2:D:241:MET:CA	2.40	0.50
2:D:2581:ARG:HG2	2:D:2582:PRO:HD2	1.92	0.50
2:D:3227:ARG:HG2	2:D:3229:THR:H	1.76	0.50
2:D:4579:HIS:HD1	2:D:4739:PHE:HE1	1.57	0.50
2:A:867:VAL:HG11	2:A:942:THR:HG23	1.91	0.50
2:A:1007:TRP:NE1	4:A:5005:ATP:O1B	2.40	0.50
2:A:2114:GLU:HG2	2:A:2115:ASP:N	2.26	0.50
2:A:2645:PHE:HZ	2:A:2970:LEU:HD21	1.75	0.50
2:A:2758:LYS:HD3	2:A:2763:LEU:HA	1.94	0.50
2:A:4579:HIS:HD1	2:A:4739:PHE:HE1	1.57	0.50
2:B:1564:MET:CE	2:B:1565:PRO:HD2	2.35	0.50
2:C:241:MET:HE2	2:C:241:MET:CA	2.41	0.50
2:C:829:LYS:NZ	2:C:1037:LEU:O	2.44	0.50
2:C:2178:VAL:HG21	2:C:2192:MET:HG3	1.92	0.50
2:C:2758:LYS:HD3	2:C:2763:LEU:HA	1.93	0.50
2:C:2768:LYS:HE3	2:C:2772:ARG:NH1	2.27	0.50
2:C:2833:LEU:HB2	2:C:2838[B]:HIS:NE2	2.25	0.50
2:C:3227:ARG:HG2	2:C:3229:THR:H	1.76	0.50
2:D:1011:ARG:HB3	2:D:1016:TRP:HB2	1.92	0.50
2:D:2681:MET:HA	2:D:2681:MET:CE	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:829:LYS:NZ	2:A:1037:LEU:O	2.44	0.50
2:A:3118:GLY:O	2:A:3122:ILE:HG22	2.11	0.50
2:A:3166:PHE:CE2	2:A:3168:VAL:HB	2.47	0.50
2:C:2114:GLU:HG2	2:C:2115:ASP:N	2.26	0.50
2:C:2389:MET:CE	2:C:2460:PHE:HD1	2.24	0.50
2:C:2788:ARG:NH1	2:C:2905:ARG:O	2.44	0.50
2:C:3117:PHE:CD2	2:C:3117:PHE:CB	2.79	0.50
2:C:3219:VAL:O	2:C:3222:ALA:HB3	2.12	0.50
2:C:4248:LEU:HG	2:C:4297:PHE:CE1	2.47	0.50
2:D:480:ARG:NH2	2:D:3678:GLU:OE2	2.44	0.50
2:D:3042:ALA:H	2:D:3117:PHE:HD2	1.58	0.50
2:D:3122:ILE:HD11	2:D:3127:GLN:HA	1.93	0.50
2:A:552:SER:HB2	2:A:588:ILE:HD12	1.93	0.50
2:A:983:LEU:CD1	2:A:1055:ARG:HB3	2.41	0.50
2:A:2610:LEU:HD23	2:A:2613:HIS:HE1	1.75	0.50
2:A:4732:GLY:HA2	2:A:4738:PHE:HB2	1.94	0.50
2:B:394:HIS:CE1	2:B:396:GLU:HG3	2.46	0.50
2:B:552:SER:HB2	2:B:588:ILE:HD12	1.93	0.50
2:B:1047:LYS:O	2:B:1051:ARG:HG3	2.12	0.50
2:B:2645:PHE:HZ	2:B:2970:LEU:HD21	1.75	0.50
2:B:2788:ARG:NH1	2:B:2905:ARG:O	2.44	0.50
2:C:983:LEU:HD13	2:C:986:ILE:HD12	1.93	0.50
2:C:3727:GLN:HG2	2:C:3730:ARG:NH2	2.26	0.50
2:D:2341:ASN:OD1	2:D:2342:GLY:N	2.44	0.50
2:D:2758:LYS:HD3	2:D:2763:LEU:HA	1.94	0.50
2:A:655:MET:HG3	2:A:1619:VAL:HG11	1.92	0.50
2:A:2580:LEU:O	2:A:2616:ARG:NH1	2.45	0.50
2:B:1943:ARG:O	2:B:1947:VAL:HG23	2.11	0.50
2:B:2956:TYR:HD2	2:B:2960:ILE:HG12	1.75	0.50
2:B:3227:ARG:HG2	2:B:3229:THR:H	1.76	0.50
2:C:983:LEU:CD1	2:C:1055:ARG:HB3	2.41	0.50
2:C:2229:LEU:HD13	2:C:2297:ARG:HB2	1.92	0.50
2:D:983:LEU:HD13	2:D:986:ILE:HD12	1.93	0.50
2:D:2741:TRP:CD1	2:D:2754:GLN:HG3	2.46	0.50
2:D:3727:GLN:HG2	2:D:3730:ARG:NH2	2.26	0.50
2:A:878:LEU:HA	2:A:881:ILE:HG12	1.94	0.50
2:A:3112:ILE:HG13	2:A:3118:GLY:HA2	1.94	0.50
2:A:4248:LEU:HG	2:A:4297:PHE:CE1	2.47	0.50
2:A:4726:MET:HB3	2:D:4291:PHE:CE1	2.46	0.50
2:C:1436:GLN:HG2	2:C:1552:VAL:HG23	1.94	0.50
2:C:3118:GLY:O	2:C:3122:ILE:HG22	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:3166:PHE:CE2	2:C:3168:VAL:HB	2.47	0.50
2:D:3043:ARG:HH22	2:D:3115:HIS:CE1	2.30	0.50
2:D:3112:ILE:HG13	2:D:3118:GLY:HA2	1.94	0.50
2:A:1047:LYS:O	2:A:1051:ARG:HG3	2.11	0.50
2:A:2686:VAL:O	2:A:2688:MET:HG2	2.12	0.50
2:A:2741:TRP:CD1	2:A:2754:GLN:HG3	2.46	0.50
2:A:3316:LYS:O	2:A:3317:THR:OG1	2.28	0.50
2:A:4203:ALA:HA	2:A:4206:ILE:HG12	1.92	0.50
2:B:3166:PHE:CE2	2:B:3168:VAL:HB	2.47	0.50
2:B:3219:VAL:O	2:B:3222:ALA:HB3	2.12	0.50
2:C:423:VAL:HG22	2:C:494:MET:HE1	1.93	0.50
2:C:1681:ASP:HB2	2:C:1684:GLN:HG3	1.93	0.50
2:D:2886:ARG:O	2:D:2890:GLN:HG2	2.12	0.50
2:D:3149:GLU:OE1	2:D:3152:ARG:NH1	2.43	0.50
2:A:3043:ARG:HH22	2:A:3115:HIS:CE1	2.30	0.50
2:B:330:THR:HG23	2:B:366:VAL:HG12	1.93	0.50
2:B:480:ARG:NH2	2:B:3678:GLU:OE2	2.44	0.50
2:B:483:LYS:NZ	2:B:543:GLY:O	2.45	0.50
2:B:1019:GLY:HA2	2:B:1028:ARG:HH21	1.77	0.50
2:B:2768:LYS:HE3	2:B:2772:ARG:NH1	2.27	0.50
2:B:3042:ALA:H	2:B:3117:PHE:HD2	1.59	0.50
2:C:15:ARG:HE	2:C:16:THR:HG22	1.77	0.50
2:C:480:ARG:NH2	2:C:3678:GLU:OE2	2.44	0.50
2:C:483:LYS:NZ	2:C:543:GLY:O	2.45	0.50
2:C:3026:ALA:O	2:C:3030:VAL:HG13	2.12	0.50
2:C:3122:ILE:HD11	2:C:3127:GLN:HA	1.93	0.50
2:D:878:LEU:HA	2:D:881:ILE:HG12	1.94	0.50
2:D:1943:ARG:O	2:D:1947:VAL:HG23	2.11	0.50
2:A:394:HIS:CE1	2:A:396:GLU:HG3	2.46	0.49
2:A:1287:GLN:NE2	2:A:1549:SER:O	2.42	0.49
2:A:3728:GLN:O	2:A:3732:HIS:ND1	2.40	0.49
2:A:4828:GLY:HA2	2:A:4843:ARG:HH22	1.77	0.49
2:B:337:LYS:NZ	2:B:371:TRP:HE1	2.10	0.49
2:B:829:LYS:NZ	2:B:1037:LEU:O	2.44	0.49
2:B:3026:ALA:O	2:B:3030:VAL:HG13	2.12	0.49
2:B:3118:GLY:O	2:B:3122:ILE:HG22	2.11	0.49
2:B:3613:ARG:O	2:B:3617:VAL:HG23	2.12	0.49
2:D:2119:LEU:HD13	2:D:2154:VAL:HG23	1.94	0.49
2:D:3699:CYS:HB2	2:D:3764:ALA:HB1	1.94	0.49
2:A:483:LYS:NZ	2:A:543:GLY:O	2.45	0.49
2:A:920:GLU:OE2	2:A:975:GLY:N	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2769:GLU:HA	2:A:2772:ARG:CG	2.38	0.49
2:B:1964:GLU:HG3	2:B:1975:MET:HE3	1.93	0.49
2:C:337:LYS:NZ	2:C:371:TRP:HE1	2.10	0.49
2:C:882:ARG:HG2	2:C:882:ARG:HH11	1.76	0.49
2:C:2580:LEU:O	2:C:2616:ARG:NH1	2.45	0.49
2:C:3293:GLY:H	2:C:3296:MET:HE1	1.77	0.49
2:C:3613:ARG:O	2:C:3617:VAL:HG23	2.13	0.49
2:D:1007:TRP:NE1	4:D:5005:ATP:O1B	2.40	0.49
2:D:1727:VAL:HG11	2:D:1926:VAL:HG21	1.93	0.49
2:D:2727:HIS:O	2:D:2731:LYS:HG2	2.12	0.49
2:D:4732:GLY:HA2	2:D:4738:PHE:HB2	1.94	0.49
1:F:25:VAL:HG12	1:F:104:LEU:HA	1.93	0.49
2:A:2964:ALA:HA	2:A:2968:LEU:HD12	1.94	0.49
2:B:983:LEU:HD13	2:B:986:ILE:HD12	1.93	0.49
2:B:2114:GLU:HG2	2:B:2115:ASP:N	2.26	0.49
2:B:2348:GLU:O	2:B:2352:LYS:HG2	2.13	0.49
2:B:3072:MET:HB3	2:B:3076:LYS:HZ2	1.76	0.49
2:B:4154:GLU:O	2:B:4158:THR:HG23	2.12	0.49
2:C:988:LEU:H	2:C:1055:ARG:NH2	2.10	0.49
2:C:1943:ARG:O	2:C:1947:VAL:HG23	2.11	0.49
2:D:290:ARG:HB2	2:D:343:ARG:HH21	1.78	0.49
2:D:483:LYS:NZ	2:D:543:GLY:O	2.45	0.49
2:D:829:LYS:NZ	2:D:1037:LEU:O	2.44	0.49
2:D:3166:PHE:CE2	2:D:3168:VAL:HB	2.47	0.49
2:D:3219:VAL:O	2:D:3222:ALA:HB3	2.12	0.49
2:D:4828:GLY:HA2	2:D:4843:ARG:HH22	1.77	0.49
2:A:3026:ALA:O	2:A:3030:VAL:HG13	2.12	0.49
2:A:3117:PHE:CD1	2:A:3117:PHE:HA	2.47	0.49
2:B:308:LEU:HD13	2:B:393:MET:HG2	1.93	0.49
2:B:2119:LEU:HD13	2:B:2154:VAL:HG23	1.94	0.49
2:B:2460:PHE:CZ	2:B:2465:LYS:HG3	2.48	0.49
2:B:2686:VAL:O	2:B:2688:MET:HG2	2.12	0.49
2:B:4732:GLY:HA2	2:B:4738:PHE:HB2	1.94	0.49
2:C:878:LEU:HA	2:C:881:ILE:HG12	1.94	0.49
2:C:3117:PHE:CD1	2:C:3117:PHE:HA	2.47	0.49
2:D:330:THR:HG23	2:D:366:VAL:HG12	1.93	0.49
2:D:521:GLU:H	2:D:521:GLU:CD	2.15	0.49
2:D:4898:PHE:O	2:D:4904:GLY:HA3	2.13	0.49
1:H:25:VAL:HG12	1:H:104:LEU:HA	1.93	0.49
2:A:290:ARG:HB2	2:A:343:ARG:HH21	1.78	0.49
2:A:330:THR:HG23	2:A:366:VAL:HG12	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1943:ARG:O	2:A:1947:VAL:HG23	2.11	0.49
2:A:1997:LEU:O	2:A:2001:GLU:HG2	2.12	0.49
2:A:2119:LEU:HD13	2:A:2154:VAL:HG23	1.94	0.49
2:A:2727:HIS:O	2:A:2731:LYS:HG2	2.13	0.49
2:A:2768:LYS:HE3	2:A:2772:ARG:NH1	2.27	0.49
2:A:2999:LYS:HZ1	2:A:3003:MET:HB3	1.78	0.49
2:B:2580:LEU:O	2:B:2616:ARG:NH1	2.45	0.49
2:B:3250:TRP:HE3	2:B:3309:LYS:HZ3	1.60	0.49
2:C:1997:LEU:O	2:C:2001:GLU:HG2	2.12	0.49
2:C:2119:LEU:HD13	2:C:2154:VAL:HG23	1.94	0.49
2:C:2348:GLU:O	2:C:2352:LYS:HG2	2.13	0.49
2:C:3699:CYS:HB2	2:C:3764:ALA:HB1	1.94	0.49
2:D:337:LYS:NZ	2:D:371:TRP:HE1	2.10	0.49
2:D:1019:GLY:HA2	2:D:1028:ARG:HH21	1.77	0.49
2:D:1964:GLU:HG3	2:D:1975:MET:HE3	1.93	0.49
2:D:2964:ALA:HA	2:D:2968:LEU:HD12	1.94	0.49
2:D:4248:LEU:HG	2:D:4297:PHE:CE1	2.47	0.49
2:A:15:ARG:HE	2:A:16:THR:HG22	1.77	0.49
2:A:3699:CYS:HB2	2:A:3764:ALA:HB1	1.94	0.49
2:A:4154:GLU:O	2:A:4158:THR:HG23	2.12	0.49
2:B:241:MET:HE2	2:B:241:MET:CA	2.40	0.49
2:B:290:ARG:HB2	2:B:343:ARG:HH21	1.78	0.49
2:B:878:LEU:HA	2:B:881:ILE:HG12	1.94	0.49
2:B:1287:GLN:NE2	2:B:1549:SER:O	2.42	0.49
2:B:3112:ILE:HG13	2:B:3118:GLY:HA2	1.94	0.49
2:B:4248:LEU:HG	2:B:4297:PHE:CE1	2.47	0.49
2:C:330:THR:HG23	2:C:366:VAL:HG12	1.93	0.49
2:C:1019:GLY:HA2	2:C:1028:ARG:HH21	1.77	0.49
2:C:2635:GLU:OE2	2:C:2680:TYR:OH	2.24	0.49
2:C:2886:ARG:O	2:C:2890:GLN:HG2	2.12	0.49
2:C:4898:PHE:O	2:C:4904:GLY:HA3	2.13	0.49
2:D:882:ARG:HG2	2:D:882:ARG:HH11	1.76	0.49
2:D:1997:LEU:O	2:D:2001:GLU:HG2	2.12	0.49
2:D:2460:PHE:CZ	2:D:2465:LYS:HG3	2.48	0.49
2:D:3316:LYS:O	2:D:3317:THR:OG1	2.28	0.49
1:G:25:VAL:HG12	1:G:104:LEU:HA	1.93	0.49
2:A:337:LYS:NZ	2:A:371:TRP:HE1	2.10	0.49
2:A:2460:PHE:CZ	2:A:2465:LYS:HG3	2.48	0.49
2:A:2886:ARG:O	2:A:2890:GLN:HG2	2.12	0.49
2:A:3218:ILE:C	2:A:3279:ASN:HD21	2.16	0.49
2:A:4800:ASP:OD1	2:A:4801:THR:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:521:GLU:H	2:B:521:GLU:CD	2.15	0.49
2:B:1436:GLN:HG2	2:B:1552:VAL:HG23	1.94	0.49
2:B:3088:LYS:HG3	2:B:3090:VAL:HG12	1.95	0.49
2:B:3117:PHE:CD1	2:B:3117:PHE:HA	2.47	0.49
2:D:987:LYS:NZ	2:D:988:LEU:O	2.44	0.49
2:D:2686:VAL:O	2:D:2688:MET:HG2	2.12	0.49
2:D:2768:LYS:HE3	2:D:2772:ARG:NH1	2.27	0.49
2:D:3209:PRO:HB3	2:D:3213:LYS:NZ	2.28	0.49
2:D:4154:GLU:O	2:D:4158:THR:HG23	2.12	0.49
2:D:4179:GLU:OE1	2:D:4179:GLU:N	2.46	0.49
2:A:3042:ALA:H	2:A:3117:PHE:HD2	1.59	0.49
2:A:3227:ARG:HG2	2:A:3229:THR:H	1.76	0.49
2:A:4181:GLY:O	2:A:4185:LYS:N	2.41	0.49
2:B:2964:ALA:HA	2:B:2968:LEU:HD12	1.94	0.49
2:B:4828:GLY:HA2	2:B:4843:ARG:HH22	1.77	0.49
2:B:4898:PHE:O	2:B:4904:GLY:HA3	2.13	0.49
2:C:2727:HIS:O	2:C:2731:LYS:HG2	2.13	0.49
2:C:3070:LYS:O	2:C:3073:GLU:HG3	2.13	0.49
2:C:3651:PRO:HB2	2:C:3652:PRO:HD3	1.95	0.49
2:C:4179:GLU:N	2:C:4179:GLU:OE1	2.46	0.49
2:C:4517:LEU:O	2:C:4520:TYR:HB2	2.13	0.49
2:C:4640:PHE:CG	2:C:4641:PRO:HD3	2.48	0.49
2:D:988:LEU:H	2:D:1055:ARG:NH2	2.10	0.49
2:D:2580:LEU:O	2:D:2616:ARG:NH1	2.45	0.49
2:D:2914:THR:N	2:D:2915:PRO:HD2	2.28	0.49
2:D:4702:ASP:HB3	2:D:4705:TYR:HB3	1.94	0.49
1:E:25:VAL:HG12	1:E:104:LEU:HA	1.93	0.49
2:A:1124:PRO:HD2	2:A:1594:VAL:HG23	1.95	0.49
2:A:2460:PHE:HZ	2:A:2465:LYS:HG3	1.78	0.49
2:B:2886:ARG:O	2:B:2890:GLN:HG2	2.12	0.49
2:B:3070:LYS:O	2:B:3073:GLU:HG3	2.13	0.49
2:B:3209:PRO:HB3	2:B:3213:LYS:NZ	2.28	0.49
2:C:1124:PRO:HD2	2:C:1594:VAL:HG23	1.95	0.49
2:C:1748:LEU:HD22	2:C:1851:PHE:HD1	1.77	0.49
2:C:2688:MET:HB2	2:C:2689:MET:HE3	1.94	0.49
2:C:3042:ALA:H	2:C:3117:PHE:HD2	1.59	0.49
2:C:3088:LYS:HG3	2:C:3090:VAL:HG12	1.95	0.49
2:D:15:ARG:HE	2:D:16:THR:HG22	1.77	0.49
2:D:3026:ALA:O	2:D:3030:VAL:HG13	2.12	0.49
2:D:3613:ARG:O	2:D:3617:VAL:HG23	2.12	0.49
2:A:2348:GLU:O	2:A:2352:LYS:HG2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:3209:PRO:HB3	2:A:3213:LYS:NZ	2.28	0.49
2:A:3613:ARG:O	2:A:3617:VAL:HG23	2.13	0.49
2:A:3665:HIS:HB2	2:A:3734:ARG:HG2	1.95	0.49
2:A:4702:ASP:HB3	2:A:4705:TYR:HB3	1.94	0.49
2:B:3043:ARG:HH22	2:B:3115:HIS:CE1	2.30	0.49
2:B:3218:ILE:C	2:B:3279:ASN:HD21	2.16	0.49
2:B:4702:ASP:HB3	2:B:4705:TYR:HB3	1.94	0.49
2:C:290:ARG:HB2	2:C:343:ARG:HH21	1.77	0.49
2:C:2460:PHE:HZ	2:C:2465:LYS:HG3	1.78	0.49
2:C:2591:ARG:NH2	2:C:2876:THR:OG1	2.45	0.49
2:C:2964:ALA:HA	2:C:2968:LEU:HD12	1.94	0.49
2:C:4828:GLY:HA2	2:C:4843:ARG:HH22	1.77	0.49
2:D:1436:GLN:HG2	2:D:1552:VAL:HG23	1.94	0.49
2:D:2659:GLN:HG3	2:D:2663:LYS:HZ1	1.76	0.49
2:A:1910:LEU:HD13	2:A:2062:ILE:HG12	1.95	0.48
2:A:3088:LYS:HG3	2:A:3090:VAL:HG12	1.95	0.48
2:A:4517:LEU:O	2:A:4520:TYR:HB2	2.13	0.48
2:B:1714:TYR:CZ	2:B:1761:MET:HG3	2.48	0.48
2:B:2769:GLU:HA	2:B:2772:ARG:CG	2.38	0.48
2:B:2914:THR:N	2:B:2915:PRO:HD2	2.28	0.48
2:C:218:SER:HB3	2:C:286:GLY:HA3	1.95	0.48
2:C:2769:GLU:HA	2:C:2772:ARG:CG	2.38	0.48
2:C:3043:ARG:HH22	2:C:3115:HIS:CE1	2.30	0.48
2:C:3218:ILE:C	2:C:3279:ASN:HD21	2.16	0.48
2:C:4154:GLU:O	2:C:4158:THR:HG23	2.12	0.48
2:C:4702:ASP:HB3	2:C:4705:TYR:HB3	1.94	0.48
2:C:4732:GLY:HA2	2:C:4738:PHE:HB2	1.94	0.48
2:D:983:LEU:CD1	2:D:1055:ARG:HB3	2.41	0.48
2:D:1910:LEU:HD13	2:D:2062:ILE:HG12	1.95	0.48
2:A:218:SER:HB3	2:A:286:GLY:HA3	1.95	0.48
2:A:2335:LEU:HD11	2:A:2343:LEU:HD13	1.96	0.48
2:A:2914:THR:N	2:A:2915:PRO:HD2	2.28	0.48
2:A:3219:VAL:O	2:A:3222:ALA:HB3	2.12	0.48
2:B:654:SER:OG	2:B:837:SER:OG	2.16	0.48
2:B:3665:HIS:HB2	2:B:3734:ARG:HG2	1.95	0.48
2:C:3665:HIS:HB2	2:C:3734:ARG:HG2	1.95	0.48
2:C:4521:LYS:HZ3	2:D:4808:ASP:CG	2.15	0.48
2:D:1714:TYR:CZ	2:D:1761:MET:HG3	2.48	0.48
2:D:2905:ARG:HH11	2:D:2906:GLY:H	1.60	0.48
2:D:4071:GLU:OE1	2:D:4086:ARG:NH2	2.30	0.48
2:A:2599:LEU:HB2	2:A:2655:LYS:HZ1	1.78	0.48

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
2:A:3070:LYS:O	2:A:3073:GLU:HG3	2.13	0.48
2:B:227:TYR:CG	2:B:352:SER:HB3	2.48	0.48
2:B:810:GLU:CD	2:B:1614:ARG:HH21	2.17	0.48
2:B:1124:PRO:HD2	2:B:1594:VAL:HG23	1.95	0.48
2:B:2460:PHE:HZ	2:B:2465:LYS:HG3	1.78	0.48
2:B:4179:GLU:OE1	2:B:4179:GLU:N	2.46	0.48
2:B:4279:MET:HE2	2:C:4484:ILE:HG22	1.94	0.48
2:B:4480:PHE:O	2:B:4484:ILE:HG23	2.13	0.48
2:C:2686:VAL:O	2:C:2688:MET:HG2	2.12	0.48
2:C:2914:THR:N	2:C:2915:PRO:HD2	2.28	0.48
2:C:3112:ILE:HG13	2:C:3118:GLY:HA2	1.94	0.48
2:C:4172:PHE:O	2:C:4176:VAL:HG22	2.14	0.48
2:C:4283:PHE:CZ	2:D:4491:LEU:HD11	2.48	0.48
2:C:4480:PHE:O	2:C:4484:ILE:HG23	2.13	0.48
2:D:308:LEU:HD13	2:D:393:MET:HG2	1.93	0.48
2:D:1711:LEU:HD22	2:D:1831:MET:HE1	1.96	0.48
2:D:2068:ARG:NH1	2:D:2072:GLU:OE2	2.47	0.48
2:D:2295:GLY:HA3	2:D:2391:PHE:HE2	1.78	0.48
2:D:2460:PHE:HZ	2:D:2465:LYS:HG3	1.78	0.48
2:D:2601:GLU:HA	2:D:2604:LYS:HZ1	1.78	0.48
2:D:2768:LYS:HB3	2:D:2772:ARG:NH1	2.29	0.48
1:H:42:ASP:OD1	2:D:688:ALA:HB1	2.12	0.48
2:A:4172:PHE:O	2:A:4176:VAL:HG22	2.14	0.48
2:B:15:ARG:HE	2:B:16:THR:HG22	1.77	0.48
2:B:4517:LEU:O	2:B:4520:TYR:HB2	2.13	0.48
2:C:3171:LEU:HD23	2:C:3214:LEU:HD13	1.96	0.48
2:C:3209:PRO:HB3	2:C:3213:LYS:NZ	2.28	0.48
2:D:3171:LEU:HD23	2:D:3214:LEU:HD13	1.96	0.48
2:D:3218:ILE:C	2:D:3279:ASN:HD21	2.16	0.48
2:A:227:TYR:CG	2:A:352:SER:HB3	2.48	0.48
2:A:810:GLU:CD	2:A:1614:ARG:HH21	2.17	0.48
2:A:1444:GLY:HA3	2:A:1487:MET:HA	1.96	0.48
2:A:2149:ILE:HD13	2:A:2167:MET:CE	2.44	0.48
2:A:2174:VAL:O	2:A:2178:VAL:HG23	2.13	0.48
2:B:1997:LEU:O	2:B:2001:GLU:HG2	2.12	0.48
2:B:2149:ILE:HD13	2:B:2167:MET:CE	2.44	0.48
2:B:2295:GLY:HA3	2:B:2391:PHE:HE2	1.78	0.48
2:B:2905:ARG:HH11	2:B:2906:GLY:H	1.60	0.48
2:B:4481:TRP:CE3	2:B:4484:ILE:HD11	2.49	0.48
2:C:15:ARG:HA	2:C:113:LEU:CD1	2.43	0.48
2:C:227:TYR:CG	2:C:352:SER:HB3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:987:LYS:NZ	2:C:988:LEU:O	2.44	0.48
2:C:1444:GLY:HA3	2:C:1487:MET:HA	1.96	0.48
2:C:2460:PHE:CZ	2:C:2465:LYS:HG3	2.48	0.48
2:D:176:ARG:HB2	2:D:179:ASP:HB2	1.96	0.48
2:D:654:SER:OG	2:D:837:SER:OG	2.15	0.48
2:D:1748:LEU:HD22	2:D:1851:PHE:HD1	1.77	0.48
2:D:1788:LYS:HG3	2:D:1834:PHE:CE1	2.49	0.48
2:D:2335:LEU:HD11	2:D:2343:LEU:HD13	1.96	0.48
2:D:2927:GLN:HB3	2:D:2931:ARG:HH22	1.79	0.48
2:D:3117:PHE:CD1	2:D:3117:PHE:HA	2.47	0.48
2:D:4481:TRP:CE3	2:D:4484:ILE:HD11	2.49	0.48
2:A:1748:LEU:HD22	2:A:1851:PHE:HD1	1.77	0.48
2:A:2601:GLU:HA	2:A:2604:LYS:HZ1	1.78	0.48
2:A:4481:TRP:CE3	2:A:4484:ILE:HD11	2.49	0.48
2:B:1748:LEU:HD22	2:B:1851:PHE:HD1	1.77	0.48
2:B:2068:ARG:NH1	2:B:2072:GLU:OE2	2.47	0.48
2:B:2335:LEU:HD11	2:B:2343:LEU:HD13	1.96	0.48
2:B:4640:PHE:CG	2:B:4641:PRO:HD3	2.48	0.48
2:B:4800:ASP:OD1	2:B:4801:THR:N	2.46	0.48
2:C:176:ARG:HB2	2:C:179:ASP:HB2	1.96	0.48
2:C:1714:TYR:CZ	2:C:1761:MET:HG3	2.48	0.48
2:C:2801:TYR:OH	2:D:1497:GLY:HA3	2.13	0.48
2:C:4272:LYS:HD2	2:C:4273:LYS:HG2	1.96	0.48
2:C:4481:TRP:CE3	2:C:4484:ILE:HD11	2.49	0.48
2:D:15:ARG:HA	2:D:113:LEU:CD1	2.44	0.48
2:D:1989:PRO:HD2	2:D:1992:ILE:HD12	1.96	0.48
2:D:3070:LYS:O	2:D:3073:GLU:HG3	2.13	0.48
2:D:4480:PHE:O	2:D:4484:ILE:HG23	2.13	0.48
1:H:9:SER:HB2	1:H:72:ARG:HB3	1.95	0.48
2:A:176:ARG:HB2	2:A:179:ASP:HB2	1.96	0.48
2:A:941:LYS:HA	2:A:944:LEU:HD12	1.96	0.48
2:A:1190:LEU:HB2	2:A:1193:LYS:HZ1	1.79	0.48
2:A:1436:GLN:HG2	2:A:1552:VAL:HG23	1.94	0.48
2:A:2768:LYS:HB3	2:A:2772:ARG:NH1	2.29	0.48
2:A:2927:GLN:HB3	2:A:2931:ARG:HH22	1.79	0.48
2:B:881:ILE:HG21	2:B:1062:TYR:CE1	2.49	0.48
2:B:988:LEU:H	2:B:1055:ARG:NH2	2.10	0.48
2:C:1788:LYS:HG3	2:C:1834:PHE:CE1	2.49	0.48
2:C:2174:VAL:O	2:C:2178:VAL:HG23	2.13	0.48
2:C:4800:ASP:OD1	2:C:4801:THR:N	2.46	0.48
2:D:218:SER:HB3	2:D:286:GLY:HA3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:227:TYR:CG	2:D:352:SER:HB3	2.48	0.48
2:D:291:TRP:CD1	2:D:353:GLU:HB3	2.49	0.48
2:D:1124:PRO:HD2	2:D:1594:VAL:HG23	1.95	0.48
2:D:3117:PHE:CD2	2:D:3117:PHE:CB	2.79	0.48
2:D:3218:ILE:HA	2:D:3221:LEU:HG	1.95	0.48
2:D:4272:LYS:HD2	2:D:4273:LYS:HG2	1.95	0.48
2:D:4517:LEU:O	2:D:4520:TYR:HB2	2.13	0.48
2:A:503:ASP:O	2:A:507:VAL:HG13	2.14	0.48
2:A:1019:GLY:HA2	2:A:1028:ARG:HH21	1.77	0.48
2:A:4179:GLU:OE1	2:A:4179:GLU:N	2.46	0.48
2:A:4480:PHE:O	2:A:4484:ILE:HG23	2.13	0.48
2:B:3171:LEU:HD23	2:B:3214:LEU:HD13	1.96	0.48
2:C:1522:ALA:O	2:C:1525:LYS:HG2	2.14	0.48
2:C:2068:ARG:NH1	2:C:2072:GLU:OE2	2.47	0.48
2:C:2455:ASP:OD2	2:C:2457:SER:OG	2.32	0.48
2:C:2927:GLN:HB3	2:C:2931:ARG:HH22	1.79	0.48
2:C:4248:LEU:HD22	2:D:4711:GLY:HA2	1.95	0.48
2:C:4822:ARG:NH2	2:D:4825:GLY:O	2.46	0.48
2:D:661:LEU:O	2:D:788:PHE:N	2.30	0.48
2:D:810:GLU:CD	2:D:1614:ARG:HH21	2.17	0.48
2:D:2348:GLU:O	2:D:2352:LYS:HG2	2.13	0.48
2:D:2788:ARG:HB2	2:D:2904:SER:OG	2.14	0.48
2:A:480:ARG:HE	2:A:3678:GLU:HG2	1.79	0.48
2:A:1522:ALA:O	2:A:1525:LYS:HG2	2.14	0.48
2:A:1714:TYR:CZ	2:A:1761:MET:HG3	2.48	0.48
2:A:2935:GLU:O	2:A:2938:GLN:HG3	2.14	0.48
2:A:3171:LEU:HD23	2:A:3214:LEU:HD13	1.96	0.48
2:B:15:ARG:HA	2:B:113:LEU:CD1	2.43	0.48
2:B:218:SER:HB3	2:B:286:GLY:HA3	1.95	0.48
2:B:1522:ALA:O	2:B:1525:LYS:HG2	2.14	0.48
2:B:1910:LEU:HD13	2:B:2062:ILE:HG12	1.95	0.48
2:B:2927:GLN:HB3	2:B:2931:ARG:HH22	1.79	0.48
2:B:2935:GLU:O	2:B:2938:GLN:HG3	2.14	0.48
2:B:3699:CYS:HB2	2:B:3764:ALA:HB1	1.94	0.48
2:C:2295:GLY:HA3	2:C:2391:PHE:HE2	1.78	0.48
2:C:3728:GLN:O	2:C:3732:HIS:ND1	2.40	0.48
2:D:503:ASP:O	2:D:507:VAL:HG13	2.14	0.48
2:D:2591:ARG:NH2	2:D:2876:THR:OG1	2.45	0.48
2:D:3067:ASP:O	2:D:3070:LYS:HG2	2.14	0.48
2:D:3088:LYS:HG3	2:D:3090:VAL:HG12	1.95	0.48
2:B:176:ARG:HB2	2:B:179:ASP:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:291:TRP:CD1	2:C:353:GLU:HB3	2.49	0.48
2:C:399:MET:SD	2:C:399:MET:N	2.87	0.48
2:C:1175:PHE:HB2	2:C:1182:LEU:HD12	1.96	0.48
2:C:1989:PRO:HD2	2:C:1992:ILE:HD12	1.96	0.48
2:C:2688:MET:HB2	2:C:2689:MET:HE2	1.94	0.48
2:C:2788:ARG:HB2	2:C:2904:SER:OG	2.14	0.48
2:D:941:LYS:HA	2:D:944:LEU:HD12	1.96	0.48
2:D:3651:PRO:HB2	2:D:3652:PRO:HD3	1.95	0.48
2:D:4640:PHE:CG	2:D:4641:PRO:HD3	2.48	0.48
2:D:4800:ASP:OD1	2:D:4801:THR:N	2.46	0.48
2:A:291:TRP:CD1	2:A:353:GLU:HB3	2.49	0.47
2:A:1989:PRO:HD2	2:A:1992:ILE:HD12	1.96	0.47
2:A:2295:GLY:HA3	2:A:2391:PHE:HE2	1.78	0.47
2:A:2551:THR:O	2:A:2555:LEU:HG	2.14	0.47
2:A:4898:PHE:O	2:A:4904:GLY:HA3	2.13	0.47
2:B:2727:HIS:O	2:B:2731:LYS:HG2	2.12	0.47
2:B:2788:ARG:HB2	2:B:2904:SER:OG	2.14	0.47
2:B:3218:ILE:HA	2:B:3221:LEU:HG	1.95	0.47
2:B:4157:ARG:O	2:B:4161:GLU:HG2	2.14	0.47
2:B:4172:PHE:O	2:B:4176:VAL:HG22	2.14	0.47
2:C:3218:ILE:HA	2:C:3221:LEU:HG	1.96	0.47
2:C:3986:LEU:HG	2:C:3999:MET:SD	2.54	0.47
2:D:895:MET:HG3	2:D:896:ASN:N	2.29	0.47
2:D:2551:THR:O	2:D:2555:LEU:HG	2.14	0.47
2:D:3986:LEU:HG	2:D:3999:MET:SD	2.54	0.47
1:G:9:SER:HB2	1:G:72:ARG:HB3	1.95	0.47
2:A:2681:MET:HG3	2:A:2914:THR:HG22	1.96	0.47
2:A:2773:TRP:HB3	2:A:2774:PRO:HD3	1.96	0.47
2:A:3234:VAL:HA	2:A:3237:VAL:HG12	1.96	0.47
2:A:3651:PRO:HB2	2:A:3652:PRO:HD3	1.95	0.47
2:A:3787:VAL:HG12	2:A:3864:ASN:HB3	1.96	0.47
2:B:291:TRP:CD1	2:B:353:GLU:HB3	2.49	0.47
2:B:480:ARG:HE	2:B:3678:GLU:HG2	1.79	0.47
2:B:1444:GLY:HA3	2:B:1487:MET:HA	1.96	0.47
2:B:3732:HIS:O	2:B:3776:LYS:NZ	2.47	0.47
2:C:810:GLU:CD	2:C:1614:ARG:HH21	2.17	0.47
2:C:1415:ASP:OD2	2:C:1559:ARG:NH2	2.35	0.47
2:C:1910:LEU:HD13	2:C:2062:ILE:HG12	1.95	0.47
2:C:3067:ASP:O	2:C:3070:LYS:HG2	2.14	0.47
2:D:2174:VAL:O	2:D:2178:VAL:HG23	2.13	0.47
2:D:2424:ARG:NH2	2:D:2476:TYR:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:9:SER:HB2	1:F:72:ARG:HB3	1.95	0.47
2:A:261:HIS:CD2	2:A:263:GLU:HG3	2.49	0.47
2:A:895:MET:HG3	2:A:896:ASN:N	2.29	0.47
2:A:1175:PHE:HB2	2:A:1182:LEU:HD12	1.97	0.47
2:A:3067:ASP:O	2:A:3070:LYS:HG2	2.14	0.47
2:A:3154:ALA:O	2:A:3157:GLU:HG3	2.15	0.47
2:A:3249:TRP:HB3	2:A:3266:THR:HG21	1.97	0.47
2:A:4587:ILE:HD13	2:A:4726:MET:HG2	1.96	0.47
2:B:261:HIS:CD2	2:B:263:GLU:HG3	2.50	0.47
2:B:412:GLU:HG3	2:B:488:LEU:HD11	1.96	0.47
2:B:941:LYS:HA	2:B:944:LEU:HD12	1.96	0.47
2:B:2768:LYS:HB3	2:B:2772:ARG:NH1	2.29	0.47
2:B:3217:GLU:O	2:B:3220:GLU:HG3	2.14	0.47
2:B:3324:GLU:HG2	2:B:3327:LYS:HE3	1.96	0.47
2:C:521:GLU:H	2:C:521:GLU:CD	2.15	0.47
2:C:2335:LEU:HD11	2:C:2343:LEU:HD13	1.96	0.47
2:C:2585:MET:O	2:C:2589:LEU:HG	2.15	0.47
2:C:2618:TRP:HD1	2:C:2619:LYS:HZ2	1.55	0.47
2:C:2905:ARG:HH11	2:C:2906:GLY:H	1.60	0.47
2:C:4522:VAL:HG13	2:D:4786:PHE:CZ	2.50	0.47
2:D:3117:PHE:CD1	2:D:3117:PHE:CB	2.79	0.47
2:D:3665:HIS:HB2	2:D:3734:ARG:HG2	1.95	0.47
2:A:988:LEU:H	2:A:1055:ARG:NH2	2.10	0.47
2:A:2627:TRP:O	2:A:2631:GLY:N	2.48	0.47
2:B:2455:ASP:OD2	2:B:2457:SER:OG	2.32	0.47
2:B:2591:ARG:NH2	2:B:2876:THR:OG1	2.45	0.47
2:B:3651:PRO:HB2	2:B:3652:PRO:HD3	1.95	0.47
2:C:1711:LEU:HD22	2:C:1831:MET:HE1	1.97	0.47
2:C:2549:LEU:HD11	2:C:2580:LEU:HD11	1.97	0.47
2:D:423:VAL:HG22	2:D:494:MET:HE1	1.95	0.47
2:D:881:ILE:HG21	2:D:1062:TYR:CE1	2.49	0.47
2:D:1444:GLY:HA3	2:D:1487:MET:HA	1.96	0.47
2:D:2935:GLU:O	2:D:2938:GLN:HG3	2.14	0.47
2:D:3187:LYS:NZ	2:D:3191:GLU:OE1	2.46	0.47
2:D:3732:HIS:O	2:D:3776:LYS:NZ	2.47	0.47
2:A:16:THR:OG1	2:A:69:LEU:O	2.22	0.47
2:A:2424:ARG:HE	2:A:2476:TYR:HA	1.80	0.47
2:A:3072:MET:HE2	2:A:3072:MET:N	2.30	0.47
2:A:4157:ARG:O	2:A:4161:GLU:HG2	2.14	0.47
2:A:4509:VAL:HG13	2:A:4575:LEU:HD22	1.97	0.47
2:A:4584:PHE:O	2:A:4588:ILE:HG13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:62:LEU:O	2:B:66:THR:HG23	2.15	0.47
2:B:3067:ASP:O	2:B:3070:LYS:HG2	2.14	0.47
2:B:3154:ALA:O	2:B:3157:GLU:HG3	2.15	0.47
2:B:3778:LEU:HD13	2:B:3854:PHE:HD1	1.80	0.47
2:C:323:ASP:OD1	2:C:324:VAL:N	2.48	0.47
2:C:808:HIS:NE2	2:C:832:LEU:HB3	2.30	0.47
2:C:2830:ASN:HD22	2:D:1435:GLY:HA3	1.79	0.47
2:D:480:ARG:HE	2:D:3678:GLU:HG2	1.79	0.47
2:D:2833:LEU:HB2	2:D:2838[A]:HIS:NE2	2.29	0.47
2:A:15:ARG:HA	2:A:113:LEU:CD1	2.44	0.47
2:A:1939:ASN:ND2	2:A:1989:PRO:HG2	2.30	0.47
2:A:2068:ARG:NH1	2:A:2072:GLU:OE2	2.46	0.47
2:A:4640:PHE:CG	2:A:4641:PRO:HD3	2.48	0.47
2:B:1989:PRO:HD2	2:B:1992:ILE:HD12	1.96	0.47
2:B:3249:TRP:HB3	2:B:3266:THR:HG21	1.97	0.47
2:B:4587:ILE:HD13	2:B:4726:MET:HG2	1.96	0.47
2:B:4694:LEU:HD23	2:B:4694:LEU:H	1.79	0.47
2:C:3324:GLU:HG2	2:C:3327:LYS:HE3	1.96	0.47
2:C:4930:GLU:OE1	2:C:4930:GLU:N	2.34	0.47
2:D:2627:TRP:O	2:D:2631:GLY:N	2.48	0.47
2:D:3249:TRP:HB3	2:D:3266:THR:HG21	1.97	0.47
2:D:3664:LEU:O	2:D:3668:ILE:HG13	2.15	0.47
2:D:4172:PHE:O	2:D:4176:VAL:HG22	2.14	0.47
2:D:4584:PHE:O	2:D:4588:ILE:HG13	2.14	0.47
2:D:4694:LEU:HD23	2:D:4694:LEU:H	1.80	0.47
2:A:412:GLU:HG3	2:A:488:LEU:HD11	1.96	0.47
2:A:808:HIS:NE2	2:A:832:LEU:HB3	2.30	0.47
2:A:824:GLU:HA	2:A:1020:ILE:HD12	1.97	0.47
2:A:877:HIS:CA	2:A:880:ARG:NH1	2.76	0.47
2:A:881:ILE:HG21	2:A:1062:TYR:CE1	2.49	0.47
2:A:1788:LYS:HG3	2:A:1834:PHE:CE1	2.49	0.47
2:A:2788:ARG:HB2	2:A:2904:SER:OG	2.14	0.47
2:A:2905:ARG:HH11	2:A:2906:GLY:H	1.60	0.47
2:A:3217:GLU:O	2:A:3220:GLU:HG3	2.14	0.47
2:A:3986:LEU:HG	2:A:3999:MET:SD	2.54	0.47
2:A:4694:LEU:HD23	2:A:4694:LEU:H	1.80	0.47
2:A:4818:TYR:CD2	2:A:4819:VAL:HG23	2.50	0.47
2:B:895:MET:HG3	2:B:896:ASN:N	2.29	0.47
2:B:993:GLU:HG2	2:B:1051:ARG:HH12	1.80	0.47
2:B:1007:TRP:NE1	4:B:5005:ATP:O1B	2.40	0.47
2:B:1175:PHE:HB2	2:B:1182:LEU:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2353:ILE:HG12	2:B:2359:ARG:HE	1.80	0.47
2:B:2551:THR:O	2:B:2555:LEU:HG	2.14	0.47
2:B:2585:MET:O	2:B:2589:LEU:HG	2.15	0.47
2:B:2609:LEU:HA	2:B:2612:ASN:HD21	1.80	0.47
2:B:2641:SER:HA	2:B:2644:LEU:HD12	1.97	0.47
2:B:2681:MET:HG3	2:B:2914:THR:HG22	1.96	0.47
2:B:3316:LYS:O	2:B:3317:THR:OG1	2.28	0.47
2:B:3986:LEU:HG	2:B:3999:MET:SD	2.54	0.47
2:B:4664:ASP:OD2	2:B:4674:LYS:NZ	2.48	0.47
2:B:4725:TYR:CD1	2:B:4742:HIS:HD2	2.33	0.47
2:C:881:ILE:HG21	2:C:1062:TYR:CE1	2.49	0.47
2:C:1006:VAL:HA	2:C:1009:ARG:HH12	1.80	0.47
2:C:2149:ILE:HD13	2:C:2167:MET:CE	2.44	0.47
2:C:2641:SER:HA	2:C:2644:LEU:HD12	1.97	0.47
2:C:2768:LYS:HB3	2:C:2772:ARG:NH1	2.29	0.47
2:C:2935:GLU:O	2:C:2938:GLN:HG3	2.14	0.47
2:C:3234:VAL:HA	2:C:3237:VAL:HG12	1.96	0.47
2:C:3664:LEU:O	2:C:3668:ILE:HG13	2.15	0.47
2:C:4157:ARG:O	2:C:4161:GLU:HG2	2.14	0.47
2:C:4818:TYR:CD2	2:C:4819:VAL:HG23	2.50	0.47
2:D:62:LEU:O	2:D:66:THR:HG23	2.15	0.47
2:D:261:HIS:CD2	2:D:263:GLU:HG3	2.49	0.47
2:D:927:GLN:HG2	2:D:928:GLU:N	2.30	0.47
2:D:3054:LYS:HB3	2:D:3058:ARG:HH12	1.80	0.47
2:D:3217:GLU:O	2:D:3220:GLU:HG3	2.14	0.47
2:D:3324:GLU:HG2	2:D:3327:LYS:HE3	1.96	0.47
2:D:4157:ARG:O	2:D:4161:GLU:HG2	2.14	0.47
2:D:4166:LYS:O	2:D:4170:ARG:HG2	2.15	0.47
2:D:4509:VAL:HG13	2:D:4575:LEU:HD22	1.97	0.47
2:A:3054:LYS:HB3	2:A:3058:ARG:HH12	1.80	0.47
2:A:3272:HIS:O	2:A:3275:THR:OG1	2.25	0.47
2:A:4272:LYS:HD2	2:A:4273:LYS:HG2	1.95	0.47
2:B:2424:ARG:HE	2:B:2476:TYR:HA	1.80	0.47
2:B:3109:PHE:CE2	2:B:3162:PHE:HD1	2.33	0.47
2:B:4584:PHE:O	2:B:4588:ILE:HG13	2.14	0.47
2:C:2681:MET:HG3	2:C:2914:THR:HG22	1.96	0.47
2:C:2773:TRP:HB3	2:C:2774:PRO:HD3	1.96	0.47
2:C:4042:VAL:HB	2:C:4077:THR:HB	1.97	0.47
2:D:824:GLU:HA	2:D:1020:ILE:HD12	1.97	0.47
2:D:1006:VAL:HA	2:D:1009:ARG:HH12	1.80	0.47
2:D:2609:LEU:HA	2:D:2612:ASN:HD21	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3154:ALA:O	2:D:3157:GLU:HG3	2.15	0.47
2:D:3778:LEU:HD13	2:D:3854:PHE:HD1	1.80	0.47
2:D:4481:TRP:HA	2:D:4484:ILE:HG12	1.97	0.47
2:D:4818:TYR:CD2	2:D:4819:VAL:HG23	2.50	0.47
1:E:9:SER:HB2	1:E:72:ARG:HB3	1.95	0.47
2:A:323:ASP:OD1	2:A:324:VAL:N	2.48	0.47
2:A:521:GLU:H	2:A:521:GLU:CD	2.15	0.47
2:A:2641:SER:HA	2:A:2644:LEU:HD12	1.97	0.47
2:A:3068:LEU:O	2:A:3072:MET:HE3	2.14	0.47
2:A:3324:GLU:OE1	2:A:3328:LYS:NZ	2.48	0.47
2:B:2174:VAL:O	2:B:2178:VAL:HG23	2.13	0.47
2:B:2601:GLU:HA	2:B:2604:LYS:HZ1	1.79	0.47
2:B:4042:VAL:HB	2:B:4077:THR:HB	1.97	0.47
2:B:4818:TYR:CD2	2:B:4819:VAL:HG23	2.50	0.47
2:C:2732:TRP:O	2:C:2732:TRP:CD1	2.67	0.47
2:D:562:LEU:HD11	2:D:600:LEU:HD22	1.97	0.47
2:D:1522:ALA:O	2:D:1525:LYS:HG2	2.14	0.47
2:D:2149:ILE:HD13	2:D:2167:MET:CE	2.44	0.47
2:D:2641:SER:HA	2:D:2644:LEU:HD12	1.97	0.47
2:A:927:GLN:HG2	2:A:928:GLU:N	2.30	0.47
2:A:2591:ARG:NH2	2:A:2876:THR:OG1	2.45	0.47
2:A:3218:ILE:HA	2:A:3221:LEU:HG	1.95	0.47
2:A:3664:LEU:O	2:A:3668:ILE:HG13	2.15	0.47
2:A:4166:LYS:O	2:A:4170:ARG:HG2	2.15	0.47
2:B:611:LEU:HD22	2:B:1660:LEU:HD22	1.97	0.47
2:B:1788:LYS:HG3	2:B:1834:PHE:CE1	2.49	0.47
2:C:674:TYR:CE1	2:C:756:SER:HB2	2.50	0.47
2:C:895:MET:HG3	2:C:896:ASN:N	2.29	0.47
2:C:941:LYS:HA	2:C:944:LEU:HD12	1.96	0.47
2:C:952:ILE:HA	2:C:1062:TYR:HA	1.97	0.47
2:C:1269:GLU:HB2	2:C:1288:LYS:HE3	1.97	0.47
2:C:3109:PHE:CE2	2:C:3162:PHE:HD1	2.33	0.47
2:C:3159:LEU:HD13	2:C:3241:MET:SD	2.55	0.47
2:C:4584:PHE:O	2:C:4588:ILE:HG13	2.14	0.47
2:C:4725:TYR:CD1	2:C:4742:HIS:HD2	2.33	0.47
2:D:611:LEU:HD22	2:D:1660:LEU:HD22	1.97	0.47
2:A:2549:LEU:HD11	2:A:2580:LEU:HD11	1.97	0.46
2:A:2732:TRP:O	2:A:2732:TRP:CD1	2.67	0.46
2:A:3324:GLU:HG2	2:A:3327:LYS:HE3	1.96	0.46
2:B:411:GLU:OE2	2:B:485:ARG:NE	2.38	0.46
2:B:987:LYS:NZ	2:B:988:LEU:O	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2773:TRP:HB3	2:B:2774:PRO:HD3	1.96	0.46
2:B:4248:LEU:HB3	2:C:4630:TRP:CH2	2.50	0.46
2:B:4272:LYS:HD2	2:B:4273:LYS:HG2	1.95	0.46
2:B:4509:VAL:HG13	2:B:4575:LEU:HD22	1.97	0.46
2:C:503:ASP:O	2:C:507:VAL:HG13	2.14	0.46
2:C:3154:ALA:O	2:C:3157:GLU:HG3	2.15	0.46
2:C:4166:LYS:O	2:C:4170:ARG:HG2	2.15	0.46
2:C:4481:TRP:HA	2:C:4484:ILE:HG12	1.97	0.46
2:D:323:ASP:OD1	2:D:324:VAL:N	2.48	0.46
2:D:494:MET:HA	2:D:494:MET:HE3	1.96	0.46
2:D:674:TYR:CE1	2:D:756:SER:HB2	2.50	0.46
2:D:808:HIS:NE2	2:D:832:LEU:HB3	2.30	0.46
2:D:1175:PHE:HB2	2:D:1182:LEU:HD12	1.97	0.46
2:D:2353:ILE:HG12	2:D:2359:ARG:HE	1.80	0.46
2:D:2681:MET:HG3	2:D:2914:THR:HG22	1.96	0.46
2:D:3787:VAL:HG12	2:D:3864:ASN:HB3	1.96	0.46
2:A:378:ASP:OD2	2:A:389:ARG:NH2	2.49	0.46
2:A:579:LEU:HD22	2:A:586:LEU:HD23	1.97	0.46
2:A:674:TYR:CE1	2:A:756:SER:HB2	2.50	0.46
2:B:15:ARG:HD3	2:B:112:THR:HA	1.98	0.46
2:B:1269:GLU:HB2	2:B:1288:LYS:HE3	1.97	0.46
2:B:3221:LEU:HD12	2:B:3283:ILE:HD11	1.98	0.46
2:C:378:ASP:OD2	2:C:389:ARG:NH2	2.49	0.46
2:C:562:LEU:HD11	2:C:600:LEU:HD22	1.97	0.46
2:C:1939:ASN:ND2	2:C:1989:PRO:HG2	2.30	0.46
2:C:2182:GLY:HA3	2:C:2185:LYS:HE2	1.98	0.46
2:C:2609:LEU:HA	2:C:2612:ASN:HD21	1.80	0.46
2:C:2975:PHE:HD2	2:C:3039:THR:HG21	1.81	0.46
2:D:399:MET:SD	2:D:399:MET:N	2.87	0.46
2:D:2732:TRP:O	2:D:2732:TRP:CD1	2.67	0.46
2:D:2975:PHE:HD2	2:D:3039:THR:HG21	1.81	0.46
2:D:3109:PHE:CE2	2:D:3162:PHE:HD1	2.33	0.46
2:A:62:LEU:O	2:A:66:THR:HG23	2.15	0.46
2:A:2353:ILE:HG12	2:A:2359:ARG:HE	1.80	0.46
2:A:2585:MET:O	2:A:2589:LEU:HG	2.15	0.46
2:A:3221:LEU:HD12	2:A:3283:ILE:HD11	1.98	0.46
2:A:4071:GLU:OE1	2:A:4086:ARG:NH2	2.30	0.46
2:A:4481:TRP:HA	2:A:4484:ILE:HG12	1.97	0.46
2:A:4725:TYR:CD1	2:A:4742:HIS:HD2	2.33	0.46
2:A:4838:GLU:OE1	2:A:4838:GLU:N	2.36	0.46
2:B:503:ASP:O	2:B:507:VAL:HG13	2.14	0.46

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
2:B:824:GLU:HA	2:B:1020:ILE:HD12	1.97	0.46
2:B:1118:SER:HB3	2:B:1204:VAL:HG11	1.98	0.46
2:B:2627:TRP:O	2:B:2631:GLY:N	2.48	0.46
2:B:3234:VAL:HA	2:B:3237:VAL:HG12	1.96	0.46
2:B:3664:LEU:O	2:B:3668:ILE:HG13	2.15	0.46
2:B:3787:VAL:HG12	2:B:3864:ASN:HB3	1.96	0.46
2:C:251:GLU:HB2	2:C:256:GLN:NE2	2.30	0.46
2:C:261:HIS:CD2	2:C:263:GLU:HG3	2.49	0.46
2:C:2551:THR:O	2:C:2555:LEU:HG	2.14	0.46
2:C:3249:TRP:HB3	2:C:3266:THR:HG21	1.97	0.46
2:C:3324:GLU:OE1	2:C:3328:LYS:NZ	2.48	0.46
2:C:4509:VAL:HG13	2:C:4575:LEU:HD22	1.97	0.46
2:D:579:LEU:HD22	2:D:586:LEU:HD23	1.97	0.46
2:D:2585:MET:O	2:D:2589:LEU:HG	2.15	0.46
2:D:2773:TRP:HB3	2:D:2774:PRO:HD3	1.96	0.46
2:D:2833:LEU:HB2	2:D:2838[B]:HIS:NE2	2.30	0.46
2:D:2956:TYR:CD2	2:D:2960:ILE:HG12	2.50	0.46
2:D:2980:LEU:HG	2:D:2990:LEU:HB2	1.97	0.46
2:A:952:ILE:HA	2:A:1062:TYR:HA	1.97	0.46
2:A:3159:LEU:HD13	2:A:3241:MET:SD	2.55	0.46
2:B:952:ILE:HA	2:B:1062:TYR:HA	1.97	0.46
2:B:3159:LEU:HD13	2:B:3241:MET:SD	2.55	0.46
2:B:3178:HIS:HD1	2:B:3260:ARG:NH2	2.13	0.46
2:B:4178:ASN:HB3	2:B:4179:GLU:OE1	2.16	0.46
2:C:541:ILE:HD13	2:C:574:VAL:HG13	1.97	0.46
2:C:3217:GLU:O	2:C:3220:GLU:HG3	2.14	0.46
2:D:15:ARG:HD3	2:D:112:THR:HA	1.98	0.46
2:D:877:HIS:CA	2:D:880:ARG:NH1	2.77	0.46
2:D:1435:GLY:N	2:D:1501:ASN:OD1	2.35	0.46
2:A:251:GLU:HB2	2:A:256:GLN:NE2	2.30	0.46
2:A:611:LEU:HD22	2:A:1660:LEU:HD22	1.97	0.46
2:A:1782:PHE:HE2	2:A:1787:LEU:HD13	1.81	0.46
2:A:2129:LEU:HD13	2:A:2142:MET:HG3	1.98	0.46
2:A:2609:LEU:HA	2:A:2612:ASN:HD21	1.80	0.46
2:A:3109:PHE:CE2	2:A:3162:PHE:HD1	2.33	0.46
2:A:3178:HIS:HD1	2:A:3260:ARG:NH2	2.13	0.46
2:A:4107:GLU:OE1	2:A:4149:TYR:OH	2.27	0.46
2:B:1939:ASN:ND2	2:B:1989:PRO:HG2	2.30	0.46
2:B:2182:GLY:HA3	2:B:2185:LYS:HE2	1.97	0.46
2:B:2549:LEU:HD11	2:B:2580:LEU:HD11	1.97	0.46
2:B:3054:LYS:HB3	2:B:3058:ARG:HH12	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4481:TRP:HA	2:B:4484:ILE:HG12	1.97	0.46
2:B:4650:LYS:HA	2:B:4653:VAL:HG22	1.98	0.46
2:C:412:GLU:HG3	2:C:488:LEU:HD11	1.96	0.46
2:C:1194:ASP:OD1	2:C:1195:PHE:N	2.48	0.46
2:C:2353:ILE:HG12	2:C:2359:ARG:HE	1.80	0.46
2:C:4038:ASP:HB3	2:C:4040:LYS:HZ2	1.80	0.46
2:D:378:ASP:OD2	2:D:389:ARG:NH2	2.49	0.46
2:D:3159:LEU:HD13	2:D:3241:MET:SD	2.55	0.46
2:A:15:ARG:HD3	2:A:112:THR:HA	1.98	0.46
2:A:993:GLU:HG2	2:A:1051:ARG:HH12	1.80	0.46
2:A:3749:GLY:HA2	2:A:3796:LEU:HG	1.98	0.46
2:A:4814:MET:CE	2:B:4841:ILE:HD13	2.45	0.46
2:B:541:ILE:HD13	2:B:574:VAL:HG13	1.97	0.46
2:B:579:LEU:HD22	2:B:586:LEU:HD23	1.97	0.46
2:B:808:HIS:NE2	2:B:832:LEU:HB3	2.30	0.46
2:B:927:GLN:HG2	2:B:928:GLU:N	2.30	0.46
2:B:2504:THR:O	2:B:2508:SER:N	2.45	0.46
2:B:3324:GLU:OE1	2:B:3328:LYS:NZ	2.48	0.46
2:C:927:GLN:HG2	2:C:928:GLU:N	2.30	0.46
2:C:1782:PHE:HE2	2:C:1787:LEU:HD13	1.81	0.46
2:C:2129:LEU:HD13	2:C:2142:MET:HG3	1.98	0.46
2:C:3787:VAL:HG12	2:C:3864:ASN:HB3	1.96	0.46
2:C:4587:ILE:HD13	2:C:4726:MET:HG2	1.97	0.46
2:D:250:GLY:HA2	2:D:257:ARG:HD3	1.98	0.46
2:D:251:GLU:HB2	2:D:256:GLN:NE2	2.30	0.46
2:D:2504:THR:O	2:D:2508:SER:N	2.45	0.46
2:D:2549:LEU:HD11	2:D:2580:LEU:HD11	1.97	0.46
2:D:4042:VAL:HB	2:D:4077:THR:HB	1.97	0.46
2:D:4650:LYS:HA	2:D:4653:VAL:HG22	1.98	0.46
2:A:1006:VAL:HA	2:A:1009:ARG:HH12	1.80	0.46
2:A:2787:TRP:CD1	2:A:2904:SER:O	2.68	0.46
2:A:3778:LEU:HD13	2:A:3854:PHE:HD1	1.80	0.46
2:A:4042:VAL:HB	2:A:4077:THR:HB	1.97	0.46
2:A:4248:LEU:HB3	2:B:4630:TRP:CZ3	2.51	0.46
2:B:251:GLU:HB2	2:B:256:GLN:NE2	2.30	0.46
2:B:674:TYR:CE1	2:B:756:SER:HB2	2.50	0.46
2:B:2980:LEU:HG	2:B:2990:LEU:HB2	1.97	0.46
2:B:4166:LYS:O	2:B:4170:ARG:HG2	2.15	0.46
2:C:824:GLU:HA	2:C:1020:ILE:HD12	1.97	0.46
2:C:877:HIS:CA	2:C:880:ARG:NH1	2.76	0.46
2:C:997:ASP:OD1	2:C:1047:LYS:NZ	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1118:SER:HB3	2:C:1204:VAL:HG11	1.98	0.46
2:C:4026:LEU:HD21	2:C:4052:MET:HG2	1.98	0.46
2:C:4078:LEU:HD23	2:C:4078:LEU:H	1.80	0.46
2:D:3324:GLU:OE1	2:D:3328:LYS:NZ	2.48	0.46
2:D:4725:TYR:CD1	2:D:4742:HIS:HD2	2.33	0.46
2:A:250:GLY:HA2	2:A:257:ARG:HD3	1.98	0.46
2:A:1118:SER:HB3	2:A:1204:VAL:HG11	1.98	0.46
2:A:2649:PHE:HZ	2:A:2967:VAL:HG22	1.80	0.46
2:B:1685:LEU:HB3	2:B:1706:LEU:HD12	1.98	0.46
2:B:2424:ARG:NH2	2:B:2476:TYR:O	2.47	0.46
2:B:2688:MET:HB2	2:B:2689:MET:HE3	1.96	0.46
2:B:2981:TYR:O	2:B:2984:SER:OG	2.21	0.46
2:C:15:ARG:HD3	2:C:112:THR:HA	1.98	0.46
2:C:62:LEU:O	2:C:66:THR:HG23	2.15	0.46
2:C:250:GLY:HA2	2:C:257:ARG:HD3	1.98	0.46
2:C:611:LEU:HD22	2:C:1660:LEU:HD22	1.97	0.46
2:C:2627:TRP:O	2:C:2631:GLY:N	2.48	0.46
2:C:2956:TYR:CD2	2:C:2960:ILE:HG12	2.50	0.46
2:C:3778:LEU:HD13	2:C:3854:PHE:HD1	1.80	0.46
2:D:1782:PHE:HE2	2:D:1787:LEU:HD13	1.81	0.46
2:D:2182:GLY:HA3	2:D:2185:LYS:HE2	1.98	0.46
2:D:3178:HIS:HD1	2:D:3260:ARG:NH2	2.13	0.46
2:D:3221:LEU:HD12	2:D:3283:ILE:HD11	1.97	0.46
2:D:4587:ILE:HD13	2:D:4726:MET:HG2	1.96	0.46
2:A:1269:GLU:HB2	2:A:1288:LYS:HE3	1.97	0.46
2:A:2833:LEU:HD23	2:A:2897:GLN:NE2	2.31	0.46
2:A:3122:ILE:HG21	2:A:3167:PRO:HG3	1.98	0.46
2:A:4178:ASN:HB3	2:A:4179:GLU:OE1	2.16	0.46
2:A:4650:LYS:HA	2:A:4653:VAL:HG22	1.98	0.46
2:B:323:ASP:OD1	2:B:324:VAL:N	2.48	0.46
2:B:378:ASP:OD2	2:B:389:ARG:NH2	2.49	0.46
2:B:2728:SER:HA	2:B:2731:LYS:HE3	1.98	0.46
2:B:2956:TYR:CD2	2:B:2960:ILE:HG12	2.50	0.46
2:B:3054:LYS:HB3	2:B:3058:ARG:NH1	2.31	0.46
2:B:3627:SER:HB2	2:B:3628:TRP:HD1	1.81	0.46
2:C:2666:LEU:HD13	2:C:2966:VAL:HA	1.97	0.46
2:C:4178:ASN:HB3	2:C:4179:GLU:OE1	2.16	0.46
2:C:4694:LEU:HD23	2:C:4694:LEU:H	1.79	0.46
2:D:412:GLU:HG3	2:D:488:LEU:HD11	1.96	0.46
2:D:993:GLU:HG2	2:D:1051:ARG:HH12	1.80	0.46
2:D:1939:ASN:ND2	2:D:1989:PRO:HG2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3234:VAL:HA	2:D:3237:VAL:HG12	1.96	0.46
2:A:2824:ARG:HH22	2:B:1502:ASN:ND2	2.13	0.46
2:A:2956:TYR:CD2	2:A:2960:ILE:HG12	2.50	0.46
2:A:3054:LYS:HB3	2:A:3058:ARG:NH1	2.31	0.46
2:A:4664:ASP:OD2	2:A:4674:LYS:NZ	2.48	0.46
2:B:399:MET:SD	2:B:399:MET:N	2.86	0.46
2:B:562:LEU:HD11	2:B:600:LEU:HD22	1.97	0.46
2:B:934:GLN:O	2:B:938:GLU:OE1	2.34	0.46
2:B:2129:LEU:HD13	2:B:2142:MET:HG3	1.98	0.46
2:B:2720:PHE:HB2	2:B:2901:TYR:CE2	2.51	0.46
2:B:2975:PHE:HD2	2:B:3039:THR:HG21	1.81	0.46
2:C:1685:LEU:HB3	2:C:1706:LEU:HD12	1.98	0.46
2:C:2649:PHE:HZ	2:C:2967:VAL:HG22	1.80	0.46
2:C:3627:SER:HB2	2:C:3628:TRP:HD1	1.81	0.46
2:C:4492:LEU:HD22	2:C:4592:CYS:SG	2.56	0.46
2:C:4818:TYR:O	2:C:4819:VAL:HB	2.16	0.46
2:D:1194:ASP:OD1	2:D:1195:PHE:N	2.48	0.46
2:D:3183:ILE:HG23	2:D:3184:TYR:CD1	2.51	0.46
2:A:1194:ASP:OD1	2:A:1195:PHE:N	2.48	0.45
2:A:2285:TYR:HA	2:A:2362:PRO:HA	1.98	0.45
2:A:2980:LEU:HG	2:A:2990:LEU:HB2	1.97	0.45
2:A:3183:ILE:HG23	2:A:3184:TYR:CD1	2.51	0.45
2:A:4078:LEU:HD23	2:A:4078:LEU:H	1.81	0.45
2:A:4631:ASP:OD1	2:A:4708:TRP:NE1	2.45	0.45
2:B:2126:ILE:HD11	2:B:2145:GLY:HA3	1.98	0.45
2:B:3183:ILE:HG23	2:B:3184:TYR:CD1	2.51	0.45
2:B:3326:LEU:HD21	2:B:3336:GLU:HB3	1.98	0.45
2:B:3749:GLY:HA2	2:B:3796:LEU:HG	1.98	0.45
2:C:514:PHE:CD2	2:C:526:TRP:HB2	2.51	0.45
2:C:629:GLN:OE1	2:C:1669:ASN:ND2	2.49	0.45
2:C:1564:MET:HE3	2:C:1565:PRO:CD	2.39	0.45
2:C:2397:ASP:O	2:C:2401:ARG:HG3	2.17	0.45
2:D:16:THR:OG1	2:D:69:LEU:O	2.22	0.45
2:D:2580:LEU:HD23	2:D:2581:ARG:O	2.16	0.45
2:D:3226:ILE:HD11	2:D:3235:MET:HB3	1.97	0.45
2:D:3749:GLY:HA2	2:D:3796:LEU:HG	1.98	0.45
2:A:541:ILE:HD13	2:A:574:VAL:HG13	1.98	0.45
2:A:934:GLN:O	2:A:938:GLU:OE1	2.34	0.45
2:A:1497:GLY:HA3	2:D:2801:TYR:OH	2.16	0.45
2:A:2182:GLY:HA3	2:A:2185:LYS:HE2	1.98	0.45
2:A:2397:ASP:O	2:A:2401:ARG:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2975:PHE:HD2	2:A:3039:THR:HG21	1.81	0.45
2:A:3170:PHE:HD2	2:A:3208:ILE:HG12	1.81	0.45
2:A:3226:ILE:HD11	2:A:3235:MET:HB3	1.97	0.45
2:B:250:GLY:HA2	2:B:257:ARG:HD3	1.98	0.45
2:B:2841:ALA:CA	2:B:2844:MET:HG2	2.41	0.45
2:B:4026:LEU:HD21	2:B:4052:MET:HG2	1.98	0.45
2:C:480:ARG:HE	2:C:3678:GLU:HG2	1.79	0.45
2:C:3054:LYS:HB3	2:C:3058:ARG:HH12	1.80	0.45
2:C:3072:MET:HB3	2:C:3076:LYS:HZ2	1.81	0.45
2:C:3226:ILE:HD11	2:C:3235:MET:HB3	1.97	0.45
2:D:1269:GLU:HB2	2:D:1288:LYS:HE3	1.97	0.45
2:D:1554:GLN:NE2	2:D:1556:GLU:OE2	2.35	0.45
2:D:2409:ILE:HD12	2:D:2420:ARG:HE	1.81	0.45
2:A:3975:GLN:O	2:A:3979:VAL:HG23	2.17	0.45
2:A:4672:MET:HE1	2:A:4677:LEU:HD21	1.99	0.45
2:A:4818:TYR:O	2:A:4819:VAL:HB	2.16	0.45
2:A:4930:GLU:OE1	2:A:4930:GLU:N	2.34	0.45
2:B:630:HIS:CE1	2:B:1671:ARG:HE	2.35	0.45
2:B:1782:PHE:HE2	2:B:1787:LEU:HD13	1.81	0.45
2:B:2652:LEU:HB3	2:B:2962:PHE:CE1	2.52	0.45
2:B:3134:LEU:HB2	2:B:3162:PHE:CE2	2.52	0.45
2:C:479:LEU:O	2:C:483:LYS:HG2	2.17	0.45
2:C:993:GLU:HG2	2:C:1051:ARG:HH12	1.80	0.45
2:C:3183:ILE:HG23	2:C:3184:TYR:CD1	2.51	0.45
2:C:3326:LEU:HD21	2:C:3336:GLU:HB3	1.98	0.45
2:D:629:GLN:OE1	2:D:1669:ASN:ND2	2.49	0.45
2:D:2129:LEU:HD13	2:D:2142:MET:HG3	1.98	0.45
2:D:2424:ARG:HE	2:D:2476:TYR:HA	1.80	0.45
2:D:3054:LYS:HB3	2:D:3058:ARG:NH1	2.31	0.45
2:D:3627:SER:HB2	2:D:3628:TRP:HD1	1.81	0.45
2:D:4078:LEU:HD23	2:D:4078:LEU:H	1.81	0.45
2:D:4492:LEU:HD22	2:D:4592:CYS:SG	2.56	0.45
2:D:4818:TYR:O	2:D:4819:VAL:HB	2.16	0.45
2:D:4838:GLU:OE1	2:D:4838:GLU:N	2.36	0.45
2:D:4840:GLU:OE2	2:D:4844:ILE:HD11	2.17	0.45
2:A:370:LEU:C	2:A:393:MET:HE3	2.37	0.45
2:A:562:LEU:HD11	2:A:600:LEU:HD22	1.97	0.45
2:A:629:GLN:OE1	2:A:1669:ASN:ND2	2.49	0.45
2:A:889:ILE:HA	2:A:892:LEU:HD12	1.98	0.45
2:A:2580:LEU:HD23	2:A:2581:ARG:O	2.16	0.45
2:A:3134:LEU:HB2	2:A:3162:PHE:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:3627:SER:HB2	2:A:3628:TRP:HD1	1.81	0.45
2:A:4818:TYR:CD1	2:A:4822:ARG:HD3	2.52	0.45
2:B:1194:ASP:OD1	2:B:1195:PHE:N	2.48	0.45
2:B:1481:LYS:HB3	2:B:1481:LYS:HE3	1.81	0.45
2:B:3122:ILE:HG21	2:B:3167:PRO:HG3	1.98	0.45
2:B:3332:THR:OG1	2:B:3336:GLU:OE2	2.34	0.45
2:C:370:LEU:C	2:C:393:MET:HE3	2.37	0.45
2:C:934:GLN:O	2:C:938:GLU:OE1	2.34	0.45
2:C:1921:ARG:O	2:C:1925:ILE:HG13	2.17	0.45
2:C:3221:LEU:HD12	2:C:3283:ILE:HD11	1.98	0.45
2:C:3281:LEU:HA	2:C:3284:ILE:HG12	1.98	0.45
2:C:3303:SER:O	2:C:3307:ILE:HG12	2.17	0.45
2:C:3808:PHE:HB2	2:C:3829:VAL:HG21	1.99	0.45
2:D:479:LEU:O	2:D:483:LYS:HG2	2.17	0.45
2:D:1921:ARG:O	2:D:1925:ILE:HG13	2.17	0.45
2:D:2285:TYR:HA	2:D:2362:PRO:HA	1.98	0.45
2:D:3281:LEU:HA	2:D:3284:ILE:HG12	1.98	0.45
2:A:399:MET:SD	2:A:399:MET:N	2.87	0.45
2:A:997:ASP:OD1	2:A:1047:LYS:NZ	2.46	0.45
2:A:2126:ILE:HD11	2:A:2145:GLY:HA3	1.98	0.45
2:A:3281:LEU:HA	2:A:3284:ILE:HG12	1.98	0.45
2:A:3303:SER:O	2:A:3307:ILE:HG12	2.17	0.45
2:B:629:GLN:OE1	2:B:1669:ASN:ND2	2.49	0.45
2:B:2409:ILE:HD12	2:B:2420:ARG:HE	1.81	0.45
2:B:4818:TYR:CD1	2:B:4822:ARG:HD3	2.52	0.45
2:C:2126:ILE:HD11	2:C:2145:GLY:HA3	1.98	0.45
2:C:3170:PHE:HD2	2:C:3208:ILE:HG12	1.81	0.45
2:C:3178:HIS:HD1	2:C:3260:ARG:NH2	2.13	0.45
2:C:3599:VAL:O	2:C:3603:PHE:HD2	2.00	0.45
2:C:4252:ILE:HD13	2:D:4710:LEU:HB2	1.98	0.45
2:C:4650:LYS:HA	2:C:4653:VAL:HG22	1.98	0.45
2:C:4818:TYR:CD1	2:C:4822:ARG:HD3	2.52	0.45
2:D:952:ILE:HA	2:D:1062:TYR:HA	1.97	0.45
2:D:2649:PHE:HZ	2:D:2967:VAL:HG22	1.80	0.45
2:D:3212:GLU:HA	2:D:3215:MET:HE3	1.99	0.45
2:A:479:LEU:O	2:A:483:LYS:HG2	2.17	0.45
2:A:2424:ARG:NH2	2:A:2476:TYR:O	2.47	0.45
2:A:3808:PHE:HB2	2:A:3829:VAL:HG21	1.99	0.45
2:B:370:LEU:C	2:B:393:MET:HE3	2.37	0.45
2:B:895:MET:O	2:B:899:GLU:N	2.44	0.45
2:B:1921:ARG:O	2:B:1925:ILE:HG13	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2285:TYR:HA	2:B:2362:PRO:HA	1.98	0.45
2:B:2580:LEU:HD23	2:B:2581:ARG:O	2.17	0.45
2:B:2701:PHE:HZ	2:B:2853:ALA:HB1	1.82	0.45
2:B:3075:LEU:HD21	2:B:3094:ILE:HD12	1.99	0.45
2:B:3303:SER:O	2:B:3307:ILE:HG12	2.17	0.45
2:B:3975:GLN:O	2:B:3979:VAL:HG23	2.17	0.45
2:C:579:LEU:HD22	2:C:586:LEU:HD23	1.97	0.45
2:C:889:ILE:HA	2:C:892:LEU:HD12	1.98	0.45
2:C:2285:TYR:HA	2:C:2362:PRO:HA	1.98	0.45
2:C:3975:GLN:O	2:C:3979:VAL:HG23	2.17	0.45
2:D:3134:LEU:HB2	2:D:3162:PHE:CE2	2.52	0.45
2:D:3137:LEU:HD21	2:D:3159:LEU:HA	1.99	0.45
2:A:630:HIS:CE1	2:A:1671:ARG:HE	2.35	0.45
2:A:904:TYR:HA	2:A:915:HIS:O	2.17	0.45
2:A:2688:MET:HB2	2:A:2689:MET:HE2	1.97	0.45
2:A:2701:PHE:HZ	2:A:2853:ALA:HB1	1.82	0.45
2:A:4822:ARG:HB3	2:B:4851:PHE:CD2	2.52	0.45
2:B:3808:PHE:HB2	2:B:3829:VAL:HG21	1.99	0.45
2:C:2599:LEU:HB2	2:C:2655:LYS:HZ2	1.81	0.45
2:C:2652:LEU:HB3	2:C:2962:PHE:CE1	2.52	0.45
2:C:3749:GLY:HA2	2:C:3796:LEU:HG	1.98	0.45
2:D:2126:ILE:HD11	2:D:2145:GLY:HA3	1.98	0.45
2:D:2455:ASP:OD2	2:D:2457:SER:OG	2.32	0.45
2:D:2666:LEU:HD13	2:D:2966:VAL:HA	1.98	0.45
2:D:2701:PHE:HZ	2:D:2853:ALA:HB1	1.82	0.45
2:D:3122:ILE:HG21	2:D:3167:PRO:HG3	1.98	0.45
2:D:3808:PHE:HB2	2:D:3829:VAL:HG21	1.99	0.45
2:A:1921:ARG:O	2:A:1925:ILE:HG13	2.17	0.45
2:A:2765:GLU:O	2:A:2769:GLU:N	2.49	0.45
2:B:932:ASN:HA	2:B:935:MET:CG	2.41	0.45
2:B:2666:LEU:HD13	2:B:2966:VAL:HA	1.98	0.45
2:B:3170:PHE:HD2	2:B:3208:ILE:HG12	1.81	0.45
2:B:3226:ILE:HD11	2:B:3235:MET:HB3	1.97	0.45
2:B:4631:ASP:OD1	2:B:4708:TRP:NE1	2.45	0.45
2:B:4818:TYR:O	2:B:4819:VAL:HB	2.16	0.45
2:C:630:HIS:CE1	2:C:1671:ARG:HE	2.34	0.45
2:C:2701:PHE:HZ	2:C:2853:ALA:HB1	1.82	0.45
2:C:2980:LEU:HG	2:C:2990:LEU:HB2	1.97	0.45
2:C:3054:LYS:HB3	2:C:3058:ARG:NH1	2.31	0.45
2:C:3137:LEU:HD21	2:C:3159:LEU:HA	1.99	0.45
2:C:3205:CYS:O	2:C:3208:ILE:HG22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:4840:GLU:OE2	2:C:4844:ILE:HD11	2.17	0.45
2:D:541:ILE:HD13	2:D:574:VAL:HG13	1.97	0.45
2:D:762:SER:OG	2:D:763:ALA:N	2.50	0.45
2:D:3170:PHE:HD2	2:D:3208:ILE:HG12	1.81	0.45
1:G:24:VAL:HG12	1:G:105:LEU:HD12	1.99	0.45
2:A:877:HIS:O	2:A:881:ILE:HG12	2.17	0.45
2:A:2743:TYR:CD1	2:A:2757:MET:HB3	2.52	0.45
2:A:2833:LEU:HB2	2:A:2838[A]:HIS:HE2	1.82	0.45
2:A:3326:LEU:HD21	2:A:3336:GLU:HB3	1.98	0.45
2:A:4279:MET:HE1	2:B:4484:ILE:HG22	1.99	0.45
2:A:4492:LEU:HD22	2:A:4592:CYS:SG	2.56	0.45
2:A:4840:GLU:OE2	2:A:4844:ILE:HD11	2.17	0.45
2:B:2295:GLY:HA3	2:B:2391:PHE:CE2	2.52	0.45
2:B:2431:ASP:O	2:B:2435:VAL:HG23	2.17	0.45
2:B:3281:LEU:HA	2:B:3284:ILE:HG12	1.98	0.45
2:B:4866:ILE:HD12	2:C:4857:ILE:HD11	1.98	0.45
2:C:2424:ARG:HE	2:C:2476:TYR:HA	1.80	0.45
2:C:2424:ARG:NH2	2:C:2476:TYR:O	2.47	0.45
2:C:2426:LEU:CD1	2:D:143:LEU:HD11	2.46	0.45
2:C:2431:ASP:O	2:C:2435:VAL:HG23	2.17	0.45
2:C:2580:LEU:HD23	2:C:2581:ARG:O	2.17	0.45
2:C:3129:SER:O	2:C:3133:ILE:HG13	2.17	0.45
2:D:877:HIS:O	2:D:881:ILE:HG12	2.17	0.45
2:D:1685:LEU:HB3	2:D:1706:LEU:HD12	1.98	0.45
2:D:2652:LEU:HB3	2:D:2962:PHE:CE1	2.52	0.45
2:D:2937:HIS:O	2:D:2940:ILE:HG22	2.17	0.45
2:D:3599:VAL:O	2:D:3603:PHE:HD2	2.00	0.45
2:D:3892:TYR:HD2	2:D:3906:PHE:HE2	1.64	0.45
1:E:24:VAL:HG12	1:E:105:LEU:HD12	1.98	0.45
1:E:50:ARG:HH21	1:E:53:LYS:NZ	2.15	0.45
2:A:335:LYS:HE3	2:A:371:TRP:CG	2.52	0.45
2:A:2431:ASP:O	2:A:2435:VAL:HG23	2.17	0.45
2:A:2827:ASP:OD2	2:B:1434:PRO:HB2	2.17	0.45
2:A:3732:HIS:O	2:A:3776:LYS:NZ	2.47	0.45
2:A:4026:LEU:HD21	2:A:4052:MET:HG2	1.98	0.45
2:B:1006:VAL:HA	2:B:1009:ARG:HH12	1.80	0.45
2:B:3137:LEU:HD21	2:B:3159:LEU:HA	1.99	0.45
2:B:3982:LEU:O	2:B:3999:MET:HE1	2.17	0.45
2:B:4488:GLN:HA	2:B:4491:LEU:HD23	1.99	0.45
2:C:515:ALA:HB2	2:C:523:GLY:HA3	1.99	0.45
2:D:3205:CYS:O	2:D:3208:ILE:HG22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4516:ILE:HG21	2:D:4572:LEU:HB2	1.99	0.45
1:F:24:VAL:HG12	1:F:105:LEU:HD12	1.99	0.44
2:A:2652:LEU:HB3	2:A:2962:PHE:CE1	2.52	0.44
2:A:2728:SER:HA	2:A:2731:LYS:HE3	1.98	0.44
2:B:479:LEU:O	2:B:483:LYS:HG2	2.17	0.44
2:B:514:PHE:CD2	2:B:526:TRP:HB2	2.51	0.44
2:B:521:GLU:OE1	2:B:521:GLU:N	2.35	0.44
2:B:2649:PHE:HZ	2:B:2967:VAL:HG22	1.80	0.44
2:B:4078:LEU:HD23	2:B:4078:LEU:H	1.81	0.44
2:C:762:SER:OG	2:C:763:ALA:N	2.50	0.44
2:C:2295:GLY:HA3	2:C:2391:PHE:CE2	2.52	0.44
2:C:2409:ILE:HD12	2:C:2420:ARG:HE	1.81	0.44
2:C:2610:LEU:HA	2:C:2613:HIS:HE1	1.80	0.44
2:D:514:PHE:CD2	2:D:526:TRP:HB2	2.51	0.44
2:D:934:GLN:O	2:D:938:GLU:OE1	2.34	0.44
2:D:1118:SER:HB3	2:D:1204:VAL:HG11	1.98	0.44
2:D:1564:MET:HE3	2:D:1565:PRO:CD	2.39	0.44
2:D:2720:PHE:HB2	2:D:2901:TYR:CE2	2.51	0.44
2:D:2723:LYS:HB3	2:D:2723:LYS:HE2	1.83	0.44
2:D:3228:TYR:O	2:D:3232:PRO:HB3	2.17	0.44
2:D:3975:GLN:O	2:D:3979:VAL:HG23	2.17	0.44
2:D:4818:TYR:CD1	2:D:4822:ARG:HD3	2.52	0.44
2:A:855:VAL:HG23	2:A:1078:CYS:HB3	1.99	0.44
2:A:1415:ASP:OD2	2:A:1559:ARG:NH2	2.35	0.44
2:A:2937:HIS:O	2:A:2940:ILE:HG22	2.17	0.44
2:A:3205:CYS:O	2:A:3208:ILE:HG22	2.17	0.44
2:A:3892:TYR:HD2	2:A:3906:PHE:HE2	1.64	0.44
2:B:904:TYR:HA	2:B:915:HIS:O	2.17	0.44
2:B:2610:LEU:HA	2:B:2613:HIS:HE1	1.80	0.44
2:B:3129:SER:O	2:B:3133:ILE:HG13	2.17	0.44
2:B:4679:PHE:HD1	2:B:4682:ALA:HB3	1.82	0.44
2:C:2728:SER:HA	2:C:2731:LYS:HE3	1.98	0.44
2:C:3212:GLU:HA	2:C:3215:MET:HE3	1.99	0.44
2:C:3228:TYR:O	2:C:3232:PRO:HB3	2.17	0.44
2:D:889:ILE:HA	2:D:892:LEU:HD12	1.98	0.44
2:D:904:TYR:HA	2:D:915:HIS:O	2.17	0.44
2:D:2082:ARG:HG3	2:D:3687:LEU:HD22	1.99	0.44
2:D:3303:SER:O	2:D:3307:ILE:HG12	2.17	0.44
2:D:3833:ASP:OD2	2:D:3908:LYS:HB3	2.18	0.44
2:D:4178:ASN:HB3	2:D:4179:GLU:OE1	2.16	0.44
2:D:4238:ILE:HG22	2:D:4242:ARG:HE	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:23:CYS:SG	1:E:51:ILE:HD11	2.58	0.44
1:H:23:CYS:SG	1:H:51:ILE:HD11	2.58	0.44
2:A:515:ALA:HB2	2:A:523:GLY:HA3	1.99	0.44
2:A:932:ASN:HA	2:A:935:MET:CG	2.41	0.44
2:A:2409:ILE:HD12	2:A:2420:ARG:HE	1.81	0.44
2:A:2824:ARG:NH2	2:B:1502:ASN:ND2	2.66	0.44
2:A:3027:THR:O	2:A:3030:VAL:HG22	2.18	0.44
2:A:4279:MET:CE	2:B:4484:ILE:HG22	2.47	0.44
2:B:515:ALA:HB2	2:B:523:GLY:HA3	1.99	0.44
2:B:877:HIS:O	2:B:881:ILE:HG12	2.17	0.44
2:B:988:LEU:HD23	2:B:1051:ARG:HH12	1.82	0.44
2:B:2397:ASP:O	2:B:2401:ARG:HG3	2.17	0.44
2:B:2937:HIS:O	2:B:2940:ILE:HG22	2.17	0.44
2:B:3228:TYR:O	2:B:3232:PRO:HB3	2.17	0.44
2:B:3239:LEU:HD12	2:B:3295:TRP:HH2	1.82	0.44
2:B:4492:LEU:HD22	2:B:4592:CYS:SG	2.56	0.44
2:C:2720:PHE:HB2	2:C:2901:TYR:CE2	2.51	0.44
2:C:4679:PHE:HD1	2:C:4682:ALA:HB3	1.82	0.44
2:D:335:LYS:HE3	2:D:371:TRP:CG	2.52	0.44
2:D:630:HIS:CE1	2:D:1671:ARG:HE	2.35	0.44
2:D:1426:TYR:CD1	2:D:1564:MET:HB3	2.52	0.44
2:D:3982:LEU:O	2:D:3999:MET:HE1	2.17	0.44
2:D:4726:MET:HA	2:D:4726:MET:CE	2.48	0.44
2:A:762:SER:OG	2:A:763:ALA:N	2.50	0.44
2:A:2666:LEU:HD13	2:A:2966:VAL:HA	1.98	0.44
2:A:2720:PHE:HB2	2:A:2901:TYR:CE2	2.51	0.44
2:A:3075:LEU:HD21	2:A:3094:ILE:HD12	1.99	0.44
2:A:3137:LEU:HD21	2:A:3159:LEU:HA	1.99	0.44
2:A:3239:LEU:HD12	2:A:3295:TRP:HH2	1.82	0.44
2:A:4739:PHE:HA	2:A:4742:HIS:ND1	2.33	0.44
2:B:889:ILE:HA	2:B:892:LEU:HD12	1.98	0.44
2:B:3027:THR:O	2:B:3030:VAL:HG22	2.18	0.44
2:B:3074:ASN:HA	2:B:3077:GLN:HG3	1.99	0.44
2:B:3728:GLN:O	2:B:3732:HIS:ND1	2.40	0.44
2:C:877:HIS:HA	2:C:880:ARG:HH11	1.80	0.44
2:C:904:TYR:HA	2:C:915:HIS:O	2.17	0.44
2:C:2743:TYR:CD1	2:C:2757:MET:HB3	2.53	0.44
2:C:3134:LEU:HB2	2:C:3162:PHE:CE2	2.52	0.44
2:C:3892:TYR:HD2	2:C:3906:PHE:HE2	1.64	0.44
2:C:4516:ILE:HG21	2:C:4572:LEU:HB2	1.99	0.44
2:D:2582:PRO:O	2:D:2585:MET:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2768:LYS:HB3	2:D:2772:ARG:CZ	2.47	0.44
2:A:1225:LYS:HB2	2:A:1225:LYS:HE2	1.84	0.44
2:A:1685:LEU:HB3	2:A:1706:LEU:HD12	1.98	0.44
2:A:2582:PRO:O	2:A:2585:MET:HG2	2.18	0.44
2:A:2791:ARG:HD2	2:A:2901:TYR:HE1	1.83	0.44
2:A:3982:LEU:O	2:A:3999:MET:HE1	2.18	0.44
2:B:335:LYS:HE3	2:B:371:TRP:CG	2.52	0.44
2:B:896:ASN:HA	2:B:899:GLU:HG2	1.99	0.44
2:B:2705:PRO:HD3	2:B:2854:LYS:HG3	2.00	0.44
2:B:3205:CYS:O	2:B:3208:ILE:HG22	2.17	0.44
2:C:335:LYS:HE3	2:C:371:TRP:CG	2.52	0.44
2:C:877:HIS:O	2:C:881:ILE:HG12	2.17	0.44
2:C:988:LEU:HD23	2:C:1051:ARG:HH12	1.82	0.44
2:C:3239:LEU:HD12	2:C:3295:TRP:HH2	1.82	0.44
2:D:3074:ASN:HA	2:D:3077:GLN:HG3	1.99	0.44
2:D:3075:LEU:HD21	2:D:3094:ILE:HD12	1.99	0.44
2:D:4026:LEU:HD21	2:D:4052:MET:HG2	1.98	0.44
1:F:50:ARG:HH21	1:F:53:LYS:NZ	2.15	0.44
2:A:271:ALA:HB2	2:A:488:LEU:HD22	1.99	0.44
2:A:1426:TYR:CD1	2:A:1564:MET:HB3	2.52	0.44
2:A:2062:ILE:HA	2:A:2065:THR:HG22	2.00	0.44
2:A:2926:LEU:CD1	2:A:2929:LEU:HD23	2.48	0.44
2:A:3129:SER:O	2:A:3133:ILE:HG13	2.17	0.44
2:A:4658:GLY:C	2:A:4663:ARG:HD2	2.38	0.44
2:B:1077:VAL:HG13	2:B:1077:VAL:O	2.18	0.44
2:B:1426:TYR:CD1	2:B:1564:MET:HB3	2.52	0.44
2:B:2062:ILE:HA	2:B:2065:THR:HG22	2.00	0.44
2:B:2841:ALA:CB	2:B:2886:ARG:HH22	2.30	0.44
2:B:3833:ASP:OD2	2:B:3908:LYS:HB3	2.18	0.44
2:B:4726:MET:HA	2:B:4726:MET:CE	2.48	0.44
2:C:1086:ARG:HH21	2:C:1251:LEU:CD1	2.24	0.44
2:C:2062:ILE:HA	2:C:2065:THR:HG22	2.00	0.44
2:C:2582:PRO:O	2:C:2585:MET:HG2	2.18	0.44
2:C:2926:LEU:HB3	2:C:3003:MET:CE	2.48	0.44
2:C:3122:ILE:HG21	2:C:3167:PRO:HG3	1.98	0.44
2:C:3250:TRP:HE3	2:C:3309:LYS:HZ3	1.66	0.44
2:C:3650:GLU:HB2	2:C:3651:PRO:HD3	2.00	0.44
2:C:4011:GLU:HG2	2:C:4121:LEU:HD13	2.00	0.44
2:C:4044:SER:HA	2:C:4076:GLU:O	2.18	0.44
2:C:4726:MET:CE	2:C:4726:MET:HA	2.48	0.44
2:D:1745:LYS:HA	2:D:1745:LYS:HD2	1.78	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2062:ILE:HA	2:D:2065:THR:HG22	2.00	0.44
2:D:2397:ASP:O	2:D:2401:ARG:HG3	2.16	0.44
2:D:3892:TYR:CD2	2:D:3906:PHE:HE2	2.35	0.44
2:D:4011:GLU:HG2	2:D:4121:LEU:HD13	2.00	0.44
2:D:4306:PHE:HD1	2:D:4309:ILE:HD11	1.82	0.44
2:D:4488:GLN:HA	2:D:4491:LEU:HD23	1.99	0.44
1:H:24:VAL:HG12	1:H:105:LEU:HD12	1.99	0.44
1:H:35:LYS:HA	2:D:647:ARG:HH22	1.82	0.44
2:A:3599:VAL:O	2:A:3603:PHE:HD2	2.00	0.44
2:A:4044:SER:HA	2:A:4076:GLU:O	2.18	0.44
2:B:2732:TRP:O	2:B:2732:TRP:CD1	2.67	0.44
2:B:2926:LEU:HB3	2:B:3003:MET:CE	2.48	0.44
2:B:3212:GLU:HA	2:B:3215:MET:HE3	1.99	0.44
2:B:3892:TYR:HD2	2:B:3906:PHE:HE2	1.64	0.44
2:B:4630:TRP:CZ2	2:B:4711:GLY:HA3	2.53	0.44
2:C:866:PRO:HB3	2:C:1009:ARG:NH1	2.33	0.44
2:C:2263:GLU:O	2:C:2267:ARG:HG3	2.18	0.44
2:C:2641:SER:HB2	2:C:2676:LEU:HD21	2.00	0.44
2:C:2705:PRO:HD3	2:C:2854:LYS:HG3	2.00	0.44
2:C:2791:ARG:HD2	2:C:2901:TYR:HE1	1.83	0.44
2:C:3224:SER:OG	2:C:3226:ILE:HG23	2.18	0.44
2:C:3982:LEU:O	2:C:3999:MET:HE1	2.17	0.44
2:C:4488:GLN:HA	2:C:4491:LEU:HD23	2.00	0.44
2:D:504:ARG:O	2:D:507:VAL:HG22	2.18	0.44
2:D:997:ASP:OD1	2:D:1047:LYS:NZ	2.46	0.44
2:D:1106:GLU:HG2	2:D:1161:VAL:HG22	2.00	0.44
2:D:2743:TYR:CD1	2:D:2757:MET:HB3	2.52	0.44
2:D:3042:ALA:O	2:D:3046:MET:HG2	2.18	0.44
2:D:3326:LEU:HD21	2:D:3336:GLU:HB3	1.98	0.44
2:D:4081:GLU:O	2:D:4085:LYS:HG2	2.17	0.44
2:D:4085:LYS:HA	2:D:4089:GLU:OE1	2.18	0.44
2:D:4602:ARG:NH1	2:D:4712:VAL:HG13	2.33	0.44
2:A:3228:TYR:O	2:A:3232:PRO:HB3	2.17	0.44
2:A:4246:PHE:O	2:A:4246:PHE:HD1	2.01	0.44
2:A:4516:ILE:HG21	2:A:4572:LEU:HB2	1.99	0.44
2:A:4602:ARG:NH1	2:A:4712:VAL:HG13	2.33	0.44
2:B:855:VAL:HG23	2:B:1078:CYS:HB3	1.99	0.44
2:B:2791:ARG:HD2	2:B:2901:TYR:HE1	1.83	0.44
2:B:3224:SER:OG	2:B:3226:ILE:HG23	2.18	0.44
2:B:3293:GLY:H	2:B:3296:MET:HE1	1.83	0.44
2:B:4011:GLU:HG2	2:B:4121:LEU:CD1	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4246:PHE:HD1	2:B:4246:PHE:O	2.01	0.44
2:B:4306:PHE:HD1	2:B:4309:ILE:HD11	1.82	0.44
2:B:4516:ILE:HG21	2:B:4572:LEU:HB2	1.99	0.44
2:C:1106:GLU:HG2	2:C:1161:VAL:HG22	2.00	0.44
2:C:2768:LYS:HB3	2:C:2772:ARG:CZ	2.48	0.44
2:C:4630:TRP:CZ2	2:C:4711:GLY:HA3	2.53	0.44
2:D:2926:LEU:HB3	2:D:3003:MET:CE	2.48	0.44
2:D:3650:GLU:HB2	2:D:3651:PRO:HD3	2.00	0.44
1:G:23:CYS:SG	1:G:51:ILE:HD11	2.58	0.44
2:A:514:PHE:CD2	2:A:526:TRP:HB2	2.51	0.44
2:A:866:PRO:HB3	2:A:1009:ARG:NH1	2.33	0.44
2:A:896:ASN:HA	2:A:899:GLU:HG2	1.99	0.44
2:A:2122:SER:O	2:A:2126:ILE:HG12	2.18	0.44
2:A:2455:ASP:OD2	2:A:2457:SER:OG	2.32	0.44
2:A:2926:LEU:HB3	2:A:3003:MET:CE	2.48	0.44
2:A:2926:LEU:HD12	2:A:2929:LEU:HD23	2.00	0.44
2:A:3833:ASP:OD2	2:A:3908:LYS:HB3	2.18	0.44
2:A:3892:TYR:CD2	2:A:3906:PHE:HE2	2.35	0.44
2:A:4630:TRP:CZ2	2:A:4711:GLY:HA3	2.53	0.44
2:B:504:ARG:O	2:B:507:VAL:HG22	2.18	0.44
2:B:762:SER:OG	2:B:763:ALA:N	2.50	0.44
2:B:885:LEU:O	2:B:889:ILE:HG23	2.18	0.44
2:B:3184:TYR:OH	2:B:3204:VAL:HG11	2.18	0.44
2:B:3599:VAL:O	2:B:3603:PHE:HD2	2.00	0.44
2:B:4081:GLU:O	2:B:4085:LYS:HG2	2.17	0.44
2:B:4840:GLU:OE2	2:B:4844:ILE:HD11	2.17	0.44
2:C:271:ALA:HB2	2:C:488:LEU:HD22	1.99	0.44
2:C:855:VAL:HG23	2:C:1078:CYS:HB3	1.99	0.44
2:C:1077:VAL:O	2:C:1077:VAL:HG13	2.18	0.44
2:C:1426:TYR:CD1	2:C:1564:MET:HB3	2.52	0.44
2:C:2981:TYR:O	2:C:2984:SER:OG	2.21	0.44
2:C:3074:ASN:HA	2:C:3077:GLN:HG3	1.99	0.44
2:A:504:ARG:O	2:A:507:VAL:HG22	2.18	0.43
2:A:1308:ILE:HD12	2:A:1445:TRP:CZ3	2.53	0.43
2:A:1435:GLY:N	2:A:1501:ASN:OD1	2.35	0.43
2:B:271:ALA:HB2	2:B:488:LEU:HD22	2.00	0.43
2:B:4839:TYR:HA	2:B:4842:TYR:HD2	1.83	0.43
2:C:253:GLY:O	2:C:257:ARG:HG2	2.18	0.43
2:C:1308:ILE:HD12	2:C:1445:TRP:CZ3	2.53	0.43
2:C:3184:TYR:OH	2:C:3204:VAL:HG11	2.18	0.43
2:C:4011:GLU:HG2	2:C:4121:LEU:CD1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:4238:ILE:HG22	2:C:4242:ARG:HE	1.83	0.43
2:C:4306:PHE:HD1	2:C:4309:ILE:HD11	1.82	0.43
2:C:4739:PHE:HA	2:C:4742:HIS:ND1	2.33	0.43
2:D:896:ASN:HA	2:D:899:GLU:HG2	1.99	0.43
2:D:2681:MET:HA	2:D:2681:MET:HE3	2.00	0.43
2:D:2926:LEU:CD1	2:D:2929:LEU:HD23	2.48	0.43
2:D:3027:THR:O	2:D:3030:VAL:HG22	2.18	0.43
2:D:4664:ASP:OD2	2:D:4674:LYS:NZ	2.48	0.43
1:G:50:ARG:HH21	1:G:53:LYS:NZ	2.15	0.43
1:H:50:ARG:HH21	1:H:53:LYS:NZ	2.15	0.43
2:A:2082:ARG:HG3	2:A:3687:LEU:HD22	1.99	0.43
2:A:3273:MET:O	2:A:3277:LEU:HD23	2.19	0.43
2:A:3650:GLU:HB2	2:A:3651:PRO:HD3	2.00	0.43
2:A:4085:LYS:HA	2:A:4089:GLU:OE1	2.18	0.43
2:A:4238:ILE:HG22	2:A:4242:ARG:HE	1.83	0.43
2:B:1963:LYS:HD2	2:B:1963:LYS:O	2.18	0.43
2:B:2263:GLU:O	2:B:2267:ARG:HG3	2.18	0.43
2:B:2642:ARG:NH1	2:B:2682:GLU:OE1	2.51	0.43
2:B:3254:PRO:HG3	2:B:3267:ALA:HA	2.01	0.43
2:B:4658:GLY:C	2:B:4663:ARG:HD2	2.38	0.43
2:C:1963:LYS:O	2:C:1963:LYS:HD2	2.18	0.43
2:C:2723:LYS:HB3	2:C:2723:LYS:HE2	1.83	0.43
2:C:2833:LEU:HD23	2:C:2897:GLN:NE2	2.31	0.43
2:C:3732:HIS:O	2:C:3776:LYS:NZ	2.47	0.43
2:C:3892:TYR:CD2	2:C:3906:PHE:HE2	2.35	0.43
2:C:4602:ARG:NH1	2:C:4712:VAL:HG13	2.33	0.43
2:D:988:LEU:HD23	2:D:1051:ARG:HH12	1.82	0.43
2:D:1308:ILE:HD12	2:D:1445:TRP:CZ3	2.53	0.43
2:D:3184:TYR:OH	2:D:3204:VAL:HG11	2.18	0.43
2:D:4044:SER:HA	2:D:4076:GLU:O	2.18	0.43
2:D:4679:PHE:HD1	2:D:4682:ALA:HB3	1.82	0.43
2:D:4839:TYR:HA	2:D:4842:TYR:HD2	1.83	0.43
2:A:872:ILE:HB	2:A:941:LYS:HD3	2.01	0.43
2:A:3042:ALA:O	2:A:3046:MET:HG2	2.18	0.43
2:A:3074:ASN:HA	2:A:3077:GLN:HG3	1.99	0.43
2:A:3182:SER:O	2:A:3186:THR:HG23	2.19	0.43
2:A:3212:GLU:HA	2:A:3215:MET:HE3	1.99	0.43
2:A:3219:VAL:O	2:A:3223:GLU:OE1	2.37	0.43
2:A:3332:THR:OG1	2:A:3336:GLU:OE2	2.34	0.43
2:A:4011:GLU:HG2	2:A:4121:LEU:CD1	2.48	0.43
2:A:4679:PHE:HD1	2:A:4682:ALA:HB3	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:4839:TYR:HA	2:A:4842:TYR:HD2	1.82	0.43
2:B:1434:PRO:HG3	2:B:1503:ASN:HA	2.00	0.43
2:B:2833:LEU:HD23	2:B:2897:GLN:NE2	2.31	0.43
2:B:2920:ARG:HD2	2:B:3000:GLU:OE2	2.18	0.43
2:B:3187:LYS:NZ	2:B:3191:GLU:OE1	2.46	0.43
2:B:3219:VAL:O	2:B:3223:GLU:OE1	2.37	0.43
2:C:885:LEU:O	2:C:889:ILE:HG23	2.18	0.43
2:C:2587:HIS:HA	2:C:2590:ARG:HG2	2.00	0.43
2:C:2756:LEU:HA	2:C:2756:LEU:HD12	1.79	0.43
2:C:2937:HIS:O	2:C:2940:ILE:HG22	2.17	0.43
2:C:2954:PHE:CD2	2:C:2961:LYS:NZ	2.87	0.43
2:C:3833:ASP:OD2	2:C:3908:LYS:HB3	2.17	0.43
2:C:4906:GLU:O	2:C:4910:LEU:HB2	2.18	0.43
2:D:2263:GLU:O	2:D:2267:ARG:HG3	2.18	0.43
2:D:2434:GLY:O	2:D:2438:ILE:HG13	2.18	0.43
2:D:2765:GLU:O	2:D:2769:GLU:N	2.49	0.43
2:D:3178:HIS:HD1	2:D:3260:ARG:HH21	1.67	0.43
2:D:4011:GLU:HG2	2:D:4121:LEU:CD1	2.48	0.43
1:E:50:ARG:HH21	1:E:53:LYS:HZ2	1.66	0.43
2:A:2894:LYS:HZ2	2:A:2894:LYS:HG3	1.70	0.43
2:A:4297:PHE:O	2:A:4301:VAL:HG23	2.19	0.43
2:B:866:PRO:HB3	2:B:1009:ARG:NH1	2.33	0.43
2:B:1435:GLY:N	2:B:1501:ASN:OD1	2.35	0.43
2:B:2122:SER:O	2:B:2126:ILE:HG12	2.18	0.43
2:B:2743:TYR:CD1	2:B:2757:MET:HB3	2.52	0.43
2:B:2768:LYS:HB3	2:B:2772:ARG:CZ	2.47	0.43
2:B:4085:LYS:HA	2:B:4089:GLU:OE1	2.18	0.43
2:B:4602:ARG:NH1	2:B:4712:VAL:HG13	2.33	0.43
2:C:504:ARG:O	2:C:507:VAL:HG22	2.18	0.43
2:C:1834:PHE:HD1	2:C:1838:ASP:HB3	1.84	0.43
2:C:2065:THR:HG23	2:C:2066:MET:HE3	1.99	0.43
2:C:2434:GLY:O	2:C:2438:ILE:HG13	2.18	0.43
2:C:2642:ARG:NH1	2:C:2682:GLU:OE1	2.51	0.43
2:C:3182:SER:O	2:C:3186:THR:HG23	2.19	0.43
2:C:3332:THR:OG1	2:C:3336:GLU:OE2	2.34	0.43
2:C:4081:GLU:O	2:C:4085:LYS:HG2	2.17	0.43
2:D:515:ALA:HB2	2:D:523:GLY:HA3	1.99	0.43
2:D:866:PRO:HB3	2:D:1009:ARG:NH1	2.33	0.43
2:D:1077:VAL:O	2:D:1077:VAL:HG13	2.18	0.43
2:D:2066:MET:HA	2:D:2066:MET:HE3	2.00	0.43
2:D:2587:HIS:HA	2:D:2590:ARG:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2769:GLU:HA	2:D:2772:ARG:CG	2.38	0.43
2:D:2954:PHE:CD2	2:D:2961:LYS:NZ	2.87	0.43
2:D:4627:LYS:HB3	2:D:4627:LYS:HE3	1.86	0.43
2:D:4630:TRP:CZ2	2:D:4711:GLY:HA3	2.53	0.43
2:D:4906:GLU:O	2:D:4910:LEU:HB2	2.18	0.43
1:F:23:CYS:SG	1:F:51:ILE:HD11	2.58	0.43
2:A:253:GLY:O	2:A:257:ARG:HG2	2.18	0.43
2:A:988:LEU:HD23	2:A:1051:ARG:HH12	1.82	0.43
2:A:1745:LYS:HA	2:A:1745:LYS:HD2	1.78	0.43
2:A:1963:LYS:HD2	2:A:1963:LYS:O	2.18	0.43
2:A:2295:GLY:HA3	2:A:2391:PHE:CE2	2.52	0.43
2:A:2841:ALA:CB	2:A:2886:ARG:HH22	2.30	0.43
2:A:3184:TYR:OH	2:A:3204:VAL:HG11	2.18	0.43
2:A:3254:PRO:HG3	2:A:3267:ALA:HA	2.01	0.43
2:A:4726:MET:HA	2:A:4726:MET:CE	2.48	0.43
2:B:76:ARG:HA	2:B:76:ARG:HD3	1.79	0.43
2:B:877:HIS:CA	2:B:880:ARG:NH1	2.77	0.43
2:B:2582:PRO:O	2:B:2585:MET:HG2	2.18	0.43
2:B:3650:GLU:HB2	2:B:3651:PRO:HD3	2.00	0.43
2:B:4044:SER:HA	2:B:4076:GLU:O	2.18	0.43
2:B:4724:TRP:O	2:B:4728:MET:HG2	2.19	0.43
2:B:4739:PHE:HA	2:B:4742:HIS:ND1	2.33	0.43
2:C:799:LYS:NZ	2:C:1620:GLN:OE1	2.52	0.43
2:C:896:ASN:HA	2:C:899:GLU:HG2	1.99	0.43
2:C:4658:GLY:C	2:C:4663:ARG:HD2	2.38	0.43
2:C:4664:ASP:OD2	2:C:4674:LYS:NZ	2.48	0.43
2:C:4839:TYR:HA	2:C:4842:TYR:HD2	1.82	0.43
2:D:678:MET:HG3	2:D:754:VAL:HG22	2.00	0.43
2:D:2642:ARG:NH1	2:D:2682:GLU:OE1	2.51	0.43
2:D:2648:ILE:O	2:D:2652:LEU:HD13	2.18	0.43
2:D:3332:THR:OG1	2:D:3336:GLU:OE2	2.34	0.43
2:D:4038:ASP:HB3	2:D:4040:LYS:HZ2	1.84	0.43
2:D:4724:TRP:O	2:D:4728:MET:HG2	2.19	0.43
2:D:4930:GLU:OE1	2:D:4930:GLU:N	2.34	0.43
2:A:799:LYS:NZ	2:A:1620:GLN:OE1	2.52	0.43
2:A:2768:LYS:HB3	2:A:2772:ARG:CZ	2.47	0.43
2:A:4081:GLU:O	2:A:4085:LYS:HG2	2.17	0.43
2:A:4480:PHE:CZ	2:D:4268:MET:HG3	2.53	0.43
2:A:4488:GLN:HA	2:A:4491:LEU:HD23	2.00	0.43
2:A:4847:ASP:OD1	2:A:4848:ILE:N	2.52	0.43
2:B:678:MET:HG3	2:B:754:VAL:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2082:ARG:HG3	2:B:3687:LEU:HD22	1.99	0.43
2:B:2641:SER:HB2	2:B:2676:LEU:HD21	2.00	0.43
2:B:2668:CYS:O	2:B:2672:VAL:HG23	2.19	0.43
2:B:2980:LEU:HD23	2:B:2990:LEU:HD13	2.01	0.43
2:B:4297:PHE:O	2:B:4301:VAL:HG23	2.19	0.43
2:C:448:PRO:O	2:C:452:VAL:HG23	2.19	0.43
2:C:895:MET:HG3	2:C:896:ASN:H	1.84	0.43
2:C:2765:GLU:O	2:C:2769:GLU:N	2.49	0.43
2:C:2893:LEU:O	2:C:2897:GLN:OE1	2.37	0.43
2:C:3027:THR:O	2:C:3030:VAL:HG22	2.18	0.43
2:C:4085:LYS:HA	2:C:4089:GLU:OE1	2.18	0.43
2:D:15:ARG:CZ	2:D:113:LEU:HD12	2.48	0.43
2:D:2122:SER:O	2:D:2126:ILE:HG12	2.18	0.43
2:D:2705:PRO:HD3	2:D:2854:LYS:HG3	2.00	0.43
2:D:2728:SER:HA	2:D:2731:LYS:HE3	1.98	0.43
2:D:2791:ARG:HD2	2:D:2901:TYR:HE1	1.83	0.43
2:D:3190:ARG:HH21	2:D:3193:ALA:CB	2.32	0.43
2:D:3224:SER:OG	2:D:3226:ILE:HG23	2.18	0.43
2:D:3239:LEU:HD12	2:D:3295:TRP:HH2	1.82	0.43
2:D:3254:PRO:HG3	2:D:3267:ALA:HA	2.00	0.43
2:D:4505:LEU:O	2:D:4509:VAL:HG23	2.19	0.43
2:A:15:ARG:CZ	2:A:113:LEU:HD12	2.48	0.43
2:A:732:LEU:HB3	2:A:779:PHE:CZ	2.53	0.43
2:A:2954:PHE:CD2	2:A:2961:LYS:NZ	2.87	0.43
2:A:3231:MET:HE3	2:A:3234:VAL:HG22	2.01	0.43
2:A:4505:LEU:O	2:A:4509:VAL:HG23	2.19	0.43
2:B:15:ARG:CZ	2:B:113:LEU:HD12	2.48	0.43
2:B:872:ILE:HB	2:B:941:LYS:HD3	2.00	0.43
2:B:2893:LEU:O	2:B:2897:GLN:OE1	2.37	0.43
2:B:3002:GLU:CD	2:B:3049:GLY:HA2	2.39	0.43
2:B:3273:MET:O	2:B:3277:LEU:HD23	2.19	0.43
2:B:4930:GLU:OE1	2:B:4930:GLU:N	2.34	0.43
2:C:2082:ARG:HG3	2:C:3687:LEU:HD22	1.99	0.43
2:C:2648:ILE:O	2:C:2652:LEU:HD13	2.18	0.43
2:C:3178:HIS:HD1	2:C:3260:ARG:HH21	1.66	0.43
2:C:3231:MET:HE3	2:C:3234:VAL:HG22	2.00	0.43
2:C:4297:PHE:O	2:C:4301:VAL:HG23	2.19	0.43
2:C:4874:ARG:HG2	2:C:4878:GLU:OE2	2.19	0.43
2:D:253:GLY:O	2:D:257:ARG:HG2	2.18	0.43
2:D:855:VAL:HG23	2:D:1078:CYS:HB3	1.99	0.43
2:D:1963:LYS:HD2	2:D:1963:LYS:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1967:SER:O	2:D:1972:GLN:NE2	2.52	0.43
2:D:2582:PRO:HG3	2:D:2627:TRP:HZ3	1.84	0.43
2:D:2981:TYR:O	2:D:2984:SER:OG	2.21	0.43
2:D:4294:LEU:O	2:D:4298:VAL:HG23	2.18	0.43
2:D:4658:GLY:C	2:D:4663:ARG:HD2	2.38	0.43
2:D:4739:PHE:HA	2:D:4742:HIS:ND1	2.33	0.43
2:D:4767:LEU:HD11	2:D:4862:ILE:HG23	2.01	0.43
2:A:1077:VAL:O	2:A:1077:VAL:HG13	2.18	0.43
2:A:2434:GLY:O	2:A:2438:ILE:HG13	2.18	0.43
2:A:2649:PHE:CZ	2:A:2967:VAL:HG22	2.54	0.43
2:A:2664:LEU:O	2:A:2667:PRO:HD2	2.19	0.43
2:A:2668:CYS:O	2:A:2672:VAL:HG23	2.19	0.43
2:A:3178:HIS:HD1	2:A:3260:ARG:HH21	1.66	0.43
2:A:4306:PHE:HD1	2:A:4309:ILE:HD11	1.82	0.43
2:B:419:ILE:O	2:B:423:VAL:HG23	2.19	0.43
2:B:799:LYS:NZ	2:B:1620:GLN:OE1	2.52	0.43
2:B:877:HIS:HA	2:B:880:ARG:HH11	1.81	0.43
2:B:1308:ILE:HD12	2:B:1445:TRP:CZ3	2.53	0.43
2:B:2434:GLY:O	2:B:2438:ILE:HG13	2.18	0.43
2:B:2756:LEU:HD12	2:B:2756:LEU:HA	1.79	0.43
2:B:2926:LEU:CD1	2:B:2929:LEU:HD23	2.48	0.43
2:B:3169:ALA:O	2:B:3172:GLU:N	2.51	0.43
2:B:4011:GLU:HG2	2:B:4121:LEU:HD13	2.00	0.43
2:C:337:LYS:HZ2	2:C:371:TRP:HE1	1.66	0.43
2:C:932:ASN:HA	2:C:935:MET:CG	2.41	0.43
2:C:2122:SER:O	2:C:2126:ILE:HG12	2.18	0.43
2:C:2668:CYS:O	2:C:2672:VAL:HG23	2.19	0.43
2:C:2761:LYS:HA	2:C:2761:LYS:HD3	1.74	0.43
2:C:2980:LEU:HD23	2:C:2990:LEU:HD13	2.01	0.43
2:C:3042:ALA:O	2:C:3046:MET:HG2	2.18	0.43
2:C:4767:LEU:HD11	2:C:4862:ILE:HG23	2.01	0.43
2:C:4818:TYR:CE1	2:C:4822:ARG:HD3	2.54	0.43
2:D:271:ALA:HB2	2:D:488:LEU:HD22	1.99	0.43
2:D:370:LEU:C	2:D:393:MET:HE3	2.38	0.43
2:D:648:LEU:HD13	2:D:1626:GLN:NE2	2.34	0.43
2:D:2295:GLY:HA3	2:D:2391:PHE:CE2	2.52	0.43
2:D:2688:MET:HB2	2:D:2689:MET:HE3	1.98	0.43
2:D:2926:LEU:HD12	2:D:2929:LEU:HD23	2.00	0.43
2:D:3273:MET:O	2:D:3277:LEU:HD23	2.19	0.43
2:D:4557:VAL:O	2:D:4557:VAL:HG13	2.19	0.43
2:D:4847:ASP:OD1	2:D:4848:ILE:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1834:PHE:HD1	2:A:1838:ASP:HB3	1.84	0.43
2:A:2920:ARG:HD2	2:A:3000:GLU:OE2	2.18	0.43
2:A:4266:LYS:O	2:A:4270:LYS:HG2	2.19	0.43
2:B:253:GLY:O	2:B:257:ARG:HG2	2.18	0.43
2:B:448:PRO:O	2:B:452:VAL:HG23	2.19	0.43
2:B:648:LEU:HD13	2:B:1626:GLN:NE2	2.34	0.43
2:B:1834:PHE:HD1	2:B:1838:ASP:HB3	1.84	0.43
2:B:3231:MET:HE3	2:B:3234:VAL:HG22	2.01	0.43
2:B:3604:ARG:HG2	2:B:3604:ARG:O	2.19	0.43
2:B:4557:VAL:O	2:B:4557:VAL:HG13	2.19	0.43
2:B:4847:ASP:OD1	2:B:4848:ILE:N	2.52	0.43
2:C:15:ARG:CZ	2:C:113:LEU:HD12	2.48	0.43
2:C:893:TRP:HD1	2:C:897:LYS:HZ1	1.66	0.43
2:C:2926:LEU:HD12	2:C:2929:LEU:HD23	2.00	0.43
2:C:3075:LEU:HD21	2:C:3094:ILE:HD12	1.99	0.43
2:C:3187:LYS:NZ	2:C:3191:GLU:OE1	2.46	0.43
2:C:3254:PRO:HG3	2:C:3267:ALA:HA	2.01	0.43
2:D:1434:PRO:HG3	2:D:1503:ASN:HA	2.00	0.43
2:D:1788:LYS:HD3	2:D:1833:ILE:HG22	2.01	0.43
2:D:2431:ASP:O	2:D:2435:VAL:HG23	2.17	0.43
2:D:2610:LEU:HA	2:D:2613:HIS:HE1	1.80	0.43
2:D:2668:CYS:O	2:D:2672:VAL:HG23	2.19	0.43
2:D:3002:GLU:CD	2:D:3049:GLY:HA2	2.39	0.43
2:D:4874:ARG:HG2	2:D:4878:GLU:OE2	2.19	0.43
2:A:885:LEU:O	2:A:889:ILE:HG23	2.18	0.43
2:A:895:MET:O	2:A:899:GLU:N	2.44	0.43
2:A:2635:GLU:OE2	2:A:2680:TYR:OH	2.24	0.43
2:A:2648:ILE:O	2:A:2652:LEU:HD13	2.18	0.43
2:A:2705:PRO:HD3	2:A:2854:LYS:HG3	2.00	0.43
2:A:3002:GLU:CD	2:A:3049:GLY:HA2	2.39	0.43
2:A:3955:GLN:NE2	2:A:3972:MET:HG2	2.34	0.43
2:B:1304:LEU:HD23	2:B:1304:LEU:HA	1.89	0.43
2:B:1757:LEU:HD22	2:B:2117:ILE:HD11	2.01	0.43
2:B:2649:PHE:CZ	2:B:2967:VAL:HG22	2.54	0.43
2:B:3210:SER:O	2:B:3214:LEU:HD12	2.19	0.43
2:B:3892:TYR:CD2	2:B:3906:PHE:HE2	2.35	0.43
2:B:4294:LEU:O	2:B:4298:VAL:HG23	2.19	0.43
2:B:4767:LEU:HD11	2:B:4862:ILE:HG23	2.01	0.43
2:C:1757:LEU:HD22	2:C:2117:ILE:HD11	2.01	0.43
2:C:2741:TRP:HB3	2:C:2754:GLN:CB	2.47	0.43
2:D:732:LEU:HB3	2:D:779:PHE:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2641:SER:HB2	2:D:2676:LEU:HD21	2.00	0.43
2:D:2787:TRP:CD1	2:D:2904:SER:O	2.68	0.43
2:D:2920:ARG:HD2	2:D:3000:GLU:OE2	2.18	0.43
2:D:3134:LEU:HB2	2:D:3162:PHE:HE2	1.84	0.43
2:A:678:MET:HG3	2:A:754:VAL:HG22	2.00	0.42
2:A:1434:PRO:HG3	2:A:1503:ASN:HA	2.00	0.42
2:A:2468:MET:HB3	2:A:2468:MET:HE3	1.97	0.42
2:A:3190:ARG:HH21	2:A:3193:ALA:CB	2.31	0.42
2:A:3224:SER:OG	2:A:3226:ILE:HG23	2.18	0.42
2:B:732:LEU:HB3	2:B:779:PHE:CZ	2.53	0.42
2:B:3190:ARG:HH21	2:B:3193:ALA:CB	2.31	0.42
2:B:3260:ARG:HE	2:B:3263:MET:HG3	1.84	0.42
2:B:4874:ARG:HG2	2:B:4878:GLU:OE2	2.19	0.42
2:C:732:LEU:HB3	2:C:779:PHE:CZ	2.53	0.42
2:C:872:ILE:HB	2:C:941:LYS:HD3	2.00	0.42
2:C:1967:SER:O	2:C:1972:GLN:NE2	2.52	0.42
2:C:2649:PHE:CZ	2:C:2967:VAL:HG22	2.54	0.42
2:C:2664:LEU:O	2:C:2667:PRO:HD2	2.19	0.42
2:C:2926:LEU:CD1	2:C:2929:LEU:HD23	2.48	0.42
2:C:4288:TRP:O	2:C:4292:MET:HG3	2.19	0.42
2:D:895:MET:HG3	2:D:896:ASN:H	1.84	0.42
2:D:988:LEU:HD23	2:D:993:GLU:HG2	2.01	0.42
2:D:2741:TRP:HB3	2:D:2754:GLN:CB	2.47	0.42
2:D:3169:ALA:O	2:D:3172:GLU:N	2.51	0.42
2:D:3604:ARG:O	2:D:3604:ARG:HG2	2.19	0.42
2:D:4246:PHE:O	2:D:4246:PHE:HD1	2.01	0.42
2:D:4818:TYR:CE1	2:D:4822:ARG:HD3	2.54	0.42
2:A:1015:GLY:HA3	2:A:1027:ARG:HH22	1.84	0.42
2:A:3633:GLU:OE1	2:A:3634:HIS:N	2.52	0.42
2:A:4011:GLU:HG2	2:A:4121:LEU:HD13	2.00	0.42
2:A:4294:LEU:O	2:A:4298:VAL:HG23	2.18	0.42
2:B:919:VAL:HG12	2:B:920:GLU:N	2.35	0.42
2:B:1106:GLU:HG2	2:B:1161:VAL:HG22	2.00	0.42
2:B:3042:ALA:O	2:B:3046:MET:HG2	2.18	0.42
2:B:3182:SER:O	2:B:3186:THR:HG23	2.19	0.42
2:C:2884:LYS:HG3	2:C:2885:ASP:H	1.85	0.42
2:C:4246:PHE:O	2:C:4246:PHE:HD1	2.01	0.42
2:D:419:ILE:O	2:D:423:VAL:HG23	2.19	0.42
2:D:448:PRO:O	2:D:452:VAL:HG23	2.18	0.42
2:D:872:ILE:HB	2:D:941:LYS:HD3	2.00	0.42
2:D:3129:SER:O	2:D:3133:ILE:HG13	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4266:LYS:O	2:D:4270:LYS:HG2	2.19	0.42
2:A:648:LEU:HD13	2:A:1626:GLN:NE2	2.34	0.42
2:A:1564:MET:HE3	2:A:1565:PRO:CD	2.41	0.42
2:A:2682:GLU:HB3	2:A:2919:LYS:HE3	2.01	0.42
2:A:3638:ASP:OD2	2:A:4683:ARG:HD3	2.19	0.42
2:A:4627:LYS:HB3	2:A:4627:LYS:HE3	1.86	0.42
2:A:4767:LEU:HD11	2:A:4862:ILE:HG23	2.01	0.42
2:B:675:TYR:HB3	2:B:822:CYS:SG	2.59	0.42
2:B:1428:TYR:HB3	2:B:1566:LEU:HD22	2.01	0.42
2:B:1951:LEU:HD23	2:B:1951:LEU:HA	1.95	0.42
2:B:2587:HIS:HA	2:B:2590:ARG:HG2	2.00	0.42
2:B:2623:LEU:HB3	2:B:2626:GLY:H	1.85	0.42
2:B:2648:ILE:O	2:B:2652:LEU:HD13	2.18	0.42
2:B:3001:LYS:HD2	2:B:3041:ASP:HB2	2.01	0.42
2:B:3072:MET:HE2	2:B:3072:MET:N	2.34	0.42
2:B:3134:LEU:HB2	2:B:3162:PHE:HE2	1.84	0.42
2:B:3954:MET:HB3	2:B:3971:LEU:CD2	2.49	0.42
2:C:648:LEU:HD13	2:C:1626:GLN:NE2	2.34	0.42
2:C:2383:HIS:CE1	2:C:2458:ALA:HB2	2.55	0.42
2:C:2920:ARG:HD2	2:C:3000:GLU:OE2	2.18	0.42
2:C:3190:ARG:HH21	2:C:3193:ALA:CB	2.31	0.42
2:C:4557:VAL:HG13	2:C:4557:VAL:O	2.19	0.42
2:D:799:LYS:NZ	2:D:1620:GLN:OE1	2.52	0.42
2:D:912:LYS:NZ	2:D:914:GLN:HB2	2.34	0.42
2:D:919:VAL:HG12	2:D:920:GLU:N	2.35	0.42
2:D:1299:ILE:HG12	2:D:1546:GLN:HB2	2.01	0.42
1:E:26:HIS:ND1	1:E:105:LEU:HD11	2.35	0.42
2:A:419:ILE:O	2:A:423:VAL:HG23	2.19	0.42
2:A:912:LYS:NZ	2:A:914:GLN:HB2	2.34	0.42
2:A:919:VAL:HG12	2:A:920:GLU:N	2.35	0.42
2:A:1299:ILE:HG12	2:A:1546:GLN:HB2	2.01	0.42
2:A:2642:ARG:NH1	2:A:2682:GLU:OE1	2.51	0.42
2:A:3210:SER:O	2:A:3214:LEU:HD12	2.19	0.42
2:A:4818:TYR:CE1	2:A:4822:ARG:HD3	2.54	0.42
2:A:4906:GLU:O	2:A:4910:LEU:HB2	2.18	0.42
2:B:4238:ILE:HG22	2:B:4242:ARG:HE	1.83	0.42
2:B:4505:LEU:O	2:B:4509:VAL:HG23	2.19	0.42
2:C:111:ARG:H	2:C:111:ARG:HG2	1.67	0.42
2:C:1929:SER:OG	2:C:3617:VAL:HG13	2.19	0.42
2:C:2248:MET:HE3	2:C:2248:MET:HB2	1.94	0.42
2:C:2582:PRO:HG3	2:C:2627:TRP:HZ3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:3002:GLU:CD	2:C:3049:GLY:HA2	2.39	0.42
2:C:3260:ARG:HE	2:C:3263:MET:HG3	1.84	0.42
2:C:3763:ILE:HD11	2:C:3838:ASP:O	2.20	0.42
2:C:3954:MET:HB3	2:C:3971:LEU:CD2	2.49	0.42
2:C:3955:GLN:NE2	2:C:3972:MET:HG2	2.34	0.42
2:C:4505:LEU:O	2:C:4509:VAL:HG23	2.19	0.42
2:C:4630:TRP:CE2	2:C:4711:GLY:HA3	2.55	0.42
2:D:885:LEU:O	2:D:889:ILE:HG23	2.18	0.42
2:D:2593:VAL:HG22	2:D:2644:LEU:HD21	2.01	0.42
2:D:3219:VAL:O	2:D:3223:GLU:OE1	2.37	0.42
2:D:3260:ARG:HE	2:D:3263:MET:HG3	1.84	0.42
2:D:3976:LYS:HG3	2:D:4097:ASN:ND2	2.35	0.42
1:F:26:HIS:ND1	1:F:105:LEU:HD11	2.35	0.42
1:G:63:GLY:O	1:G:67:MET:HG3	2.19	0.42
2:A:2263:GLU:O	2:A:2267:ARG:HG3	2.18	0.42
2:A:2582:PRO:HG3	2:A:2627:TRP:HZ3	1.84	0.42
2:A:2623:LEU:HB3	2:A:2626:GLY:H	1.85	0.42
2:A:2681:MET:HA	2:A:2681:MET:HE3	2.00	0.42
2:A:2893:LEU:O	2:A:2897:GLN:OE1	2.37	0.42
2:A:2980:LEU:HD23	2:A:2990:LEU:HD13	2.01	0.42
2:A:3260:ARG:HE	2:A:3263:MET:HG3	1.84	0.42
2:B:15:ARG:HH22	2:B:72:SER:HB3	1.84	0.42
2:B:228:LEU:HD21	2:B:277:LEU:HD13	2.01	0.42
2:B:1549:SER:OG	2:B:1551:ASN:O	2.37	0.42
2:B:2754:GLN:HA	2:B:2755:PRO:HD3	1.88	0.42
2:B:3178:HIS:HD1	2:B:3260:ARG:HH21	1.67	0.42
2:B:3955:GLN:NE2	2:B:3972:MET:HG2	2.34	0.42
2:B:4603:GLU:HA	2:B:4606:VAL:HG12	2.02	0.42
2:C:419:ILE:O	2:C:423:VAL:HG23	2.19	0.42
2:C:678:MET:HG3	2:C:754:VAL:HG22	2.00	0.42
2:C:713:TRP:CH2	2:C:1251:LEU:HD21	2.51	0.42
2:C:2966:VAL:O	2:C:2970:LEU:N	2.47	0.42
2:C:4672:MET:HE1	2:C:4677:LEU:HD21	2.02	0.42
2:D:228:LEU:HD21	2:D:277:LEU:HD13	2.01	0.42
2:D:932:ASN:HA	2:D:935:MET:CG	2.41	0.42
2:A:329:PHE:HB3	2:A:363:ILE:HD11	2.01	0.42
2:A:1172:THR:HB	2:A:1190:LEU:HD22	2.02	0.42
2:A:1304:LEU:HD23	2:A:1304:LEU:HA	1.89	0.42
2:A:2587:HIS:HA	2:A:2590:ARG:HG2	2.00	0.42
2:A:3169:ALA:O	2:A:3172:GLU:N	2.51	0.42
2:A:3325:LYS:HA	2:A:3328:LYS:CE	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:3976:LYS:HG3	2:A:4097:ASN:ND2	2.35	0.42
2:A:4024:LYS:HB2	2:A:4088:HIS:CD2	2.55	0.42
2:A:4197:ILE:HG13	2:A:4919:LEU:HD11	2.02	0.42
2:A:4791:LYS:HE3	2:A:4791:LYS:HB3	1.87	0.42
2:A:4874:ARG:HG2	2:A:4878:GLU:OE2	2.19	0.42
2:B:895:MET:HG3	2:B:896:ASN:H	1.84	0.42
2:B:1015:GLY:HA3	2:B:1027:ARG:HH22	1.84	0.42
2:B:2682:GLU:HB3	2:B:2919:LYS:HE3	2.02	0.42
2:B:2918:GLU:OE1	2:B:2918:GLU:N	2.51	0.42
2:B:2926:LEU:HD12	2:B:2929:LEU:HD23	2.00	0.42
2:B:2954:PHE:CD2	2:B:2961:LYS:NZ	2.87	0.42
2:B:4256:MET:SD	2:C:4703:VAL:HG23	2.60	0.42
2:B:4765:LYS:HD2	2:B:4765:LYS:HA	1.82	0.42
2:C:675:TYR:HB3	2:C:822:CYS:SG	2.60	0.42
2:C:972:LEU:HD13	2:C:978:PRO:HD3	2.02	0.42
2:C:3134:LEU:HB2	2:C:3162:PHE:HE2	1.84	0.42
2:C:3604:ARG:O	2:C:3604:ARG:HG2	2.19	0.42
2:C:3790:PHE:HE1	2:C:3858:LEU:HD23	1.85	0.42
2:C:3976:LYS:HG3	2:C:4097:ASN:ND2	2.35	0.42
2:C:4024:LYS:HB2	2:C:4088:HIS:CD2	2.55	0.42
2:C:4266:LYS:O	2:C:4270:LYS:HG2	2.19	0.42
2:C:4294:LEU:O	2:C:4298:VAL:HG23	2.18	0.42
2:C:4847:ASP:OD1	2:C:4848:ILE:N	2.52	0.42
2:D:877:HIS:HA	2:D:880:ARG:HH11	1.80	0.42
2:D:2841:ALA:CB	2:D:2886:ARG:HH22	2.30	0.42
2:D:3182:SER:O	2:D:3186:THR:HG23	2.19	0.42
2:D:3231:MET:HE3	2:D:3234:VAL:HG22	2.00	0.42
2:D:4058:TYR:HD2	2:D:4062:GLU:HB3	1.85	0.42
1:F:63:GLY:O	1:F:67:MET:HG3	2.20	0.42
2:A:448:PRO:O	2:A:452:VAL:HG23	2.18	0.42
2:A:3134:LEU:HB2	2:A:3162:PHE:HE2	1.84	0.42
2:A:4288:TRP:O	2:A:4292:MET:HG3	2.19	0.42
2:A:4630:TRP:CE2	2:A:4711:GLY:HA3	2.55	0.42
2:B:1929:SER:OG	2:B:3617:VAL:HG13	2.19	0.42
2:B:2593:VAL:HG22	2:B:2644:LEU:HD21	2.01	0.42
2:B:3633:GLU:OE1	2:B:3634:HIS:N	2.52	0.42
2:B:3713:SER:OG	2:B:3715:GLU:OE1	2.33	0.42
2:B:4818:TYR:CE1	2:B:4822:ARG:HD3	2.54	0.42
2:C:1714:TYR:CE2	2:C:1761:MET:HG3	2.55	0.42
2:C:2678:PRO:HB2	2:C:2981:TYR:CZ	2.55	0.42
2:C:4743:LEU:CD2	2:D:4776:VAL:HG13	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:329:PHE:HB3	2:D:363:ILE:HD11	2.01	0.42
2:D:675:TYR:HB3	2:D:822:CYS:SG	2.60	0.42
2:D:1016:TRP:CE3	2:D:1029:ASN:HB2	2.54	0.42
2:D:2649:PHE:CZ	2:D:2967:VAL:HG22	2.54	0.42
2:D:2833:LEU:HD23	2:D:2897:GLN:NE2	2.31	0.42
2:D:3210:SER:O	2:D:3214:LEU:HD12	2.19	0.42
2:D:3712:LYS:HB3	2:D:3716:GLU:HB2	2.02	0.42
2:D:3954:MET:HB3	2:D:3971:LEU:CD2	2.49	0.42
2:D:4024:LYS:HB2	2:D:4088:HIS:CD2	2.55	0.42
2:D:4297:PHE:O	2:D:4301:VAL:HG23	2.19	0.42
2:A:988:LEU:HD23	2:A:993:GLU:HG2	2.01	0.42
2:A:1106:GLU:HG2	2:A:1161:VAL:HG22	2.00	0.42
2:A:1825:PHE:CE1	2:A:1842:ILE:HG12	2.55	0.42
2:A:1967:SER:O	2:A:1972:GLN:NE2	2.52	0.42
2:A:2325:ILE:CD1	2:A:2426:LEU:HD11	2.50	0.42
2:A:2538:THR:HG21	2:A:2545:ILE:HD12	2.02	0.42
2:B:1788:LYS:HD3	2:B:1833:ILE:HG22	2.01	0.42
2:B:2319:VAL:O	2:B:2323:LEU:HG	2.20	0.42
2:B:2659:GLN:HG3	2:B:2663:LYS:HZ1	1.85	0.42
2:B:2664:LEU:O	2:B:2667:PRO:HD2	2.19	0.42
2:B:4197:ILE:HG13	2:B:4919:LEU:HD11	2.02	0.42
2:C:411:GLU:OE2	2:C:485:ARG:NE	2.38	0.42
2:C:919:VAL:HG12	2:C:920:GLU:N	2.35	0.42
2:C:1016:TRP:CE3	2:C:1029:ASN:HB2	2.54	0.42
2:C:1435:GLY:N	2:C:1501:ASN:OD1	2.35	0.42
2:C:2782:MET:HG2	2:C:2787:TRP:CE3	2.55	0.42
2:C:3273:MET:O	2:C:3277:LEU:HD23	2.19	0.42
2:C:4603:GLU:HA	2:C:4606:VAL:HG12	2.02	0.42
2:C:4631:ASP:OD1	2:C:4708:TRP:NE1	2.45	0.42
2:C:4724:TRP:O	2:C:4728:MET:HG2	2.19	0.42
2:D:1172:THR:HB	2:D:1190:LEU:HD22	2.02	0.42
2:D:1834:PHE:HD1	2:D:1838:ASP:HB3	1.84	0.42
2:D:2325:ILE:CD1	2:D:2426:LEU:HD11	2.50	0.42
2:D:2893:LEU:O	2:D:2897:GLN:OE1	2.37	0.42
2:D:2980:LEU:HD23	2:D:2990:LEU:HD13	2.01	0.42
2:D:3208:ILE:HA	2:D:3209:PRO:HD3	1.88	0.42
2:D:3638:ASP:OD2	2:D:4683:ARG:HD3	2.20	0.42
2:D:4288:TRP:O	2:D:4292:MET:HG3	2.19	0.42
2:A:15:ARG:HH11	2:A:112:THR:C	2.23	0.42
2:A:334:SER:OG	2:A:338:LEU:HD22	2.20	0.42
2:A:372:LEU:HD11	2:A:391:ALA:HB1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2641:SER:HB2	2:A:2676:LEU:HD21	2.00	0.42
2:A:2973:GLN:HA	2:A:2976:LYS:HE2	2.02	0.42
2:A:3712:LYS:HB3	2:A:3716:GLU:HB2	2.02	0.42
2:A:3763:ILE:HD11	2:A:3838:ASP:O	2.20	0.42
2:A:4061:SER:O	2:A:4064:GLU:HG3	2.20	0.42
2:A:4786:PHE:CE2	2:D:4520:TYR:HD2	2.38	0.42
2:B:334:SER:OG	2:B:338:LEU:HD22	2.20	0.42
2:B:2444:THR:O	2:B:2452:VAL:HG12	2.20	0.42
2:B:3763:ILE:HD11	2:B:3838:ASP:O	2.20	0.42
2:B:3976:LYS:HG3	2:B:4097:ASN:ND2	2.35	0.42
2:B:4024:LYS:HB2	2:B:4088:HIS:CD2	2.55	0.42
2:B:4288:TRP:O	2:B:4292:MET:HG3	2.19	0.42
2:B:4630:TRP:CE2	2:B:4711:GLY:HA3	2.55	0.42
2:B:4906:GLU:O	2:B:4910:LEU:HB2	2.18	0.42
2:C:895:MET:O	2:C:899:GLU:N	2.44	0.42
2:C:1825:PHE:CE1	2:C:1842:ILE:HG12	2.55	0.42
2:C:2444:THR:O	2:C:2452:VAL:HG12	2.20	0.42
2:C:2538:THR:HG21	2:C:2545:ILE:HD12	2.02	0.42
2:C:2841:ALA:CB	2:C:2886:ARG:HH22	2.30	0.42
2:C:3633:GLU:OE1	2:C:3634:HIS:N	2.52	0.42
2:D:2383:HIS:CE1	2:D:2458:ALA:HB2	2.55	0.42
2:D:2444:THR:O	2:D:2452:VAL:HG12	2.20	0.42
2:D:2678:PRO:HB2	2:D:2981:TYR:CZ	2.55	0.42
1:E:63:GLY:O	1:E:67:MET:HG3	2.19	0.42
1:G:26:HIS:ND1	1:G:105:LEU:HD11	2.35	0.42
2:A:228:LEU:HD21	2:A:277:LEU:HD13	2.01	0.42
2:A:895:MET:HG3	2:A:896:ASN:H	1.84	0.42
2:A:1427:TYR:HB2	2:A:1563:VAL:HG11	2.02	0.42
2:A:3790:PHE:HE1	2:A:3858:LEU:HD23	1.85	0.42
2:A:3954:MET:HB3	2:A:3971:LEU:CD2	2.49	0.42
2:B:1299:ILE:HG12	2:B:1546:GLN:HB2	2.01	0.42
2:B:1745:LYS:HA	2:B:1745:LYS:HD2	1.78	0.42
2:B:1796:THR:HG22	2:B:1800:LYS:HZ1	1.85	0.42
2:B:2383:HIS:CE1	2:B:2458:ALA:HB2	2.55	0.42
2:B:2741:TRP:HB3	2:B:2754:GLN:CB	2.47	0.42
2:B:3231:MET:O	2:B:3235:MET:HG3	2.20	0.42
2:B:3325:LYS:HA	2:B:3328:LYS:CE	2.50	0.42
2:C:988:LEU:HD23	2:C:993:GLU:HG2	2.01	0.42
2:C:1283:LEU:HB2	2:C:1555:PHE:HB2	2.02	0.42
2:C:1788:LYS:HD3	2:C:1833:ILE:HG22	2.01	0.42
2:C:2319:VAL:O	2:C:2323:LEU:HG	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2468:MET:HB3	2:C:2468:MET:HE3	1.97	0.42
2:C:2593:VAL:HG22	2:C:2644:LEU:HD21	2.01	0.42
2:C:2682:GLU:HB3	2:C:2919:LYS:HE3	2.02	0.42
2:C:3210:SER:O	2:C:3214:LEU:HD12	2.19	0.42
2:C:4197:ILE:HG13	2:C:4919:LEU:HD11	2.02	0.42
2:C:4838:GLU:OE1	2:C:4838:GLU:N	2.36	0.42
2:D:1427:TYR:HB2	2:D:1563:VAL:HG11	2.02	0.42
2:D:1714:TYR:CE2	2:D:1761:MET:HG3	2.55	0.42
2:D:2664:LEU:O	2:D:2667:PRO:HD2	2.19	0.42
2:D:3324:GLU:O	2:D:3327:LYS:HB3	2.20	0.42
2:D:4061:SER:O	2:D:4064:GLU:HG3	2.20	0.42
2:D:4197:ILE:HG13	2:D:4919:LEU:HD11	2.02	0.42
2:D:4603:GLU:HA	2:D:4606:VAL:HG12	2.02	0.42
2:D:4630:TRP:CE2	2:D:4711:GLY:HA3	2.55	0.42
2:A:15:ARG:HH22	2:A:72:SER:HB3	1.84	0.41
2:A:125:TYR:O	2:A:414:ARG:NH1	2.53	0.41
2:A:1283:LEU:HB2	2:A:1555:PHE:HB2	2.02	0.41
2:A:1554:GLN:NE2	2:A:1556:GLU:OE2	2.35	0.41
2:A:2171:VAL:HG21	2:A:2199:PHE:CE2	2.55	0.41
2:A:2646:TRP:HA	2:A:2646:TRP:CE3	2.55	0.41
2:A:4277:LYS:O	2:A:4281:THR:HG23	2.20	0.41
2:A:4603:GLU:HA	2:A:4606:VAL:HG12	2.02	0.41
2:A:4660:PHE:HA	2:D:4056:LYS:NZ	2.34	0.41
2:A:4724:TRP:O	2:A:4728:MET:HG2	2.19	0.41
2:B:844:ARG:HB2	2:B:847:THR:OG1	2.20	0.41
2:B:1016:TRP:CE3	2:B:1029:ASN:HB2	2.54	0.41
2:B:1714:TYR:CE2	2:B:1761:MET:HG3	2.55	0.41
2:B:2782:MET:HG2	2:B:2787:TRP:CE3	2.55	0.41
2:B:3122:ILE:HG12	2:B:3167:PRO:HG3	2.02	0.41
2:C:562:LEU:HD21	2:C:600:LEU:HD22	2.02	0.41
2:C:626:ARG:NH2	2:C:1667:LEU:O	2.53	0.41
2:C:2826:ILE:HG13	2:C:2828:MET:CE	2.50	0.41
2:C:3122:ILE:HG12	2:C:3167:PRO:HG3	2.02	0.41
2:C:3219:VAL:O	2:C:3223:GLU:OE1	2.37	0.41
2:C:3231:MET:O	2:C:3235:MET:HG3	2.20	0.41
2:C:3638:ASP:OD2	2:C:4683:ARG:HD3	2.20	0.41
2:C:4058:TYR:HD2	2:C:4062:GLU:HB3	1.85	0.41
2:C:4587:ILE:CD1	2:C:4726:MET:HG2	2.50	0.41
2:C:4708:TRP:O	2:C:4712:VAL:HG23	2.20	0.41
2:D:1428:TYR:HB3	2:D:1566:LEU:HD22	2.01	0.41
2:D:2761:LYS:HA	2:D:2761:LYS:HD3	1.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2782:MET:HG2	2:D:2787:TRP:CE3	2.55	0.41
2:D:3001:LYS:HD2	2:D:3041:ASP:HB2	2.01	0.41
2:D:3763:ILE:HD11	2:D:3838:ASP:O	2.20	0.41
2:D:4107:GLU:OE1	2:D:4149:TYR:OH	2.27	0.41
2:D:4575:LEU:HD23	2:D:4575:LEU:HA	1.95	0.41
2:D:4587:ILE:CD1	2:D:4726:MET:HG2	2.50	0.41
2:D:4631:ASP:OD1	2:D:4708:TRP:NE1	2.45	0.41
2:D:4806:CYS:HA	2:D:4812:CYS:HB2	2.02	0.41
2:A:675:TYR:HB3	2:A:822:CYS:SG	2.60	0.41
2:A:1714:TYR:CE2	2:A:1761:MET:HG3	2.55	0.41
2:A:2592:LEU:HD22	2:A:2606:PRO:HB3	2.02	0.41
2:A:2826:ILE:HG13	2:A:2828:MET:CE	2.50	0.41
2:A:3604:ARG:O	2:A:3604:ARG:HG2	2.19	0.41
2:A:4806:CYS:HA	2:A:4812:CYS:HB2	2.02	0.41
2:B:15:ARG:HH11	2:B:112:THR:C	2.23	0.41
2:B:329:PHE:HB3	2:B:363:ILE:HD11	2.01	0.41
2:B:372:LEU:HD11	2:B:391:ALA:HB1	2.02	0.41
2:B:562:LEU:HD21	2:B:600:LEU:HD22	2.02	0.41
2:B:988:LEU:HD23	2:B:993:GLU:HG2	2.01	0.41
2:B:997:ASP:OD1	2:B:1047:LYS:NZ	2.46	0.41
2:B:2468:MET:HB3	2:B:2468:MET:HE3	1.98	0.41
2:B:2538:THR:HG21	2:B:2545:ILE:HD12	2.02	0.41
2:B:2791:ARG:HE	2:B:2792:THR:N	2.18	0.41
2:B:4266:LYS:O	2:B:4270:LYS:HG2	2.19	0.41
2:B:4708:TRP:O	2:B:4712:VAL:HG23	2.20	0.41
2:C:372:LEU:HD11	2:C:391:ALA:HB1	2.02	0.41
2:C:1428:TYR:HB3	2:C:1566:LEU:HD22	2.02	0.41
2:C:1434:PRO:HG3	2:C:1503:ASN:HA	2.00	0.41
2:C:2066:MET:SD	2:C:2087:LEU:HD23	2.61	0.41
2:C:2754:GLN:HA	2:C:2755:PRO:HD3	1.88	0.41
2:C:2999:LYS:HZ2	2:C:3003:MET:HB3	1.85	0.41
2:C:3301:VAL:HA	2:C:3304:GLN:OE1	2.20	0.41
2:C:4664:ASP:HA	2:C:4674:LYS:HZ1	1.84	0.41
2:D:125:TYR:O	2:D:414:ARG:NH1	2.53	0.41
2:D:895:MET:O	2:D:899:GLU:N	2.44	0.41
2:D:919:VAL:HG12	2:D:920:GLU:H	1.85	0.41
2:D:1718:ARG:HD3	2:D:1831:MET:HA	2.03	0.41
2:D:2171:VAL:HG21	2:D:2199:PHE:CE2	2.55	0.41
2:D:2319:VAL:O	2:D:2323:LEU:HG	2.20	0.41
2:D:2849:HIS:CD2	2:D:2874:TYR:HB2	2.55	0.41
2:D:3955:GLN:NE2	2:D:3972:MET:HG2	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4708:TRP:O	2:D:4712:VAL:HG23	2.20	0.41
1:H:63:GLY:O	1:H:67:MET:HG3	2.19	0.41
2:A:670:TYR:O	2:A:673:TRP:NE1	2.54	0.41
2:A:2319:VAL:O	2:A:2323:LEU:HG	2.20	0.41
2:A:2480:VAL:HB	2:A:2483:PHE:HB3	2.02	0.41
2:A:2596:VAL:O	2:A:2599:LEU:HD22	2.21	0.41
2:A:3778:LEU:HD11	2:A:3782:LYS:HE3	2.02	0.41
2:A:4557:VAL:HG13	2:A:4557:VAL:O	2.19	0.41
2:B:242:ASP:OD1	2:B:243:GLU:N	2.53	0.41
2:B:912:LYS:NZ	2:B:914:GLN:HB2	2.34	0.41
2:B:1177:LEU:HB2	2:B:1182:LEU:HD21	2.03	0.41
2:B:2066:MET:SD	2:B:2087:LEU:HD23	2.61	0.41
2:B:2480:VAL:HB	2:B:2483:PHE:HB3	2.02	0.41
2:B:2557:LYS:HB2	2:B:2557:LYS:HE2	1.85	0.41
2:B:2582:PRO:HG3	2:B:2627:TRP:HZ3	1.84	0.41
2:B:2826:ILE:HG13	2:B:2828:MET:CE	2.50	0.41
2:B:2849:HIS:CD2	2:B:2874:TYR:HB2	2.55	0.41
2:C:125:TYR:O	2:C:414:ARG:NH1	2.53	0.41
2:C:258:ARG:NH1	2:C:317:MET:HA	2.36	0.41
2:C:2623:LEU:HB3	2:C:2626:GLY:H	1.85	0.41
2:C:3001:LYS:HD2	2:C:3041:ASP:HB2	2.01	0.41
2:C:3324:GLU:O	2:C:3327:LYS:HB3	2.20	0.41
2:C:4277:LYS:O	2:C:4281:THR:HG23	2.21	0.41
2:D:674:TYR:HE1	2:D:756:SER:HB2	1.85	0.41
2:D:844:ARG:HB2	2:D:847:THR:OG1	2.21	0.41
2:D:2232:PRO:C	2:D:2234:MET:H	2.24	0.41
2:D:2623:LEU:HB3	2:D:2626:GLY:H	1.85	0.41
1:E:18:LYS:HA	1:E:18:LYS:HE3	2.03	0.41
1:F:18:LYS:HA	1:F:18:LYS:HE3	2.02	0.41
2:A:674:TYR:HE1	2:A:756:SER:HB2	1.85	0.41
2:A:1549:SER:OG	2:A:1551:ASN:O	2.37	0.41
2:A:1718:ARG:HD3	2:A:1831:MET:HA	2.02	0.41
2:A:1788:LYS:HD3	2:A:1833:ILE:HG22	2.01	0.41
2:A:1958:THR:O	2:A:1962:THR:HG22	2.21	0.41
2:A:2385:GLY:O	2:A:2389:MET:HG3	2.20	0.41
2:A:2593:VAL:HG22	2:A:2644:LEU:HD21	2.01	0.41
2:A:2678:PRO:HB2	2:A:2981:TYR:CZ	2.55	0.41
2:A:2754:GLN:HA	2:A:2755:PRO:HD3	1.88	0.41
2:A:3122:ILE:HG12	2:A:3167:PRO:HG3	2.02	0.41
2:A:3324:GLU:O	2:A:3327:LYS:HB3	2.20	0.41
2:B:520:ARG:HG2	2:B:524:GLU:HG2	2.03	0.41

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
2:B:936:SER:O	2:B:939:THR:HB	2.20	0.41
2:B:1825:PHE:CE1	2:B:1842:ILE:HG12	2.55	0.41
2:B:2884:LYS:HG3	2:B:2885:ASP:H	1.85	0.41
2:B:2888:LYS:HE2	2:B:2888:LYS:HB2	1.92	0.41
2:B:3301:VAL:HA	2:B:3304:GLN:OE1	2.21	0.41
2:B:4061:SER:O	2:B:4064:GLU:HG3	2.20	0.41
2:C:15:ARG:HH11	2:C:112:THR:C	2.23	0.41
2:C:334:SER:OG	2:C:338:LEU:HD22	2.20	0.41
2:C:489:PHE:CD2	2:C:494:MET:HG3	2.56	0.41
2:C:972:LEU:HD23	2:C:972:LEU:H	1.86	0.41
2:C:1299:ILE:HG12	2:C:1546:GLN:HB2	2.01	0.41
2:C:3068:LEU:O	2:C:3072:MET:HE3	2.21	0.41
2:D:15:ARG:HH22	2:D:72:SER:HB3	1.84	0.41
2:D:111:ARG:H	2:D:111:ARG:HG2	1.67	0.41
2:D:520:ARG:HG2	2:D:524:GLU:HG2	2.03	0.41
2:D:872:ILE:C	2:D:941:LYS:HZ2	2.24	0.41
2:D:948:CYS:HA	2:D:1067:PRO:HD3	2.02	0.41
2:D:1825:PHE:CE1	2:D:1842:ILE:HG12	2.55	0.41
2:D:1929:SER:OG	2:D:3617:VAL:HG13	2.19	0.41
2:D:2066:MET:SD	2:D:2087:LEU:HD23	2.61	0.41
2:D:2538:THR:HG21	2:D:2545:ILE:HD12	2.02	0.41
2:D:2705:PRO:HD2	2:D:2854:LYS:HZ2	1.85	0.41
2:D:2726:GLU:OE2	2:D:2821:TYR:OH	2.24	0.41
2:D:3068:LEU:O	2:D:3072:MET:HE3	2.21	0.41
2:D:3261:ALA:C	2:D:3263:MET:H	2.24	0.41
2:D:3273:MET:HB3	2:D:3273:MET:HE2	1.81	0.41
2:D:4277:LYS:O	2:D:4281:THR:HG23	2.21	0.41
2:D:4611:GLU:HA	2:D:4653:VAL:HG12	2.03	0.41
2:D:4726:MET:O	2:D:4730:VAL:HG13	2.21	0.41
2:A:411:GLU:OE2	2:A:485:ARG:NE	2.38	0.41
2:A:520:ARG:HG2	2:A:524:GLU:HG2	2.03	0.41
2:A:737:ILE:HG21	2:A:1534:GLU:OE2	2.21	0.41
2:A:919:VAL:HG12	2:A:920:GLU:H	1.85	0.41
2:A:1016:TRP:CE3	2:A:1029:ASN:HB2	2.54	0.41
2:A:2383:HIS:CE1	2:A:2458:ALA:HB2	2.55	0.41
2:A:2849:HIS:CD2	2:A:2874:TYR:HB2	2.55	0.41
2:A:3001:LYS:HD2	2:A:3041:ASP:HB2	2.01	0.41
2:A:3607:PRO:HD2	2:A:3610:ASN:OD1	2.21	0.41
2:A:4252:ILE:HD12	2:B:4707:MET:CE	2.50	0.41
2:A:4587:ILE:CD1	2:A:4726:MET:HG2	2.50	0.41
2:B:489:PHE:CD2	2:B:494:MET:HG3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1958:THR:O	2:B:1962:THR:HG22	2.21	0.41
2:B:3757:ALA:HA	2:B:3760:LYS:HE2	2.03	0.41
2:C:15:ARG:HH22	2:C:72:SER:HB3	1.84	0.41
2:C:737:ILE:HG21	2:C:1534:GLU:OE2	2.21	0.41
2:C:912:LYS:NZ	2:C:914:GLN:HB2	2.34	0.41
2:C:936:SER:O	2:C:939:THR:HB	2.20	0.41
2:C:1284:LYS:HE2	2:C:1433:PHE:CZ	2.56	0.41
2:C:2480:VAL:HB	2:C:2483:PHE:HB3	2.02	0.41
2:C:2592:LEU:HD22	2:C:2606:PRO:HB3	2.02	0.41
2:C:2787:TRP:CD1	2:C:2904:SER:O	2.68	0.41
2:C:4611:GLU:HA	2:C:4653:VAL:HG12	2.03	0.41
2:D:242:ASP:OD1	2:D:243:GLU:N	2.53	0.41
2:D:1284:LYS:HE2	2:D:1433:PHE:CZ	2.56	0.41
2:D:1757:LEU:HD22	2:D:2117:ILE:HD11	2.01	0.41
2:D:2618:TRP:CH2	2:D:2977:ASN:HB3	2.56	0.41
2:D:4706:GLN:O	2:D:4710:LEU:HG	2.21	0.41
2:A:785:ASP:OD2	2:A:786:GLY:N	2.54	0.41
2:A:936:SER:O	2:A:939:THR:HB	2.20	0.41
2:A:956:HIS:O	2:A:960:LYS:HG2	2.21	0.41
2:A:972:LEU:HD23	2:A:972:LEU:H	1.86	0.41
2:A:1765:SER:HA	2:A:1766:PRO:HD3	1.93	0.41
2:A:1929:SER:OG	2:A:3617:VAL:HG13	2.20	0.41
2:A:2566:ARG:HA	2:A:2569:ILE:HG22	2.03	0.41
2:A:3231:MET:O	2:A:3235:MET:HG3	2.20	0.41
2:A:4858:LEU:HD23	2:A:4861:ILE:HD12	2.02	0.41
2:B:692:HIS:H	2:B:795:SER:HG	1.69	0.41
2:B:919:VAL:HG12	2:B:920:GLU:H	1.85	0.41
2:B:1415:ASP:OD2	2:B:1559:ARG:NH2	2.35	0.41
2:B:1967:SER:O	2:B:1972:GLN:NE2	2.52	0.41
2:B:2385:GLY:O	2:B:2389:MET:HG3	2.20	0.41
2:B:2526:PRO:O	2:B:2530:ARG:HG3	2.21	0.41
2:B:2678:PRO:HB2	2:B:2981:TYR:CZ	2.55	0.41
2:B:3638:ASP:OD2	2:B:4683:ARG:HD3	2.20	0.41
2:C:1108:VAL:HB	2:C:1212:VAL:HB	2.02	0.41
2:C:1172:THR:HB	2:C:1190:LEU:HD22	2.02	0.41
2:C:1745:LYS:HA	2:C:1745:LYS:HD2	1.78	0.41
2:C:1796:THR:HG22	2:C:1800:LYS:HZ1	1.86	0.41
2:C:2566:ARG:HA	2:C:2569:ILE:HG22	2.03	0.41
2:C:2618:TRP:CH2	2:C:2977:ASN:HB3	2.56	0.41
2:C:2646:TRP:CE3	2:C:2646:TRP:HA	2.55	0.41
2:C:3261:ALA:C	2:C:3263:MET:H	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:3677:THR:O	2:C:3679:LYS:NZ	2.54	0.41
2:C:3757:ALA:HA	2:C:3760:LYS:HE2	2.03	0.41
2:C:3778:LEU:HD13	2:C:3854:PHE:CD1	2.56	0.41
2:D:956:HIS:O	2:D:960:LYS:HG2	2.21	0.41
2:D:1415:ASP:OD2	2:D:1559:ARG:NH2	2.35	0.41
2:D:2566:ARG:HA	2:D:2569:ILE:HG22	2.03	0.41
2:D:2826:ILE:HG13	2:D:2828:MET:CE	2.50	0.41
2:D:3778:LEU:HD11	2:D:3782:LYS:HE3	2.02	0.41
2:A:844:ARG:HB2	2:A:847:THR:OG1	2.20	0.41
2:A:877:HIS:HA	2:A:880:ARG:HH11	1.80	0.41
2:A:1284:LYS:HE2	2:A:1433:PHE:CZ	2.56	0.41
2:A:1428:TYR:HB3	2:A:1566:LEU:HD22	2.01	0.41
2:A:1444:GLY:CA	2:A:1487:MET:HG2	2.51	0.41
2:A:1914:CYS:SG	2:A:2091:GLN:NE2	2.88	0.41
2:A:2066:MET:SD	2:A:2087:LEU:HD23	2.61	0.41
2:A:2504:THR:O	2:A:2508:SER:N	2.45	0.41
2:A:2782:MET:HG2	2:A:2787:TRP:CE3	2.55	0.41
2:B:125:TYR:O	2:B:414:ARG:NH1	2.53	0.41
2:B:258:ARG:NH1	2:B:317:MET:HA	2.36	0.41
2:B:737:ILE:HG21	2:B:1534:GLU:OE2	2.21	0.41
2:B:785:ASP:OD2	2:B:786:GLY:N	2.54	0.41
2:B:948:CYS:HA	2:B:1067:PRO:HD3	2.02	0.41
2:B:956:HIS:O	2:B:960:LYS:HG2	2.21	0.41
2:B:1718:ARG:HD3	2:B:1831:MET:HA	2.02	0.41
2:B:2596:VAL:O	2:B:2599:LEU:HD22	2.21	0.41
2:B:3677:THR:O	2:B:3679:LYS:NZ	2.54	0.41
2:B:3790:PHE:HE1	2:B:3858:LEU:HD23	1.85	0.41
2:B:4250:TYR:HE1	2:B:4257:ARG:HE	1.69	0.41
2:B:4753:LEU:HD21	2:C:4769:LEU:HB3	2.03	0.41
2:C:670:TYR:O	2:C:673:TRP:NE1	2.53	0.41
2:C:785:ASP:OD2	2:C:786:GLY:N	2.54	0.41
2:C:1177:LEU:HB2	2:C:1182:LEU:HD21	2.03	0.41
2:C:2385:GLY:O	2:C:2389:MET:HG3	2.20	0.41
2:C:3208:ILE:HA	2:C:3209:PRO:HD3	1.88	0.41
2:C:3325:LYS:HA	2:C:3328:LYS:CE	2.50	0.41
2:C:4291:PHE:CZ	2:D:4726:MET:HB3	2.56	0.41
2:C:4858:LEU:HD23	2:C:4861:ILE:HD12	2.02	0.41
2:D:334:SER:OG	2:D:338:LEU:HD22	2.20	0.41
2:D:785:ASP:OD2	2:D:786:GLY:N	2.54	0.41
2:D:1129:GLY:H	2:D:1134:ALA:HB3	1.86	0.41
2:D:1177:LEU:HB2	2:D:1182:LEU:HD21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2682:GLU:HB3	2:D:2919:LYS:HE3	2.01	0.41
2:D:2884:LYS:HG3	2:D:2885:ASP:H	1.85	0.41
2:D:3231:MET:O	2:D:3235:MET:HG3	2.20	0.41
2:D:3325:LYS:HA	2:D:3328:LYS:CE	2.50	0.41
2:D:4306:PHE:HA	2:D:4309:ILE:HG12	2.03	0.41
2:D:4765:LYS:HD2	2:D:4765:LYS:HA	1.82	0.41
1:H:26:HIS:ND1	1:H:105:LEU:HD11	2.35	0.41
2:A:948:CYS:HA	2:A:1067:PRO:HD3	2.02	0.41
2:A:972:LEU:HD13	2:A:978:PRO:HD3	2.02	0.41
2:A:2886:ARG:HE	2:A:2890:GLN:HG2	1.86	0.41
2:A:2888:LYS:HE2	2:A:2888:LYS:HB2	1.92	0.41
2:A:3301:VAL:HA	2:A:3304:GLN:OE1	2.21	0.41
2:A:4306:PHE:HA	2:A:4309:ILE:HG12	2.03	0.41
2:A:4599:ILE:HG13	2:A:4709:LYS:NZ	2.36	0.41
2:A:4611:GLU:HA	2:A:4653:VAL:HG12	2.03	0.41
2:B:1427:TYR:HB2	2:B:1563:VAL:HG11	2.02	0.41
2:B:1957:LEU:HD21	2:B:1960:ARG:HH21	1.86	0.41
2:B:2646:TRP:HA	2:B:2646:TRP:CE3	2.55	0.41
2:B:2787:TRP:CD1	2:B:2904:SER:O	2.68	0.41
2:B:4587:ILE:HD11	2:B:4722:LEU:O	2.21	0.41
2:B:4611:GLU:HA	2:B:4653:VAL:HG12	2.03	0.41
2:B:4858:LEU:HD23	2:B:4861:ILE:HD12	2.02	0.41
2:C:228:LEU:HD21	2:C:277:LEU:HD13	2.01	0.41
2:C:242:ASP:OD1	2:C:243:GLU:N	2.53	0.41
2:C:329:PHE:HB3	2:C:363:ILE:HD11	2.01	0.41
2:C:844:ARG:HB2	2:C:847:THR:OG1	2.21	0.41
2:C:2232:PRO:C	2:C:2234:MET:H	2.24	0.41
2:C:3725:LEU:HD23	2:C:3725:LEU:HA	1.96	0.41
2:D:15:ARG:HH11	2:D:112:THR:C	2.23	0.41
2:D:670:TYR:O	2:D:673:TRP:NE1	2.53	0.41
2:D:936:SER:O	2:D:939:THR:HB	2.20	0.41
2:D:1015:GLY:HA3	2:D:1027:ARG:HH22	1.85	0.41
2:D:2403:ALA:HB2	2:D:2475:VAL:HG22	2.02	0.41
2:D:2468:MET:HB3	2:D:2468:MET:HE3	1.97	0.41
2:D:2585:MET:CE	2:D:2613:HIS:HD2	2.34	0.41
2:D:2618:TRP:HD1	2:D:2619:LYS:HZ2	1.62	0.41
2:D:2646:TRP:HA	2:D:2646:TRP:CE3	2.55	0.41
2:D:2926:LEU:O	2:D:2930:ILE:HG12	2.21	0.41
2:D:3306:ILE:O	2:D:3310:VAL:HG23	2.21	0.41
2:D:3677:THR:O	2:D:3679:LYS:NZ	2.54	0.41
2:D:3778:LEU:HD13	2:D:3854:PHE:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3846:LEU:HB3	2:D:3854:PHE:HE2	1.86	0.41
2:D:4587:ILE:HD11	2:D:4722:LEU:O	2.21	0.41
1:G:18:LYS:HE3	1:G:18:LYS:HA	2.03	0.41
1:G:85:ALA:O	1:G:94:PRO:HB3	2.21	0.41
2:A:215:ALA:HA	2:A:216:PRO:HD3	1.98	0.41
2:A:436:LEU:HD23	2:A:436:LEU:HA	1.92	0.41
2:A:750:ARG:HH11	2:A:750:ARG:HG2	1.85	0.41
2:A:872:ILE:C	2:A:941:LYS:HZ2	2.24	0.41
2:A:924:LEU:HD22	2:A:929:ARG:HB2	2.03	0.41
2:A:1129:GLY:H	2:A:1134:ALA:HB3	1.86	0.41
2:A:1138:ASP:OD2	2:A:1141:LYS:HE2	2.21	0.41
2:A:1177:LEU:HB2	2:A:1182:LEU:HD21	2.03	0.41
2:A:1644:LEU:HB3	2:A:1651:LEU:HD13	2.03	0.41
2:A:1757:LEU:HD22	2:A:2117:ILE:HD11	2.01	0.41
2:A:1957:LEU:HD21	2:A:1960:ARG:HH21	1.86	0.41
2:A:2232:PRO:C	2:A:2234:MET:H	2.24	0.41
2:A:2471:PHE:CE2	2:A:2475:VAL:HG21	2.56	0.41
2:A:2526:PRO:O	2:A:2530:ARG:HG3	2.21	0.41
2:A:2759:PRO:HB3	2:A:2821:TYR:CD1	2.56	0.41
2:A:2884:LYS:HG3	2:A:2885:ASP:H	1.85	0.41
2:A:3191:GLU:HA	2:A:3194:ALA:HB3	2.03	0.41
2:A:4250:TYR:HE1	2:A:4257:ARG:HE	1.69	0.41
2:A:4726:MET:O	2:A:4730:VAL:HG13	2.21	0.41
2:A:4924:TYR:CZ	2:A:4928:LYS:HD2	2.56	0.41
2:B:670:TYR:O	2:B:673:TRP:NE1	2.54	0.41
2:B:881:ILE:HD13	2:B:1062:TYR:CZ	2.56	0.41
2:B:924:LEU:HD22	2:B:929:ARG:HB2	2.03	0.41
2:B:1172:THR:HB	2:B:1190:LEU:HD22	2.02	0.41
2:B:1284:LYS:HE2	2:B:1433:PHE:CZ	2.56	0.41
2:B:1444:GLY:HA3	2:B:1487:MET:HG2	2.03	0.41
2:B:2171:VAL:HG21	2:B:2199:PHE:CE2	2.56	0.41
2:B:2232:PRO:C	2:B:2234:MET:H	2.24	0.41
2:B:2325:ILE:CD1	2:B:2426:LEU:HD11	2.50	0.41
2:B:2585:MET:CE	2:B:2613:HIS:HD2	2.34	0.41
2:B:2765:GLU:O	2:B:2769:GLU:N	2.49	0.41
2:B:3195:LEU:HD23	2:B:3195:LEU:HA	1.93	0.41
2:B:3712:LYS:HB3	2:B:3716:GLU:HB2	2.02	0.41
2:B:4289:SER:O	2:B:4293:THR:HG23	2.21	0.41
2:B:4627:LYS:HB3	2:B:4627:LYS:HE3	1.86	0.41
2:B:4706:GLN:O	2:B:4710:LEU:HG	2.21	0.41
2:B:4726:MET:O	2:B:4730:VAL:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4806:CYS:HA	2:B:4812:CYS:HB2	2.02	0.41
2:B:4924:TYR:CZ	2:B:4928:LYS:HD2	2.56	0.41
2:C:520:ARG:HG2	2:C:524:GLU:HG2	2.03	0.41
2:C:750:ARG:HG2	2:C:750:ARG:HH11	1.85	0.41
2:C:1427:TYR:HB2	2:C:1563:VAL:HG11	2.02	0.41
2:C:1644:LEU:HB3	2:C:1651:LEU:HD13	2.03	0.41
2:C:1718:ARG:HD3	2:C:1831:MET:HA	2.03	0.41
2:C:2171:VAL:HG21	2:C:2199:PHE:CE2	2.56	0.41
2:C:2403:ALA:HB2	2:C:2475:VAL:HG22	2.02	0.41
2:C:2471:PHE:CE2	2:C:2475:VAL:HG21	2.56	0.41
2:C:2596:VAL:O	2:C:2599:LEU:HD22	2.21	0.41
2:C:2791:ARG:HE	2:C:2792:THR:N	2.18	0.41
2:C:2973:GLN:HA	2:C:2976:LYS:HE2	2.02	0.41
2:C:3250:TRP:CZ2	2:C:3270:SER:HB2	2.56	0.41
2:C:4250:TYR:HE1	2:C:4257:ARG:HE	1.69	0.41
2:C:4306:PHE:HA	2:C:4309:ILE:HG12	2.03	0.41
2:C:4726:MET:O	2:C:4730:VAL:HG13	2.21	0.41
2:C:4765:LYS:HD2	2:C:4765:LYS:HA	1.82	0.41
2:C:4806:CYS:HA	2:C:4812:CYS:HB2	2.02	0.41
2:D:76:ARG:HA	2:D:76:ARG:HD3	1.79	0.41
2:D:161:THR:HG23	2:D:186:VAL:HG22	2.03	0.41
2:D:258:ARG:NH1	2:D:317:MET:HA	2.36	0.41
2:D:372:LEU:HD11	2:D:391:ALA:HB1	2.02	0.41
2:D:737:ILE:HG21	2:D:1534:GLU:OE2	2.21	0.41
2:D:750:ARG:HG2	2:D:750:ARG:HH11	1.85	0.41
2:D:972:LEU:HD23	2:D:972:LEU:H	1.85	0.41
2:D:972:LEU:HD13	2:D:978:PRO:HD3	2.02	0.41
2:D:1303:ARG:HA	2:D:1542:ALA:HA	2.03	0.41
2:D:2471:PHE:CE2	2:D:2475:VAL:HG21	2.56	0.41
2:D:2596:VAL:O	2:D:2599:LEU:HD22	2.21	0.41
2:D:2635:GLU:OE2	2:D:2680:TYR:OH	2.24	0.41
2:D:2658:GLU:OE1	2:D:2661:LEU:N	2.30	0.41
2:D:2756:LEU:HD12	2:D:2756:LEU:HA	1.79	0.41
2:D:2826:ILE:HG13	2:D:2828:MET:HE3	2.02	0.41
2:D:3301:VAL:HA	2:D:3304:GLN:OE1	2.21	0.41
2:D:3633:GLU:OE1	2:D:3634:HIS:N	2.52	0.41
2:D:3725:LEU:HD23	2:D:3725:LEU:HA	1.96	0.41
2:A:881:ILE:HD13	2:A:1062:TYR:CZ	2.56	0.41
2:A:2830:ASN:CB	2:B:1435:GLY:HA3	2.50	0.41
2:A:3187:LYS:NZ	2:A:3191:GLU:OE1	2.46	0.41
2:A:3757:ALA:HA	2:A:3760:LYS:HE2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:4058:TYR:HD2	2:A:4062:GLU:HB3	1.85	0.41
2:A:4587:ILE:HD11	2:A:4722:LEU:O	2.21	0.41
2:B:674:TYR:HE1	2:B:756:SER:HB2	1.85	0.41
2:B:2403:ALA:HB2	2:B:2475:VAL:HG22	2.02	0.41
2:B:2566:ARG:HA	2:B:2569:ILE:HG22	2.03	0.41
2:B:2618:TRP:CH2	2:B:2977:ASN:HB3	2.56	0.41
2:B:3324:GLU:O	2:B:3327:LYS:HB3	2.20	0.41
2:B:4035:TYR:CZ	2:B:4050:LYS:HB3	2.56	0.41
2:C:881:ILE:HD13	2:C:1062:TYR:CZ	2.56	0.41
2:C:1138:ASP:OD2	2:C:1141:LYS:HE2	2.21	0.41
2:C:1190:LEU:HB2	2:C:1193:LYS:HZ1	1.84	0.41
2:C:1303:ARG:HA	2:C:1542:ALA:HA	2.03	0.41
2:C:1444:GLY:CA	2:C:1487:MET:HG2	2.51	0.41
2:C:2418:ARG:HD3	2:D:189:GLU:CD	2.41	0.41
2:C:2849:HIS:CD2	2:C:2874:TYR:HB2	2.55	0.41
2:C:4587:ILE:HD11	2:C:4722:LEU:O	2.21	0.41
2:C:4943:MET:HB3	2:C:4948:CYS:HB2	2.03	0.41
2:D:436:LEU:HD23	2:D:436:LEU:HA	1.92	0.41
2:D:489:PHE:CD2	2:D:494:MET:HG3	2.56	0.41
2:D:1283:LEU:HB2	2:D:1555:PHE:HB2	2.02	0.41
2:D:2480:VAL:HB	2:D:2483:PHE:HB3	2.02	0.41
2:D:2759:PRO:HB3	2:D:2821:TYR:CD1	2.56	0.41
2:D:2760:TYR:OH	2:D:2772:ARG:NH1	2.54	0.41
2:D:3790:PHE:HE1	2:D:3858:LEU:HD23	1.85	0.41
2:A:489:PHE:CD2	2:A:494:MET:HG3	2.56	0.40
2:A:1828:LEU:HA	2:A:1831:MET:HE2	2.03	0.40
2:A:2403:ALA:HB2	2:A:2475:VAL:HG22	2.02	0.40
2:A:2444:THR:O	2:A:2452:VAL:HG12	2.20	0.40
2:A:2760:TYR:OH	2:A:2772:ARG:NH1	2.54	0.40
2:A:3743:THR:HB	2:A:3758:THR:HG21	2.03	0.40
2:B:1944:TYR:O	2:B:1948:MET:HG3	2.21	0.40
2:B:2471:PHE:CE2	2:B:2475:VAL:HG21	2.56	0.40
2:B:2592:LEU:HD22	2:B:2606:PRO:HB3	2.03	0.40
2:B:2610:LEU:HD23	2:B:2613:HIS:CE1	2.55	0.40
2:B:2886:ARG:HE	2:B:2890:GLN:HG2	1.86	0.40
2:B:4058:TYR:HD2	2:B:4062:GLU:HB3	1.85	0.40
2:C:956:HIS:O	2:C:960:LYS:HG2	2.21	0.40
2:C:1444:GLY:HA3	2:C:1487:MET:HG2	2.03	0.40
2:C:1944:TYR:O	2:C:1948:MET:HG3	2.21	0.40
2:C:2325:ILE:CD1	2:C:2426:LEU:HD11	2.50	0.40
2:C:2504:THR:O	2:C:2508:SER:N	2.45	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2884:LYS:O	2:C:2887:GLU:HG3	2.22	0.40
2:C:2926:LEU:O	2:C:2930:ILE:HG12	2.21	0.40
2:C:3712:LYS:HB3	2:C:3716:GLU:HB2	2.02	0.40
2:C:4706:GLN:O	2:C:4710:LEU:HG	2.21	0.40
2:C:4827:ILE:HG13	2:C:4831:ILE:HG12	2.04	0.40
2:C:4942:LYS:O	2:C:4946:GLU:HG3	2.22	0.40
2:D:881:ILE:HD13	2:D:1062:TYR:CZ	2.56	0.40
2:D:1944:TYR:O	2:D:1948:MET:HG3	2.21	0.40
2:D:2385:GLY:O	2:D:2389:MET:HG3	2.20	0.40
2:D:2610:LEU:HD23	2:D:2613:HIS:CE1	2.55	0.40
2:D:2884:LYS:HG3	2:D:2885:ASP:N	2.36	0.40
2:D:3757:ALA:HA	2:D:3760:LYS:HE2	2.03	0.40
1:G:63:GLY:HA3	1:G:75:LEU:HD21	2.03	0.40
1:H:32:GLN:HA	1:H:99:ILE:HD13	2.03	0.40
2:A:242:ASP:OD1	2:A:243:GLU:N	2.53	0.40
2:A:881:ILE:HD13	2:A:1062:TYR:CE1	2.57	0.40
2:A:1166:VAL:HA	2:A:1173:MET:HG2	2.03	0.40
2:A:1303:ARG:HA	2:A:1542:ALA:HA	2.03	0.40
2:A:1979:PHE:CG	2:A:1993:ARG:HG2	2.56	0.40
2:A:4660:PHE:HA	2:D:4056:LYS:HZ2	1.87	0.40
2:B:750:ARG:HH11	2:B:750:ARG:HG2	1.85	0.40
2:B:920:GLU:N	2:B:974:SER:HB3	2.37	0.40
2:B:972:LEU:H	2:B:972:LEU:HD23	1.86	0.40
2:B:1138:ASP:OD2	2:B:1141:LYS:HE2	2.21	0.40
2:B:1166:VAL:HA	2:B:1173:MET:HG2	2.03	0.40
2:B:2973:GLN:HA	2:B:2976:LYS:HE2	2.02	0.40
2:B:3172:GLU:HG2	2:B:3175:LEU:HB2	2.03	0.40
2:B:3176:ASP:HB3	2:B:3201:VAL:HG21	2.04	0.40
2:B:3306:ILE:O	2:B:3310:VAL:HG23	2.21	0.40
2:B:4306:PHE:HA	2:B:4309:ILE:HG12	2.03	0.40
2:B:4484:ILE:HG13	2:B:4485:ILE:N	2.36	0.40
2:C:270:HIS:CD2	2:C:491:GLU:HG3	2.56	0.40
2:C:919:VAL:HG12	2:C:920:GLU:H	1.85	0.40
2:C:948:CYS:HA	2:C:1067:PRO:HD3	2.02	0.40
2:C:1129:GLY:H	2:C:1134:ALA:HB3	1.86	0.40
2:C:1166:VAL:HA	2:C:1173:MET:HG2	2.03	0.40
2:C:2759:PRO:HB3	2:C:2821:TYR:CD1	2.56	0.40
2:C:3306:ILE:O	2:C:3310:VAL:HG23	2.21	0.40
2:D:1549:SER:OG	2:D:1551:ASN:O	2.37	0.40
2:D:2841:ALA:HA	2:D:2844:MET:CG	2.43	0.40
2:D:2888:LYS:HE2	2:D:2888:LYS:HB2	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3122:ILE:HG12	2:D:3167:PRO:HG3	2.02	0.40
2:D:4599:ILE:HG13	2:D:4709:LYS:NZ	2.36	0.40
2:D:4891:CYS:HB3	2:D:4913:HIS:CE1	2.57	0.40
1:G:32:GLN:HA	1:G:99:ILE:HD13	2.04	0.40
2:A:258:ARG:NH1	2:A:317:MET:HA	2.36	0.40
2:A:562:LEU:HD21	2:A:600:LEU:HD22	2.02	0.40
2:A:877:HIS:HB3	2:A:880:ARG:HH12	1.86	0.40
2:A:1108:VAL:HB	2:A:1212:VAL:HB	2.02	0.40
2:A:1766:PRO:HG3	2:A:1780:PRO:HB3	2.03	0.40
2:A:2585:MET:CE	2:A:2613:HIS:HD2	2.33	0.40
2:A:2601:GLU:HA	2:A:2604:LYS:NZ	2.36	0.40
2:A:2756:LEU:HD12	2:A:2756:LEU:HA	1.79	0.40
2:A:3176:ASP:HB3	2:A:3201:VAL:HG21	2.03	0.40
2:A:3250:TRP:HE3	2:A:3309:LYS:HZ3	1.68	0.40
2:A:4706:GLN:O	2:A:4710:LEU:HG	2.21	0.40
2:B:1108:VAL:HB	2:B:1212:VAL:HB	2.02	0.40
2:B:1444:GLY:CA	2:B:1487:MET:HG2	2.51	0.40
2:B:1828:LEU:HA	2:B:1831:MET:HE2	2.03	0.40
2:B:2884:LYS:HG3	2:B:2885:ASP:N	2.36	0.40
2:B:3607:PRO:HD2	2:B:3610:ASN:OD1	2.21	0.40
2:B:3778:LEU:HD13	2:B:3854:PHE:CD1	2.56	0.40
2:B:3882:GLN:HE21	2:B:3882:GLN:HB3	1.74	0.40
2:B:4587:ILE:CD1	2:B:4726:MET:HG2	2.50	0.40
2:B:4599:ILE:HG13	2:B:4709:LYS:NZ	2.36	0.40
2:C:161:THR:HG23	2:C:186:VAL:HG22	2.03	0.40
2:C:290:ARG:HH21	2:C:350:GLY:HA3	1.87	0.40
2:C:872:ILE:C	2:C:941:LYS:HZ2	2.24	0.40
2:C:924:LEU:HD22	2:C:929:ARG:HB2	2.03	0.40
2:C:2526:PRO:O	2:C:2530:ARG:HG3	2.21	0.40
2:C:2884:LYS:HG3	2:C:2885:ASP:N	2.36	0.40
2:C:3778:LEU:HD11	2:C:3782:LYS:HE3	2.02	0.40
2:C:4522:VAL:HG22	2:D:4807:ASP:O	2.22	0.40
2:D:1086:ARG:HH21	2:D:1251:LEU:CD1	2.24	0.40
2:D:1444:GLY:CA	2:D:1487:MET:HG2	2.51	0.40
2:D:2884:LYS:O	2:D:2887:GLU:HG3	2.21	0.40
2:D:2886:ARG:HE	2:D:2890:GLN:HG2	1.86	0.40
2:D:3191:GLU:HA	2:D:3194:ALA:HB3	2.02	0.40
2:D:4728:MET:HE2	2:D:4741:ALA:HB3	2.03	0.40
1:F:32:GLN:HA	1:F:99:ILE:HD13	2.03	0.40
2:A:1017:THR:HG23	2:A:1028:ARG:HG2	2.04	0.40
2:A:1444:GLY:HA3	2:A:1487:MET:HG2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2618:TRP:CH2	2:A:2977:ASN:HB3	2.56	0.40
2:A:3007:LEU:HD23	2:A:3036:LEU:HD11	2.04	0.40
2:A:3208:ILE:HA	2:A:3209:PRO:HD3	1.88	0.40
2:A:3677:THR:O	2:A:3679:LYS:NZ	2.54	0.40
2:A:4035:TYR:CZ	2:A:4050:LYS:HB3	2.56	0.40
2:A:4708:TRP:O	2:A:4712:VAL:HG23	2.20	0.40
2:B:893:TRP:HD1	2:B:897:LYS:HZ1	1.69	0.40
2:B:972:LEU:HD13	2:B:978:PRO:HD3	2.02	0.40
2:B:1283:LEU:HB2	2:B:1555:PHE:HB2	2.02	0.40
2:B:1554:GLN:NE2	2:B:1556:GLU:OE2	2.35	0.40
2:B:1914:CYS:SG	2:B:2091:GLN:NE2	2.88	0.40
2:B:2065:THR:HG23	2:B:2066:MET:HE3	2.03	0.40
2:B:2926:LEU:O	2:B:2930:ILE:HG12	2.21	0.40
2:B:3778:LEU:HD11	2:B:3782:LYS:HE3	2.02	0.40
2:B:4942:LYS:O	2:B:4946:GLU:HG3	2.22	0.40
2:C:16:THR:OG1	2:C:69:LEU:O	2.22	0.40
2:C:674:TYR:HE1	2:C:756:SER:HB2	1.86	0.40
2:C:713:TRP:CE2	2:C:1600:PRO:HD3	2.56	0.40
2:C:920:GLU:N	2:C:974:SER:HB3	2.37	0.40
2:C:1015:GLY:HA3	2:C:1027:ARG:HH22	1.85	0.40
2:C:1979:PHE:CG	2:C:1993:ARG:HG2	2.56	0.40
2:C:3007:LEU:HD23	2:C:3036:LEU:HD11	2.04	0.40
2:C:3175:LEU:HB3	2:C:3178:HIS:NE2	2.37	0.40
2:C:3760:LYS:HE2	2:C:3760:LYS:HB2	1.94	0.40
2:D:562:LEU:HD21	2:D:600:LEU:HD22	2.02	0.40
2:D:881:ILE:HD13	2:D:1062:TYR:CE1	2.57	0.40
2:D:924:LEU:HD22	2:D:929:ARG:HB2	2.04	0.40
2:D:992:GLN:HA	2:D:995:MET:HE2	2.03	0.40
2:D:1166:VAL:HA	2:D:1173:MET:HG2	2.03	0.40
2:D:2526:PRO:O	2:D:2530:ARG:HG3	2.21	0.40
2:D:2592:LEU:HD22	2:D:2606:PRO:HB3	2.02	0.40
2:D:2756:LEU:HD11	2:D:2763:LEU:CD1	2.52	0.40
2:D:3007:LEU:HD23	2:D:3036:LEU:HD11	2.04	0.40
2:D:4921:PHE:HE2	2:D:4940:VAL:HG11	1.87	0.40
1:F:85:ALA:O	1:F:94:PRO:HB3	2.21	0.40
2:A:290:ARG:HH21	2:A:350:GLY:HA3	1.87	0.40
2:A:337:LYS:HZ2	2:A:371:TRP:HE1	1.69	0.40
2:A:2202:TYR:O	2:A:2206:ILE:HG12	2.22	0.40
2:A:2756:LEU:HD11	2:A:2763:LEU:CD1	2.52	0.40
2:A:2756:LEU:HD11	2:A:2763:LEU:HD11	2.03	0.40
2:A:2884:LYS:O	2:A:2887:GLU:HG3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2926:LEU:O	2:A:2930:ILE:HG12	2.21	0.40
2:B:713:TRP:CE2	2:B:1600:PRO:HD3	2.56	0.40
2:B:980:PRO:HB2	2:B:981:MET:SD	2.62	0.40
2:B:1177:LEU:HD12	2:B:1177:LEU:HA	1.91	0.40
2:B:1697:LEU:HD23	2:B:1697:LEU:HA	1.91	0.40
2:B:1979:PHE:CG	2:B:1993:ARG:HG2	2.56	0.40
2:B:2443:PRO:HB3	2:B:2452:VAL:O	2.22	0.40
2:B:2756:LEU:HD11	2:B:2763:LEU:CD1	2.52	0.40
2:B:2870:LEU:HD21	2:B:2881:GLU:HB2	2.04	0.40
2:B:3007:LEU:HD23	2:B:3036:LEU:HD11	2.04	0.40
2:B:3042:ALA:O	2:B:3046:MET:HE2	2.22	0.40
2:B:3191:GLU:HA	2:B:3194:ALA:HB3	2.03	0.40
2:B:4791:LYS:HE3	2:B:4791:LYS:HB3	1.87	0.40
2:B:4943:MET:HB3	2:B:4948:CYS:HB2	2.03	0.40
2:C:1957:LEU:HD21	2:C:1960:ARG:HH21	1.86	0.40
2:C:1958:THR:O	2:C:1962:THR:HG22	2.21	0.40
2:C:2756:LEU:HD11	2:C:2763:LEU:HD11	2.03	0.40
2:C:2759:PRO:HB3	2:C:2821:TYR:CE1	2.56	0.40
2:C:2760:TYR:OH	2:C:2772:ARG:NH1	2.54	0.40
2:C:2886:ARG:HE	2:C:2890:GLN:HG2	1.86	0.40
2:C:3607:PRO:HD2	2:C:3610:ASN:OD1	2.21	0.40
2:C:4891:CYS:HB3	2:C:4913:HIS:CE1	2.57	0.40
2:C:4924:TYR:CZ	2:C:4928:LYS:HD2	2.56	0.40
2:D:713:TRP:CE2	2:D:1600:PRO:HD3	2.56	0.40
2:D:1108:VAL:HB	2:D:1212:VAL:HB	2.02	0.40
2:D:1828:LEU:HA	2:D:1831:MET:HE2	2.04	0.40
2:D:2186:GLU:CD	2:D:2187:ILE:H	2.25	0.40
2:D:4034:GLU:O	2:D:4037:PRO:HD3	2.22	0.40
2:D:4035:TYR:CZ	2:D:4050:LYS:HB3	2.56	0.40
2:D:4289:SER:O	2:D:4293:THR:HG23	2.21	0.40
2:D:4520:TYR:HD1	2:D:4561:LEU:HD13	1.87	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	E	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
1	F	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
1	G	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
1	H	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
2	A	4198/4967 (84%)	4064 (97%)	131 (3%)	3 (0%)	51	83
2	B	4198/4967 (84%)	4064 (97%)	131 (3%)	3 (0%)	51	83
2	C	4198/4967 (84%)	4062 (97%)	133 (3%)	3 (0%)	51	83
2	D	4198/4967 (84%)	4064 (97%)	131 (3%)	3 (0%)	51	83
All	All	17212/20300 (85%)	16666 (97%)	534 (3%)	12 (0%)	54	83

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	1553	PHE
2	A	2988	ARG
2	A	4641	PRO
2	B	1553	PHE
2	B	2988	ARG
2	B	4641	PRO
2	C	1553	PHE
2	C	2988	ARG
2	C	4641	PRO
2	D	1553	PHE
2	D	2988	ARG
2	D	4641	PRO

5.3.2 Protein sidechains ⓘ

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	E	88/89 (99%)	85 (97%)	3 (3%)	37	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	88/89 (99%)	85 (97%)	3 (3%)	37	69
1	G	88/89 (99%)	85 (97%)	3 (3%)	37	69
1	H	88/89 (99%)	85 (97%)	3 (3%)	37	69
2	A	3708/4358 (85%)	3633 (98%)	75 (2%)	55	79
2	B	3708/4358 (85%)	3633 (98%)	75 (2%)	55	79
2	C	3708/4358 (85%)	3633 (98%)	75 (2%)	55	79
2	D	3708/4358 (85%)	3633 (98%)	75 (2%)	55	79
All	All	15184/17788 (85%)	14872 (98%)	312 (2%)	56	78

All (312) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	4	GLU
1	E	19	LYS
1	E	58	LYS
1	F	4	GLU
1	F	19	LYS
1	F	58	LYS
1	G	4	GLU
1	G	19	LYS
1	G	58	LYS
1	H	4	GLU
1	H	19	LYS
1	H	58	LYS
2	A	153	THR
2	A	203	VAL
2	A	241	MET
2	A	309	MET
2	A	343	ARG
2	A	393	MET
2	A	403	ILE
2	A	469	HIS
2	A	494	MET
2	A	765	SER
2	A	880	ARG
2	A	895	MET
2	A	929	ARG
2	A	1013	ARG
2	A	1249	MET
2	A	1481	LYS

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Mol	Chain	Res	Type
2	A	1564	MET
2	A	1694	MET
2	A	1720	MET
2	A	1729	MET
2	A	1751	ILE
2	A	1896	MET
2	A	1933	VAL
2	A	2066	MET
2	A	2142	MET
2	A	2192	MET
2	A	2234	MET
2	A	2248	MET
2	A	2279	MET
2	A	2303	ARG
2	A	2347	MET
2	A	2406	MET
2	A	2581	ARG
2	A	2589	LEU
2	A	2681	MET
2	A	2688	MET
2	A	2689	MET
2	A	2729	HIS
2	A	2754	GLN
2	A	2758	LYS
2	A	2761	LYS
2	A	2772	ARG
2	A	2788	ARG
2	A	2828	MET
2	A	2894	LYS
2	A	2905	ARG
2	A	3018	ARG
2	A	3072	MET
2	A	3201	VAL
2	A	3235	MET
2	A	3241	MET
2	A	3242	LEU
2	A	3277	LEU
2	A	3322	LEU
2	A	3819	MET
2	A	3882	GLN
2	A	3954	MET
2	A	3981	MET

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Mol	Chain	Res	Type
2	A	3985	MET
2	A	4012	MET
2	A	4246	PHE
2	A	4251	ASN
2	A	4271	VAL
2	A	4272	LYS
2	A	4279	MET
2	A	4491	LEU
2	A	4626	ILE
2	A	4654	MET
2	A	4707	MET
2	A	4726	MET
2	A	4748	MET
2	A	4771	VAL
2	A	4804	MET
2	A	4884	MET
2	A	4903	HIS
2	B	153	THR
2	B	203	VAL
2	B	241	MET
2	B	309	MET
2	B	343	ARG
2	B	393	MET
2	B	403	ILE
2	B	469	HIS
2	B	494	MET
2	B	765	SER
2	B	880	ARG
2	B	895	MET
2	B	929	ARG
2	B	1013	ARG
2	B	1249	MET
2	B	1481	LYS
2	B	1564	MET
2	B	1694	MET
2	B	1720	MET
2	B	1729	MET
2	B	1751	ILE
2	B	1896	MET
2	B	1933	VAL
2	B	2066	MET
2	B	2142	MET

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Mol	Chain	Res	Type
2	B	2192	MET
2	B	2234	MET
2	B	2248	MET
2	B	2279	MET
2	B	2303	ARG
2	B	2347	MET
2	B	2406	MET
2	B	2581	ARG
2	B	2589	LEU
2	B	2681	MET
2	B	2688	MET
2	B	2689	MET
2	B	2729	HIS
2	B	2754	GLN
2	B	2758	LYS
2	B	2761	LYS
2	B	2772	ARG
2	B	2788	ARG
2	B	2828	MET
2	B	2894	LYS
2	B	2905	ARG
2	B	3018	ARG
2	B	3072	MET
2	B	3201	VAL
2	B	3235	MET
2	B	3241	MET
2	B	3242	LEU
2	B	3277	LEU
2	B	3322	LEU
2	B	3819	MET
2	B	3882	GLN
2	B	3954	MET
2	B	3981	MET
2	B	3985	MET
2	B	4012	MET
2	B	4246	PHE
2	B	4251	ASN
2	B	4271	VAL
2	B	4272	LYS
2	B	4279	MET
2	B	4491	LEU
2	B	4626	ILE

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Mol	Chain	Res	Type
2	B	4654	MET
2	B	4707	MET
2	B	4726	MET
2	B	4748	MET
2	B	4771	VAL
2	B	4804	MET
2	B	4884	MET
2	B	4903	HIS
2	C	153	THR
2	C	203	VAL
2	C	241	MET
2	C	309	MET
2	C	343	ARG
2	C	393	MET
2	C	403	ILE
2	C	469	HIS
2	C	494	MET
2	C	765	SER
2	C	880	ARG
2	C	895	MET
2	C	929	ARG
2	C	1013	ARG
2	C	1249	MET
2	C	1481	LYS
2	C	1564	MET
2	C	1694	MET
2	C	1720	MET
2	C	1729	MET
2	C	1751	ILE
2	C	1896	MET
2	C	1933	VAL
2	C	2066	MET
2	C	2142	MET
2	C	2192	MET
2	C	2234	MET
2	C	2248	MET
2	C	2279	MET
2	C	2303	ARG
2	C	2347	MET
2	C	2406	MET
2	C	2581	ARG
2	C	2589	LEU

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Mol	Chain	Res	Type
2	C	2681	MET
2	C	2688	MET
2	C	2689	MET
2	C	2729	HIS
2	C	2754	GLN
2	C	2758	LYS
2	C	2761	LYS
2	C	2772	ARG
2	C	2788	ARG
2	C	2828	MET
2	C	2894	LYS
2	C	2905	ARG
2	C	3018	ARG
2	C	3072	MET
2	C	3201	VAL
2	C	3235	MET
2	C	3241	MET
2	C	3242	LEU
2	C	3277	LEU
2	C	3322	LEU
2	C	3819	MET
2	C	3882	GLN
2	C	3954	MET
2	C	3981	MET
2	C	3985	MET
2	C	4012	MET
2	C	4246	PHE
2	C	4251	ASN
2	C	4271	VAL
2	C	4272	LYS
2	C	4279	MET
2	C	4491	LEU
2	C	4626	ILE
2	C	4654	MET
2	C	4707	MET
2	C	4726	MET
2	C	4748	MET
2	C	4771	VAL
2	C	4804	MET
2	C	4884	MET
2	C	4903	HIS
2	D	153	THR

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Mol	Chain	Res	Type
2	D	203	VAL
2	D	241	MET
2	D	309	MET
2	D	343	ARG
2	D	393	MET
2	D	403	ILE
2	D	469	HIS
2	D	494	MET
2	D	765	SER
2	D	880	ARG
2	D	895	MET
2	D	929	ARG
2	D	1013	ARG
2	D	1249	MET
2	D	1481	LYS
2	D	1564	MET
2	D	1694	MET
2	D	1720	MET
2	D	1729	MET
2	D	1751	ILE
2	D	1896	MET
2	D	1933	VAL
2	D	2066	MET
2	D	2142	MET
2	D	2192	MET
2	D	2234	MET
2	D	2248	MET
2	D	2279	MET
2	D	2303	ARG
2	D	2347	MET
2	D	2406	MET
2	D	2581	ARG
2	D	2589	LEU
2	D	2681	MET
2	D	2688	MET
2	D	2689	MET
2	D	2729	HIS
2	D	2754	GLN
2	D	2758	LYS
2	D	2761	LYS
2	D	2772	ARG
2	D	2788	ARG

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Mol	Chain	Res	Type
2	D	2828	MET
2	D	2894	LYS
2	D	2905	ARG
2	D	3018	ARG
2	D	3072	MET
2	D	3201	VAL
2	D	3235	MET
2	D	3241	MET
2	D	3242	LEU
2	D	3277	LEU
2	D	3322	LEU
2	D	3819	MET
2	D	3882	GLN
2	D	3954	MET
2	D	3981	MET
2	D	3985	MET
2	D	4012	MET
2	D	4246	PHE
2	D	4251	ASN
2	D	4271	VAL
2	D	4272	LYS
2	D	4279	MET
2	D	4491	LEU
2	D	4626	ILE
2	D	4654	MET
2	D	4707	MET
2	D	4726	MET
2	D	4748	MET
2	D	4771	VAL
2	D	4804	MET
2	D	4884	MET
2	D	4903	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	934	GLN
2	A	1581	GLN
2	A	1656	HIS
2	A	2654	GLN
2	A	2684	ASN
2	A	2830	ASN

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Mol	Chain	Res	Type
2	A	2849	HIS
2	A	3174	HIS
2	A	3850	HIS
2	A	4489	GLN
2	A	4493	ASN
2	A	4629	GLN
2	A	4642	ASN
2	B	934	GLN
2	B	1581	GLN
2	B	1656	HIS
2	B	2654	GLN
2	B	2684	ASN
2	B	2849	HIS
2	B	3174	HIS
2	B	3850	HIS
2	B	4489	GLN
2	B	4493	ASN
2	B	4629	GLN
2	B	4642	ASN
2	C	934	GLN
2	C	1581	GLN
2	C	1656	HIS
2	C	2654	GLN
2	C	2684	ASN
2	C	2849	HIS
2	C	3174	HIS
2	C	3850	HIS
2	C	4489	GLN
2	C	4493	ASN
2	C	4629	GLN
2	C	4642	ASN
2	C	4903	HIS
2	D	934	GLN
2	D	1581	GLN
2	D	1656	HIS
2	D	2654	GLN
2	D	2684	ASN
2	D	2849	HIS
2	D	3174	HIS
2	D	3850	HIS
2	D	4489	GLN
2	D	4493	ASN

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Mol	Chain	Res	Type
2	D	4629	GLN
2	D	4642	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 20 ligands modelled in this entry, 8 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\lvert Z\rvert > 2$	Counts	RMSZ	$\#\lvert Z\rvert > 2$
6	XAN	C	5004	-	8,12,12	1.51	2 (25%)	4,17,17	3.25	2 (50%)
6	XAN	B	5004	-	8,12,12	1.51	2 (25%)	4,17,17	3.28	2 (50%)
4	ATP	B	5002	-	26,33,33	0.59	0	31,52,52	0.73	2 (6%)
4	ATP	C	5005	-	26,33,33	0.60	0	31,52,52	0.75	2 (6%)
4	ATP	C	5002	-	26,33,33	0.60	0	31,52,52	0.73	2 (6%)
4	ATP	D	5005	-	26,33,33	0.61	0	31,52,52	0.75	2 (6%)
6	XAN	D	5004	-	8,12,12	1.51	2 (25%)	4,17,17	3.26	2 (50%)
4	ATP	B	5005	-	26,33,33	0.60	0	31,52,52	0.75	2 (6%)
4	ATP	D	5002	-	26,33,33	0.59	0	31,52,52	0.73	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
4	ATP	A	5005	-	26,33,33	0.60	0	31,52,52	0.75	2 (6%)
4	ATP	A	5002	-	26,33,33	0.60	0	31,52,52	0.73	2 (6%)
6	XAN	A	5004	-	8,12,12	1.51	2 (25%)	4,17,17	3.25	2 (50%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	XAN	C	5004	-	-	-	0/2/2/2
6	XAN	B	5004	-	-	-	0/2/2/2
4	ATP	B	5002	-	-	9/18/38/38	0/3/3/3
4	ATP	C	5005	-	-	4/18/38/38	0/3/3/3
4	ATP	C	5002	-	-	9/18/38/38	0/3/3/3
4	ATP	D	5005	-	-	4/18/38/38	0/3/3/3
6	XAN	D	5004	-	-	-	0/2/2/2
4	ATP	B	5005	-	-	4/18/38/38	0/3/3/3
4	ATP	D	5002	-	-	9/18/38/38	0/3/3/3
4	ATP	A	5005	-	-	4/18/38/38	0/3/3/3
4	ATP	A	5002	-	-	9/18/38/38	0/3/3/3
6	XAN	A	5004	-	-	-	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	5004	XAN	C5-C4	-2.63	1.34	1.40
6	C	5004	XAN	C5-C4	-2.63	1.34	1.40
6	A	5004	XAN	C5-C4	-2.63	1.34	1.40
6	B	5004	XAN	C5-C4	-2.62	1.34	1.40
6	B	5004	XAN	O6-C6	-2.25	1.18	1.24
6	C	5004	XAN	O6-C6	-2.25	1.18	1.24
6	D	5004	XAN	O6-C6	-2.22	1.19	1.24
6	A	5004	XAN	O6-C6	-2.21	1.19	1.24

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	5004	XAN	C2-N1-C6	5.83	120.06	115.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	5004	XAN	C2-N1-C6	5.78	120.03	115.14
6	A	5004	XAN	C2-N1-C6	5.77	120.01	115.14
6	C	5004	XAN	C2-N1-C6	5.76	120.00	115.14
6	B	5004	XAN	C5-C6-N1	-2.53	119.97	123.43
6	C	5004	XAN	C5-C6-N1	-2.51	120.00	123.43
6	D	5004	XAN	C5-C6-N1	-2.50	120.02	123.43
6	A	5004	XAN	C5-C6-N1	-2.49	120.02	123.43
4	C	5005	ATP	C5-C6-N6	2.31	123.86	120.35
4	A	5002	ATP	C5-C6-N6	2.30	123.85	120.35
4	A	5005	ATP	C5-C6-N6	2.28	123.82	120.35
4	C	5002	ATP	C5-C6-N6	2.28	123.81	120.35
4	B	5002	ATP	C5-C6-N6	2.28	123.81	120.35
4	B	5005	ATP	C5-C6-N6	2.27	123.81	120.35
4	D	5005	ATP	C5-C6-N6	2.27	123.81	120.35
4	D	5002	ATP	C5-C6-N6	2.26	123.78	120.35
4	A	5002	ATP	PB-O3B-PG	2.05	139.87	132.83
4	C	5005	ATP	PB-O3B-PG	2.05	139.87	132.83
4	B	5002	ATP	PB-O3B-PG	2.05	139.86	132.83
4	D	5002	ATP	PB-O3B-PG	2.05	139.85	132.83
4	A	5005	ATP	PB-O3B-PG	2.04	139.83	132.83
4	B	5005	ATP	PB-O3B-PG	2.04	139.82	132.83
4	C	5002	ATP	PB-O3B-PG	2.04	139.81	132.83
4	D	5005	ATP	PB-O3B-PG	2.03	139.79	132.83

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	5002	ATP	PB-O3B-PG-O2G
4	A	5002	ATP	C5'-O5'-PA-O1A
4	A	5002	ATP	C5'-O5'-PA-O2A
4	A	5002	ATP	C5'-O5'-PA-O3A
4	B	5002	ATP	PB-O3B-PG-O2G
4	B	5002	ATP	C5'-O5'-PA-O1A
4	B	5002	ATP	C5'-O5'-PA-O2A
4	B	5002	ATP	C5'-O5'-PA-O3A
4	C	5002	ATP	PB-O3B-PG-O2G
4	C	5002	ATP	C5'-O5'-PA-O1A
4	C	5002	ATP	C5'-O5'-PA-O2A
4	C	5002	ATP	C5'-O5'-PA-O3A
4	D	5002	ATP	PB-O3B-PG-O2G
4	D	5002	ATP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
4	D	5002	ATP	C5'-O5'-PA-O2A
4	D	5002	ATP	C5'-O5'-PA-O3A
4	A	5002	ATP	C4'-C5'-O5'-PA
4	B	5002	ATP	C4'-C5'-O5'-PA
4	C	5002	ATP	C4'-C5'-O5'-PA
4	D	5002	ATP	C4'-C5'-O5'-PA
4	A	5005	ATP	C3'-C4'-C5'-O5'
4	B	5005	ATP	C3'-C4'-C5'-O5'
4	C	5005	ATP	C3'-C4'-C5'-O5'
4	D	5005	ATP	C3'-C4'-C5'-O5'
4	A	5005	ATP	O4'-C4'-C5'-O5'
4	B	5005	ATP	O4'-C4'-C5'-O5'
4	C	5005	ATP	O4'-C4'-C5'-O5'
4	D	5005	ATP	O4'-C4'-C5'-O5'
4	A	5002	ATP	PA-O3A-PB-O3B
4	B	5002	ATP	PA-O3A-PB-O3B
4	C	5002	ATP	PA-O3A-PB-O3B
4	D	5002	ATP	PA-O3A-PB-O3B
4	A	5005	ATP	PB-O3A-PA-O2A
4	B	5005	ATP	PB-O3A-PA-O2A
4	C	5005	ATP	PB-O3A-PA-O2A
4	D	5005	ATP	PB-O3A-PA-O2A
4	A	5005	ATP	PB-O3A-PA-O1A
4	B	5005	ATP	PB-O3A-PA-O1A
4	C	5005	ATP	PB-O3A-PA-O1A
4	D	5005	ATP	PB-O3A-PA-O1A
4	A	5002	ATP	PB-O3B-PG-O1G
4	B	5002	ATP	PB-O3B-PG-O1G
4	C	5002	ATP	PB-O3B-PG-O1G
4	D	5002	ATP	PB-O3B-PG-O1G
4	A	5002	ATP	PB-O3B-PG-O3G
4	B	5002	ATP	PB-O3B-PG-O3G
4	C	5002	ATP	PB-O3B-PG-O3G
4	D	5002	ATP	PB-O3B-PG-O3G
4	A	5002	ATP	PA-O3A-PB-O1B
4	B	5002	ATP	PA-O3A-PB-O1B
4	C	5002	ATP	PA-O3A-PB-O1B
4	D	5002	ATP	PA-O3A-PB-O1B

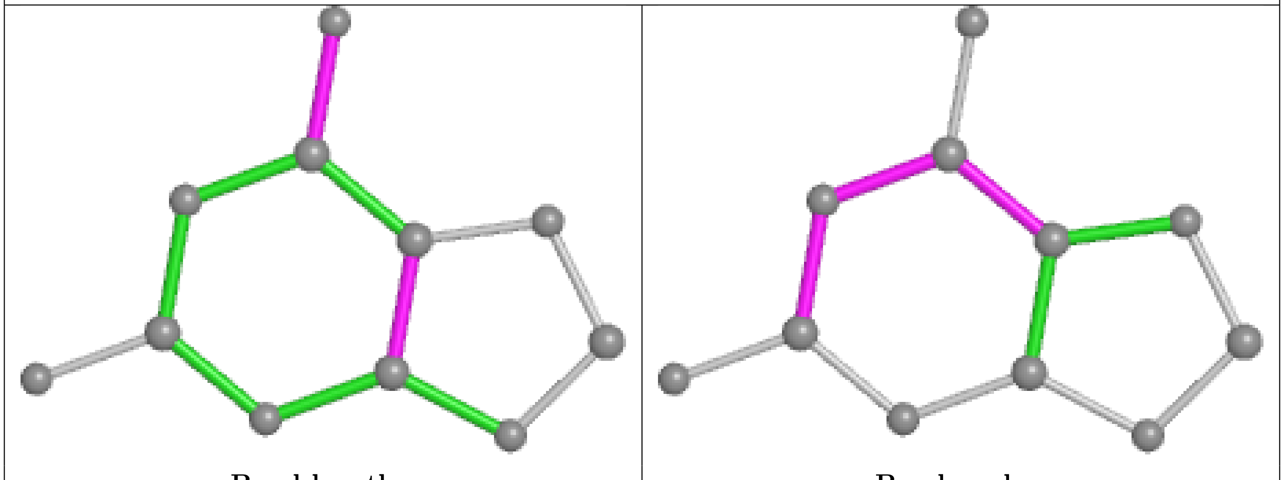
There are no ring outliers.

4 monomers are involved in 8 short contacts:

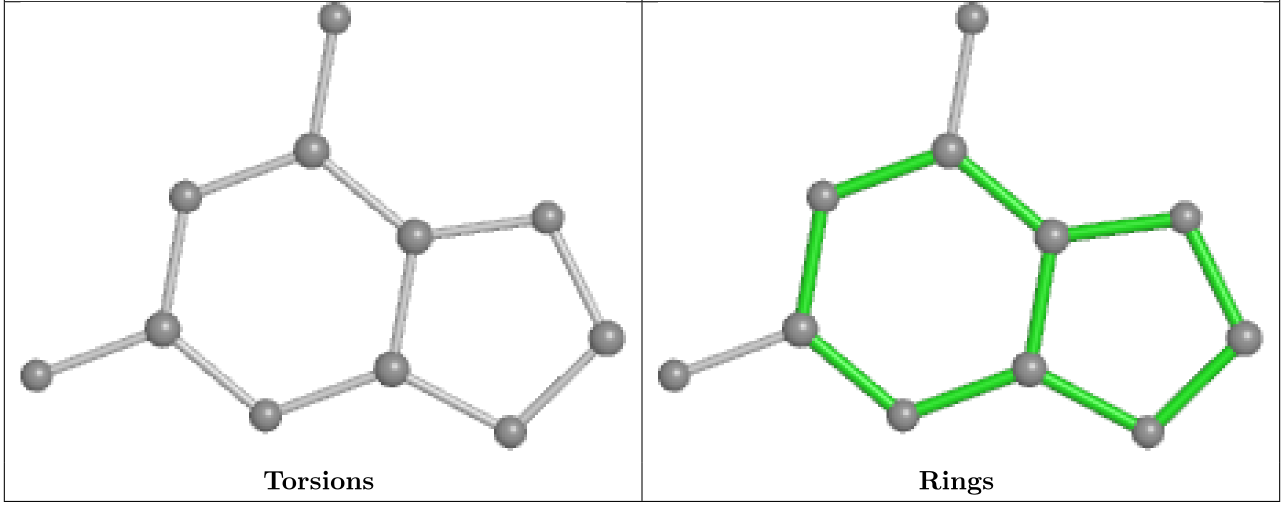
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	5005	ATP	2	0
4	D	5005	ATP	2	0
4	B	5005	ATP	2	0
4	A	5005	ATP	2	0

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

Ligand XAN C 5004

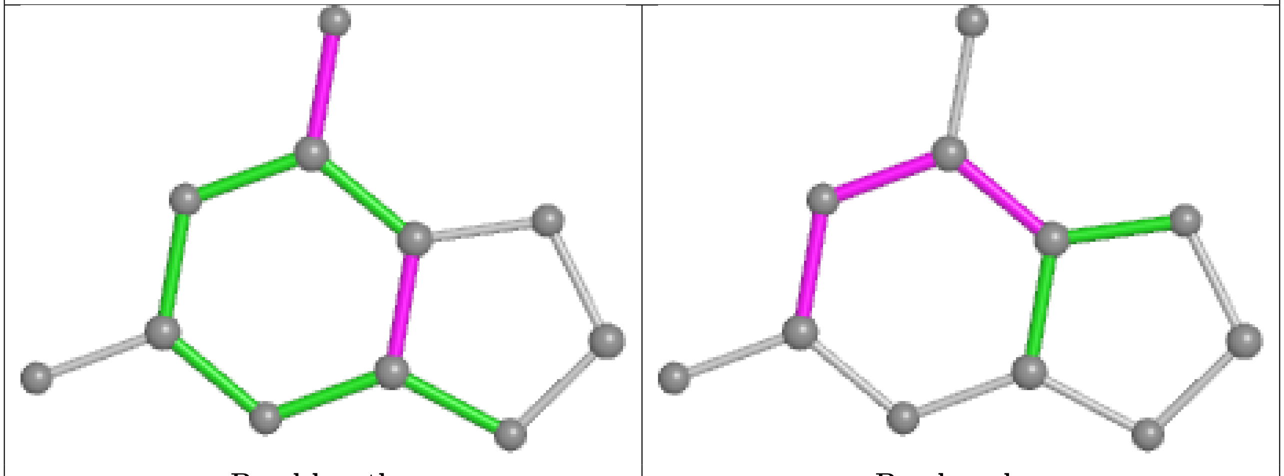


Bond lengths **Bond angles**



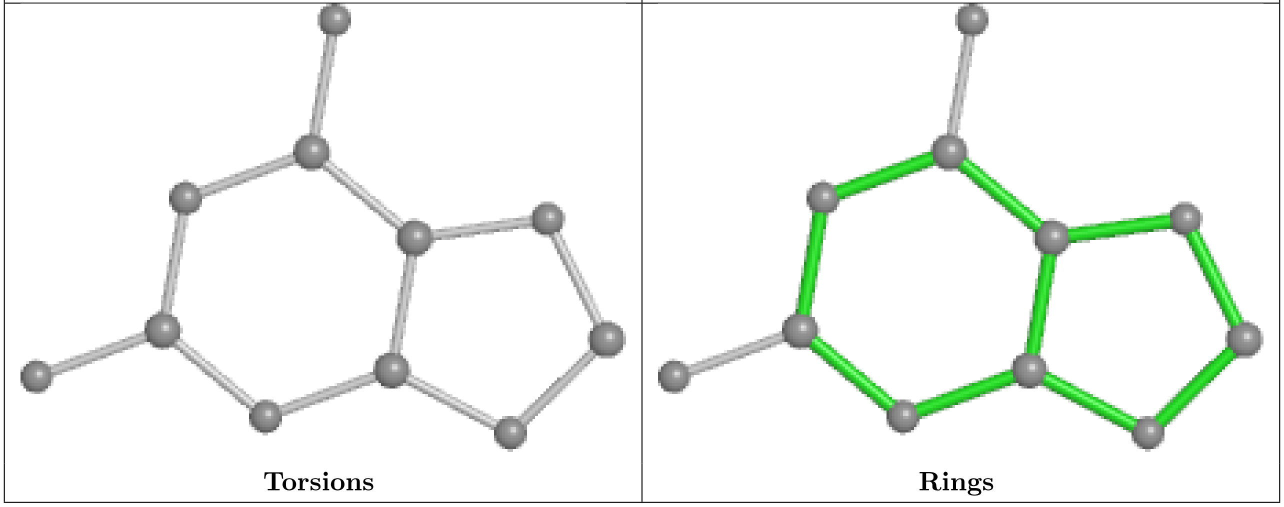
Torsions **Rings**

Ligand XAN B 5004



Bond lengths

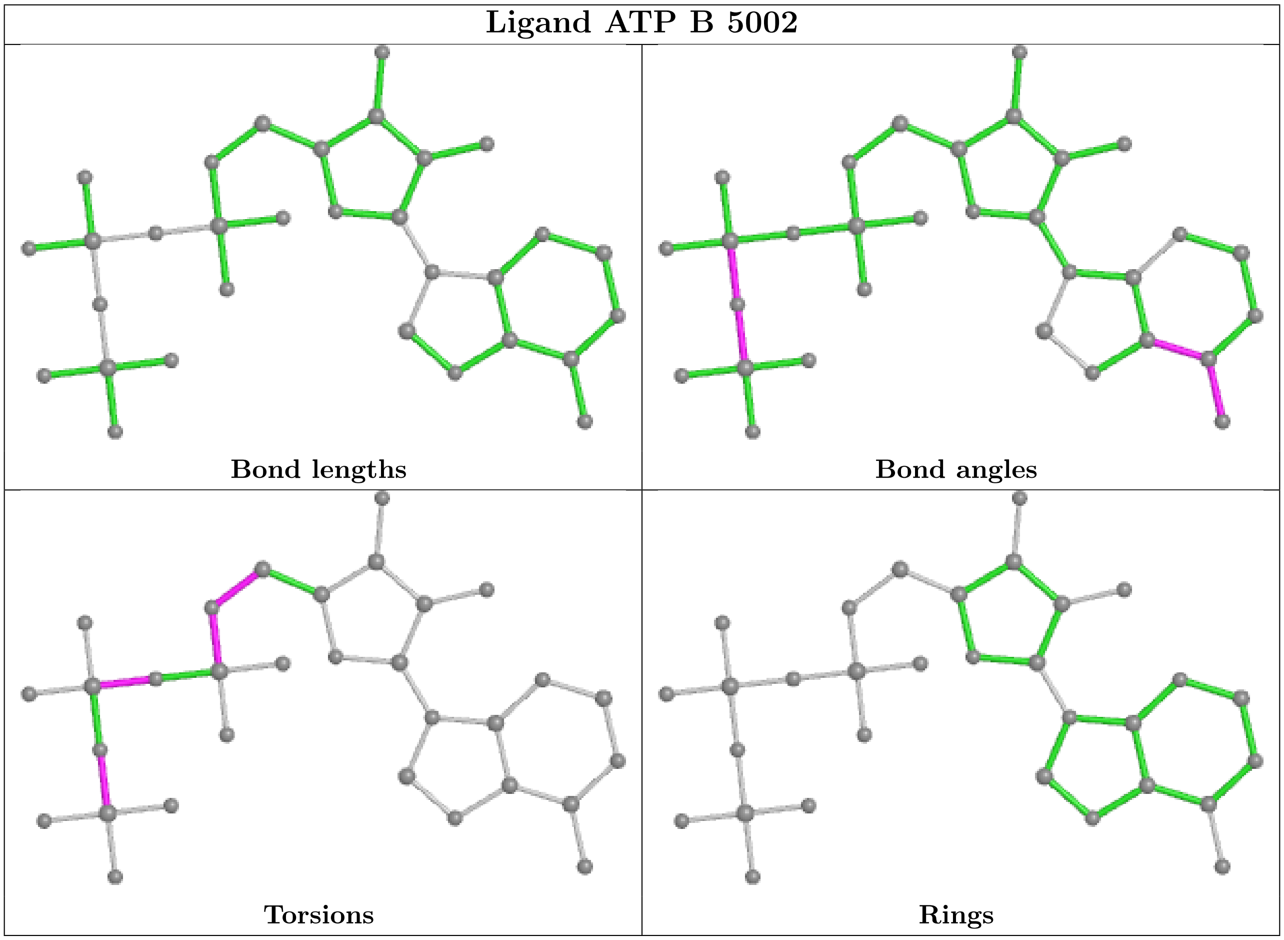
Bond angles



Torsions

Rings

Ligand ATP B 5002



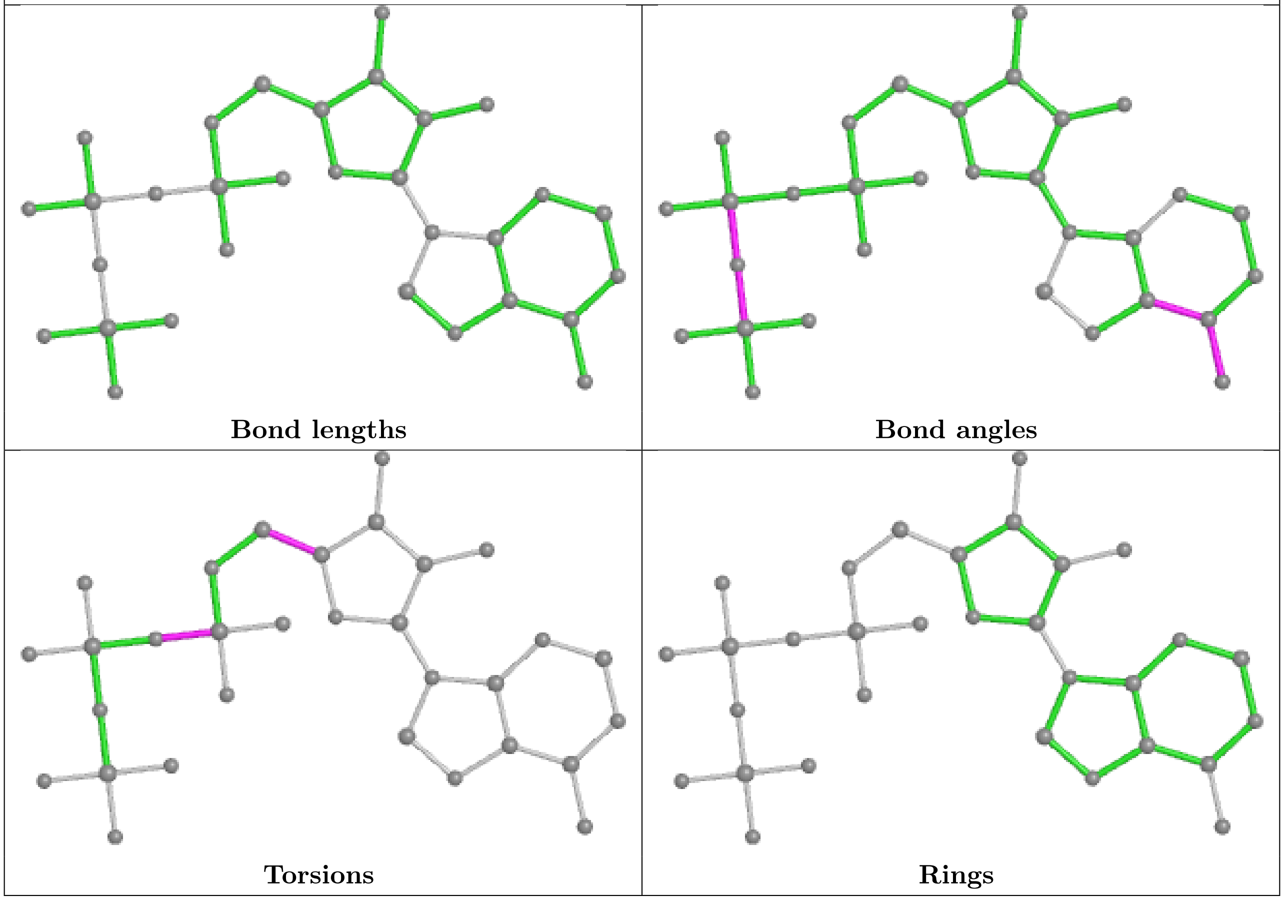
Bond lengths

Bond angles

Torsions

Rings

Ligand ATP C 5005

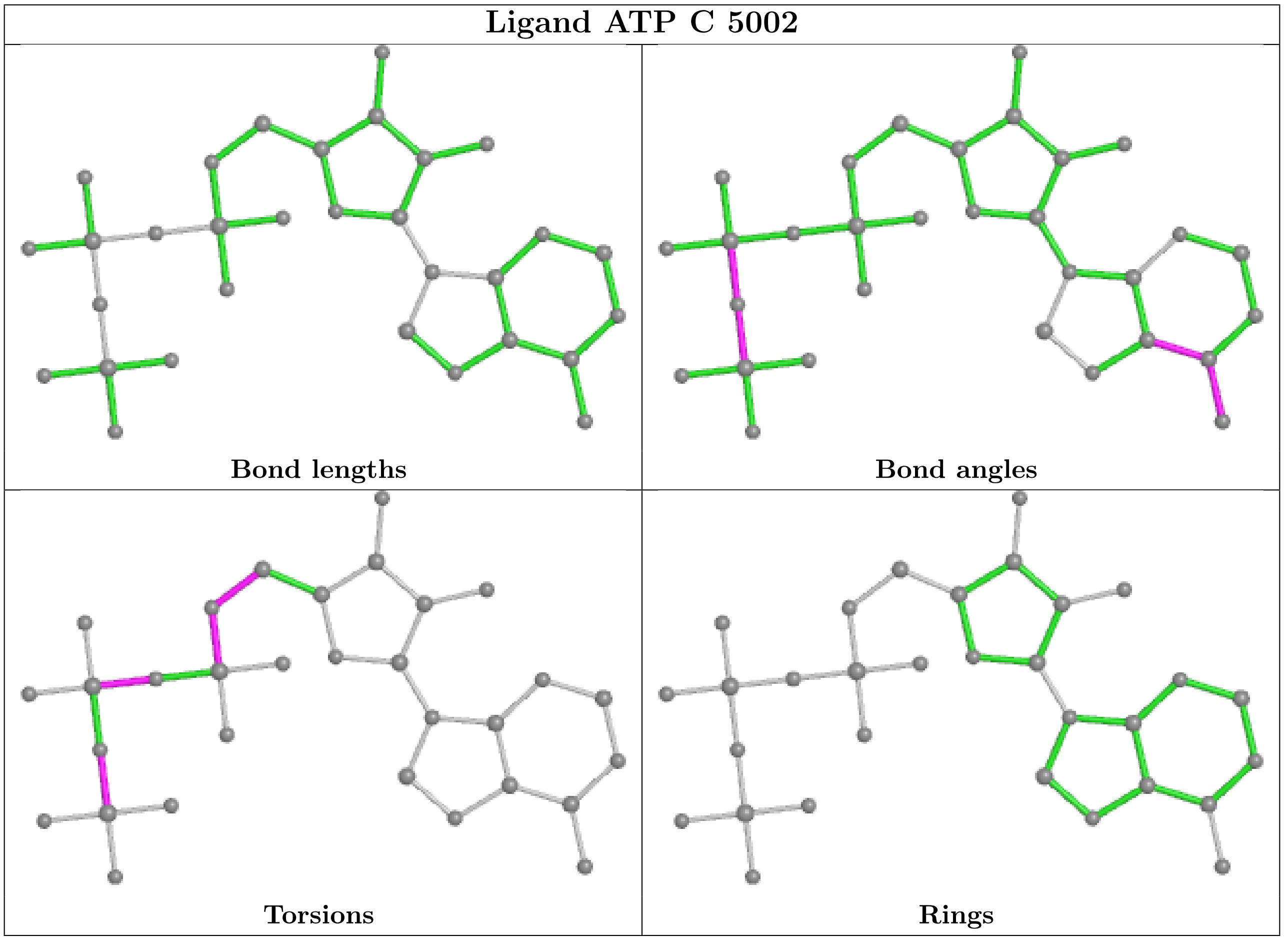


Bond lengths

Bond angles

Torsions

Rings



Ligand ATP C 5002

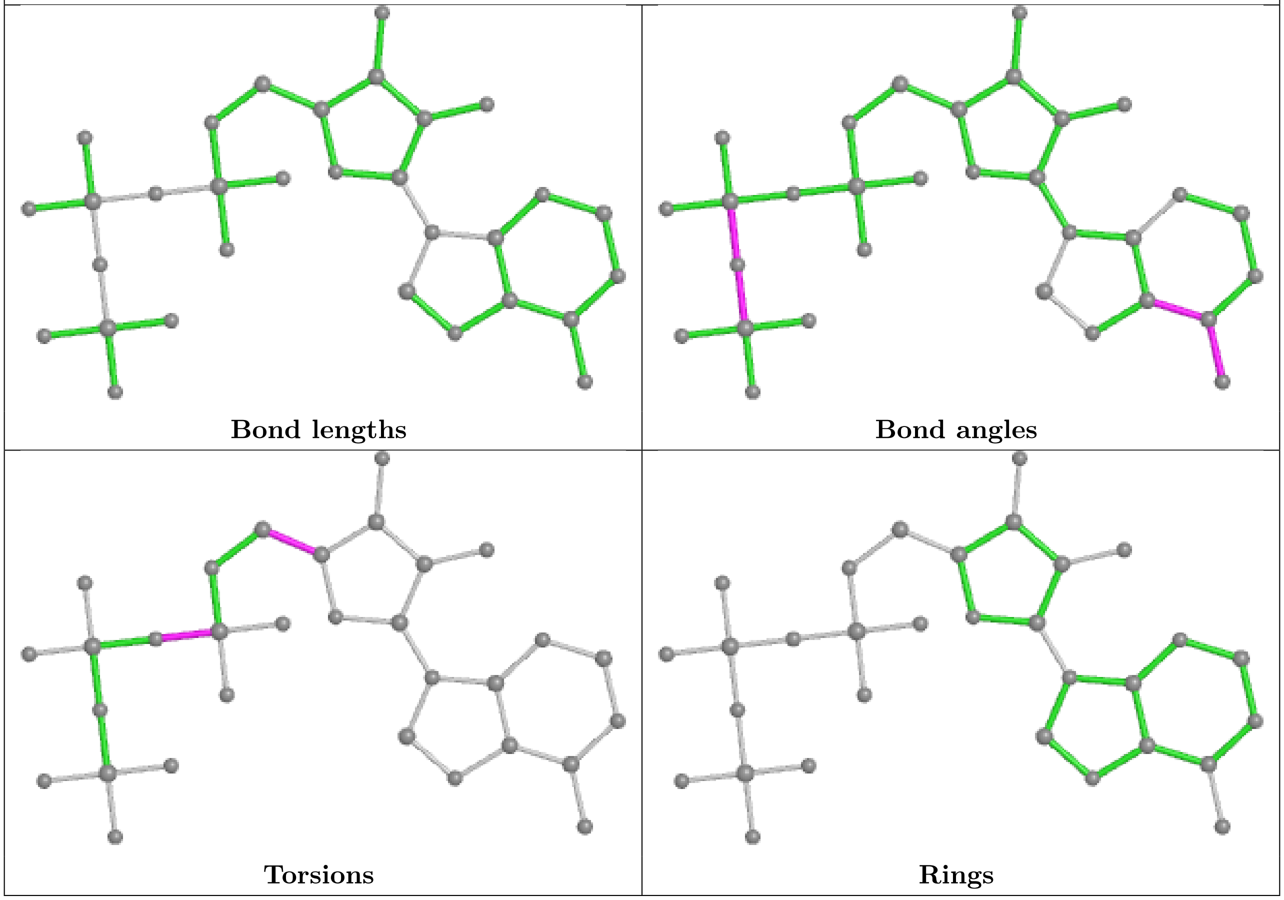
Bond lengths

Bond angles

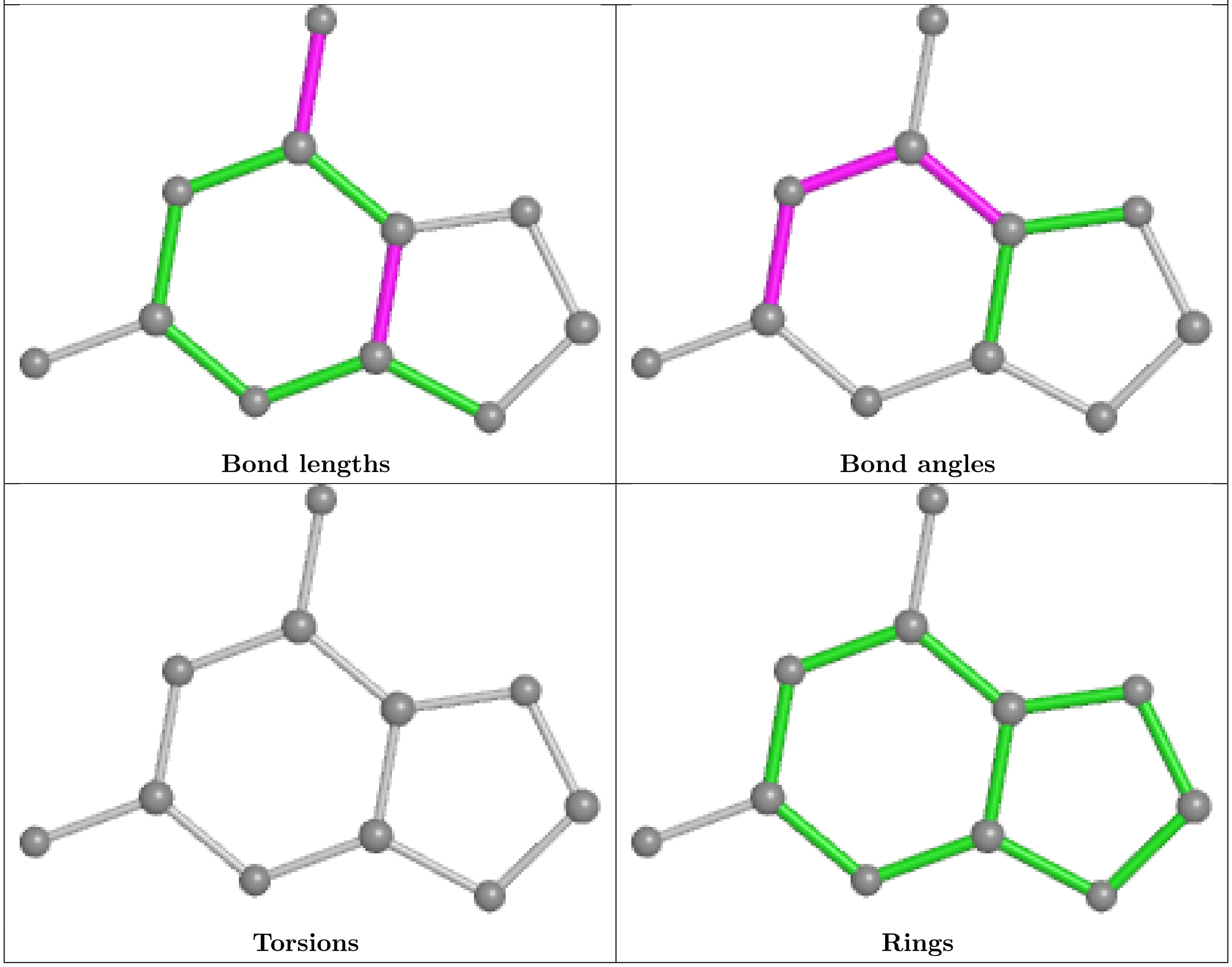
Torsions

Rings

Ligand ATP D 5005



Ligand XAN D 5004



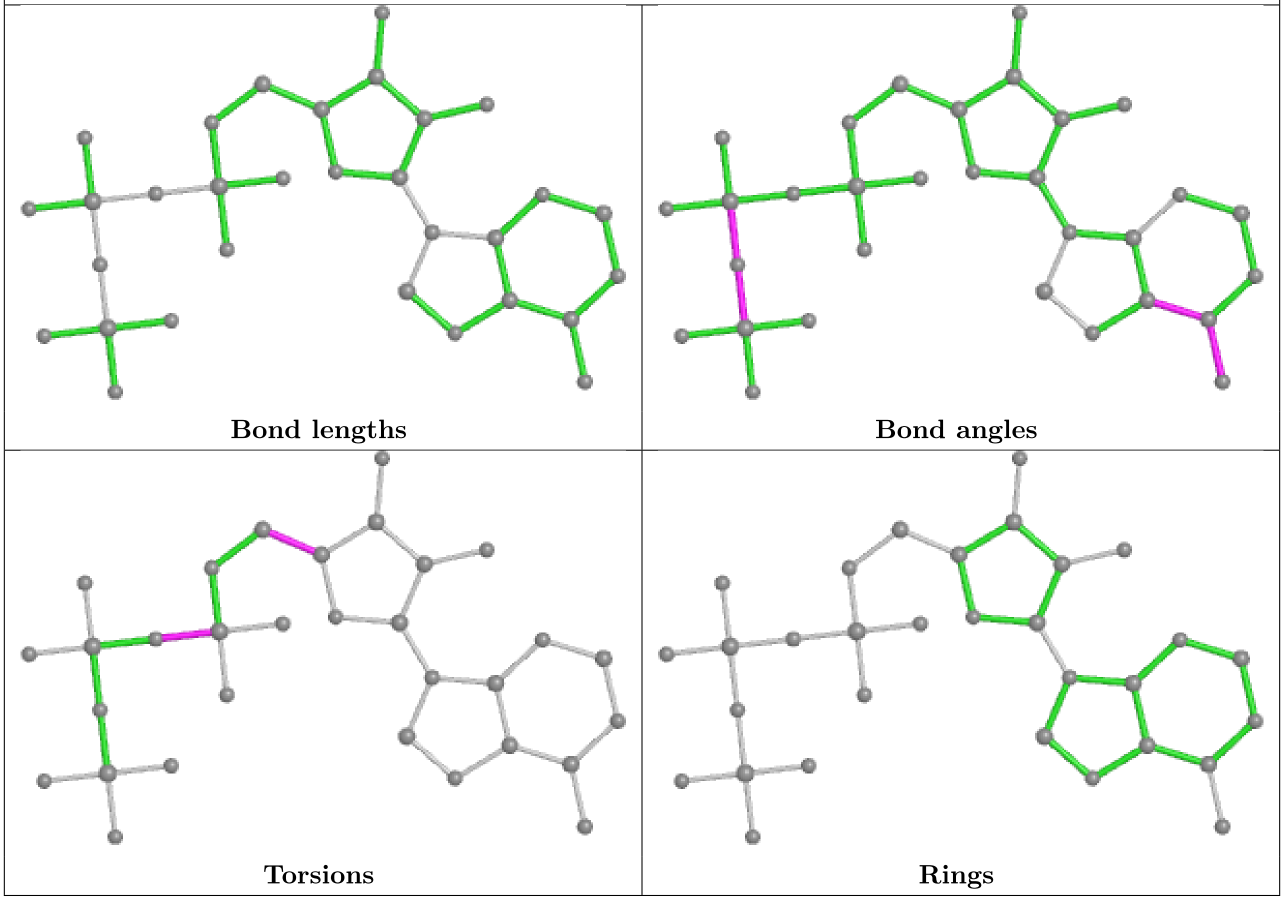
Bond lengths

Bond angles

Torsions

Rings

Ligand ATP B 5005



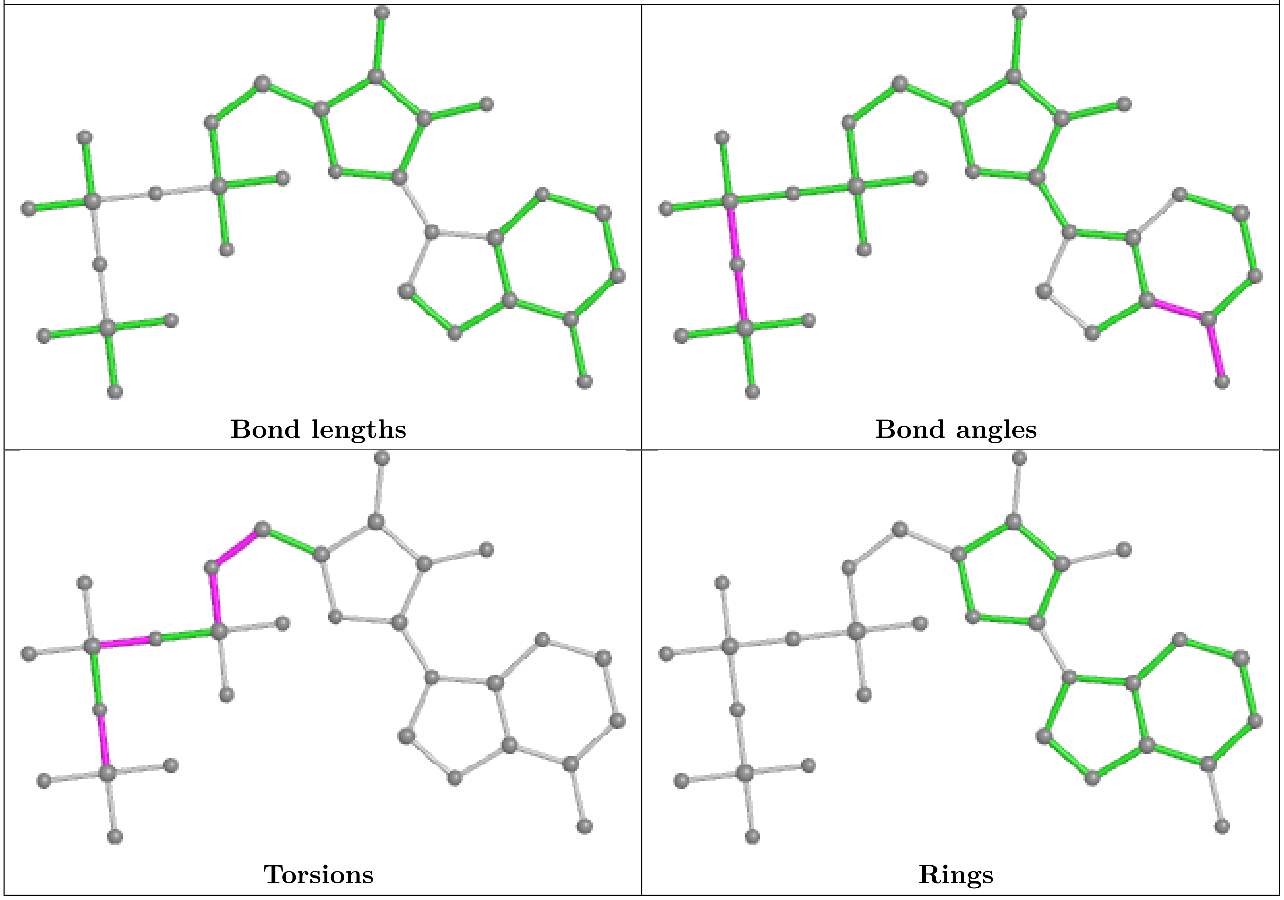
Bond lengths

Bond angles

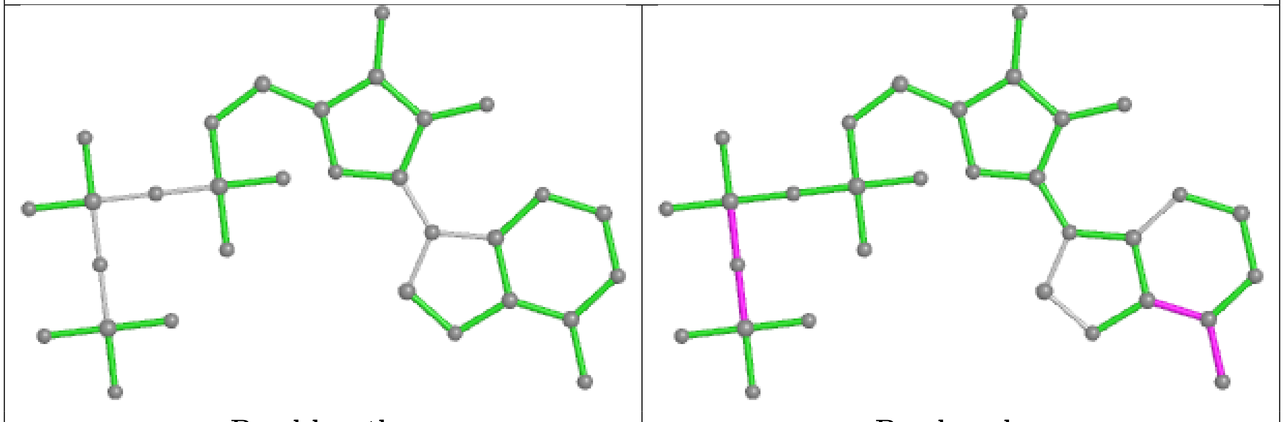
Torsions

Rings

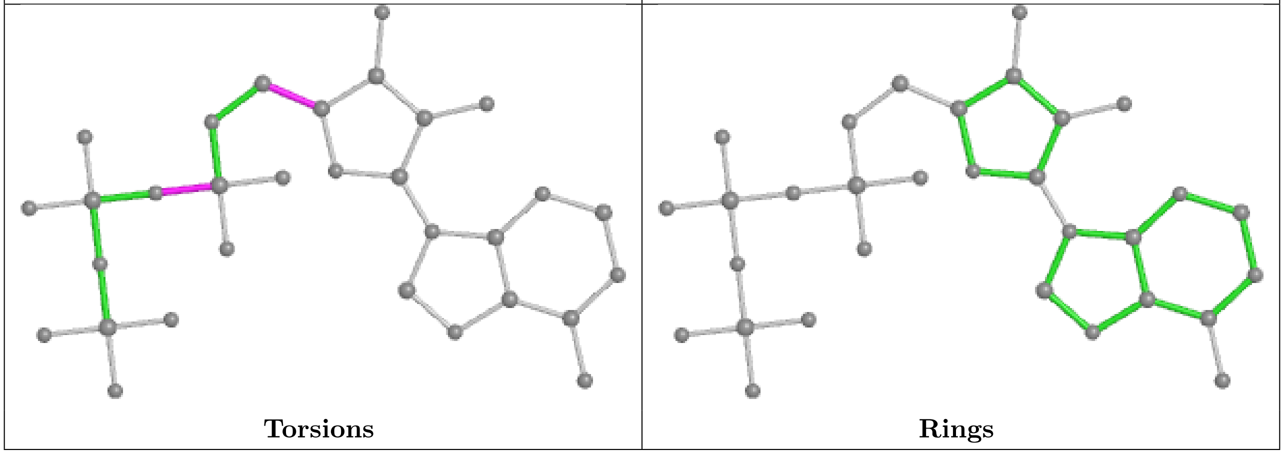
Ligand ATP D 5002



Ligand ATP A 5005

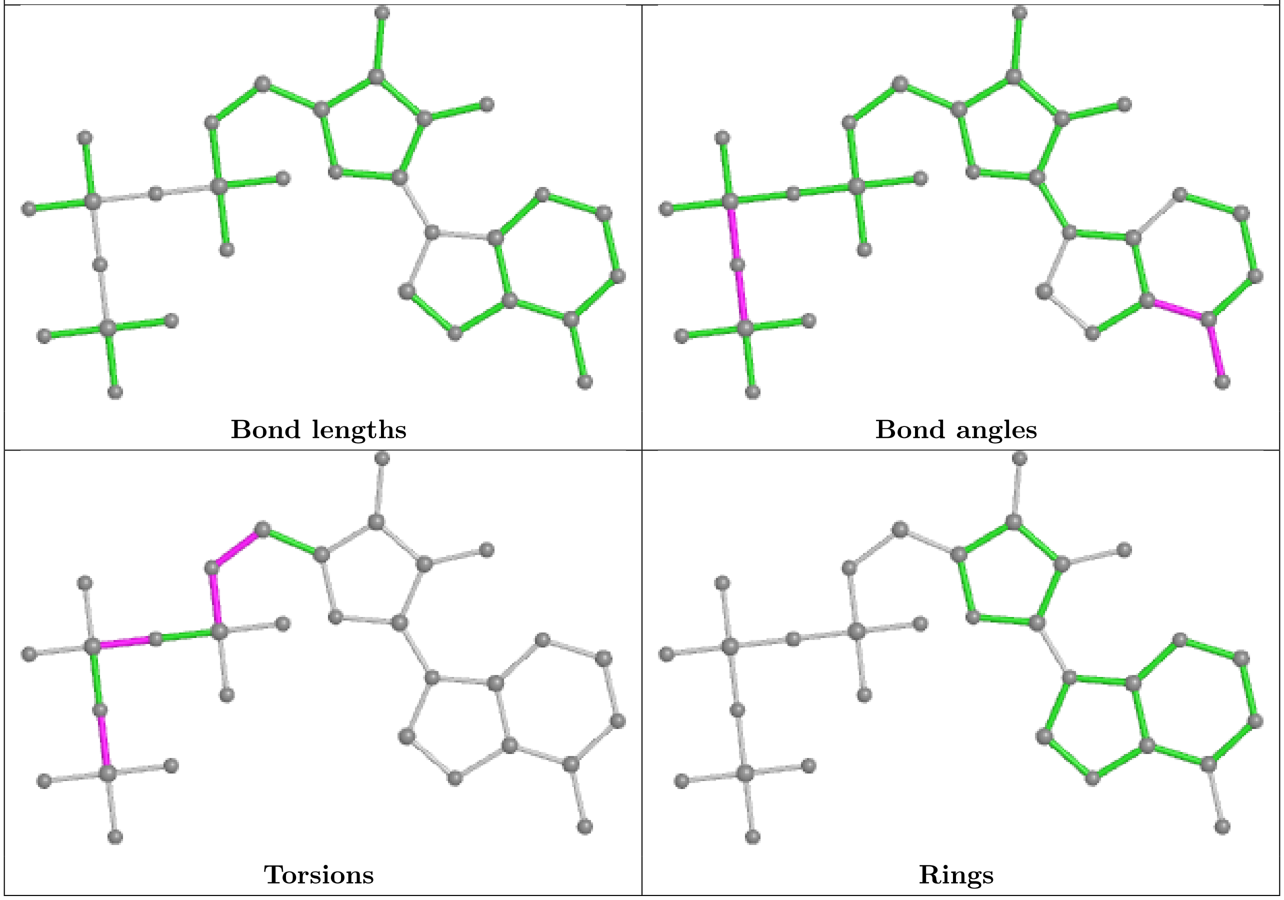


Bond lengths **Bond angles**



Torsions **Rings**

Ligand ATP A 5002

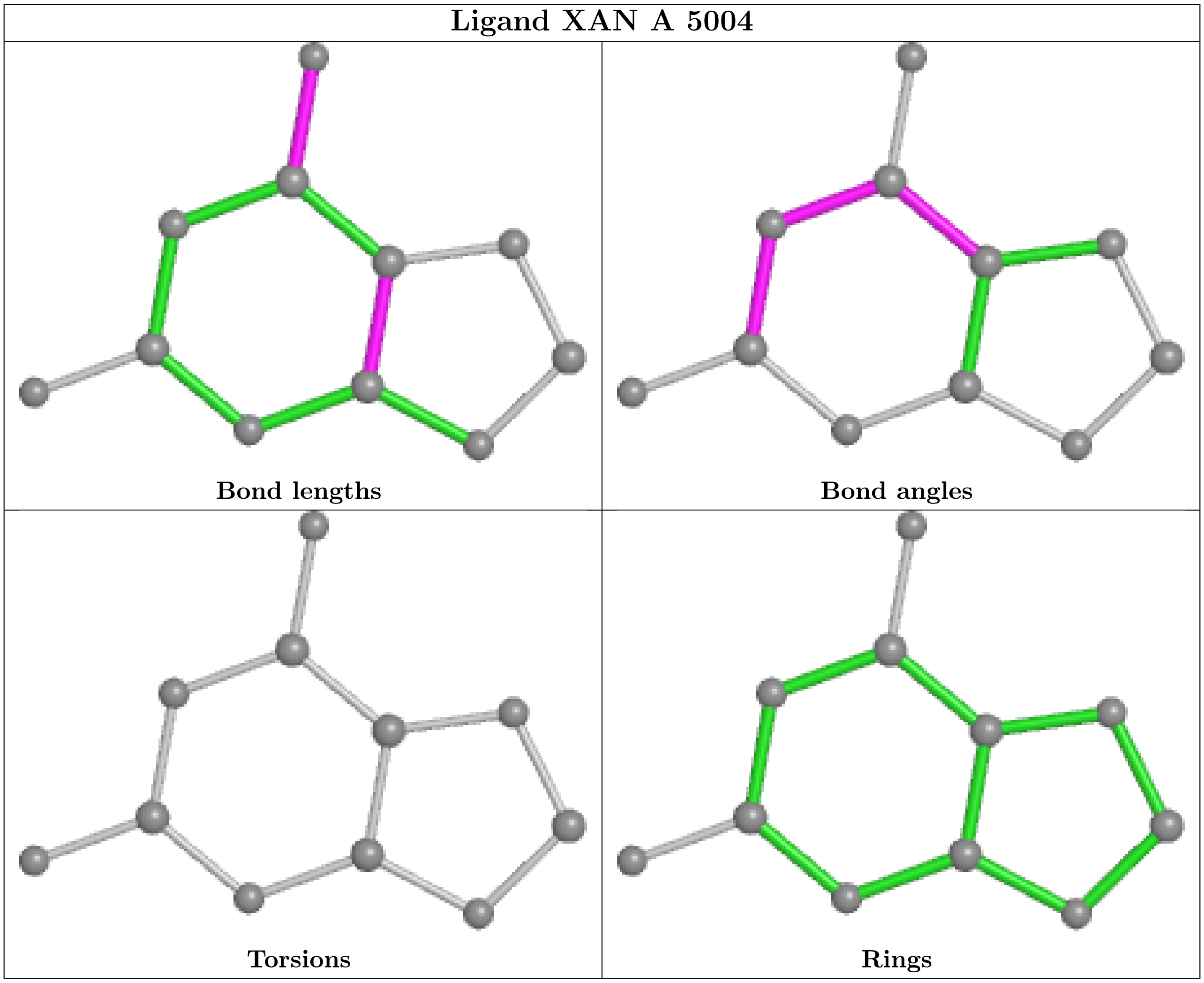


Bond lengths

Bond angles

Torsions

Rings



Ligand XAN A 5004

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

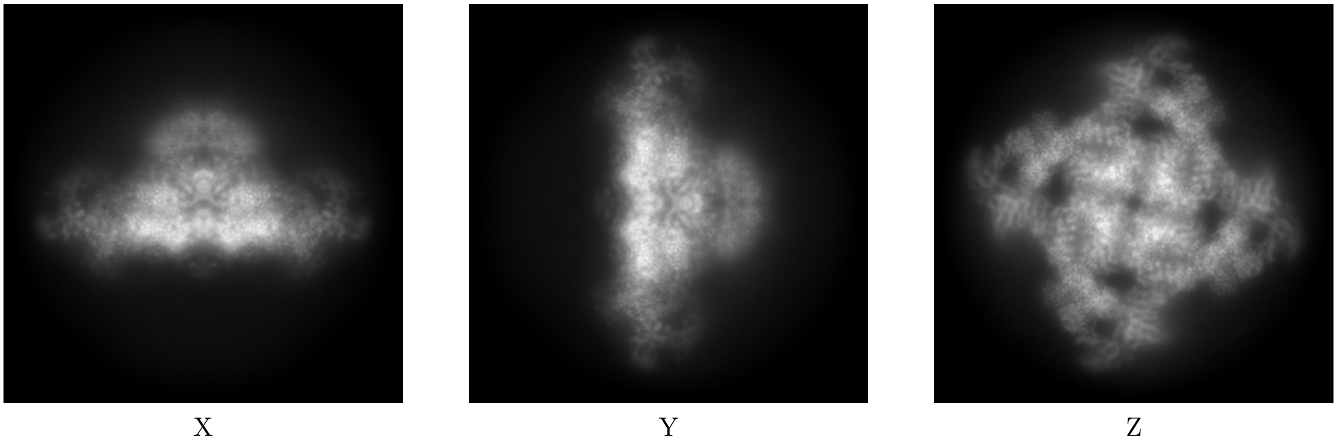
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-26416. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections

6.1.1 Primary map

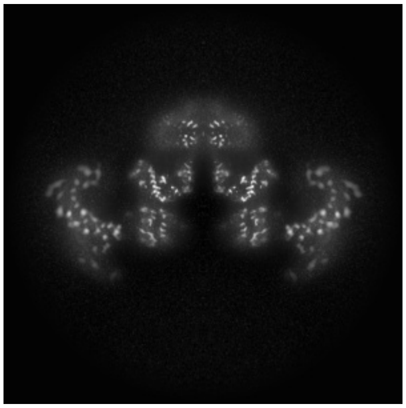


X Y Z

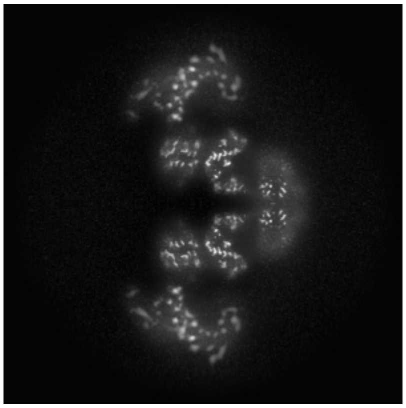
The images above show the map projected in three orthogonal directions.

6.2 Central slices

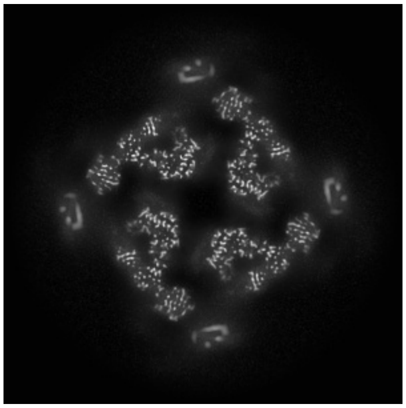
6.2.1 Primary map



X Index: 256



Y Index: 256

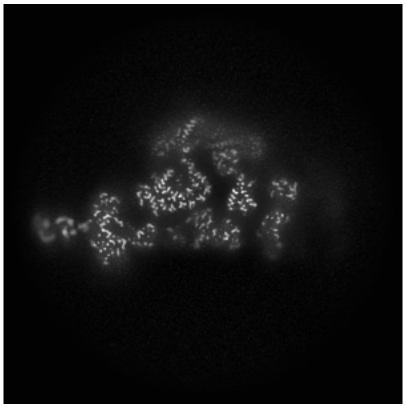


Z Index: 256

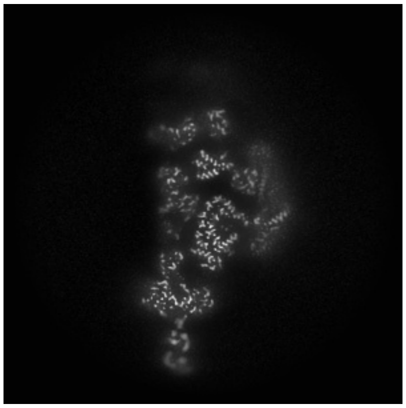
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices

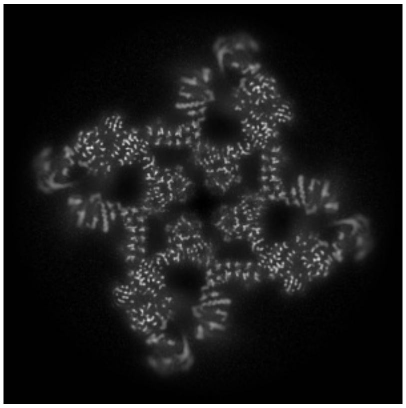
6.3.1 Primary map



X Index: 206



Y Index: 306



Z Index: 227

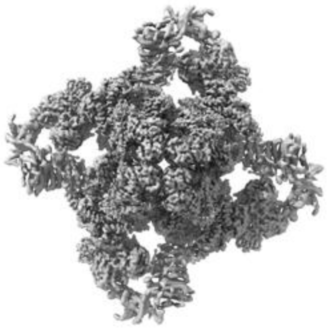
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views

6.4.1 Primary map

X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.13. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

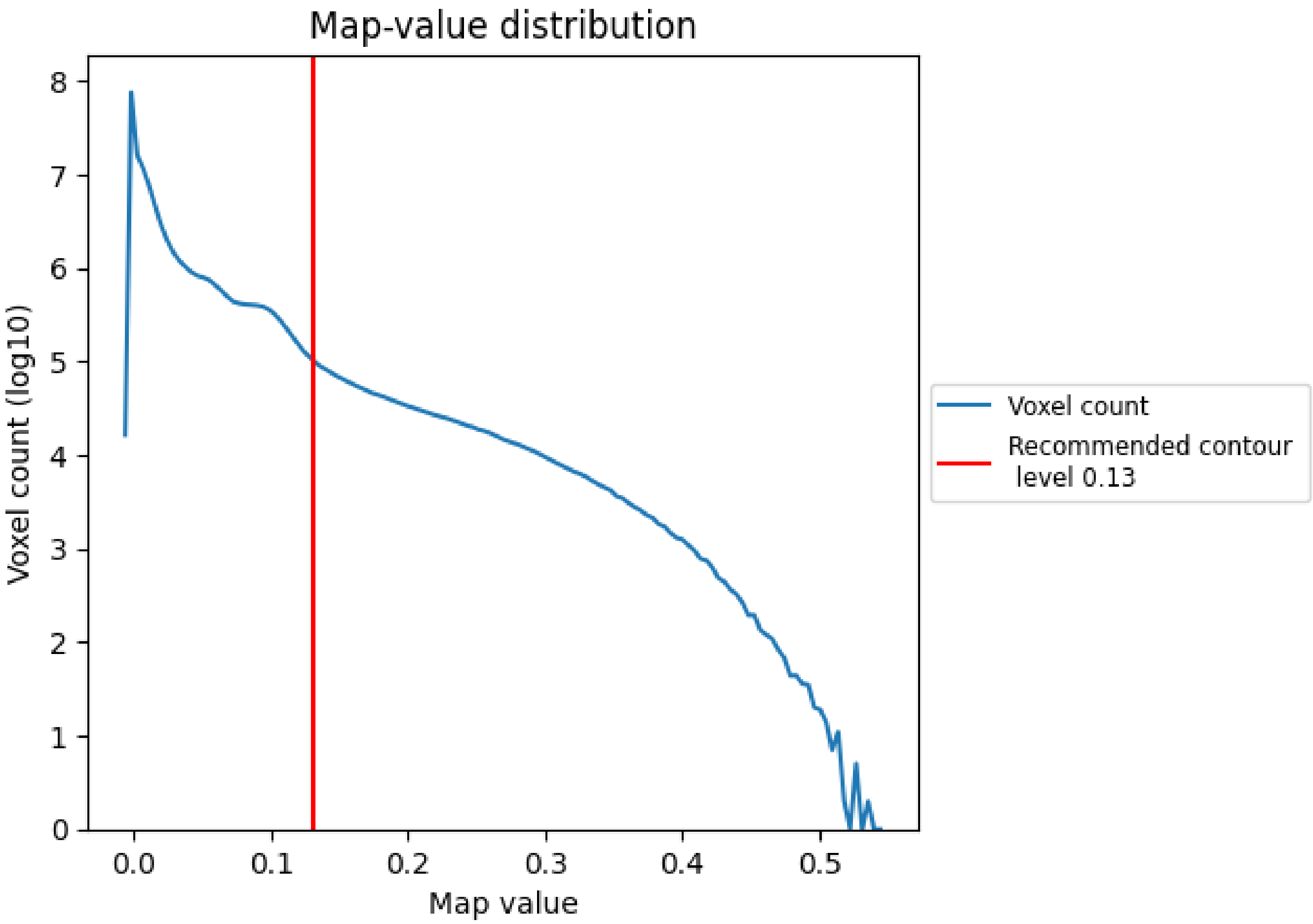
6.5 Mask visualisation ⓘ

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

7 Map analysis ⓘ

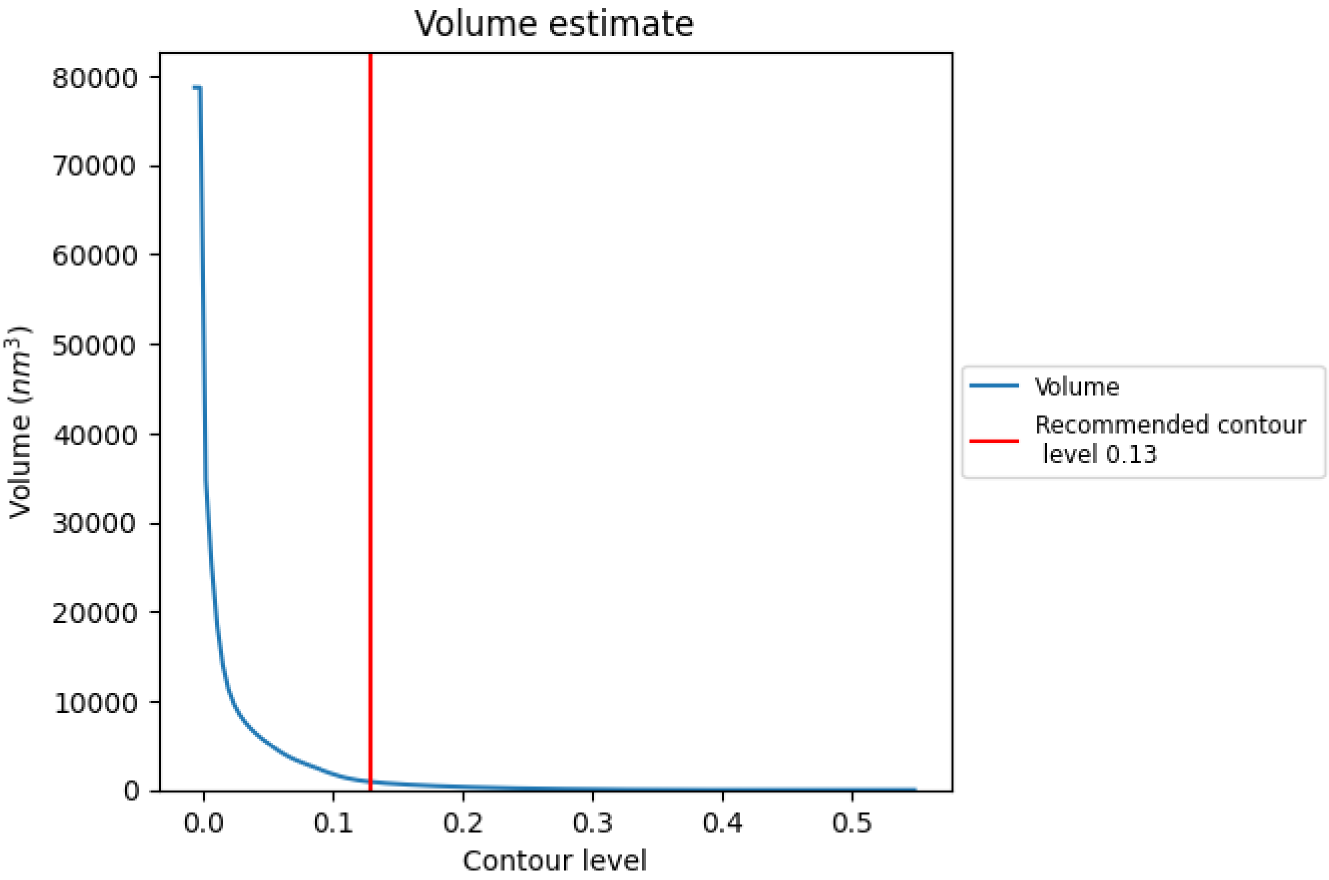
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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

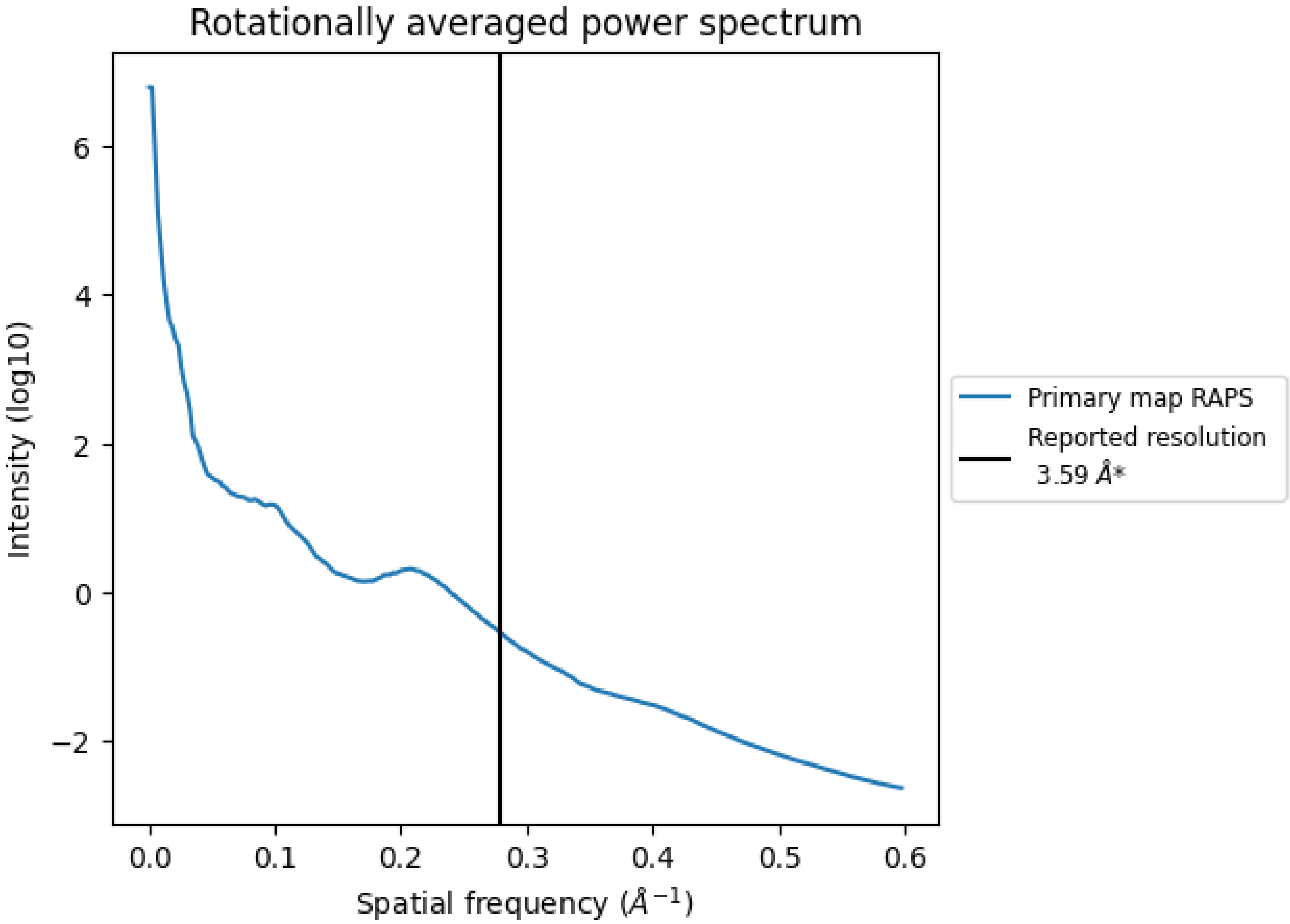
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 901 nm^3; this corresponds to an approximate mass of 814 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.279 $Å^{-1}$

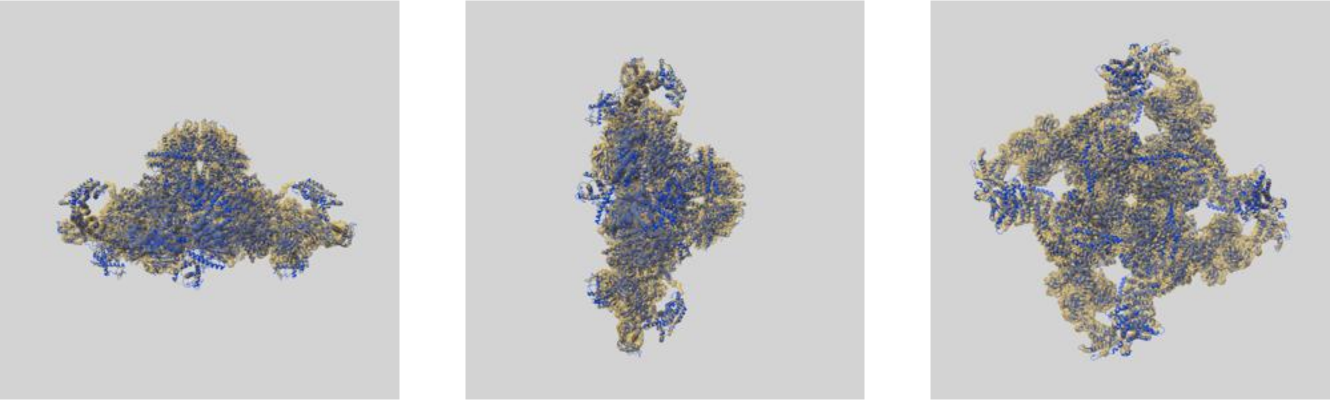
8 Fourier-Shell correlation (i)

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

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-26416 and PDB model 7UA9. Per-residue inclusion information can be found in section 3 on page 6.

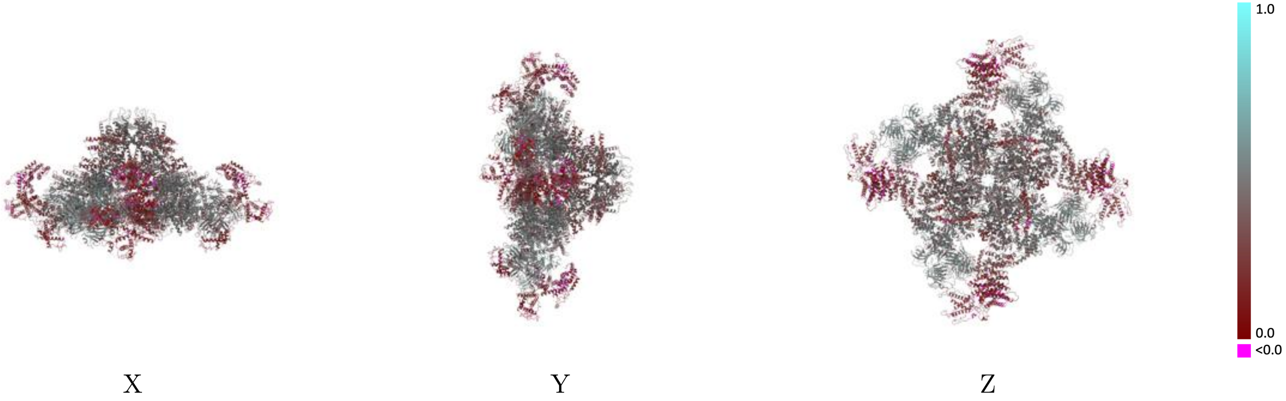
9.1 Map-model overlay



X Y Z

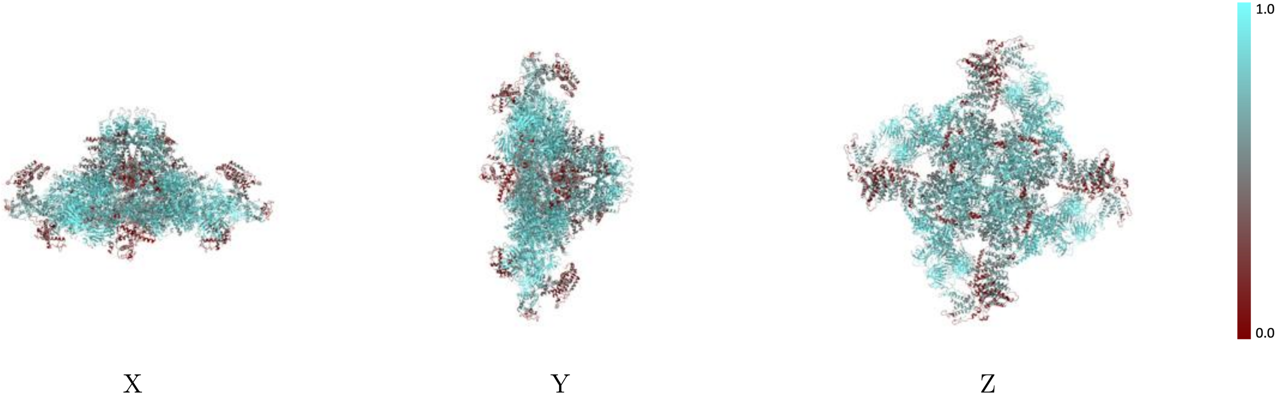
The images above show the 3D surface view of the map at the recommended contour level 0.13 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ



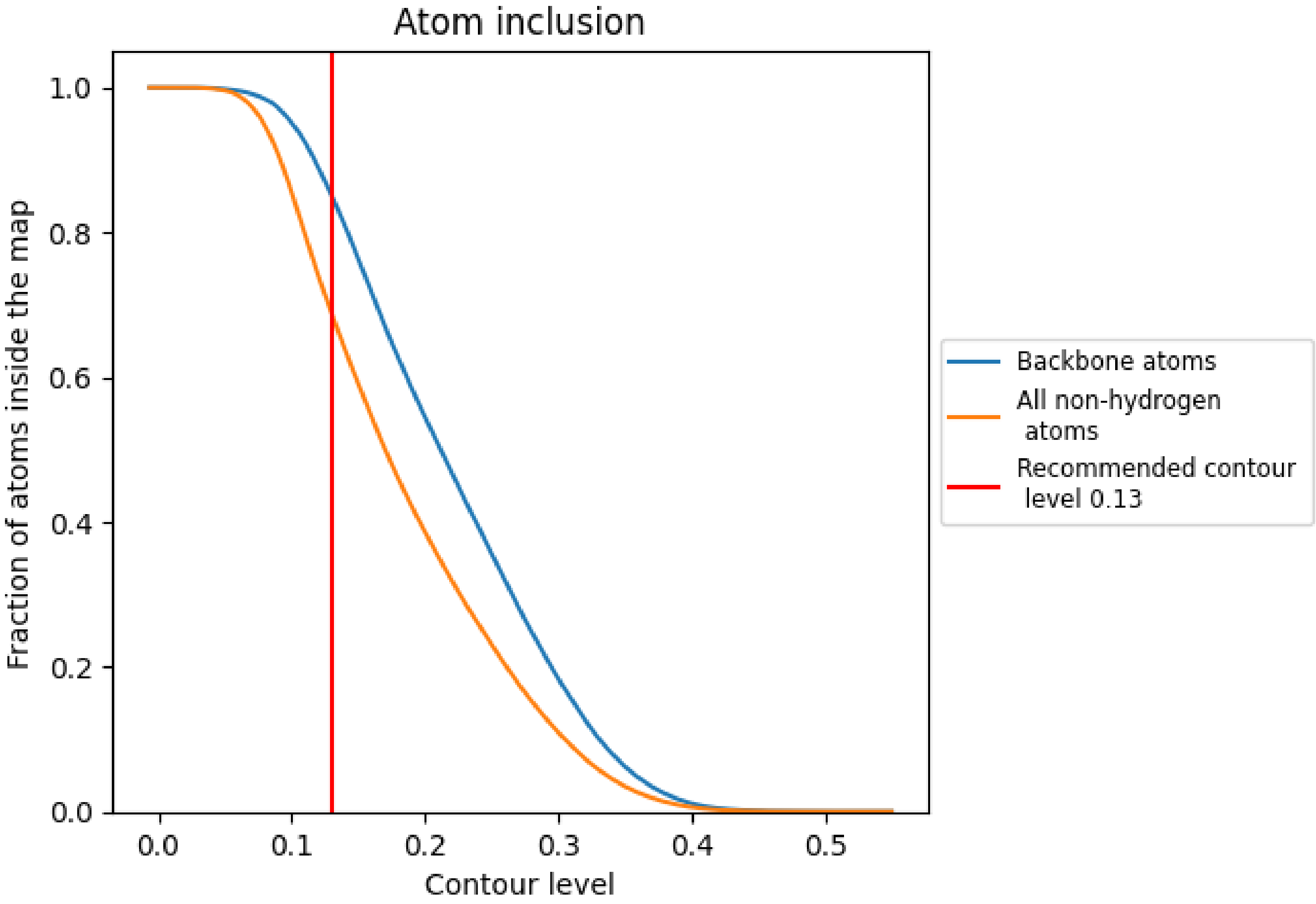
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model ⓘ



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.13).

9.4 Atom inclusion ⓘ



At the recommended contour level, 85% of all backbone atoms, 69% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	▬ 0.6866	▬ 0.3670
A	▬ 0.6900	▬ 0.3740
B	▬ 0.6769	▬ 0.3560
C	▬ 0.6862	▬ 0.3720
D	▬ 0.6771	▬ 0.3530
E	▬ 0.8610	▬ 0.5070
F	▬ 0.8623	▬ 0.4990
G	▬ 0.8474	▬ 0.5000
H	▬ 0.8511	▬ 0.5010