Full wwPDB EM Validation Report ⓘ

Mar 3, 2024 – 08:02 AM EST

PDB ID	:	6BQ1
EMDB ID	:	EMD-7129
Title	:	Human PI4KIIIa lipid kinase complex
Authors	:	Lees, J.A.; Zhang, Y.; Oh, M.; Schauder, C.M.; Yu, X.; Baskin, J.; Dobbs, K.; Notarangelo, L.D.; Camilli, P.D.; Walz, T.; Reinisch, K.M.
Deposited on	:	2017-11-27
Resolution	:	3.60 Å(reported)

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

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

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

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

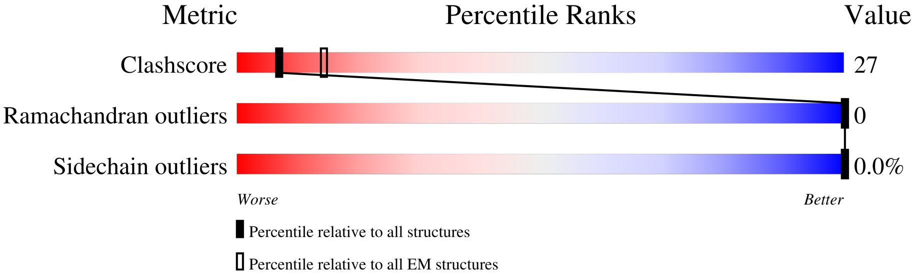
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance

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

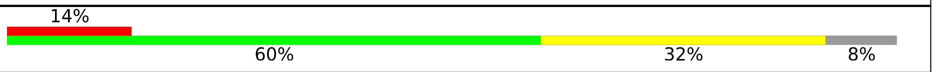
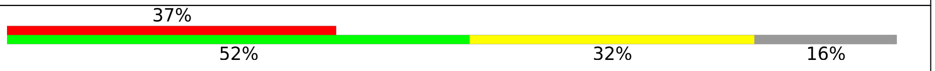
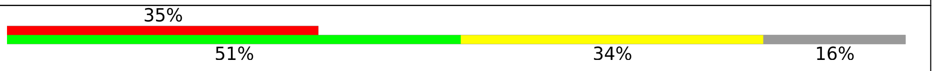
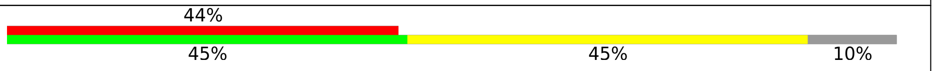
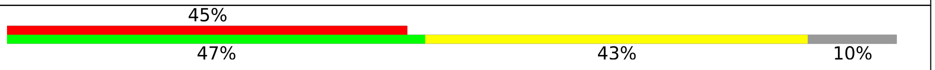
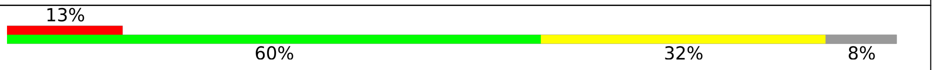
The reported resolution of this entry is 3.60 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	1647	
2	B	863	
2	F	863	
3	C	292	
3	G	292	
4	E	1648	

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 37217 atoms, of which 54 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 Phosphatidylinositol 4-kinase III alpha (PI4KA).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1509	10673	6767	1872	1972	62	0	0

- Molecule 2 is a protein called Tetratricopeptide repeat protein 7B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	728	5774	3670	1007	1065	32	0	0
2	F	728	5774	3670	1007	1065	32	0	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	expression tag	UNP Q86TV6
B	-18	TYR	-	expression tag	UNP Q86TV6
B	-17	PRO	-	expression tag	UNP Q86TV6
B	-16	TYR	-	expression tag	UNP Q86TV6
B	-15	ASP	-	expression tag	UNP Q86TV6
B	-14	VAL	-	expression tag	UNP Q86TV6
B	-13	PRO	-	expression tag	UNP Q86TV6
B	-12	ASP	-	expression tag	UNP Q86TV6
B	-11	TYR	-	expression tag	UNP Q86TV6
B	-10	ALA	-	expression tag	UNP Q86TV6
B	-9	ALA	-	expression tag	UNP Q86TV6
B	-8	ILE	-	expression tag	UNP Q86TV6
B	-7	ALA	-	expression tag	UNP Q86TV6
B	-6	GLY	-	expression tag	UNP Q86TV6
B	-5	ALA	-	expression tag	UNP Q86TV6
B	-4	PRO	-	expression tag	UNP Q86TV6
B	-3	ASP	-	expression tag	UNP Q86TV6
B	-2	LEU	-	expression tag	UNP Q86TV6
B	-1	LYS	-	expression tag	UNP Q86TV6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	LEU	-	expression tag	UNP Q86TV6
F	-19	MET	-	expression tag	UNP Q86TV6
F	-18	TYR	-	expression tag	UNP Q86TV6
F	-17	PRO	-	expression tag	UNP Q86TV6
F	-16	TYR	-	expression tag	UNP Q86TV6
F	-15	ASP	-	expression tag	UNP Q86TV6
F	-14	VAL	-	expression tag	UNP Q86TV6
F	-13	PRO	-	expression tag	UNP Q86TV6
F	-12	ASP	-	expression tag	UNP Q86TV6
F	-11	TYR	-	expression tag	UNP Q86TV6
F	-10	ALA	-	expression tag	UNP Q86TV6
F	-9	ALA	-	expression tag	UNP Q86TV6
F	-8	ILE	-	expression tag	UNP Q86TV6
F	-7	ALA	-	expression tag	UNP Q86TV6
F	-6	GLY	-	expression tag	UNP Q86TV6
F	-5	ALA	-	expression tag	UNP Q86TV6
F	-4	PRO	-	expression tag	UNP Q86TV6
F	-3	ASP	-	expression tag	UNP Q86TV6
F	-2	LEU	-	expression tag	UNP Q86TV6
F	-1	LYS	-	expression tag	UNP Q86TV6
F	0	LEU	-	expression tag	UNP Q86TV6

- Molecule 3 is a protein called Protein FAM126A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	264	Total 2091	C 1357	N 338	O 383	S 13	0	0
3	G	264	Total 2091	C 1357	N 338	O 383	S 13	0	0

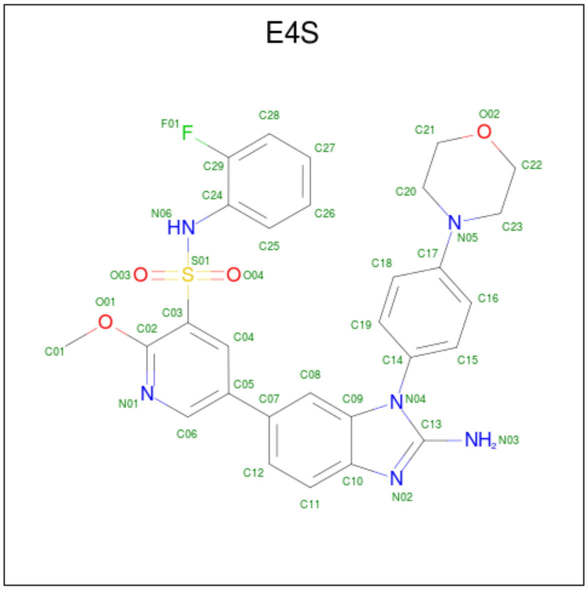
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP Q9BYI3
C	-1	PRO	-	expression tag	UNP Q9BYI3
C	0	GLY	-	expression tag	UNP Q9BYI3
C	1	SER	-	expression tag	UNP Q9BYI3
G	-2	GLY	-	expression tag	UNP Q9BYI3
G	-1	PRO	-	expression tag	UNP Q9BYI3
G	0	GLY	-	expression tag	UNP Q9BYI3
G	1	SER	-	expression tag	UNP Q9BYI3

- Molecule 4 is a protein called Phosphatidylinositol 4-kinase III alpha (PI4KA).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	1510	10678	6770	1873	1973	62	0	0

- Molecule 5 is 5-{2-amino-1-[4-(morpholin-4-yl)phenyl]-1H-benzimidazol-6-yl}-N-(2-fluorophenyl)-2-methoxypyridine-3-sulfonamide (three-letter code: E4S) (formula: $C_{29}H_{27}FN_6O_4S$).


E4S
F01 F
C28
C27
C29
C24
C26
N06
HN
C25
S01
O03 O
S
O O04
O01
O
C03
C01
C02
C04
N
N01
C06
C05
C07
C08
C09
C12
C11
C10
N
N02
N
N04
C13
NH2 N03
C14
C15
C19
C16
C18
C17
N
N05
C20
C23
C21
O
O02
C22

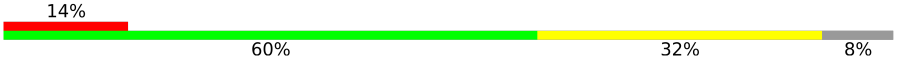
Mol	Chain	Residues	Atoms							AltConf
			Total	C	F	H	N	O	S	
5	A	1	68	29	1	27	6	4	1	0
5	E	1	68	29	1	27	6	4	1	0

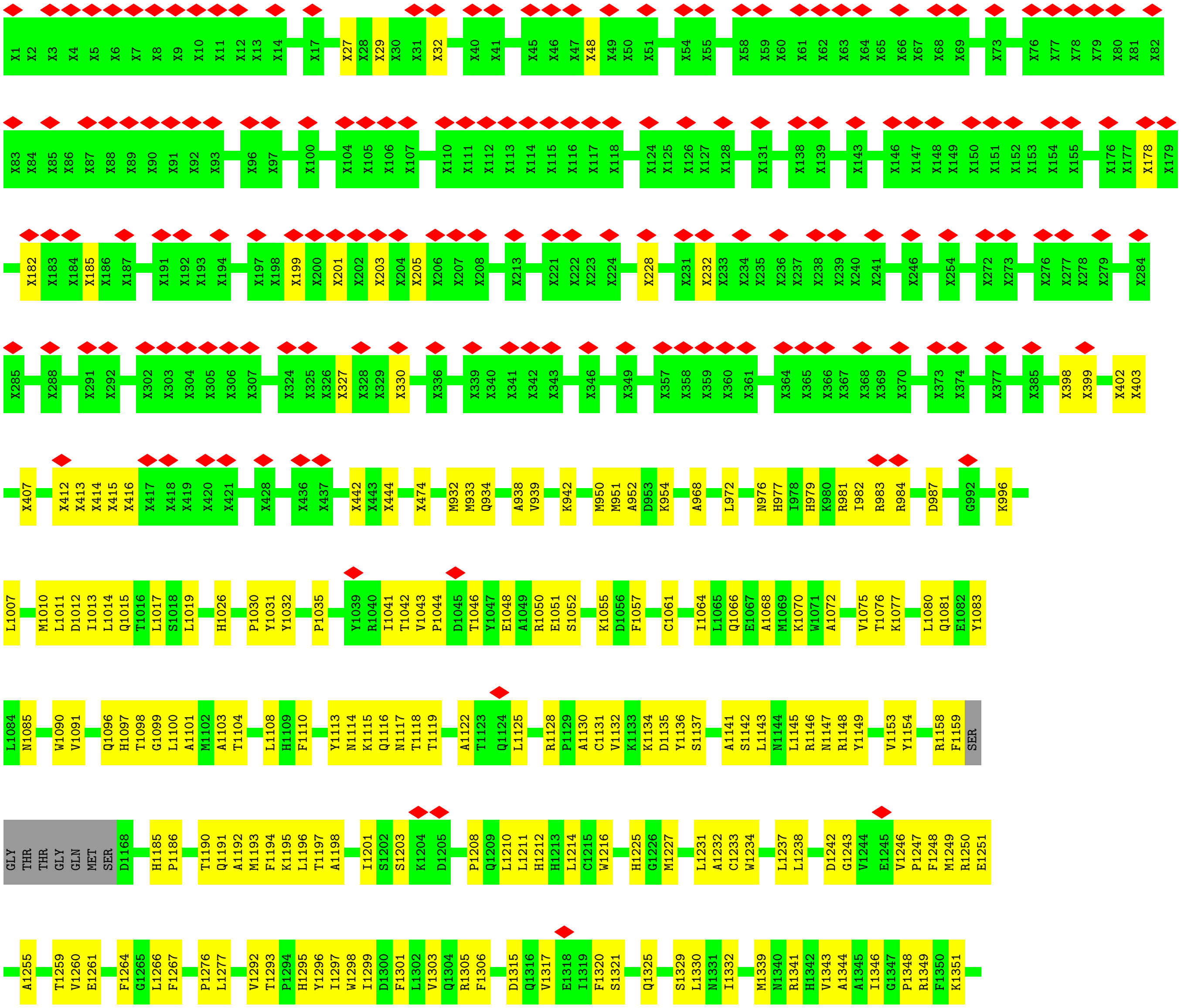
3 Residue-property plots

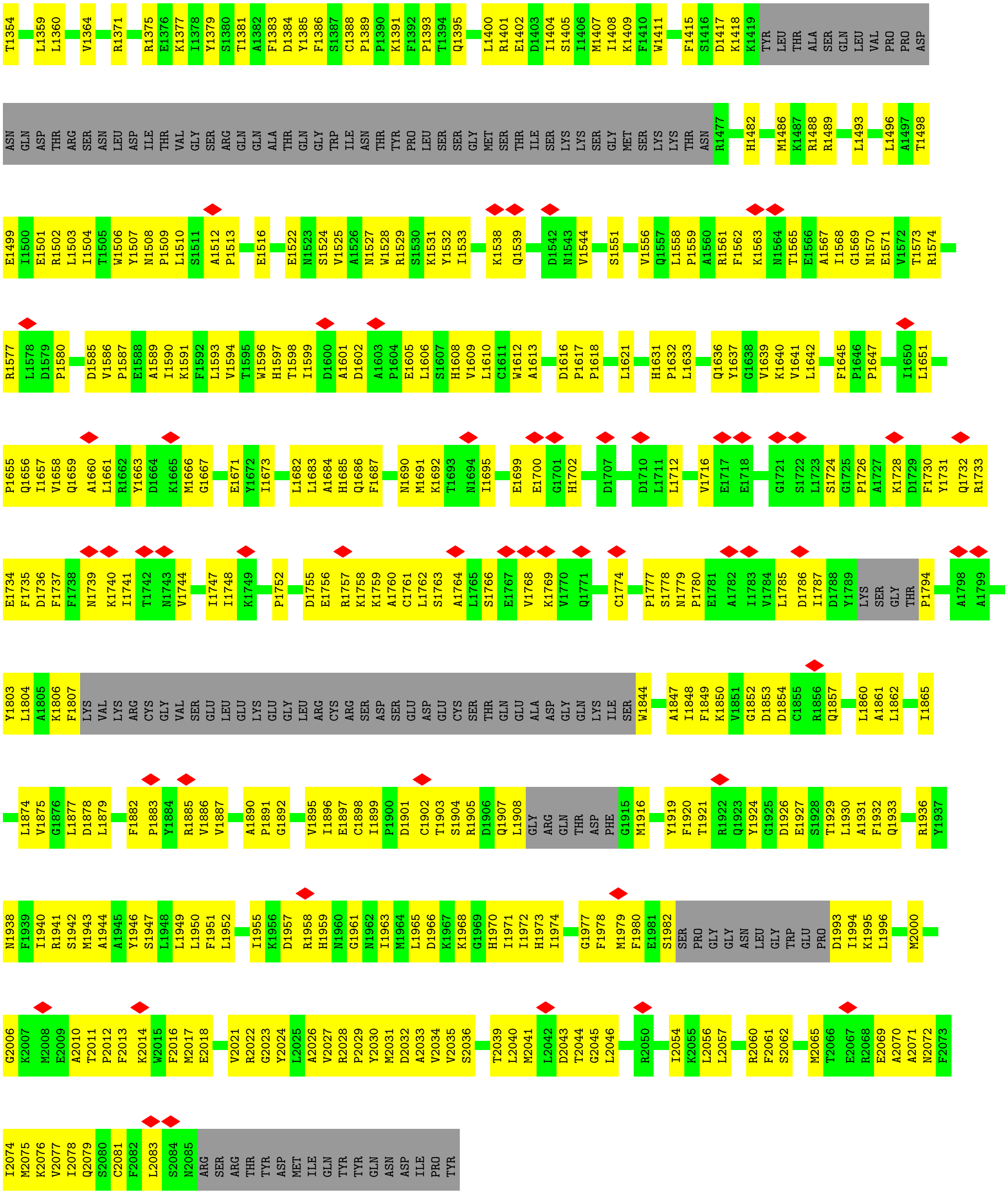
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Phosphatidylinositol 4-kinase III alpha (PI4KA)

Chain A:

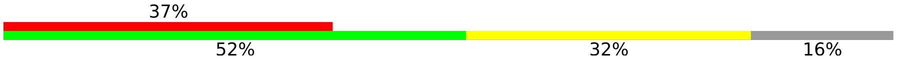


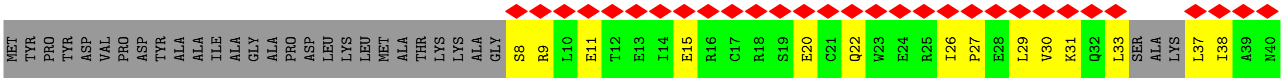



T1354 L1359 L1360 V1364 R1371 R1375 E1376 K1377 I1378 Y1379 S1380 T1381 A1382 F1383 D1384 Y1385 F1386 S1387 C1388 P1389 P1390 K1391 F1392 P1393 T1394 Q1395 L1400 R1401 E1402 D1403 I1404 S1405 I1406 M1407 I1408 K1409 F1410 W1411 F1415 S1416 D1417 K1418 K1419 TYR LEU THR ALA SER GLN LEU VAL PRO PRO ASP
ASN GLN ASP THR ARG SER ASN LEU ASP ILE THR VAL GLY SER ARG GLN GLN ALA THR GLN GLY TRP ILE ASN THR TYR PRO LEU SER SER GLY MET SER THR ILE SER LYS LYS SER GLY MET SER LYS LYS THR ASN R1477 H1482 M1486 K1487 R1488 R1489 L1493 L1496 A1497 T1498
E1499 I1500 E1501 R1502 L1503 I1504 T1505 W1506 Y1507 N1508 P1509 L1510 S1511 A1512 P1513 E1516 E1522 N1523 S1524 V1525 A1526 N1527 W1528 R1529 S1530 K1531 Y1532 I1533 K1538 Q1539 D1542 N1543 V1544 S1551 V1556 Q1557 L1558 P1559 A1560 R1561 F1562 K1563 N1564 T1565 E1566 A1567 I1568 G1569 N1570 E1571 V1572 T1573 R1574
R1577 L1578 D1579 P1580 D1585 V1586 P1587 E1588 A1589 I1590 K1591 F1592 L1593 V1594 T1595 W1596 H1597 T1598 I1599 D1600 A1601 D1602 A1603 P1604 E1605 L1606 S1607 H1608 V1609 L1610 C1611 W1612 A1613 D1616 P1617 P1618 L1621 H1631 P1632 L1633 Q1636 Y1637 G1638 V1639 K1640 V1641 L1642 F1645 P1646 P1647 I1650 L1651
P1655 Q1656 I1657 V1658 Q1659 A1660 L1661 R1662 Y1663 D1664 K1665 M1666 G1667 E1671 Y1672 I1673 L1682 L1683 A1684 H1685 Q1686 F1687 N1690 M1691 K1692 T1693 N1694 I1695 E1699 E1700 G1701 H1702 D1707 D1710 L1711 L1712 V1716 E1717 E1718 G1721 S1722 L1723 S1724 G1725 P1726 A1727 K1728 D1729 F1730 Y1731 Q1732 R1733
E1734 F1735 D1736 F1737 F1738 N1739 K1740 I1741 T1742 N1743 V1744 I1747 I1748 K1749 P1752 D1755 E1756 R1757 K1758 K1759 A1760 C1761 L1762 S1763 A1764 L1765 S1766 E1767 V1768 K1769 V1770 Q1771 C1774 P1777 S1778 N1779 P1780 E1781 A1782 I1783 V1784 L1785 D1786 I1787 D1788 Y1789 LYS SER GLY THR P1794 A1798 A1799
Y1803 L1804 A1805 K1806 F1807 LYS VAL LYS ARG CYS GLY VAL SER GLU LEU GLU LYS GLU GLY LEU ARG CYS ARG SER ASP SER GLU ASP GLU CYS SER THR GLN GLU ALA ASP GLY GLN LYS ILE SER W1844 A1847 I1848 F1849 K1850 V1851 G1852 D1853 D1854 C1855 R1856 Q1857 L1860 A1861 L1862 I1865
L1874 V1875 G1876 L1877 D1878 L1879 F1882 P1883 Y1884 R1885 V1886 V1887 A1890 P1891 G1892 V1895 I1896 E1897 C1898 I1899 P1900 D1901 C1902 T1903 S1904 R1905 D1906 Q1907 L1908 GLY ARG GLN THR ASP PHE G1915 M1916 Y1919 F1920 T1921 R1922 Q1923 Y1924 G1925 D1926 E1927 S1928 T1929 L1930 A1931 F1932 Q1933 R1936 Y1937
N1938 F1939 I1940 R1941 S1942 M1943 A1944 A1945 Y1946 S1947 L1948 L1949 L1950 F1951 L1952 I1955 K1956 D1957 R1958 H1959 N1960 G1961 N1962 I1963 M1964 L1965 D1966 K1967 K1968 G1969 H1970 I1971 I1972 H1973 I1974 G1977 F1978 M1979 F1980 E1981 S1982 SER PRO GLY GLY ASN LEU GLY TRP GLU PRO D1993 I1994 K1995 L1996 M2000
G2006 K2007 M2008 E2009 A2010 T2011 P2012 F2013 K2014 W2015 F2016 M2017 E2018 V2021 R2022 G2023 Y2024 L2025 A2026 V2027 R2028 P2029 Y2030 M2031 D2032 A2033 V2034 V2035 S2036 T2039 L2040 M2041 L2042 D2043 T2044 G2045 L2046 R2050 I2054 K2055 L2056 L2057 R2060 F2061 S2062 M2065 T2066 E2067 R2068 E2069 A2070 A2071 N2072 F2073
I2074 M2075 K2076 V2077 I2078 Q2079 S2080 C2081 F2082 L2083 S2084 N2085 ARG SER ARG THR TYR ASP MET ILE GLN TYR TYR GLN ASN ASP ILE PRO TYR

- Molecule 2: Tetratricopeptide repeat protein 7B

Chain B:

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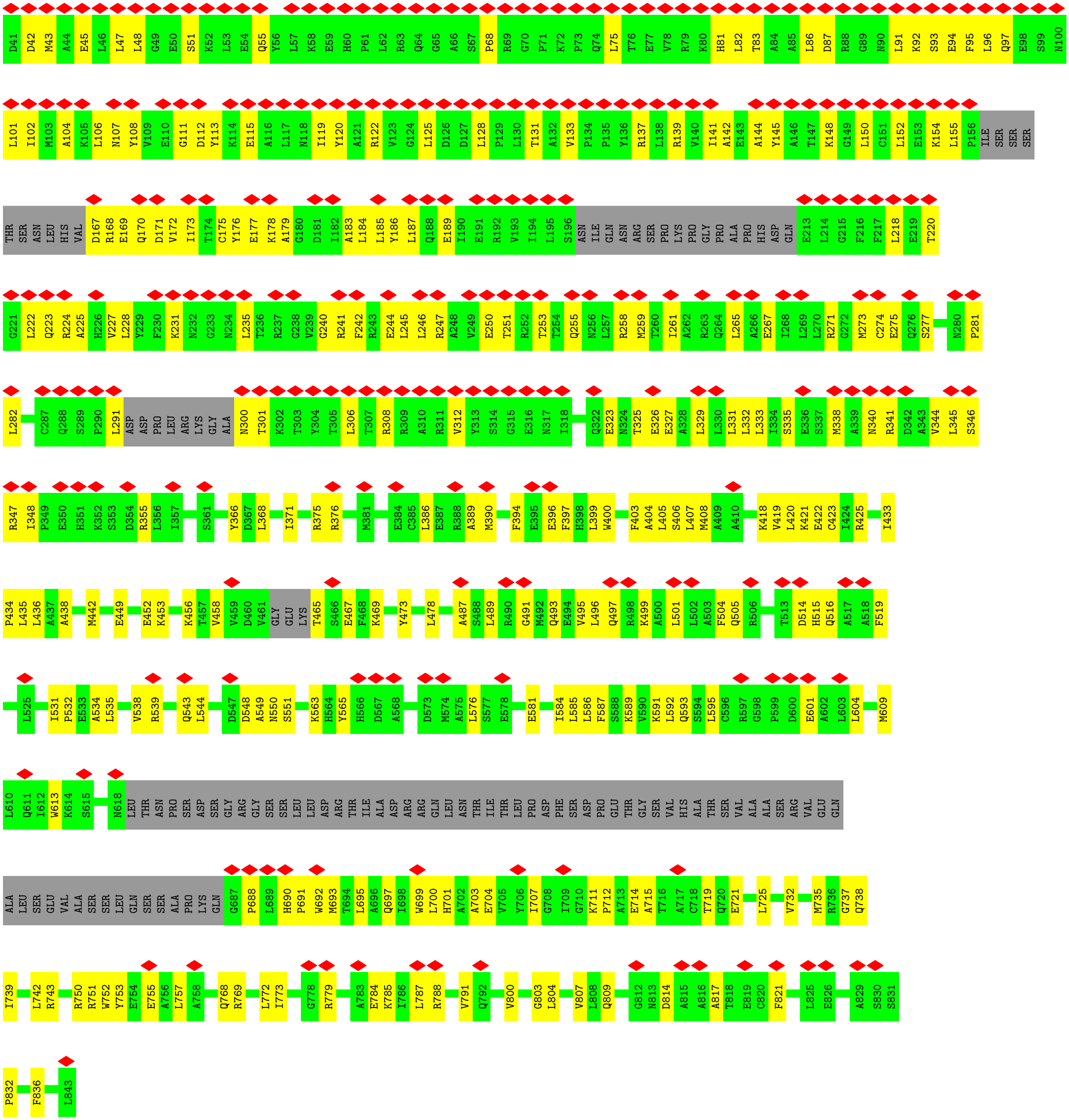
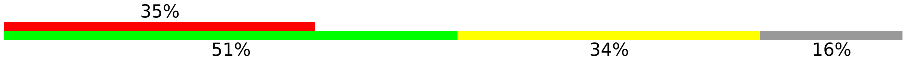
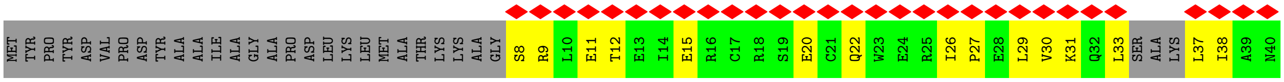
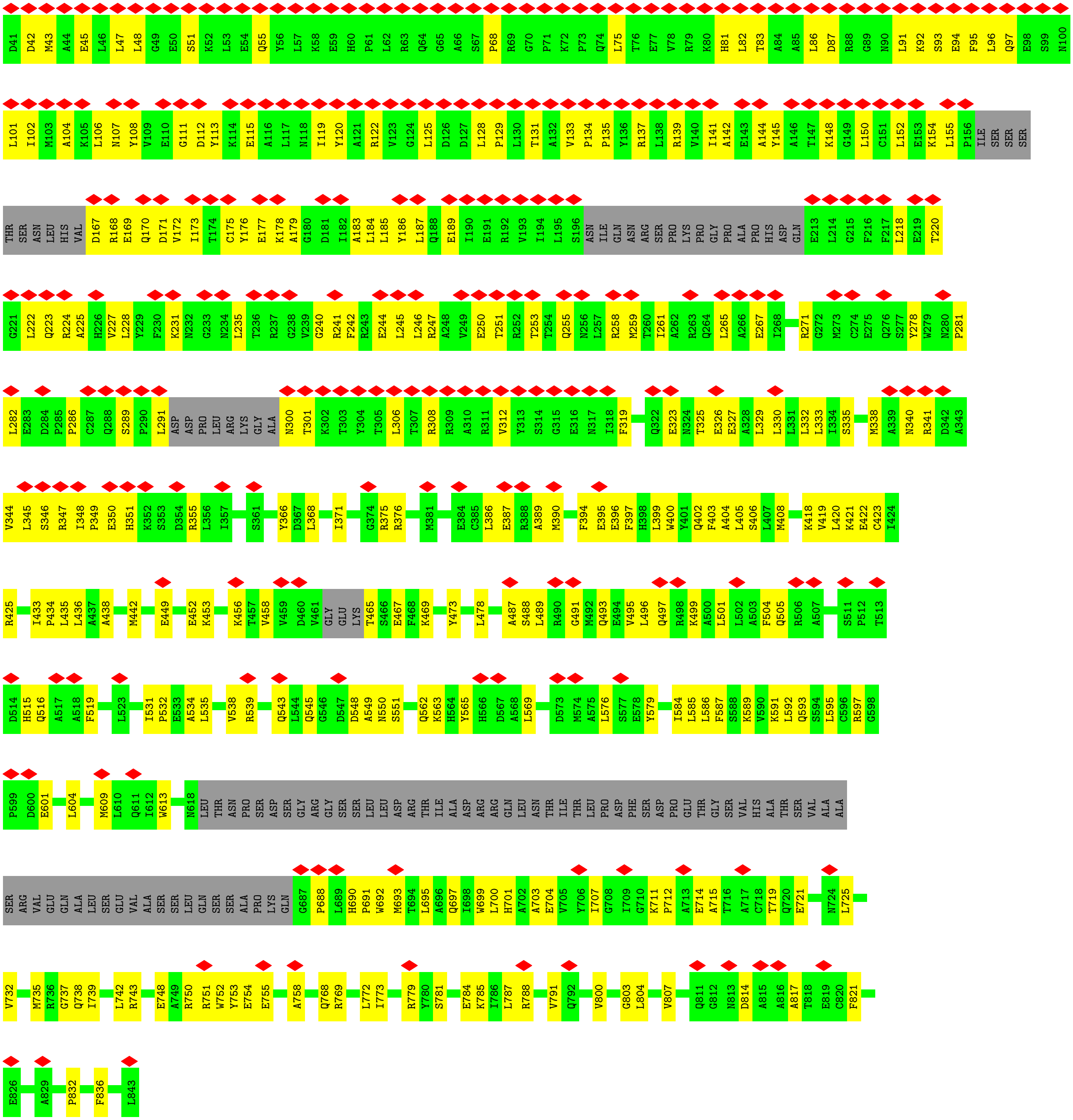


- Molecule 2: Tetratricopeptide repeat protein 7B

Chain F:

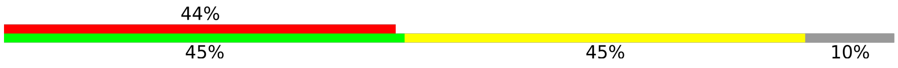


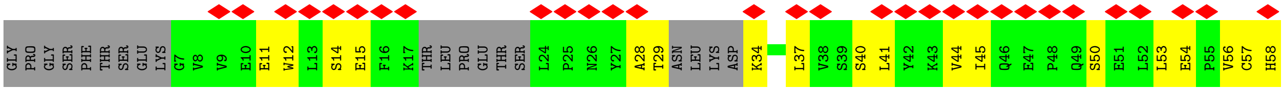


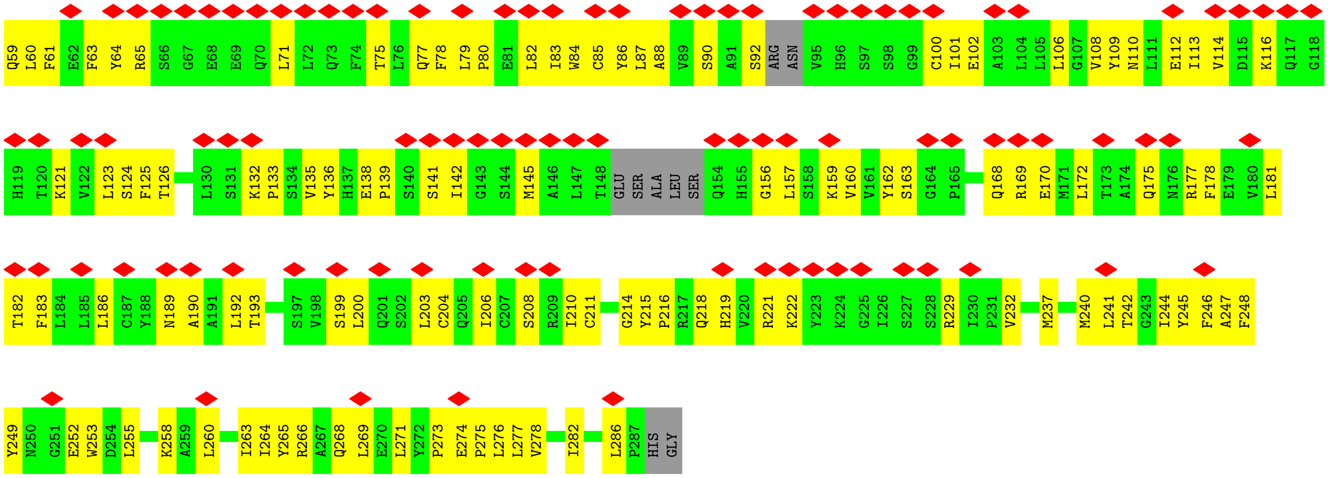

D41 D42 M43 A44 E45 L46 L47 L48 G49 E50 S51 K52 L53 E54 Q55 Y56 L57 K58 E59 H60 P61 L62 R63 Q64 G65 A66 S67 P68 R69 G70 P71 K72 P73 Q74 L75 T76 E77 V78 R79 K80 H81 L82 T83 A84 A85 L86 D87 R88 G89 N90 L91 K92 S93 E94 F95 L96 Q97 E98 S99 N100
L101 I102 M103 A104 K105 L106 N107 Y108 V109 E110 G111 D112 Y113 K114 E115 A116 L117 N118 I119 Y120 A121 R122 V123 G124 L125 D126 D127 L128 P129 L130 T131 A132 V133 P134 P135 Y136 R137 L138 R139 V140 I141 A142 E143 A144 Y145 A146 T147 K148 G149 L150 C151 L152 E153 K154 L155 P156 ILE SER SER SER
THR SER ASN LEU HIS VAL D167 R168 E169 Q170 D171 V172 I173 T174 C175 Y176 E177 K178 A179 G180 D181 I182 A183 L184 L185 Y186 L187 Q188 E189 I190 E191 R192 V193 I194 L195 S196 ASN ILE GLN ASN ARG SER PRO LYS PRO GLY PRO ALA PRO HIS ASP GLN E213 L214 G215 F216 F217 L218 E219 T220
G221 L222 Q223 R224 A225 H226 V227 L228 Y229 F230 K231 R232 G233 N234 L235 T236 R237 G238 V239 G240 R241 F242 R243 E244 L245 L246 R247 A248 V249 E250 T251 R252 T253 T254 Q255 N256 L257 R258 M259 T260 I261 A262 R263 Q264 L265 A266 E267 I268 R271 G272 M273 C274 E275 Q276 S277 Y278 W279 N280 P281
L282 E283 D284 P285 P286 C287 Q288 S289 P290 L291 ASP ASP PRO LEU ARG LYS GLY ALA N300 T301 K302 T303 Y304 T305 L306 T307 R308 R309 A310 R311 V312 Y313 S314 G315 E316 N317 I318 F319 Q322 E323 N324 T325 E326 E327 A328 L329 L330 L331 L332 L333 I334 S335 M338 A339 N340 R341 D342 A343
V344 L345 S346 R347 I348 P349 E350 H351 K352 S353 D354 R355 L356 I357 S361 Y366 D367 L368 I371 G374 R375 R376 M381 E384 C385 L386 E387 R388 A389 M390 F394 E395 E396 F397 H398 L399 W400 Y401 Q402 F403 A404 L405 S406 L407 M408 K418 V419 L420 K421 E422 C423 I424
R425 I433 P434 L435 L436 A437 A438 M442 E449 E452 K453 K456 T457 V458 V459 D460 V461 GLY GLU LYS T465 S466 E467 F468 K469 Y473 L478 A487 S488 L489 R490 G491 M492 Q493 E494 V495 L496 Q497 R498 K499 A500 L501 L502 A503 F504 Q505 R506 A507 S511 P512 T513
D514 H515 Q516 A517 A518 F519 L523 I531 P532 E533 A534 L535 V538 R539 Q543 L544 Q545 G546 D547 D548 A549 N550 S551 Q562 K563 H564 Y565 H566 D567 A568 L569 D573 M574 A575 L576 S577 E578 Y579 I584 L585 L586 F587 S588 K589 V590 K591 L592 Q593 S594 L595 C596 R597 G598
P599 D600 E601 L604 M609 L610 Q611 I612 W613 N618 LEU THR ASN PRO SER ASP SER GLY ARG GLY SER SER LEU LEU ASP ARG THR ILE ALA ASP ARG ARG GLN LEU ASN THR ILE THR LEU PRO ASP PHE SER ASP PRO GLU THR GLY SER VAL HIS ALA THR SER VAL ALA ALA
SER ARG VAL GLU GLN ALA LEU SER GLU VAL ALA SER SER LEU GLN SER SER ALA PRO LYS GLN G687 P688 L689 H690 P691 W692 M693 T694 L695 A696 Q697 I698 W699 L700 H701 A702 A703 E704 V705 Y706 I707 G708 I709 G710 K711 P712 A713 E714 A715 T716 A717 C718 T719 Q720 E721 N724 L725
V732 M735 R736 G737 Q738 I739 L742 R743 E748 A749 R750 R751 W752 Y753 E754 E755 A758 Q768 R769 L772 I773 R779 Y780 S781 E784 K785 I786 L787 R788 V791 Q792 V800 G803 L804 V807 Q811 G812 N813 D814 A815 A816 A817 T818 E819 C820 F821
E826 A829 P832 F836 L843

- Molecule 3: Protein FAM126A

Chain C:

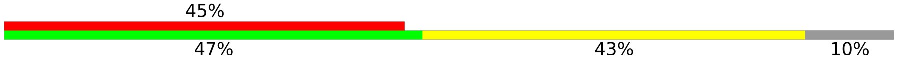


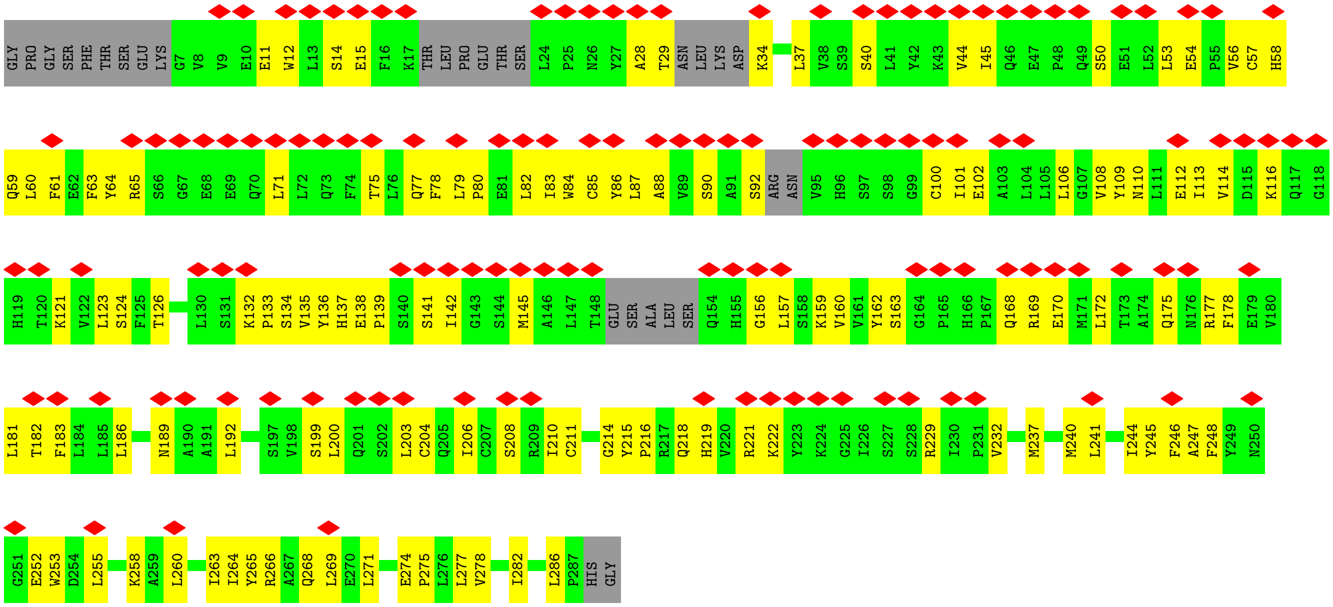

GLY PRO GLY SER PHE THR SER GLU LYS G7 V8 V9 E10 E11 W12 L13 S14 E15 F16 K17 THR LEU PRO GLU THR SER L24 P25 N26 Y27 A28 T29 ASN LEU LYS ASP K34 L37 V38 S39 S40 L41 Y42 K43 V44 I45 Q46 E47 P48 Q49 S50 E51 L52 L53 E54 P55 V56 C57 H58



- Molecule 3: Protein FAM126A

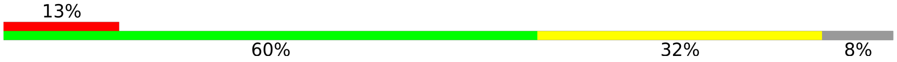
Chain G:

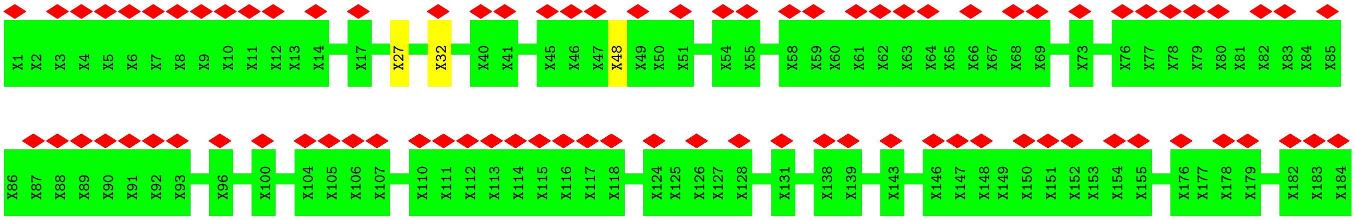


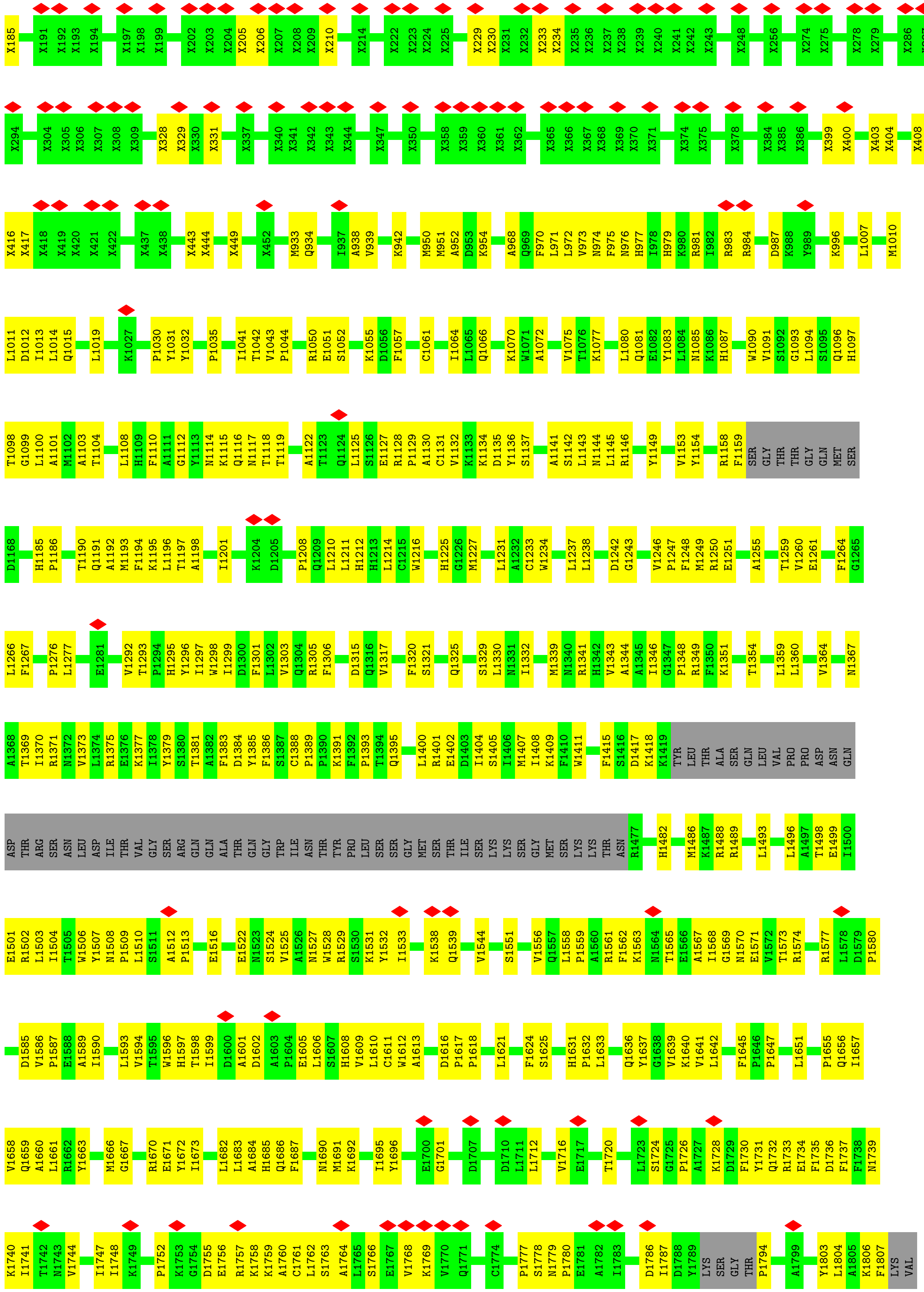


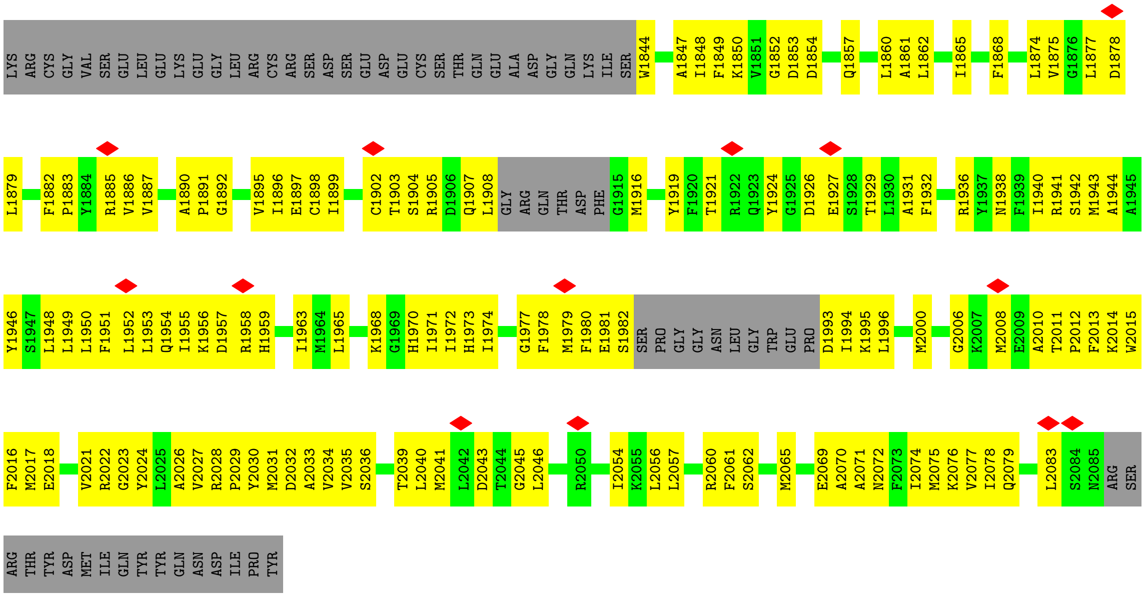
- Molecule 4: Phosphatidylinositol 4-kinase III alpha (PI4KA)

Chain E:






X185 X191 X192 X193 X194 X197 X198 X199 X202 X203 X204 X205 X206 X207 X208 X209 X210 X214 X222 X223 X224 X225 X229 X230 X231 X232 X233 X234 X235 X236 X237 X238 X239 X240 X241 X242 X243 X248 X256 X274 X275 X278 X279 X286 X287 X290 X293
X294 X304 X305 X306 X307 X308 X309 X328 X329 X330 X331 X337 X340 X341 X342 X343 X344 X347 X350 X358 X359 X360 X361 X362 X365 X366 X367 X368 X369 X370 X371 X374 X375 X378 X384 X385 X386 X399 X400 X403 X404 X408 X413 X414 X415
X416 X417 X418 X419 X420 X421 X422 X437 X438 X443 X444 X449 X452 M933 Q934 I937 A938 V939 K942 M950 M951 A952 D953 K954 A968 Q969 F970 L971 L972 V973 N974 F975 N976 H977 I978 H979 K980 R981 I982 R983 R984 D987 K988 Y989 K996 L1007 M1010
L1011 D1012 I1013 L1014 Q1015 L1019 K1027 P1030 Y1031 Y1032 P1035 I1041 T1042 V1043 P1044 R1050 E1051 S1052 K1055 D1056 F1057 C1061 I1064 L1065 Q1066 K1070 W1071 A1072 V1075 T1076 K1077 L1080 Q1081 E1082 Y1083 L1084 N1085 K1086 H1087 W1090 V1091 S1092 G1093 L1094 S1095 Q1096 H1097
T1098 G1099 L1100 A1101 M1102 A1103 T1104 L1108 H1109 F1110 A1111 G1112 Y1113 N1114 K1115 Q1116 N1117 T1118 T1119 A1122 T1123 Q1124 L1125 S1126 E1127 R1128 P1129 A1130 C1131 V1132 K1133 K1134 D1135 Y1136 S1137 A1141 S1142 L1143 N1144 L1145 R1146 Y1149 V1153 Y1154 R1158 F1159 SER GLY THR THR GLY GLN MET SER
D1168 H1185 P1186 T1190 Q1191 A1192 M1193 F1194 K1195 L1196 T1197 A1198 I1201 K1204 D1205 P1208 Q1209 L1210 L1211 H1212 H1213 L1214 C1215 W1216 H1225 G1226 M1227 L1231 A1232 C1233 W1234 L1237 L1238 D1242 G1243 V1246 P1247 F1248 M1249 R1250 E1251 A1255 T1259 V1260 E1261 F1264 G1265
L1266 F1267 P1276 L1277 E1281 V1292 T1293 P1294 H1295 Y1296 I1297 W1298 I1299 D1300 F1301 L1302 V1303 Q1304 R1305 F1306 D1315 Q1316 V1317 F1320 S1321 Q1325 S1329 L1330 N1331 I1332 M1339 N1340 R1341 H1342 V1343 A1344 A1345 L1346 G1347 P1348 R1349 F1350 K1351 T1354 L1359 L1360 V1364 N1367
A1368 T1369 I1370 R1371 N1372 V1373 L1374 R1375 E1376 K1377 I1378 Y1379 S1380 T1381 A1382 F1383 D1384 Y1385 F1386 S1387 C1388 P1389 P1390 K1391 F1392 P1393 T1394 Q1395 L1400 R1401 E1402 D1403 I1404 S1405 I1406 M1407 I1408 K1409 F1410 W1411 F1415 S1416 D1417 K1418 K1419 TYR LEU THR ALA SER GLN LEU VAL PRO PRO ASP ASN GLN
ASP THR ARG SER ASN LEU ASP ILE THR VAL GLY SER ARG GLN GLN ALA THR GLN GLY TRP ILE ASN THR TYR PRO LEU SER SER GLY MET SER THR ILE SER LYS LYS SER GLY MET SER LYS LYS THR ASN R1477 H1482 M1486 K1487 R1488 R1489 L1493 L1496 A1497 T1498 E1499 I1500
E1501 R1502 L1503 I1504 T1505 W1506 Y1507 N1508 P1509 L1510 S1511 A1512 P1513 E1516 E1522 N1523 S1524 V1525 A1526 N1527 W1528 R1529 S1530 K1531 Y1532 I1533 K1538 Q1539 V1544 S1551 V1556 Q1557 L1558 P1559 A1560 R1561 F1562 K1563 N1564 T1565 E1566 A1567 I1568 G1569 N1570 E1571 V1572 T1573 R1574 R1577 L1578 D1579 P1580
D1585 V1586 P1587 E1588 A1589 I1590 L1593 V1594 T1595 W1596 H1597 T1598 I1599 D1600 A1601 D1602 A1603 P1604 E1605 L1606 S1607 H1608 V1609 L1610 C1611 W1612 A1613 D1616 P1617 P1618 L1621 F1624 S1625 H1631 P1632 L1633 Q1636 Y1637 G1638 V1639 K1640 V1641 L1642 F1645 P1646 P1647 L1651 P1655 Q1656 I1657
V1658 Q1659 A1660 L1661 R1662 Y1663 M1666 G1667 R1670 E1671 Y1672 I1673 L1682 L1683 A1684 H1685 Q1686 F1687 N1690 M1691 K1692 I1695 Y1696 E1700 G1701 D1707 D1710 L1711 L1712 V1716 E1717 T1720 L1723 S1724 G1725 P1726 A1727 K1728 D1729 F1730 Y1731 Q1732 R1733 E1734 F1735 D1736 F1737 F1738 N1739
K1740 I1741 T1742 N1743 V1744 I1747 I1748 K1749 P1752 K1753 G1754 D1755 E1756 R1757 K1758 K1759 A1760 C1761 L1762 S1763 A1764 L1765 S1766 E1767 V1768 K1769 V1770 Q1771 C1774 P1777 S1778 N1779 P1780 E1781 A1782 I1783 D1786 I1787 D1788 Y1789 LYS SER GLY THR P1794 A1799 Y1803 L1804 A1805 K1806 F1807 LYS VAL


LYS
ARG
CYS
GLY
VAL
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ARG
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ASP
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GLU
ASP
GLU
CYS
SER
THR
GLN
GLU
ALA
ASP
GLY
GLN
LYS
ILE
SER
W1844
A1847
I1848
F1849
K1850
V1851
G1852
D1853
D1854
Q1857
L1860
A1861
L1862
I1865
F1868
L1874
V1875
G1876
L1877
D1878
L1879
F1882
P1883
Y1884
R1885
V1886
V1887
A1890
P1891
G1892
V1895
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E1897
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C1902
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Q1907
L1908
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M1916
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F1920
T1921
R1922
Q1923
Y1924
G1925
D1926
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L1930
A1931
F1932
R1936
Y1937
N1938
F1939
I1940
R1941
S1942
M1943
A1944
A1945
Y1946
S1947
L1948
L1949
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F1951
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L1953
Q1954
I1955
K1956
D1957
R1958
H1959
I1963
M1964
L1965
K1968
G1969
H1970
I1971
I1972
H1973
I1974
G1977
F1978
M1979
F1980
E1981
S1982
SER
PRO
GLY
GLY
ASN
LEU
GLY
TRP
GLU
PRO
D1993
I1994
K1995
L1996
M2000
G2006
K2007
M2008
E2009
A2010
T2011
P2012
F2013
K2014
W2015
F2016
M2017
E2018
V2021
R2022
G2023
Y2024
L2025
A2026
V2027
R2028
P2029
Y2030
M2031
D2032
A2033
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V2035
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M2041
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D2043
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G2045
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I2078
Q2079
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N2085
ARG
SER
ARG
THR
TYR
ASP
MET
ILE
GLN
TYR
TYR
GLN
ASN
ASP
ILE
PRO
TYR

4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	64104	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 $(e^-/\text{Å}^2)$	47	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	3700	Depositor
Magnification	38461	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.287	Depositor
Minimum map value	-0.167	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	416.0, 416.0, 416.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3, 1.3, 1.3	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: E4S

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.41	0/8500	0.56	0/11506
2	B	0.32	0/5877	0.45	0/7948
2	F	0.32	0/5877	0.46	0/7948
3	C	0.31	0/2140	0.48	0/2903
3	G	0.31	0/2140	0.47	0/2903
4	E	0.41	0/8500	0.56	0/11506
All	All	0.37	0/33034	0.52	0/44714

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10673	0	8799	623	0
2	B	5774	0	5852	262	0
2	F	5774	0	5852	273	0
3	C	2091	0	2096	156	0
3	G	2091	0	2096	135	0
4	E	10678	0	8800	619	0
5	A	41	27	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	41	27	0	3	0
All	All	37163	54	33495	1915	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 27.

All (1915) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1932:PHE:CZ	1:A:1936:ARG:HD3	1.30	1.60
4:E:1696:TYR:CD1	4:E:1701:GLY:HA2	1.34	1.58
4:E:1860:LEU:HD22	4:E:1979:MET:CE	1.50	1.40
1:A:1404:ILE:HD12	1:A:1507:TYR:CE2	1.55	1.40
1:A:1932:PHE:CE2	1:A:1936:ARG:HD3	1.55	1.38
3:C:178:PHE:CD1	3:C:181:LEU:HD12	1.57	1.37
1:A:1404:ILE:CD1	1:A:1507:TYR:HE2	1.36	1.35
1:A:1860:LEU:HD22	1:A:1979:MET:CE	1.56	1.33
3:C:177:ARG:O	3:C:181:LEU:HG	1.26	1.31
4:E:1404:ILE:HD12	4:E:1507:TYR:CE2	1.66	1.29
4:E:1404:ILE:CD1	4:E:1507:TYR:HE2	1.45	1.28
3:G:178:PHE:CD1	3:G:181:LEU:HD12	1.70	1.27
1:A:1932:PHE:CZ	1:A:1936:ARG:CD	2.20	1.23
4:E:1696:TYR:CD1	4:E:1701:GLY:CA	2.20	1.23
4:E:1955:ILE:HD12	4:E:1959:HIS:CD2	1.70	1.23
3:G:177:ARG:O	3:G:181:LEU:HG	1.35	1.21
1:A:1932:PHE:CE2	1:A:1936:ARG:CD	2.28	1.17
1:A:182:UNK:CB	1:A:201:UNK:CB	2.23	1.16
1:A:1950:LEU:HD23	1:A:1955:ILE:HD13	1.26	1.16
1:A:1860:LEU:HD22	1:A:1979:MET:HE1	1.20	1.14
1:A:1860:LEU:CD2	1:A:1979:MET:HE1	1.77	1.13
1:A:1590:ILE:HA	1:A:1612:TRP:CZ3	1.83	1.12
3:C:60:LEU:HD22	3:C:75:THR:HG22	1.34	1.10
1:A:1632:PRO:HG2	2:B:345:LEU:HD13	1.34	1.08
1:A:933:MET:HE3	1:A:981:ARG:HD2	1.16	1.08
2:B:346:SER:CB	2:B:355:ARG:HH11	1.66	1.08
4:E:1666:MET:HG2	2:F:347:ARG:HG2	1.11	1.07
1:A:1098:THR:HG23	4:E:1131:CYS:HB2	1.35	1.06
4:E:1950:LEU:HB3	4:E:1994:ILE:HD12	1.34	1.06
1:A:1950:LEU:HG	1:A:1955:ILE:HG21	1.36	1.06
4:E:1666:MET:CG	2:F:347:ARG:HG2	1.84	1.06
4:E:1590:ILE:HD11	4:E:1594:VAL:HG21	1.38	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:1590:ILE:HG13	4:E:1594:VAL:HG23	1.37	1.04
1:A:1699:GLU:HB3	1:A:1702:HIS:HD2	1.20	1.04
3:G:60:LEU:HD22	3:G:75:THR:HG22	1.34	1.04
2:B:587:PHE:CD1	2:B:701:HIS:CE1	2.46	1.04
4:E:1404:ILE:HD12	4:E:1507:TYR:HE2	0.88	1.04
4:E:1666:MET:HG2	2:F:347:ARG:CG	1.87	1.04
4:E:1865:ILE:HG12	4:E:1949:LEU:HD23	1.39	1.03
1:A:1108:LEU:HD22	4:E:1108:LEU:HD22	1.40	1.03
3:C:178:PHE:CD1	3:C:181:LEU:CD1	2.40	1.03
4:E:1955:ILE:HD12	4:E:1959:HIS:HD2	1.21	1.03
2:F:346:SER:HB2	2:F:355:ARG:NH1	1.74	1.02
2:F:587:PHE:CD1	2:F:701:HIS:CE1	2.46	1.02
2:F:346:SER:CB	2:F:355:ARG:HH11	1.71	1.02
1:A:933:MET:HE1	1:A:981:ARG:HB2	1.41	1.01
2:B:346:SER:HB2	2:B:355:ARG:NH1	1.75	1.01
3:G:211:CYS:O	3:G:266:ARG:HD2	1.61	1.01
4:E:1696:TYR:HD1	4:E:1701:GLY:HA2	1.19	1.00
4:E:1860:LEU:CD2	4:E:1979:MET:CE	2.40	0.99
1:A:1860:LEU:HD22	1:A:1979:MET:HE2	1.42	0.99
4:E:933:MET:HE3	4:E:981:ARG:HD2	1.45	0.99
4:E:1860:LEU:HD22	4:E:1979:MET:HE1	0.99	0.98
1:A:1590:ILE:HA	1:A:1612:TRP:HZ3	1.20	0.98
1:A:1699:GLU:HB3	1:A:1702:HIS:CD2	1.99	0.98
4:E:1590:ILE:HG13	4:E:1612:TRP:HZ3	1.25	0.97
3:C:178:PHE:HD1	3:C:181:LEU:CD1	1.76	0.97
4:E:1860:LEU:CD2	4:E:1979:MET:HE1	1.93	0.97
1:A:1632:PRO:CG	2:B:345:LEU:HD13	1.94	0.96
4:E:185:UNK:CB	4:E:205:UNK:CB	2.42	0.96
1:A:1404:ILE:CD1	1:A:1507:TYR:CE2	2.27	0.96
4:E:933:MET:CE	4:E:981:ARG:HD2	1.97	0.95
1:A:182:UNK:CB	1:A:201:UNK:CA	2.43	0.95
4:E:1590:ILE:HG13	4:E:1594:VAL:CG2	1.97	0.94
1:A:1404:ILE:HD12	1:A:1507:TYR:HE2	0.77	0.94
3:G:83:ILE:O	3:G:87:LEU:HB3	1.68	0.94
3:C:83:ILE:O	3:C:87:LEU:HB3	1.68	0.93
4:E:1404:ILE:CD1	4:E:1507:TYR:CE2	2.36	0.93
4:E:1586:VAL:CG1	4:E:1613:ALA:HB3	1.99	0.93
1:A:1590:ILE:CA	1:A:1612:TRP:HZ3	1.82	0.93
1:A:1929:THR:O	1:A:1933:GLN:HG3	1.68	0.93
4:E:1586:VAL:HG13	4:E:1613:ALA:HB3	1.50	0.93
1:A:1131:CYS:SG	4:E:1101:ALA:HB3	2.09	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1277:LEU:HD23	1:A:1618:PRO:HG2	1.51	0.92
4:E:1590:ILE:CG1	4:E:1612:TRP:HZ3	1.83	0.92
3:G:60:LEU:HD22	3:G:75:THR:CG2	2.00	0.92
2:B:346:SER:CB	2:B:355:ARG:NH1	2.32	0.92
1:A:933:MET:CE	1:A:981:ARG:HD2	2.00	0.92
3:C:211:CYS:O	3:C:266:ARG:HD2	1.69	0.91
4:E:1860:LEU:HD22	4:E:1979:MET:HE3	1.50	0.91
4:E:1590:ILE:CD1	4:E:1594:VAL:HG21	1.99	0.91
3:C:60:LEU:HD22	3:C:75:THR:CG2	2.00	0.91
1:A:1671:GLU:OE1	2:B:348:ILE:HD11	1.71	0.91
3:G:60:LEU:CD2	3:G:75:THR:CG2	2.49	0.91
3:C:82:LEU:O	3:C:86:TYR:HB3	1.70	0.90
4:E:1667:GLY:HA3	2:F:347:ARG:O	1.69	0.90
1:A:1128:ARG:HD3	4:E:1051:GLU:HG3	1.51	0.90
3:G:82:LEU:O	3:G:86:TYR:HB3	1.70	0.90
4:E:1112:GLY:O	4:E:1135:ASP:OD1	1.90	0.90
1:A:1905:ARG:HB3	1:A:1961:GLY:HA2	1.53	0.90
3:C:60:LEU:CD2	3:C:75:THR:CG2	2.49	0.89
1:A:1699:GLU:HG3	1:A:1700:GLU:H	1.38	0.89
1:A:1860:LEU:CD2	1:A:1979:MET:CE	2.43	0.89
3:G:178:PHE:CD1	3:G:181:LEU:CD1	2.56	0.89
4:E:1277:LEU:HD23	4:E:1618:PRO:HG2	1.51	0.89
4:E:1696:TYR:CE1	4:E:1701:GLY:CA	2.56	0.89
1:A:1804:LEU:HA	1:A:1848:ILE:HG22	1.54	0.89
1:A:1131:CYS:HB2	4:E:1098:THR:HG23	1.55	0.89
4:E:1565:THR:HG22	4:E:1567:ALA:H	1.38	0.89
1:A:1565:THR:HG22	1:A:1567:ALA:H	1.38	0.89
1:A:1946:TYR:O	1:A:1950:LEU:HD13	1.71	0.88
3:G:178:PHE:HD1	3:G:181:LEU:HD12	1.16	0.88
4:E:1585:ASP:OD1	4:E:1589:ALA:HB2	1.74	0.88
4:E:1955:ILE:CD1	4:E:1959:HIS:HD2	1.85	0.88
1:A:1865:ILE:HG12	1:A:1949:LEU:HD23	1.53	0.88
1:A:1586:VAL:HG23	1:A:1587:PRO:HD3	1.56	0.88
4:E:1696:TYR:CE1	4:E:1701:GLY:HA2	2.08	0.88
4:E:1950:LEU:CB	4:E:1994:ILE:HD12	2.03	0.88
4:E:1250:ARG:HH22	2:F:781:SER:HB3	1.38	0.87
1:A:1590:ILE:CA	1:A:1612:TRP:CZ3	2.56	0.86
3:G:211:CYS:O	3:G:266:ARG:CD	2.23	0.86
4:E:1954:GLN:HG2	4:E:2060:ARG:CZ	2.05	0.86
3:C:84:TRP:O	3:C:88:ALA:HB3	1.76	0.86
4:E:1804:LEU:HA	4:E:1848:ILE:HG22	1.54	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1950:LEU:HG	1:A:1955:ILE:CG2	2.05	0.85
1:A:1344:ALA:HA	1:A:1395:GLN:HE21	1.40	0.85
1:A:977:HIS:O	1:A:983:ARG:HD3	1.75	0.85
1:A:1860:LEU:HB3	1:A:1979:MET:HE1	1.57	0.85
3:G:84:TRP:O	3:G:88:ALA:HB3	1.76	0.85
4:E:1590:ILE:CG1	4:E:1594:VAL:CG2	2.54	0.85
4:E:1344:ALA:HA	4:E:1395:GLN:HE21	1.40	0.84
1:A:1978:PHE:HD1	1:A:1982:SER:CB	1.91	0.84
3:C:178:PHE:HD1	3:C:181:LEU:HD12	1.02	0.84
2:F:346:SER:HB2	2:F:355:ARG:HH11	1.29	0.84
1:A:933:MET:HE3	1:A:981:ARG:CD	2.06	0.84
1:A:1052:SER:HA	1:A:1055:LYS:HE2	1.59	0.84
3:C:178:PHE:CE1	3:C:181:LEU:HD12	2.12	0.84
1:A:1122:ALA:HB3	1:A:1125:LEU:HD23	1.60	0.84
1:A:1134:LYS:HG3	1:A:1136:TYR:CE2	2.12	0.83
4:E:1052:SER:HA	4:E:1055:LYS:HE2	1.59	0.83
1:A:1400:LEU:CD2	1:A:1507:TYR:CD2	2.61	0.83
1:A:1651:LEU:HD11	1:A:1686:GLN:HG3	1.60	0.83
4:E:1122:ALA:HB3	4:E:1125:LEU:HD23	1.60	0.83
3:C:211:CYS:O	3:C:266:ARG:CD	2.26	0.83
1:A:1944:ALA:HB2	1:A:2016:PHE:CD1	2.14	0.82
4:E:1666:MET:HA	2:F:347:ARG:HG2	1.61	0.82
2:F:319:PHE:H	3:G:134:SER:HA	1.43	0.82
3:G:274:GLU:HG2	3:G:275:PRO:HD3	1.62	0.82
4:E:1586:VAL:CG1	4:E:1613:ALA:CB	2.57	0.82
2:B:346:SER:HB3	2:B:355:ARG:HH11	1.44	0.82
3:C:274:GLU:HG2	3:C:275:PRO:HD3	1.62	0.82
4:E:1950:LEU:HB3	4:E:1994:ILE:CD1	2.10	0.81
1:A:1978:PHE:HD1	1:A:1982:SER:HB2	1.43	0.81
4:E:1651:LEU:HD11	4:E:1686:GLN:HG3	1.61	0.81
4:E:1666:MET:HA	2:F:347:ARG:CG	2.09	0.81
2:F:587:PHE:CD1	2:F:701:HIS:HE1	1.98	0.81
1:A:1994:ILE:H	1:A:1994:ILE:HD12	1.43	0.81
4:E:977:HIS:O	4:E:983:ARG:HD3	1.79	0.81
2:F:142:ALA:HA	2:F:145:TYR:HD2	1.46	0.81
2:B:274:CYS:HB3	3:C:192:LEU:HB2	1.62	0.81
1:A:1098:THR:HG23	4:E:1131:CYS:CB	2.11	0.81
1:A:1963:ILE:CD1	1:A:1995:LYS:HD2	2.10	0.81
3:G:178:PHE:HD1	3:G:181:LEU:CD1	1.93	0.81
2:B:142:ALA:HA	2:B:145:TYR:HD2	1.46	0.80
1:A:1944:ALA:HA	1:A:2016:PHE:CE1	2.16	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:UNK:CB	1:A:981:ARG:NH1	2.45	0.80
1:A:1666:MET:HG2	2:B:347:ARG:HG2	1.61	0.80
4:E:1860:LEU:CD2	4:E:1979:MET:HE3	2.08	0.80
1:A:976:ASN:OD1	1:A:1017:LEU:HD11	1.83	0.80
3:G:178:PHE:CE1	3:G:181:LEU:HD12	2.16	0.80
3:C:178:PHE:CE1	3:C:181:LEU:CD1	2.65	0.79
4:E:933:MET:HE1	4:E:981:ARG:HB2	1.62	0.79
1:A:1684:ALA:HA	1:A:1687:PHE:HD2	1.47	0.79
4:E:1684:ALA:HA	4:E:1687:PHE:HD2	1.47	0.79
4:E:1586:VAL:HG23	4:E:1587:PRO:HD3	1.64	0.79
2:B:587:PHE:CD1	2:B:701:HIS:ND1	2.50	0.79
2:F:587:PHE:CD1	2:F:701:HIS:ND1	2.50	0.79
1:A:1101:ALA:HB3	4:E:1131:CYS:SG	2.22	0.79
1:A:1932:PHE:CE2	1:A:1936:ARG:NE	2.50	0.79
2:B:37:LEU:HB3	2:B:38:ILE:HD12	1.65	0.79
1:A:1153:VAL:HG21	1:A:1198:ALA:HB3	1.65	0.78
4:E:1696:TYR:CE1	4:E:1701:GLY:HA3	2.18	0.78
1:A:1101:ALA:HB1	4:E:1136:TYR:HB2	1.64	0.78
4:E:1958:ARG:O	4:E:1959:HIS:CG	2.36	0.78
4:E:1726:PRO:O	4:E:1730:PHE:HB2	1.84	0.78
1:A:1944:ALA:CA	1:A:2016:PHE:CE1	2.67	0.78
1:A:1978:PHE:CD1	1:A:1982:SER:HB2	2.18	0.78
2:B:587:PHE:HD1	2:B:701:HIS:ND1	1.82	0.78
1:A:1943:MET:HB3	1:A:1971:ILE:HG21	1.65	0.77
2:B:587:PHE:CD1	2:B:701:HIS:HE1	1.98	0.77
1:A:933:MET:HE1	1:A:981:ARG:CB	2.12	0.77
1:A:1132:VAL:O	1:A:1134:LYS:HG2	1.85	0.77
2:F:346:SER:HA	2:F:355:ARG:HG3	1.66	0.77
1:A:1586:VAL:HG12	1:A:1613:ALA:CB	2.15	0.77
1:A:1924:TYR:HB3	1:A:1931:ALA:HB1	1.66	0.77
1:A:2034:VAL:HG12	1:A:2057:LEU:HD21	1.67	0.77
2:B:405:LEU:HB2	3:C:277:LEU:HD13	1.66	0.77
1:A:1726:PRO:O	1:A:1730:PHE:HB2	1.84	0.77
1:A:1861:ALA:HB2	1:A:1979:MET:HB2	1.64	0.77
4:E:1130:ALA:O	4:E:1131:CYS:HB3	1.83	0.77
4:E:1932:PHE:O	4:E:1936:ARG:HB2	1.85	0.77
4:E:1955:ILE:CD1	4:E:1959:HIS:CD2	2.58	0.77
2:F:587:PHE:HD1	2:F:701:HIS:ND1	1.82	0.77
4:E:2034:VAL:HG12	4:E:2057:LEU:HD21	1.67	0.77
1:A:1098:THR:CG2	4:E:1131:CYS:HB2	2.15	0.77
4:E:1153:VAL:HG21	4:E:1198:ALA:HB3	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:1191:GLN:HG2	4:E:1195:LYS:HE3	1.67	0.77
4:E:1590:ILE:HG13	4:E:1612:TRP:CZ3	2.16	0.77
4:E:1400:LEU:CD2	4:E:1507:TYR:CD2	2.67	0.76
4:E:1886:VAL:HG22	4:E:1896:ILE:HG22	1.67	0.76
1:A:1055:LYS:HB3	4:E:1128:ARG:HA	1.67	0.76
4:E:1666:MET:CB	2:F:347:ARG:HG2	2.14	0.76
1:A:1904:SER:HB2	1:A:1907:GLN:HG2	1.68	0.76
1:A:1950:LEU:CG	1:A:1955:ILE:HG21	2.13	0.76
4:E:1904:SER:HB2	4:E:1907:GLN:HG2	1.68	0.76
2:F:37:LEU:HB3	2:F:38:ILE:HD12	1.65	0.76
4:E:1590:ILE:CB	4:E:1612:TRP:CZ3	2.68	0.76
4:E:1667:GLY:CA	2:F:347:ARG:O	2.34	0.76
1:A:1077:LYS:O	1:A:1081:GLN:HB2	1.86	0.76
1:A:1259:THR:HG23	1:A:1264:PHE:HB2	1.68	0.76
4:E:1954:GLN:CG	4:E:2060:ARG:CZ	2.63	0.76
1:A:1735:PHE:O	1:A:1739:ASN:HB2	1.86	0.76
4:E:1507:TYR:C	4:E:1509:PRO:HD3	2.05	0.76
4:E:1640:LYS:HE2	2:F:425:ARG:HH22	1.51	0.75
4:E:1077:LYS:O	4:E:1081:GLN:HB2	1.86	0.75
3:C:112:GLU:O	3:C:116:LYS:NZ	2.20	0.75
2:B:83:THR:O	2:B:87:ASP:HB2	1.87	0.75
2:F:83:THR:O	2:F:87:ASP:HB2	1.87	0.75
1:A:1191:GLN:HG2	1:A:1195:LYS:HE3	1.67	0.75
1:A:1944:ALA:HB2	1:A:2016:PHE:CE1	2.21	0.74
1:A:1886:VAL:HG22	1:A:1896:ILE:HG22	1.67	0.74
3:G:241:LEU:HD21	3:G:263:ILE:HG21	1.69	0.74
1:A:1699:GLU:HG3	1:A:1700:GLU:N	2.02	0.74
2:B:346:SER:HA	2:B:355:ARG:HG3	1.67	0.74
2:B:712:PRO:HB2	2:B:743:ARG:HE	1.52	0.74
1:A:182:UNK:CB	1:A:201:UNK:C	2.66	0.74
1:A:1667:GLY:N	2:B:347:ARG:O	2.20	0.74
4:E:1590:ILE:CG1	4:E:1594:VAL:HG21	2.16	0.74
4:E:1926:ASP:OD1	4:E:1927:GLU:HG3	1.87	0.74
1:A:1371:ARG:O	1:A:1375:ARG:HB2	1.88	0.74
4:E:1371:ARG:O	4:E:1375:ARG:HB2	1.88	0.74
4:E:1655:PRO:O	4:E:1659:GLN:NE2	2.20	0.74
3:G:60:LEU:CD2	3:G:75:THR:HG22	2.12	0.74
3:G:112:GLU:O	3:G:116:LYS:NZ	2.20	0.74
3:G:237:MET:HA	3:G:240:MET:HG2	1.69	0.74
4:E:1259:THR:HG23	4:E:1264:PHE:HB2	1.68	0.74
3:C:84:TRP:O	3:C:88:ALA:CB	2.36	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:1735:PHE:O	4:E:1739:ASN:HB2	1.86	0.74
4:E:1954:GLN:HG3	4:E:2060:ARG:NH2	2.03	0.73
1:A:1507:TYR:C	1:A:1509:PRO:HD3	2.08	0.73
1:A:1598:THR:HG22	1:A:1599:ILE:HG23	1.70	0.73
4:E:1590:ILE:HB	4:E:1612:TRP:CE3	2.22	0.73
1:A:1593:LEU:HB3	1:A:1612:TRP:HH2	1.53	0.73
1:A:1993:ASP:HB3	1:A:2081:CYS:SG	2.29	0.73
3:C:237:MET:HA	3:C:240:MET:HG2	1.69	0.73
3:C:241:LEU:HD21	3:C:263:ILE:HG21	1.69	0.73
2:F:587:PHE:CE1	2:F:701:HIS:CE1	2.76	0.73
1:A:1667:GLY:HA3	2:B:347:ARG:O	1.88	0.73
3:G:84:TRP:O	3:G:88:ALA:CB	2.36	0.73
1:A:1655:PRO:O	1:A:1659:GLN:NE2	2.20	0.73
1:A:1946:TYR:O	1:A:1950:LEU:CD1	2.37	0.73
2:B:587:PHE:CE1	2:B:701:HIS:CE1	2.76	0.73
1:A:413:UNK:O	1:A:416:UNK:N	2.22	0.73
2:B:587:PHE:HD1	2:B:701:HIS:CE1	2.05	0.73
4:E:414:UNK:O	4:E:417:UNK:N	2.21	0.73
1:A:1586:VAL:CG1	1:A:1613:ALA:CB	2.66	0.73
3:C:177:ARG:O	3:C:181:LEU:CG	2.22	0.73
1:A:1994:ILE:HD12	1:A:1994:ILE:N	2.04	0.72
1:A:1920:PHE:HE2	1:A:1932:PHE:CD1	2.06	0.72
2:B:241:ARG:NH1	2:B:244:GLU:OE1	2.22	0.72
3:C:113:ILE:HG13	3:C:114:VAL:HG23	1.72	0.72
4:E:1943:MET:HE1	4:E:2000:MET:HG2	1.70	0.72
2:F:241:ARG:NH1	2:F:244:GLU:OE1	2.22	0.72
2:F:712:PRO:HB2	2:F:743:ARG:HE	1.52	0.72
1:A:1586:VAL:CG2	1:A:1587:PRO:HD3	2.19	0.72
1:A:1586:VAL:CG1	1:A:1613:ALA:HB3	2.20	0.72
1:A:1667:GLY:CA	2:B:347:ARG:O	2.38	0.72
1:A:2028:ARG:NH1	1:A:2065:MET:O	2.22	0.72
4:E:1261:GLU:OE2	2:F:489:LEU:HG	1.88	0.72
4:E:1636:GLN:HG2	2:F:394:PHE:HD1	1.54	0.72
4:E:2028:ARG:NH1	4:E:2065:MET:O	2.22	0.72
1:A:1586:VAL:HG12	1:A:1613:ALA:HB3	1.71	0.72
4:E:1611:CYS:HB3	2:F:418:LYS:HB3	1.72	0.72
2:B:246:LEU:HD21	2:B:261:ILE:HG23	1.72	0.71
3:C:106:LEU:HD11	3:C:169:ARG:HB3	1.72	0.71
1:A:1926:ASP:OD1	1:A:1927:GLU:HG3	1.90	0.71
2:F:185:LEU:O	2:F:189:GLU:HB2	1.90	0.71
2:F:246:LEU:HD21	2:F:261:ILE:HG23	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:1250:ARG:NE	2:F:785:LYS:HB2	2.06	0.71
4:E:1950:LEU:HD22	4:E:1955:ILE:HG21	1.72	0.71
4:E:1598:THR:HG22	4:E:1599:ILE:HG23	1.70	0.71
1:A:178:UNK:O	1:A:201:UNK:CB	2.38	0.71
4:E:1861:ALA:HB2	4:E:1979:MET:HB2	1.71	0.71
1:A:1586:VAL:HG23	1:A:1587:PRO:CD	2.21	0.71
2:F:51:SER:O	2:F:55:GLN:HB2	1.91	0.71
3:G:86:TYR:OH	3:G:100:CYS:N	2.24	0.71
2:B:51:SER:O	2:B:55:GLN:HB2	1.91	0.70
4:E:1185:HIS:HD2	4:E:1186:PRO:HD2	1.56	0.70
4:E:1732:GLN:NE2	4:E:1736:ASP:OD2	2.24	0.70
1:A:1404:ILE:HD13	1:A:1507:TYR:HE2	1.51	0.70
4:E:408:UNK:CB	4:E:413:UNK:CB	2.70	0.70
4:E:1955:ILE:HD12	4:E:1959:HIS:NE2	2.06	0.70
3:G:113:ILE:HG13	3:G:114:VAL:HG23	1.72	0.70
1:A:1486:MET:HE3	1:A:1489:ARG:HH21	1.55	0.70
2:B:185:LEU:O	2:B:189:GLU:HB2	1.90	0.70
1:A:1732:GLN:NE2	1:A:1736:ASP:OD2	2.24	0.70
1:A:1926:ASP:OD1	1:A:1927:GLU:N	2.25	0.70
1:A:1996:LEU:HA	1:A:2000:MET:CE	2.22	0.70
1:A:1963:ILE:HG22	1:A:1971:ILE:HD11	1.73	0.70
4:E:1590:ILE:CG1	4:E:1612:TRP:CZ3	2.71	0.70
3:G:106:LEU:HD11	3:G:169:ARG:HB3	1.72	0.70
1:A:1185:HIS:HD2	1:A:1186:PRO:HD2	1.56	0.70
2:B:587:PHE:HD1	2:B:701:HIS:HD1	1.40	0.70
4:E:1586:VAL:HG13	4:E:1613:ALA:CB	2.19	0.69
2:B:591:LYS:NZ	2:B:704:GLU:OE1	2.26	0.69
4:E:1369:THR:HG21	2:F:755:GLU:HA	1.72	0.69
1:A:1128:ARG:HD3	4:E:1051:GLU:CG	2.21	0.69
4:E:1593:LEU:HB3	4:E:1612:TRP:HH2	1.57	0.69
2:F:33:LEU:HA	2:F:37:LEU:HD12	1.74	0.69
1:A:1499:GLU:OE2	1:A:1561:ARG:NE	2.25	0.69
2:F:591:LYS:NZ	2:F:704:GLU:OE1	2.26	0.69
2:B:291:LEU:HD23	3:C:193:THR:HG21	1.73	0.69
4:E:1489:ARG:O	4:E:1493:LEU:HD13	1.93	0.69
1:A:1590:ILE:HG13	1:A:1594:VAL:CG2	2.22	0.69
1:A:1860:LEU:CB	1:A:1979:MET:HE1	2.22	0.69
3:C:86:TYR:OH	3:C:100:CYS:N	2.24	0.69
4:E:2075:MET:HA	4:E:2078:ILE:HG22	1.75	0.69
3:G:178:PHE:CE1	3:G:181:LEU:CD1	2.76	0.69
1:A:407:UNK:CB	1:A:412:UNK:CB	2.70	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1978:PHE:CD1	1:A:1982:SER:CB	2.74	0.68
4:E:1666:MET:CA	2:F:347:ARG:HG2	2.23	0.68
4:E:1938:ASN:HB3	4:E:1970:HIS:CD2	2.28	0.68
4:E:1963:ILE:HG22	4:E:1971:ILE:HD11	1.73	0.68
2:F:228:LEU:HD23	2:F:231:LYS:HD2	1.75	0.68
1:A:1938:ASN:HB3	1:A:1970:HIS:CD2	2.28	0.68
2:B:33:LEU:HA	2:B:37:LEU:HD12	1.74	0.68
2:B:228:LEU:HD23	2:B:231:LYS:HD2	1.75	0.68
4:E:1590:ILE:HB	4:E:1612:TRP:CZ3	2.28	0.68
1:A:1590:ILE:CB	1:A:1612:TRP:HZ3	2.06	0.68
4:E:449:UNK:CB	4:E:939:VAL:HG11	2.24	0.68
1:A:1946:TYR:HB3	1:A:1973:HIS:CE1	2.28	0.68
4:E:1994:ILE:HG22	4:E:1995:LYS:N	2.08	0.68
1:A:933:MET:CE	1:A:981:ARG:HB2	2.20	0.68
2:F:587:PHE:HD1	2:F:701:HIS:HD1	1.40	0.68
1:A:1114:ASN:HB3	1:A:1135:ASP:HB3	1.73	0.68
1:A:1489:ARG:O	1:A:1493:LEU:HD13	1.93	0.68
4:E:1571:GLU:OE1	4:E:1574:ARG:NH1	2.25	0.68
1:A:1014:LEU:HD21	1:A:1098:THR:HG22	1.74	0.68
1:A:1081:GLN:HE22	1:A:1142:SER:HB2	1.59	0.68
4:E:1954:GLN:HG2	4:E:2060:ARG:NH1	2.09	0.68
4:E:1014:LEU:HD21	4:E:1098:THR:HG22	1.74	0.68
4:E:1590:ILE:HA	4:E:1612:TRP:CZ3	2.29	0.68
1:A:2075:MET:HA	1:A:2078:ILE:HG22	1.75	0.68
2:B:531:ILE:HB	2:B:532:PRO:HD3	1.76	0.68
2:F:531:ILE:HB	2:F:532:PRO:HD3	1.76	0.68
2:F:346:SER:HB3	2:F:355:ARG:HH11	1.59	0.67
1:A:182:UNK:CB	1:A:201:UNK:HA	2.24	0.67
1:A:1671:GLU:OE1	2:B:348:ILE:CD1	2.43	0.67
1:A:1932:PHE:O	1:A:1936:ARG:CB	2.43	0.67
4:E:1610:LEU:HB3	2:F:400:TRP:HH2	1.60	0.67
2:B:11:GLU:O	2:B:15:GLU:HB2	1.94	0.67
4:E:1486:MET:HE3	4:E:1489:ARG:HH21	1.58	0.67
1:A:1571:GLU:OE1	1:A:1574:ARG:NH1	2.25	0.67
2:F:133:VAL:HG13	2:F:137:ARG:HD3	1.77	0.67
1:A:1994:ILE:H	1:A:1994:ILE:CD1	2.07	0.67
4:E:1978:PHE:CD1	4:E:1982:SER:HB2	2.30	0.67
2:B:323:GLU:OE2	2:B:325:THR:HB	1.95	0.67
4:E:1696:TYR:CG	4:E:1701:GLY:HA2	2.21	0.67
2:F:11:GLU:O	2:F:15:GLU:HB2	1.94	0.67
4:E:1227:MET:CB	4:E:1297:ILE:HD11	2.24	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:2072:ASN:O	4:E:2076:LYS:HB2	1.95	0.66
1:A:1227:MET:CB	1:A:1297:ILE:HD11	2.24	0.66
2:B:125:LEU:HD22	2:B:141:ILE:HG23	1.78	0.66
4:E:414:UNK:O	4:E:415:UNK:C	2.42	0.66
4:E:933:MET:HE1	4:E:981:ARG:CB	2.24	0.66
4:E:1590:ILE:CB	4:E:1612:TRP:HZ3	2.06	0.66
1:A:199:UNK:O	1:A:203:UNK:N	2.28	0.66
1:A:1924:TYR:O	1:A:1931:ALA:HB3	1.95	0.66
3:C:60:LEU:CD2	3:C:75:THR:HG22	2.12	0.66
4:E:1369:THR:HG23	4:E:1370:ILE:N	2.11	0.66
1:A:1944:ALA:CB	1:A:2016:PHE:CE1	2.79	0.66
4:E:979:HIS:O	4:E:983:ARG:HG2	1.95	0.66
4:E:1590:ILE:CG1	4:E:1594:VAL:HG23	2.15	0.66
4:E:976:ASN:ND2	4:E:1013:ILE:CG2	2.58	0.66
2:F:125:LEU:HD22	2:F:141:ILE:HG23	1.78	0.66
2:F:323:GLU:OE2	2:F:325:THR:HB	1.95	0.66
1:A:1131:CYS:SG	4:E:1101:ALA:CB	2.83	0.66
1:A:2072:ASN:O	1:A:2076:LYS:HB2	1.95	0.66
2:B:346:SER:HB2	2:B:355:ARG:HH12	1.61	0.66
3:C:206:ILE:O	3:C:210:ILE:HG23	1.96	0.66
2:B:133:VAL:HG13	2:B:137:ARG:HD3	1.77	0.66
2:B:271:ARG:HD2	3:C:249:TYR:CG	2.31	0.66
2:F:465:THR:HG23	2:F:467:GLU:H	1.61	0.65
4:E:1779:ASN:HD21	4:E:1897:GLU:HG3	1.61	0.65
4:E:1958:ARG:O	4:E:1959:HIS:ND1	2.29	0.65
4:E:1081:GLN:HE22	4:E:1142:SER:HB2	1.59	0.65
1:A:1882:PHE:CE2	1:A:1899:ILE:HG12	2.32	0.65
1:A:2024:TYR:HE2	1:A:2070:ALA:HB1	1.61	0.65
4:E:1882:PHE:CE2	4:E:1899:ILE:HG12	2.32	0.65
4:E:1212:HIS:ND1	4:E:1251:GLU:OE2	2.29	0.65
4:E:1926:ASP:OD1	4:E:1927:GLU:N	2.30	0.65
1:A:1212:HIS:ND1	1:A:1251:GLU:OE2	2.29	0.65
1:A:1544:VAL:HG22	1:A:1558:LEU:HD23	1.78	0.65
4:E:1752:PRO:HA	4:E:1755:ASP:OD2	1.97	0.65
3:C:126:THR:HG22	3:C:159:LYS:HA	1.79	0.65
4:E:1499:GLU:OE2	4:E:1561:ARG:NE	2.25	0.65
4:E:1544:VAL:HG22	4:E:1558:LEU:HD23	1.78	0.65
1:A:1691:MET:O	1:A:1695:ILE:HD12	1.97	0.65
1:A:1752:PRO:HA	1:A:1755:ASP:OD2	1.97	0.65
4:E:1586:VAL:HG23	4:E:1587:PRO:CD	2.27	0.65
4:E:1586:VAL:CG2	4:E:1587:PRO:HD3	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:126:THR:HG22	3:G:159:LYS:HA	1.79	0.65
1:A:1944:ALA:HA	1:A:2016:PHE:CZ	2.32	0.65
4:E:1994:ILE:CG2	4:E:1995:LYS:N	2.60	0.64
1:A:1590:ILE:CB	1:A:1612:TRP:CZ3	2.80	0.64
1:A:1905:ARG:CB	1:A:1961:GLY:HA2	2.26	0.64
2:B:465:THR:HG23	2:B:467:GLU:H	1.61	0.64
2:F:267:GLU:O	2:F:271:ARG:HG2	1.98	0.64
1:A:1902:CYS:O	1:A:1903:THR:OG1	2.15	0.64
2:B:397:PHE:HZ	2:B:433:ILE:HD11	1.62	0.64
2:B:267:GLU:O	2:B:271:ARG:HG2	1.98	0.64
2:F:152:LEU:HD13	2:F:171:ASP:HB3	1.80	0.64
4:E:2024:TYR:HE2	4:E:2070:ALA:HB1	1.61	0.64
1:A:1748:ILE:HG12	1:A:1758:LYS:HB3	1.80	0.64
1:A:1276:PRO:HD3	1:A:1874:LEU:HD22	1.80	0.64
4:E:1748:ILE:HG12	4:E:1758:LYS:HB3	1.80	0.64
1:A:1131:CYS:CB	4:E:1098:THR:HG23	2.26	0.64
1:A:1779:ASN:HD21	1:A:1897:GLU:HG3	1.61	0.64
1:A:1804:LEU:CA	1:A:1848:ILE:HG22	2.27	0.64
4:E:1276:PRO:HD3	4:E:1874:LEU:HD22	1.80	0.64
1:A:1974:ILE:HG21	5:A:2201:E4S:C05	2.28	0.64
3:C:109:TYR:HE1	3:C:183:PHE:HB2	1.63	0.64
4:E:1404:ILE:HD13	4:E:1507:TYR:HE2	1.55	0.64
4:E:1524:SER:HA	4:E:1527:ASN:HD22	1.63	0.64
1:A:1524:SER:HA	1:A:1527:ASN:HD22	1.63	0.63
4:E:1655:PRO:HA	4:E:1690:ASN:ND2	2.13	0.63
4:E:1952:LEU:O	4:E:1953:LEU:HD23	1.98	0.63
3:G:206:ILE:O	3:G:210:ILE:HG23	1.96	0.63
1:A:1655:PRO:HA	1:A:1690:ASN:ND2	2.13	0.63
2:F:86:LEU:HD23	2:F:96:LEU:HD22	1.81	0.63
1:A:1134:LYS:HG3	1:A:1136:TYR:CZ	2.33	0.63
4:E:1932:PHE:O	4:E:1936:ARG:CB	2.46	0.63
1:A:1585:ASP:OD1	1:A:1589:ALA:HB2	1.97	0.63
2:B:152:LEU:HD13	2:B:171:ASP:HB3	1.80	0.63
4:E:951:MET:HE1	4:E:954:LYS:HE3	1.79	0.63
1:A:1250:ARG:HE	2:B:785:LYS:HD3	1.62	0.63
4:E:1956:LYS:HG3	4:E:1982:SER:OG	1.98	0.63
3:G:216:PRO:HA	3:G:219:HIS:ND1	2.13	0.63
1:A:1400:LEU:HD21	1:A:1507:TYR:CD2	2.32	0.63
1:A:1632:PRO:HG3	2:B:345:LEU:HD13	1.81	0.63
4:E:1344:ALA:HA	4:E:1395:GLN:NE2	2.13	0.63
4:E:1691:MET:O	4:E:1695:ILE:HD12	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:1886:VAL:CG2	4:E:1896:ILE:HG22	2.29	0.63
2:F:397:PHE:HZ	2:F:433:ILE:HD11	1.62	0.63
4:E:1952:LEU:C	4:E:1953:LEU:HD23	2.20	0.63
4:E:1954:GLN:CG	4:E:2060:ARG:NH2	2.62	0.63
1:A:1979:MET:HE3	1:A:1980:PHE:CE2	2.34	0.63
3:C:216:PRO:HA	3:C:219:HIS:ND1	2.13	0.63
2:F:167:ASP:OD2	2:F:170:GLN:N	2.31	0.63
1:A:27:UNK:HA	2:B:821:PHE:CD2	2.34	0.62
4:E:1957:ASP:HB2	4:E:1993:ASP:O	1.99	0.62
4:E:2021:VAL:HG12	4:E:2074:ILE:HG23	1.81	0.62
2:F:173:ILE:O	2:F:177:GLU:HB2	1.98	0.62
1:A:2032:ASP:O	1:A:2036:SER:HB3	1.99	0.62
1:A:413:UNK:O	1:A:414:UNK:C	2.42	0.62
1:A:976:ASN:ND2	1:A:1013:ILE:HG21	2.14	0.62
4:E:1631:HIS:HD2	4:E:1632:PRO:HD2	1.64	0.62
2:B:544:LEU:HD13	3:C:229:ARG:NH2	2.14	0.62
4:E:1405:SER:OG	4:E:1409:LYS:NZ	2.33	0.62
4:E:1804:LEU:CA	4:E:1848:ILE:HG22	2.27	0.62
1:A:1349:ARG:NH2	1:A:1381:THR:O	2.32	0.62
1:A:1963:ILE:HD13	1:A:1995:LYS:HD2	1.82	0.62
4:E:1586:VAL:HG12	4:E:1613:ALA:HB3	1.80	0.62
2:F:131:THR:HA	2:F:308:ARG:HH11	1.64	0.62
2:F:184:LEU:HD11	2:F:245:LEU:HD23	1.81	0.62
1:A:951:MET:HE1	1:A:954:LYS:HE3	1.80	0.62
1:A:1632:PRO:HG2	2:B:345:LEU:CD1	2.21	0.62
1:A:2021:VAL:HG12	1:A:2074:ILE:HG23	1.81	0.62
2:B:131:THR:HA	2:B:308:ARG:HH11	1.64	0.62
2:B:173:ILE:O	2:B:177:GLU:HB2	1.98	0.62
3:C:63:PHE:HD2	3:C:75:THR:HG21	1.64	0.62
3:G:63:PHE:HD2	3:G:75:THR:HG21	1.64	0.62
2:B:184:LEU:HD11	2:B:245:LEU:HD23	1.81	0.62
4:E:1250:ARG:HE	2:F:785:LYS:HB2	1.64	0.62
4:E:1349:ARG:NH2	4:E:1381:THR:O	2.32	0.62
3:G:109:TYR:HE1	3:G:183:PHE:HB2	1.63	0.62
1:A:1529:ARG:HA	1:A:1532:TYR:CE2	2.35	0.62
1:A:1344:ALA:HA	1:A:1395:GLN:NE2	2.13	0.62
2:B:86:LEU:HD23	2:B:96:LEU:HD22	1.81	0.62
2:B:167:ASP:OD2	2:B:170:GLN:N	2.31	0.62
3:C:116:LYS:NZ	3:C:121:LYS:HB2	2.15	0.62
2:F:330:LEU:HD11	3:G:137:HIS:HE1	1.64	0.62
3:G:116:LYS:NZ	3:G:121:LYS:HB2	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1405:SER:OG	1:A:1409:LYS:NZ	2.33	0.61
4:E:1527:ASN:O	4:E:1531:LYS:HG2	1.99	0.61
1:A:1077:LYS:O	1:A:1081:GLN:CB	2.48	0.61
1:A:1227:MET:HB3	1:A:1297:ILE:HD11	1.81	0.61
1:A:1886:VAL:CG2	1:A:1896:ILE:HG22	2.29	0.61
4:E:1130:ALA:O	4:E:1131:CYS:CB	2.48	0.61
4:E:1339:MET:HE1	4:E:1349:ARG:HA	1.82	0.61
4:E:1666:MET:HA	2:F:347:ARG:CB	2.30	0.61
1:A:1586:VAL:CG1	1:A:1613:ALA:HB1	2.30	0.61
4:E:1401:ARG:HH22	4:E:1516:GLU:HB2	1.65	0.61
4:E:2032:ASP:O	4:E:2036:SER:HB3	1.99	0.61
2:F:323:GLU:OE2	2:F:326:GLU:HG3	2.00	0.61
1:A:1527:ASN:O	1:A:1531:LYS:HG2	1.99	0.61
1:A:1778:SER:O	1:A:1885:ARG:NH2	2.34	0.61
3:C:138:GLU:OE2	3:C:141:SER:HB2	2.00	0.61
4:E:1610:LEU:HB3	2:F:400:TRP:CH2	2.35	0.61
3:G:138:GLU:OE2	3:G:141:SER:HB2	2.00	0.61
1:A:1131:CYS:HB2	4:E:1098:THR:HA	1.83	0.61
1:A:1886:VAL:HG13	1:A:1896:ILE:HG22	1.82	0.61
1:A:1159:PHE:HD2	4:E:1159:PHE:HD2	1.48	0.61
1:A:1932:PHE:O	1:A:1936:ARG:HB2	2.01	0.61
4:E:1227:MET:HB3	4:E:1297:ILE:HD11	1.81	0.61
4:E:1250:ARG:NH2	2:F:781:SER:HB3	2.15	0.61
4:E:1667:GLY:N	2:F:347:ARG:O	2.33	0.61
2:B:346:SER:O	2:B:348:ILE:HG12	2.01	0.61
2:B:700:LEU:HD22	2:B:735:MET:HG3	1.83	0.61
4:E:1529:ARG:HA	4:E:1532:TYR:CE2	2.35	0.61
1:A:1401:ARG:HH22	1:A:1516:GLU:HB2	1.65	0.61
4:E:1639:VAL:HG21	2:F:394:PHE:HE1	1.66	0.61
2:F:700:LEU:HD22	2:F:735:MET:HG3	1.83	0.61
1:A:1631:HIS:HD2	1:A:1632:PRO:HD2	1.64	0.61
1:A:1860:LEU:HB3	1:A:1979:MET:CE	2.30	0.61
4:E:1132:VAL:O	4:E:1132:VAL:HG12	2.01	0.61
4:E:1886:VAL:HG13	4:E:1896:ILE:HG22	1.82	0.61
4:E:1077:LYS:O	4:E:1081:GLN:CB	2.48	0.60
4:E:1778:SER:O	4:E:1885:ARG:NH2	2.34	0.60
4:E:1953:LEU:HD22	4:E:1980:PHE:CE1	2.35	0.60
4:E:1586:VAL:HG12	4:E:1613:ALA:C	2.22	0.60
1:A:977:HIS:HD2	1:A:982:ILE:HB	1.65	0.60
3:G:75:THR:HG22	3:G:75:THR:O	2.01	0.60
3:C:214:GLY:HA3	3:C:229:ARG:HG3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:277:SER:OG	3:C:193:THR:HB	2.01	0.60
3:C:12:TRP:O	3:C:15:GLU:HG3	2.02	0.60
3:C:58:HIS:O	3:C:61:PHE:HB3	2.02	0.60
4:E:1538:LYS:HG3	4:E:1539:GLN:OE1	2.02	0.60
2:F:113:TYR:HB3	2:F:155:LEU:HD21	1.82	0.60
2:F:348:ILE:HG13	2:F:348:ILE:O	2.01	0.60
4:E:1332:ILE:HG21	4:E:1551:SER:HB2	1.84	0.60
4:E:1655:PRO:HA	4:E:1690:ASN:HD21	1.67	0.60
2:F:539:ARG:O	2:F:543:GLN:HB2	2.01	0.60
3:G:12:TRP:O	3:G:15:GLU:HG3	2.02	0.60
2:B:94:GLU:HB2	2:B:137:ARG:HH12	1.67	0.60
3:G:58:HIS:O	3:G:61:PHE:HB3	2.02	0.60
2:B:172:VAL:O	2:B:176:TYR:HB2	2.02	0.60
3:C:75:THR:HG22	3:C:75:THR:O	2.01	0.60
2:F:330:LEU:HD11	3:G:137:HIS:CE1	2.36	0.60
2:B:275:GLU:OE1	3:C:190:ALA:HA	2.01	0.60
1:A:1128:ARG:CD	4:E:1051:GLU:HG3	2.28	0.60
1:A:1852:GLY:N	1:A:1892:GLY:O	2.33	0.60
4:E:1522:GLU:OE1	4:E:1522:GLU:N	2.32	0.59
2:F:172:VAL:O	2:F:176:TYR:HB2	2.02	0.59
4:E:2010:ALA:O	4:E:2014:LYS:N	2.28	0.59
1:A:1128:ARG:NH1	1:A:1130:ALA:HB2	2.17	0.59
1:A:2071:ALA:O	1:A:2075:MET:HG2	2.02	0.59
3:C:123:LEU:HB3	3:C:162:TYR:CZ	2.37	0.59
2:F:452:GLU:HG2	2:F:456:LYS:HE2	1.83	0.59
2:F:751:ARG:O	2:F:755:GLU:HG2	2.02	0.59
2:B:113:TYR:HB3	2:B:155:LEU:HD21	1.82	0.59
2:B:539:ARG:O	2:B:543:GLN:HB2	2.01	0.59
3:G:123:LEU:HB3	3:G:162:TYR:CZ	2.37	0.59
1:A:1655:PRO:HA	1:A:1690:ASN:HD21	1.67	0.59
2:B:452:GLU:HG2	2:B:456:LYS:HE2	1.83	0.59
2:B:751:ARG:O	2:B:755:GLU:HG2	2.02	0.59
2:B:11:GLU:O	2:B:15:GLU:CB	2.50	0.59
2:B:496:LEU:HD23	2:B:499:LYS:HD2	1.85	0.59
4:E:1756:GLU:O	4:E:1759:LYS:HG2	2.03	0.59
2:F:341:ARG:HH22	3:G:145:MET:HE2	1.68	0.59
1:A:29:UNK:CB	2:B:809:GLN:HE22	2.16	0.59
1:A:1538:LYS:HG3	1:A:1539:GLN:OE1	2.02	0.59
1:A:1132:VAL:O	1:A:1132:VAL:HG12	2.01	0.59
1:A:1590:ILE:HG13	1:A:1594:VAL:HG21	1.83	0.59
4:E:1963:ILE:HG12	4:E:1973:HIS:CD2	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:2071:ALA:O	4:E:2075:MET:HG2	2.02	0.59
1:A:1562:PHE:O	1:A:1563:LYS:HE2	2.03	0.59
1:A:1685:HIS:HE1	1:A:1730:PHE:HD2	1.51	0.59
1:A:1857:GLN:O	1:A:1979:MET:SD	2.61	0.59
1:A:1963:ILE:HG12	1:A:1973:HIS:CD2	2.38	0.59
1:A:442:UNK:C	1:A:444:UNK:N	2.65	0.58
1:A:1756:GLU:O	1:A:1759:LYS:HG2	2.02	0.58
1:A:1943:MET:HG3	1:A:2016:PHE:HE1	1.67	0.58
4:E:1953:LEU:HD22	4:E:1980:PHE:HE1	1.65	0.58
1:A:1128:ARG:HA	4:E:1055:LYS:HB3	1.84	0.58
1:A:27:UNK:HA	2:B:821:PHE:HD2	1.68	0.58
1:A:1332:ILE:HG21	1:A:1551:SER:HB2	1.84	0.58
4:E:1277:LEU:HD22	4:E:1616:ASP:OD2	2.03	0.58
4:E:1902:CYS:O	4:E:1903:THR:OG1	2.15	0.58
2:F:319:PHE:HB2	3:G:132:LYS:HE2	1.85	0.58
1:A:1386:PHE:HZ	1:A:1496:LEU:HD23	1.69	0.58
2:B:422:GLU:OE1	2:B:425:ARG:NH2	2.36	0.58
4:E:1014:LEU:HB2	4:E:1057:PHE:HE2	1.67	0.58
4:E:1685:HIS:HE1	4:E:1730:PHE:HD2	1.51	0.58
4:E:1862:LEU:HD11	4:E:1883:PRO:O	2.03	0.58
3:G:186:LEU:HD12	3:G:189:ASN:HB3	1.86	0.58
1:A:1590:ILE:HG13	1:A:1594:VAL:HG23	1.85	0.58
1:A:1651:LEU:CD1	1:A:1686:GLN:HG3	2.33	0.58
4:E:1044:PRO:HD2	4:E:1050:ARG:HG2	1.85	0.58
1:A:1317:VAL:HG11	1:A:1364:VAL:HG11	1.85	0.58
2:F:11:GLU:O	2:F:15:GLU:CB	2.50	0.58
4:E:1010:MET:HE2	4:E:1061:CYS:HA	1.86	0.58
4:E:1360:LEU:HD21	4:E:1375:ARG:CZ	2.33	0.58
4:E:1896:ILE:HD12	4:E:1896:ILE:O	2.04	0.58
2:F:422:GLU:OE1	2:F:425:ARG:NH2	2.36	0.58
1:A:1196:LEU:HD23	1:A:1214:LEU:HD13	1.85	0.58
1:A:1360:LEU:HD21	1:A:1375:ARG:CZ	2.33	0.58
1:A:2006:GLY:HA2	1:A:2010:ALA:HB3	1.86	0.58
4:E:1400:LEU:HD21	4:E:1507:TYR:CD2	2.39	0.58
4:E:1501:GLU:HA	4:E:1504:ILE:HG22	1.86	0.58
4:E:2006:GLY:HA2	4:E:2010:ALA:HB3	1.84	0.58
2:F:346:SER:CB	2:F:355:ARG:NH1	2.43	0.58
1:A:1404:ILE:HD11	1:A:1503:LEU:HB3	1.86	0.58
1:A:1896:ILE:O	1:A:1896:ILE:HD12	2.04	0.58
4:E:1386:PHE:HZ	4:E:1496:LEU:HD23	1.69	0.58
4:E:1404:ILE:HD11	4:E:1503:LEU:HB3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:1562:PHE:O	4:E:1563:LYS:HE2	2.03	0.58
1:A:1794:PRO:HA	1:A:1804:LEU:H	1.69	0.57
4:E:1141:ALA:O	4:E:1145:LEU:HG	2.04	0.57
1:A:1014:LEU:HB2	1:A:1057:PHE:HE2	1.67	0.57
2:F:94:GLU:HB2	2:F:137:ARG:HH12	1.67	0.57
1:A:1862:LEU:HD11	1:A:1883:PRO:O	2.03	0.57
4:E:1370:ILE:HG12	2:F:758:ALA:HB2	1.85	0.57
2:F:247:ARG:NH1	2:F:281:PRO:O	2.38	0.57
2:F:496:LEU:HD23	2:F:499:LYS:HD2	1.85	0.57
1:A:939:VAL:HA	1:A:942:LYS:HZ3	1.70	0.57
1:A:1044:PRO:HD2	1:A:1050:ARG:HG2	1.85	0.57
1:A:1501:GLU:HA	1:A:1504:ILE:HG22	1.86	0.57
2:B:112:ASP:OD2	2:B:115:GLU:HB3	2.05	0.57
1:A:1921:THR:HG23	1:A:1926:ASP:HA	1.87	0.57
2:B:175:CYS:O	2:B:179:ALA:HB2	2.04	0.57
2:B:247:ARG:NH1	2:B:281:PRO:O	2.38	0.57
4:E:1299:ILE:O	4:E:1303:VAL:HG23	2.04	0.57
1:A:1113:TYR:O	1:A:1135:ASP:HB3	2.04	0.57
4:E:1852:GLY:N	4:E:1892:GLY:O	2.33	0.57
1:A:1277:LEU:HD22	1:A:1616:ASP:OD2	2.03	0.57
1:A:1512:ALA:HB3	1:A:1513:PRO:HD3	1.86	0.57
2:B:389:ALA:O	2:B:399:LEU:HD21	2.05	0.57
2:F:112:ASP:OD2	2:F:115:GLU:HB3	2.05	0.57
2:F:408:MET:HE1	2:F:436:LEU:HB3	1.86	0.57
1:A:1141:ALA:O	1:A:1145:LEU:HG	2.04	0.57
4:E:1317:VAL:HG11	4:E:1364:VAL:HG11	1.85	0.57
1:A:1299:ILE:O	1:A:1303:VAL:HG23	2.04	0.57
1:A:1683:LEU:HG	1:A:1687:PHE:HE2	1.70	0.57
4:E:1196:LEU:HD23	4:E:1214:LEU:HD13	1.85	0.57
2:F:175:CYS:O	2:F:179:ALA:HB2	2.04	0.57
2:F:402:GLN:NE2	3:G:277:LEU:HD12	2.19	0.57
1:A:1786:ASP:OD1	1:A:1787:ILE:N	2.38	0.56
2:B:491:GLY:O	2:B:495:VAL:HG23	2.05	0.56
4:E:1779:ASN:ND2	4:E:1897:GLU:HG3	2.20	0.56
2:F:487:ALA:O	2:F:493:GLN:NE2	2.33	0.56
1:A:1924:TYR:O	1:A:1931:ALA:CB	2.53	0.56
2:B:340:ASN:OD1	2:B:340:ASN:O	2.23	0.56
3:C:253:TRP:CH2	3:C:286:LEU:HD22	2.40	0.56
4:E:1950:LEU:HD22	4:E:1955:ILE:CG2	2.36	0.56
3:G:245:TYR:HA	3:G:248:PHE:HD2	1.70	0.56
1:A:182:UNK:CB	1:A:201:UNK:O	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1590:ILE:HB	1:A:1612:TRP:CE3	2.39	0.56
1:A:1860:LEU:CG	1:A:1979:MET:HE1	2.34	0.56
1:A:1896:ILE:HD13	5:A:2201:E4S:C06	2.35	0.56
3:C:186:LEU:HD12	3:C:189:ASN:HB3	1.86	0.56
4:E:1512:ALA:HB3	4:E:1513:PRO:HD3	1.86	0.56
4:E:1590:ILE:CA	4:E:1612:TRP:CZ3	2.88	0.56
4:E:1786:ASP:OD1	4:E:1787:ILE:N	2.38	0.56
2:F:587:PHE:HD1	2:F:701:HIS:CE1	2.05	0.56
2:B:784:GLU:O	2:B:788:ARG:HG2	2.05	0.56
3:C:245:TYR:HA	3:C:248:PHE:HD2	1.70	0.56
2:F:784:GLU:O	2:F:788:ARG:HG2	2.05	0.56
3:G:253:TRP:CH2	3:G:286:LEU:HD22	2.41	0.56
1:A:1192:ALA:HA	1:A:1195:LYS:NZ	2.21	0.56
4:E:976:ASN:HD21	4:E:1013:ILE:HG23	1.71	0.56
2:F:389:ALA:O	2:F:399:LEU:HD21	2.05	0.56
2:F:737:GLY:HA3	2:F:753:TYR:CE1	2.41	0.56
1:A:1779:ASN:ND2	1:A:1897:GLU:HG3	2.20	0.56
4:E:2011:THR:N	4:E:2012:PRO:HD2	2.21	0.56
1:A:1227:MET:HB2	1:A:1297:ILE:HD11	1.87	0.56
1:A:1486:MET:HE3	1:A:1489:ARG:NH2	2.21	0.56
2:F:491:GLY:O	2:F:495:VAL:HG23	2.05	0.56
1:A:1580:PRO:HG2	1:A:1608:HIS:NE2	2.21	0.56
1:A:1586:VAL:CG2	1:A:1587:PRO:CD	2.83	0.56
1:A:1979:MET:CE	1:A:1980:PHE:CE2	2.89	0.56
4:E:1946:TYR:HB3	4:E:1973:HIS:CE1	2.41	0.56
1:A:1098:THR:HA	4:E:1131:CYS:HB2	1.87	0.55
2:B:144:ALA:O	2:B:148:LYS:HB2	2.06	0.55
2:B:155:LEU:O	2:B:168:ARG:NH2	2.40	0.55
2:B:271:ARG:HD2	3:C:249:TYR:CD1	2.41	0.55
4:E:1261:GLU:OE2	2:F:488:SER:OG	2.22	0.55
4:E:1921:THR:HG23	4:E:1926:ASP:HA	1.87	0.55
1:A:1400:LEU:HD21	1:A:1507:TYR:HD2	1.72	0.55
1:A:1687:PHE:O	1:A:1691:MET:HG2	2.06	0.55
2:B:107:ASN:HB3	2:B:112:ASP:HB3	1.89	0.55
2:F:82:LEU:HD11	2:F:102:ILE:HG22	1.89	0.55
1:A:1522:GLU:OE1	1:A:1522:GLU:N	2.32	0.55
2:B:82:LEU:HD11	2:B:102:ILE:HG22	1.88	0.55
4:E:1586:VAL:HG12	4:E:1613:ALA:CB	2.36	0.55
4:E:1896:ILE:HD13	5:E:2201:E4S:C06	2.37	0.55
2:F:26:ILE:HD13	2:F:29:LEU:HD12	1.87	0.55
1:A:1330:LEU:O	1:A:1330:LEU:HD23	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:1508:ASN:N	4:E:1509:PRO:HD3	2.21	0.55
4:E:1621:LEU:CD2	4:E:1642:LEU:HD11	2.36	0.55
3:G:237:MET:O	3:G:241:LEU:HG	2.07	0.55
2:B:493:GLN:O	2:B:497:GLN:HG3	2.07	0.55
4:E:1192:ALA:HA	4:E:1195:LYS:NZ	2.21	0.55
4:E:1651:LEU:CD1	4:E:1686:GLN:HG3	2.34	0.55
2:F:787:LEU:O	2:F:791:VAL:HG23	2.06	0.55
2:B:26:ILE:HD13	2:B:29:LEU:HD12	1.87	0.55
2:B:104:ALA:HA	2:B:107:ASN:HD22	1.70	0.55
2:B:752:TRP:HA	2:B:755:GLU:CG	2.37	0.55
4:E:976:ASN:ND2	4:E:1013:ILE:HG23	2.21	0.55
4:E:1227:MET:HB2	4:E:1297:ILE:HD11	1.87	0.55
4:E:1371:ARG:O	4:E:1375:ARG:CB	2.55	0.55
1:A:1030:PRO:O	1:A:1043:VAL:HG22	2.07	0.55
1:A:1647:PRO:O	1:A:1651:LEU:HB2	2.07	0.55
1:A:1759:LYS:O	1:A:1762:LEU:HB3	2.06	0.55
2:B:737:GLY:HA3	2:B:753:TYR:CE1	2.41	0.55
4:E:1580:PRO:HG2	4:E:1608:HIS:NE2	2.21	0.55
4:E:1944:ALA:CA	4:E:2016:PHE:CE1	2.89	0.55
4:E:2024:TYR:CE2	4:E:2070:ALA:HB1	2.42	0.55
1:A:1993:ASP:CG	1:A:1994:ILE:HD12	2.27	0.55
2:B:42:ASP:HB2	2:B:91:LEU:HG	1.89	0.55
4:E:1661:LEU:HD21	4:E:1673:ILE:HD12	1.89	0.55
2:B:274:CYS:HB3	3:C:192:LEU:H	1.71	0.55
4:E:1216:TRP:CH2	4:E:1255:ALA:HA	2.42	0.55
2:F:104:ALA:HA	2:F:107:ASN:HD22	1.70	0.55
2:B:534:ALA:O	2:B:538:VAL:HG23	2.07	0.55
4:E:1683:LEU:HG	4:E:1687:PHE:HE2	1.70	0.55
4:E:1794:PRO:HA	4:E:1804:LEU:H	1.70	0.55
2:F:155:LEU:O	2:F:168:ARG:NH2	2.40	0.55
2:F:707:ILE:HD11	2:F:739:ILE:HG12	1.88	0.55
1:A:1261:GLU:OE2	2:B:489:LEU:HG	2.06	0.54
1:A:1339:MET:HE1	1:A:1349:ARG:HA	1.87	0.54
1:A:1661:LEU:HD21	1:A:1673:ILE:HD12	1.89	0.54
2:B:420:LEU:HD22	2:B:433:ILE:HG23	1.88	0.54
2:B:787:LEU:O	2:B:791:VAL:HG23	2.06	0.54
3:C:116:LYS:HZ2	3:C:121:LYS:HB2	1.72	0.54
4:E:1639:VAL:HG21	2:F:394:PHE:CE1	2.43	0.54
3:G:85:CYS:SG	3:G:86:TYR:N	2.81	0.54
4:E:1687:PHE:O	4:E:1691:MET:HG2	2.06	0.54
2:F:493:GLN:O	2:F:497:GLN:HG3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:752:TRP:HA	2:F:755:GLU:CG	2.37	0.54
3:G:28:ALA:HA	3:G:71:LEU:HD21	1.89	0.54
1:A:182:UNK:CA	1:A:201:UNK:CB	2.85	0.54
1:A:1114:ASN:OD1	1:A:1117:ASN:N	2.38	0.54
2:B:707:ILE:HD11	2:B:739:ILE:HG12	1.88	0.54
4:E:1621:LEU:HD21	4:E:1642:LEU:HD11	1.88	0.54
4:E:1759:LYS:O	4:E:1762:LEU:HB3	2.07	0.54
2:F:144:ALA:O	2:F:148:LYS:HB2	2.06	0.54
3:G:60:LEU:CD2	3:G:75:THR:HG21	2.37	0.54
1:A:1201:ILE:HD11	1:A:1237:LEU:HA	1.89	0.54
1:A:1216:TRP:CH2	1:A:1255:ALA:HA	2.42	0.54
2:B:341:ARG:HH12	3:C:145:MET:HE2	1.73	0.54
4:E:939:VAL:HA	4:E:942:LYS:HZ3	1.72	0.54
4:E:1636:GLN:HG2	2:F:394:PHE:CD1	2.41	0.54
2:F:42:ASP:HB2	2:F:91:LEU:HG	1.89	0.54
2:F:176:TYR:HB3	2:F:225:ALA:HB2	1.90	0.54
1:A:182:UNK:N	1:A:201:UNK:CB	2.70	0.54
1:A:1849:PHE:CD1	1:A:1895:VAL:HG22	2.43	0.54
1:A:2010:ALA:O	1:A:2014:LYS:HG3	2.07	0.54
4:E:1367:ASN:ND2	4:E:1369:THR:HG22	2.22	0.54
4:E:1569:GLY:O	4:E:1573:THR:CB	2.55	0.54
4:E:1952:LEU:O	4:E:2060:ARG:NH1	2.40	0.54
2:F:101:LEU:HD11	2:F:125:LEU:HD21	1.90	0.54
1:A:1154:TYR:O	1:A:1158:ARG:HG2	2.08	0.54
1:A:1621:LEU:HD21	1:A:1642:LEU:HD11	1.88	0.54
2:B:224:ARG:CZ	2:B:228:LEU:HD21	2.38	0.54
2:B:768:GLN:HE21	2:B:800:VAL:HG23	1.73	0.54
3:C:237:MET:O	3:C:241:LEU:HG	2.07	0.54
4:E:1647:PRO:O	4:E:1651:LEU:HB2	2.07	0.54
4:E:1974:ILE:HG21	5:E:2201:E4S:C05	2.37	0.54
2:F:246:LEU:HD21	2:F:261:ILE:CG2	2.38	0.54
1:A:1621:LEU:CD2	1:A:1642:LEU:HD11	2.36	0.54
1:A:1682:LEU:HD11	1:A:1780:PRO:HB3	1.89	0.54
1:A:1877:LEU:HB3	1:A:1879:LEU:HD13	1.89	0.54
2:B:251:THR:HG22	2:B:253:THR:H	1.73	0.54
3:C:135:VAL:HG13	3:C:136:TYR:CD1	2.43	0.54
4:E:1030:PRO:O	4:E:1043:VAL:HG22	2.07	0.54
4:E:1201:ILE:HD11	4:E:1237:LEU:HA	1.89	0.54
4:E:1849:PHE:CD1	4:E:1895:VAL:HG22	2.43	0.54
4:E:968:ALA:O	4:E:972:LEU:HG	2.08	0.54
2:F:242:PHE:HD2	2:F:265:LEU:HD13	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:515:HIS:CD2	3:G:229:ARG:NH1	2.75	0.54
4:E:1617:PRO:HD3	4:E:1645:PHE:HE2	1.72	0.54
2:F:107:ASN:HB3	2:F:112:ASP:HB3	1.89	0.54
2:F:224:ARG:CZ	2:F:228:LEU:HD21	2.38	0.54
2:F:534:ALA:O	2:F:538:VAL:HG23	2.07	0.54
1:A:1339:MET:CE	1:A:1349:ARG:HA	2.37	0.54
1:A:1617:PRO:HD3	1:A:1645:PHE:HE2	1.72	0.54
4:E:1330:LEU:HD23	4:E:1330:LEU:O	2.07	0.54
4:E:1339:MET:CE	4:E:1349:ARG:HA	2.37	0.54
4:E:1951:PHE:HD2	4:E:1952:LEU:HD22	1.74	0.54
1:A:1890:ALA:HB1	1:A:1891:PRO:HD2	1.89	0.53
4:E:1757:ARG:O	4:E:1760:ALA:HB3	2.08	0.53
4:E:1877:LEU:HB3	4:E:1879:LEU:HD13	1.89	0.53
2:F:137:ARG:HG2	2:F:141:ILE:HD12	1.89	0.53
2:F:250:GLU:OE2	2:F:255:GLN:HG2	2.09	0.53
2:F:420:LEU:HD22	2:F:433:ILE:HG23	1.88	0.53
3:G:156:GLY:O	3:G:157:LEU:HD23	2.08	0.53
3:G:211:CYS:O	3:G:266:ARG:NH2	2.37	0.53
1:A:1509:PRO:HG2	1:A:2022:ARG:HE	1.73	0.53
1:A:2011:THR:N	1:A:2012:PRO:HD2	2.22	0.53
2:B:137:ARG:HG2	2:B:141:ILE:HD12	1.89	0.53
2:B:176:TYR:HB3	2:B:225:ALA:HB2	1.90	0.53
3:C:85:CYS:SG	3:C:86:TYR:N	2.80	0.53
4:E:975:PHE:O	4:E:983:ARG:HB2	2.08	0.53
4:E:1682:LEU:HD11	4:E:1780:PRO:HB3	1.89	0.53
4:E:1794:PRO:HA	4:E:1804:LEU:N	2.24	0.53
1:A:1339:MET:HE2	1:A:1349:ARG:HG3	1.90	0.53
1:A:1569:GLY:O	1:A:1573:THR:CB	2.55	0.53
1:A:1747:ILE:HD12	1:A:1748:ILE:HG13	1.91	0.53
2:B:487:ALA:O	2:B:493:GLN:NE2	2.33	0.53
3:C:83:ILE:O	3:C:87:LEU:CB	2.50	0.53
3:C:199:SER:O	3:C:203:LEU:HB3	2.09	0.53
4:E:1238:LEU:HD11	4:E:1248:PHE:CD2	2.44	0.53
4:E:1332:ILE:CG2	4:E:1551:SER:HB2	2.38	0.53
4:E:1942:SER:OG	4:E:1971:ILE:HG22	2.08	0.53
3:G:126:THR:HG22	3:G:159:LYS:CB	2.39	0.53
1:A:1411:TRP:CE3	1:A:1525:VAL:HG22	2.43	0.53
2:B:814:ASP:HA	2:B:817:ALA:HB3	1.91	0.53
1:A:1371:ARG:O	1:A:1375:ARG:CB	2.55	0.53
1:A:1905:ARG:HG2	1:A:1961:GLY:H	1.72	0.53
2:B:242:PHE:HD2	2:B:265:LEU:HD13	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1091:VAL:HG13	4:E:1225:HIS:HE1	1.73	0.53
1:A:1332:ILE:CG2	1:A:1551:SER:HB2	2.38	0.53
1:A:1568:ILE:HD12	1:A:1569:GLY:N	2.24	0.53
1:A:1794:PRO:HA	1:A:1804:LEU:N	2.23	0.53
1:A:2011:THR:OG1	1:A:2012:PRO:HD3	2.08	0.53
4:E:1154:TYR:O	4:E:1158:ARG:HG2	2.08	0.53
4:E:1569:GLY:O	4:E:1573:THR:HB	2.09	0.53
2:F:119:ILE:HG12	2:F:122:ARG:HH22	1.74	0.53
2:F:251:THR:HG22	2:F:253:THR:H	1.73	0.53
2:F:405:LEU:HB2	3:G:277:LEU:HD13	1.91	0.53
3:G:50:SER:O	3:G:53:LEU:HD13	2.09	0.53
1:A:1569:GLY:O	1:A:1573:THR:HB	2.09	0.53
1:A:1636:GLN:O	1:A:1640:LYS:HG3	2.09	0.53
4:E:1636:GLN:O	4:E:1640:LYS:HG3	2.09	0.53
2:F:768:GLN:HE21	2:F:800:VAL:HG23	1.73	0.53
1:A:968:ALA:O	1:A:972:LEU:HG	2.08	0.53
1:A:1943:MET:HG3	1:A:2016:PHE:CE1	2.43	0.53
1:A:1951:PHE:HD2	1:A:1952:LEU:HD22	1.74	0.53
2:B:101:LEU:HD11	2:B:125:LEU:HD21	1.90	0.53
2:B:120:TYR:HB3	2:B:148:LYS:HE3	1.91	0.53
3:C:28:ALA:HA	3:C:71:LEU:HD21	1.90	0.53
4:E:1193:MET:HG2	4:E:1233:CYS:SG	2.49	0.53
4:E:1857:GLN:O	4:E:1979:MET:SD	2.67	0.53
1:A:1757:ARG:O	1:A:1760:ALA:HB3	2.09	0.53
2:B:119:ILE:HG12	2:B:122:ARG:HH22	1.74	0.53
2:B:246:LEU:HD21	2:B:261:ILE:CG2	2.38	0.53
2:B:469:LYS:HE2	2:B:473:TYR:HE2	1.74	0.53
3:C:156:GLY:O	3:C:157:LEU:HD23	2.08	0.53
4:E:1890:ALA:HB1	4:E:1891:PRO:HD2	1.89	0.53
4:E:1974:ILE:HG21	5:E:2201:E4S:C07	2.39	0.53
4:E:2032:ASP:O	4:E:2036:SER:CB	2.56	0.53
3:G:135:VAL:HG13	3:G:136:TYR:CD1	2.43	0.53
1:A:1010:MET:HE2	1:A:1061:CYS:HA	1.91	0.52
2:B:544:LEU:HD13	3:C:229:ARG:HH22	1.74	0.52
4:E:1190:THR:HG23	4:E:1194:PHE:HE2	1.74	0.52
4:E:1411:TRP:CE3	4:E:1525:VAL:HG22	2.43	0.52
4:E:1568:ILE:HD12	4:E:1569:GLY:N	2.24	0.52
4:E:1632:PRO:CG	2:F:345:LEU:HD13	2.39	0.52
4:E:1908:LEU:HD13	4:E:1919:TYR:HB2	1.90	0.52
4:E:2010:ALA:O	4:E:2014:LYS:HG3	2.08	0.52
1:A:1250:ARG:HD3	2:B:785:LYS:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1292:VAL:HB	1:A:1348:PRO:HG2	1.91	0.52
2:B:703:ALA:O	2:B:707:ILE:HG12	2.09	0.52
3:C:221:ARG:NH1	3:C:258:LYS:HB3	2.25	0.52
1:A:1908:LEU:HD13	1:A:1919:TYR:HB2	1.90	0.52
1:A:2024:TYR:CE2	1:A:2070:ALA:HB1	2.42	0.52
1:A:2032:ASP:O	1:A:2036:SER:CB	2.56	0.52
3:C:60:LEU:CD2	3:C:75:THR:HG21	2.37	0.52
4:E:1683:LEU:HG	4:E:1687:PHE:CE2	2.44	0.52
1:A:1238:LEU:HD11	1:A:1248:PHE:CD2	2.44	0.52
1:A:1486:MET:O	1:A:1489:ARG:HG2	2.10	0.52
1:A:1932:PHE:CE1	1:A:1936:ARG:HD3	2.24	0.52
1:A:2024:TYR:OH	1:A:2061:PHE:O	2.23	0.52
3:C:126:THR:HG22	3:C:159:LYS:CB	2.39	0.52
4:E:1012:ASP:HB3	4:E:1035:PRO:HD2	1.91	0.52
4:E:1014:LEU:HB2	4:E:1057:PHE:CE2	2.44	0.52
4:E:1486:MET:O	4:E:1489:ARG:HG2	2.10	0.52
2:F:131:THR:HA	2:F:308:ARG:NH1	2.24	0.52
3:G:84:TRP:HZ3	3:G:210:ILE:HG22	1.75	0.52
3:G:199:SER:O	3:G:203:LEU:HB3	2.09	0.52
1:A:1012:ASP:HB3	1:A:1035:PRO:HD2	1.91	0.52
1:A:2023:GLY:O	1:A:2027:VAL:HG23	2.10	0.52
4:E:1369:THR:CG2	4:E:1370:ILE:N	2.73	0.52
3:G:221:ARG:NH1	3:G:258:LYS:HB3	2.25	0.52
1:A:1190:THR:HG23	1:A:1194:PHE:HE2	1.74	0.52
1:A:1246:VAL:HG21	1:A:1315:ASP:OD2	2.09	0.52
2:B:563:LYS:HD2	2:B:565:TYR:OH	2.09	0.52
4:E:1671:GLU:OE1	2:F:348:ILE:HD11	2.10	0.52
2:F:814:ASP:HA	2:F:817:ALA:HB3	1.91	0.52
1:A:1942:SER:OG	1:A:1971:ILE:HG22	2.09	0.52
1:A:1950:LEU:CD2	1:A:1955:ILE:HD13	2.18	0.52
1:A:2072:ASN:O	1:A:2076:LYS:CB	2.58	0.52
2:B:142:ALA:HA	2:B:145:TYR:CD2	2.37	0.52
2:B:515:HIS:O	2:B:519:PHE:HB2	2.10	0.52
2:B:750:ARG:HH22	2:B:779:ARG:HH11	1.57	0.52
3:C:50:SER:O	3:C:53:LEU:HD13	2.09	0.52
4:E:1208:PRO:O	4:E:1212:HIS:HB3	2.10	0.52
4:E:1666:MET:HA	2:F:347:ARG:HB3	1.90	0.52
4:E:1978:PHE:CD1	4:E:1982:SER:CB	2.93	0.52
4:E:1418:LYS:HE2	4:E:1486:MET:HE1	1.91	0.52
4:E:1886:VAL:CG1	4:E:1896:ILE:HG22	2.40	0.52
2:F:172:VAL:HA	2:F:176:TYR:HD2	1.75	0.52

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
2:F:469:LYS:HE2	2:F:473:TYR:HE2	1.74	0.52
2:F:548:ASP:HB3	2:F:551:SER:HB2	1.92	0.52
1:A:1193:MET:HG2	1:A:1233:CYS:SG	2.49	0.52
4:E:1246:VAL:HG21	4:E:1315:ASP:OD2	2.09	0.52
2:F:563:LYS:HD2	2:F:565:TYR:OH	2.09	0.52
2:F:703:ALA:O	2:F:707:ILE:HG12	2.09	0.52
3:G:126:THR:HG22	3:G:159:LYS:CA	2.40	0.52
1:A:1683:LEU:HG	1:A:1687:PHE:CE2	2.44	0.52
2:B:250:GLU:OE2	2:B:255:GLN:HG2	2.09	0.52
2:B:274:CYS:CB	3:C:192:LEU:H	2.22	0.52
4:E:973:VAL:O	4:E:976:ASN:OD1	2.28	0.52
3:G:215:TYR:O	3:G:218:GLN:HG3	2.10	0.52
2:B:366:TYR:CE1	2:B:389:ALA:HB2	2.46	0.51
3:C:211:CYS:O	3:C:266:ARG:HD3	2.09	0.51
4:E:933:MET:CE	4:E:981:ARG:CD	2.80	0.51
4:E:1586:VAL:HG12	4:E:1613:ALA:O	2.09	0.51
4:E:1606:LEU:HA	2:F:387:GLU:OE2	2.10	0.51
2:F:120:TYR:HB3	2:F:148:LYS:HE3	1.91	0.51
3:G:82:LEU:HA	3:G:85:CYS:SG	2.50	0.51
1:A:1131:CYS:CA	4:E:1098:THR:HG23	2.40	0.51
1:A:1952:LEU:O	1:A:2060:ARG:NH1	2.40	0.51
1:A:1958:ARG:O	1:A:1959:HIS:CG	2.63	0.51
1:A:1963:ILE:HD13	1:A:1995:LYS:CD	2.40	0.51
4:E:1114:ASN:OD1	4:E:1117:ASN:N	2.38	0.51
2:F:30:VAL:HG21	2:F:48:LEU:HD21	1.92	0.51
1:A:1122:ALA:H	1:A:1125:LEU:HD21	1.75	0.51
2:B:172:VAL:HA	2:B:176:TYR:HD2	1.75	0.51
3:C:199:SER:O	3:C:203:LEU:CB	2.59	0.51
4:E:1509:PRO:HG2	4:E:2022:ARG:HE	1.73	0.51
1:A:1104:THR:HG22	4:E:1108:LEU:HD21	1.93	0.51
1:A:1208:PRO:O	1:A:1212:HIS:HB3	2.10	0.51
4:E:1192:ALA:HA	4:E:1195:LYS:HZ2	1.76	0.51
4:E:1486:MET:HE3	4:E:1489:ARG:NH2	2.25	0.51
4:E:1747:ILE:HD12	4:E:1748:ILE:HG13	1.91	0.51
2:F:179:ALA:O	2:F:183:ALA:HB2	2.11	0.51
1:A:1072:ALA:HB1	1:A:1075:VAL:HG12	1.93	0.51
1:A:1136:TYR:HB2	4:E:1101:ALA:HB1	1.92	0.51
1:A:1763:SER:O	1:A:1766:SER:HB2	2.11	0.51
2:B:548:ASP:HB3	2:B:551:SER:HB2	1.92	0.51
4:E:1292:VAL:HB	4:E:1348:PRO:HG2	1.91	0.51
4:E:1758:LYS:O	4:E:1761:CYS:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:933:MET:CE	1:A:981:ARG:CD	2.75	0.51
1:A:1758:LYS:O	1:A:1761:CYS:HB2	2.10	0.51
1:A:1886:VAL:CG1	1:A:1896:ILE:HG22	2.40	0.51
1:A:1898:CYS:HA	5:A:2201:E4S:C11	2.41	0.51
1:A:1932:PHE:O	1:A:1936:ARG:HB3	2.11	0.51
2:B:30:VAL:HG21	2:B:48:LEU:HD21	1.92	0.51
2:B:375:ARG:CZ	3:C:242:THR:HG23	2.41	0.51
2:B:403:PHE:O	2:B:406:SER:OG	2.24	0.51
4:E:1014:LEU:CD2	4:E:1098:THR:HG22	2.41	0.51
4:E:1339:MET:HE2	4:E:1349:ARG:HG3	1.93	0.51
4:E:1370:ILE:HD11	2:F:754:GLU:HB3	1.92	0.51
4:E:2079:GLN:O	4:E:2083:LEU:HG	2.11	0.51
2:F:366:TYR:CE1	2:F:389:ALA:HB2	2.46	0.51
2:B:515:HIS:O	2:B:519:PHE:CB	2.59	0.51
4:E:1383:PHE:HE2	4:E:1488:ARG:HE	1.58	0.51
4:E:2072:ASN:O	4:E:2076:LYS:CB	2.58	0.51
1:A:1197:THR:O	1:A:1201:ILE:HG12	2.11	0.51
1:A:1293:THR:O	1:A:1296:TYR:HB3	2.11	0.51
1:A:1538:LYS:HE2	1:A:1539:GLN:NE2	2.26	0.51
1:A:1940:ILE:HG23	1:A:2016:PHE:HD1	1.75	0.51
2:B:173:ILE:HG23	2:B:177:GLU:OE1	2.11	0.51
3:C:84:TRP:HZ3	3:C:210:ILE:HG22	1.75	0.51
3:C:215:TYR:O	3:C:218:GLN:HG3	2.10	0.51
4:E:1763:SER:O	4:E:1766:SER:HB2	2.10	0.51
4:E:1944:ALA:HB2	4:E:2016:PHE:CD1	2.46	0.51
4:E:1944:ALA:HA	4:E:2016:PHE:CE1	2.46	0.51
4:E:2056:LEU:O	4:E:2060:ARG:HG3	2.11	0.51
2:F:173:ILE:HG23	2:F:177:GLU:OE1	2.11	0.51
2:B:45:GLU:OE1	2:B:81:HIS:ND1	2.44	0.51
2:B:131:THR:HA	2:B:308:ARG:NH1	2.25	0.51
4:E:1197:THR:O	4:E:1201:ILE:HG12	2.11	0.51
4:E:1957:ASP:CG	4:E:1957:ASP:O	2.49	0.51
2:F:515:HIS:O	2:F:519:PHE:HB2	2.10	0.51
2:F:750:ARG:HH22	2:F:779:ARG:HH11	1.58	0.51
4:E:1072:ALA:HB1	4:E:1075:VAL:HG12	1.93	0.51
4:E:1940:ILE:HG23	4:E:2016:PHE:HD1	1.75	0.51
2:F:258:ARG:HA	2:F:261:ILE:HG22	1.92	0.51
2:F:278:TYR:HE1	2:F:327:GLU:OE1	1.94	0.51
2:F:515:HIS:O	2:F:519:PHE:CB	2.59	0.51
1:A:1014:LEU:CD2	1:A:1098:THR:HG22	2.41	0.50
1:A:1944:ALA:CA	1:A:2016:PHE:HE1	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:495:VAL:HG12	2:B:499:LYS:HE3	1.93	0.50
4:E:328:UNK:O	4:E:331:UNK:N	2.43	0.50
4:E:1954:GLN:HG3	4:E:2060:ARG:CZ	2.38	0.50
2:F:495:VAL:HG12	2:F:499:LYS:HE3	1.93	0.50
1:A:1996:LEU:HD12	1:A:2081:CYS:SG	2.52	0.50
3:C:123:LEU:HB2	3:C:163:SER:HB3	1.93	0.50
3:C:126:THR:HG22	3:C:159:LYS:CA	2.40	0.50
4:E:934:GLN:O	4:E:938:ALA:CB	2.59	0.50
4:E:1122:ALA:H	4:E:1125:LEU:HD21	1.75	0.50
4:E:2023:GLY:O	4:E:2027:VAL:HG23	2.10	0.50
2:F:403:PHE:O	2:F:406:SER:OG	2.24	0.50
3:G:84:TRP:CZ3	3:G:210:ILE:HG22	2.47	0.50
1:A:327:UNK:O	1:A:330:UNK:N	2.45	0.50
1:A:1007:LEU:O	1:A:1011:LEU:HD13	2.12	0.50
1:A:1556:VAL:O	1:A:1559:PRO:HD2	2.11	0.50
1:A:1631:HIS:CD2	1:A:1632:PRO:HD2	2.45	0.50
1:A:1920:PHE:CE2	1:A:1932:PHE:CD1	2.95	0.50
2:B:179:ALA:O	2:B:183:ALA:HB2	2.11	0.50
4:E:1556:VAL:O	4:E:1559:PRO:HD2	2.10	0.50
4:E:1605:GLU:O	4:E:1606:LEU:HG	2.11	0.50
4:E:1944:ALA:HB2	4:E:2016:PHE:CE1	2.46	0.50
2:F:579:TYR:HA	3:G:175:GLN:HG3	1.93	0.50
3:G:199:SER:O	3:G:203:LEU:CB	2.59	0.50
1:A:1508:ASN:N	1:A:1509:PRO:HD3	2.22	0.50
4:E:1128:ARG:NH1	4:E:1130:ALA:HB3	2.26	0.50
4:E:1849:PHE:HD1	4:E:1895:VAL:HG22	1.76	0.50
2:F:45:GLU:OE1	2:F:81:HIS:ND1	2.44	0.50
2:F:170:GLN:HA	2:F:173:ILE:HD12	1.93	0.50
2:F:478:LEU:HD23	2:F:504:PHE:HZ	1.76	0.50
1:A:1400:LEU:HD13	1:A:1506:TRP:HZ3	1.76	0.50
1:A:1596:TRP:HE1	1:A:1601:ALA:HA	1.77	0.50
1:A:2056:LEU:O	1:A:2060:ARG:HG3	2.11	0.50
2:B:408:MET:CE	2:B:436:LEU:HB3	2.42	0.50
3:C:88:ALA:O	3:C:92:SER:OG	2.29	0.50
3:C:178:PHE:CD2	3:C:232:VAL:HA	2.47	0.50
4:E:1586:VAL:CG1	4:E:1613:ALA:HB1	2.41	0.50
4:E:1860:LEU:HB3	4:E:1979:MET:SD	2.50	0.50
4:E:1908:LEU:H	4:E:1908:LEU:HD23	1.77	0.50
1:A:1014:LEU:HB2	1:A:1057:PHE:CE2	2.44	0.50
1:A:1101:ALA:CB	4:E:1131:CYS:SG	2.96	0.50
1:A:2031:MET:HG3	1:A:2061:PHE:HD2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2079:GLN:O	1:A:2083:LEU:HG	2.11	0.50
2:B:170:GLN:HA	2:B:173:ILE:HD12	1.93	0.50
4:E:1137:SER:O	4:E:1141:ALA:CB	2.60	0.50
4:E:1293:THR:O	4:E:1296:TYR:HB3	2.11	0.50
4:E:1400:LEU:HD13	4:E:1506:TRP:HZ3	1.76	0.50
4:E:1538:LYS:HE2	4:E:1539:GLN:NE2	2.26	0.50
4:E:1978:PHE:HB3	4:E:1982:SER:HB3	1.93	0.50
2:F:113:TYR:HB3	2:F:155:LEU:HD11	1.94	0.50
3:G:79:LEU:HD12	3:G:80:PRO:HD3	1.93	0.50
3:G:116:LYS:HZ1	3:G:121:LYS:HB2	1.74	0.50
1:A:934:GLN:O	1:A:938:ALA:CB	2.59	0.50
1:A:1249:MET:HE2	1:A:1320:PHE:CE1	2.47	0.50
1:A:1590:ILE:HG13	1:A:1612:TRP:HZ3	1.77	0.50
1:A:1908:LEU:HD23	1:A:1908:LEU:H	1.77	0.50
4:E:1848:ILE:CG1	4:E:1896:ILE:HD11	2.42	0.50
4:E:2045:GLY:C	4:E:2046:LEU:HD12	2.32	0.50
3:G:88:ALA:O	3:G:92:SER:OG	2.29	0.50
1:A:1104:THR:HG22	4:E:1108:LEU:CD2	2.41	0.50
1:A:1130:ALA:HB1	4:E:1096:GLN:HE22	1.76	0.50
1:A:1137:SER:O	1:A:1141:ALA:CB	2.60	0.50
2:B:478:LEU:HD23	2:B:504:PHE:HZ	1.76	0.50
3:C:82:LEU:HA	3:C:85:CYS:SG	2.50	0.50
4:E:1596:TRP:HE1	4:E:1601:ALA:HA	1.77	0.50
1:A:1031:TYR:CE1	1:A:1042:THR:HG22	2.47	0.50
1:A:1081:GLN:HG3	1:A:1143:LEU:HD13	1.94	0.50
1:A:1383:PHE:HE2	1:A:1488:ARG:HE	1.58	0.50
1:A:1586:VAL:HG13	1:A:1613:ALA:HB3	1.94	0.50
2:B:258:ARG:HA	2:B:261:ILE:HG22	1.92	0.50
2:B:273:MET:HA	3:C:193:THR:OG1	2.12	0.50
2:B:326:GLU:OE2	3:C:125:PHE:HB2	2.11	0.50
3:C:84:TRP:CZ3	3:C:210:ILE:HG22	2.47	0.50
3:C:169:ARG:HH11	3:C:170:GLU:H	1.60	0.50
3:C:264:ILE:O	3:C:268:GLN:HG3	2.12	0.50
4:E:1007:LEU:O	4:E:1011:LEU:HD13	2.12	0.50
4:E:1373:VAL:HG11	2:F:758:ALA:O	2.11	0.50
1:A:1848:ILE:CG1	1:A:1896:ILE:HD11	2.42	0.49
1:A:1849:PHE:HD1	1:A:1895:VAL:HG22	1.76	0.49
4:E:1128:ARG:HD2	4:E:1128:ARG:O	2.12	0.49
4:E:1401:ARG:NH2	4:E:1516:GLU:OE1	2.45	0.49
2:F:141:ILE:HG22	2:F:145:TYR:CE2	2.47	0.49
2:F:787:LEU:HD13	2:F:804:LEU:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:123:LEU:HB2	3:G:163:SER:HB3	1.93	0.49
1:A:1590:ILE:HG13	1:A:1612:TRP:CZ3	2.47	0.49
1:A:1605:GLU:O	1:A:1606:LEU:HG	2.11	0.49
1:A:1916:MET:HE3	1:A:1965:LEU:HD23	1.94	0.49
1:A:1996:LEU:CD1	1:A:2081:CYS:SG	3.00	0.49
4:E:1114:ASN:O	4:E:1118:THR:OG1	2.20	0.49
4:E:2031:MET:HG3	4:E:2061:PHE:HD2	1.77	0.49
2:F:752:TRP:O	2:F:755:GLU:HB2	2.12	0.49
3:G:274:GLU:HG2	3:G:275:PRO:CD	2.37	0.49
1:A:1208:PRO:O	1:A:1212:HIS:CB	2.61	0.49
1:A:1735:PHE:O	1:A:1739:ASN:CB	2.59	0.49
1:A:1862:LEU:HD21	1:A:1885:ARG:HA	1.93	0.49
2:B:752:TRP:O	2:B:755:GLU:HB2	2.12	0.49
3:C:214:GLY:HA3	3:C:229:ARG:CG	2.43	0.49
4:E:1081:GLN:HG3	4:E:1143:LEU:HD13	1.94	0.49
4:E:1259:THR:HG21	4:E:1295:HIS:NE2	2.27	0.49
4:E:1777:PRO:O	4:E:1887:VAL:HG21	2.12	0.49
4:E:1932:PHE:CE2	4:E:1936:ARG:HD3	2.48	0.49
4:E:2065:MET:HE2	4:E:2069:GLU:HG3	1.93	0.49
1:A:1114:ASN:CB	1:A:1135:ASP:HB3	2.40	0.49
4:E:1321:SER:O	4:E:1325:GLN:HB3	2.13	0.49
4:E:1944:ALA:N	4:E:2016:PHE:HE1	2.11	0.49
1:A:1741:ILE:HG23	1:A:1803:TYR:OH	2.13	0.49
2:B:141:ILE:HG22	2:B:145:TYR:CE2	2.47	0.49
2:B:408:MET:SD	3:C:273:PRO:HG3	2.52	0.49
4:E:1031:TYR:CE1	4:E:1042:THR:HG22	2.48	0.49
4:E:1119:THR:HG21	4:E:1402:GLU:HA	1.94	0.49
4:E:1503:LEU:O	4:E:1506:TRP:N	2.46	0.49
4:E:1924:TYR:HD1	4:E:1931:ALA:HB1	1.78	0.49
4:E:1948:LEU:O	4:E:1952:LEU:HD23	2.11	0.49
2:F:75:LEU:HD22	2:F:106:LEU:HD13	1.95	0.49
3:G:264:ILE:O	3:G:268:GLN:HG3	2.12	0.49
1:A:1401:ARG:NH2	1:A:1516:GLU:OE1	2.46	0.49
2:B:75:LEU:HD22	2:B:106:LEU:HD13	1.95	0.49
2:B:587:PHE:CE1	2:B:701:HIS:ND1	2.80	0.49
3:C:79:LEU:HD12	3:C:80:PRO:HD3	1.94	0.49
4:E:1741:ILE:HG23	4:E:1803:TYR:OH	2.13	0.49
2:F:281:PRO:HB2	3:G:135:VAL:HG21	1.94	0.49
2:F:548:ASP:OD1	2:F:549:ALA:N	2.46	0.49
1:A:1978:PHE:HD1	1:A:1982:SER:HB3	1.72	0.49
2:B:469:LYS:HE2	2:B:473:TYR:CE2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:1806:LYS:HZ3	4:E:1844:TRP:N	2.11	0.49
2:F:128:LEU:HD22	2:F:137:ARG:NH2	2.27	0.49
2:F:240:GLY:O	2:F:244:GLU:HG3	2.13	0.49
3:G:178:PHE:CD2	3:G:232:VAL:HA	2.47	0.49
1:A:1098:THR:HG23	4:E:1131:CYS:CA	2.42	0.49
2:B:113:TYR:HB3	2:B:155:LEU:HD11	1.94	0.49
4:E:1321:SER:O	4:E:1325:GLN:CB	2.61	0.49
4:E:1346:ILE:HD12	4:E:1407:MET:SD	2.53	0.49
4:E:1631:HIS:CD2	4:E:1632:PRO:HD2	2.45	0.49
4:E:1862:LEU:HD21	4:E:1885:ARG:HA	1.93	0.49
2:B:128:LEU:HD22	2:B:137:ARG:NH2	2.27	0.49
4:E:939:VAL:HG13	4:E:942:LYS:HZ1	1.78	0.49
4:E:1208:PRO:O	4:E:1212:HIS:CB	2.61	0.49
4:E:1573:THR:O	4:E:1577:ARG:HB2	2.13	0.49
4:E:1860:LEU:HB3	4:E:1979:MET:CE	2.43	0.49
4:E:1877:LEU:HB3	4:E:1879:LEU:CD1	2.43	0.49
4:E:2006:GLY:HA2	4:E:2010:ALA:CB	2.42	0.49
3:G:237:MET:CA	3:G:240:MET:HG2	2.40	0.49
3:G:245:TYR:HA	3:G:248:PHE:CD2	2.48	0.49
1:A:1321:SER:O	1:A:1325:GLN:CB	2.61	0.49
1:A:1559:PRO:HB3	1:A:1568:ILE:HD13	1.95	0.49
1:A:1699:GLU:CB	1:A:1702:HIS:CD2	2.86	0.49
1:A:1882:PHE:HE2	1:A:1899:ILE:HG12	1.78	0.49
1:A:1940:ILE:HG23	1:A:2016:PHE:CD1	2.48	0.49
1:A:2017:MET:O	1:A:2021:VAL:HG22	2.13	0.49
2:B:576:LEU:HD13	2:B:586:LEU:HD23	1.95	0.49
2:B:787:LEU:HD13	2:B:804:LEU:N	2.27	0.49
4:E:1381:THR:O	4:E:1384:ASP:HB3	2.12	0.49
4:E:1685:HIS:CE1	4:E:1731:TYR:HB3	2.47	0.49
4:E:1940:ILE:HG23	4:E:2016:PHE:CD1	2.48	0.49
2:F:601:GLU:HA	2:F:604:LEU:HD12	1.95	0.49
3:G:169:ARG:HH11	3:G:170:GLU:H	1.60	0.49
1:A:1507:TYR:O	1:A:1509:PRO:HD3	2.13	0.48
1:A:1806:LYS:HZ3	1:A:1844:TRP:N	2.11	0.48
4:E:1590:ILE:O	4:E:1593:LEU:N	2.46	0.48
4:E:1954:GLN:OE1	4:E:1954:GLN:HA	2.12	0.48
3:G:54:GLU:HA	3:G:101:ILE:HD11	1.95	0.48
3:G:221:ARG:HH12	3:G:258:LYS:HD3	1.78	0.48
1:A:1119:THR:HG21	1:A:1402:GLU:HA	1.95	0.48
1:A:1259:THR:HG21	1:A:1295:HIS:NE2	2.27	0.48
1:A:1346:ILE:HD12	1:A:1407:MET:SD	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1777:PRO:O	1:A:1887:VAL:HG21	2.12	0.48
1:A:2045:GLY:C	1:A:2046:LEU:HD12	2.33	0.48
4:E:1944:ALA:HA	4:E:2016:PHE:CZ	2.48	0.48
2:F:139:ARG:HB2	2:F:186:TYR:CE1	2.48	0.48
2:F:408:MET:CE	2:F:436:LEU:HB3	2.42	0.48
2:F:576:LEU:HD13	2:F:586:LEU:HD23	1.95	0.48
2:B:218:LEU:O	2:B:222:LEU:HD13	2.14	0.48
2:B:548:ASP:OD1	2:B:549:ALA:N	2.46	0.48
2:B:601:GLU:HA	2:B:604:LEU:HD12	1.96	0.48
3:C:245:TYR:HA	3:C:248:PHE:CD2	2.48	0.48
3:C:274:GLU:HG2	3:C:275:PRO:CD	2.37	0.48
4:E:27:UNK:HA	2:F:821:PHE:CD2	2.48	0.48
4:E:1231:LEU:HD22	4:E:1301:PHE:CD1	2.48	0.48
4:E:1631:HIS:CE1	4:E:1633:LEU:HD12	2.49	0.48
1:A:1381:THR:O	1:A:1384:ASP:HB3	2.12	0.48
1:A:1685:HIS:CE1	1:A:1731:TYR:HB3	2.48	0.48
2:B:220:THR:O	2:B:224:ARG:HB3	2.13	0.48
4:E:1214:LEU:HG	4:E:1234:TRP:HE1	1.78	0.48
4:E:1878:ASP:O	4:E:1941:ARG:HG3	2.14	0.48
4:E:2011:THR:OG1	4:E:2012:PRO:HD3	2.13	0.48
2:F:218:LEU:O	2:F:222:LEU:HD13	2.14	0.48
1:A:1321:SER:O	1:A:1325:GLN:HB3	2.12	0.48
1:A:1731:TYR:HA	1:A:1734:GLU:HB3	1.96	0.48
2:B:178:LYS:HE2	2:B:306:LEU:HD21	1.96	0.48
2:B:227:VAL:HG12	2:B:231:LYS:HE3	1.94	0.48
2:B:592:LEU:HD23	2:B:595:LEU:HD12	1.96	0.48
4:E:1981:GLU:HA	4:E:1981:GLU:OE1	2.14	0.48
2:F:51:SER:O	2:F:55:GLN:CB	2.61	0.48
2:F:227:VAL:HG12	2:F:231:LYS:HE3	1.94	0.48
2:F:519:PHE:CE1	2:F:551:SER:HA	2.48	0.48
1:A:1503:LEU:O	1:A:1506:TRP:N	2.46	0.48
2:B:240:GLY:O	2:B:244:GLU:HG3	2.13	0.48
3:C:86:TYR:O	3:C:90:SER:CB	2.61	0.48
4:E:1031:TYR:HA	4:E:1041:ILE:O	2.14	0.48
4:E:1586:VAL:CG2	4:E:1587:PRO:CD	2.89	0.48
4:E:1670:ARG:NH1	2:F:349:PRO:HB2	2.28	0.48
4:E:1735:PHE:O	4:E:1739:ASN:CB	2.59	0.48
2:F:178:LYS:HE2	2:F:306:LEU:HD21	1.96	0.48
2:F:227:VAL:O	2:F:231:LYS:HG3	2.14	0.48
2:B:113:TYR:CB	2:B:155:LEU:HD21	2.43	0.48
2:B:179:ALA:O	2:B:183:ALA:CB	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:1249:MET:HE2	4:E:1320:PHE:CE1	2.49	0.48
4:E:1349:ARG:NE	4:E:1385:TYR:HB2	2.29	0.48
4:E:1692:LYS:HA	4:E:1695:ILE:CD1	2.44	0.48
2:F:179:ALA:O	2:F:183:ALA:CB	2.61	0.48
2:F:469:LYS:HE2	2:F:473:TYR:CE2	2.48	0.48
1:A:1214:LEU:HG	1:A:1234:TRP:HE1	1.78	0.48
1:A:1231:LEU:HD22	1:A:1301:PHE:CD1	2.48	0.48
1:A:1692:LYS:HA	1:A:1695:ILE:CD1	2.44	0.48
2:B:139:ARG:HB2	2:B:186:TYR:CE1	2.48	0.48
4:E:1731:TYR:HA	4:E:1734:GLU:HB3	1.96	0.48
4:E:1978:PHE:HD1	4:E:1982:SER:CB	2.27	0.48
4:E:2061:PHE:O	4:E:2062:SER:OG	2.32	0.48
2:F:92:LYS:HB2	2:F:95:PHE:HD2	1.79	0.48
3:G:83:ILE:O	3:G:87:LEU:CB	2.50	0.48
1:A:1031:TYR:HA	1:A:1041:ILE:O	2.14	0.48
1:A:1979:MET:HE3	1:A:1980:PHE:HE2	1.76	0.48
2:B:227:VAL:O	2:B:231:LYS:HG3	2.14	0.48
2:B:584:ILE:HA	2:B:587:PHE:HD2	1.79	0.48
3:C:265:TYR:CZ	3:C:269:LEU:HD11	2.49	0.48
4:E:1994:ILE:CG2	4:E:1995:LYS:H	2.26	0.48
2:F:142:ALA:HA	2:F:145:TYR:CD2	2.37	0.48
2:F:178:LYS:HG2	2:F:306:LEU:HD21	1.96	0.48
2:F:220:THR:O	2:F:224:ARG:HB3	2.13	0.48
2:F:587:PHE:CE1	2:F:701:HIS:ND1	2.80	0.48
3:G:86:TYR:O	3:G:90:SER:CB	2.61	0.48
3:G:265:TYR:CZ	3:G:269:LEU:HD11	2.49	0.48
1:A:1351:LYS:O	1:A:1354:THR:HB	2.14	0.48
1:A:1590:ILE:HG23	1:A:1591:LYS:N	2.29	0.48
2:F:584:ILE:HA	2:F:587:PHE:HD2	1.79	0.48
1:A:939:VAL:HG13	1:A:942:LYS:NZ	2.29	0.47
1:A:1853:ASP:OD1	1:A:1854:ASP:N	2.47	0.47
2:B:519:PHE:CE1	2:B:551:SER:HA	2.48	0.47
3:C:221:ARG:HH12	3:C:258:LYS:HD3	1.78	0.47
4:E:951:MET:HE1	4:E:954:LYS:CE	2.44	0.47
4:E:1559:PRO:HB3	4:E:1568:ILE:HD13	1.95	0.47
2:F:113:TYR:CB	2:F:155:LEU:HD21	2.44	0.47
1:A:1128:ARG:HB3	4:E:1051:GLU:HG3	1.96	0.47
1:A:1573:THR:O	1:A:1577:ARG:HB2	2.13	0.47
4:E:2017:MET:O	4:E:2021:VAL:HG22	2.13	0.47
2:F:592:LEU:HD23	2:F:595:LEU:HD12	1.96	0.47
1:A:1570:ASN:O	1:A:1574:ARG:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:260:LEU:HD13	3:C:282:ILE:HG21	1.96	0.47
4:E:1569:GLY:O	4:E:1573:THR:OG1	2.31	0.47
4:E:1570:ASN:O	4:E:1574:ARG:HB2	2.14	0.47
2:F:325:THR:OG1	2:F:376:ARG:NH2	2.47	0.47
2:F:519:PHE:CZ	2:F:550:ASN:HB3	2.49	0.47
1:A:1090:TRP:CZ2	4:E:1144:ASN:HB3	2.50	0.47
1:A:1249:MET:HE2	1:A:1320:PHE:HE1	1.78	0.47
1:A:1349:ARG:NE	1:A:1385:TYR:HB2	2.29	0.47
1:A:1938:ASN:HA	1:A:1941:ARG:HG2	1.95	0.47
2:B:92:LYS:HB2	2:B:95:PHE:HD2	1.79	0.47
2:B:690:HIS:CG	2:B:691:PRO:HD3	2.49	0.47
3:C:54:GLU:HA	3:C:101:ILE:HD11	1.95	0.47
4:E:1351:LYS:O	4:E:1354:THR:HB	2.14	0.47
2:F:224:ARG:NE	2:F:228:LEU:HD11	2.29	0.47
1:A:1051:GLU:O	1:A:1055:LYS:HG2	2.15	0.47
2:B:371:ILE:HD11	3:C:282:ILE:CD1	2.45	0.47
2:B:519:PHE:CZ	2:B:550:ASN:HB3	2.49	0.47
2:B:752:TRP:HA	2:B:755:GLU:HG3	1.96	0.47
4:E:939:VAL:HG13	4:E:942:LYS:NZ	2.29	0.47
1:A:1317:VAL:HG11	1:A:1364:VAL:CG1	2.45	0.47
1:A:1529:ARG:O	1:A:1533:ILE:HG13	2.15	0.47
1:A:1590:ILE:HB	1:A:1612:TRP:CZ3	2.50	0.47
1:A:2061:PHE:O	1:A:2062:SER:OG	2.32	0.47
2:B:51:SER:O	2:B:55:GLN:CB	2.61	0.47
3:C:237:MET:CA	3:C:240:MET:HG2	2.40	0.47
4:E:1507:TYR:O	4:E:1509:PRO:HD3	2.12	0.47
1:A:1101:ALA:CB	4:E:1136:TYR:HB2	2.39	0.47
1:A:1137:SER:O	1:A:1141:ALA:HB2	2.15	0.47
1:A:1266:LEU:H	1:A:1295:HIS:CE1	2.33	0.47
1:A:1404:ILE:O	1:A:1408:ILE:HG13	2.15	0.47
1:A:1877:LEU:HB3	1:A:1879:LEU:CD1	2.43	0.47
1:A:1904:SER:HB2	1:A:1907:GLN:CG	2.42	0.47
3:C:252:GLU:OE1	3:C:255:LEU:HD12	2.15	0.47
4:E:1051:GLU:O	4:E:1055:LYS:HG2	2.15	0.47
4:E:1266:LEU:H	4:E:1295:HIS:CE1	2.33	0.47
4:E:1317:VAL:HG11	4:E:1364:VAL:CG1	2.45	0.47
4:E:1737:PHE:CE2	4:E:1741:ILE:HD11	2.50	0.47
4:E:1853:ASP:OD1	4:E:1854:ASP:N	2.47	0.47
2:F:83:THR:O	2:F:87:ASP:CB	2.61	0.47
2:F:688:PRO:HG2	2:F:691:PRO:HG2	1.97	0.47
3:G:221:ARG:NH1	3:G:258:LYS:HD3	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:252:GLU:OE1	3:G:255:LEU:HD12	2.15	0.47
1:A:1631:HIS:CE1	1:A:1633:LEU:HD12	2.48	0.47
1:A:1951:PHE:HE1	1:A:2077:VAL:HG11	1.79	0.47
1:A:2006:GLY:HA2	1:A:2010:ALA:CB	2.45	0.47
2:B:178:LYS:HG2	2:B:306:LEU:HD21	1.96	0.47
2:B:325:THR:OG1	2:B:376:ARG:NH2	2.47	0.47
3:C:178:PHE:CE1	3:C:181:LEU:HD11	2.49	0.47
4:E:206:UNK:O	4:E:210:UNK:N	2.48	0.47
4:E:1404:ILE:O	4:E:1408:ILE:HG13	2.15	0.47
1:A:1737:PHE:CE2	1:A:1741:ILE:HD11	2.50	0.47
2:B:224:ARG:NE	2:B:228:LEU:HD11	2.29	0.47
2:B:434:PRO:HG2	2:B:458:VAL:HG22	1.97	0.47
3:C:139:PRO:O	3:C:142:ILE:HG22	2.15	0.47
3:C:159:LYS:HD2	3:C:160:VAL:N	2.30	0.47
4:E:1529:ARG:O	4:E:1533:ILE:HG13	2.15	0.47
4:E:1597:HIS:ND1	4:E:1602:ASP:OD2	2.45	0.47
4:E:1712:LEU:O	4:E:1716:VAL:HG23	2.15	0.47
1:A:1010:MET:HG3	1:A:1064:ILE:HD11	1.96	0.47
1:A:1015:GLN:NE2	1:A:1099:GLY:H	2.13	0.47
1:A:1250:ARG:NE	2:B:785:LYS:HB2	2.30	0.47
1:A:1768:VAL:HG23	1:A:1769:LYS:H	1.80	0.47
3:C:274:GLU:CG	3:C:275:PRO:HD3	2.40	0.47
4:E:1658:VAL:O	4:E:1661:LEU:HB2	2.15	0.47
4:E:1768:VAL:HG23	4:E:1769:LYS:H	1.80	0.47
3:G:260:LEU:HD13	3:G:282:ILE:HG21	1.96	0.47
1:A:1493:LEU:HB3	1:A:1528:TRP:NE1	2.31	0.46
1:A:1544:VAL:HG22	1:A:1558:LEU:CD2	2.45	0.46
1:A:1875:VAL:HG21	1:A:2026:ALA:HB1	1.98	0.46
2:B:8:SER:OG	2:B:9:ARG:N	2.48	0.46
4:E:1015:GLN:NE2	4:E:1099:GLY:H	2.13	0.46
4:E:1276:PRO:HG2	4:E:1277:LEU:HD12	1.97	0.46
4:E:1544:VAL:HG22	4:E:1558:LEU:CD2	2.45	0.46
4:E:1731:TYR:HB2	4:E:1735:PHE:CE1	2.50	0.46
4:E:2034:VAL:CG1	4:E:2057:LEU:HD21	2.43	0.46
2:F:346:SER:HB2	2:F:355:ARG:HH12	1.72	0.46
3:G:204:CYS:O	3:G:208:SER:HB2	2.15	0.46
1:A:1114:ASN:O	1:A:1118:THR:OG1	2.20	0.46
2:B:576:LEU:HD21	2:B:585:LEU:HB2	1.97	0.46
3:C:204:CYS:O	3:C:208:SER:HB2	2.15	0.46
4:E:1761:CYS:O	4:E:1764:ALA:HB3	2.16	0.46
4:E:1951:PHE:HE1	4:E:2077:VAL:HG11	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:436:LEU:HD23	3:G:271:LEU:HD23	1.98	0.46
2:F:690:HIS:CG	2:F:691:PRO:HD3	2.50	0.46
3:G:172:LEU:HD21	3:G:177:ARG:CB	2.45	0.46
1:A:1238:LEU:HD22	1:A:1305:ARG:CZ	2.46	0.46
1:A:1632:PRO:O	1:A:1636:GLN:HG3	2.16	0.46
1:A:1944:ALA:N	1:A:2016:PHE:HE1	2.13	0.46
2:B:515:HIS:H	3:C:229:ARG:HH12	1.62	0.46
2:B:832:PRO:HB3	2:B:836:PHE:CZ	2.51	0.46
3:G:156:GLY:C	3:G:157:LEU:HD23	2.36	0.46
4:E:1010:MET:HG3	4:E:1064:ILE:HD11	1.96	0.46
2:F:340:ASN:OD1	2:F:340:ASN:O	2.34	0.46
2:F:576:LEU:HD21	2:F:585:LEU:HB2	1.97	0.46
1:A:1647:PRO:HB3	1:A:1683:LEU:HD22	1.96	0.46
1:A:1658:VAL:O	1:A:1661:LEU:HB2	2.15	0.46
3:C:218:GLN:O	3:C:222:LYS:N	2.43	0.46
4:E:2035:VAL:HG13	4:E:2054:ILE:HG23	1.97	0.46
1:A:939:VAL:HG13	1:A:942:LYS:HZ1	1.81	0.46
2:B:688:PRO:HG2	2:B:691:PRO:HG2	1.97	0.46
3:C:37:LEU:HA	3:C:40:SER:HG	1.80	0.46
4:E:1137:SER:O	4:E:1141:ALA:HB2	2.15	0.46
4:E:1924:TYR:OH	4:E:1968:LYS:N	2.48	0.46
3:G:139:PRO:O	3:G:142:ILE:HG22	2.15	0.46
1:A:951:MET:HE1	1:A:954:LYS:CE	2.45	0.46
2:B:220:THR:O	2:B:224:ARG:CB	2.64	0.46
3:C:260:LEU:CD1	3:C:282:ILE:HG21	2.46	0.46
4:E:1011:LEU:HD21	4:E:1103:ALA:HB2	1.97	0.46
4:E:1498:THR:O	4:E:1501:GLU:HG2	2.15	0.46
4:E:1916:MET:HE3	4:E:1965:LEU:HD23	1.97	0.46
4:E:1950:LEU:HD12	4:E:1994:ILE:HG23	1.96	0.46
2:F:8:SER:OG	2:F:9:ARG:N	2.48	0.46
2:F:519:PHE:HE1	2:F:551:SER:HA	1.80	0.46
3:G:124:SER:HB2	3:G:159:LYS:HD3	1.97	0.46
3:G:159:LYS:HD2	3:G:160:VAL:N	2.30	0.46
1:A:1096:GLN:NE2	4:E:1130:ALA:O	2.47	0.46
1:A:1192:ALA:HA	1:A:1195:LYS:HZ2	1.80	0.46
1:A:1731:TYR:HB2	1:A:1735:PHE:CE1	2.50	0.46
1:A:1924:TYR:OH	1:A:1968:LYS:N	2.48	0.46
1:A:1958:ARG:O	1:A:1959:HIS:CD2	2.69	0.46
1:A:2018:GLU:OE2	1:A:2022:ARG:NH1	2.49	0.46
1:A:2028:ARG:HH12	1:A:2065:MET:C	2.16	0.46
2:B:20:GLU:OE1	2:B:22:GLN:NE2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:712:PRO:HB3	2:B:742:LEU:HD23	1.97	0.46
3:C:124:SER:HB2	3:C:159:LYS:HD3	1.97	0.46
4:E:1128:ARG:HH11	4:E:1130:ALA:HB3	1.80	0.46
4:E:1400:LEU:HD21	4:E:1507:TYR:HD2	1.77	0.46
4:E:1647:PRO:HB3	4:E:1683:LEU:HD22	1.96	0.46
4:E:1724:SER:HA	4:E:1728:LYS:HB2	1.98	0.46
2:F:20:GLU:OE1	2:F:22:GLN:NE2	2.49	0.46
3:G:260:LEU:CD1	3:G:282:ILE:HG21	2.46	0.46
1:A:1104:THR:CG2	4:E:1108:LEU:HD21	2.45	0.46
1:A:1498:THR:O	1:A:1501:GLU:HG2	2.15	0.46
1:A:1712:LEU:O	1:A:1716:VAL:HG23	2.15	0.46
3:C:156:GLY:C	3:C:157:LEU:HD23	2.36	0.46
3:C:221:ARG:NH1	3:C:258:LYS:HD3	2.30	0.46
4:E:1529:ARG:HD2	4:E:1533:ILE:CD1	2.46	0.46
2:F:220:THR:O	2:F:224:ARG:CB	2.64	0.46
2:F:344:VAL:HG11	2:F:351:HIS:CE1	2.50	0.46
2:F:545:GLN:NE2	3:G:229:ARG:O	2.49	0.46
1:A:1232:ALA:HB2	4:E:1094:LEU:HD21	1.96	0.46
1:A:2035:VAL:HG13	1:A:2054:ILE:HG23	1.97	0.46
1:A:2036:SER:O	1:A:2039:THR:HG22	2.16	0.46
2:B:271:ARG:HD2	3:C:249:TYR:CD2	2.51	0.46
2:F:423:CYS:HB3	2:F:433:ILE:HD13	1.98	0.46
3:G:37:LEU:HA	3:G:40:SER:HG	1.80	0.46
1:A:1098:THR:HG23	4:E:1131:CYS:N	2.31	0.45
1:A:1108:LEU:HD21	4:E:1104:THR:HG22	1.98	0.45
1:A:1569:GLY:O	1:A:1573:THR:OG1	2.31	0.45
2:B:167:ASP:OD2	2:B:169:GLU:HB3	2.16	0.45
4:E:1238:LEU:HD22	4:E:1305:ARG:CZ	2.46	0.45
4:E:1529:ARG:HD2	4:E:1533:ILE:HD11	1.98	0.45
2:F:235:LEU:HB2	2:F:291:LEU:C	2.36	0.45
3:G:108:VAL:O	3:G:112:GLU:HG2	2.16	0.45
1:A:185:UNK:CB	1:A:205:UNK:CB	2.94	0.45
1:A:1276:PRO:HG2	1:A:1277:LEU:HD12	1.97	0.45
1:A:1510:LEU:CD2	1:A:2017:MET:HB3	2.46	0.45
1:A:1529:ARG:HD2	1:A:1533:ILE:CD1	2.46	0.45
1:A:1724:SER:HA	1:A:1728:LYS:HB2	1.98	0.45
4:E:1950:LEU:CD2	4:E:1955:ILE:HG21	2.45	0.45
2:F:434:PRO:HG2	2:F:458:VAL:HG22	1.97	0.45
1:A:1306:PHE:HA	1:A:1320:PHE:HE2	1.81	0.45
2:B:235:LEU:HB2	2:B:291:LEU:C	2.36	0.45
3:C:172:LEU:HD21	3:C:177:ARG:CB	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:1848:ILE:HD11	4:E:1896:ILE:HD11	1.98	0.45
4:E:1875:VAL:HG21	4:E:2026:ALA:HB1	1.97	0.45
4:E:2018:GLU:OE2	4:E:2022:ARG:NH1	2.49	0.45
2:F:242:PHE:CD2	2:F:265:LEU:HD13	2.51	0.45
2:F:832:PRO:HB3	2:F:836:PHE:CZ	2.51	0.45
3:G:45:ILE:O	3:G:45:ILE:HG22	2.17	0.45
3:G:64:TYR:CZ	3:G:108:VAL:HG13	2.51	0.45
1:A:1051:GLU:HG3	4:E:1128:ARG:HB3	1.97	0.45
1:A:1128:ARG:HD3	4:E:1051:GLU:CD	2.36	0.45
1:A:1211:LEU:HD11	1:A:1248:PHE:HD1	1.82	0.45
1:A:1932:PHE:CZ	1:A:1936:ARG:HD2	2.40	0.45
2:B:327:GLU:O	2:B:331:LEU:HG	2.16	0.45
2:B:423:CYS:HB3	2:B:433:ILE:HD13	1.98	0.45
4:E:1493:LEU:HB3	4:E:1528:TRP:NE1	2.31	0.45
4:E:1510:LEU:CD2	4:E:2017:MET:HB3	2.46	0.45
4:E:1632:PRO:O	4:E:1636:GLN:HG3	2.16	0.45
4:E:1878:ASP:C	4:E:1879:LEU:HD12	2.37	0.45
1:A:1134:LYS:CG	1:A:1136:TYR:CE2	2.92	0.45
1:A:1137:SER:N	4:E:1101:ALA:HB2	2.31	0.45
1:A:1234:TRP:O	1:A:1238:LEU:HD13	2.17	0.45
1:A:1298:TRP:O	1:A:1301:PHE:N	2.49	0.45
1:A:1639:VAL:HG21	2:B:394:PHE:HE1	1.82	0.45
1:A:2011:THR:OG1	1:A:2012:PRO:CD	2.64	0.45
2:B:613:TRP:CE3	2:B:695:LEU:HD13	2.52	0.45
2:B:711:LYS:HB3	2:B:714:GLU:OE1	2.17	0.45
3:C:108:VAL:O	3:C:112:GLU:HG2	2.16	0.45
2:F:535:LEU:O	2:F:539:ARG:HG2	2.17	0.45
2:F:586:LEU:HD13	2:F:609:MET:HG2	1.98	0.45
2:F:752:TRP:HA	2:F:755:GLU:HG3	1.96	0.45
1:A:1411:TRP:O	1:A:1415:PHE:HB2	2.17	0.45
1:A:1761:CYS:O	1:A:1764:ALA:HB3	2.16	0.45
2:B:185:LEU:O	2:B:189:GLU:CB	2.63	0.45
2:B:435:LEU:HG	3:C:271:LEU:HD21	1.99	0.45
2:B:693:MET:O	2:B:697:GLN:HG2	2.16	0.45
3:C:79:LEU:N	3:C:80:PRO:HD2	2.32	0.45
4:E:1904:SER:HB2	4:E:1907:GLN:CG	2.42	0.45
2:F:712:PRO:HB3	2:F:742:LEU:HD23	1.97	0.45
3:G:79:LEU:N	3:G:80:PRO:HD2	2.32	0.45
1:A:1131:CYS:HB2	4:E:1098:THR:CG2	2.34	0.45
1:A:1637:TYR:O	1:A:1641:VAL:HG23	2.16	0.45
1:A:1699:GLU:HG2	1:A:1702:HIS:NE2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2010:ALA:O	1:A:2014:LYS:N	2.30	0.45
1:A:2072:ASN:HA	1:A:2075:MET:HG2	1.99	0.45
2:B:271:ARG:HB2	3:C:249:TYR:CD2	2.52	0.45
2:B:519:PHE:HE1	2:B:551:SER:HA	1.80	0.45
4:E:1196:LEU:HD11	4:E:1210:LEU:HD22	1.99	0.45
4:E:1400:LEU:HD13	4:E:1506:TRP:CZ3	2.52	0.45
4:E:1861:ALA:N	4:E:1979:MET:HE3	2.32	0.45
2:F:693:MET:O	2:F:697:GLN:HG2	2.16	0.45
3:G:274:GLU:CG	3:G:275:PRO:HD3	2.40	0.45
1:A:1011:LEU:HD21	1:A:1103:ALA:HB2	1.97	0.45
1:A:1878:ASP:C	1:A:1879:LEU:HD12	2.37	0.45
2:B:83:THR:O	2:B:87:ASP:CB	2.61	0.45
2:B:418:LYS:O	2:B:421:LYS:HB2	2.17	0.45
2:B:535:LEU:O	2:B:539:ARG:HG2	2.17	0.45
4:E:414:UNK:C	4:E:416:UNK:N	2.80	0.45
4:E:1298:TRP:O	4:E:1301:PHE:N	2.50	0.45
4:E:1329:SER:HA	4:E:1377:LYS:NZ	2.32	0.45
4:E:1637:TYR:O	4:E:1641:VAL:HG23	2.16	0.45
2:F:247:ARG:NH2	2:F:282:LEU:HD23	2.32	0.45
2:F:449:GLU:HG2	2:F:453:LYS:NZ	2.32	0.45
1:A:1066:GLN:HA	1:A:1110:PHE:CZ	2.52	0.45
1:A:1590:ILE:CG1	1:A:1594:VAL:HG21	2.46	0.45
2:B:247:ARG:HB3	2:B:312:VAL:HG13	1.98	0.45
2:F:167:ASP:OD2	2:F:169:GLU:HB3	2.16	0.45
3:G:11:GLU:HA	3:G:14:SER:OG	2.17	0.45
3:G:211:CYS:O	3:G:266:ARG:HD3	2.15	0.45
1:A:1225:HIS:HE1	4:E:1091:VAL:HG13	1.82	0.45
1:A:1306:PHE:HD1	1:A:1320:PHE:HD2	1.64	0.45
1:A:1963:ILE:CD1	1:A:1995:LYS:CD	2.89	0.45
3:C:64:TYR:CZ	3:C:108:VAL:HG13	2.51	0.45
3:C:200:LEU:O	3:C:204:CYS:HB2	2.16	0.45
4:E:1211:LEU:HD11	4:E:1248:PHE:HD1	1.82	0.45
1:A:1590:ILE:CG1	1:A:1612:TRP:HZ3	2.28	0.44
1:A:1657:ILE:O	1:A:1660:ALA:HB3	2.18	0.44
3:C:86:TYR:HH	3:C:100:CYS:N	2.12	0.44
3:C:178:PHE:O	3:C:182:THR:OG1	2.34	0.44
4:E:1501:GLU:HA	4:E:1504:ILE:CG2	2.47	0.44
2:F:435:LEU:HG	3:G:271:LEU:HD21	1.98	0.44
2:F:613:TRP:CE3	2:F:695:LEU:HD13	2.52	0.44
1:A:1277:LEU:HD21	1:A:2033:ALA:HB2	1.99	0.44
1:A:1329:SER:HA	1:A:1377:LYS:NZ	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2006:GLY:HA3	1:A:2013:PHE:HB2	1.98	0.44
1:A:2034:VAL:CG1	1:A:2057:LEU:HD21	2.43	0.44
2:B:247:ARG:NH2	2:B:282:LEU:HD23	2.32	0.44
2:B:452:GLU:O	2:B:456:LYS:HG3	2.17	0.44
2:B:489:LEU:O	2:B:493:GLN:HG3	2.17	0.44
3:C:110:ASN:OD1	3:C:168:GLN:HB2	2.18	0.44
4:E:1379:TYR:OH	4:E:1417:ASP:OD2	2.33	0.44
4:E:1667:GLY:H	2:F:347:ARG:HA	1.82	0.44
4:E:2006:GLY:HA3	4:E:2013:PHE:HB2	1.98	0.44
4:E:2036:SER:O	4:E:2039:THR:HG22	2.16	0.44
2:F:452:GLU:O	2:F:456:LYS:HG3	2.17	0.44
2:F:738:GLN:HE22	2:F:769:ARG:HG3	1.83	0.44
1:A:1196:LEU:HD11	1:A:1210:LEU:HD22	1.99	0.44
1:A:1929:THR:O	1:A:1933:GLN:CG	2.53	0.44
1:A:1943:MET:CB	1:A:1971:ILE:HG21	2.40	0.44
4:E:1369:THR:HG23	4:E:1370:ILE:HG13	1.98	0.44
4:E:1411:TRP:O	4:E:1415:PHE:HB2	2.17	0.44
2:F:108:TYR:CZ	2:F:150:LEU:HB3	2.53	0.44
3:G:110:ASN:OD1	3:G:168:GLN:HB2	2.18	0.44
3:G:200:LEU:O	3:G:204:CYS:HB2	2.16	0.44
3:G:237:MET:HA	3:G:240:MET:CG	2.43	0.44
1:A:934:GLN:O	1:A:938:ALA:HB2	2.18	0.44
1:A:1051:GLU:HG3	4:E:1128:ARG:HG2	2.00	0.44
1:A:1246:VAL:HG13	1:A:1247:PRO:HD3	1.99	0.44
1:A:1260:VAL:HG22	1:A:1267:PHE:CE2	2.53	0.44
1:A:1404:ILE:HD13	1:A:1507:TYR:CE2	2.35	0.44
1:A:1905:ARG:HD3	1:A:1963:ILE:O	2.18	0.44
2:B:108:TYR:CZ	2:B:150:LEU:HB3	2.53	0.44
3:C:11:GLU:HA	3:C:14:SER:OG	2.17	0.44
4:E:1066:GLN:HA	4:E:1110:PHE:CZ	2.52	0.44
4:E:1400:LEU:CD2	4:E:1507:TYR:HD2	2.26	0.44
2:B:715:ALA:O	2:B:719:THR:HG22	2.18	0.44
2:B:738:GLN:HE22	2:B:769:ARG:HG3	1.83	0.44
4:E:1306:PHE:HA	4:E:1320:PHE:HE2	1.81	0.44
2:F:715:ALA:O	2:F:719:THR:HG22	2.18	0.44
3:G:109:TYR:CE1	3:G:183:PHE:HB2	2.50	0.44
1:A:1242:ASP:OD1	1:A:1243:GLY:N	2.50	0.44
1:A:1260:VAL:HG22	1:A:1267:PHE:CZ	2.53	0.44
1:A:1359:LEU:HD23	1:A:1359:LEU:O	2.18	0.44
1:A:1848:ILE:HD11	1:A:1896:ILE:HD11	1.98	0.44
1:A:1930:LEU:HD12	1:A:1930:LEU:HA	1.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:246:LEU:HA	2:B:246:LEU:HD23	1.83	0.44
2:B:300:ASN:OD1	2:B:301:THR:N	2.50	0.44
2:B:405:LEU:HB3	3:C:277:LEU:HB2	1.99	0.44
2:B:586:LEU:HD13	2:B:609:MET:HG2	1.98	0.44
4:E:1246:VAL:HG13	4:E:1247:PRO:HD3	1.99	0.44
4:E:1260:VAL:HG22	4:E:1267:PHE:CE2	2.53	0.44
4:E:1260:VAL:HG22	4:E:1267:PHE:CZ	2.53	0.44
2:F:246:LEU:HD23	2:F:246:LEU:HA	1.83	0.44
3:G:86:TYR:HH	3:G:100:CYS:N	2.15	0.44
1:A:1529:ARG:HD2	1:A:1533:ILE:HD11	1.98	0.44
1:A:1861:ALA:CB	1:A:1979:MET:HB2	2.41	0.44
1:A:1947:SER:OG	1:A:1994:ILE:HG21	2.18	0.44
1:A:2075:MET:HA	1:A:2078:ILE:CG2	2.46	0.44
2:B:242:PHE:CD2	2:B:265:LEU:HD13	2.51	0.44
2:B:341:ARG:HH12	3:C:145:MET:CE	2.30	0.44
2:B:589:LYS:HE2	2:B:593:GLN:NE2	2.33	0.44
3:C:45:ILE:HG22	3:C:45:ILE:O	2.17	0.44
4:E:1154:TYR:CE2	4:E:1158:ARG:HD3	2.53	0.44
4:E:1242:ASP:OD1	4:E:1243:GLY:N	2.50	0.44
4:E:1733:ARG:O	4:E:1737:PHE:HB2	2.18	0.44
4:E:1905:ARG:HD3	4:E:1963:ILE:O	2.18	0.44
4:E:2024:TYR:OH	4:E:2061:PHE:O	2.23	0.44
4:E:2072:ASN:HA	4:E:2075:MET:HG2	1.99	0.44
2:F:418:LYS:O	2:F:421:LYS:HB2	2.17	0.44
2:F:711:LYS:HB3	2:F:714:GLU:OE1	2.17	0.44
3:G:75:THR:CG2	3:G:75:THR:O	2.66	0.44
3:G:79:LEU:O	3:G:83:ILE:HG13	2.18	0.44
3:G:218:GLN:O	3:G:222:LYS:N	2.43	0.44
1:A:1594:VAL:O	1:A:1594:VAL:HG12	2.18	0.44
2:B:150:LEU:O	2:B:154:LYS:HG2	2.18	0.44
3:C:79:LEU:O	3:C:83:ILE:HG13	2.18	0.44
4:E:1142:SER:O	4:E:1146:ARG:HG3	2.18	0.44
3:G:214:GLY:HA3	3:G:229:ARG:HB3	2.00	0.44
1:A:1010:MET:SD	1:A:1064:ILE:HD11	2.58	0.44
1:A:1400:LEU:HD13	1:A:1506:TRP:CZ3	2.52	0.44
2:B:329:LEU:O	2:B:333:LEU:HG	2.18	0.44
4:E:970:PHE:CE2	4:E:974:ASN:ND2	2.86	0.44
4:E:1234:TRP:O	4:E:1238:LEU:HD13	2.17	0.44
4:E:1306:PHE:HD1	4:E:1320:PHE:HD2	1.64	0.44
4:E:1957:ASP:OD1	4:E:1993:ASP:O	2.36	0.44
4:E:2075:MET:HA	4:E:2078:ILE:CG2	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:175:CYS:O	2:F:179:ALA:CB	2.66	0.44
2:F:247:ARG:HB3	2:F:312:VAL:HG13	1.98	0.44
2:F:341:ARG:NH2	3:G:145:MET:HE2	2.33	0.44
1:A:1055:LYS:NZ	4:E:1127:GLU:HB3	2.33	0.43
1:A:1147:ASN:ND2	4:E:1144:ASN:OD1	2.51	0.43
3:C:75:THR:CG2	3:C:75:THR:O	2.66	0.43
4:E:1010:MET:SD	4:E:1064:ILE:HD11	2.58	0.43
4:E:1359:LEU:O	4:E:1359:LEU:HD23	2.18	0.43
3:G:56:VAL:O	3:G:59:GLN:HB3	2.18	0.43
3:G:86:TYR:O	3:G:90:SER:HB2	2.18	0.43
1:A:1019:LEU:O	1:A:1019:LEU:HD23	2.19	0.43
1:A:1996:LEU:CA	1:A:2000:MET:CE	2.95	0.43
2:B:449:GLU:HG2	2:B:453:LYS:NZ	2.32	0.43
3:C:86:TYR:O	3:C:90:SER:HB2	2.18	0.43
4:E:1924:TYR:CD1	4:E:1931:ALA:HB1	2.53	0.43
4:E:1957:ASP:CB	4:E:1993:ASP:O	2.66	0.43
2:F:68:PRO:HB3	2:F:111:GLY:HA3	2.00	0.43
2:F:613:TRP:CH2	2:F:695:LEU:HD22	2.53	0.43
1:A:1594:VAL:HG22	1:A:1609:VAL:HG11	2.01	0.43
1:A:1663:TYR:OH	1:A:2043:ASP:OD2	2.36	0.43
1:A:2065:MET:HE2	1:A:2069:GLU:HG3	2.00	0.43
2:B:408:MET:HG2	3:C:273:PRO:CG	2.49	0.43
2:B:581:GLU:N	3:C:175:GLN:HE22	2.16	0.43
3:C:56:VAL:O	3:C:59:GLN:HB3	2.18	0.43
4:E:1594:VAL:O	4:E:1594:VAL:HG12	2.18	0.43
2:F:489:LEU:O	2:F:493:GLN:HG3	2.17	0.43
2:F:589:LYS:HE2	2:F:593:GLN:NE2	2.33	0.43
1:A:1142:SER:O	1:A:1146:ARG:HG3	2.18	0.43
1:A:1154:TYR:CE2	1:A:1158:ARG:HD3	2.53	0.43
1:A:1482:HIS:O	1:A:1486:MET:HB2	2.18	0.43
1:A:1730:PHE:HE1	1:A:1774:CYS:HG	1.66	0.43
1:A:1733:ARG:O	1:A:1737:PHE:HB2	2.18	0.43
1:A:2065:MET:CE	1:A:2069:GLU:HG3	2.48	0.43
2:B:613:TRP:CH2	2:B:695:LEU:HD22	2.53	0.43
3:C:29:THR:HA	3:C:34:LYS:HG3	2.00	0.43
3:C:77:GLN:HG3	3:C:78:PHE:CE2	2.54	0.43
4:E:2036:SER:HA	4:E:2039:THR:HG22	2.00	0.43
2:F:329:LEU:O	2:F:333:LEU:HG	2.18	0.43
2:F:341:ARG:HH12	3:G:145:MET:HG3	1.82	0.43
2:F:438:ALA:O	2:F:442:MET:HG2	2.19	0.43
1:A:1097:HIS:CE1	1:A:1100:LEU:HB2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:68:PRO:HB3	2:B:111:GLY:HA3	2.00	0.43
3:C:182:THR:HG22	3:C:183:PHE:CD1	2.54	0.43
4:E:443:UNK:O	4:E:444:UNK:C	2.62	0.43
4:E:1277:LEU:HD21	4:E:2033:ALA:HB2	1.99	0.43
4:E:1482:HIS:O	4:E:1486:MET:HB2	2.18	0.43
4:E:1663:TYR:OH	4:E:2043:ASP:OD2	2.36	0.43
4:E:1850:LYS:HB3	4:E:1850:LYS:HE3	1.74	0.43
4:E:1868:PHE:HD2	4:E:1949:LEU:HG	1.83	0.43
4:E:1944:ALA:N	4:E:2016:PHE:CE1	2.87	0.43
1:A:1418:LYS:HE2	1:A:1486:MET:HE1	1.99	0.43
1:A:1597:HIS:ND1	1:A:1602:ASP:OD2	2.45	0.43
2:B:769:ARG:NH1	2:B:772:LEU:HD13	2.34	0.43
4:E:1097:HIS:CE1	4:E:1100:LEU:HB2	2.53	0.43
4:E:1115:LYS:NZ	4:E:1116:GLN:HE21	2.17	0.43
4:E:1249:MET:HE2	4:E:1320:PHE:HE1	1.83	0.43
4:E:1391:LYS:C	4:E:1502:ARG:HH22	2.22	0.43
4:E:1908:LEU:CD1	4:E:1919:TYR:HB2	2.49	0.43
2:F:300:ASN:OD1	2:F:301:THR:N	2.50	0.43
1:A:1137:SER:OG	4:E:1093:GLY:O	2.31	0.43
1:A:1190:THR:HG23	1:A:1194:PHE:CE2	2.53	0.43
1:A:1656:GLN:HB3	1:A:2040:LEU:CD1	2.49	0.43
1:A:2036:SER:HA	1:A:2039:THR:HG22	2.00	0.43
2:B:175:CYS:O	2:B:179:ALA:CB	2.65	0.43
2:B:449:GLU:HG2	2:B:453:LYS:HZ3	1.84	0.43
4:E:1594:VAL:HG22	4:E:1609:VAL:HG11	2.01	0.43
4:E:1658:VAL:HG23	4:E:1659:GLN:OE1	2.19	0.43
4:E:1899:ILE:CD1	4:E:1972:ILE:HG21	2.49	0.43
4:E:2028:ARG:HH12	4:E:2065:MET:C	2.16	0.43
4:E:2065:MET:CE	4:E:2069:GLU:HG3	2.48	0.43
3:G:182:THR:HG22	3:G:183:PHE:CD1	2.53	0.43
1:A:1586:VAL:HG13	1:A:1613:ALA:CB	2.45	0.43
1:A:1656:GLN:HB3	1:A:2040:LEU:HD13	2.01	0.43
1:A:1699:GLU:CG	1:A:1700:GLU:H	2.10	0.43
4:E:1122:ALA:O	4:E:1125:LEU:HG	2.19	0.43
3:G:61:PHE:O	3:G:65:ARG:N	2.52	0.43
1:A:1122:ALA:HB3	1:A:1125:LEU:CD2	2.40	0.43
1:A:1401:ARG:NH2	1:A:1516:GLU:HB2	2.33	0.43
2:B:173:ILE:HG23	2:B:177:GLU:CD	2.39	0.43
2:B:438:ALA:O	2:B:442:MET:HG2	2.19	0.43
2:B:501:LEU:O	2:B:505:GLN:HG3	2.19	0.43
4:E:1080:LEU:O	4:E:1083:TYR:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:1656:GLN:HB3	4:E:2040:LEU:HD13	2.01	0.43
4:E:2026:ALA:O	4:E:2029:PRO:HD2	2.19	0.43
2:F:150:LEU:O	2:F:154:LYS:HG2	2.18	0.43
1:A:979:HIS:O	1:A:983:ARG:HG2	2.18	0.43
1:A:1068:ALA:O	1:A:1076:THR:OG1	2.31	0.43
1:A:1250:ARG:CD	2:B:785:LYS:HB2	2.48	0.43
1:A:1899:ILE:CD1	1:A:1972:ILE:HG21	2.49	0.43
2:B:467:GLU:OE2	3:C:216:PRO:HG2	2.19	0.43
2:B:750:ARG:HB2	2:B:773:ILE:HG21	2.01	0.43
4:E:1586:VAL:HG23	4:E:1587:PRO:N	2.34	0.43
3:G:29:THR:HA	3:G:34:LYS:HG3	2.00	0.43
3:G:77:GLN:HG3	3:G:78:PHE:CE2	2.54	0.43
1:A:950:MET:HG2	1:A:954:LYS:HE3	2.01	0.42
1:A:1115:LYS:NZ	1:A:1116:GLN:HE21	2.17	0.42
1:A:1577:ARG:NH2	1:A:1596:TRP:O	2.52	0.42
1:A:1658:VAL:HG23	1:A:1659:GLN:OE1	2.19	0.42
2:B:699:TRP:CE3	2:B:721:GLU:HB2	2.54	0.42
4:E:934:GLN:O	4:E:938:ALA:HB2	2.18	0.42
4:E:1577:ARG:NH2	4:E:1596:TRP:O	2.52	0.42
2:F:173:ILE:HG23	2:F:177:GLU:CD	2.39	0.42
1:A:1055:LYS:CB	4:E:1128:ARG:HA	2.44	0.42
1:A:1659:GLN:NE2	1:A:2041:MET:HG2	2.34	0.42
2:B:344:VAL:O	2:B:347:ARG:HG3	2.18	0.42
3:C:221:ARG:CZ	3:C:258:LYS:HB3	2.50	0.42
4:E:1190:THR:HG23	4:E:1194:PHE:CE2	2.53	0.42
2:F:223:GLN:O	2:F:227:VAL:HG23	2.19	0.42
1:A:1391:LYS:C	1:A:1502:ARG:HH22	2.22	0.42
1:A:1501:GLU:HA	1:A:1504:ILE:CG2	2.47	0.42
1:A:1946:TYR:CB	1:A:1973:HIS:CE1	3.00	0.42
2:B:26:ILE:HB	2:B:27:PRO:HD3	2.02	0.42
2:B:223:GLN:O	2:B:227:VAL:HG23	2.19	0.42
3:C:12:TRP:CG	3:C:37:LEU:HD11	2.54	0.42
4:E:1019:LEU:HD23	4:E:1019:LEU:O	2.19	0.42
4:E:1259:THR:CG2	4:E:1295:HIS:NE2	2.83	0.42
4:E:1659:GLN:NE2	4:E:2041:MET:HG2	2.34	0.42
4:E:1780:PRO:HD3	4:E:1885:ARG:HH22	1.84	0.42
2:F:43:MET:HG3	2:F:47:LEU:CD1	2.50	0.42
1:A:1586:VAL:HG23	1:A:1587:PRO:N	2.35	0.42
1:A:1957:ASP:OD1	1:A:1993:ASP:N	2.52	0.42
2:B:242:PHE:HA	2:B:261:ILE:HD11	2.01	0.42
2:B:700:LEU:HD11	2:B:732:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:950:MET:HG2	4:E:954:LYS:HE3	2.01	0.42
4:E:1081:GLN:HE21	4:E:1143:LEU:N	2.18	0.42
4:E:1657:ILE:O	4:E:1660:ALA:HB3	2.18	0.42
4:E:1882:PHE:HE2	4:E:1899:ILE:HG12	1.78	0.42
2:F:769:ARG:NH1	2:F:772:LEU:HD13	2.34	0.42
3:G:64:TYR:OH	3:G:112:GLU:HG2	2.19	0.42
3:G:79:LEU:O	3:G:82:LEU:HG	2.20	0.42
3:G:102:GLU:HB3	3:G:172:LEU:HB3	2.00	0.42
3:G:244:ILE:HG22	3:G:248:PHE:CE2	2.55	0.42
1:A:1341:ARG:HG3	1:A:1385:TYR:HA	2.01	0.42
1:A:1850:LYS:HE3	1:A:1850:LYS:HB3	1.74	0.42
2:B:187:LEU:HB3	2:B:251:THR:HG21	2.00	0.42
3:C:60:LEU:HD23	3:C:75:THR:HG21	2.02	0.42
3:C:61:PHE:O	3:C:65:ARG:N	2.52	0.42
3:C:80:PRO:HA	3:C:83:ILE:HD12	2.02	0.42
3:C:102:GLU:HB3	3:C:172:LEU:HB3	2.01	0.42
3:C:178:PHE:HE1	3:C:181:LEU:CD1	2.29	0.42
4:E:328:UNK:O	4:E:329:UNK:C	2.67	0.42
4:E:1375:ARG:O	4:E:1379:TYR:HD2	2.03	0.42
2:F:699:TRP:CE3	2:F:721:GLU:HB2	2.54	0.42
1:A:228:UNK:O	1:A:232:UNK:CB	2.68	0.42
1:A:1010:MET:CE	1:A:1061:CYS:HA	2.49	0.42
1:A:1920:PHE:CE2	1:A:1932:PHE:HD1	2.36	0.42
2:B:404:ALA:HB2	2:B:419:VAL:HG12	2.02	0.42
2:B:465:THR:HG23	2:B:467:GLU:N	2.32	0.42
3:C:40:SER:O	3:C:44:VAL:HB	2.20	0.42
4:E:27:UNK:HA	2:F:821:PHE:HD2	1.83	0.42
4:E:1656:GLN:HB3	4:E:2040:LEU:CD1	2.49	0.42
4:E:1787:ILE:HD12	4:E:1807:PHE:CE1	2.55	0.42
4:E:1865:ILE:HG23	4:E:1949:LEU:CD2	2.49	0.42
3:G:12:TRP:CG	3:G:37:LEU:HD11	2.54	0.42
1:A:1787:ILE:HD12	1:A:1807:PHE:CE1	2.55	0.42
1:A:2026:ALA:O	1:A:2029:PRO:HD2	2.19	0.42
2:B:757:LEU:HD23	2:B:757:LEU:HA	1.90	0.42
3:C:192:LEU:HD12	3:C:246:PHE:CG	2.54	0.42
4:E:1149:TYR:O	4:E:1153:VAL:HG23	2.20	0.42
2:F:26:ILE:HB	2:F:27:PRO:HD3	2.02	0.42
2:F:187:LEU:HB3	2:F:251:THR:HG21	2.00	0.42
2:F:332:LEU:HA	2:F:335:SER:HB2	2.02	0.42
2:F:700:LEU:HD11	2:F:732:VAL:HG22	2.01	0.42
1:A:398:UNK:O	1:A:402:UNK:CB	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1232:ALA:HB2	4:E:1094:LEU:CD2	2.50	0.42
1:A:1259:THR:CG2	1:A:1295:HIS:NE2	2.83	0.42
1:A:1780:PRO:HD3	1:A:1885:ARG:HH22	1.84	0.42
1:A:1847:ALA:HA	1:A:1898:CYS:H	1.85	0.42
4:E:399:UNK:O	4:E:403:UNK:CB	2.68	0.42
4:E:1956:LYS:CG	4:E:1982:SER:OG	2.66	0.42
2:F:404:ALA:HB2	2:F:419:VAL:HG12	2.02	0.42
3:G:63:PHE:CD1	3:G:71:LEU:HD13	2.55	0.42
1:A:1080:LEU:O	1:A:1083:TYR:N	2.52	0.42
1:A:1081:GLN:HE21	1:A:1143:LEU:N	2.18	0.42
1:A:1098:THR:CA	4:E:1131:CYS:HB2	2.50	0.42
1:A:1128:ARG:HH11	1:A:1130:ALA:HB2	1.83	0.42
1:A:1375:ARG:O	1:A:1379:TYR:HD2	2.03	0.42
4:E:1066:GLN:O	4:E:1070:LYS:HG2	2.19	0.42
4:E:1538:LYS:HG3	4:E:1539:GLN:CD	2.40	0.42
2:F:371:ILE:CG2	2:F:375:ARG:HH21	2.33	0.42
2:F:386:LEU:HD23	2:F:386:LEU:HA	1.85	0.42
1:A:413:UNK:C	1:A:415:UNK:N	2.81	0.42
1:A:984:ARG:O	1:A:987:ASP:HB3	2.20	0.42
1:A:1149:TYR:O	1:A:1153:VAL:HG23	2.20	0.42
1:A:1993:ASP:CG	1:A:1994:ILE:CD1	2.88	0.42
2:B:371:ILE:CG2	2:B:375:ARG:HH21	2.33	0.42
4:E:1388:CYS:SG	4:E:1389:PRO:HD2	2.60	0.42
4:E:1903:THR:HB	4:E:1965:LEU:O	2.20	0.42
2:F:27:PRO:O	2:F:31:LYS:HB2	2.20	0.42
2:F:242:PHE:HA	2:F:261:ILE:HD11	2.01	0.42
2:F:692:TRP:HE3	2:F:725:LEU:HD22	1.85	0.42
1:A:1046:THR:HG22	1:A:1048:GLU:H	1.86	0.41
1:A:1128:ARG:HB3	4:E:1051:GLU:CG	2.50	0.41
1:A:1379:TYR:OH	1:A:1417:ASP:OD2	2.33	0.41
2:B:386:LEU:HA	2:B:386:LEU:HD23	1.85	0.41
2:B:408:MET:HE1	2:B:436:LEU:HB3	2.01	0.41
3:C:64:TYR:OH	3:C:112:GLU:HG2	2.19	0.41
3:C:132:LYS:HG2	3:C:133:PRO:O	2.20	0.41
4:E:1950:LEU:CB	4:E:1994:ILE:CD1	2.83	0.41
2:F:501:LEU:O	2:F:505:GLN:HG3	2.19	0.41
2:F:787:LEU:HD23	2:F:787:LEU:HA	1.81	0.41
3:G:79:LEU:HD12	3:G:80:PRO:CD	2.49	0.41
1:A:950:MET:O	1:A:954:LYS:HG3	2.20	0.41
1:A:972:LEU:HD22	1:A:1010:MET:SD	2.60	0.41
1:A:1277:LEU:HD23	1:A:1618:PRO:CG	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1940:ILE:O	1:A:1944:ALA:HB2	2.20	0.41
2:B:43:MET:HG3	2:B:47:LEU:CD1	2.50	0.41
3:C:278:VAL:O	3:C:282:ILE:HG12	2.20	0.41
4:E:1696:TYR:CG	4:E:1701:GLY:CA	2.93	0.41
2:F:286:PRO:HG2	2:F:289:SER:HB3	2.02	0.41
1:A:1277:LEU:HD11	1:A:2030:TYR:CD1	2.55	0.41
1:A:1590:ILE:HB	1:A:1612:TRP:HE3	1.83	0.41
1:A:1748:ILE:HG12	1:A:1758:LYS:CB	2.48	0.41
1:A:1860:LEU:HB3	1:A:1979:MET:SD	2.60	0.41
4:E:1585:ASP:O	4:E:1589:ALA:HB3	2.21	0.41
4:E:1847:ALA:HA	4:E:1898:CYS:H	1.85	0.41
2:F:695:LEU:HD23	2:F:725:LEU:HD11	2.02	0.41
3:G:40:SER:O	3:G:44:VAL:HB	2.20	0.41
1:A:1122:ALA:O	1:A:1125:LEU:HG	2.19	0.41
1:A:2043:ASP:O	1:A:2044:THR:OG1	2.35	0.41
2:B:346:SER:HB3	2:B:355:ARG:NH1	2.18	0.41
2:B:487:ALA:HB3	2:B:493:GLN:HG2	2.01	0.41
3:C:79:LEU:O	3:C:82:LEU:HG	2.20	0.41
3:C:237:MET:HA	3:C:240:MET:CG	2.43	0.41
4:E:950:MET:O	4:E:954:LYS:HG3	2.20	0.41
4:E:952:ALA:HB2	4:E:996:LYS:HE3	2.02	0.41
4:E:1085:ASN:HA	4:E:1090:TRP:HZ2	1.85	0.41
4:E:1343:VAL:HG11	4:E:1393:PRO:HG3	2.03	0.41
4:E:1529:ARG:CD	4:E:1533:ILE:HD11	2.51	0.41
4:E:1857:GLN:NE2	4:E:1977:GLY:O	2.54	0.41
2:F:93:SER:O	2:F:97:GLN:HG3	2.21	0.41
3:G:278:VAL:O	3:G:282:ILE:HG12	2.20	0.41
1:A:32:UNK:HA	1:A:48:UNK:CB	2.50	0.41
1:A:1066:GLN:O	1:A:1070:LYS:HG2	2.19	0.41
1:A:1388:CYS:SG	1:A:1389:PRO:HD2	2.60	0.41
1:A:1590:ILE:CG1	1:A:1594:VAL:CG2	2.97	0.41
2:B:695:LEU:HD23	2:B:725:LEU:HD11	2.02	0.41
3:C:79:LEU:HD12	3:C:80:PRO:CD	2.50	0.41
2:F:128:LEU:HA	2:F:129:PRO:HD3	1.93	0.41
2:F:259:MET:HB2	2:F:338:MET:HG2	2.02	0.41
2:F:390:MET:SD	2:F:399:LEU:HG	2.61	0.41
3:G:192:LEU:HD12	3:G:246:PHE:CG	2.54	0.41
3:G:200:LEU:HD13	3:G:247:ALA:HA	2.01	0.41
1:A:1085:ASN:HA	1:A:1090:TRP:HZ2	1.86	0.41
2:B:27:PRO:O	2:B:31:LYS:HB2	2.20	0.41
2:B:332:LEU:HA	2:B:335:SER:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:57:CYS:O	3:C:60:LEU:HB2	2.21	0.41
3:C:63:PHE:CD1	3:C:71:LEU:HD13	2.55	0.41
4:E:1277:LEU:HD11	4:E:2030:TYR:CD1	2.55	0.41
4:E:1305:ARG:HD3	4:E:1305:ARG:HA	1.81	0.41
4:E:1329:SER:HA	4:E:1377:LYS:HZ1	1.85	0.41
3:G:221:ARG:CZ	3:G:258:LYS:HB3	2.50	0.41
1:A:1529:ARG:CD	1:A:1533:ILE:HD11	2.51	0.41
2:B:259:MET:HB2	2:B:338:MET:HG2	2.02	0.41
2:B:515:HIS:CE1	2:B:516:GLN:HG3	2.56	0.41
3:C:79:LEU:HD12	3:C:80:PRO:N	2.36	0.41
3:C:244:ILE:HG22	3:C:248:PHE:CE2	2.55	0.41
4:E:1953:LEU:HD23	4:E:1953:LEU:N	2.32	0.41
2:F:449:GLU:HG2	2:F:453:LYS:HZ3	1.86	0.41
2:F:803:GLY:O	2:F:807:VAL:HG23	2.20	0.41
1:A:1032:TYR:HE2	1:A:1043:VAL:HG21	1.86	0.41
1:A:1343:VAL:HG11	1:A:1393:PRO:HG3	2.03	0.41
1:A:1617:PRO:HD3	1:A:1645:PHE:CE2	2.54	0.41
1:A:1908:LEU:CD1	1:A:1919:TYR:HB2	2.49	0.41
2:B:695:LEU:HG	2:B:699:TRP:CD1	2.56	0.41
3:C:200:LEU:HD13	3:C:247:ALA:HA	2.01	0.41
4:E:1032:TYR:HE2	4:E:1043:VAL:HG21	1.86	0.41
4:E:1341:ARG:HG3	4:E:1385:TYR:HA	2.01	0.41
4:E:1367:ASN:ND2	4:E:1369:THR:CG2	2.83	0.41
4:E:1720:THR:HG23	4:E:1731:TYR:OH	2.20	0.41
4:E:1740:LYS:O	4:E:1744:VAL:HG23	2.21	0.41
4:E:1996:LEU:HA	4:E:2000:MET:CE	2.50	0.41
2:F:139:ARG:HD3	2:F:186:TYR:OH	2.21	0.41
2:F:185:LEU:O	2:F:189:GLU:CB	2.63	0.41
2:F:750:ARG:HB2	2:F:773:ILE:HG21	2.01	0.41
2:F:787:LEU:HD13	2:F:804:LEU:CA	2.51	0.41
1:A:976:ASN:ND2	1:A:1013:ILE:CG2	2.83	0.41
1:A:1026:HIS:HE1	4:E:2015:TRP:CE3	2.39	0.41
1:A:1185:HIS:CD2	1:A:1186:PRO:HD2	2.46	0.41
1:A:1538:LYS:HG3	1:A:1539:GLN:CD	2.40	0.41
1:A:1586:VAL:N	1:A:1587:PRO:HD2	2.36	0.41
1:A:1740:LYS:O	1:A:1744:VAL:HG23	2.21	0.41
1:A:1785:LEU:HD12	1:A:1786:ASP:HB2	2.03	0.41
1:A:1901:ASP:HB3	1:A:1966:ASP:HB2	2.03	0.41
1:A:1951:PHE:CE1	1:A:2077:VAL:HG11	2.55	0.41
2:B:544:LEU:HB3	3:C:229:ARG:HH21	1.85	0.41
2:B:787:LEU:HD13	2:B:804:LEU:CA	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:159:LYS:HE2	3:C:159:LYS:HB3	1.95	0.41
4:E:972:LEU:HD22	4:E:1010:MET:SD	2.60	0.41
2:F:134:PRO:HA	2:F:135:PRO:HD3	1.96	0.41
2:F:394:PHE:CD2	2:F:395:GLU:HG2	2.56	0.41
2:F:531:ILE:HG21	2:F:562:GLN:HG3	2.03	0.41
2:F:576:LEU:CD1	2:F:586:LEU:HD23	2.51	0.41
1:A:1499:GLU:OE1	1:A:1502:ARG:HD3	2.21	0.41
1:A:1943:MET:HB3	1:A:1971:ILE:CG2	2.43	0.41
2:B:139:ARG:HD3	2:B:186:TYR:OH	2.21	0.41
2:B:576:LEU:CD1	2:B:586:LEU:HD23	2.51	0.41
3:C:29:THR:HA	3:C:34:LYS:HE3	2.03	0.41
4:E:229:UNK:O	4:E:233:UNK:CB	2.68	0.41
4:E:1401:ARG:NH2	4:E:1516:GLU:HB2	2.33	0.41
4:E:1632:PRO:HG2	2:F:345:LEU:HD13	2.03	0.41
4:E:1632:PRO:HG3	2:F:345:LEU:HD13	2.02	0.41
4:E:1951:PHE:CE1	4:E:2077:VAL:HG11	2.55	0.41
2:F:350:GLU:HG2	2:F:350:GLU:O	2.21	0.41
2:F:569:LEU:CD2	2:F:597:ARG:HE	2.34	0.41
1:A:952:ALA:HB2	1:A:996:LYS:HE3	2.02	0.40
1:A:1857:GLN:NE2	1:A:1977:GLY:O	2.54	0.40
3:C:109:TYR:CE1	3:C:183:PHE:HB2	2.50	0.40
4:E:984:ARG:O	4:E:987:ASP:HB3	2.20	0.40
4:E:1122:ALA:HB3	4:E:1125:LEU:CD2	2.40	0.40
4:E:1191:GLN:HG2	4:E:1195:LYS:CE	2.44	0.40
4:E:1624:PHE:O	4:E:1663:TYR:HB2	2.21	0.40
4:E:1642:LEU:O	4:E:1672:TYR:OH	2.39	0.40
2:F:172:VAL:HA	2:F:176:TYR:CD2	2.55	0.40
3:G:80:PRO:HA	3:G:83:ILE:HD12	2.02	0.40
1:A:932:MET:HG3	1:A:934:GLN:H	1.86	0.40
1:A:1148:ARG:HD2	4:E:1087:HIS:NE2	2.35	0.40
1:A:1610:LEU:HB3	2:B:400:TRP:HH2	1.86	0.40
2:B:93:SER:O	2:B:97:GLN:HG3	2.21	0.40
2:B:390:MET:SD	2:B:399:LEU:HG	2.61	0.40
2:B:403:PHE:CE2	2:B:407:LEU:HD11	2.57	0.40
2:B:514:ASP:HA	3:C:229:ARG:HH12	1.86	0.40
4:E:32:UNK:HA	4:E:48:UNK:CB	2.51	0.40
4:E:2008:MET:CE	4:E:2083:LEU:HD21	2.51	0.40
4:E:2011:THR:OG1	4:E:2012:PRO:CD	2.69	0.40
2:F:515:HIS:CE1	2:F:516:GLN:HG3	2.56	0.40
2:F:748:GLU:HA	2:F:751:ARG:CZ	2.51	0.40
3:G:57:CYS:O	3:G:60:LEU:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:79:LEU:HD12	3:G:80:PRO:N	2.36	0.40
3:G:132:LYS:HG2	3:G:133:PRO:O	2.20	0.40
1:A:1055:LYS:CB	4:E:1129:PRO:HD2	2.52	0.40
1:A:1134:LYS:HB2	1:A:1136:TYR:CD2	2.56	0.40
1:A:1563:LYS:O	1:A:1565:THR:N	2.53	0.40
1:A:1570:ASN:O	1:A:1574:ARG:CB	2.69	0.40
1:A:1616:ASP:OD1	1:A:1616:ASP:N	2.54	0.40
1:A:1903:THR:HB	1:A:1965:LEU:O	2.20	0.40
1:A:1924:TYR:CB	1:A:1931:ALA:HB1	2.45	0.40
4:E:400:UNK:O	4:E:404:UNK:CB	2.70	0.40
4:E:1237:LEU:CD1	4:E:1238:LEU:HD12	2.52	0.40
4:E:1570:ASN:O	4:E:1574:ARG:CB	2.69	0.40
2:F:487:ALA:HB3	2:F:493:GLN:HG2	2.01	0.40
3:G:60:LEU:HD23	3:G:75:THR:HG21	2.01	0.40
1:A:1191:GLN:HG2	1:A:1195:LYS:CE	2.44	0.40
1:A:1201:ILE:O	1:A:1203:SER:N	2.55	0.40
1:A:1636:GLN:HG2	2:B:394:PHE:HD1	1.86	0.40
2:B:692:TRP:HE3	2:B:725:LEU:HD22	1.85	0.40
2:B:803:GLY:O	2:B:807:VAL:HG23	2.20	0.40
4:E:971:LEU:HD23	4:E:971:LEU:HA	1.91	0.40
4:E:1625:SER:HB3	4:E:2040:LEU:HD21	2.04	0.40
2:F:9:ARG:O	2:F:12:THR:OG1	2.30	0.40
1:A:399:UNK:O	1:A:403:UNK:CB	2.70	0.40
1:A:1011:LEU:CD2	1:A:1103:ALA:HB2	2.52	0.40
1:A:1938:ASN:HB3	1:A:1970:HIS:HD2	1.84	0.40
2:B:368:LEU:HD23	2:B:368:LEU:HA	1.86	0.40
2:B:396:GLU:O	2:B:400:TRP:HD1	2.04	0.40
2:B:495:VAL:CG1	2:B:499:LYS:HE3	2.52	0.40
2:B:589:LYS:HE2	2:B:593:GLN:HE22	1.86	0.40
3:C:41:LEU:HG	3:C:45:ILE:HB	2.04	0.40
3:C:264:ILE:HG23	3:C:276:LEU:CD1	2.52	0.40
4:E:230:UNK:O	4:E:234:UNK:CB	2.70	0.40
4:E:1132:VAL:O	4:E:1134:LYS:HG2	2.22	0.40
4:E:1227:MET:HB3	4:E:1227:MET:HE3	1.96	0.40
4:E:1499:GLU:OE1	4:E:1502:ARG:HD3	2.21	0.40
4:E:1958:ARG:C	4:E:1959:HIS:CG	2.95	0.40
2:F:368:LEU:HD23	2:F:368:LEU:HA	1.86	0.40
2:F:396:GLU:O	2:F:400:TRP:HD1	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1019/1647 (62%)	949 (93%)	70 (7%)	0	100	100
2	B	714/863 (83%)	691 (97%)	23 (3%)	0	100	100
2	F	714/863 (83%)	692 (97%)	22 (3%)	0	100	100
3	C	254/292 (87%)	242 (95%)	12 (5%)	0	100	100
3	G	254/292 (87%)	242 (95%)	12 (5%)	0	100	100
4	E	1019/1648 (62%)	951 (93%)	68 (7%)	0	100	100
All	All	3974/5605 (71%)	3767 (95%)	207 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	A	901/1022 (88%)	901 (100%)	0	100	100
2	B	616/727 (85%)	616 (100%)	0	100	100
2	F	616/727 (85%)	616 (100%)	0	100	100
3	C	236/260 (91%)	236 (100%)	0	100	100
3	G	236/260 (91%)	236 (100%)	0	100	100
4	E	901/1022 (88%)	900 (100%)	1 (0%)	93	98
All	All	3506/4018 (87%)	3505 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	E	1929	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	977	HIS
1	A	979	HIS
1	A	1015	GLN
1	A	1026	HIS
1	A	1081	GLN
1	A	1116	GLN
1	A	1147	ASN
1	A	1527	ASN
1	A	1557	GLN
1	A	1631	HIS
1	A	1685	HIS
1	A	1690	ASN
1	A	1779	ASN
1	A	1796	GLN
1	A	2072	ASN
2	B	107	ASN
2	B	446	HIS
2	B	515	HIS
2	B	701	HIS
2	B	738	GLN
2	B	809	GLN
4	E	1015	GLN
4	E	1026	HIS
4	E	1081	GLN
4	E	1096	GLN
4	E	1116	GLN
4	E	1147	ASN
4	E	1225	HIS
4	E	1527	ASN
4	E	1557	GLN
4	E	1631	HIS
4	E	1685	HIS
4	E	1690	ASN
4	E	1779	ASN
4	E	1796	GLN
4	E	1959	HIS

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Mol	Chain	Res	Type
4	E	1973	HIS
4	E	2072	ASN
2	F	107	ASN
2	F	351	HIS
2	F	402	GLN
2	F	446	HIS
2	F	701	HIS
2	F	738	GLN
3	G	137	HIS
3	G	175	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	E4S	E	2201	-	45,46,46	4.38	29 (64%)	59,67,67	2.71	18 (30%)
5	E4S	A	2201	-	45,46,46	4.17	28 (62%)	59,67,67	2.63	19 (32%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	E4S	E	2201	-	-	8/25/33/33	0/6/6/6
5	E4S	A	2201	-	-	10/25/33/33	0/6/6/6

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	2201	E4S	C24-C29	10.88	1.52	1.38
5	A	2201	E4S	C24-C29	10.68	1.52	1.38
5	E	2201	E4S	C04-C03	-9.49	1.24	1.39
5	E	2201	E4S	C06-N01	8.05	1.51	1.34
5	E	2201	E4S	C19-C14	7.57	1.53	1.38
5	A	2201	E4S	C04-C03	-7.39	1.28	1.39
5	E	2201	E4S	C09-N04	-7.27	1.29	1.39
5	A	2201	E4S	C09-N04	-7.23	1.29	1.39
5	E	2201	E4S	C16-C15	7.15	1.51	1.38
5	A	2201	E4S	C19-C14	7.04	1.52	1.38
5	A	2201	E4S	C27-C28	6.80	1.53	1.38
5	A	2201	E4S	C16-C15	6.79	1.51	1.38
5	E	2201	E4S	C27-C28	6.77	1.53	1.38
5	A	2201	E4S	C18-C17	6.68	1.52	1.39
5	A	2201	E4S	C26-C25	6.52	1.52	1.38
5	E	2201	E4S	C26-C25	6.46	1.52	1.38
5	A	2201	E4S	C06-N01	6.36	1.47	1.34
5	E	2201	E4S	C18-C17	6.35	1.51	1.39
5	A	2201	E4S	C04-C05	6.09	1.50	1.39
5	E	2201	E4S	C04-C05	6.06	1.50	1.39
5	E	2201	E4S	C13-N03	5.95	1.46	1.33
5	A	2201	E4S	C13-N03	5.94	1.45	1.33
5	E	2201	E4S	C25-C24	-5.28	1.30	1.39
5	A	2201	E4S	C25-C24	-5.07	1.31	1.39
5	E	2201	E4S	C19-C18	-5.00	1.29	1.38
5	E	2201	E4S	S01-N06	4.89	1.71	1.63
5	A	2201	E4S	C19-C18	-4.68	1.30	1.38
5	A	2201	E4S	S01-N06	4.45	1.71	1.63
5	E	2201	E4S	C16-C17	-4.38	1.30	1.39
5	A	2201	E4S	C16-C17	-4.28	1.30	1.39
5	A	2201	E4S	C06-C05	-4.24	1.31	1.39
5	E	2201	E4S	C06-C05	-3.96	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	2201	E4S	C13-N04	-3.95	1.29	1.37
5	A	2201	E4S	C11-C10	-3.61	1.35	1.41
5	A	2201	E4S	C13-N04	-3.45	1.30	1.37
5	A	2201	E4S	C15-C14	-3.38	1.31	1.38
5	A	2201	E4S	C10-N02	3.37	1.49	1.38
5	E	2201	E4S	C10-N02	3.11	1.49	1.38
5	E	2201	E4S	C15-C14	-3.07	1.32	1.38
5	E	2201	E4S	C08-C09	-3.04	1.34	1.40
5	E	2201	E4S	C11-C10	-2.96	1.36	1.41
5	E	2201	E4S	O03-S01	2.88	1.46	1.43
5	E	2201	E4S	C28-C29	-2.82	1.32	1.37
5	A	2201	E4S	C28-C29	-2.80	1.32	1.37
5	E	2201	E4S	O04-S01	2.80	1.46	1.43
5	A	2201	E4S	O04-S01	2.75	1.46	1.43
5	A	2201	E4S	C02-N01	-2.64	1.27	1.32
5	A	2201	E4S	O01-C02	2.61	1.39	1.35
5	A	2201	E4S	O03-S01	2.53	1.46	1.43
5	E	2201	E4S	O01-C02	2.52	1.39	1.35
5	E	2201	E4S	C27-C26	-2.37	1.31	1.38
5	A	2201	E4S	C27-C26	-2.36	1.31	1.38
5	E	2201	E4S	C02-N01	-2.31	1.28	1.32
5	A	2201	E4S	C03-S01	2.28	1.80	1.77
5	A	2201	E4S	C20-N05	-2.12	1.43	1.46
5	E	2201	E4S	C03-S01	2.06	1.80	1.77
5	E	2201	E4S	C11-C12	2.02	1.40	1.36

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	2201	E4S	O04-S01-O03	-14.41	101.83	119.55
5	A	2201	E4S	O04-S01-O03	-13.79	102.60	119.55
5	E	2201	E4S	C25-C24-C29	4.47	121.68	117.17
5	A	2201	E4S	O01-C02-C03	4.32	123.59	117.29
5	E	2201	E4S	C23-N05-C20	4.12	120.60	111.52
5	A	2201	E4S	C25-C24-C29	4.03	121.24	117.17
5	E	2201	E4S	C03-S01-N06	3.89	111.82	107.27
5	E	2201	E4S	C28-C29-C24	-3.75	118.98	123.24
5	A	2201	E4S	C23-N05-C20	3.62	119.52	111.52
5	E	2201	E4S	C15-C14-N04	3.59	122.58	119.24
5	A	2201	E4S	C28-C29-C24	-3.51	119.25	123.24
5	E	2201	E4S	C05-C06-N01	-3.48	118.59	124.32
5	A	2201	E4S	C14-N04-C09	-3.46	119.97	125.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	2201	E4S	C24-N06-S01	-3.32	112.62	123.41
5	A	2201	E4S	O01-C02-N01	-3.29	116.52	120.35
5	E	2201	E4S	C12-C07-C05	3.17	126.85	121.36
5	A	2201	E4S	C13-N02-C10	-3.16	102.36	106.73
5	E	2201	E4S	O03-S01-C03	3.11	112.78	107.66
5	A	2201	E4S	C01-O01-C02	-3.01	114.23	117.21
5	A	2201	E4S	C07-C08-C09	-2.92	118.75	121.87
5	A	2201	E4S	C18-C17-N05	-2.89	117.39	121.38
5	E	2201	E4S	C18-C17-N05	-2.88	117.41	121.38
5	E	2201	E4S	C04-C03-S01	-2.83	113.53	118.51
5	E	2201	E4S	C22-C23-N05	-2.75	104.95	110.02
5	A	2201	E4S	C24-N06-S01	-2.69	114.65	123.41
5	A	2201	E4S	C03-S01-N06	2.53	110.22	107.27
5	A	2201	E4S	O03-S01-N06	2.51	113.03	106.73
5	E	2201	E4S	N03-C13-N02	-2.50	120.03	123.28
5	A	2201	E4S	C08-C09-C10	2.47	122.99	120.54
5	A	2201	E4S	C04-C05-C06	2.35	119.44	117.11
5	A	2201	E4S	C05-C06-N01	-2.26	120.59	124.32
5	E	2201	E4S	C14-N04-C09	-2.21	122.09	125.84
5	E	2201	E4S	O03-S01-N06	2.20	112.24	106.73
5	A	2201	E4S	C19-C18-C17	-2.17	117.46	120.32
5	E	2201	E4S	C08-C07-C05	-2.14	116.15	121.05
5	E	2201	E4S	C01-O01-C02	-2.13	115.10	117.21
5	A	2201	E4S	C08-C09-N04	2.09	136.59	132.04

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2201	E4S	C03-C02-O01-C01
5	A	2201	E4S	N01-C02-O01-C01
5	A	2201	E4S	C02-C03-S01-N06
5	A	2201	E4S	C24-N06-S01-C03
5	E	2201	E4S	C03-C02-O01-C01
5	E	2201	E4S	N01-C02-O01-C01
5	E	2201	E4S	C02-C03-S01-N06
5	E	2201	E4S	C02-C03-S01-O03
5	E	2201	E4S	C02-C03-S01-O04
5	E	2201	E4S	C24-N06-S01-C03
5	E	2201	E4S	C04-C03-S01-N06
5	E	2201	E4S	C04-C03-S01-O03
5	A	2201	E4S	C04-C03-S01-N06

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Mol	Chain	Res	Type	Atoms
5	A	2201	E4S	C24-N06-S01-O04
5	A	2201	E4S	C04-C03-S01-O03
5	A	2201	E4S	C02-C03-S01-O03
5	A	2201	E4S	C25-C24-N06-S01
5	A	2201	E4S	C02-C03-S01-O04

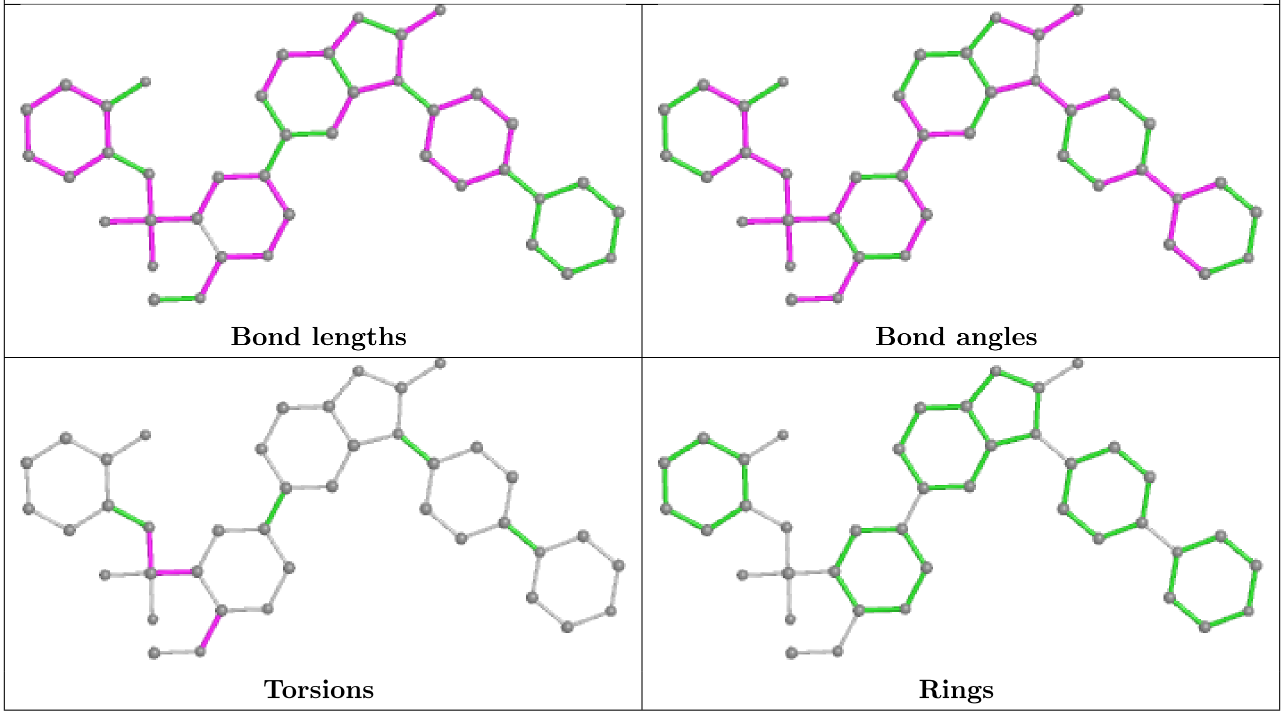
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	2201	E4S	3	0
5	A	2201	E4S	3	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 E4S E 2201



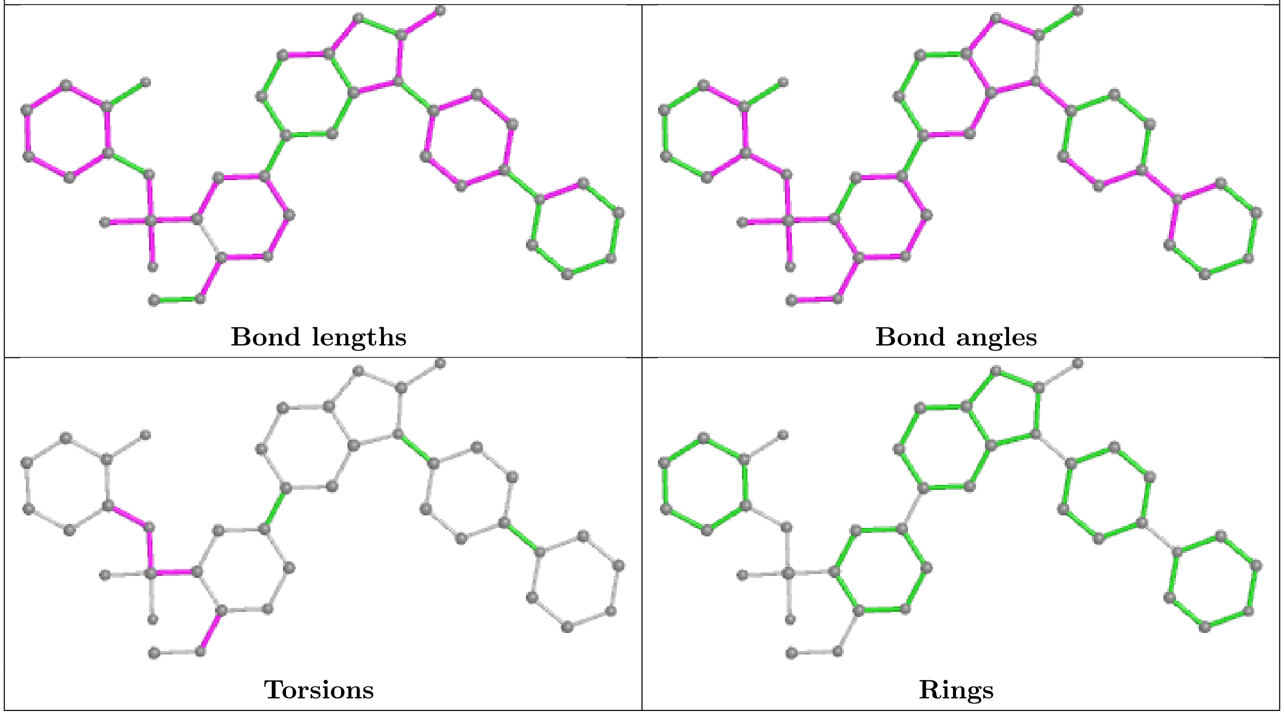
Bond lengths

Bond angles

Torsions

Rings

Ligand E4S A 2201



Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	E	27
1	A	27

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	194:UNK	C	195:UNK	N	33.07
1	A	175:UNK	C	176:UNK	N	30.98
1	E	175:UNK	C	176:UNK	N	30.98
1	A	437:UNK	C	438:UNK	N	29.73
1	E	438:UNK	C	439:UNK	N	29.73
1	A	52:UNK	C	53:UNK	N	29.41
1	E	52:UNK	C	53:UNK	N	29.40
1	A	194:UNK	C	195:UNK	N	28.74
1	A	139:UNK	C	140:UNK	N	27.98
1	E	139:UNK	C	140:UNK	N	27.98
1	E	33:UNK	C	34:UNK	N	25.84
1	A	307:UNK	C	308:UNK	N	25.79
1	E	309:UNK	C	310:UNK	N	25.78
1	A	33:UNK	C	34:UNK	N	25.75
1	E	120:UNK	C	121:UNK	N	25.68
1	A	120:UNK	C	121:UNK	N	25.67
1	A	17:UNK	C	18:UNK	N	22.92
1	E	17:UNK	C	18:UNK	N	22.91
1	A	69:UNK	C	70:UNK	N	19.19
1	E	69:UNK	C	70:UNK	N	19.17
1	A	288:UNK	C	289:UNK	N	17.30
1	E	290:UNK	C	291:UNK	N	17.30
1	A	155:UNK	C	156:UNK	N	14.99
1	E	155:UNK	C	156:UNK	N	14.99
1	E	210:UNK	C	211:UNK	N	14.50
1	A	269:UNK	C	270:UNK	N	13.05
1	E	422:UNK	C	423:UNK	N	13.02
1	A	421:UNK	C	422:UNK	N	13.01
1	E	271:UNK	C	272:UNK	N	12.93
1	A	237:UNK	C	238:UNK	N	12.26
1	E	255:UNK	C	256:UNK	N	12.00
1	A	253:UNK	C	254:UNK	N	11.99
1	E	103:UNK	C	104:UNK	N	11.96
1	A	209:UNK	C	210:UNK	N	11.95

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	103:UNK	C	104:UNK	N	11.94
1	A	342:UNK	C	343:UNK	N	11.91
1	E	343:UNK	C	344:UNK	N	11.91
1	A	324:UNK	C	325:UNK	N	11.51
1	A	89:UNK	C	90:UNK	N	10.36
1	E	396:UNK	C	397:UNK	N	10.36
1	A	395:UNK	C	396:UNK	N	10.35
1	E	89:UNK	C	90:UNK	N	10.35
1	A	379:UNK	C	380:UNK	N	10.03
1	E	380:UNK	C	381:UNK	N	10.03
1	E	238:UNK	C	239:UNK	N	9.90
1	A	407:UNK	C	408:UNK	N	8.93
1	E	408:UNK	C	409:UNK	N	8.92
1	A	361:UNK	C	362:UNK	N	8.65
1	E	362:UNK	C	363:UNK	N	8.65
1	E	326:UNK	C	327:UNK	N	8.10
1	A	476:UNK	C	932:MET	N	7.70
1	E	477:UNK	C	932:MET	N	7.20
1	A	224:UNK	C	225:UNK	N	6.17
1	E	225:UNK	C	226:UNK	N	6.15

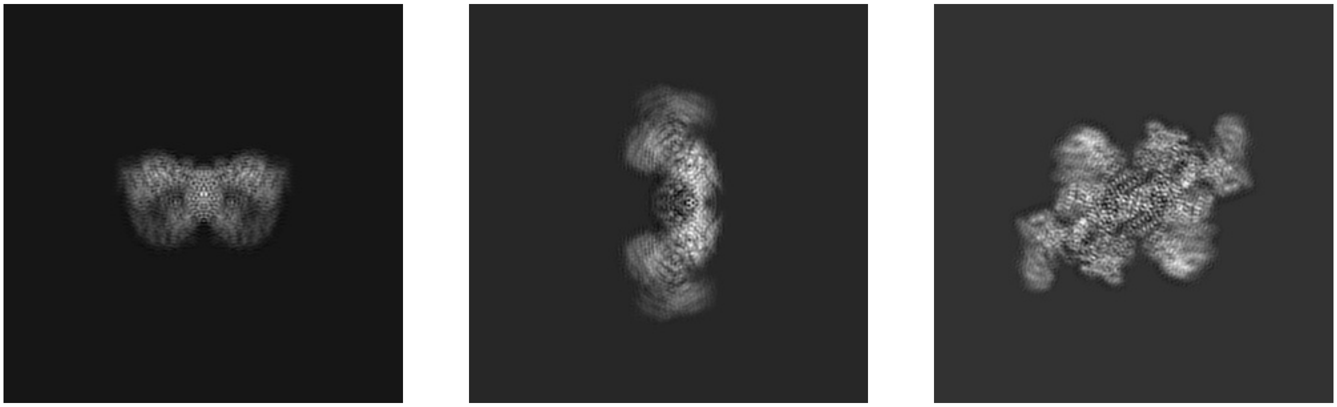
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-7129. 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



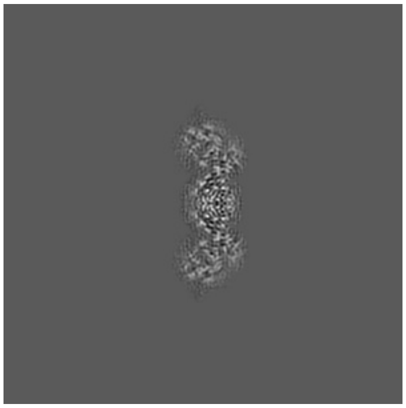
X Y Z

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

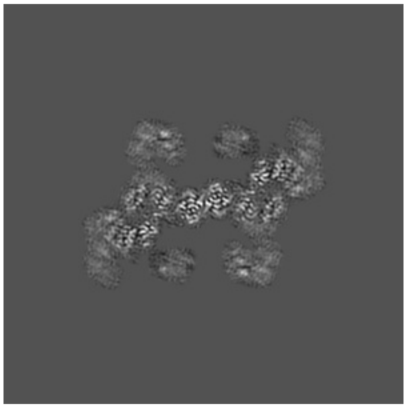
6.2 Central slices

6.2.1 Primary map

X Index: 160



Y Index: 160



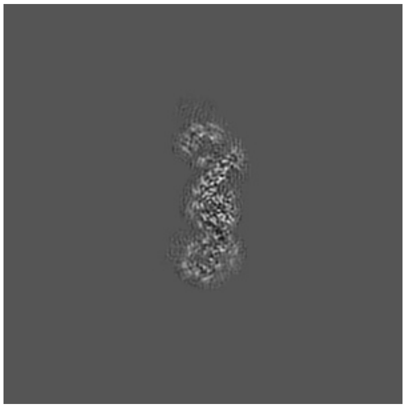
Z Index: 160

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

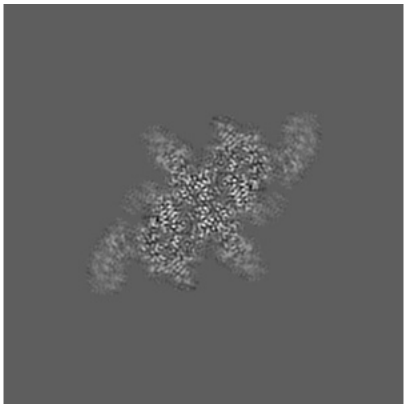
6.3 Largest variance slices

6.3.1 Primary map

X Index: 136



Y Index: 163

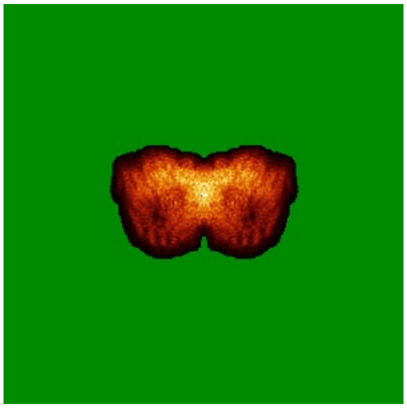


Z Index: 178

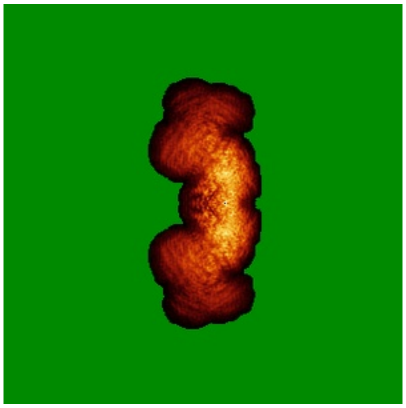
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color)

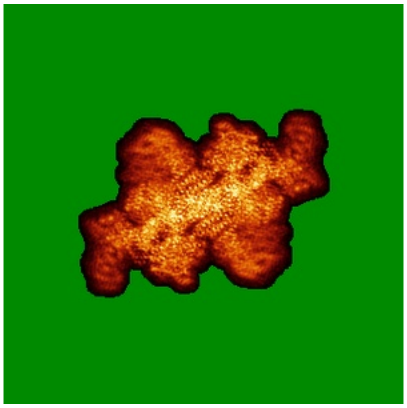
6.4.1 Primary map



X



Y

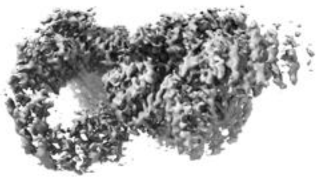


Z

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

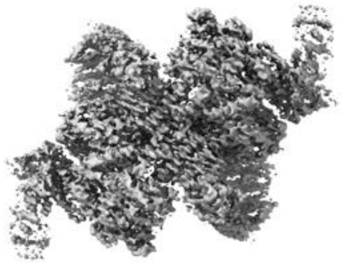
6.5 Orthogonal surface views

6.5.1 Primary map



X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

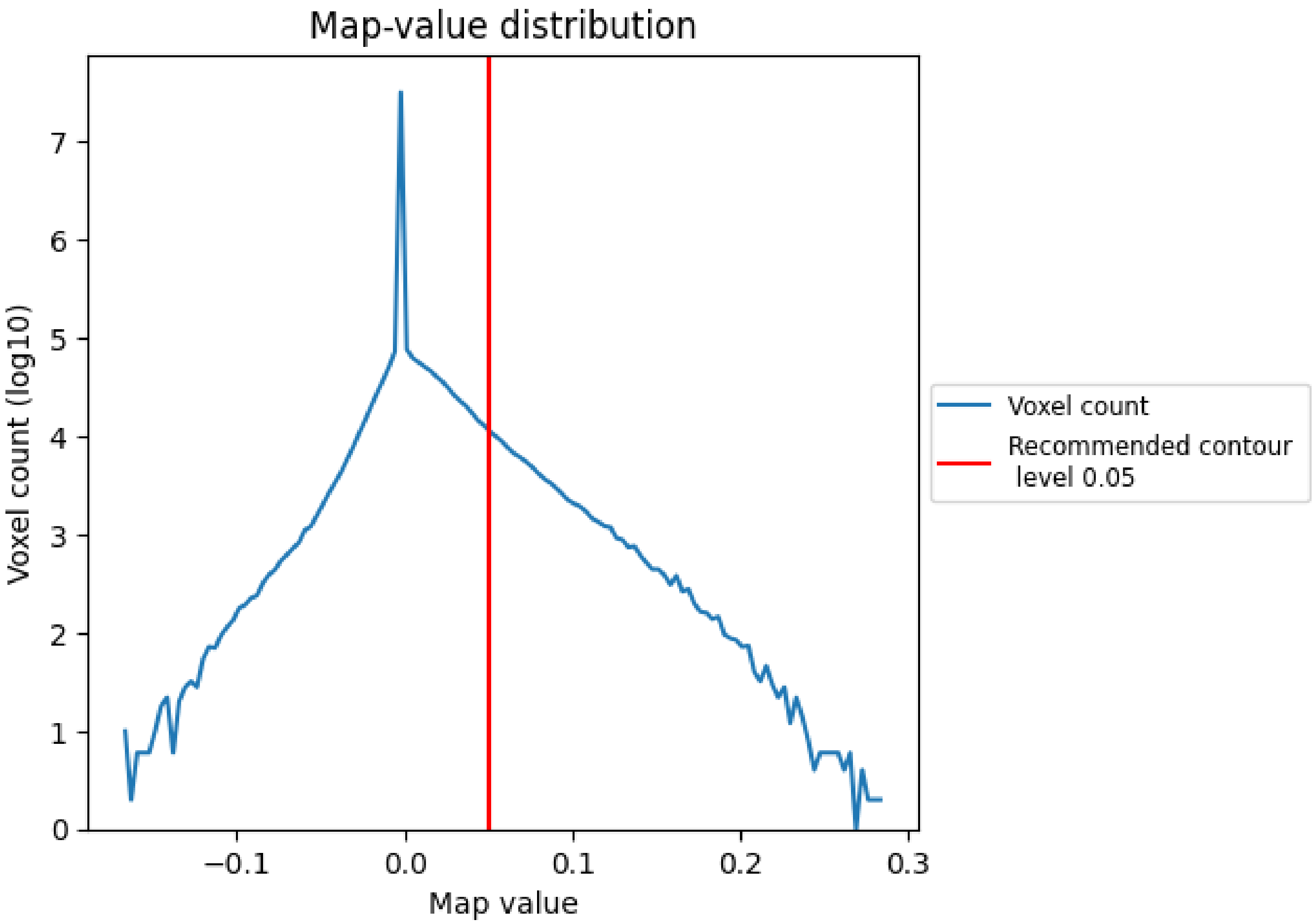
6.6 Mask visualisation

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

7 Map analysis ⓘ

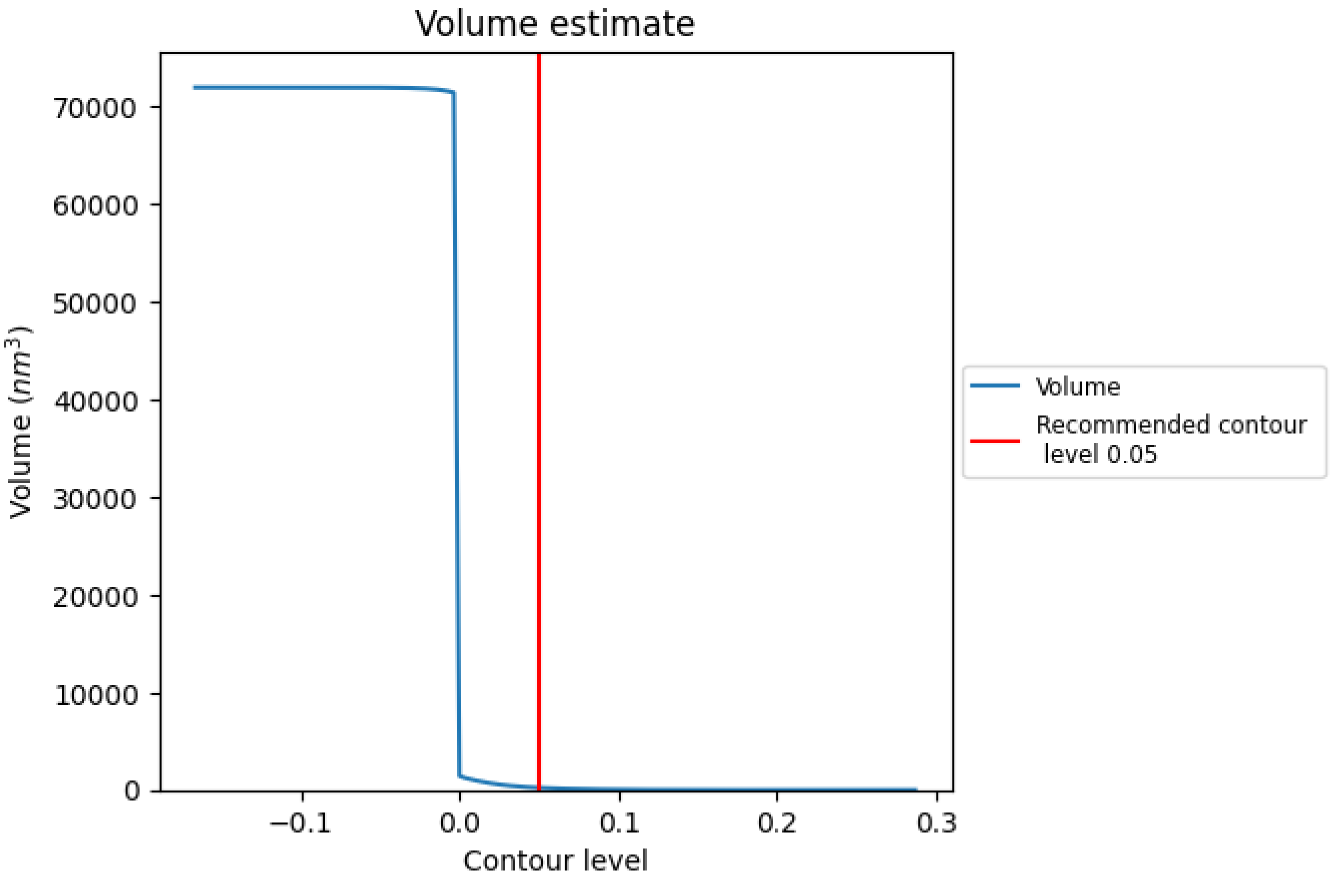
This section contains the results of statistical analysis of the map.

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.

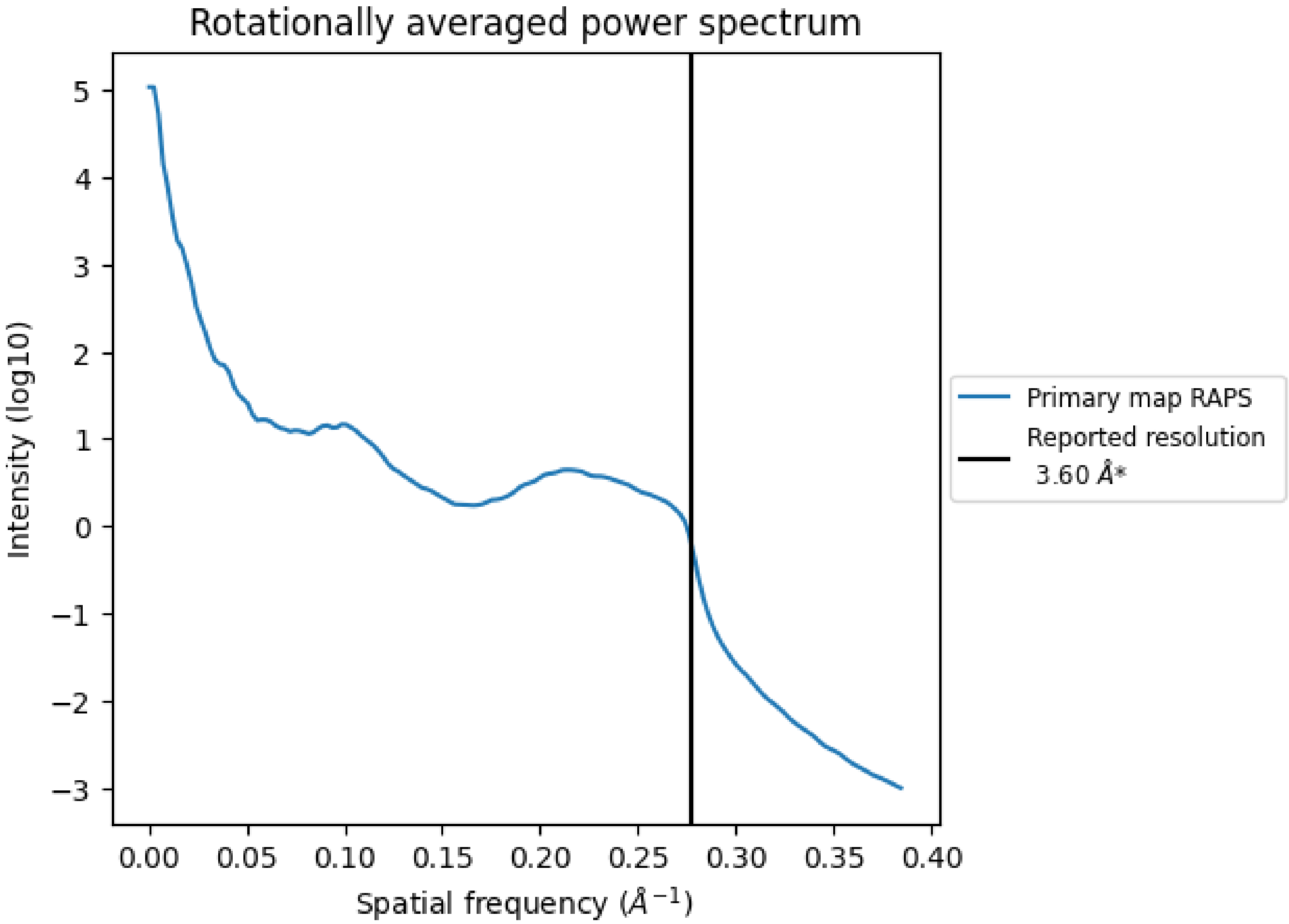
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 227 nm^3; this corresponds to an approximate mass of 205 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 ⓘ

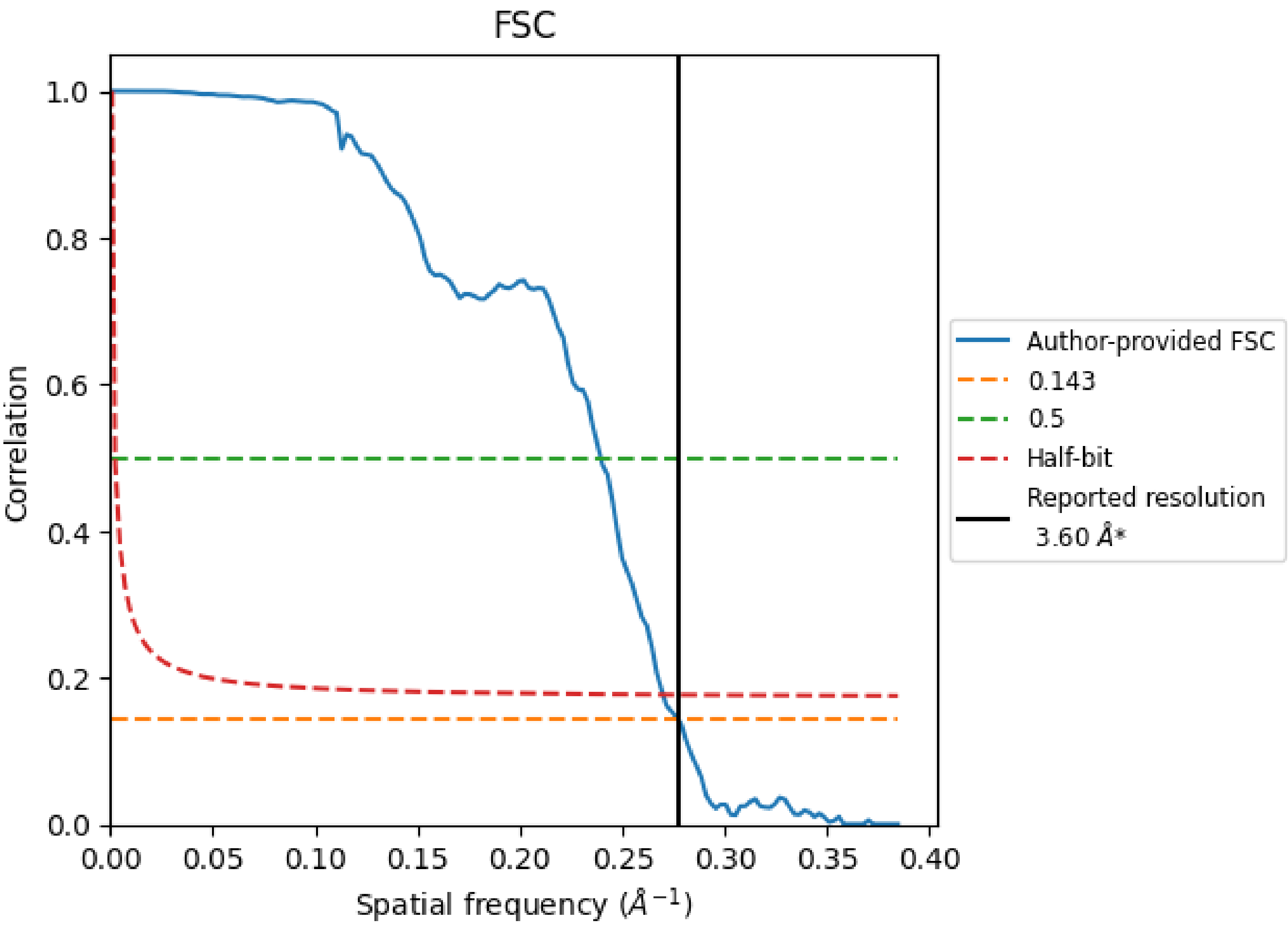


*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8 Fourier-Shell correlation ⓘ

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

8.1 FSC ⓘ



*Reported resolution corresponds to spatial frequency of 0.278 $Å^{-1}$

8.2 Resolution estimates ⓘ

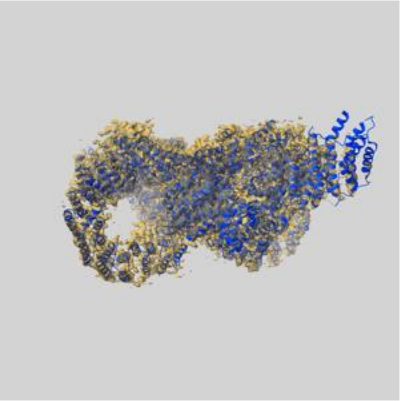
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.61	4.18	3.70
Unmasked-calculated*	-	-	-

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

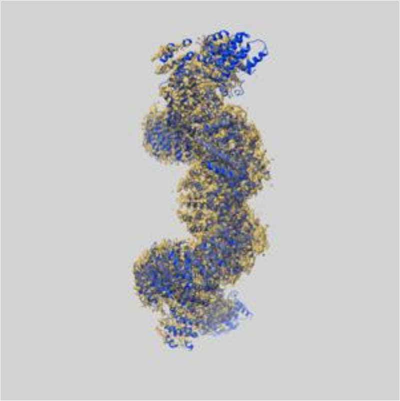
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-7129 and PDB model 6BQ1. Per-residue inclusion information can be found in section 3 on page 6.

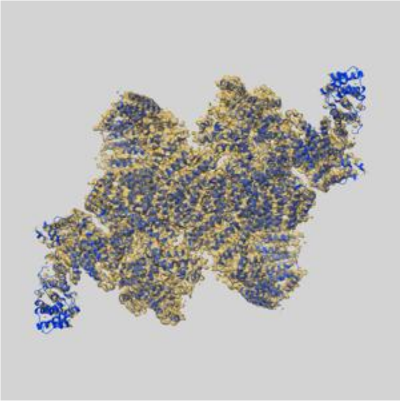
9.1 Map-model overlay (i)



X



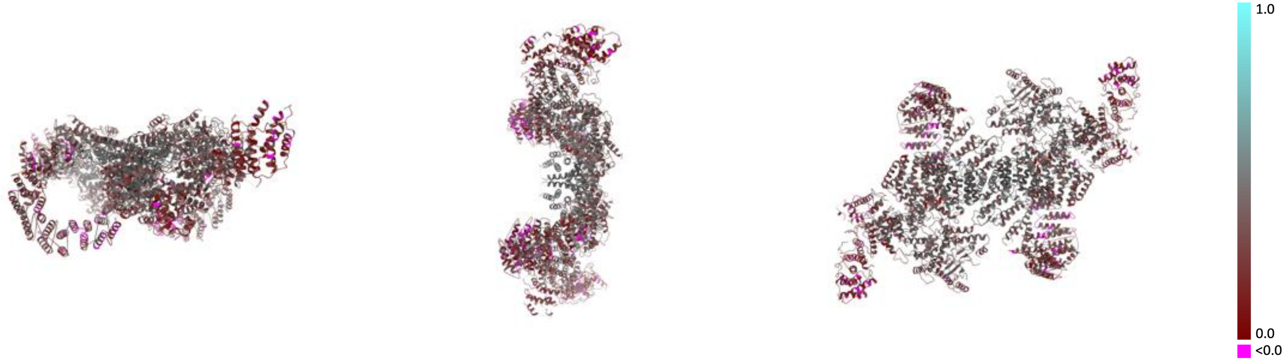
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05 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.

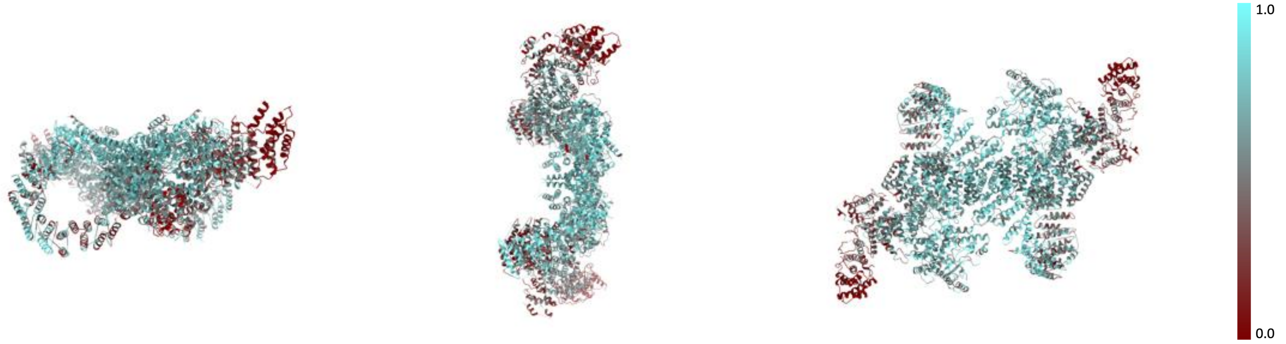
9.2 Q-score mapped to coordinate model ⓘ



X Y Z

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

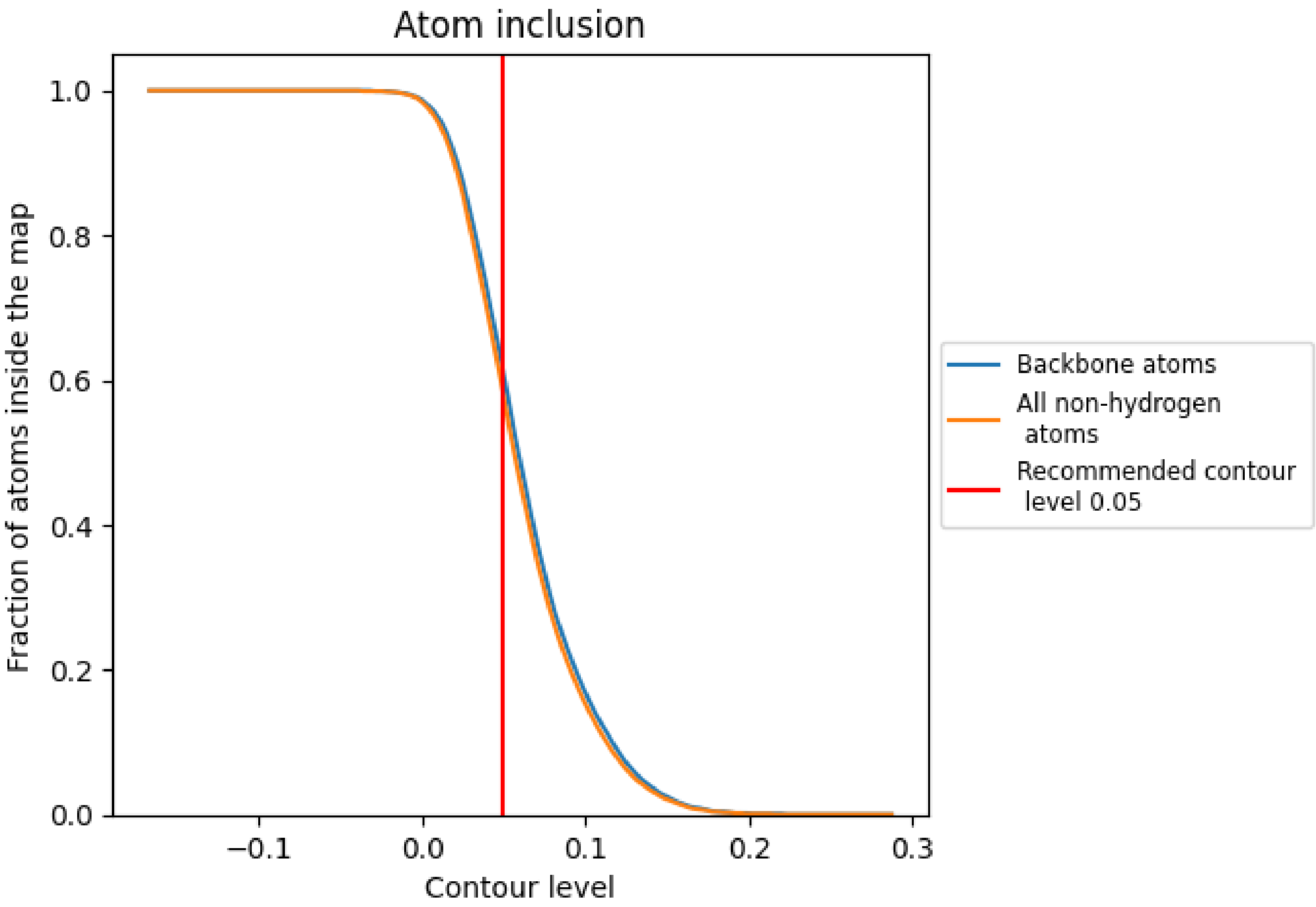
9.3 Atom inclusion mapped to coordinate model ⓘ



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).

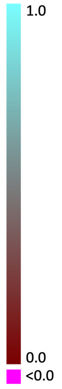
9.4 Atom inclusion ⓘ



At the recommended contour level, 61% of all backbone atoms, 58% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	▬ 0.5780	▬ 0.3410
A	▬ 0.6900	▬ 0.3680
B	▬ 0.4340	▬ 0.2940
C	▬ 0.3910	▬ 0.2800
E	▬ 0.7020	▬ 0.3820
F	▬ 0.4370	▬ 0.3040
G	▬ 0.3970	▬ 0.2830