Full wwPDB EM Validation Report ⓘ

Dec 11, 2022 – 08:41 pm GMT

PDB ID	:	6TA1
EMDB ID	:	EMD-10420
Title	:	Fatty acid synthase of S. cerevisiae
Authors	:	Vonck, J.; D'Imprima, E.; Joppe, M.; Grininger, M.
Deposited on	:	2019-10-29
Resolution	:	3.10 Å(reported)
Based on initial model	:	3HMJ

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:

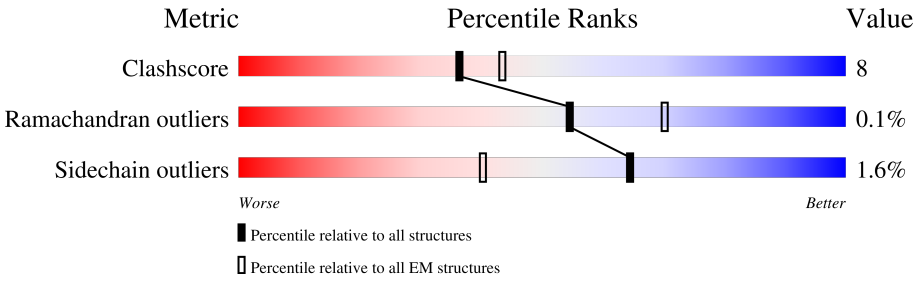
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 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	1887	15% 77% 15% 7%
1	B	1887	15% 78% 15% • 7%
1	D	1887	15% 78% 15% 7%
1	F	1887	15% 78% 14% 7%
1	I	1887	15% 78% 15% 7%
1	K	1887	15% 78% 15% 7%
2	C	2051	8% 81% 17% ••
2	E	2051	8% 81% 17% ••

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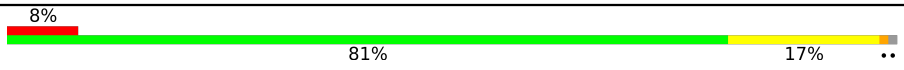
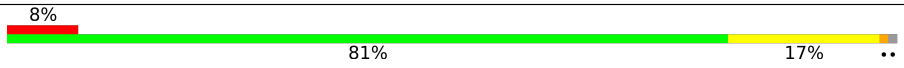
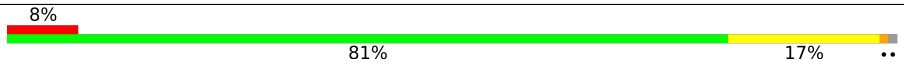
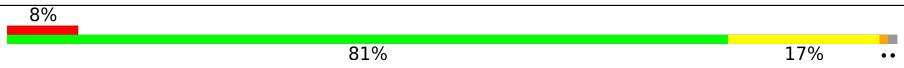
Mol	Chain	Length	Quality of chain
2	G	2051	
2	H	2051	
2	J	2051	
2	L	2051	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 178206 atoms, of which 156 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.

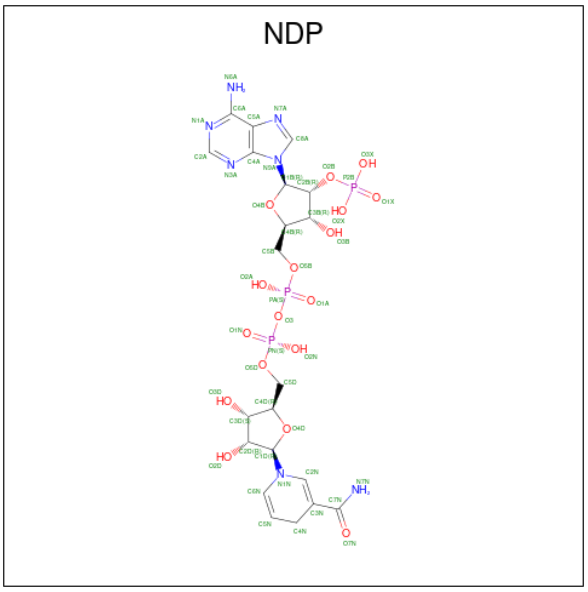
- Molecule 1 is a protein called Fatty acid synthase subunit alpha.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1750	Total	C	N	O	P	S	0	0
			13619	8620	2297	2650	1	51		
1	B	1750	Total	C	N	O	P	S	0	0
			13619	8620	2297	2650	1	51		
1	D	1750	Total	C	N	O	P	S	0	0
			13619	8620	2297	2650	1	51		
1	K	1750	Total	C	N	O	P	S	0	0
			13619	8620	2297	2650	1	51		
1	F	1750	Total	C	N	O	P	S	0	0
			13619	8620	2297	2650	1	51		
1	I	1750	Total	C	N	O	P	S	0	0
			13619	8620	2297	2650	1	51		

- Molecule 2 is a protein called Fatty acid synthase subunit beta.

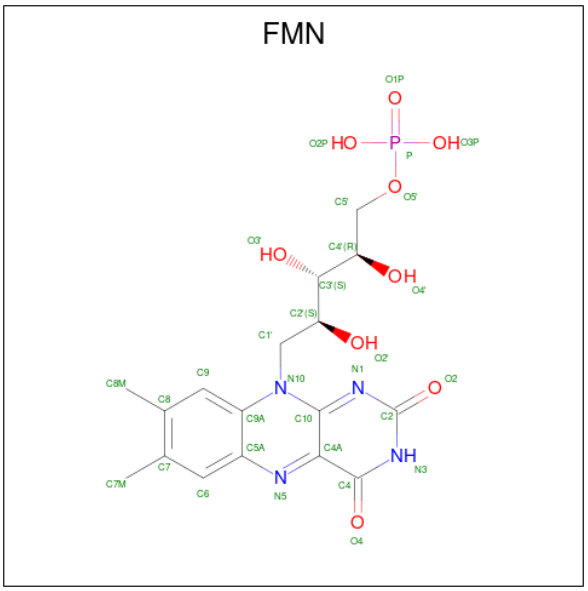
Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	2031	Total	C	N	O	S	0	0
			15977	10243	2657	3021	56		
2	C	2031	Total	C	N	O	S	0	0
			15977	10243	2657	3021	56		
2	E	2031	Total	C	N	O	S	0	0
			15977	10243	2657	3021	56		
2	L	2031	Total	C	N	O	S	0	0
			15977	10243	2657	3021	56		
2	H	2031	Total	C	N	O	S	0	0
			15977	10243	2657	3021	56		
2	J	2031	Total	C	N	O	S	0	0
			15977	10243	2657	3021	56		

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms						AltConf
3	A	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	
3	B	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	
3	D	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	
3	K	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	
3	F	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	
3	I	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	

- Molecule 4 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



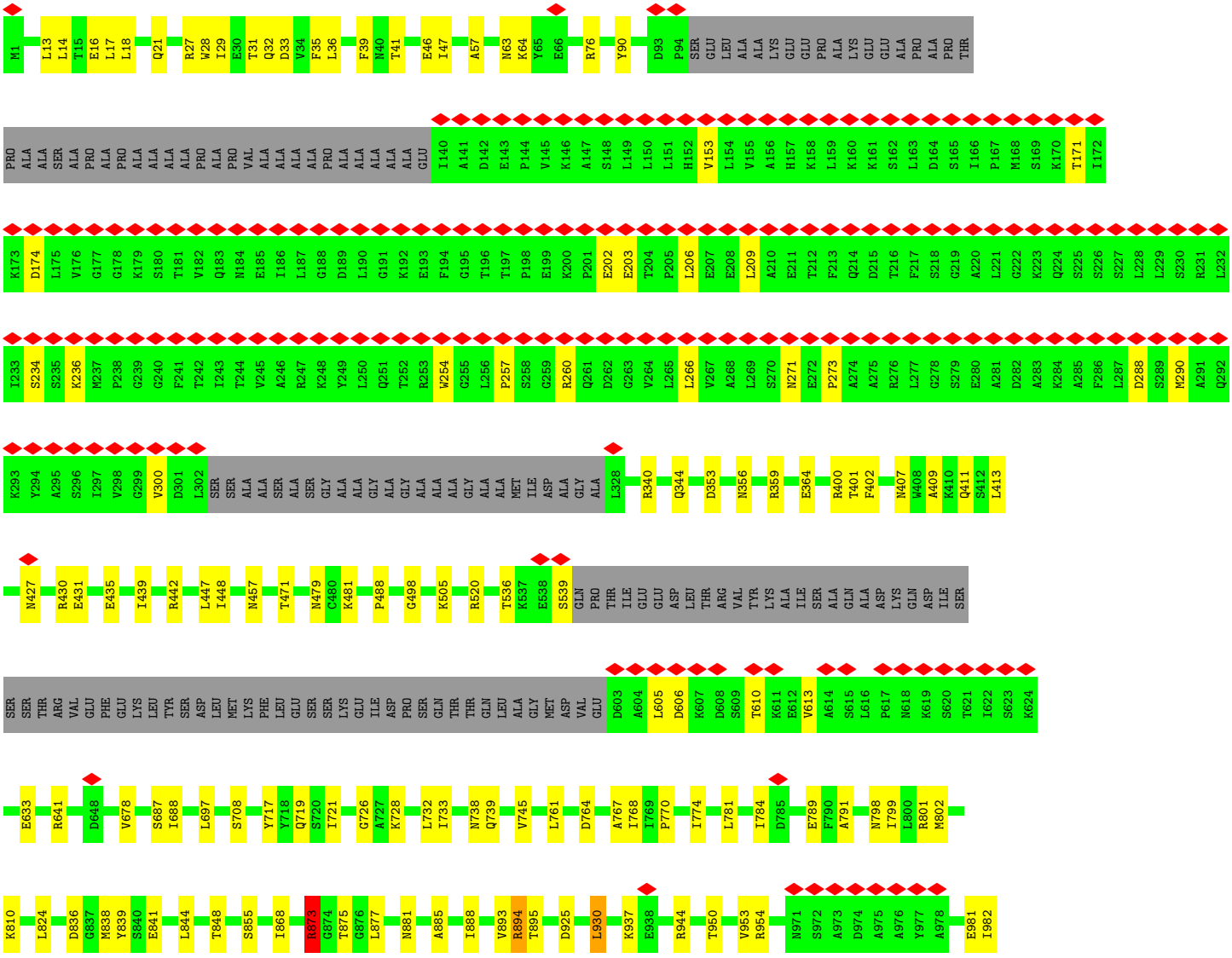
Mol	Chain	Residues	Atoms					AltConf
4	G	1	Total	C	N	O	P	0
			31	17	4	9	1	
4	C	1	Total	C	N	O	P	0
			31	17	4	9	1	
4	E	1	Total	C	N	O	P	0
			31	17	4	9	1	
4	L	1	Total	C	N	O	P	0
			31	17	4	9	1	
4	H	1	Total	C	N	O	P	0
			31	17	4	9	1	
4	J	1	Total	C	N	O	P	0
			31	17	4	9	1	

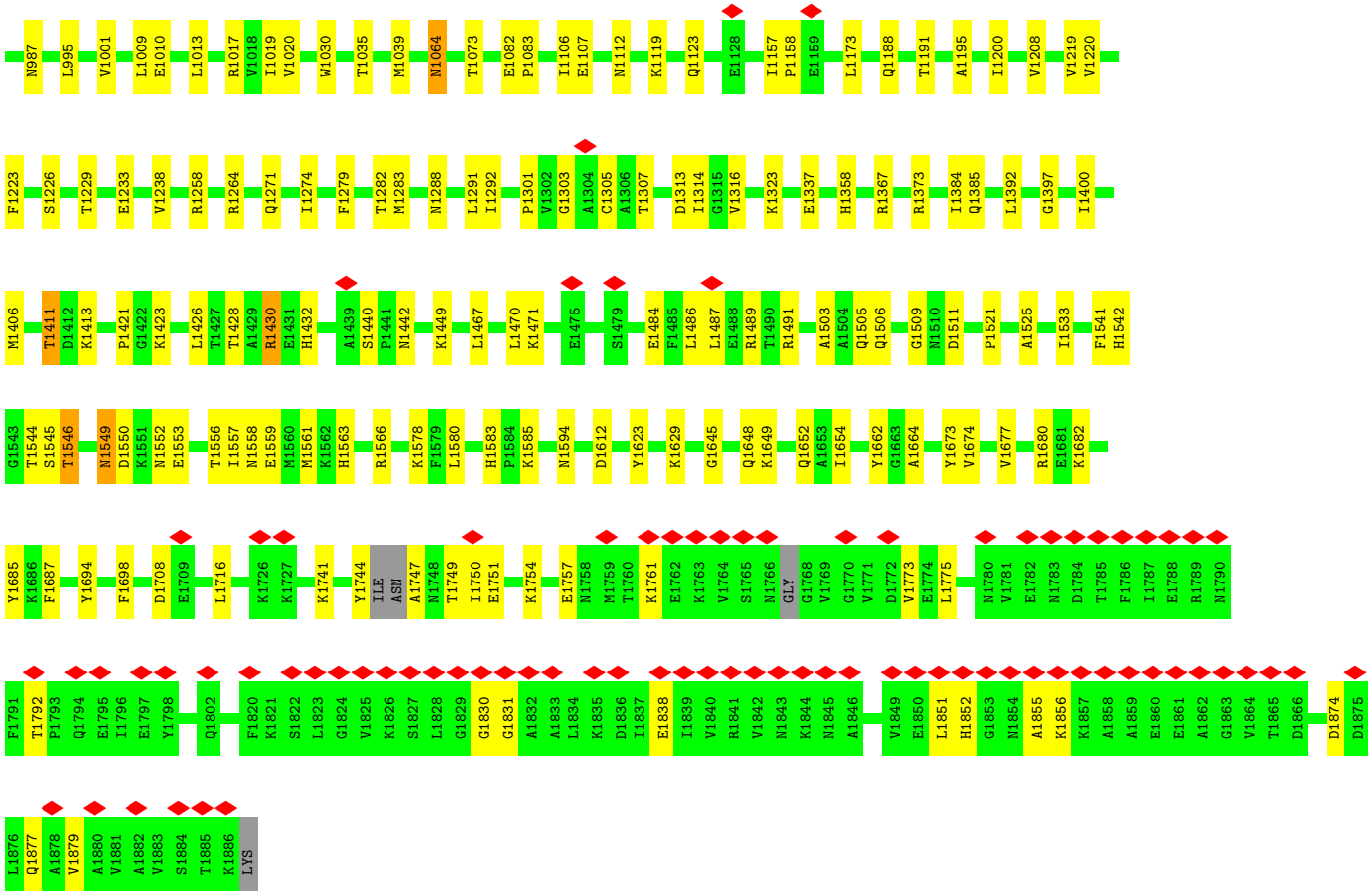
3 Residue-property plots (i)

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

• Molecule 1: Fatty acid synthase subunit alpha

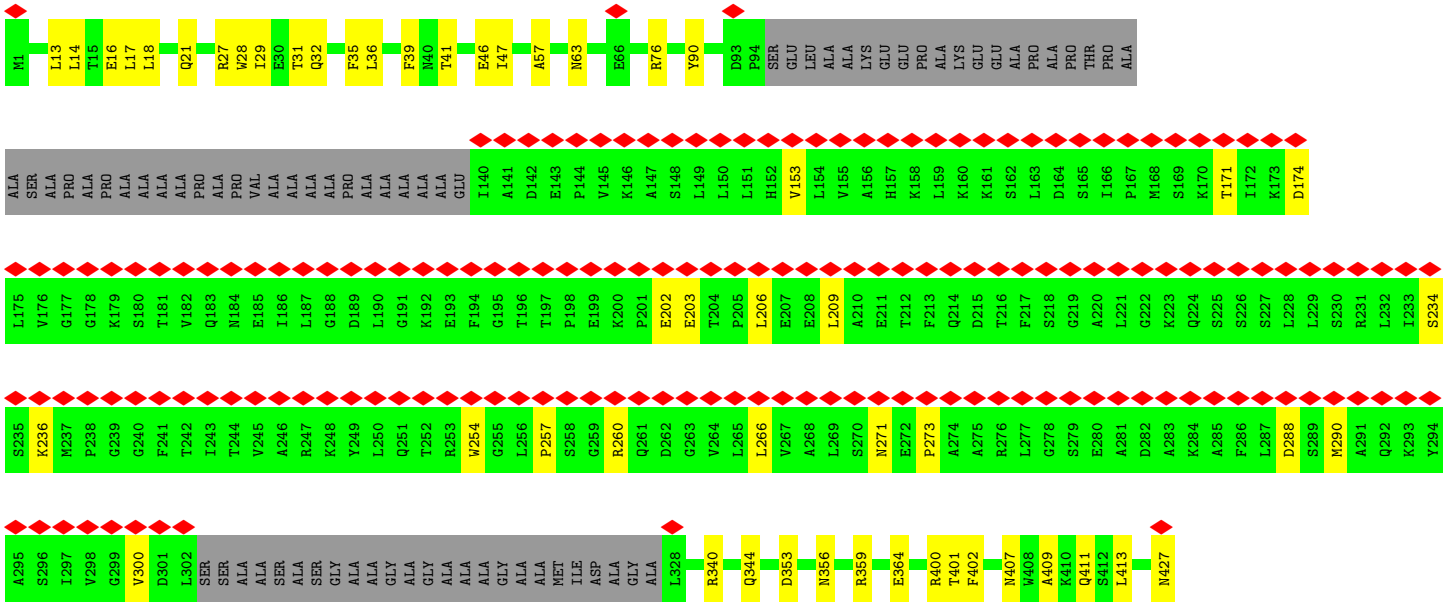
Chain A:

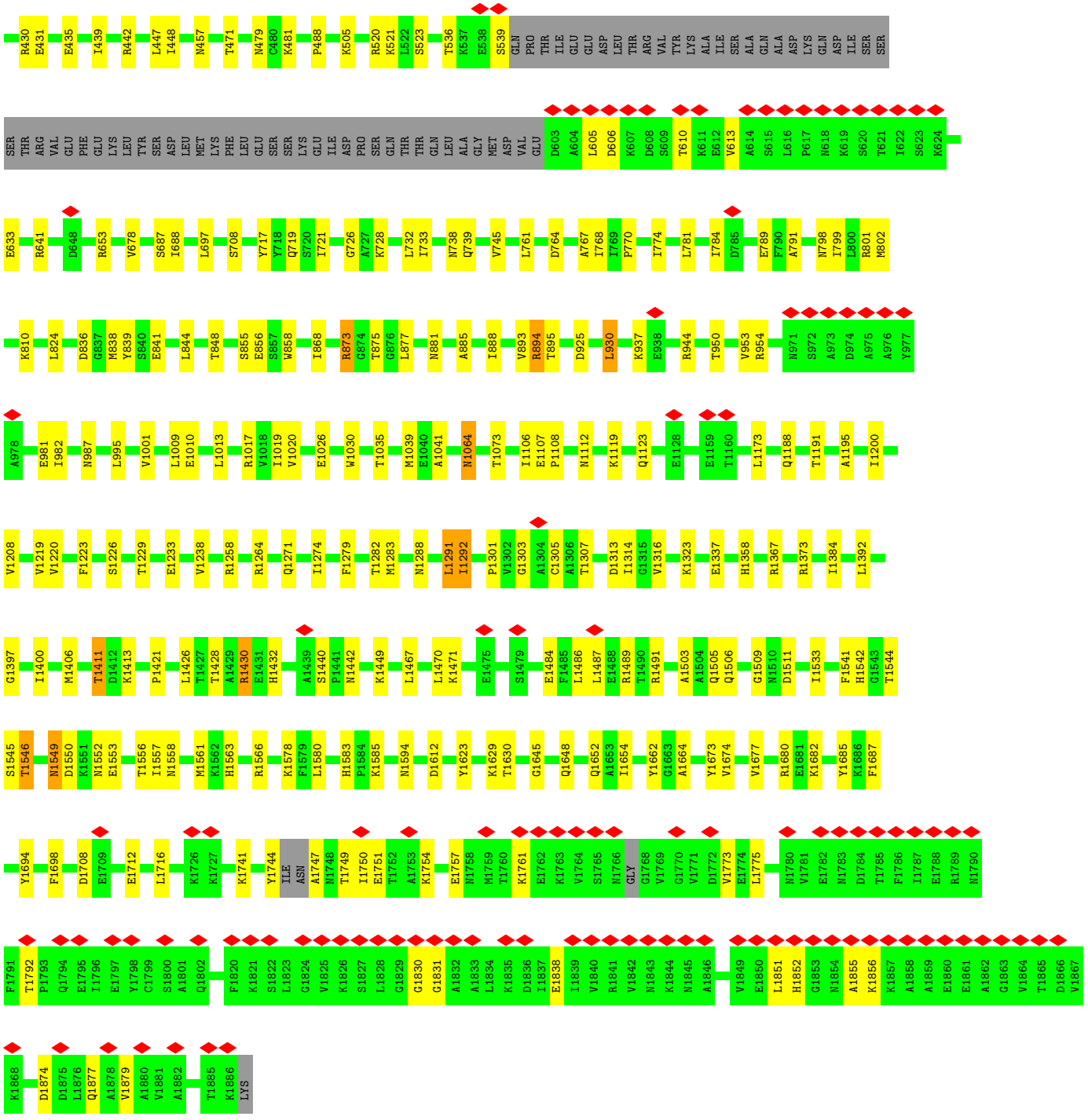




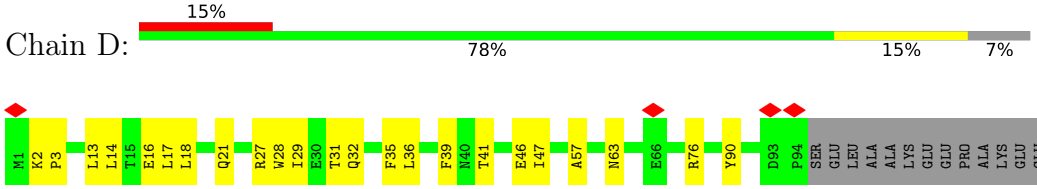
• Molecule 1: Fatty acid synthase subunit alpha

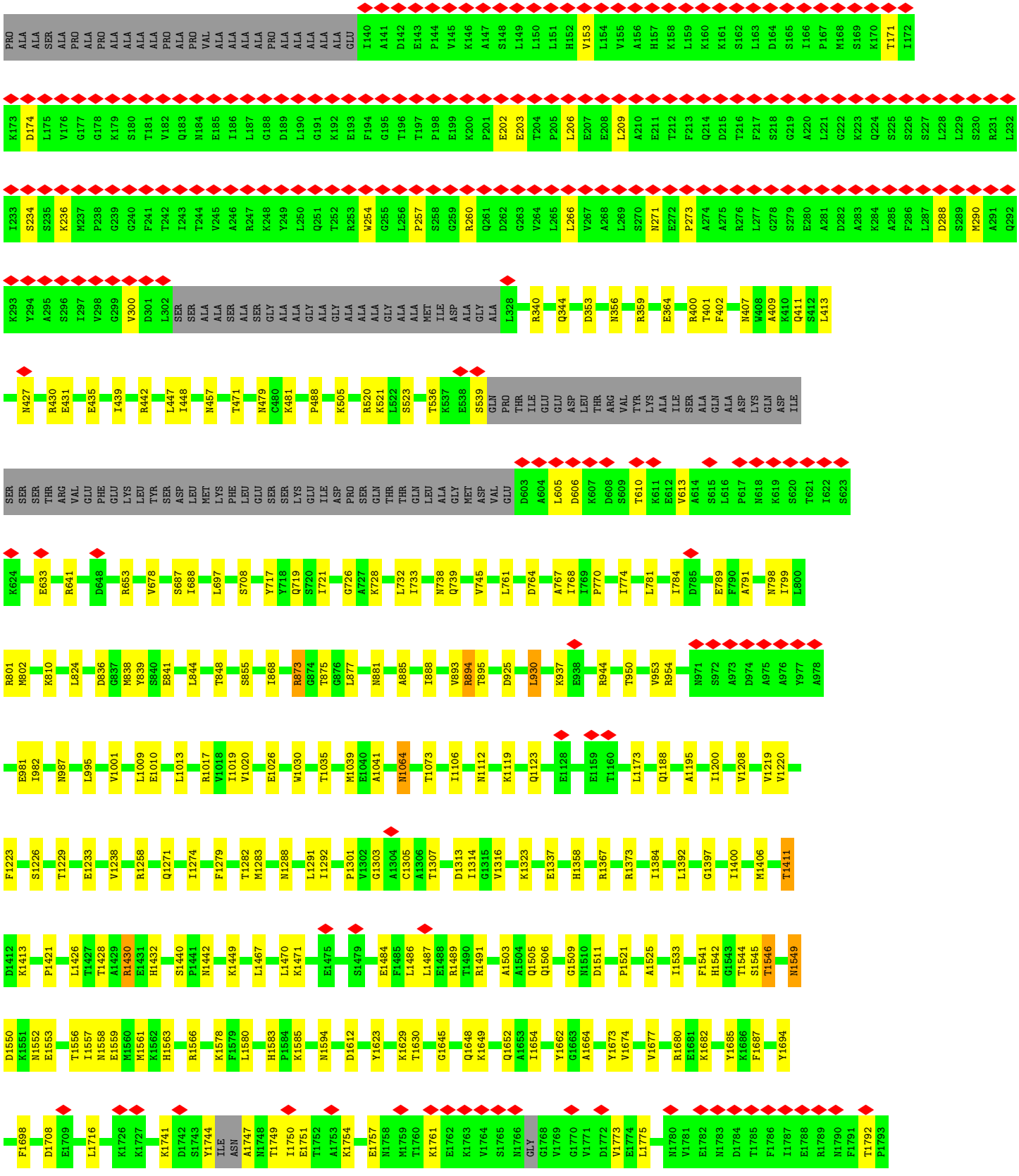
Chain B:





• Molecule 1: Fatty acid synthase subunit alpha

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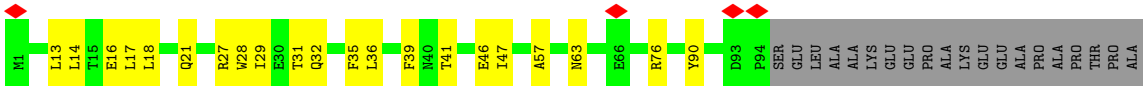
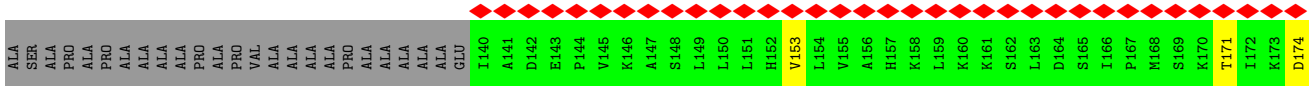
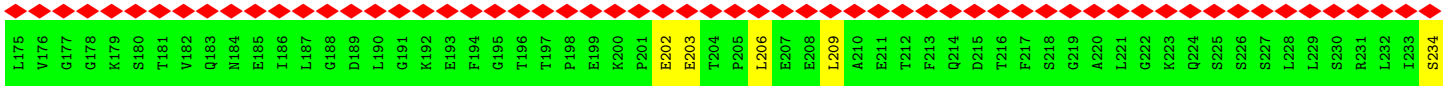
K173 D174 L175 V176 G177 G178 K179 S180 T181 V182 Q183 N184 E185 I186 L187 G188 D189 L190 G191 K192 E193 F194 G195 T196 T197 P198 E199 K200 P201 E202 E203 T204 P205 L206 E207 E208 L209 A210 E211 T212 F213 Q214 D215 T216 F217 S218 G219 A220 L221 G222 K223 Q224 S225 S226 S227 L228 L229 S230 R231 L232
I233 S234 S235 K236 M237 P238 G239 G240 F241 T242 I243 T244 V245 A246 R247 K248 Y249 L250 Q251 T252 R253 W254 G255 L256 P257 S258 G259 R260 Q261 D262 G263 V264 L265 L266 V267 A268 L269 S270 N271 E272 P273 A274 A275 R276 L277 G278 S279 E280 A281 D282 A283 K284 A285 F286 L287 D288 S289 M290 A291 Q292
K293 Y294 A295 S296 I297 V298 G299 V300 D301 L302 SER SER ALA ALA SER ALA SER GLY ALA ALA GLY ALA GLY ALA ALA GLY ALA ALA ALA MET ILE ASP ALA GLY ALA L328 R340 Q344 D353 N356 R359 E364 R400 T401 F402 N407 W408 A409 K410 Q411 S412 L413
N427 R430 E431 E435 I439 R442 L447 I448 N457 T471 N479 C480 K481 P488 K505 R520 K521 L522 S523 T536 K537 E538 S539 GLN PRO THR ILE GLU GLU ASP LEU THR ARG VAL TYR LYS ALA ILE SER ALA GLN ALA ASP LYS GLN ASP ILE
SER SER SER THR ARG VAL GLU PHE GLU LYS LEU TYR SER ASP LEU MET LYS PHE LEU GLU SER SER LYS GLU ILE ASP PRO SER GLN THR THR GLN LEU ALA GLY MET ASP VAL GLU D603 A604 L605 D606 K607 D608 S609 T610 K611 E612 V613 A614 S615 L616 P617 N618 K619 S620 T621 I622 S623
K624 E633 R641 D648 R653 V678 S687 I688 L697 S708 Y717 Y718 Q719 S720 I721 G726 A727 K728 L732 I733 N738 Q739 V745 L761 D764 A767 I768 I769 P770 I774 L781 I784 D785 E789 F790 A791 N798 I799 L800
R801 M802 K810 L824 D836 G837 M838 Y839 S840 E841 L844 T848 S855 I868 R873 G874 T875 G876 L877 N881 A885 I888 V893 R894 T895 D925 L930 K937 E938 R944 T950 V953 R954 N971 S972 A973 D974 A975 A976 Y977 A978
E981 I982 N987 L995 V1001 L1009 E1010 L1013 R1017 V1018 I1019 V1020 E1026 W1030 T1035 M1039 E1040 A1041 N1064 T1073 I1106 N1112 K1119 Q1123 E1128 E1159 T1160 L1173 Q1188 A1195 I1200 V1208 V1219 V1220
F1223 S1226 T1229 E1233 V1238 R1258 Q1271 I1274 F1279 T1282 M1283 N1288 L1291 I1292 P1301 V1302 G1303 A1304 C1305 A1306 T1307 D1313 I1314 G1315 V1316 K1323 E1337 H1358 R1367 R1373 I1384 L1392 G1397 I1400 M1406 T1411
D1412 K1413 P1421 L1426 T1427 T1428 A1429 R1430 E1431 H1432 S1440 P1441 N1442 K1449 L1467 L1470 K1471 E1475 S1479 E1484 F1485 L1486 L1487 E1488 R1489 T1490 R1491 A1503 A1504 Q1505 Q1506 G1509 N1510 D1511 P1521 A1525 I1533 F1541 H1542 G1543 T1544 S1545 T1546 N1549
D1550 K1551 N1552 E1553 T1556 I1557 N1558 E1559 M1560 M1561 K1562 H1563 R1566 K1578 F1579 L1580 H1583 P1584 K1585 N1594 D1612 Y1623 K1629 T1630 G1645 Q1648 K1649 Q1652 A1653 I1654 Y1662 G1663 A1664 Y1673 V1674 V1677 R1680 E1681 K1682 Y1685 K1686 F1687 Y1694
F1698 D1708 E1709 L1716 K1726 K1727 K1741 D1742 S1743 Y1744 ILE ASN A1747 N1748 T1749 I1750 E1751 T1752 A1753 K1754 E1757 N1758 M1759 T1760 K1761 E1762 K1763 V1764 S1765 N1766 GLY G1768 V1769 G1770 V1771 D1772 V1773 E1774 L1775 N1780 V1781 E1782 N1783 D1784 T1785 F1786 I1787 E1788 R1789 N1790 F1791 T1792 P1793

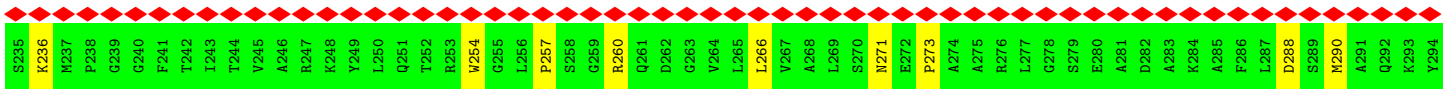
• Molecule 1: Fatty acid synthase subunit alpha

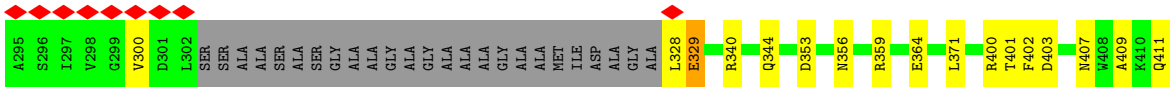
Chain K:

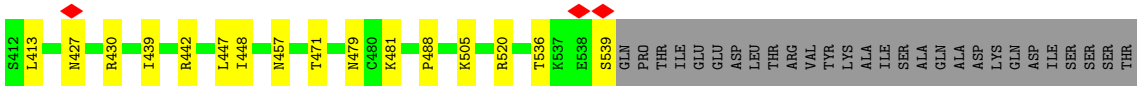


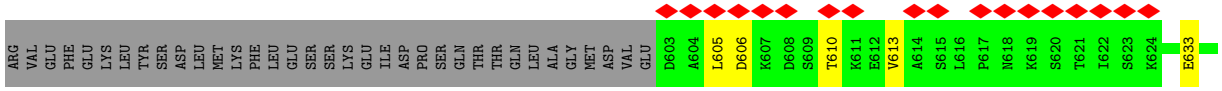


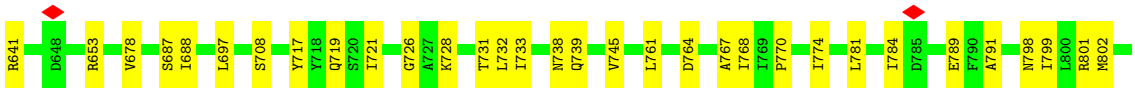


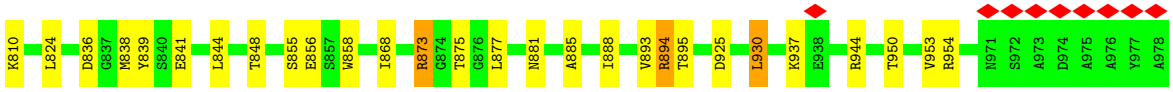


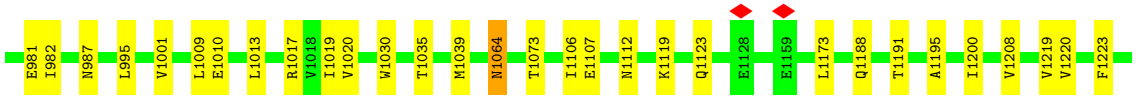


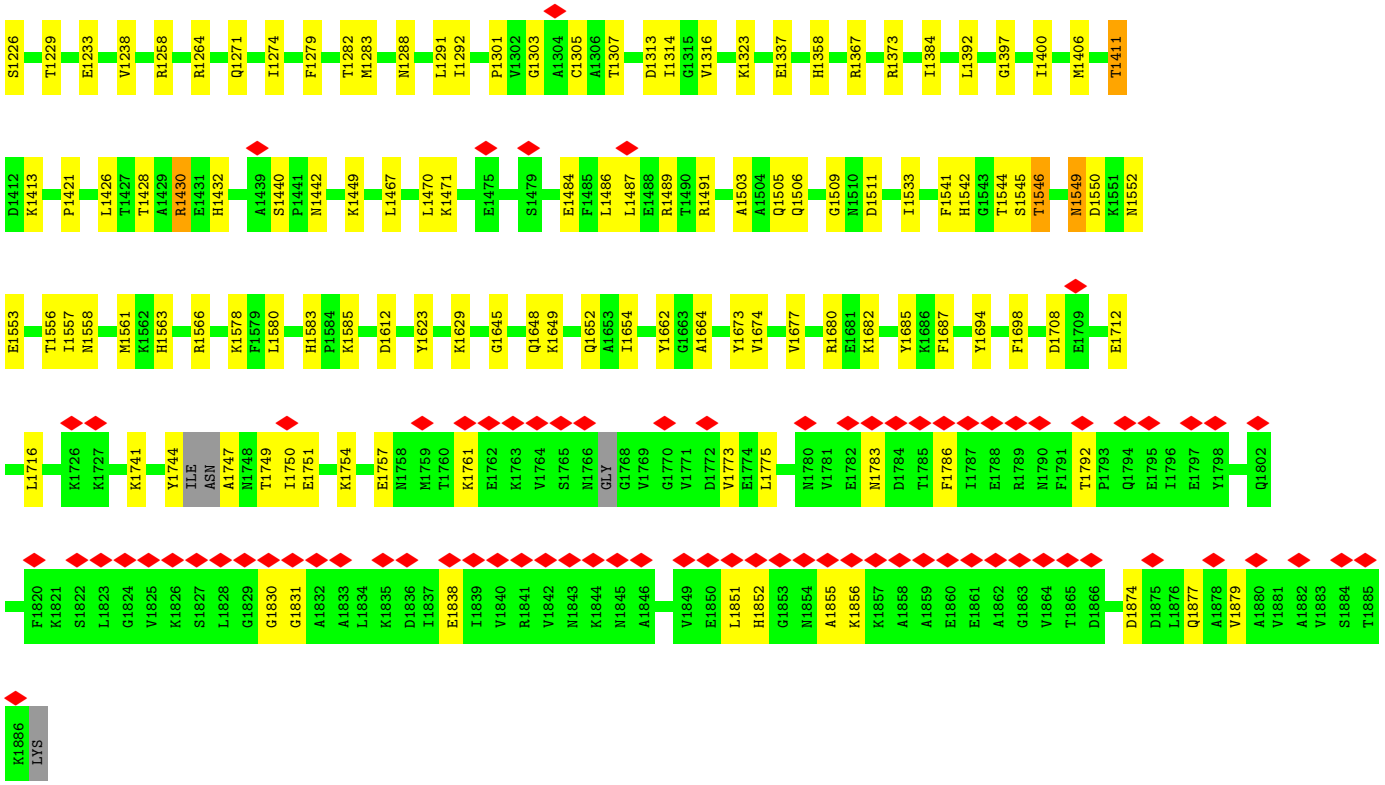






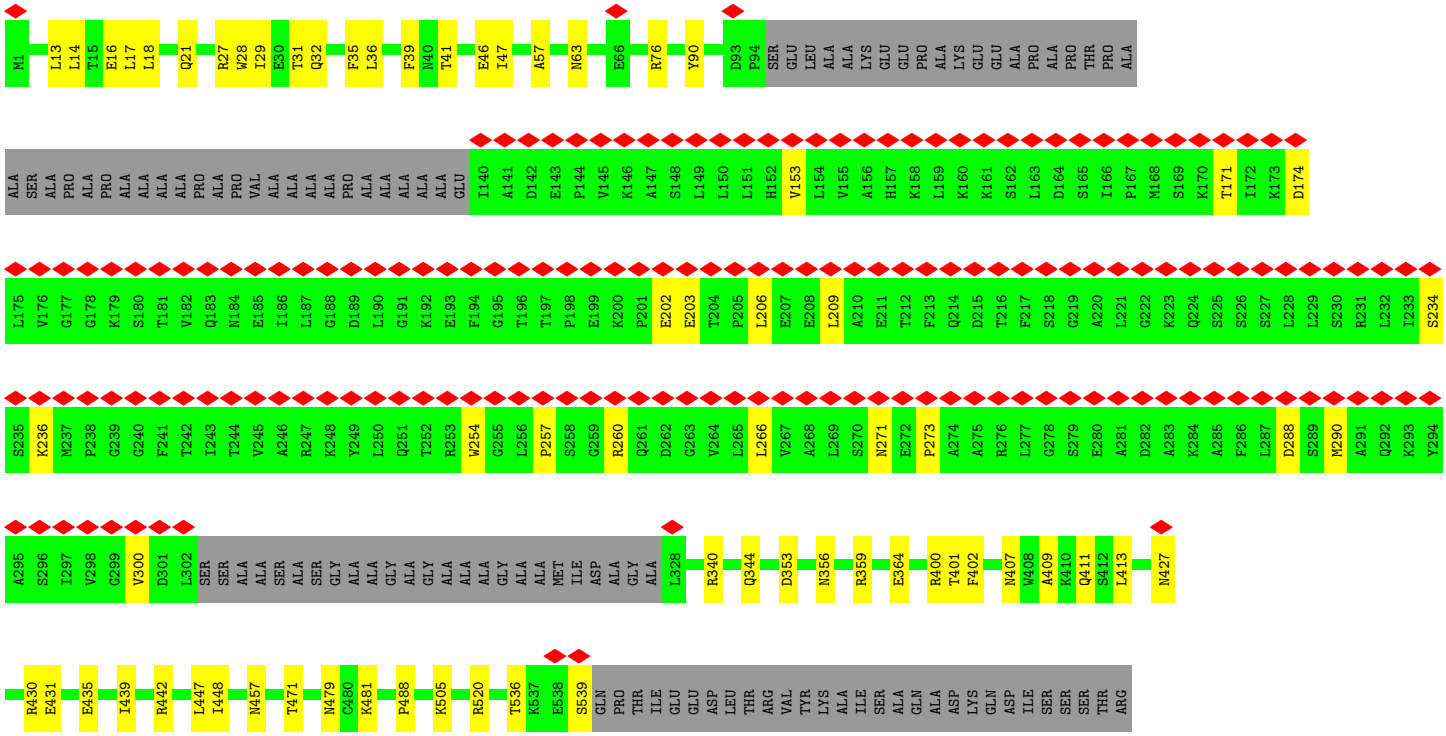


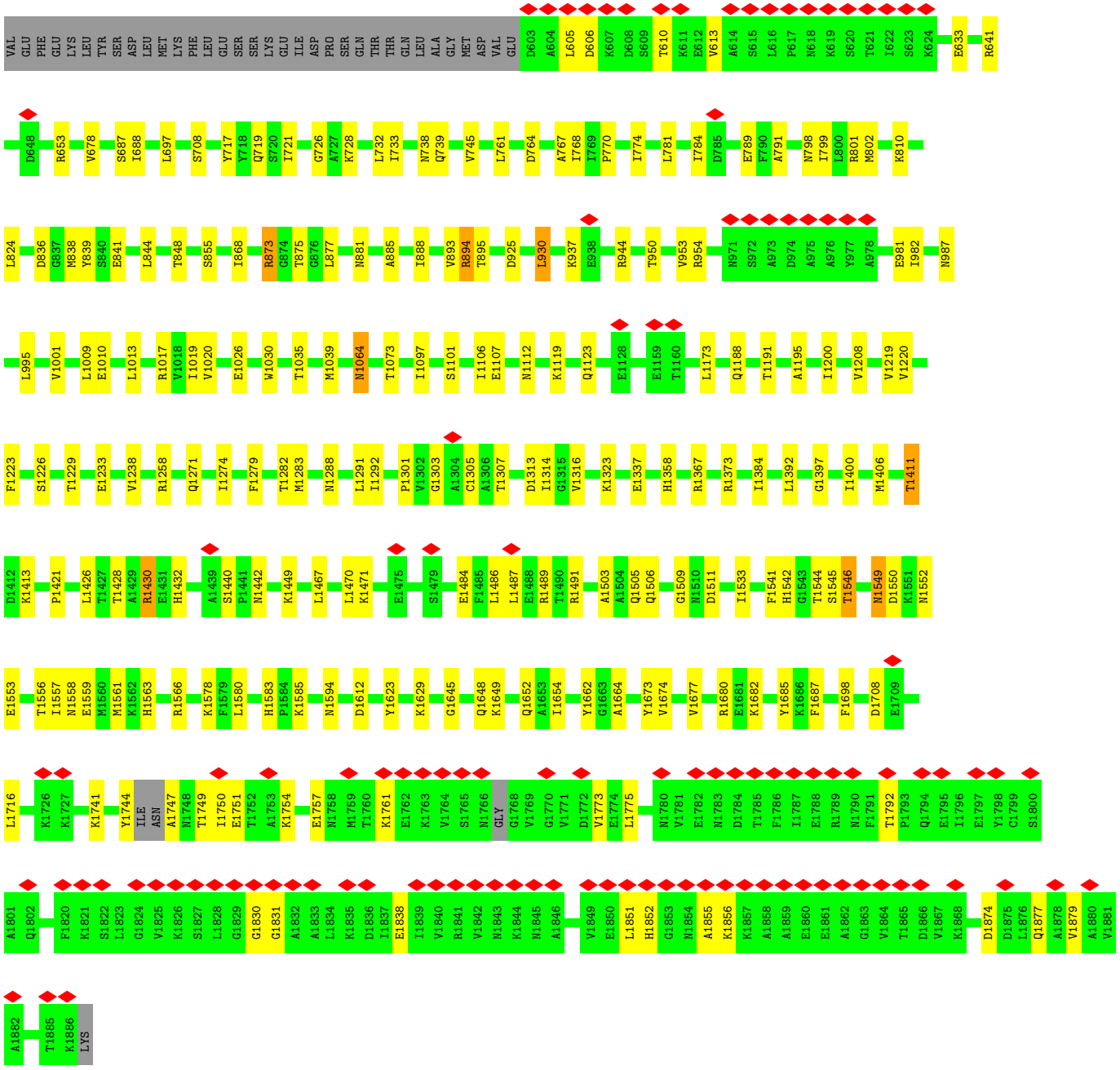




- Molecule 1: Fatty acid synthase subunit alpha

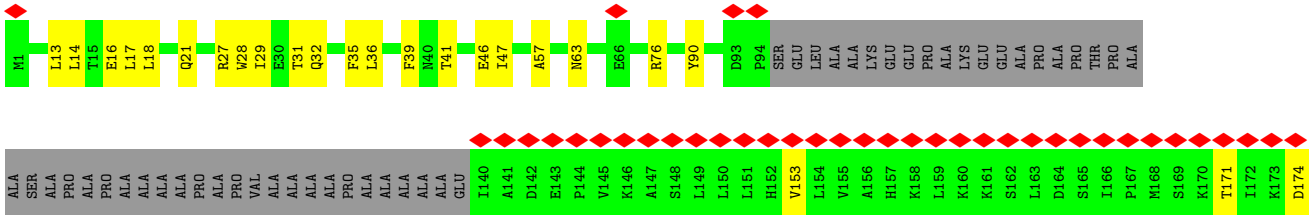
Chain F:

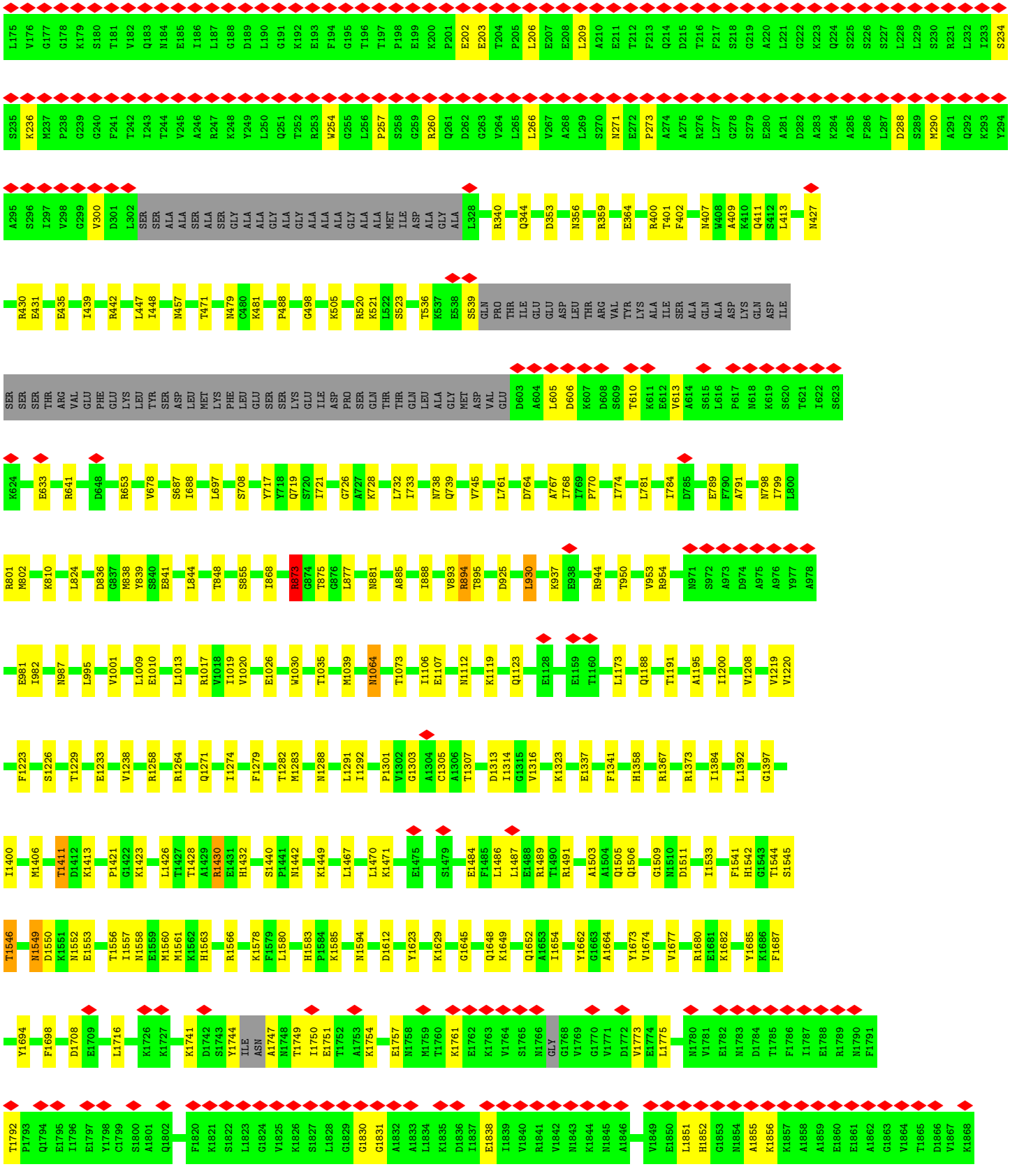




• Molecule 1: Fatty acid synthase subunit alpha

Chain I:

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S235 K236 M237 P238 G239 G240 F241 T242 I243 T244 V245 A246 R247 K248 Y249 L250 Q251 T252 R253 W254 G255 L256 P257 S258 G259 R260 Q261 D262 G263 V264 L265 L266 V267 A268 L269 S270 N271 E272 P273 A274 A275 R276 L277 G278 S279 E280 A281 D282 A283 K284 A285 F286 L287 D288 S289 M290 A291 Q292 K293 Y294
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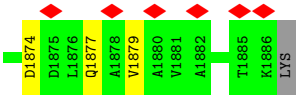
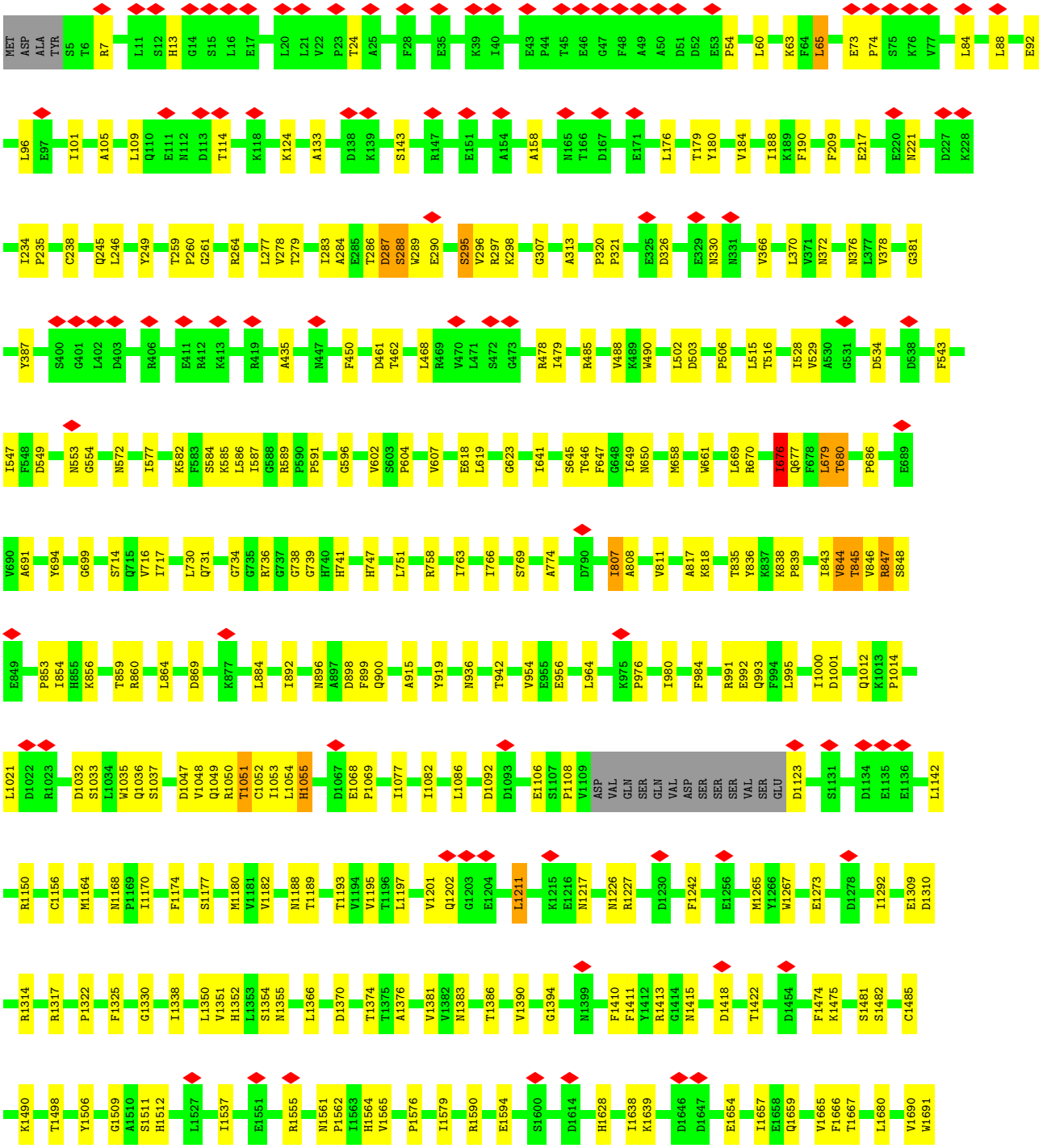
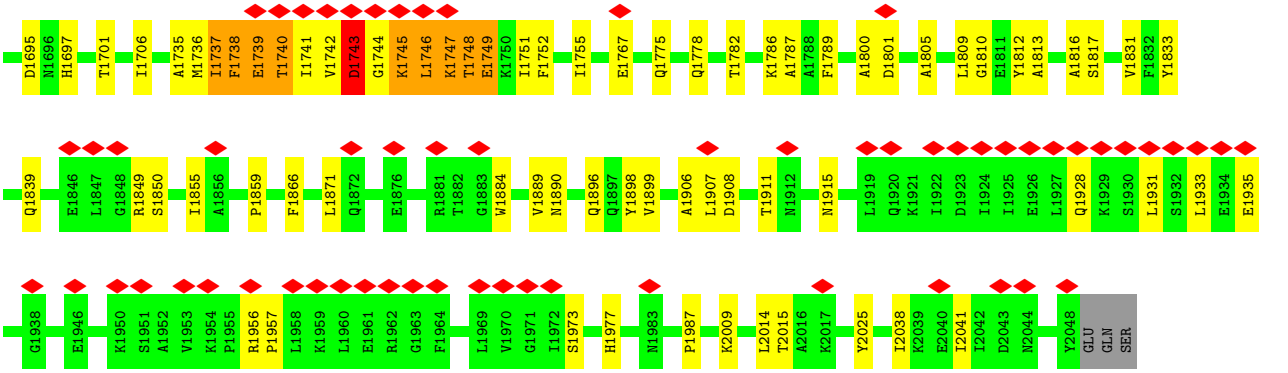
R430 E431 E435 I439 R442 L447 I448 N457 T471 N479 C480 K481 P488 G498 K505 R520 K521 L522 S523 T536 K537 E538 S539 GLN PRO THR ILE GLU GLU ASP LEU THR ARG VAL TYR LYS ALA ILE SER ALA GLN ALA ASP LYS GLN ASP ILE
SER SER SER THR ARG VAL GLU PHE GLU LYS LEU TYR SER ASP LEU MET LYS PHE LEU GLU SER SER LYS GLU ILE ASP PRO SER GLN THR THR GLN LEU ALA GLY MET ASP VAL GLU D603 A604 L605 D606 K607 D608 S609 T610 K611 E612 V613 A614 S615 L616 P617 N618 K619 S620 T621 I622 S623
K624 E633 R641 D648 R653 V678 S687 I688 L697 S708 Y717 Y718 Q719 S720 I721 G726 A727 K728 L732 I733 N738 Q739 V745 L761 D764 A767 I768 I769 P770 I774 L781 I784 D785 E789 F790 A791 N798 I799 L800
R801 M802 K810 L824 D836 G837 M838 Y839 S840 E841 L844 T848 S855 I868 R873 G874 T875 G876 L877 N881 A885 I888 V893 R894 T895 D925 L930 K937 E938 R944 T950 V953 R954 N971 S972 A973 D974 A975 A976 Y977 A978
E981 I982 N987 L995 V1001 L1009 E1010 L1013 R1017 V1018 I1019 V1020 E1026 W1030 T1035 M1039 N1064 T1073 I1106 E1107 N1112 K1119 Q1123 E1128 E1159 T1160 L1173 Q1188 T1191 A1195 I1200 V1208 V1219 V1220
F1223 S1226 T1229 E1233 V1238 R1258 R1264 Q1271 I1274 F1279 T1282 M1283 N1288 L1291 I1292 P1301 V1302 G1303 A1304 C1305 A1306 T1307 D1313 I1314 G1315 V1316 K1323 E1337 F1341 H1358 R1367 R1373 I1384 L1392 G1397
I1400 M1406 T1411 D1412 K1413 P1421 G1422 K1423 L1426 T1427 T1428 A1429 R1430 E1431 H1432 S1440 P1441 N1442 K1449 L1467 L1470 K1471 E1475 S1479 E1484 F1485 L1486 L1487 E1488 R1489 T1490 R1491 A1503 A1504 Q1505 Q1506 G1509 N1510 D1511 I1533 F1541 H1542 G1543 T1544 S1545
T1546 N1549 D1550 K1551 N1552 E1553 T1556 I1557 N1558 E1559 M1560 M1561 K1562 H1563 R1566 K1578 F1579 L1580 H1583 P1584 K1585 N1594 D1612 Y1623 K1629 G1645 Q1648 K1649 Q1652 A1653 I1654 Y1662 G1663 A1664 Y1673 V1674 V1677 R1680 E1681 K1682 Y1685 K1686 F1687
Y1694 F1698 D1708 E1709 L1716 K1726 K1727 K1741 D1742 S1743 Y1744 ILE ASN A1747 N1748 T1749 I1750 E1751 T1752 A1753 K1754 E1757 N1758 M1759 T1760 K1761 E1762 K1763 V1764 S1765 N1766 GLY G1768 V1769 G1770 V1771 D1772 V1773 E1774 L1775 N1780 V1781 E1782 N1783 D1784 T1785 F1786 I1787 E1788 R1789 N1790 F1791
T1792 P1793 Q1794 E1795 I1796 E1797 Y1798 C1799 S1800 A1801 Q1802 F1820 K1821 S1822 L1823 G1824 V1825 K1826 S1827 I1750 L1828 G1829 G1830 G1831 A1832 A1833 L1834 K1835 D1836 I1837 E1838 I1839 V1840 R1841 V1842 N1843 K1844 N1845 A1846 V1849 E1850 L1851 H1852 G1853 N1854 A1855 K1856 K1857 K1858 A1859 E1860 E1861 A1862 G1863 V1864 T1865 D1866 V1867 K1868



• Molecule 2: Fatty acid synthase subunit beta

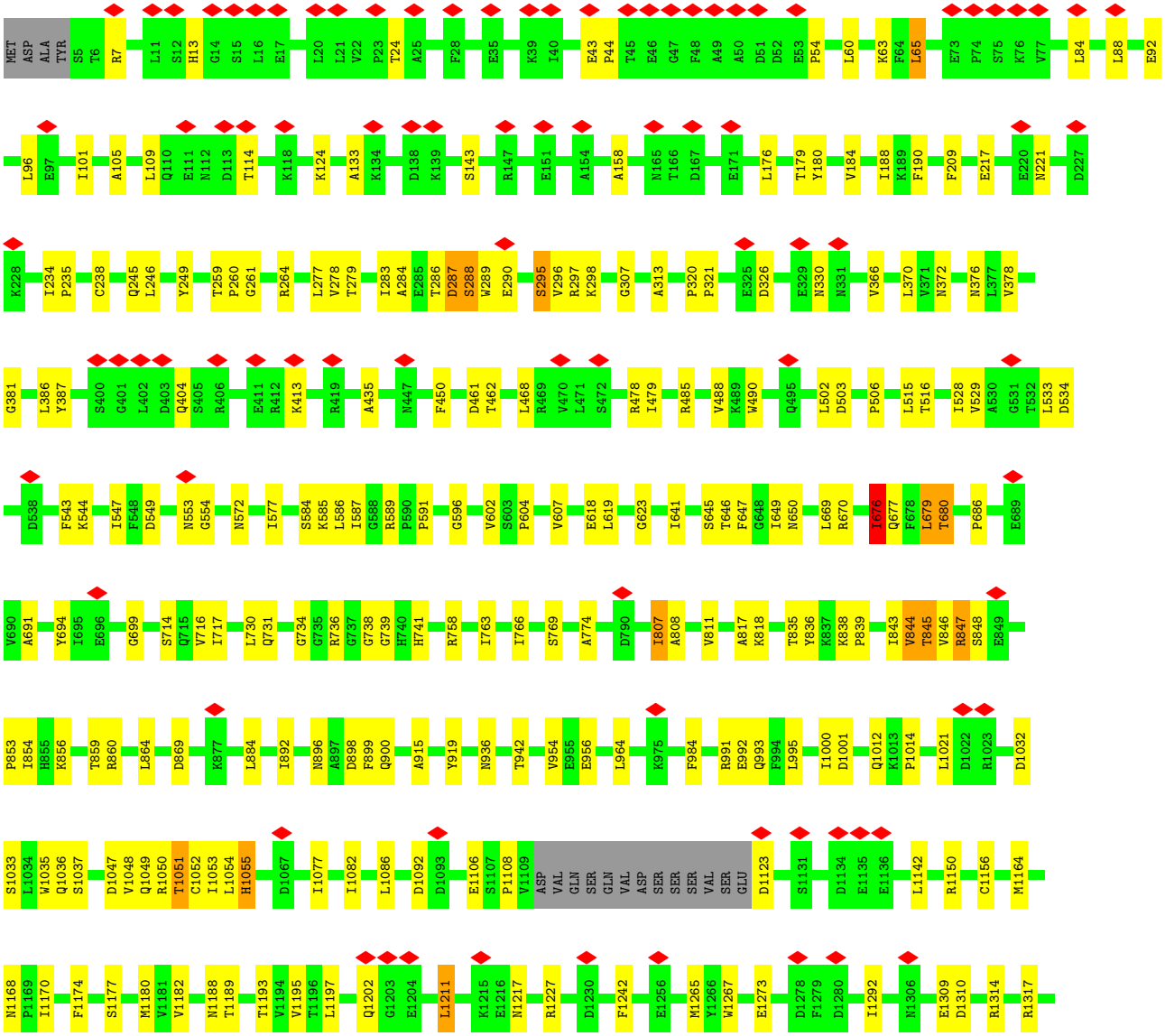
Chain G:

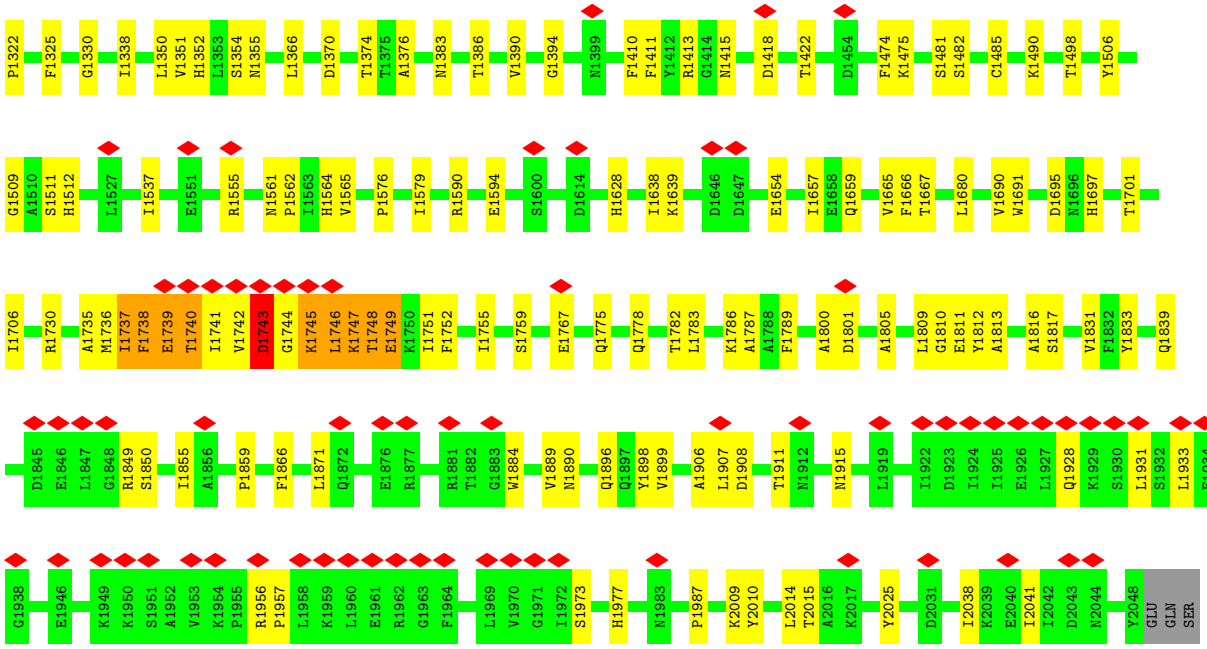




• Molecule 2: Fatty acid synthase subunit beta

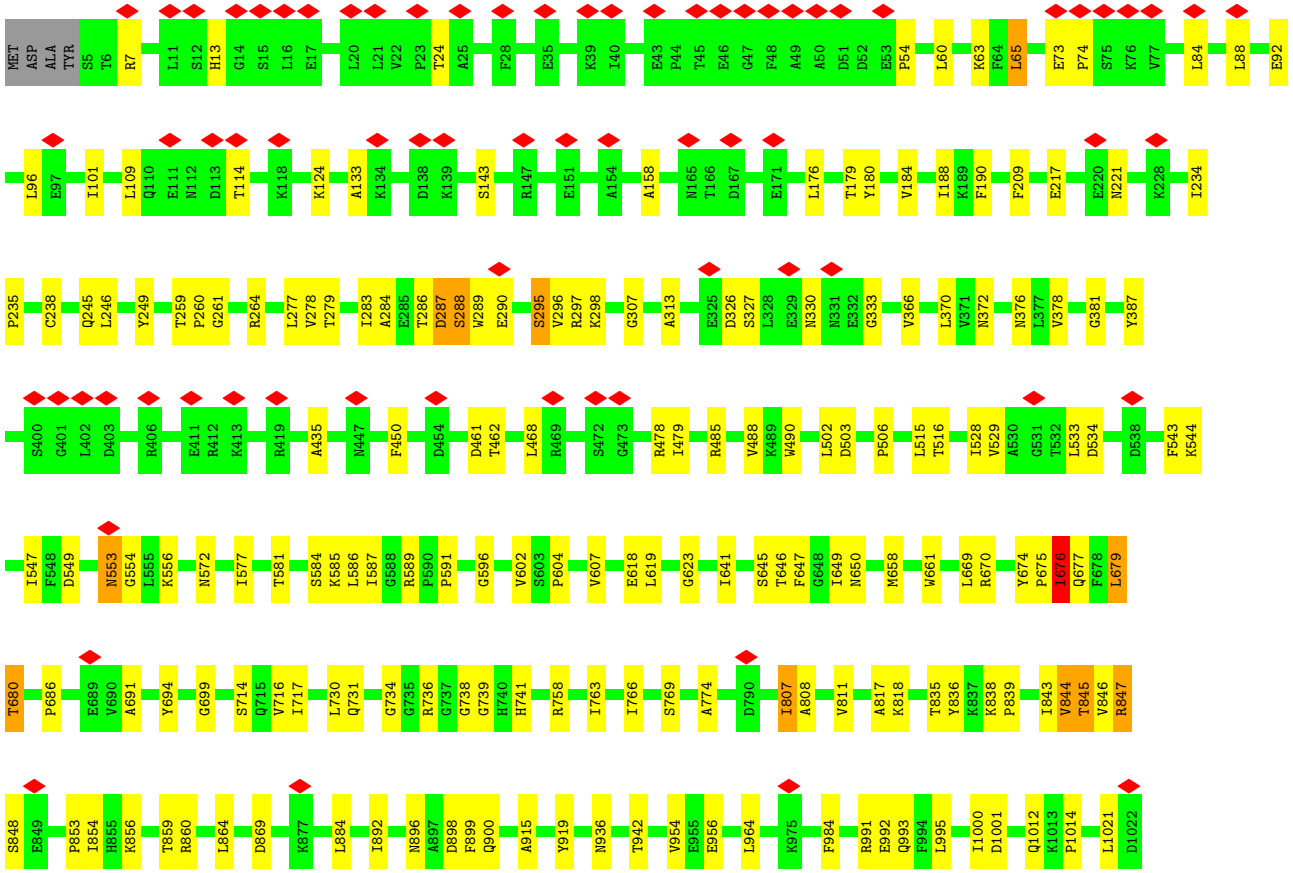
Chain C:

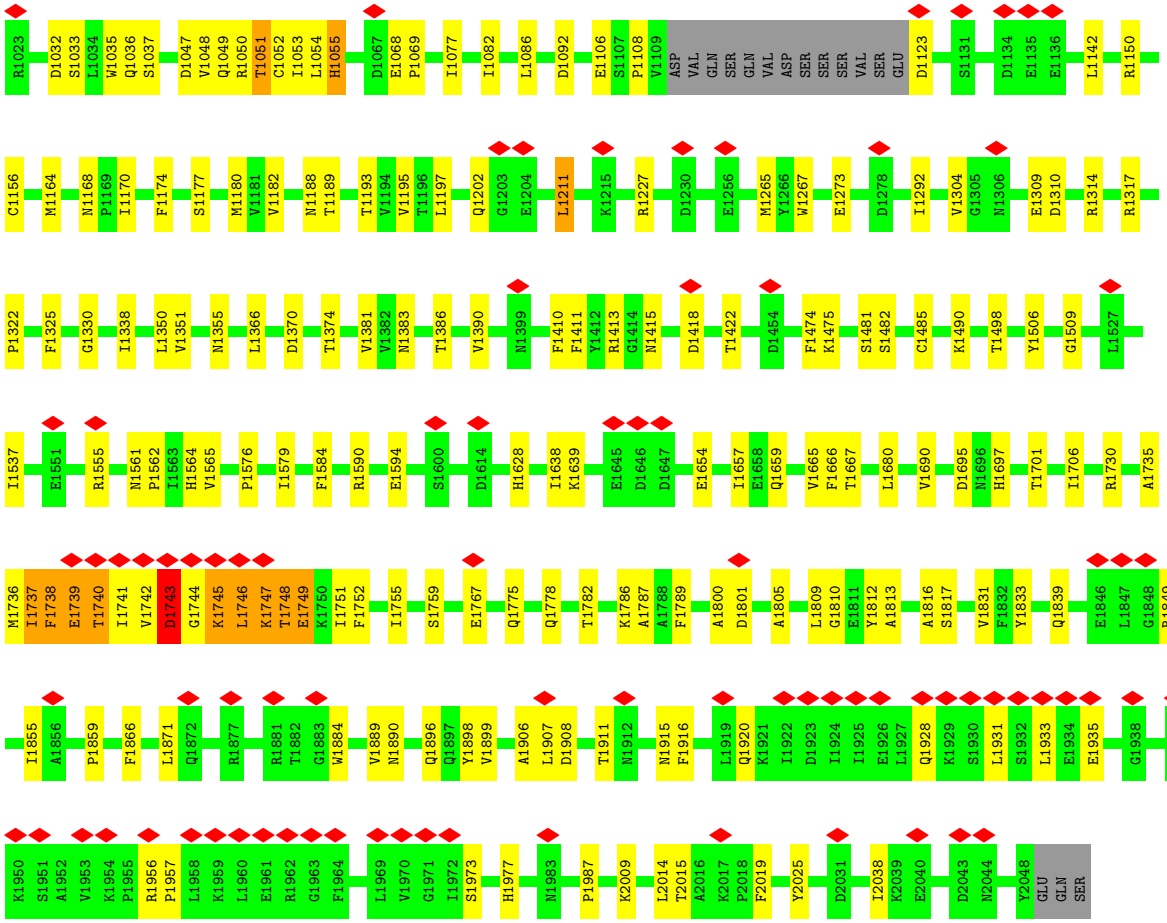




• Molecule 2: Fatty acid synthase subunit beta

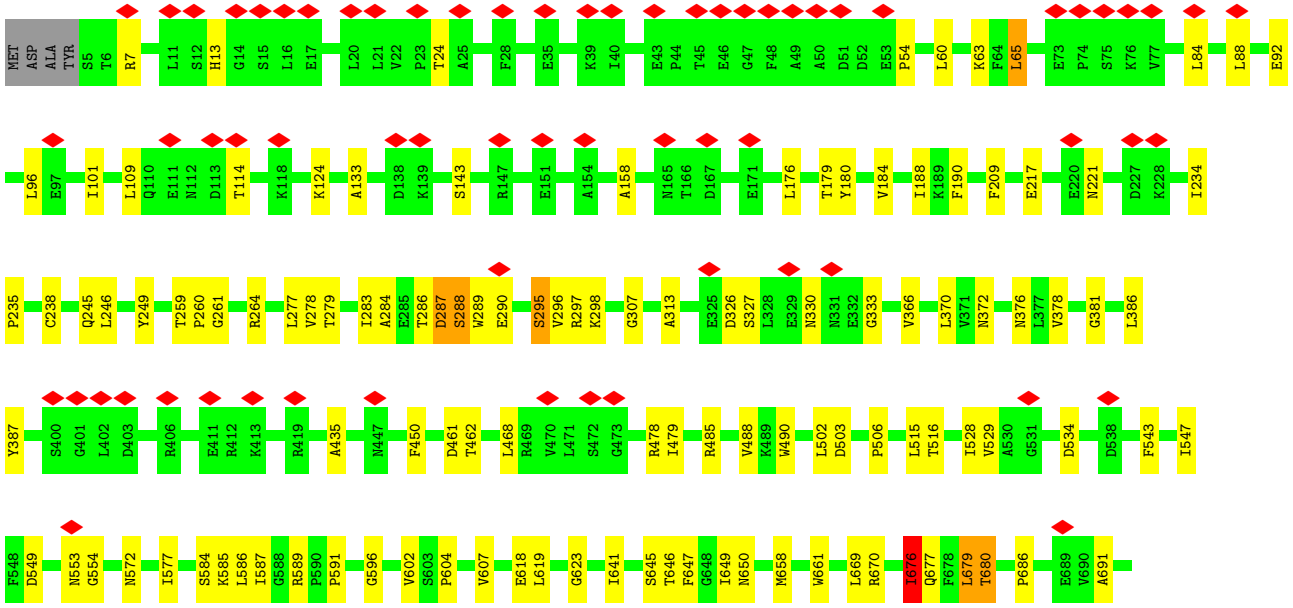
Chain E:

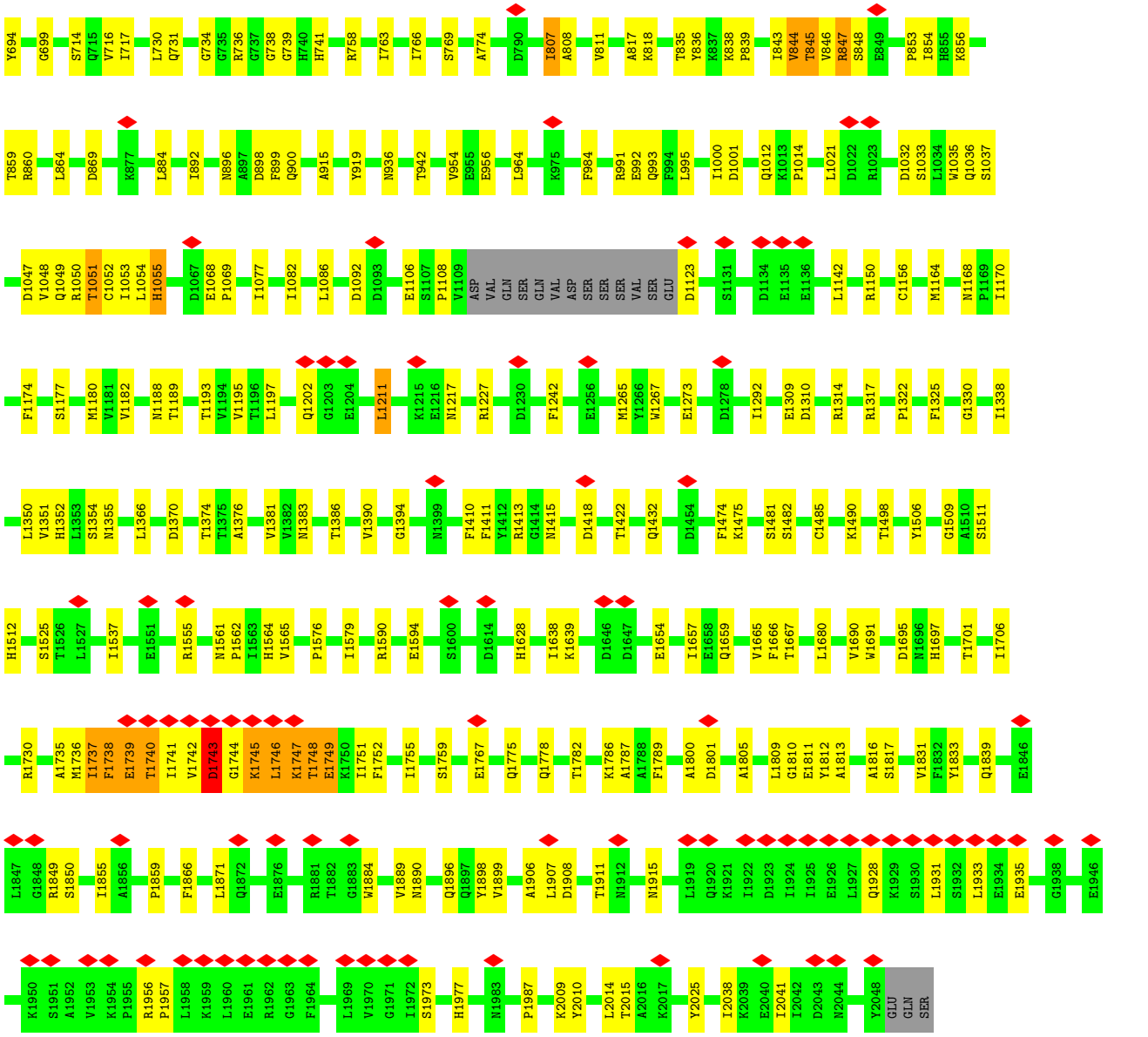




• Molecule 2: Fatty acid synthase subunit beta

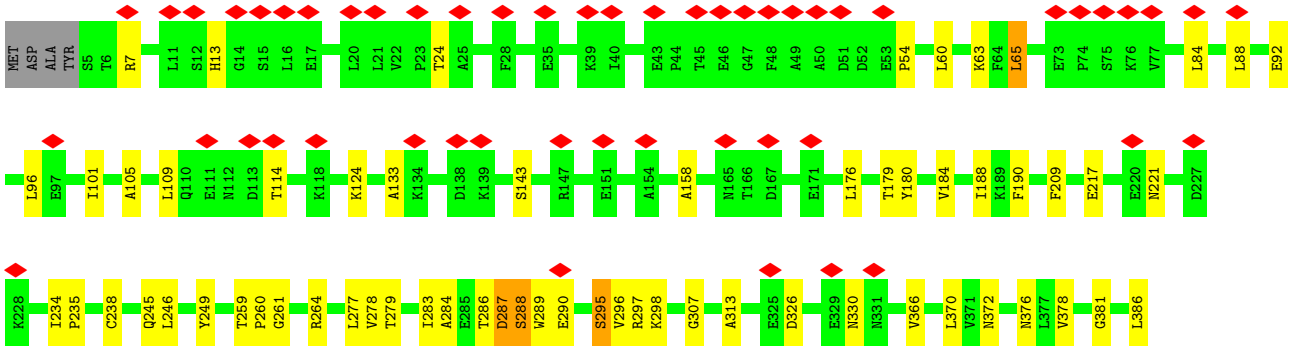
Chain L:

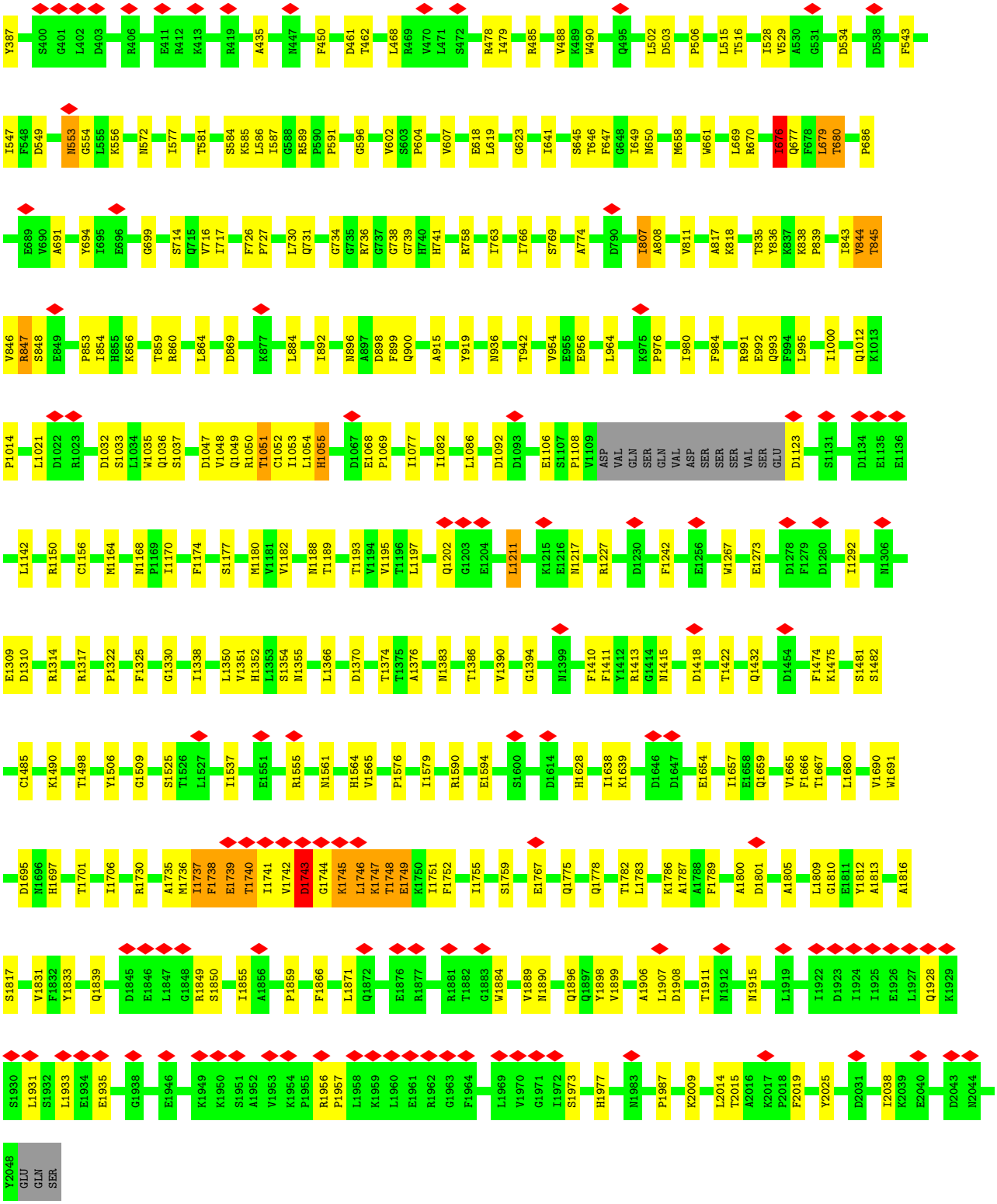




• Molecule 2: Fatty acid synthase subunit beta

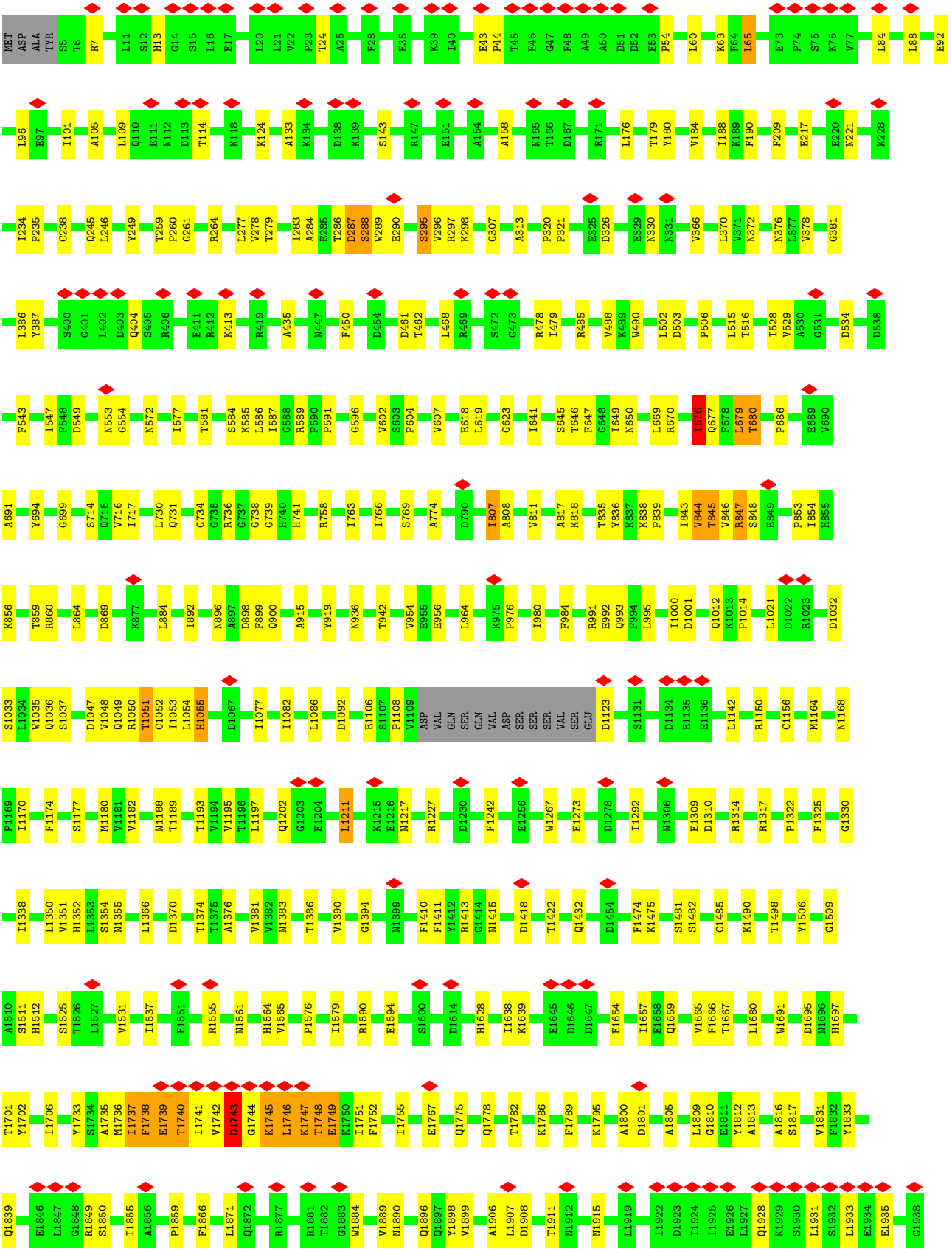
Chain H:





• Molecule 2: Fatty acid synthase subunit beta

Chain J: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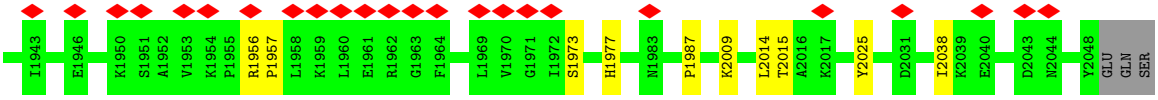
L96 E97 I101 A105 L109 Q110 E111 N112 D113 T114 K118 K124 A133 K134 D138 K139 S143 R147 E151 A154 A158 N165 T166 D167 E171 L176 T179 Y180 V184 I188 K189 F190 F209 E217 E220 N221 K228
I234 P235 C238 Q245 L246 Y249 T259 P260 G261 R264 L277 V278 T279 I283 A284 E285 T286 D287 S288 W289 E290 S295 V296 R297 K298 G307 A313 P320 P321 E325 D326 E329 N330 N331 V366 L370 V371 N372 N376 L377 V378 G381
L386 Y387 S400 G401 L402 D403 Q404 S405 R406 E411 R412 K413 R419 A435 N447 F450 D454 D461 T462 L468 R469 S472 G473 R478 I479 R485 V488 K489 W490 L502 D503 P506 L515 T516 I528 V529 A530 G531 D534 D538
F543 I547 F548 D549 N553 G554 N572 I577 T581 S584 K585 L586 I587 G588 R589 P590 P591 G596 V602 S603 P604 V607 E618 L619 G623 I641 S645 T646 F647 G648 I649 N650 L669 R670 I676 Q677 F678 L679 T680 P686 E689 V690
A691 Y694 G699 S714 Q715 V716 I717 L730 Q731 G734 G735 R736 G737 G738 G739 H740 H741 R758 I763 I766 S769 A774 D790 I807 A808 V811 A817 K818 T835 Y836 K837 K838 P839 I843 V844 T845 V846 R847 S848 E849 P853 I854 H855
K856 T859 R860 L864 D869 K877 L884 I892 N896 A897 D898 F899 Q900 A915 Y919 N936 T942 V954 E955 E956 L964 K975 P976 I980 F984 R991 E992 Q993 F994 L995 I1000 D1001 Q1012 K1013 P1014 L1021 D1022 R1023 D1032
S1033 L1034 W1035 Q1036 S1037 D1047 V1048 Q1049 R1050 T1051 C1052 I1053 L1054 H1055 D1067 I1077 I1082 L1086 D1092 E1106 S1107 P1108 V1109 ASP VAL GLN SER GLN VAL ASP SER SER SER VAL SER GLU D1123 S1131 D1134 E1135 E1136 L1142 R1150 C1156 M1164 N1168
P1169 I1170 F1174 S1177 M1180 V1181 V1182 N1188 T1189 T1193 V1194 V1195 T1196 L1197 Q1202 G1203 E1204 L1211 K1215 E1216 N1217 R1227 D1230 F1242 E1256 W1267 E1273 D1278 I1292 N1306 E1309 D1310 R1314 R1317 P1322 F1325 G1330
I1338 L1350 V1351 H1352 L1353 S1354 N1355 L1366 D1370 T1374 T1375 A1376 V1381 V1382 N1383 T1386 V1390 G1394 N1399 F1410 F1411 Y1412 R1413 G1414 N1415 D1418 T1422 Q1432 D1454 F1474 K1475 S1481 S1482 C1485 K1490 T1498 Y1506 G1509
A1510 S1511 H1512 S1525 T1526 L1527 V1531 I1537 E1551 R1555 N1561 H1564 V1565 P1576 I1579 R1590 E1594 S1600 D1614 H1628 I1638 K1639 E1645 D1646 D1647 E1654 I1657 E1658 Q1659 V1665 F1666 T1667 L1680 W1691 D1695 N1696 H1697
T1701 Y1702 I1706 Y1733 S1734 A1735 M1736 I1737 F1738 E1739 T1740 I1741 V1742 D1743 G1744 K1745 L1746 K1747 T1748 E1749 K1750 I1751 F1752 I1755 E1767 Q1775 Q1778 T1782 K1786 F1789 K1795 A1800 D1801 A1805 L1809 G1810 E1811 Y1812 A1813 A1816 S1817 V1831 F1832 Y1833
Q1839 E1846 L1847 G1848 R1849 S1850 I1855 A1856 P1859 F1866 L1871 Q1872 R1877 R1881 T1882 G1883 W1884 V1889 N1890 Q1896 Q1897 Y1898 V1899 A1906 L1907 D1908 T1911 N1912 N1915 L1919 I1922 D1923 I1924 I1925 E1926 L1927 Q1928 K1929 S1930 L1931 S1932 L1933 E1934 E1935 G1938


I1943
E1946
K1950
S1951
A1952
V1953
K1954
P1955
R1956
P1957
L1958
K1959
L1960
E1961
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F1964
L1969
V1970
G1971
I1972
S1973
H1977
N1983
P1987
K2009
L2014
T2015
A2016
K2017
Y2025
D2031
I2038
K2039
E2040
D2043
N2044
Y2048
GLU
GLN
SER

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D3	Depositor
Number of particles used	15320	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	32	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	5.293	Depositor
Minimum map value	-3.098	Depositor
Average map value	0.011	Depositor
Map value standard deviation	0.187	Depositor
Recommended contour level	0.6	Depositor
Map size (Å)	399.84, 399.84, 399.84	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.833, 0.833, 0.833	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, NDP, SEP

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	0.51	0/13859	0.62	7/18724 (0.0%)
1	B	0.51	0/13859	0.62	7/18724 (0.0%)
1	D	0.51	0/13859	0.62	7/18724 (0.0%)
1	F	0.51	0/13859	0.62	7/18724 (0.0%)
1	I	0.51	0/13859	0.62	7/18724 (0.0%)
1	K	0.51	0/13859	0.64	9/18724 (0.0%)
2	C	0.39	0/16342	0.58	4/22174 (0.0%)
2	E	0.39	0/16342	0.58	4/22174 (0.0%)
2	G	0.39	0/16342	0.58	4/22174 (0.0%)
2	H	0.39	0/16342	0.58	4/22174 (0.0%)
2	J	0.39	0/16342	0.58	4/22174 (0.0%)
2	L	0.39	0/16342	0.58	4/22174 (0.0%)
All	All	0.45	0/181206	0.60	68/245388 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	1
2	E	0	1
2	G	0	1
2	H	0	1
2	J	0	1
2	L	0	1
All	All	0	6

There are no bond length outliers.

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	329	GLU	N-CA-CB	15.05	137.69	110.60
1	K	328	LEU	N-CA-C	-14.18	72.71	111.00
1	B	873	ARG	NE-CZ-NH1	-6.19	117.21	120.30
1	F	873	ARG	NE-CZ-NH1	-6.19	117.21	120.30
1	D	873	ARG	NE-CZ-NH1	-6.16	117.22	120.30
1	I	873	ARG	NE-CZ-NH1	-6.16	117.22	120.30
1	A	873	ARG	NE-CZ-NH1	-6.11	117.25	120.30
1	K	873	ARG	NE-CZ-NH1	-6.11	117.25	120.30
1	A	930	LEU	CA-CB-CG	5.96	129.01	115.30
1	K	930	LEU	CA-CB-CG	5.96	129.01	115.30
1	D	930	LEU	CA-CB-CG	5.96	129.00	115.30
1	I	930	LEU	CA-CB-CG	5.96	129.00	115.30
1	B	930	LEU	CA-CB-CG	5.96	129.00	115.30
1	F	930	LEU	CA-CB-CG	5.96	129.00	115.30
2	E	65	LEU	CA-CB-CG	5.75	128.51	115.30
2	J	65	LEU	CA-CB-CG	5.75	128.51	115.30
2	G	65	LEU	CA-CB-CG	5.74	128.49	115.30
2	C	65	LEU	CA-CB-CG	5.74	128.49	115.30
2	L	65	LEU	CA-CB-CG	5.74	128.49	115.30
2	H	65	LEU	CA-CB-CG	5.74	128.49	115.30
1	D	1013	LEU	CA-CB-CG	5.71	128.42	115.30
1	I	1013	LEU	CA-CB-CG	5.71	128.42	115.30
1	B	1013	LEU	CA-CB-CG	5.70	128.42	115.30
1	F	1013	LEU	CA-CB-CG	5.70	128.42	115.30
1	A	1013	LEU	CA-CB-CG	5.70	128.40	115.30
1	K	1013	LEU	CA-CB-CG	5.70	128.40	115.30
1	B	824	LEU	CA-CB-CG	5.46	127.85	115.30
1	F	824	LEU	CA-CB-CG	5.46	127.85	115.30
1	D	824	LEU	CA-CB-CG	5.45	127.84	115.30
1	I	824	LEU	CA-CB-CG	5.45	127.84	115.30
1	A	824	LEU	CA-CB-CG	5.45	127.83	115.30
1	K	824	LEU	CA-CB-CG	5.45	127.83	115.30
2	C	1680	LEU	CA-CB-CG	5.41	127.75	115.30
2	H	1680	LEU	CA-CB-CG	5.41	127.75	115.30
2	E	1680	LEU	CA-CB-CG	5.39	127.71	115.30
2	J	1680	LEU	CA-CB-CG	5.39	127.71	115.30
2	G	1680	LEU	CA-CB-CG	5.39	127.70	115.30
2	L	1680	LEU	CA-CB-CG	5.39	127.70	115.30
1	B	447	LEU	CB-CG-CD1	-5.37	101.88	111.00
1	F	447	LEU	CB-CG-CD1	-5.37	101.88	111.00
1	A	447	LEU	CB-CG-CD1	-5.36	101.88	111.00
1	K	447	LEU	CB-CG-CD1	-5.36	101.88	111.00
1	D	447	LEU	CB-CG-CD1	-5.36	101.89	111.00

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Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	447	LEU	CB-CG-CD1	-5.36	101.89	111.00
2	G	1211	LEU	CA-CB-CG	5.35	127.61	115.30
2	C	1211	LEU	CA-CB-CG	5.35	127.61	115.30
2	L	1211	LEU	CA-CB-CG	5.35	127.61	115.30
2	H	1211	LEU	CA-CB-CG	5.35	127.61	115.30
2	E	1211	LEU	CA-CB-CG	5.35	127.61	115.30
2	J	1211	LEU	CA-CB-CG	5.35	127.61	115.30
2	G	807	ILE	CG1-CB-CG2	-5.17	100.03	111.40
2	L	807	ILE	CG1-CB-CG2	-5.17	100.03	111.40
2	C	807	ILE	CG1-CB-CG2	-5.17	100.03	111.40
2	H	807	ILE	CG1-CB-CG2	-5.17	100.03	111.40
2	E	807	ILE	CG1-CB-CG2	-5.15	100.06	111.40
2	J	807	ILE	CG1-CB-CG2	-5.15	100.06	111.40
1	B	1426	LEU	CA-CB-CG	5.10	127.02	115.30
1	F	1426	LEU	CA-CB-CG	5.10	127.02	115.30
1	A	1426	LEU	CA-CB-CG	5.09	127.01	115.30
1	K	1426	LEU	CA-CB-CG	5.09	127.01	115.30
1	D	1426	LEU	CA-CB-CG	5.09	127.00	115.30
1	I	1426	LEU	CA-CB-CG	5.09	127.00	115.30
1	A	1430	ARG	CA-CB-CG	5.04	124.48	113.40
1	K	1430	ARG	CA-CB-CG	5.04	124.48	113.40
1	B	1430	ARG	CA-CB-CG	5.02	124.44	113.40
1	D	1430	ARG	CA-CB-CG	5.02	124.44	113.40
1	F	1430	ARG	CA-CB-CG	5.02	124.44	113.40
1	I	1430	ARG	CA-CB-CG	5.02	124.44	113.40

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	1014	PRO	Peptide
2	E	1014	PRO	Peptide
2	G	1014	PRO	Peptide
2	H	1014	PRO	Peptide
2	J	1014	PRO	Peptide
2	L	1014	PRO	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	13619	0	13602	244	0
1	B	13619	0	13602	241	0
1	D	13619	0	13602	242	0
1	F	13619	0	13602	242	0
1	I	13619	0	13602	243	0
1	K	13619	0	13602	240	0
2	C	15977	0	15964	290	0
2	E	15977	0	15964	289	0
2	G	15977	0	15964	294	0
2	H	15977	0	15964	287	0
2	J	15977	0	15964	293	0
2	L	15977	0	15964	288	0
3	A	48	26	26	8	0
3	B	48	26	26	7	0
3	D	48	26	26	7	0
3	F	48	26	26	7	0
3	I	48	26	26	8	0
3	K	48	26	26	7	0
4	C	31	0	19	0	0
4	E	31	0	19	0	0
4	G	31	0	19	0	0
4	H	31	0	19	0	0
4	J	31	0	19	0	0
4	L	31	0	19	0	0
All	All	178050	156	177666	2989	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (2989) 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:K:1491:ARG:CD	1:K:1750:ILE:HD11	1.37	1.55
1:D:1491:ARG:HD3	1:D:1750:ILE:CD1	1.34	1.54
1:D:1491:ARG:CD	1:D:1750:ILE:HD11	1.37	1.54
1:F:1491:ARG:CD	1:F:1750:ILE:HD11	1.37	1.54
1:A:1491:ARG:HD3	1:A:1750:ILE:CD1	1.34	1.54
1:F:1491:ARG:HD3	1:F:1750:ILE:CD1	1.34	1.54
1:B:1491:ARG:HD3	1:B:1750:ILE:CD1	1.34	1.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1491:ARG:CD	1:B:1750:ILE:HD11	1.37	1.53
1:A:1491:ARG:CD	1:A:1750:ILE:HD11	1.37	1.52
1:K:1491:ARG:HD3	1:K:1750:ILE:CD1	1.34	1.51
1:I:1491:ARG:HD3	1:I:1750:ILE:CD1	1.34	1.50
1:I:1491:ARG:CD	1:I:1750:ILE:HD11	1.37	1.49
2:H:847:ARG:HG3	2:H:869:ASP:OD2	1.21	1.38
1:I:1491:ARG:CD	1:I:1750:ILE:CD1	1.97	1.35
2:C:847:ARG:HG3	2:C:869:ASP:OD2	1.21	1.35
1:A:1491:ARG:CD	1:A:1750:ILE:CD1	1.97	1.34
1:K:1491:ARG:CD	1:K:1750:ILE:CD1	1.97	1.33
2:E:847:ARG:HG3	2:E:869:ASP:OD2	1.21	1.33
2:J:847:ARG:HG3	2:J:869:ASP:OD2	1.21	1.33
1:A:1491:ARG:CB	1:A:1750:ILE:HD13	1.60	1.32
1:D:1491:ARG:CB	1:D:1750:ILE:HD13	1.60	1.32
1:F:1491:ARG:CD	1:F:1750:ILE:CD1	1.97	1.32
1:I:1491:ARG:CB	1:I:1750:ILE:HD13	1.60	1.31
1:D:1491:ARG:CD	1:D:1750:ILE:CD1	1.97	1.30
1:K:1491:ARG:CB	1:K:1750:ILE:HD13	1.60	1.30
1:F:1491:ARG:CB	1:F:1750:ILE:HD13	1.60	1.30
1:B:1491:ARG:CB	1:B:1750:ILE:HD13	1.60	1.29
2:L:847:ARG:HG3	2:L:869:ASP:OD2	1.21	1.27
2:G:847:ARG:HG3	2:G:869:ASP:OD2	1.21	1.26
1:B:1491:ARG:CD	1:B:1750:ILE:CD1	1.97	1.26
1:F:1744:TYR:O	1:F:1747:ALA:CB	1.85	1.25
1:B:1744:TYR:O	1:B:1747:ALA:CB	1.85	1.25
1:K:1744:TYR:O	1:K:1747:ALA:CB	1.85	1.25
1:I:1744:TYR:O	1:I:1747:ALA:CB	1.85	1.24
1:D:1744:TYR:O	1:D:1747:ALA:CB	1.85	1.23
1:A:1744:TYR:O	1:A:1747:ALA:CB	1.85	1.23
1:A:1744:TYR:O	1:A:1747:ALA:HB2	1.03	1.21
1:F:1744:TYR:O	1:F:1747:ALA:HB2	1.03	1.20
1:K:1744:TYR:O	1:K:1747:ALA:HB2	1.03	1.19
1:I:1744:TYR:O	1:I:1747:ALA:HB2	1.03	1.19
1:D:1744:TYR:O	1:D:1747:ALA:HB2	1.03	1.19
1:A:1491:ARG:HD2	1:A:1750:ILE:HD11	1.20	1.18
1:B:1744:TYR:O	1:B:1747:ALA:HB2	1.03	1.18
2:E:1737:ILE:HB	2:E:1748:THR:HB	1.21	1.17
1:D:1491:ARG:HD3	1:D:1750:ILE:HD12	1.24	1.16
2:G:1735:ALA:O	2:G:1736:MET:HE2	1.45	1.16
2:L:1735:ALA:O	2:L:1736:MET:HE2	1.47	1.15
1:I:1491:ARG:HD2	1:I:1750:ILE:HD11	1.20	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1735:ALA:O	2:C:1736:MET:HE2	1.46	1.15
2:H:1737:ILE:HB	2:H:1748:THR:HB	1.20	1.15
2:J:1735:ALA:O	2:J:1736:MET:HE2	1.44	1.14
2:E:234:ILE:HG23	2:E:238:CYS:SG	1.87	1.14
1:F:1491:ARG:HD3	1:F:1750:ILE:HD12	1.24	1.14
2:H:234:ILE:HG23	2:H:238:CYS:SG	1.87	1.14
2:J:234:ILE:HG23	2:J:238:CYS:SG	1.87	1.14
2:C:234:ILE:HG23	2:C:238:CYS:SG	1.87	1.14
2:J:847:ARG:CG	2:J:869:ASP:OD2	1.97	1.13
2:L:1737:ILE:HB	2:L:1748:THR:HB	1.21	1.13
1:F:1491:ARG:HD2	1:F:1750:ILE:HD11	1.20	1.13
2:H:1735:ALA:O	2:H:1736:MET:HE2	1.47	1.13
1:A:848:THR:HG22	1:F:844:LEU:HD22	1.24	1.13
2:G:234:ILE:HG23	2:G:238:CYS:SG	1.87	1.13
2:G:847:ARG:CG	2:G:869:ASP:OD2	1.97	1.13
2:G:1737:ILE:HB	2:G:1748:THR:HB	1.21	1.12
2:L:234:ILE:HG23	2:L:238:CYS:SG	1.87	1.12
2:H:847:ARG:CG	2:H:869:ASP:OD2	1.97	1.12
1:D:844:LEU:HD22	1:I:848:THR:HG22	1.24	1.12
2:E:847:ARG:CG	2:E:869:ASP:OD2	1.97	1.11
2:L:847:ARG:CG	2:L:869:ASP:OD2	1.97	1.11
1:I:1491:ARG:HD3	1:I:1750:ILE:HD12	1.24	1.11
1:B:1491:ARG:HD2	1:B:1750:ILE:HD11	1.20	1.11
1:K:1491:ARG:HD3	1:K:1750:ILE:HD12	1.25	1.11
2:C:847:ARG:CG	2:C:869:ASP:OD2	1.97	1.10
2:J:1737:ILE:HB	2:J:1748:THR:HB	1.21	1.10
2:E:836:TYR:CD1	2:E:845:THR:HG21	1.87	1.10
2:E:1735:ALA:O	2:E:1736:MET:HE2	1.48	1.10
1:F:1751:GLU:HA	1:F:1754:LYS:HE3	1.32	1.10
2:H:836:TYR:CD1	2:H:845:THR:HG21	1.87	1.10
1:A:1491:ARG:HD3	1:A:1750:ILE:HD12	1.25	1.10
1:D:1491:ARG:HD2	1:D:1750:ILE:HD11	1.20	1.09
2:E:739:GLY:HA2	2:E:1054:LEU:HD23	1.10	1.09
2:L:739:GLY:HA2	2:L:1054:LEU:HD23	1.10	1.09
2:H:739:GLY:HA2	2:H:1054:LEU:HD23	1.10	1.09
2:C:1737:ILE:HB	2:C:1748:THR:HB	1.20	1.09
2:G:836:TYR:CD1	2:G:845:THR:HG21	1.87	1.09
1:B:848:THR:HG22	1:K:844:LEU:HD22	1.24	1.09
1:D:848:THR:HG22	1:I:844:LEU:HD22	1.24	1.09
2:L:836:TYR:CD1	2:L:845:THR:HG21	1.87	1.09
2:C:739:GLY:HA2	2:C:1054:LEU:HD23	1.10	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1751:GLU:HA	1:D:1754:LYS:HE3	1.32	1.08
1:I:1751:GLU:HA	1:I:1754:LYS:HE3	1.32	1.08
1:B:1491:ARG:HD3	1:B:1750:ILE:HD12	1.24	1.08
1:K:1491:ARG:HD2	1:K:1750:ILE:HD11	1.20	1.08
2:J:836:TYR:CD1	2:J:845:THR:HG21	1.87	1.08
1:B:844:LEU:HD22	1:K:848:THR:HG22	1.24	1.07
2:E:1036:GLN:HB3	2:E:1051:THR:HG23	1.36	1.07
2:J:739:GLY:HA2	2:J:1054:LEU:HD23	1.10	1.07
1:A:844:LEU:HD22	1:F:848:THR:HG22	1.24	1.07
2:G:646:THR:HB	2:G:677:GLN:HB2	1.36	1.07
2:G:1036:GLN:HB3	2:G:1051:THR:HG23	1.36	1.07
2:J:646:THR:HB	2:J:677:GLN:HB2	1.36	1.07
2:L:646:THR:HB	2:L:677:GLN:HB2	1.36	1.07
2:H:646:THR:HB	2:H:677:GLN:HB2	1.36	1.07
2:G:739:GLY:HA2	2:G:1054:LEU:HD23	1.10	1.07
2:C:646:THR:HB	2:C:677:GLN:HB2	1.36	1.07
2:C:836:TYR:CD1	2:C:845:THR:HG21	1.87	1.07
2:E:646:THR:HB	2:E:677:GLN:HB2	1.36	1.07
1:B:1751:GLU:HA	1:B:1754:LYS:HE3	1.32	1.06
2:H:1036:GLN:HB3	2:H:1051:THR:HG23	1.36	1.06
2:J:1036:GLN:HB3	2:J:1051:THR:HG23	1.36	1.06
2:L:1036:GLN:HB3	2:L:1051:THR:HG23	1.36	1.05
1:A:1751:GLU:HA	1:A:1754:LYS:HE3	1.32	1.04
2:C:1036:GLN:HB3	2:C:1051:THR:HG23	1.36	1.04
1:K:1751:GLU:HA	1:K:1754:LYS:HE3	1.32	1.04
1:A:1487:LEU:CD1	1:A:1754:LYS:HE2	1.89	1.02
1:F:1487:LEU:CD1	1:F:1754:LYS:HE2	1.89	1.02
1:I:1487:LEU:HD12	1:I:1754:LYS:HE2	1.41	1.02
1:B:1487:LEU:HD12	1:B:1754:LYS:HE2	1.41	1.02
1:F:1491:ARG:HB2	1:F:1750:ILE:HD13	1.02	1.01
1:I:1487:LEU:CD1	1:I:1754:LYS:HE2	1.90	1.01
1:D:1487:LEU:CD1	1:D:1754:LYS:HE2	1.90	1.01
1:D:1491:ARG:HB2	1:D:1750:ILE:HD13	1.02	1.01
1:K:1487:LEU:CD1	1:K:1754:LYS:HE2	1.89	1.01
2:J:1735:ALA:O	2:J:1736:MET:CE	2.09	1.01
1:B:1487:LEU:CD1	1:B:1754:LYS:HE2	1.89	1.01
2:E:1735:ALA:C	2:E:1736:MET:HE3	1.81	1.01
1:A:1491:ARG:HB2	1:A:1750:ILE:HD13	1.02	1.01
2:C:1735:ALA:O	2:C:1736:MET:CE	2.09	1.01
2:G:1735:ALA:O	2:G:1736:MET:CE	2.09	1.00
2:E:1735:ALA:O	2:E:1736:MET:CE	2.09	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1487:LEU:HD12	1:F:1754:LYS:HE2	1.41	1.00
2:H:1735:ALA:O	2:H:1736:MET:CE	2.09	1.00
1:D:1487:LEU:HD12	1:D:1754:LYS:HE2	1.41	1.00
2:L:1735:ALA:O	2:L:1736:MET:CE	2.09	1.00
1:I:1491:ARG:HB2	1:I:1750:ILE:HD13	1.02	0.99
1:K:1491:ARG:HB2	1:K:1750:ILE:HD13	1.02	0.99
1:K:1487:LEU:HD12	1:K:1754:LYS:HE2	1.41	0.99
1:A:1487:LEU:HD12	1:A:1754:LYS:HE2	1.41	0.99
2:L:1735:ALA:C	2:L:1736:MET:HE3	1.83	0.98
1:B:1491:ARG:HB2	1:B:1750:ILE:HD13	1.02	0.98
2:H:1735:ALA:C	2:H:1736:MET:HE3	1.83	0.98
2:L:1036:GLN:CB	2:L:1051:THR:HG23	1.94	0.97
2:E:1036:GLN:CB	2:E:1051:THR:HG23	1.94	0.96
2:C:1036:GLN:CB	2:C:1051:THR:HG23	1.95	0.96
2:H:1036:GLN:CB	2:H:1051:THR:HG23	1.95	0.96
2:J:1036:GLN:CB	2:J:1051:THR:HG23	1.94	0.96
2:C:1735:ALA:C	2:C:1736:MET:HE3	1.86	0.95
2:G:1036:GLN:CB	2:G:1051:THR:HG23	1.94	0.95
1:A:1751:GLU:HG3	1:A:1754:LYS:NZ	1.83	0.94
1:D:1751:GLU:HG3	1:D:1754:LYS:NZ	1.83	0.94
2:L:1735:ALA:C	2:L:1736:MET:CE	2.36	0.94
2:C:1735:ALA:C	2:C:1736:MET:CE	2.36	0.94
2:E:1735:ALA:C	2:E:1736:MET:CE	2.36	0.93
2:E:1739:GLU:HB3	2:E:1746:LEU:HD11	1.50	0.93
1:F:1751:GLU:HG3	1:F:1754:LYS:NZ	1.83	0.93
2:H:1735:ALA:C	2:H:1736:MET:CE	2.36	0.93
1:K:1751:GLU:HG3	1:K:1754:LYS:NZ	1.83	0.93
2:G:1735:ALA:C	2:G:1736:MET:CE	2.36	0.93
2:J:1735:ALA:C	2:J:1736:MET:CE	2.36	0.93
2:J:1735:ALA:C	2:J:1736:MET:HE3	1.89	0.93
2:G:1735:ALA:C	2:G:1736:MET:HE3	1.87	0.93
1:I:1751:GLU:HG3	1:I:1754:LYS:NZ	1.83	0.92
1:B:1751:GLU:HG3	1:B:1754:LYS:NZ	1.83	0.92
1:F:1491:ARG:CB	1:F:1750:ILE:CD1	2.47	0.92
2:H:1739:GLU:HB3	2:H:1746:LEU:HD11	1.51	0.92
1:D:1491:ARG:CB	1:D:1750:ILE:CD1	2.47	0.92
2:G:739:GLY:HA2	2:G:1054:LEU:CD2	2.00	0.92
2:L:1739:GLU:HB3	2:L:1746:LEU:HD11	1.50	0.92
1:A:1491:ARG:CB	1:A:1750:ILE:CD1	2.47	0.91
1:B:848:THR:CG2	1:K:844:LEU:HD22	2.01	0.91
1:D:844:LEU:HD22	1:I:848:THR:CG2	2.01	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1491:ARG:HB2	1:I:1750:ILE:CD1	1.98	0.91
1:K:1491:ARG:CB	1:K:1750:ILE:CD1	2.47	0.91
1:I:1491:ARG:CB	1:I:1750:ILE:CD1	2.47	0.91
1:F:1491:ARG:HB2	1:F:1750:ILE:CD1	1.98	0.91
2:H:739:GLY:HA2	2:H:1054:LEU:CD2	2.00	0.91
1:D:848:THR:CG2	1:I:844:LEU:HD22	2.01	0.91
1:A:848:THR:CG2	1:F:844:LEU:HD22	2.01	0.90
2:C:1739:GLU:HB3	2:C:1746:LEU:HD11	1.51	0.90
2:L:739:GLY:HA2	2:L:1054:LEU:CD2	2.00	0.90
2:J:1739:GLU:HB3	2:J:1746:LEU:HD11	1.50	0.90
1:A:844:LEU:HD22	1:F:848:THR:CG2	2.01	0.90
2:E:739:GLY:HA2	2:E:1054:LEU:CD2	2.00	0.90
1:B:844:LEU:HD22	1:K:848:THR:CG2	2.01	0.90
2:C:739:GLY:HA2	2:C:1054:LEU:CD2	2.00	0.90
1:K:1373:ARG:NE	1:K:1550:ASP:OD2	2.05	0.90
1:F:1373:ARG:NE	1:F:1550:ASP:OD2	2.05	0.90
1:D:1491:ARG:HB2	1:D:1750:ILE:CD1	1.98	0.89
2:G:1739:GLU:HB3	2:G:1746:LEU:HD11	1.50	0.89
1:B:1373:ARG:NE	1:B:1550:ASP:OD2	2.05	0.89
1:A:1373:ARG:NE	1:A:1550:ASP:OD2	2.05	0.89
1:D:1373:ARG:NE	1:D:1550:ASP:OD2	2.05	0.89
1:B:1491:ARG:CB	1:B:1750:ILE:CD1	2.47	0.89
2:C:847:ARG:HG3	2:C:869:ASP:CG	1.93	0.89
2:J:1738:PHE:CZ	2:J:1749:GLU:HG2	2.08	0.89
2:G:1738:PHE:CZ	2:G:1749:GLU:HG2	2.08	0.89
2:G:646:THR:CB	2:G:677:GLN:HB2	2.03	0.89
2:E:847:ARG:HG3	2:E:869:ASP:CG	1.93	0.89
2:H:847:ARG:HG3	2:H:869:ASP:CG	1.93	0.89
2:J:847:ARG:HG3	2:J:869:ASP:CG	1.93	0.89
2:E:1738:PHE:CZ	2:E:1749:GLU:HG2	2.08	0.89
2:L:847:ARG:HG3	2:L:869:ASP:CG	1.93	0.88
1:I:1373:ARG:NE	1:I:1550:ASP:OD2	2.05	0.88
2:C:646:THR:CB	2:C:677:GLN:HB2	2.03	0.88
2:H:646:THR:CB	2:H:677:GLN:HB2	2.03	0.88
2:H:1738:PHE:CZ	2:H:1749:GLU:HG2	2.08	0.88
2:L:1738:PHE:CZ	2:L:1749:GLU:HG2	2.08	0.88
2:L:646:THR:CB	2:L:677:GLN:HB2	2.03	0.88
2:C:1738:PHE:CZ	2:C:1749:GLU:HG2	2.08	0.88
2:J:646:THR:CB	2:J:677:GLN:HB2	2.03	0.88
2:E:234:ILE:CG2	2:E:238:CYS:SG	2.62	0.87
2:G:847:ARG:HG3	2:G:869:ASP:CG	1.93	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:234:ILE:CG2	2:H:238:CYS:SG	2.62	0.87
1:A:1491:ARG:HB2	1:A:1750:ILE:CD1	1.98	0.87
2:C:1737:ILE:HB	2:C:1748:THR:CB	2.05	0.87
2:G:234:ILE:CG2	2:G:238:CYS:SG	2.62	0.87
2:C:234:ILE:CG2	2:C:238:CYS:SG	2.62	0.87
1:K:1491:ARG:HB2	1:K:1750:ILE:CD1	1.98	0.87
2:J:234:ILE:CG2	2:J:238:CYS:SG	2.62	0.87
2:J:246:LEU:HD23	2:J:296:VAL:HG22	1.57	0.87
2:L:234:ILE:CG2	2:L:238:CYS:SG	2.62	0.86
2:E:646:THR:CB	2:E:677:GLN:HB2	2.03	0.86
2:C:246:LEU:HD23	2:C:296:VAL:HG22	1.57	0.86
2:L:1737:ILE:HB	2:L:1748:THR:CB	2.05	0.86
2:J:739:GLY:HA2	2:J:1054:LEU:CD2	2.00	0.86
2:G:1737:ILE:HB	2:G:1748:THR:CB	2.05	0.86
2:H:1737:ILE:HB	2:H:1748:THR:CB	2.05	0.86
2:G:246:LEU:HD23	2:G:296:VAL:HG22	1.57	0.86
2:L:246:LEU:HD23	2:L:296:VAL:HG22	1.57	0.86
2:J:1737:ILE:HB	2:J:1748:THR:CB	2.05	0.85
2:E:246:LEU:HD23	2:E:296:VAL:HG22	1.57	0.85
1:B:1491:ARG:HB2	1:B:1750:ILE:CD1	1.98	0.84
1:B:1491:ARG:CG	1:B:1750:ILE:CD1	2.55	0.84
2:E:1737:ILE:HB	2:E:1748:THR:CB	2.05	0.84
1:D:1491:ARG:CG	1:D:1750:ILE:CD1	2.55	0.84
1:K:1491:ARG:CG	1:K:1750:ILE:CD1	2.55	0.84
2:H:246:LEU:HD23	2:H:296:VAL:HG22	1.57	0.84
1:I:1751:GLU:HG3	1:I:1754:LYS:HZ1	1.43	0.84
1:I:1491:ARG:CG	1:I:1750:ILE:CD1	2.55	0.84
1:F:1491:ARG:CG	1:F:1750:ILE:CD1	2.55	0.84
1:K:1561:MET:HE2	1:K:1561:MET:HA	1.60	0.83
1:D:844:LEU:CD2	1:I:848:THR:HG22	2.08	0.83
1:A:1491:ARG:CG	1:A:1750:ILE:CD1	2.55	0.83
1:B:848:THR:HG22	1:K:844:LEU:CD2	2.08	0.83
1:K:1373:ARG:CD	1:K:1550:ASP:OD2	2.27	0.83
1:B:1373:ARG:CD	1:B:1550:ASP:OD2	2.27	0.83
1:I:1373:ARG:CD	1:I:1550:ASP:OD2	2.27	0.83
1:I:1561:MET:HE2	1:I:1561:MET:HA	1.60	0.83
1:A:848:THR:HG22	1:F:844:LEU:CD2	2.08	0.83
2:E:234:ILE:HG23	2:E:238:CYS:HG	1.41	0.83
1:D:1373:ARG:CD	1:D:1550:ASP:OD2	2.27	0.82
1:B:844:LEU:CD2	1:K:848:THR:HG22	2.08	0.82
1:F:1373:ARG:CD	1:F:1550:ASP:OD2	2.27	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:844:LEU:CD2	1:F:848:THR:HG22	2.08	0.82
1:B:1561:MET:HA	1:B:1561:MET:HE2	1.60	0.82
1:A:1373:ARG:CD	1:A:1550:ASP:OD2	2.27	0.82
1:D:848:THR:HG22	1:I:844:LEU:CD2	2.08	0.81
1:D:1541:PHE:HE1	1:D:1557:ILE:HG13	1.45	0.81
1:F:877:LEU:CD1	3:F:2001:NDP:H2D	2.10	0.81
1:D:1491:ARG:CG	1:D:1750:ILE:HD13	2.10	0.81
1:F:1541:PHE:HE1	1:F:1557:ILE:HG13	1.45	0.81
1:B:838:MET:HA	1:B:841:GLU:OE1	1.81	0.81
1:D:877:LEU:CD1	3:D:2001:NDP:H2D	2.10	0.81
1:A:1561:MET:HE2	1:A:1561:MET:HA	1.63	0.81
1:B:1541:PHE:HE1	1:B:1557:ILE:HG13	1.45	0.81
1:K:1541:PHE:HE1	1:K:1557:ILE:HG13	1.45	0.81
2:J:260:PRO:HD3	2:J:289:TRP:CZ2	2.16	0.81
1:A:1491:ARG:CG	1:A:1750:ILE:HD13	2.10	0.81
1:A:1541:PHE:HE1	1:A:1557:ILE:HG13	1.45	0.81
2:G:1737:ILE:CB	2:G:1748:THR:HB	2.09	0.81
1:K:1491:ARG:CG	1:K:1750:ILE:HD13	2.10	0.81
1:K:1751:GLU:CA	1:K:1754:LYS:HE3	2.11	0.81
1:I:1491:ARG:CG	1:I:1750:ILE:HD13	2.10	0.81
1:B:1491:ARG:CG	1:B:1750:ILE:HD13	2.10	0.81
1:K:838:MET:HA	1:K:841:GLU:OE1	1.81	0.81
1:A:838:MET:HA	1:A:841:GLU:OE1	1.81	0.81
1:A:877:LEU:CD1	3:A:2001:NDP:H2D	2.10	0.81
1:A:1673:TYR:CZ	1:A:1677:VAL:HG21	2.16	0.81
1:B:1751:GLU:CA	1:B:1754:LYS:HE3	2.11	0.81
2:C:260:PRO:HD3	2:C:289:TRP:CZ2	2.16	0.81
1:K:877:LEU:CD1	3:K:2001:NDP:H2D	2.10	0.81
1:F:1673:TYR:CZ	1:F:1677:VAL:HG21	2.16	0.81
1:D:1751:GLU:CA	1:D:1754:LYS:HE3	2.11	0.80
2:G:260:PRO:HD3	2:G:289:TRP:CZ2	2.16	0.80
2:L:260:PRO:HD3	2:L:289:TRP:CZ2	2.16	0.80
1:F:1491:ARG:CG	1:F:1750:ILE:HD13	2.10	0.80
1:B:877:LEU:CD1	3:B:2001:NDP:H2D	2.10	0.80
1:D:838:MET:HA	1:D:841:GLU:OE1	1.81	0.80
1:F:1751:GLU:CA	1:F:1754:LYS:HE3	2.11	0.80
2:H:260:PRO:HD3	2:H:289:TRP:CZ2	2.16	0.80
1:I:1673:TYR:CZ	1:I:1677:VAL:HG21	2.16	0.80
1:I:838:MET:HA	1:I:841:GLU:OE1	1.81	0.80
1:I:1491:ARG:HD3	1:I:1750:ILE:HD11	1.06	0.80
1:I:1751:GLU:CA	1:I:1754:LYS:HE3	2.11	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1673:TYR:CZ	1:B:1677:VAL:HG21	2.16	0.80
1:D:1673:TYR:CZ	1:D:1677:VAL:HG21	2.16	0.80
2:E:260:PRO:HD3	2:E:289:TRP:CZ2	2.16	0.80
1:I:877:LEU:CD1	3:I:2001:NDP:H2D	2.10	0.79
1:F:838:MET:HA	1:F:841:GLU:OE1	1.81	0.79
1:A:1751:GLU:CA	1:A:1754:LYS:HE3	2.11	0.79
2:G:295:SER:O	2:G:298:LYS:HB2	1.82	0.79
1:B:1751:GLU:HG3	1:B:1754:LYS:HZ1	1.48	0.79
1:K:1673:TYR:CZ	1:K:1677:VAL:HG21	2.16	0.79
1:I:1541:PHE:HE1	1:I:1557:ILE:HG13	1.45	0.79
2:J:1737:ILE:HG12	2:J:1748:THR:HG21	1.64	0.79
2:C:1737:ILE:HG12	2:C:1748:THR:HG21	1.64	0.79
2:H:1737:ILE:CB	2:H:1748:THR:HB	2.09	0.79
2:G:1737:ILE:H	2:G:1737:ILE:HD13	1.48	0.79
2:H:295:SER:O	2:H:298:LYS:HB2	1.82	0.79
1:B:1558:ASN:OD1	1:B:1623:TYR:HB2	1.84	0.78
2:C:295:SER:O	2:C:298:LYS:HB2	1.82	0.78
2:C:1737:ILE:HD13	2:C:1737:ILE:H	1.48	0.78
2:E:1737:ILE:HD13	2:E:1737:ILE:H	1.48	0.78
2:L:295:SER:O	2:L:298:LYS:HB2	1.82	0.78
2:L:1737:ILE:H	2:L:1737:ILE:HD13	1.48	0.78
2:J:295:SER:O	2:J:298:LYS:HB2	1.82	0.78
2:G:1737:ILE:HG12	2:G:1748:THR:HG21	1.64	0.78
1:F:1558:ASN:OD1	1:F:1623:TYR:HB2	1.84	0.78
2:E:1737:ILE:HG12	2:E:1748:THR:HG21	1.64	0.78
1:K:1558:ASN:OD1	1:K:1623:TYR:HB2	1.83	0.78
2:L:836:TYR:CD1	2:L:845:THR:CG2	2.67	0.78
2:J:1737:ILE:HD13	2:J:1737:ILE:H	1.48	0.78
1:D:1558:ASN:OD1	1:D:1623:TYR:HB2	1.84	0.78
2:E:1737:ILE:CB	2:E:1748:THR:HB	2.09	0.78
2:E:836:TYR:CD1	2:E:845:THR:CG2	2.67	0.77
1:I:1558:ASN:OD1	1:I:1623:TYR:HB2	1.84	0.77
1:A:1491:ARG:HD3	1:A:1750:ILE:HD11	1.06	0.77
2:L:1737:ILE:HG12	2:L:1748:THR:HG21	1.64	0.77
2:H:1737:ILE:HG12	2:H:1748:THR:HG21	1.64	0.77
2:G:1737:ILE:HG12	2:G:1748:THR:CG2	2.14	0.77
1:A:1558:ASN:OD1	1:A:1623:TYR:HB2	1.83	0.77
1:D:848:THR:CG2	1:I:844:LEU:CD2	2.63	0.77
2:L:1737:ILE:HG12	2:L:1748:THR:CG2	2.14	0.77
2:C:836:TYR:CD1	2:C:845:THR:CG2	2.67	0.77
2:E:295:SER:O	2:E:298:LYS:HB2	1.82	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:1737:ILE:HG12	2:J:1748:THR:CG2	2.14	0.77
1:A:844:LEU:CD2	1:F:848:THR:CG2	2.63	0.77
2:H:1737:ILE:HD13	2:H:1737:ILE:H	1.48	0.77
2:C:1737:ILE:HG12	2:C:1748:THR:CG2	2.14	0.77
2:E:1737:ILE:HG12	2:E:1748:THR:CG2	2.14	0.77
2:G:836:TYR:CD1	2:G:845:THR:CG2	2.67	0.77
2:J:836:TYR:CD1	2:J:845:THR:CG2	2.67	0.77
2:H:1737:ILE:HG12	2:H:1748:THR:CG2	2.14	0.76
2:E:1037:SER:CB	2:E:1053:ILE:HG12	2.16	0.76
2:L:1737:ILE:CB	2:L:1748:THR:HB	2.09	0.76
1:B:848:THR:CG2	1:K:844:LEU:CD2	2.63	0.76
2:H:1037:SER:CB	2:H:1053:ILE:HG12	2.16	0.76
1:D:844:LEU:CD2	1:I:848:THR:CG2	2.63	0.76
1:B:844:LEU:CD2	1:K:848:THR:CG2	2.63	0.76
1:D:1487:LEU:CG	1:D:1754:LYS:HE2	2.16	0.76
1:K:1487:LEU:CG	1:K:1754:LYS:HE2	2.16	0.76
1:F:1487:LEU:CG	1:F:1754:LYS:HE2	2.16	0.75
2:H:836:TYR:CD1	2:H:845:THR:CG2	2.67	0.75
1:A:848:THR:CG2	1:F:844:LEU:CD2	2.63	0.75
2:L:1037:SER:CB	2:L:1053:ILE:HG12	2.16	0.75
2:J:1737:ILE:CB	2:J:1748:THR:HB	2.09	0.75
2:G:1037:SER:CB	2:G:1053:ILE:HG12	2.16	0.75
1:D:1561:MET:HA	1:D:1561:MET:CE	2.17	0.75
2:C:1737:ILE:CB	2:C:1748:THR:HB	2.09	0.75
1:B:1487:LEU:HD12	1:B:1754:LYS:CE	2.17	0.75
1:B:1487:LEU:CG	1:B:1754:LYS:HE2	2.16	0.75
1:F:1561:MET:HA	1:F:1561:MET:CE	2.17	0.75
1:I:1561:MET:HA	1:I:1561:MET:CE	2.17	0.75
1:A:1487:LEU:CG	1:A:1754:LYS:HE2	2.16	0.74
1:B:1561:MET:HA	1:B:1561:MET:CE	2.17	0.74
1:A:1561:MET:HA	1:A:1561:MET:CE	2.16	0.74
2:C:1037:SER:CB	2:C:1053:ILE:HG12	2.16	0.74
1:K:1561:MET:HA	1:K:1561:MET:CE	2.16	0.74
2:J:1739:GLU:HB3	2:J:1746:LEU:CD1	2.18	0.74
2:J:1037:SER:CB	2:J:1053:ILE:HG12	2.16	0.74
2:H:246:LEU:CD2	2:H:296:VAL:HG22	2.18	0.74
2:G:246:LEU:CD2	2:G:296:VAL:HG22	2.18	0.74
2:C:1739:GLU:HB3	2:C:1746:LEU:CD1	2.18	0.74
1:D:1487:LEU:HD12	1:D:1754:LYS:CE	2.17	0.74
1:K:1487:LEU:HD12	1:K:1754:LYS:CE	2.17	0.74
2:G:1739:GLU:HB3	2:G:1746:LEU:CD1	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:246:LEU:CD2	2:E:296:VAL:HG22	2.18	0.73
2:L:839:PRO:HA	2:L:844:VAL:HG13	1.70	0.73
2:J:246:LEU:CD2	2:J:296:VAL:HG22	2.18	0.73
1:K:1751:GLU:HG3	1:K:1754:LYS:HZ1	1.53	0.73
1:A:1487:LEU:HD12	1:A:1754:LYS:CE	2.17	0.73
2:G:1036:GLN:CB	2:G:1051:THR:CG2	2.66	0.73
2:L:246:LEU:CD2	2:L:296:VAL:HG22	2.18	0.73
2:C:839:PRO:HA	2:C:844:VAL:HG13	1.70	0.73
1:I:1487:LEU:CG	1:I:1754:LYS:HE2	2.16	0.73
2:C:246:LEU:CD2	2:C:296:VAL:HG22	2.18	0.73
1:F:1487:LEU:HD12	1:F:1754:LYS:CE	2.17	0.73
1:F:1561:MET:HA	1:F:1561:MET:HE2	1.70	0.73
2:H:1739:GLU:HB3	2:H:1746:LEU:CD1	2.18	0.73
2:E:839:PRO:HA	2:E:844:VAL:HG13	1.70	0.73
2:E:1739:GLU:HB3	2:E:1746:LEU:CD1	2.18	0.73
2:H:1036:GLN:CB	2:H:1051:THR:CG2	2.66	0.73
2:E:1736:MET:HB3	2:E:1751:ILE:HD12	1.71	0.73
2:L:1736:MET:HB3	2:L:1751:ILE:HD12	1.71	0.73
2:J:234:ILE:HG23	2:J:238:CYS:HG	1.53	0.73
2:H:739:GLY:CA	2:H:1054:LEU:HD23	2.05	0.72
2:L:1739:GLU:HB3	2:L:1746:LEU:CD1	2.18	0.72
1:I:1487:LEU:HD12	1:I:1754:LYS:CE	2.17	0.72
2:J:1036:GLN:CB	2:J:1051:THR:CG2	2.66	0.72
2:E:1737:ILE:CG1	2:E:1748:THR:HG21	2.19	0.72
2:J:839:PRO:HA	2:J:844:VAL:HG13	1.70	0.72
2:H:1736:MET:HB3	2:H:1751:ILE:HD12	1.71	0.72
2:C:1737:ILE:CG1	2:C:1748:THR:HG21	2.19	0.72
2:E:1036:GLN:CB	2:E:1051:THR:CG2	2.66	0.72
2:L:1170:ILE:HG23	2:L:1174:PHE:HE2	1.55	0.72
1:B:1491:ARG:HD3	1:B:1750:ILE:HD11	1.06	0.72
2:L:1737:ILE:CG1	2:L:1748:THR:HG21	2.19	0.72
2:J:1736:MET:HB3	2:J:1751:ILE:HD12	1.71	0.72
2:G:1735:ALA:C	2:G:1736:MET:HE2	2.07	0.72
2:G:1736:MET:HB3	2:G:1751:ILE:HD12	1.71	0.72
2:C:1170:ILE:HG23	2:C:1174:PHE:HE2	1.55	0.72
2:G:1737:ILE:CG1	2:G:1748:THR:HG21	2.19	0.71
2:C:1738:PHE:HZ	2:C:1749:GLU:HG2	1.55	0.71
2:C:1736:MET:HB3	2:C:1751:ILE:HD12	1.71	0.71
2:G:839:PRO:HA	2:G:844:VAL:HG13	1.70	0.71
2:G:1738:PHE:HZ	2:G:1749:GLU:HG2	1.55	0.71
1:D:340:ARG:HH12	1:D:344:GLN:HE21	1.38	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:340:ARG:HH12	1:F:344:GLN:HE21	1.38	0.71
1:A:877:LEU:HD11	3:A:2001:NDP:H2D	1.73	0.71
1:F:1373:ARG:NH2	1:F:1550:ASP:HB2	2.06	0.71
2:H:1737:ILE:CG1	2:H:1748:THR:HG21	2.19	0.71
2:G:1170:ILE:HG23	2:G:1174:PHE:HE2	1.55	0.71
1:D:1561:MET:HA	1:D:1561:MET:HE2	1.71	0.71
2:L:1036:GLN:CB	2:L:1051:THR:CG2	2.66	0.71
2:J:1737:ILE:CG1	2:J:1748:THR:HG21	2.19	0.71
1:D:1373:ARG:NH2	1:D:1550:ASP:HB2	2.06	0.71
2:H:839:PRO:HA	2:H:844:VAL:HG13	1.70	0.71
2:H:1170:ILE:HG23	2:H:1174:PHE:HE2	1.55	0.71
2:J:836:TYR:HD1	2:J:845:THR:HG21	1.55	0.71
2:C:1036:GLN:CB	2:C:1051:THR:CG2	2.66	0.71
1:A:1373:ARG:NH2	1:A:1550:ASP:HB2	2.06	0.71
1:B:877:LEU:HD11	3:B:2001:NDP:H2D	1.73	0.70
1:D:1751:GLU:HG3	1:D:1754:LYS:HZ1	1.53	0.70
2:E:1170:ILE:HG23	2:E:1174:PHE:HE2	1.55	0.70
2:J:1170:ILE:HG23	2:J:1174:PHE:HE2	1.55	0.70
1:B:1373:ARG:NH2	1:B:1550:ASP:HB2	2.06	0.70
2:H:1738:PHE:HB2	2:H:1987:PRO:CB	2.22	0.70
2:C:836:TYR:HD1	2:C:845:THR:HG21	1.55	0.70
1:I:877:LEU:HD11	3:I:2001:NDP:H2D	1.73	0.70
1:A:340:ARG:HH12	1:A:344:GLN:HE21	1.38	0.70
2:G:1738:PHE:HB2	2:G:1987:PRO:CB	2.22	0.70
1:B:340:ARG:HH12	1:B:344:GLN:HE21	1.38	0.70
2:E:1738:PHE:HB2	2:E:1987:PRO:CB	2.22	0.70
1:K:340:ARG:HH12	1:K:344:GLN:HE21	1.38	0.70
2:L:836:TYR:HD1	2:L:845:THR:HG21	1.55	0.70
2:L:589:ARG:NH2	2:L:677:GLN:OE1	2.25	0.70
1:K:1373:ARG:NH2	1:K:1550:ASP:HB2	2.06	0.70
1:I:1373:ARG:NH2	1:I:1550:ASP:HB2	2.06	0.70
2:L:1738:PHE:HZ	2:L:1749:GLU:HG2	1.55	0.69
1:I:340:ARG:HH12	1:I:344:GLN:HE21	1.38	0.69
2:J:1738:PHE:HB2	2:J:1987:PRO:CB	2.22	0.69
2:L:838:LYS:O	2:L:844:VAL:CG1	2.41	0.69
2:G:838:LYS:O	2:G:844:VAL:CG1	2.41	0.69
2:C:1738:PHE:HB2	2:C:1987:PRO:CB	2.22	0.69
2:E:838:LYS:O	2:E:844:VAL:CG1	2.41	0.69
2:J:1736:MET:HE2	2:J:1736:MET:HA	1.73	0.69
2:G:589:ARG:NH2	2:G:677:GLN:OE1	2.25	0.69
1:D:877:LEU:HD11	3:D:2001:NDP:H2D	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:836:TYR:HD1	2:E:845:THR:HG21	1.55	0.69
1:K:877:LEU:HD11	3:K:2001:NDP:H2D	1.73	0.69
2:L:1738:PHE:HB2	2:L:1987:PRO:CB	2.22	0.69
2:J:838:LYS:O	2:J:844:VAL:CG1	2.41	0.69
2:J:1735:ALA:C	2:J:1736:MET:HE2	2.05	0.69
2:J:1738:PHE:HZ	2:J:1749:GLU:HG2	1.55	0.69
2:E:739:GLY:CA	2:E:1054:LEU:HD23	2.05	0.69
2:H:589:ARG:NH2	2:H:677:GLN:OE1	2.25	0.69
2:J:589:ARG:NH2	2:J:677:GLN:OE1	2.25	0.69
2:G:676:ILE:O	2:G:676:ILE:HG12	1.93	0.69
2:G:838:LYS:O	2:G:844:VAL:HG12	1.93	0.69
2:E:838:LYS:O	2:E:844:VAL:HG12	1.93	0.69
2:H:1738:PHE:HZ	2:H:1749:GLU:HG2	1.55	0.69
2:C:589:ARG:NH2	2:C:677:GLN:OE1	2.25	0.69
2:H:838:LYS:O	2:H:844:VAL:HG12	1.93	0.69
2:E:589:ARG:NH2	2:E:677:GLN:OE1	2.25	0.69
1:F:1751:GLU:HA	1:F:1754:LYS:CE	2.19	0.69
2:G:1736:MET:HE2	2:G:1736:MET:HA	1.76	0.68
2:J:676:ILE:O	2:J:676:ILE:HG12	1.93	0.68
2:E:1737:ILE:H	2:E:1737:ILE:CD1	2.07	0.68
2:J:838:LYS:O	2:J:844:VAL:HG12	1.93	0.68
2:G:1738:PHE:HB2	2:G:1987:PRO:HB3	1.76	0.68
2:C:838:LYS:O	2:C:844:VAL:CG1	2.41	0.68
1:K:1491:ARG:HD3	1:K:1750:ILE:HD11	1.06	0.68
2:L:1737:ILE:H	2:L:1737:ILE:CD1	2.07	0.68
1:F:877:LEU:HD11	3:F:2001:NDP:H2D	1.73	0.68
2:H:838:LYS:O	2:H:844:VAL:CG1	2.41	0.68
2:H:1170:ILE:HG23	2:H:1174:PHE:CE2	2.28	0.68
1:A:1563:HIS:ND1	1:K:1716:LEU:HD13	2.09	0.68
1:B:1716:LEU:HD13	1:I:1563:HIS:ND1	2.09	0.68
2:C:1170:ILE:HG23	2:C:1174:PHE:CE2	2.28	0.68
1:D:1716:LEU:HD13	1:F:1563:HIS:ND1	2.09	0.68
2:E:1738:PHE:HB2	2:E:1987:PRO:HB3	1.76	0.68
2:H:676:ILE:O	2:H:676:ILE:HG12	1.93	0.68
2:H:1737:ILE:H	2:H:1737:ILE:CD1	2.07	0.68
1:I:1751:GLU:HG3	1:I:1754:LYS:CE	2.24	0.68
1:A:16:GLU:HG3	2:G:2038:ILE:HD11	1.76	0.68
2:E:1170:ILE:HG23	2:E:1174:PHE:CE2	2.28	0.68
2:L:1170:ILE:HG23	2:L:1174:PHE:CE2	2.28	0.68
2:J:1170:ILE:HG23	2:J:1174:PHE:CE2	2.28	0.68
1:B:1751:GLU:HG3	1:B:1754:LYS:CE	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:817:ALA:HB1	2:E:1053:ILE:HD11	1.75	0.68
2:H:1738:PHE:HB2	2:H:1987:PRO:HB3	1.76	0.68
2:J:1738:PHE:HB2	2:J:1987:PRO:HB3	1.76	0.68
1:A:1751:GLU:HG3	1:A:1754:LYS:CE	2.24	0.68
2:C:676:ILE:O	2:C:676:ILE:HG12	1.93	0.68
2:C:1737:ILE:H	2:C:1737:ILE:CD1	2.07	0.68
1:F:16:GLU:HG3	2:H:2038:ILE:HD11	1.76	0.68
1:B:1563:HIS:ND1	1:I:1716:LEU:HD13	2.09	0.68
2:L:817:ALA:HB1	2:L:1053:ILE:HD11	1.75	0.68
1:I:1751:GLU:HA	1:I:1754:LYS:CE	2.19	0.68
3:B:2001:NDP:H51N	3:B:2001:NDP:H2N	1.77	0.67
1:D:1563:HIS:ND1	1:F:1716:LEU:HD13	2.09	0.67
1:D:1751:GLU:HA	1:D:1754:LYS:CE	2.19	0.67
2:E:676:ILE:O	2:E:676:ILE:HG12	1.93	0.67
1:F:1373:ARG:HD2	1:F:1550:ASP:OD2	1.94	0.67
2:H:817:ALA:HB1	2:H:1053:ILE:HD11	1.75	0.67
2:G:817:ALA:HB1	2:G:1053:ILE:HD11	1.75	0.67
2:C:838:LYS:O	2:C:844:VAL:HG12	1.93	0.67
2:E:1738:PHE:HZ	2:E:1749:GLU:HG2	1.55	0.67
2:L:1738:PHE:HB2	2:L:1987:PRO:HB3	1.76	0.67
3:A:2001:NDP:H2N	3:A:2001:NDP:H51N	1.77	0.67
2:C:1738:PHE:HB2	2:C:1987:PRO:HB3	1.76	0.67
1:I:16:GLU:HG3	2:J:2038:ILE:HD11	1.76	0.67
2:G:1737:ILE:H	2:G:1737:ILE:CD1	2.07	0.67
3:K:2001:NDP:H2N	3:K:2001:NDP:H51N	1.77	0.67
2:L:1742:VAL:HB	2:L:1745:LYS:HB2	1.77	0.67
1:K:1751:GLU:HG3	1:K:1754:LYS:CE	2.24	0.67
2:L:676:ILE:HG12	2:L:676:ILE:O	1.93	0.67
3:I:2001:NDP:H2N	3:I:2001:NDP:H51N	1.77	0.67
1:A:1716:LEU:HD13	1:K:1563:HIS:ND1	2.09	0.67
2:G:1170:ILE:HG23	2:G:1174:PHE:CE2	2.28	0.67
2:C:817:ALA:HB1	2:C:1053:ILE:HD11	1.75	0.67
3:D:2001:NDP:H2N	3:D:2001:NDP:H51N	1.77	0.67
1:K:16:GLU:HG3	2:L:2038:ILE:HD11	1.76	0.67
1:F:1751:GLU:HG3	1:F:1754:LYS:CE	2.24	0.67
1:I:1373:ARG:HD2	1:I:1550:ASP:OD2	1.94	0.67
2:C:1742:VAL:HB	2:C:1745:LYS:HB2	1.76	0.67
2:L:739:GLY:CA	2:L:1054:LEU:HD23	2.05	0.67
2:L:838:LYS:O	2:L:844:VAL:HG12	1.93	0.67
2:L:1036:GLN:HB2	2:L:1051:THR:CG2	2.26	0.67
3:F:2001:NDP:H2N	3:F:2001:NDP:H51N	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1742:VAL:O	2:C:1745:LYS:N	2.29	0.66
2:E:1742:VAL:O	2:E:1745:LYS:N	2.29	0.66
2:H:124:LYS:HG2	2:H:179:THR:HA	1.77	0.66
2:G:124:LYS:HG2	2:G:179:THR:HA	1.77	0.66
2:G:1036:GLN:HB2	2:G:1051:THR:CG2	2.26	0.66
2:J:1737:ILE:H	2:J:1737:ILE:CD1	2.07	0.66
1:B:1373:ARG:HD2	1:B:1550:ASP:OD2	1.94	0.66
2:J:1036:GLN:HB2	2:J:1051:THR:CG2	2.25	0.66
2:C:124:LYS:HG2	2:C:179:THR:HA	1.77	0.66
1:D:1751:GLU:HG3	1:D:1754:LYS:CE	2.24	0.66
1:K:1373:ARG:HD2	1:K:1550:ASP:OD2	1.94	0.66
2:J:817:ALA:HB1	2:J:1053:ILE:HD11	1.75	0.66
1:D:16:GLU:HG3	2:E:2038:ILE:HD11	1.76	0.66
1:D:1373:ARG:HD2	1:D:1550:ASP:OD2	1.94	0.66
2:L:234:ILE:HG23	2:L:238:CYS:HG	1.56	0.66
2:H:1742:VAL:HB	2:H:1745:LYS:HB2	1.76	0.66
1:A:1373:ARG:HD2	1:A:1550:ASP:OD2	1.94	0.66
2:L:124:LYS:HG2	2:L:179:THR:HA	1.77	0.66
2:E:1036:GLN:HB2	2:E:1051:THR:CG2	2.25	0.66
2:J:1742:VAL:O	2:J:1745:LYS:N	2.29	0.66
2:G:1742:VAL:O	2:G:1745:LYS:N	2.29	0.66
2:E:124:LYS:HG2	2:E:179:THR:HA	1.77	0.66
2:G:1742:VAL:HB	2:G:1745:LYS:HB2	1.77	0.66
2:C:1736:MET:HE2	2:C:1736:MET:HA	1.77	0.65
1:K:32:GLN:HE22	1:K:57:ALA:HA	1.61	0.65
2:E:1742:VAL:HB	2:E:1745:LYS:HB2	1.76	0.65
2:L:1742:VAL:O	2:L:1745:LYS:N	2.29	0.65
1:F:1751:GLU:HG3	1:F:1754:LYS:HZ1	1.57	0.65
2:J:1742:VAL:HB	2:J:1745:LYS:HB2	1.76	0.65
1:K:1751:GLU:HA	1:K:1754:LYS:CE	2.19	0.65
2:H:836:TYR:HD1	2:H:845:THR:HG21	1.55	0.65
2:H:1742:VAL:O	2:H:1745:LYS:N	2.29	0.65
2:J:124:LYS:HG2	2:J:179:THR:HA	1.77	0.65
1:B:16:GLU:HG3	2:C:2038:ILE:HD11	1.76	0.65
2:C:1036:GLN:HB2	2:C:1051:THR:CG2	2.25	0.65
2:E:7:ARG:NH2	2:E:24:THR:O	2.30	0.65
1:D:1491:ARG:HD3	1:D:1750:ILE:HD11	1.06	0.65
1:A:1541:PHE:CE1	1:A:1557:ILE:HG13	2.31	0.65
1:F:1541:PHE:CE1	1:F:1557:ILE:HG13	2.31	0.65
1:B:987:ASN:HD21	2:C:993:GLN:HE22	1.45	0.65
1:D:32:GLN:HE22	1:D:57:ALA:HA	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1036:GLN:HB2	2:H:1051:THR:CG2	2.25	0.65
2:H:1736:MET:HE2	2:H:1736:MET:HA	1.79	0.65
2:J:7:ARG:NH2	2:J:24:THR:O	2.30	0.65
1:A:1542:HIS:HB3	1:A:1553:GLU:OE1	1.97	0.65
1:B:32:GLN:HE22	1:B:57:ALA:HA	1.61	0.65
1:A:1751:GLU:HA	1:A:1754:LYS:CE	2.19	0.65
1:D:1542:HIS:HB3	1:D:1553:GLU:OE1	1.97	0.65
1:F:32:GLN:HE22	1:F:57:ALA:HA	1.61	0.65
1:F:1552:ASN:O	1:F:1556:THR:HG22	1.97	0.65
1:B:1552:ASN:O	1:B:1556:THR:HG22	1.97	0.65
1:F:1542:HIS:HB3	1:F:1553:GLU:OE1	1.97	0.65
1:I:987:ASN:HD21	2:J:993:GLN:HE22	1.45	0.65
1:A:1552:ASN:O	1:A:1556:THR:HG22	1.97	0.64
2:L:7:ARG:NH2	2:L:24:THR:O	2.30	0.64
2:H:7:ARG:NH2	2:H:24:THR:O	2.30	0.64
2:C:1174:PHE:HE1	2:C:1197:LEU:HB2	1.63	0.64
2:H:1036:GLN:HB2	2:H:1051:THR:HG23	1.80	0.64
2:H:1735:ALA:C	2:H:1736:MET:HE2	2.11	0.64
1:I:1542:HIS:HB3	1:I:1553:GLU:OE1	1.97	0.64
2:J:1174:PHE:HE1	2:J:1197:LEU:HB2	1.63	0.64
2:G:7:ARG:NH2	2:G:24:THR:O	2.30	0.64
1:K:987:ASN:HD21	2:L:993:GLN:HE22	1.45	0.64
2:L:1174:PHE:HE1	2:L:1197:LEU:HB2	1.63	0.64
2:L:1736:MET:HE2	2:L:1736:MET:HA	1.79	0.64
1:I:32:GLN:HE22	1:I:57:ALA:HA	1.61	0.64
1:K:1552:ASN:O	1:K:1556:THR:HG22	1.97	0.64
2:J:1037:SER:OG	2:J:1053:ILE:HG12	1.98	0.64
2:C:7:ARG:NH2	2:C:24:THR:O	2.30	0.64
1:D:1541:PHE:CE1	1:D:1557:ILE:HG13	2.31	0.64
2:G:739:GLY:CA	2:G:1054:LEU:HD23	2.05	0.64
1:B:1542:HIS:HB3	1:B:1553:GLU:OE1	1.97	0.64
2:E:1174:PHE:HE1	2:E:1197:LEU:HB2	1.63	0.64
2:J:647:PHE:O	2:J:677:GLN:N	2.31	0.64
1:A:32:GLN:HE22	1:A:57:ALA:HA	1.61	0.64
2:G:647:PHE:O	2:G:677:GLN:N	2.31	0.64
2:E:1036:GLN:HB2	2:E:1051:THR:HG23	1.80	0.64
2:H:647:PHE:O	2:H:677:GLN:N	2.31	0.64
2:H:848:SER:HB3	2:H:854:ILE:CD1	2.28	0.64
2:H:1747:LYS:HG3	2:H:1747:LYS:O	1.98	0.64
2:J:739:GLY:CA	2:J:1054:LEU:HD23	2.05	0.64
1:A:987:ASN:HD21	2:G:993:GLN:HE22	1.45	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:848:SER:HB3	2:E:854:ILE:CD1	2.28	0.64
1:I:1541:PHE:CE1	1:I:1557:ILE:HG13	2.31	0.64
1:D:1552:ASN:O	1:D:1556:THR:HG22	1.97	0.64
2:E:647:PHE:O	2:E:677:GLN:N	2.31	0.64
1:F:1491:ARG:HD3	1:F:1750:ILE:HD11	1.06	0.64
1:A:844:LEU:HG	1:F:844:LEU:HG	1.80	0.63
2:G:848:SER:HB3	2:G:854:ILE:CD1	2.28	0.63
2:C:1037:SER:OG	2:C:1053:ILE:HG12	1.98	0.63
2:E:1747:LYS:HG3	2:E:1747:LYS:O	1.98	0.63
2:G:836:TYR:HD1	2:G:845:THR:CG2	2.10	0.63
2:G:1174:PHE:HE1	2:G:1197:LEU:HB2	1.63	0.63
2:E:1037:SER:OG	2:E:1053:ILE:HG12	1.98	0.63
2:H:1737:ILE:CG1	2:H:1748:THR:CG2	2.76	0.63
1:K:687:SER:HB2	3:K:2001:NDP:O1N	1.99	0.63
1:A:1491:ARG:CA	1:A:1750:ILE:HD13	2.29	0.63
2:G:1747:LYS:HG3	2:G:1747:LYS:O	1.98	0.63
2:C:647:PHE:O	2:C:677:GLN:N	2.31	0.63
2:E:1737:ILE:CG1	2:E:1748:THR:CG2	2.76	0.63
2:L:848:SER:HB3	2:L:854:ILE:CD1	2.28	0.63
2:C:739:GLY:CA	2:C:1054:LEU:HD23	2.05	0.63
2:C:1747:LYS:HG3	2:C:1747:LYS:O	1.98	0.63
2:E:1742:VAL:O	2:E:1744:GLY:N	2.32	0.63
1:K:1542:HIS:HB3	1:K:1553:GLU:OE1	1.97	0.63
1:B:1751:GLU:HA	1:B:1754:LYS:CE	2.19	0.63
2:C:848:SER:HB3	2:C:854:ILE:CD1	2.28	0.63
1:I:687:SER:HB2	3:I:2001:NDP:O1N	1.99	0.63
1:I:1552:ASN:O	1:I:1556:THR:HG22	1.97	0.63
2:J:1747:LYS:HG3	2:J:1747:LYS:O	1.98	0.63
2:G:1742:VAL:O	2:G:1744:GLY:N	2.32	0.63
1:D:1685:TYR:OH	2:E:993:GLN:NE2	2.32	0.63
2:E:1736:MET:HE2	2:E:1736:MET:HA	1.81	0.63
2:E:1739:GLU:CB	2:E:1746:LEU:HD11	2.27	0.63
2:L:1037:SER:OG	2:L:1053:ILE:HG12	1.98	0.63
2:H:1174:PHE:HE1	2:H:1197:LEU:HB2	1.63	0.63
2:J:848:SER:HB3	2:J:854:ILE:CD1	2.28	0.63
2:J:1742:VAL:O	2:J:1744:GLY:N	2.32	0.63
1:A:32:GLN:HE21	1:A:57:ALA:HB2	1.64	0.63
1:A:1751:GLU:HG3	1:A:1754:LYS:HZ1	1.59	0.63
1:K:1541:PHE:CE1	1:K:1557:ILE:HG13	2.31	0.63
2:H:1742:VAL:O	2:H:1744:GLY:N	2.32	0.63
2:G:1037:SER:HB2	2:G:1053:ILE:HG12	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1037:SER:OG	2:G:1053:ILE:HG12	1.98	0.62
1:D:844:LEU:HG	1:I:844:LEU:HG	1.80	0.62
2:L:647:PHE:O	2:L:677:GLN:N	2.31	0.62
1:F:987:ASN:HD21	2:H:993:GLN:HE22	1.45	0.62
1:A:687:SER:HB2	3:A:2001:NDP:O1N	1.99	0.62
2:H:1037:SER:OG	2:H:1053:ILE:HG12	1.98	0.62
2:H:1739:GLU:CB	2:H:1746:LEU:HD11	2.27	0.62
2:G:817:ALA:HB1	2:G:1053:ILE:CD1	2.29	0.62
2:C:1737:ILE:CG1	2:C:1748:THR:CG2	2.76	0.62
2:C:1742:VAL:O	2:C:1744:GLY:N	2.32	0.62
1:D:987:ASN:HD21	2:E:993:GLN:HE22	1.45	0.62
1:K:32:GLN:HE21	1:K:57:ALA:HB2	1.64	0.62
2:L:1737:ILE:CG1	2:L:1748:THR:CG2	2.76	0.62
2:L:1739:GLU:CB	2:L:1746:LEU:HD11	2.27	0.62
2:E:817:ALA:HB1	2:E:1053:ILE:CD1	2.30	0.62
2:E:1037:SER:HB2	2:E:1053:ILE:HG12	1.81	0.62
2:L:1747:LYS:O	2:L:1747:LYS:HG3	1.98	0.62
1:I:32:GLN:HE21	1:I:57:ALA:HB2	1.64	0.62
2:G:1737:ILE:CG1	2:G:1748:THR:CG2	2.76	0.62
1:B:32:GLN:HE21	1:B:57:ALA:HB2	1.64	0.62
2:C:836:TYR:HD1	2:C:845:THR:CG2	2.10	0.62
1:D:32:GLN:HE21	1:D:57:ALA:HB2	1.64	0.62
1:D:687:SER:HB2	3:D:2001:NDP:O1N	1.99	0.62
1:K:1751:GLU:O	1:K:1754:LYS:HG2	2.00	0.62
2:L:1742:VAL:O	2:L:1744:GLY:N	2.32	0.62
2:H:1037:SER:HB2	2:H:1053:ILE:HG12	1.81	0.62
1:B:687:SER:HB2	3:B:2001:NDP:O1N	1.99	0.62
2:C:1576:PRO:HD2	2:C:1579:ILE:HD11	1.82	0.62
1:F:28:TRP:HA	1:F:31:THR:HB	1.82	0.62
2:J:1037:SER:HB2	2:J:1053:ILE:HG12	1.81	0.62
1:A:28:TRP:HA	1:A:31:THR:HB	1.82	0.62
1:B:844:LEU:HG	1:K:844:LEU:HG	1.80	0.62
1:B:1751:GLU:O	1:B:1754:LYS:HG2	2.00	0.62
1:D:1229:THR:OG1	1:D:1687:PHE:CD1	2.53	0.62
1:K:1685:TYR:OH	2:L:993:GLN:NE2	2.32	0.62
2:L:1036:GLN:HB2	2:L:1051:THR:HG23	1.80	0.62
2:J:817:ALA:HB1	2:J:1053:ILE:CD1	2.30	0.62
1:B:1229:THR:OG1	1:B:1687:PHE:CD1	2.53	0.62
2:E:836:TYR:HD1	2:E:845:THR:CG2	2.10	0.62
1:K:1301:PRO:HG3	1:K:1314:ILE:HD12	1.82	0.62
1:F:32:GLN:HE21	1:F:57:ALA:HB2	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1685:TYR:OH	2:H:993:GLN:NE2	2.32	0.62
2:G:1156:CYS:O	2:G:1168:ASN:ND2	2.33	0.62
1:B:1301:PRO:HG3	1:B:1314:ILE:HD12	1.82	0.62
1:B:1685:TYR:OH	2:C:993:GLN:NE2	2.32	0.62
2:E:1156:CYS:O	2:E:1168:ASN:ND2	2.33	0.62
2:L:1576:PRO:HD2	2:L:1579:ILE:HD11	1.82	0.62
2:H:817:ALA:HB1	2:H:1053:ILE:CD1	2.29	0.62
2:J:1737:ILE:CG1	2:J:1748:THR:CG2	2.76	0.62
1:B:1541:PHE:CE1	1:B:1557:ILE:HG13	2.31	0.61
2:C:1739:GLU:CB	2:C:1746:LEU:HD11	2.27	0.61
2:C:1036:GLN:HB2	2:C:1051:THR:HG23	1.80	0.61
1:D:1751:GLU:O	1:D:1754:LYS:HG2	2.00	0.61
2:L:1037:SER:HB2	2:L:1053:ILE:HG12	1.81	0.61
1:I:1751:GLU:O	1:I:1754:LYS:HG2	2.00	0.61
2:L:817:ALA:HB1	2:L:1053:ILE:CD1	2.29	0.61
2:L:1735:ALA:C	2:L:1736:MET:HE2	2.11	0.61
2:H:1156:CYS:O	2:H:1168:ASN:ND2	2.33	0.61
1:I:1685:TYR:OH	2:J:993:GLN:NE2	2.32	0.61
2:C:817:ALA:HB1	2:C:1053:ILE:CD1	2.29	0.61
2:E:1889:VAL:HG13	2:E:1977:HIS:HB2	1.82	0.61
1:F:687:SER:HB2	3:F:2001:NDP:O1N	1.99	0.61
1:F:1491:ARG:CA	1:F:1750:ILE:HD13	2.29	0.61
2:H:836:TYR:HD1	2:H:845:THR:CG2	2.10	0.61
1:A:1751:GLU:O	1:A:1754:LYS:HG2	2.00	0.61
1:F:1751:GLU:O	1:F:1754:LYS:HG2	2.00	0.61
2:J:836:TYR:HD1	2:J:845:THR:CG2	2.10	0.61
2:J:1576:PRO:HD2	2:J:1579:ILE:HD11	1.82	0.61
1:A:1229:THR:OG1	1:A:1687:PHE:CD1	2.53	0.61
2:C:1156:CYS:O	2:C:1168:ASN:ND2	2.33	0.61
1:D:1301:PRO:HG3	1:D:1314:ILE:HD12	1.82	0.61
1:A:1685:TYR:OH	2:G:993:GLN:NE2	2.32	0.61
1:B:442:ARG:NH1	1:B:726:GLY:O	2.34	0.61
1:D:1682:LYS:HE2	2:E:992:GLU:O	2.01	0.61
1:K:1229:THR:OG1	1:K:1687:PHE:CD1	2.53	0.61
2:H:1576:PRO:HD2	2:H:1579:ILE:HD11	1.82	0.61
1:A:1301:PRO:HG3	1:A:1314:ILE:HD12	1.82	0.61
2:G:1889:VAL:HG13	2:G:1977:HIS:HB2	1.82	0.61
1:I:28:TRP:HA	1:I:31:THR:HB	1.82	0.61
1:D:28:TRP:HA	1:D:31:THR:HB	1.82	0.60
2:E:1735:ALA:C	2:E:1736:MET:HE2	2.14	0.60
2:L:1889:VAL:HG13	2:L:1977:HIS:HB2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1301:PRO:HG3	1:F:1314:ILE:HD12	1.82	0.60
1:F:1682:LYS:HE2	2:H:992:GLU:O	2.01	0.60
2:G:1739:GLU:CB	2:G:1746:LEU:HD11	2.27	0.60
1:B:28:TRP:HA	1:B:31:THR:HB	1.82	0.60
1:K:1682:LYS:HE2	2:L:992:GLU:O	2.01	0.60
1:I:442:ARG:NH1	1:I:726:GLY:O	2.34	0.60
2:J:1156:CYS:O	2:J:1168:ASN:ND2	2.33	0.60
2:G:1576:PRO:HD2	2:G:1579:ILE:HD11	1.82	0.60
1:B:1491:ARG:CA	1:B:1750:ILE:HD13	2.29	0.60
2:C:1037:SER:HB2	2:C:1053:ILE:HG12	1.81	0.60
1:K:442:ARG:NH1	1:K:726:GLY:O	2.34	0.60
2:L:1156:CYS:O	2:L:1168:ASN:ND2	2.33	0.60
1:I:1301:PRO:HG3	1:I:1314:ILE:HD12	1.82	0.60
2:E:1736:MET:HE3	2:E:1736:MET:N	2.16	0.60
1:K:28:TRP:HA	1:K:31:THR:HB	1.82	0.60
1:I:1682:LYS:HE2	2:J:992:GLU:O	2.01	0.60
2:J:1036:GLN:HB2	2:J:1051:THR:HG23	1.80	0.60
1:A:442:ARG:NH1	1:A:726:GLY:O	2.34	0.60
1:B:1323:LYS:NZ	1:I:1313:ASP:OD1	2.35	0.60
1:K:1491:ARG:CA	1:K:1750:ILE:HD13	2.29	0.60
2:J:1889:VAL:HG13	2:J:1977:HIS:HB2	1.82	0.60
1:B:1749:THR:HB	1:B:1874:ASP:HB3	1.83	0.60
1:F:442:ARG:NH1	1:F:726:GLY:O	2.34	0.60
2:H:1350:LEU:HD11	2:H:1410:PHE:HB3	1.84	0.60
1:I:1749:THR:HB	1:I:1874:ASP:HB3	1.83	0.60
1:A:1313:ASP:OD1	1:K:1323:LYS:NZ	2.35	0.60
1:B:1682:LYS:HE2	2:C:992:GLU:O	2.01	0.60
1:D:442:ARG:NH1	1:D:726:GLY:O	2.34	0.60
2:E:1576:PRO:HD2	2:E:1579:ILE:HD11	1.82	0.60
2:L:584:SER:HB3	2:L:591:PRO:HG3	1.84	0.60
1:A:1487:LEU:HA	1:A:1754:LYS:HD3	1.84	0.60
2:C:1123:ASP:OD1	2:C:1188:ASN:ND2	2.35	0.60
1:I:1487:LEU:HA	1:I:1754:LYS:HD3	1.84	0.60
1:A:479:ASN:ND2	1:A:613:VAL:O	2.35	0.60
2:G:584:SER:HB3	2:G:591:PRO:HG3	1.84	0.60
1:B:1313:ASP:OD1	1:I:1323:LYS:NZ	2.35	0.60
2:C:295:SER:O	2:C:298:LYS:N	2.35	0.60
1:D:1313:ASP:OD1	1:F:1323:LYS:NZ	2.35	0.60
1:D:1487:LEU:HA	1:D:1754:LYS:HD3	1.84	0.60
1:K:479:ASN:ND2	1:K:613:VAL:O	2.35	0.60
1:F:1229:THR:OG1	1:F:1687:PHE:CD1	2.53	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1889:VAL:HG13	2:H:1977:HIS:HB2	1.82	0.60
1:A:1305:CYS:HB2	1:A:1645:GLY:HA2	1.84	0.60
1:B:1487:LEU:HA	1:B:1754:LYS:HD3	1.84	0.60
2:C:584:SER:HB3	2:C:591:PRO:HG3	1.84	0.60
1:D:1323:LYS:NZ	1:F:1313:ASP:OD1	2.35	0.60
1:D:1491:ARG:CA	1:D:1750:ILE:HD13	2.29	0.60
2:L:1741:ILE:O	2:L:1741:ILE:HG22	2.02	0.60
1:F:479:ASN:ND2	1:F:613:VAL:O	2.35	0.60
1:I:982:ILE:HG23	2:J:956:GLU:HG2	1.84	0.60
1:I:1229:THR:OG1	1:I:1687:PHE:CD1	2.53	0.60
2:J:1123:ASP:OD1	2:J:1188:ASN:ND2	2.35	0.60
1:B:479:ASN:ND2	1:B:613:VAL:O	2.35	0.59
2:C:1475:LYS:HB2	2:C:1481:SER:HB2	1.84	0.59
2:J:584:SER:HB3	2:J:591:PRO:HG3	1.84	0.59
1:A:1682:LYS:HE2	2:G:992:GLU:O	2.01	0.59
2:C:1889:VAL:HG13	2:C:1977:HIS:HB2	1.82	0.59
2:E:584:SER:HB3	2:E:591:PRO:HG3	1.84	0.59
2:J:1739:GLU:CB	2:J:1746:LEU:HD11	2.27	0.59
1:A:1323:LYS:NZ	1:K:1313:ASP:OD1	2.35	0.59
2:G:1741:ILE:O	2:G:1741:ILE:HG22	2.02	0.59
2:C:1741:ILE:O	2:C:1741:ILE:HG22	2.02	0.59
1:K:1749:THR:HB	1:K:1874:ASP:HB3	1.83	0.59
1:A:1749:THR:HB	1:A:1874:ASP:HB3	1.83	0.59
2:G:1350:LEU:HD11	2:G:1410:PHE:HB3	1.84	0.59
1:F:1305:CYS:HB2	1:F:1645:GLY:HA2	1.84	0.59
2:H:584:SER:HB3	2:H:591:PRO:HG3	1.84	0.59
2:H:1741:ILE:HG22	2:H:1741:ILE:O	2.02	0.59
2:J:1741:ILE:HG22	2:J:1741:ILE:O	2.02	0.59
1:B:894:ARG:NH1	1:B:895:THR:O	2.36	0.59
1:D:27:ARG:HH11	2:E:2015:THR:HA	1.68	0.59
1:D:894:ARG:NH1	1:D:895:THR:O	2.36	0.59
2:E:1350:LEU:HD11	2:E:1410:PHE:HB3	1.84	0.59
2:E:1741:ILE:HG22	2:E:1741:ILE:O	2.02	0.59
2:L:836:TYR:HD1	2:L:845:THR:CG2	2.10	0.59
1:I:479:ASN:ND2	1:I:613:VAL:O	2.35	0.59
1:I:894:ARG:NH1	1:I:895:THR:O	2.36	0.59
1:I:1305:CYS:HB2	1:I:1645:GLY:HA2	1.84	0.59
2:G:295:SER:O	2:G:298:LYS:N	2.35	0.59
1:B:1305:CYS:HB2	1:B:1645:GLY:HA2	1.84	0.59
2:J:295:SER:O	2:J:298:LYS:N	2.35	0.59
2:J:1475:LYS:HB2	2:J:1481:SER:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:VAL:HG21	1:A:266:LEU:HB3	1.85	0.59
1:A:982:ILE:HG23	2:G:956:GLU:HG2	1.84	0.59
1:D:479:ASN:ND2	1:D:613:VAL:O	2.35	0.59
1:D:1749:THR:HB	1:D:1874:ASP:HB3	1.83	0.59
2:L:1475:LYS:HB2	2:L:1481:SER:HB2	1.84	0.59
1:A:894:ARG:NH1	1:A:895:THR:O	2.36	0.59
2:C:1350:LEU:HD11	2:C:1410:PHE:HB3	1.84	0.59
1:K:894:ARG:NH1	1:K:895:THR:O	2.36	0.59
2:L:1123:ASP:OD1	2:L:1188:ASN:ND2	2.35	0.59
2:H:835:THR:HG22	2:H:844:VAL:HA	1.85	0.59
2:G:670:ARG:HG2	2:G:699:GLY:H	1.68	0.59
2:C:326:ASP:O	2:C:330:ASN:ND2	2.36	0.59
2:L:1350:LEU:HD11	2:L:1410:PHE:HB3	1.84	0.59
1:D:153:VAL:HG21	1:D:266:LEU:HB3	1.85	0.59
1:D:1487:LEU:HG	1:D:1754:LYS:HE2	1.84	0.59
1:K:982:ILE:HG23	2:L:956:GLU:HG2	1.84	0.59
1:K:1487:LEU:HG	1:K:1754:LYS:HE2	1.84	0.59
2:L:670:ARG:HG2	2:L:699:GLY:H	1.68	0.59
2:H:295:SER:O	2:H:298:LYS:N	2.35	0.59
2:G:1123:ASP:OD1	2:G:1188:ASN:ND2	2.35	0.58
2:C:670:ARG:HG2	2:C:699:GLY:H	1.68	0.58
1:K:153:VAL:HG21	1:K:266:LEU:HB3	1.85	0.58
1:F:1487:LEU:HA	1:F:1754:LYS:HD3	1.84	0.58
2:H:326:ASP:O	2:H:330:ASN:ND2	2.36	0.58
2:J:835:THR:HG22	2:J:844:VAL:HA	1.85	0.58
1:B:36:LEU:O	1:B:76:ARG:NH2	2.36	0.58
2:L:326:ASP:O	2:L:330:ASN:ND2	2.36	0.58
2:C:835:THR:HG22	2:C:844:VAL:HA	1.85	0.58
1:F:894:ARG:NH1	1:F:895:THR:O	2.36	0.58
1:F:1195:ALA:HB1	1:F:1200:ILE:HD12	1.85	0.58
2:H:261:GLY:N	2:H:287:ASP:O	2.37	0.58
2:G:1786:LYS:NZ	2:G:1816:ALA:O	2.35	0.58
1:B:982:ILE:HG23	2:C:956:GLU:HG2	1.84	0.58
1:D:1413:LYS:NZ	1:F:1708:ASP:OD1	2.37	0.58
1:K:1487:LEU:HA	1:K:1754:LYS:HD3	1.84	0.58
2:L:1786:LYS:NZ	2:L:1816:ALA:O	2.35	0.58
1:F:1749:THR:HB	1:F:1874:ASP:HB3	1.83	0.58
2:H:1123:ASP:OD1	2:H:1188:ASN:ND2	2.35	0.58
2:H:1475:LYS:HB2	2:H:1481:SER:HB2	1.84	0.58
1:I:27:ARG:HH11	2:J:2015:THR:HA	1.68	0.58
1:A:27:ARG:HH11	2:G:2015:THR:HA	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1475:LYS:HB2	2:G:1481:SER:HB2	1.84	0.58
1:B:1487:LEU:HG	1:B:1754:LYS:HE2	1.84	0.58
1:D:982:ILE:HG23	2:E:956:GLU:HG2	1.84	0.58
1:D:1708:ASP:OD1	1:F:1413:LYS:NZ	2.37	0.58
2:L:261:GLY:N	2:L:287:ASP:O	2.37	0.58
2:J:864:LEU:HD23	2:J:899:PHE:HB2	1.86	0.58
1:B:27:ARG:HH11	2:C:2015:THR:HA	1.68	0.58
2:C:836:TYR:CE1	2:C:845:THR:HG21	2.37	0.58
2:C:864:LEU:HD23	2:C:899:PHE:HB2	1.86	0.58
2:E:1123:ASP:OD1	2:E:1188:ASN:ND2	2.35	0.58
2:L:864:LEU:HD23	2:L:899:PHE:HB2	1.86	0.58
2:H:670:ARG:HG2	2:H:699:GLY:H	1.68	0.58
1:I:153:VAL:HG21	1:I:266:LEU:HB3	1.85	0.58
2:G:261:GLY:N	2:G:287:ASP:O	2.37	0.58
2:G:326:ASP:O	2:G:330:ASN:ND2	2.36	0.58
2:G:836:TYR:CE1	2:G:845:THR:HG21	2.37	0.58
2:E:835:THR:HG22	2:E:844:VAL:HA	1.85	0.58
1:K:27:ARG:HH11	2:L:2015:THR:HA	1.68	0.58
1:F:982:ILE:HG23	2:H:956:GLU:HG2	1.84	0.58
2:H:1742:VAL:O	2:H:1743:ASP:C	2.42	0.58
1:I:1491:ARG:CA	1:I:1750:ILE:HD13	2.29	0.58
1:I:1749:THR:HB	1:I:1874:ASP:CG	2.24	0.58
1:A:1413:LYS:NZ	1:K:1708:ASP:OD1	2.37	0.58
1:A:1487:LEU:HG	1:A:1754:LYS:HE2	1.84	0.58
1:A:1749:THR:HB	1:A:1874:ASP:CG	2.24	0.58
2:G:864:LEU:HD23	2:G:899:PHE:HB2	1.86	0.58
2:G:1737:ILE:HD13	2:G:1737:ILE:O	2.04	0.58
1:B:1413:LYS:NZ	1:I:1708:ASP:OD1	2.37	0.58
1:D:260:ARG:HH12	1:D:300:VAL:HG21	1.69	0.58
1:K:260:ARG:HH12	1:K:300:VAL:HG21	1.69	0.58
1:K:1305:CYS:HB2	1:K:1645:GLY:HA2	1.84	0.58
2:L:1736:MET:HE3	2:L:1736:MET:N	2.18	0.58
1:F:27:ARG:HH11	2:H:2015:THR:HA	1.68	0.58
1:F:260:ARG:HH12	1:F:300:VAL:HG21	1.69	0.58
1:F:1487:LEU:HG	1:F:1754:LYS:HE2	1.84	0.58
2:J:1350:LEU:HD11	2:J:1410:PHE:HB3	1.84	0.58
1:A:1708:ASP:OD1	1:K:1413:LYS:NZ	2.37	0.58
1:D:202:GLU:HG2	1:D:203:GLU:HG3	1.86	0.58
2:E:295:SER:O	2:E:298:LYS:N	2.35	0.58
2:E:864:LEU:HD23	2:E:899:PHE:HB2	1.86	0.58
2:L:295:SER:O	2:L:298:LYS:N	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1036:GLN:HB3	2:G:1051:THR:CG2	2.24	0.58
2:E:326:ASP:O	2:E:330:ASN:ND2	2.36	0.58
2:E:670:ARG:HG2	2:E:699:GLY:H	1.68	0.58
2:E:1475:LYS:HB2	2:E:1481:SER:HB2	1.84	0.58
1:K:1195:ALA:HB1	1:K:1200:ILE:HD12	1.85	0.58
1:F:153:VAL:HG21	1:F:266:LEU:HB3	1.85	0.58
1:F:202:GLU:HG2	1:F:203:GLU:HG3	1.86	0.58
1:I:838:MET:CA	1:I:841:GLU:OE1	2.52	0.58
2:C:261:GLY:N	2:C:287:ASP:O	2.37	0.57
2:E:261:GLY:N	2:E:287:ASP:O	2.37	0.57
2:E:1786:LYS:NZ	2:E:1816:ALA:O	2.35	0.57
1:F:36:LEU:O	1:F:76:ARG:NH2	2.36	0.57
2:H:864:LEU:HD23	2:H:899:PHE:HB2	1.86	0.57
1:I:1487:LEU:HG	1:I:1754:LYS:HE2	1.84	0.57
1:A:260:ARG:HH12	1:A:300:VAL:HG21	1.69	0.57
2:G:1590:ARG:NH1	2:G:1594:GLU:OE1	2.38	0.57
1:B:153:VAL:HG21	1:B:266:LEU:HB3	1.85	0.57
1:B:1195:ALA:HB1	1:B:1200:ILE:HD12	1.85	0.57
1:B:1533:ILE:O	1:B:1566:ARG:NH1	2.37	0.57
1:D:1305:CYS:HB2	1:D:1645:GLY:HA2	1.84	0.57
2:E:1742:VAL:O	2:E:1743:ASP:C	2.42	0.57
1:F:1749:THR:HB	1:F:1874:ASP:CG	2.24	0.57
2:H:1036:GLN:HB3	2:H:1051:THR:CG2	2.24	0.57
1:A:202:GLU:HG2	1:A:203:GLU:HG3	1.86	0.57
2:J:261:GLY:N	2:J:287:ASP:O	2.37	0.57
2:J:1590:ARG:NH1	2:J:1594:GLU:OE1	2.38	0.57
1:A:1195:ALA:HB1	1:A:1200:ILE:HD12	1.85	0.57
2:G:835:THR:HG22	2:G:844:VAL:HA	1.85	0.57
1:B:1708:ASP:OD1	1:I:1413:LYS:NZ	2.37	0.57
1:D:32:GLN:NE2	1:D:57:ALA:HB2	2.19	0.57
2:H:1590:ARG:NH1	2:H:1594:GLU:OE1	2.37	0.57
2:J:1737:ILE:HD13	2:J:1737:ILE:O	2.04	0.57
2:J:1786:LYS:NZ	2:J:1816:ALA:O	2.35	0.57
2:G:1742:VAL:O	2:G:1743:ASP:C	2.42	0.57
1:D:36:LEU:O	1:D:76:ARG:NH2	2.36	0.57
2:E:1737:ILE:HD13	2:E:1737:ILE:O	2.04	0.57
1:K:1533:ILE:O	1:K:1566:ARG:NH1	2.37	0.57
1:F:32:GLN:NE2	1:F:57:ALA:HB2	2.19	0.57
2:H:190:PHE:HZ	2:H:297:ARG:HD2	1.69	0.57
2:J:326:ASP:O	2:J:330:ASN:ND2	2.36	0.57
1:D:1019:ILE:HG13	1:D:1316:VAL:HG13	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1195:ALA:HB1	1:D:1200:ILE:HD12	1.85	0.57
1:D:1749:THR:HB	1:D:1874:ASP:CG	2.24	0.57
2:L:1351:VAL:HG21	2:L:1413:ARG:HH21	1.70	0.57
1:I:260:ARG:HH12	1:I:300:VAL:HG21	1.69	0.57
1:I:1195:ALA:HB1	1:I:1200:ILE:HD12	1.85	0.57
1:A:36:LEU:O	1:A:76:ARG:NH2	2.36	0.57
2:G:190:PHE:HZ	2:G:297:ARG:HD2	1.69	0.57
1:B:260:ARG:HH12	1:B:300:VAL:HG21	1.69	0.57
1:B:838:MET:CA	1:B:841:GLU:OE1	2.52	0.57
1:D:1010:GLU:O	1:D:1449:LYS:NZ	2.38	0.57
2:E:1351:VAL:HG21	2:E:1413:ARG:HH21	1.70	0.57
2:L:835:THR:HG22	2:L:844:VAL:HA	1.85	0.57
2:L:1737:ILE:HD13	2:L:1737:ILE:O	2.04	0.57
2:L:1742:VAL:O	2:L:1743:ASP:C	2.42	0.57
1:A:1533:ILE:O	1:A:1566:ARG:NH1	2.37	0.57
2:C:1351:VAL:HG21	2:C:1413:ARG:HH21	1.70	0.57
2:H:619:LEU:HB3	2:H:649:ILE:HG12	1.87	0.57
2:H:1737:ILE:HD13	2:H:1737:ILE:O	2.04	0.57
2:C:859:THR:HB	2:C:1049:GLN:HA	1.87	0.57
1:D:41:THR:O	1:D:76:ARG:NH1	2.38	0.57
1:K:838:MET:CA	1:K:841:GLU:OE1	2.52	0.57
2:H:1736:MET:HE3	2:H:1736:MET:N	2.18	0.57
2:J:670:ARG:HG2	2:J:699:GLY:H	1.68	0.57
2:J:1036:GLN:HB3	2:J:1051:THR:CG2	2.24	0.57
2:G:859:THR:HB	2:G:1049:GLN:HA	1.87	0.57
2:C:1737:ILE:HD13	2:C:1737:ILE:O	2.04	0.57
1:K:202:GLU:HG2	1:K:203:GLU:HG3	1.86	0.57
1:K:1019:ILE:HG13	1:K:1316:VAL:HG13	1.87	0.57
1:K:1749:THR:HB	1:K:1874:ASP:CG	2.24	0.57
2:H:1736:MET:CE	2:H:1736:MET:HA	2.35	0.57
1:I:41:THR:O	1:I:76:ARG:NH1	2.38	0.57
1:A:764:ASP:OD1	1:A:810:LYS:NZ	2.38	0.56
2:G:619:LEU:HB3	2:G:649:ILE:HG12	1.87	0.56
2:C:1590:ARG:NH1	2:C:1594:GLU:OE1	2.37	0.56
2:C:1742:VAL:O	2:C:1743:ASP:C	2.42	0.56
1:D:764:ASP:OD1	1:D:810:LYS:NZ	2.38	0.56
1:F:1010:GLU:O	1:F:1449:LYS:NZ	2.38	0.56
2:J:1911:THR:O	2:J:1915:ASN:ND2	2.38	0.56
2:G:1911:THR:O	2:G:1915:ASN:ND2	2.38	0.56
1:B:32:GLN:NE2	1:B:57:ALA:HB2	2.19	0.56
1:B:234:SER:OG	1:K:1123:GLN:NE2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1749:THR:HB	1:B:1874:ASP:CG	2.24	0.56
1:D:234:SER:OG	1:I:1123:GLN:NE2	2.38	0.56
1:D:1533:ILE:O	1:D:1566:ARG:NH1	2.37	0.56
2:E:1590:ARG:NH1	2:E:1594:GLU:OE1	2.38	0.56
1:K:41:THR:O	1:K:76:ARG:NH1	2.38	0.56
1:K:764:ASP:OD1	1:K:810:LYS:NZ	2.38	0.56
2:L:96:LEU:HD11	2:L:101:ILE:HG22	1.88	0.56
1:F:1019:ILE:HG13	1:F:1316:VAL:HG13	1.87	0.56
2:H:1911:THR:O	2:H:1915:ASN:ND2	2.38	0.56
1:A:41:THR:O	1:A:76:ARG:NH1	2.38	0.56
1:A:1106:ILE:HA	1:A:1188:GLN:HE22	1.70	0.56
1:A:1123:GLN:NE2	1:F:234:SER:OG	2.38	0.56
2:G:84:LEU:HD12	2:G:133:ALA:HB2	1.88	0.56
2:G:96:LEU:HD11	2:G:101:ILE:HG22	1.88	0.56
2:G:1736:MET:CE	2:G:1736:MET:HA	2.35	0.56
1:K:32:GLN:NE2	1:K:57:ALA:HB2	2.19	0.56
1:K:1010:GLU:O	1:K:1449:LYS:NZ	2.38	0.56
1:F:764:ASP:OD1	1:F:810:LYS:NZ	2.38	0.56
1:F:1106:ILE:HA	1:F:1188:GLN:HE22	1.70	0.56
1:F:1533:ILE:O	1:F:1566:ARG:NH1	2.37	0.56
2:H:84:LEU:HD12	2:H:133:ALA:HB2	1.88	0.56
2:H:1351:VAL:HG21	2:H:1413:ARG:HH21	1.70	0.56
1:I:202:GLU:HG2	1:I:203:GLU:HG3	1.86	0.56
1:I:1533:ILE:O	1:I:1566:ARG:NH1	2.37	0.56
2:J:619:LEU:HB3	2:J:649:ILE:HG12	1.87	0.56
2:J:1742:VAL:O	2:J:1743:ASP:C	2.42	0.56
1:B:764:ASP:OD1	1:B:810:LYS:NZ	2.38	0.56
2:E:619:LEU:HB3	2:E:649:ILE:HG12	1.87	0.56
1:I:32:GLN:HE22	1:I:57:ALA:CA	2.18	0.56
2:J:1351:VAL:HG21	2:J:1413:ARG:HH21	1.70	0.56
2:C:190:PHE:HZ	2:C:297:ARG:HD2	1.69	0.56
2:C:619:LEU:HB3	2:C:649:ILE:HG12	1.87	0.56
1:A:32:GLN:NE2	1:A:57:ALA:HB2	2.19	0.56
1:B:32:GLN:HE22	1:B:57:ALA:CA	2.19	0.56
1:B:41:THR:O	1:B:76:ARG:NH1	2.38	0.56
1:B:1019:ILE:HG13	1:B:1316:VAL:HG13	1.87	0.56
1:B:1491:ARG:HB2	1:B:1750:ILE:HG21	1.87	0.56
2:C:96:LEU:HD11	2:C:101:ILE:HG22	1.87	0.56
1:D:1123:GLN:NE2	1:I:234:SER:OG	2.38	0.56
1:K:1491:ARG:HB2	1:K:1750:ILE:HG21	1.87	0.56
2:L:1590:ARG:NH1	2:L:1594:GLU:OE1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:GLU:HG2	1:B:203:GLU:HG3	1.86	0.56
1:D:1106:ILE:HA	1:D:1188:GLN:HE22	1.70	0.56
2:E:1036:GLN:HB3	2:E:1051:THR:CG2	2.24	0.56
2:E:1736:MET:CE	2:E:1736:MET:HA	2.35	0.56
1:K:36:LEU:O	1:K:76:ARG:NH2	2.36	0.56
2:L:1736:MET:CE	2:L:1736:MET:HA	2.35	0.56
2:H:96:LEU:HD11	2:H:101:ILE:HG22	1.87	0.56
2:H:859:THR:HB	2:H:1049:GLN:HA	1.87	0.56
2:J:836:TYR:CE1	2:J:845:THR:HG21	2.37	0.56
1:A:844:LEU:O	1:F:844:LEU:HD23	2.06	0.56
1:B:1123:GLN:NE2	1:K:234:SER:OG	2.38	0.56
2:C:1911:THR:O	2:C:1915:ASN:ND2	2.38	0.56
2:E:190:PHE:HZ	2:E:297:ARG:HD2	1.69	0.56
2:E:1911:THR:O	2:E:1915:ASN:ND2	2.38	0.56
1:I:764:ASP:OD1	1:I:810:LYS:NZ	2.38	0.56
1:A:844:LEU:HD23	1:F:844:LEU:O	2.06	0.56
2:G:1736:MET:HB3	2:G:1751:ILE:CD1	2.36	0.56
2:C:1736:MET:CE	2:C:1736:MET:HA	2.35	0.56
2:C:1786:LYS:NZ	2:C:1816:ALA:O	2.35	0.56
1:I:32:GLN:NE2	1:I:57:ALA:HB2	2.19	0.56
2:J:190:PHE:HZ	2:J:297:ARG:HD2	1.69	0.56
1:B:844:LEU:HD23	1:K:844:LEU:O	2.06	0.56
1:K:836:ASP:HB3	1:K:839:TYR:HB3	1.88	0.56
1:K:1106:ILE:HA	1:K:1188:GLN:HE22	1.70	0.56
2:L:1911:THR:O	2:L:1915:ASN:ND2	2.38	0.56
1:A:1010:GLU:O	1:A:1449:LYS:NZ	2.38	0.55
1:A:1019:ILE:HG13	1:A:1316:VAL:HG13	1.87	0.55
2:G:1351:VAL:HG21	2:G:1413:ARG:HH21	1.70	0.55
1:B:1106:ILE:HA	1:B:1188:GLN:HE22	1.70	0.55
1:D:708:SER:HB3	3:D:2001:NDP:O2X	2.07	0.55
1:K:1471:LYS:HA	1:K:1761:LYS:HE2	1.89	0.55
2:L:619:LEU:HB3	2:L:649:ILE:HG12	1.87	0.55
2:L:836:TYR:CE1	2:L:845:THR:HG21	2.37	0.55
2:L:859:THR:HB	2:L:1049:GLN:HA	1.87	0.55
1:A:234:SER:OG	1:F:1123:GLN:NE2	2.38	0.55
1:A:838:MET:CA	1:A:841:GLU:OE1	2.52	0.55
2:C:461:ASP:OD2	2:C:478:ARG:NH2	2.39	0.55
2:E:84:LEU:HD12	2:E:133:ALA:HB2	1.88	0.55
1:K:32:GLN:NE2	1:K:57:ALA:HA	2.22	0.55
2:L:1737:ILE:HD13	2:L:1737:ILE:N	2.19	0.55
1:A:32:GLN:HE22	1:A:57:ALA:CA	2.19	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1010:GLU:O	1:B:1449:LYS:NZ	2.38	0.55
2:C:1736:MET:HB3	2:C:1751:ILE:CD1	2.36	0.55
2:L:84:LEU:HD12	2:L:133:ALA:HB2	1.88	0.55
2:J:859:THR:HB	2:J:1049:GLN:HA	1.87	0.55
1:B:836:ASP:HB3	1:B:839:TYR:HB3	1.88	0.55
2:C:84:LEU:HD12	2:C:133:ALA:HB2	1.88	0.55
2:C:1736:MET:HE3	2:C:1736:MET:N	2.21	0.55
1:D:32:GLN:HE22	1:D:57:ALA:CA	2.18	0.55
1:D:32:GLN:NE2	1:D:57:ALA:HA	2.22	0.55
1:D:1471:LYS:HA	1:D:1761:LYS:HE2	1.89	0.55
2:E:96:LEU:HD11	2:E:101:ILE:HG22	1.88	0.55
1:F:32:GLN:HE22	1:F:57:ALA:CA	2.19	0.55
1:F:838:MET:CA	1:F:841:GLU:OE1	2.52	0.55
1:I:1010:GLU:O	1:I:1449:LYS:NZ	2.38	0.55
1:I:1019:ILE:HG13	1:I:1316:VAL:HG13	1.87	0.55
2:J:84:LEU:HD12	2:J:133:ALA:HB2	1.88	0.55
1:B:708:SER:HB3	3:B:2001:NDP:O2X	2.07	0.55
1:B:844:LEU:O	1:K:844:LEU:HD23	2.06	0.55
1:D:353:ASP:OD2	1:D:359:ARG:NH2	2.40	0.55
2:E:836:TYR:CE1	2:E:845:THR:HG21	2.37	0.55
2:E:1202:GLN:HE22	2:E:1555:ARG:HH21	1.54	0.55
2:E:1928:GLN:HE22	2:E:1933:LEU:HD23	1.71	0.55
1:F:41:THR:O	1:F:76:ARG:NH1	2.38	0.55
2:H:13:HIS:HB3	2:H:60:LEU:HD11	1.89	0.55
2:H:461:ASP:OD2	2:H:478:ARG:NH2	2.39	0.55
2:G:13:HIS:HB3	2:G:60:LEU:HD11	1.89	0.55
1:D:844:LEU:HD23	1:I:844:LEU:O	2.06	0.55
1:K:32:GLN:HE22	1:K:57:ALA:CA	2.19	0.55
1:K:63:ASN:ND2	2:L:1896:GLN:OE1	2.40	0.55
2:L:461:ASP:OD2	2:L:478:ARG:NH2	2.39	0.55
2:J:1736:MET:CE	2:J:1736:MET:HA	2.35	0.55
1:D:1491:ARG:HB2	1:D:1750:ILE:HG21	1.87	0.55
2:L:13:HIS:HB3	2:L:60:LEU:HD11	1.89	0.55
2:L:190:PHE:HZ	2:L:297:ARG:HD2	1.69	0.55
1:F:708:SER:HB3	3:F:2001:NDP:O2X	2.07	0.55
1:I:1491:ARG:HB2	1:I:1750:ILE:HG21	1.87	0.55
2:J:461:ASP:OD2	2:J:478:ARG:NH2	2.39	0.55
2:J:1738:PHE:HB2	2:J:1987:PRO:HB2	1.89	0.55
1:B:1471:LYS:HA	1:B:1761:LYS:HE2	1.89	0.55
1:D:844:LEU:O	1:I:844:LEU:HD23	2.06	0.55
2:L:1482:SER:HA	2:L:1509:GLY:HA2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:1736:MET:HB3	2:L:1751:ILE:CD1	2.36	0.55
2:L:1928:GLN:HE22	2:L:1933:LEU:HD23	1.71	0.55
1:F:353:ASP:OD2	1:F:359:ARG:NH2	2.40	0.55
2:H:1739:GLU:CB	2:H:1746:LEU:CD1	2.85	0.55
1:I:708:SER:HB3	3:I:2001:NDP:O2X	2.07	0.55
1:I:1106:ILE:HA	1:I:1188:GLN:HE22	1.70	0.55
1:I:1219:VAL:HG22	1:I:1384:ILE:HD13	1.89	0.55
1:A:353:ASP:OD2	1:A:359:ARG:NH2	2.40	0.55
2:G:461:ASP:OD2	2:G:478:ARG:NH2	2.39	0.55
1:B:63:ASN:ND2	2:C:1896:GLN:OE1	2.40	0.55
1:B:877:LEU:HD12	3:B:2001:NDP:H2D	1.88	0.55
1:D:838:MET:CA	1:D:841:GLU:OE1	2.52	0.55
2:E:859:THR:HB	2:E:1049:GLN:HA	1.87	0.55
1:F:836:ASP:HB3	1:F:839:TYR:HB3	1.88	0.55
2:J:96:LEU:HD11	2:J:101:ILE:HG22	1.88	0.55
1:A:257:PRO:HD2	1:A:260:ARG:HD2	1.89	0.55
1:D:836:ASP:HB3	1:D:839:TYR:HB3	1.88	0.55
1:K:877:LEU:HD12	3:K:2001:NDP:H2D	1.88	0.55
2:H:1786:LYS:NZ	2:H:1816:ALA:O	2.35	0.55
2:J:13:HIS:HB3	2:J:60:LEU:HD11	1.89	0.55
1:A:32:GLN:NE2	1:A:57:ALA:HA	2.22	0.54
1:D:257:PRO:HD2	1:D:260:ARG:HD2	1.89	0.54
2:E:1482:SER:HA	2:E:1509:GLY:HA2	1.89	0.54
2:E:1739:GLU:CB	2:E:1746:LEU:CD1	2.84	0.54
2:L:366:VAL:HG12	2:L:381:GLY:HA3	1.89	0.54
2:L:1202:GLN:HE22	2:L:1555:ARG:HH21	1.54	0.54
1:F:1471:LYS:HA	1:F:1761:LYS:HE2	1.89	0.54
1:I:36:LEU:O	1:I:76:ARG:NH2	2.36	0.54
1:A:708:SER:HB3	3:A:2001:NDP:O2X	2.07	0.54
1:A:1219:VAL:HG22	1:A:1384:ILE:HD13	1.89	0.54
1:A:1491:ARG:HB2	1:A:1750:ILE:HG21	1.87	0.54
2:C:1736:MET:CE	2:C:1736:MET:CA	2.86	0.54
1:D:63:ASN:ND2	2:E:1896:GLN:OE1	2.40	0.54
2:E:1736:MET:HB3	2:E:1751:ILE:CD1	2.36	0.54
2:L:1736:MET:CE	2:L:1736:MET:CA	2.86	0.54
1:F:1491:ARG:HB2	1:F:1750:ILE:HG21	1.87	0.54
2:H:1202:GLN:HE22	2:H:1555:ARG:HH21	1.54	0.54
1:A:836:ASP:HB3	1:A:839:TYR:HB3	1.88	0.54
2:C:1482:SER:HA	2:C:1509:GLY:HA2	1.89	0.54
2:C:1928:GLN:HE22	2:C:1933:LEU:HD23	1.71	0.54
1:I:1471:LYS:HA	1:I:1761:LYS:HE2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:13:HIS:HB3	2:C:60:LEU:HD11	1.89	0.54
1:D:1219:VAL:HG22	1:D:1384:ILE:HD13	1.89	0.54
2:E:366:VAL:HG12	2:E:381:GLY:HA3	1.89	0.54
1:K:1219:VAL:HG22	1:K:1384:ILE:HD13	1.89	0.54
1:I:1561:MET:CE	1:I:1561:MET:CA	2.85	0.54
2:G:260:PRO:HD3	2:G:289:TRP:CH2	2.43	0.54
1:B:353:ASP:OD2	1:B:359:ARG:NH2	2.40	0.54
1:K:708:SER:HB3	3:K:2001:NDP:O2X	2.07	0.54
1:F:1219:VAL:HG22	1:F:1384:ILE:HD13	1.89	0.54
1:I:836:ASP:HB3	1:I:839:TYR:HB3	1.88	0.54
2:J:260:PRO:HD3	2:J:289:TRP:CH2	2.43	0.54
2:J:758:ARG:NH2	2:J:763:ILE:O	2.41	0.54
2:J:1736:MET:CE	2:J:1736:MET:CA	2.86	0.54
2:C:286:THR:HG23	2:C:286:THR:O	2.08	0.54
2:L:758:ARG:NH2	2:L:763:ILE:O	2.41	0.54
1:F:257:PRO:HD2	1:F:260:ARG:HD2	1.89	0.54
2:H:836:TYR:CE1	2:H:845:THR:HG21	2.37	0.54
1:I:32:GLN:NE2	1:I:57:ALA:HA	2.22	0.54
1:I:257:PRO:HD2	1:I:260:ARG:HD2	1.89	0.54
1:I:353:ASP:OD2	1:I:359:ARG:NH2	2.40	0.54
2:J:1202:GLN:HE22	2:J:1555:ARG:HH21	1.54	0.54
2:J:1736:MET:HB3	2:J:1751:ILE:CD1	2.36	0.54
1:A:1471:LYS:HA	1:A:1761:LYS:HE2	1.89	0.54
2:C:1738:PHE:HB2	2:C:1987:PRO:HB2	1.89	0.54
1:K:1561:MET:CE	1:K:1561:MET:CA	2.85	0.54
1:F:32:GLN:NE2	1:F:57:ALA:HA	2.22	0.54
1:I:63:ASN:ND2	2:J:1896:GLN:OE1	2.40	0.54
2:J:1383:ASN:ND2	2:J:1418:ASP:O	2.41	0.54
2:G:1383:ASN:ND2	2:G:1418:ASP:O	2.41	0.54
2:C:366:VAL:HG12	2:C:381:GLY:HA3	1.89	0.54
2:C:1383:ASN:ND2	2:C:1418:ASP:O	2.41	0.54
2:E:758:ARG:NH2	2:E:763:ILE:O	2.41	0.54
2:L:1739:GLU:CB	2:L:1746:LEU:CD1	2.84	0.54
2:H:1736:MET:CE	2:H:1736:MET:CA	2.86	0.54
2:J:1928:GLN:HE22	2:J:1933:LEU:HD23	1.71	0.54
2:G:1738:PHE:HB2	2:G:1987:PRO:HB2	1.89	0.54
2:G:1739:GLU:CB	2:G:1746:LEU:CD1	2.84	0.54
2:C:758:ARG:NH2	2:C:763:ILE:O	2.41	0.54
1:K:353:ASP:OD2	1:K:359:ARG:NH2	2.40	0.54
2:L:286:THR:HG23	2:L:286:THR:O	2.08	0.54
2:H:1383:ASN:ND2	2:H:1418:ASP:O	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1482:SER:HA	2:G:1509:GLY:HA2	1.89	0.54
1:B:257:PRO:HD2	1:B:260:ARG:HD2	1.89	0.54
2:E:461:ASP:OD2	2:E:478:ARG:NH2	2.39	0.54
1:F:63:ASN:ND2	2:H:1896:GLN:OE1	2.40	0.54
2:J:1032:ASP:OD2	2:J:1035:TRP:NE1	2.41	0.54
2:G:1202:GLN:HE22	2:G:1555:ARG:HH21	1.54	0.53
2:E:13:HIS:HB3	2:E:60:LEU:HD11	1.89	0.53
2:H:758:ARG:NH2	2:H:763:ILE:O	2.41	0.53
1:A:63:ASN:ND2	2:G:1896:GLN:OE1	2.40	0.53
1:A:1751:GLU:HG3	1:A:1754:LYS:HZ2	1.71	0.53
1:B:1219:VAL:HG22	1:B:1384:ILE:HD13	1.89	0.53
2:C:734:GLY:H	2:C:769:SER:HB3	1.74	0.53
2:C:1177:SER:OG	2:C:1180:MET:SD	2.63	0.53
1:D:1561:MET:CE	1:D:1561:MET:CA	2.85	0.53
2:H:1736:MET:HB3	2:H:1751:ILE:CD1	2.36	0.53
2:G:1928:GLN:HE22	2:G:1933:LEU:HD23	1.71	0.53
1:B:739:GLN:O	1:B:798:ASN:ND2	2.42	0.53
2:E:1736:MET:CE	2:E:1736:MET:CA	2.86	0.53
2:H:734:GLY:H	2:H:769:SER:HB3	1.74	0.53
2:J:366:VAL:HG12	2:J:381:GLY:HA3	1.89	0.53
2:G:758:ARG:NH2	2:G:763:ILE:O	2.41	0.53
2:G:1736:MET:CE	2:G:1736:MET:CA	2.86	0.53
1:F:1561:MET:CE	1:F:1561:MET:CA	2.86	0.53
1:I:236:LYS:HG2	1:I:273:PRO:HD2	1.90	0.53
1:I:877:LEU:HD12	3:I:2001:NDP:H2D	1.88	0.53
2:J:286:THR:HG23	2:J:286:THR:O	2.08	0.53
2:J:734:GLY:H	2:J:769:SER:HB3	1.74	0.53
2:G:602:VAL:HG21	2:G:623:GLY:HA3	1.91	0.53
2:G:734:GLY:H	2:G:769:SER:HB3	1.74	0.53
2:C:1202:GLN:HE22	2:C:1555:ARG:HH21	1.54	0.53
1:D:1019:ILE:HG21	1:D:1316:VAL:HG22	1.90	0.53
1:K:257:PRO:HD2	1:K:260:ARG:HD2	1.89	0.53
1:K:739:GLN:O	1:K:798:ASN:ND2	2.42	0.53
2:H:1928:GLN:HE22	2:H:1933:LEU:HD23	1.71	0.53
2:G:286:THR:HG23	2:G:286:THR:O	2.08	0.53
2:G:650:ASN:OD1	2:G:680:THR:HG22	2.09	0.53
2:L:1383:ASN:ND2	2:L:1418:ASP:O	2.41	0.53
2:H:366:VAL:HG12	2:H:381:GLY:HA3	1.89	0.53
2:H:1695:ASP:OD1	2:H:1706:ILE:N	2.42	0.53
2:J:1482:SER:HA	2:J:1509:GLY:HA2	1.89	0.53
1:A:1544:THR:HG21	1:A:1546:THR:OG1	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:260:PRO:HD3	2:C:289:TRP:CH2	2.43	0.53
1:D:877:LEU:HD12	3:D:2001:NDP:H2D	1.88	0.53
2:E:260:PRO:HD3	2:E:289:TRP:CH2	2.43	0.53
2:E:650:ASN:OD1	2:E:680:THR:HG22	2.09	0.53
2:E:1383:ASN:ND2	2:E:1418:ASP:O	2.41	0.53
1:K:1544:THR:HG21	1:K:1546:THR:OG1	2.09	0.53
2:H:602:VAL:HG21	2:H:623:GLY:HA3	1.91	0.53
2:H:650:ASN:OD1	2:H:680:THR:HG22	2.09	0.53
2:G:366:VAL:HG12	2:G:381:GLY:HA3	1.89	0.53
2:G:774:ALA:HB2	2:G:1077:ILE:HA	1.91	0.53
2:E:1738:PHE:HB2	2:E:1987:PRO:HB2	1.89	0.53
2:L:602:VAL:HG21	2:L:623:GLY:HA3	1.91	0.53
1:F:1019:ILE:HG21	1:F:1316:VAL:HG22	1.90	0.53
2:H:286:THR:HG23	2:H:286:THR:O	2.08	0.53
1:I:1544:THR:HG21	1:I:1546:THR:OG1	2.09	0.53
1:A:774:ILE:HG22	3:A:2001:NDP:N7A	2.24	0.53
1:A:1544:THR:CG2	1:A:1546:THR:OG1	2.57	0.53
1:F:1544:THR:CG2	1:F:1546:THR:OG1	2.57	0.53
2:H:260:PRO:HD3	2:H:289:TRP:CH2	2.43	0.53
2:H:774:ALA:HB2	2:H:1077:ILE:HA	1.91	0.53
1:I:1544:THR:CG2	1:I:1546:THR:OG1	2.57	0.53
2:J:1739:GLU:CB	2:J:1746:LEU:CD1	2.84	0.53
1:A:236:LYS:HG2	1:A:273:PRO:HD2	1.90	0.53
1:A:1545:SER:O	1:A:1545:SER:OG	2.27	0.53
1:B:32:GLN:NE2	1:B:57:ALA:HA	2.22	0.53
2:C:1032:ASP:OD2	2:C:1035:TRP:NE1	2.41	0.53
1:K:236:LYS:HG2	1:K:273:PRO:HD2	1.90	0.53
2:L:260:PRO:HD3	2:L:289:TRP:CH2	2.43	0.53
1:F:1545:SER:O	1:F:1545:SER:OG	2.27	0.53
2:J:602:VAL:HG21	2:J:623:GLY:HA3	1.91	0.53
2:J:1695:ASP:OD1	2:J:1706:ILE:N	2.42	0.53
1:A:413:LEU:HD12	1:A:439:ILE:HG21	1.91	0.52
1:A:697:LEU:HD21	1:A:732:LEU:HD23	1.91	0.52
1:A:1561:MET:CE	1:A:1561:MET:CA	2.85	0.52
2:G:1736:MET:HE3	2:G:1736:MET:N	2.23	0.52
1:B:1544:THR:HG21	1:B:1546:THR:OG1	2.09	0.52
2:C:1739:GLU:CB	2:C:1746:LEU:CD1	2.85	0.52
1:D:774:ILE:HG22	3:D:2001:NDP:N7A	2.24	0.52
2:E:286:THR:HG23	2:E:286:THR:O	2.08	0.52
2:E:734:GLY:H	2:E:769:SER:HB3	1.74	0.52
1:F:413:LEU:HD12	1:F:439:ILE:HG21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:650:ASN:OD1	2:J:680:THR:HG22	2.09	0.52
2:G:297:ARG:HG2	2:G:297:ARG:HH11	1.74	0.52
2:L:649:ILE:O	2:L:679:LEU:HD22	2.09	0.52
2:L:650:ASN:OD1	2:L:680:THR:HG22	2.09	0.52
1:F:774:ILE:HG22	3:F:2001:NDP:N7A	2.24	0.52
2:H:1309:GLU:O	2:H:1317:ARG:NH1	2.42	0.52
2:H:1482:SER:HA	2:H:1509:GLY:HA2	1.89	0.52
1:I:739:GLN:O	1:I:798:ASN:ND2	2.42	0.52
2:J:297:ARG:HG2	2:J:297:ARG:HH11	1.74	0.52
2:G:1695:ASP:OD1	2:G:1706:ILE:N	2.42	0.52
1:B:774:ILE:HG22	3:B:2001:NDP:N7A	2.24	0.52
1:B:1019:ILE:HG21	1:B:1316:VAL:HG22	1.90	0.52
1:B:1561:MET:CE	1:B:1561:MET:CA	2.86	0.52
2:C:1309:GLU:O	2:C:1317:ARG:NH1	2.42	0.52
1:D:1749:THR:HB	1:D:1874:ASP:CB	2.39	0.52
2:E:1695:ASP:OD1	2:E:1706:ILE:N	2.42	0.52
1:K:1749:THR:HB	1:K:1874:ASP:CB	2.39	0.52
2:L:1738:PHE:HB2	2:L:1987:PRO:HB2	1.89	0.52
2:G:1490:LYS:HB3	2:G:1498:THR:HB	1.92	0.52
1:B:236:LYS:HG2	1:B:273:PRO:HD2	1.90	0.52
2:C:602:VAL:HG21	2:C:623:GLY:HA3	1.91	0.52
1:D:236:LYS:HG2	1:D:273:PRO:HD2	1.90	0.52
1:K:1544:THR:CG2	1:K:1546:THR:OG1	2.57	0.52
2:L:734:GLY:H	2:L:769:SER:HB3	1.74	0.52
1:F:1749:THR:HB	1:F:1874:ASP:CB	2.39	0.52
2:H:1490:LYS:HB3	2:H:1498:THR:HB	1.92	0.52
2:E:649:ILE:O	2:E:679:LEU:HD22	2.09	0.52
2:L:847:ARG:HG2	2:L:869:ASP:OD2	2.03	0.52
2:L:1736:MET:CE	2:L:1736:MET:N	2.73	0.52
1:F:1544:THR:HG21	1:F:1546:THR:OG1	2.09	0.52
2:H:1738:PHE:HB2	2:H:1987:PRO:HB2	1.89	0.52
1:I:206:LEU:HD23	1:I:209:LEU:HD12	1.92	0.52
1:A:1749:THR:HB	1:A:1874:ASP:CB	2.39	0.52
2:E:1177:SER:OG	2:E:1180:MET:SD	2.63	0.52
2:E:1490:LYS:HB3	2:E:1498:THR:HB	1.92	0.52
2:E:1736:MET:CE	2:E:1736:MET:N	2.73	0.52
1:K:1019:ILE:HG21	1:K:1316:VAL:HG22	1.90	0.52
1:A:1491:ARG:NH1	1:A:1744:TYR:O	2.43	0.52
2:G:649:ILE:O	2:G:679:LEU:HD22	2.09	0.52
2:G:1736:MET:CE	2:G:1736:MET:N	2.73	0.52
1:D:1544:THR:CG2	1:D:1546:THR:OG1	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1544:THR:HG21	1:D:1546:THR:OG1	2.09	0.52
2:E:847:ARG:HG2	2:E:869:ASP:OD2	2.03	0.52
2:E:1032:ASP:OD2	2:E:1035:TRP:NE1	2.41	0.52
1:F:236:LYS:HG2	1:F:273:PRO:HD2	1.90	0.52
1:F:471:THR:HG22	1:F:610:THR:HG21	1.92	0.52
1:I:1491:ARG:NH1	1:I:1744:TYR:O	2.43	0.52
2:J:217:GLU:OE2	2:J:221:ASN:ND2	2.37	0.52
1:A:206:LEU:HD23	1:A:209:LEU:HD12	1.92	0.52
1:B:1544:THR:CG2	1:B:1546:THR:OG1	2.57	0.52
2:C:649:ILE:O	2:C:679:LEU:HD22	2.09	0.52
2:C:1737:ILE:CD1	2:C:1737:ILE:N	2.73	0.52
1:K:1744:TYR:C	1:K:1747:ALA:CB	2.75	0.52
2:L:774:ALA:HB2	2:L:1077:ILE:HA	1.91	0.52
1:I:774:ILE:HG22	3:I:2001:NDP:N7A	2.24	0.52
2:J:1490:LYS:HB3	2:J:1498:THR:HB	1.92	0.52
1:B:1749:THR:HB	1:B:1874:ASP:CB	2.39	0.52
2:C:1695:ASP:OD1	2:C:1706:ILE:N	2.42	0.52
2:C:1736:MET:CE	2:C:1736:MET:N	2.73	0.52
1:D:90:TYR:OH	2:E:1659:GLN:NE2	2.43	0.52
1:D:697:LEU:HD21	1:D:732:LEU:HD23	1.91	0.52
1:D:844:LEU:HD23	1:I:848:THR:HG23	1.92	0.52
1:D:881:ASN:HB3	1:D:944:ARG:HH22	1.75	0.52
1:K:774:ILE:HG22	3:K:2001:NDP:N7A	2.24	0.52
2:L:1695:ASP:OD1	2:L:1706:ILE:N	2.42	0.52
1:F:881:ASN:HB3	1:F:944:ARG:HH22	1.75	0.52
2:H:1032:ASP:OD2	2:H:1035:TRP:NE1	2.41	0.52
2:H:1189:THR:O	2:H:1193:THR:OG1	2.28	0.52
2:H:1736:MET:CE	2:H:1736:MET:N	2.73	0.52
1:A:29:ILE:HD11	2:G:1898:TYR:HE1	1.75	0.52
1:A:877:LEU:HD12	3:A:2001:NDP:H2D	1.88	0.52
1:A:1019:ILE:HG21	1:A:1316:VAL:HG22	1.90	0.52
2:G:1737:ILE:HD13	2:G:1737:ILE:N	2.19	0.52
1:B:206:LEU:HD23	1:B:209:LEU:HD12	1.92	0.52
2:C:650:ASN:OD1	2:C:680:THR:HG22	2.09	0.52
1:D:29:ILE:HD11	2:E:1898:TYR:HE1	1.75	0.52
1:D:1064:ASN:ND2	1:D:1073:THR:OG1	2.43	0.52
2:E:1738:PHE:HB3	2:E:1833:TYR:OH	2.10	0.52
1:K:29:ILE:HD11	2:L:1898:TYR:HE1	1.75	0.52
1:K:271:ASN:HB2	1:K:290:MET:HE1	1.92	0.52
1:F:206:LEU:HD23	1:F:209:LEU:HD12	1.92	0.52
1:F:739:GLN:O	1:F:798:ASN:ND2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1064:ASN:ND2	1:F:1073:THR:OG1	2.43	0.52
2:J:1736:MET:CE	2:J:1736:MET:N	2.73	0.52
1:A:739:GLN:O	1:A:798:ASN:ND2	2.42	0.51
1:B:413:LEU:HD12	1:B:439:ILE:HG21	1.91	0.51
1:B:505:LYS:HA	1:B:954:ARG:HD3	1.92	0.51
2:C:297:ARG:HG2	2:C:297:ARG:HH11	1.74	0.51
1:D:471:THR:HG22	1:D:610:THR:HG21	1.92	0.51
1:K:90:TYR:OH	2:L:1659:GLN:NE2	2.43	0.51
1:K:505:LYS:HA	1:K:954:ARG:HD3	1.92	0.51
1:K:697:LEU:HD21	1:K:732:LEU:HD23	1.91	0.51
2:L:1032:ASP:OD2	2:L:1035:TRP:NE1	2.41	0.51
1:F:877:LEU:HD12	3:F:2001:NDP:H2D	1.88	0.51
1:I:505:LYS:HA	1:I:954:ARG:HD3	1.92	0.51
2:J:649:ILE:O	2:J:679:LEU:HD22	2.09	0.51
1:A:801:ARG:NH2	1:F:789:GLU:OE1	2.43	0.51
1:B:789:GLU:OE1	1:K:801:ARG:NH2	2.43	0.51
1:B:848:THR:HG23	1:K:844:LEU:HD23	1.92	0.51
1:B:1491:ARG:NH1	1:B:1744:TYR:O	2.43	0.51
2:C:774:ALA:HB2	2:C:1077:ILE:HA	1.91	0.51
2:C:1037:SER:OG	2:C:1053:ILE:CD1	2.59	0.51
2:C:1037:SER:HB2	2:C:1053:ILE:CG1	2.40	0.51
1:F:90:TYR:OH	2:H:1659:GLN:NE2	2.43	0.51
2:H:297:ARG:HG2	2:H:297:ARG:HH11	1.74	0.51
1:I:1019:ILE:HG21	1:I:1316:VAL:HG22	1.90	0.51
1:I:1749:THR:HB	1:I:1874:ASP:CB	2.39	0.51
1:A:789:GLU:OE1	1:F:801:ARG:NH2	2.43	0.51
1:A:848:THR:HG23	1:F:844:LEU:HD23	1.92	0.51
2:C:209:PHE:HE1	2:C:235:PRO:HB2	1.75	0.51
2:E:1931:LEU:HD22	2:E:1935:GLU:HG2	1.92	0.51
2:L:1037:SER:HB2	2:L:1053:ILE:CG1	2.41	0.51
2:L:1738:PHE:HB3	2:L:1833:TYR:OH	2.11	0.51
1:F:1491:ARG:NH1	1:F:1744:TYR:O	2.43	0.51
1:I:14:LEU:HD13	1:I:14:LEU:C	2.31	0.51
1:I:1545:SER:O	1:I:1545:SER:OG	2.27	0.51
2:J:1037:SER:HB2	2:J:1053:ILE:CG1	2.41	0.51
2:J:1738:PHE:HB3	2:J:1833:TYR:OH	2.10	0.51
2:J:1931:LEU:HD22	2:J:1935:GLU:HG2	1.92	0.51
1:A:881:ASN:HB3	1:A:944:ARG:HH22	1.75	0.51
1:A:1064:ASN:ND2	1:A:1073:THR:OG1	2.43	0.51
1:B:29:ILE:HD11	2:C:1898:TYR:HE1	1.75	0.51
1:D:206:LEU:HD23	1:D:209:LEU:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:602:VAL:HG21	2:E:623:GLY:HA3	1.91	0.51
2:E:774:ALA:HB2	2:E:1077:ILE:HA	1.91	0.51
1:K:206:LEU:HD23	1:K:209:LEU:HD12	1.92	0.51
1:K:413:LEU:HD12	1:K:439:ILE:HG21	1.91	0.51
2:L:1931:LEU:HD22	2:L:1935:GLU:HG2	1.92	0.51
1:F:29:ILE:HD11	2:H:1898:TYR:HE1	1.75	0.51
1:F:271:ASN:HB2	1:F:290:MET:HE1	1.93	0.51
1:F:697:LEU:HD21	1:F:732:LEU:HD23	1.91	0.51
2:H:209:PHE:HE1	2:H:235:PRO:HB2	1.75	0.51
1:I:90:TYR:OH	2:J:1659:GLN:NE2	2.43	0.51
2:J:1189:THR:O	2:J:1193:THR:OG1	2.28	0.51
2:G:143:SER:OG	2:G:547:ILE:O	2.29	0.51
2:G:217:GLU:OE2	2:G:221:ASN:ND2	2.37	0.51
1:B:697:LEU:HD21	1:B:732:LEU:HD23	1.91	0.51
1:D:801:ARG:NH2	1:I:789:GLU:OE1	2.43	0.51
2:L:297:ARG:HG2	2:L:297:ARG:HH11	1.74	0.51
2:L:1037:SER:OG	2:L:1053:ILE:CD1	2.59	0.51
2:H:848:SER:HB3	2:H:854:ILE:HD11	1.93	0.51
2:H:1738:PHE:HB3	2:H:1833:TYR:OH	2.10	0.51
1:I:1505:GLN:O	1:I:1509:GLY:N	2.43	0.51
2:J:297:ARG:HG2	2:J:297:ARG:NH1	2.26	0.51
1:A:271:ASN:HB2	1:A:290:MET:HE1	1.93	0.51
2:G:1738:PHE:HB3	2:G:1833:TYR:OH	2.11	0.51
1:B:271:ASN:HB2	1:B:290:MET:HE1	1.92	0.51
2:C:1752:PHE:HB3	2:C:1755:ILE:HD13	1.92	0.51
2:E:297:ARG:NH1	2:E:297:ARG:HG2	2.26	0.51
2:L:1177:SER:OG	2:L:1180:MET:SD	2.63	0.51
2:H:649:ILE:O	2:H:679:LEU:HD22	2.09	0.51
1:A:14:LEU:HD13	1:A:14:LEU:C	2.31	0.51
1:A:471:THR:HG22	1:A:610:THR:HG21	1.92	0.51
1:B:801:ARG:NH2	1:K:789:GLU:OE1	2.43	0.51
1:B:1505:GLN:O	1:B:1509:GLY:N	2.43	0.51
1:D:789:GLU:OE1	1:I:801:ARG:NH2	2.43	0.51
1:K:1064:ASN:ND2	1:K:1073:THR:OG1	2.43	0.51
1:F:14:LEU:C	1:F:14:LEU:HD13	2.31	0.51
1:I:413:LEU:HD12	1:I:439:ILE:HG21	1.91	0.51
1:A:505:LYS:HA	1:A:954:ARG:HD3	1.92	0.51
2:G:848:SER:HB3	2:G:854:ILE:HD11	1.93	0.51
1:B:14:LEU:HD13	1:B:14:LEU:C	2.31	0.51
1:B:1064:ASN:ND2	1:B:1073:THR:OG1	2.43	0.51
2:E:848:SER:HB3	2:E:854:ILE:HD11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1309:GLU:O	2:E:1317:ARG:NH1	2.42	0.51
2:L:217:GLU:OE2	2:L:221:ASN:ND2	2.37	0.51
2:L:1490:LYS:HB3	2:L:1498:THR:HB	1.92	0.51
2:L:1775:GLN:OE1	2:L:1839:GLN:NE2	2.44	0.51
2:H:297:ARG:HG2	2:H:297:ARG:NH1	2.26	0.51
1:I:1064:ASN:ND2	1:I:1073:THR:OG1	2.43	0.51
2:J:774:ALA:HB2	2:J:1077:ILE:HA	1.91	0.51
2:J:1037:SER:OG	2:J:1053:ILE:CD1	2.59	0.51
1:A:950:THR:HA	1:A:953:VAL:HG12	1.93	0.51
1:A:995:LEU:HD13	1:A:1674:VAL:HG22	1.93	0.51
1:D:271:ASN:HB2	1:D:290:MET:HE1	1.93	0.51
1:D:739:GLN:O	1:D:798:ASN:ND2	2.42	0.51
2:E:1037:SER:OG	2:E:1053:ILE:CD1	2.59	0.51
2:E:1037:SER:HB2	2:E:1053:ILE:CG1	2.41	0.51
2:E:1322:PRO:HG2	2:E:1325:PHE:HB2	1.93	0.51
2:L:297:ARG:HG2	2:L:297:ARG:NH1	2.26	0.51
2:H:1037:SER:OG	2:H:1053:ILE:CD1	2.59	0.51
2:H:1037:SER:HB2	2:H:1053:ILE:CG1	2.40	0.51
1:I:471:THR:HG22	1:I:610:THR:HG21	1.92	0.51
1:I:697:LEU:HD21	1:I:732:LEU:HD23	1.91	0.51
1:I:1039:MET:HG3	1:I:1580:LEU:HD11	1.93	0.51
2:J:1752:PHE:HB3	2:J:1755:ILE:HD13	1.92	0.51
1:A:90:TYR:OH	2:G:1659:GLN:NE2	2.43	0.51
2:G:209:PHE:HE1	2:G:235:PRO:HB2	1.75	0.51
2:G:297:ARG:HG2	2:G:297:ARG:NH1	2.26	0.51
2:G:1037:SER:OG	2:G:1053:ILE:CD1	2.59	0.51
1:B:90:TYR:OH	2:C:1659:GLN:NE2	2.43	0.51
1:B:471:THR:HG22	1:B:610:THR:HG21	1.92	0.51
2:C:297:ARG:HG2	2:C:297:ARG:NH1	2.26	0.51
2:C:1189:THR:O	2:C:1193:THR:OG1	2.28	0.51
2:C:1738:PHE:HB3	2:C:1833:TYR:OH	2.10	0.51
1:D:413:LEU:HD12	1:D:439:ILE:HG21	1.91	0.51
2:E:209:PHE:HE1	2:E:235:PRO:HB2	1.75	0.51
2:E:1752:PHE:HB3	2:E:1755:ILE:HD13	1.92	0.51
1:K:881:ASN:HB3	1:K:944:ARG:HH22	1.75	0.51
1:K:1491:ARG:NH1	1:K:1744:TYR:O	2.43	0.51
2:L:209:PHE:HE1	2:L:235:PRO:HB2	1.75	0.51
2:L:1036:GLN:HB3	2:L:1051:THR:CG2	2.24	0.51
2:L:1189:THR:O	2:L:1193:THR:OG1	2.28	0.51
2:L:1267:TRP:NE1	2:L:1273:GLU:O	2.39	0.51
2:J:209:PHE:HE1	2:J:235:PRO:HB2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:1322:PRO:HG2	2:J:1325:PHE:HB2	1.93	0.51
2:J:1775:GLN:OE1	2:J:1839:GLN:NE2	2.44	0.51
1:A:364:GLU:OE1	1:F:364:GLU:OE1	2.29	0.50
1:B:1406:MET:HB3	1:B:1654:ILE:HG22	1.93	0.50
2:C:1490:LYS:HB3	2:C:1498:THR:HB	1.92	0.50
1:D:1491:ARG:NH1	1:D:1744:TYR:O	2.43	0.50
2:L:848:SER:HB3	2:L:854:ILE:HD11	1.93	0.50
1:A:844:LEU:HD23	1:F:848:THR:HG23	1.92	0.50
2:G:1931:LEU:HD22	2:G:1935:GLU:HG2	1.92	0.50
1:B:844:LEU:HD23	1:K:848:THR:HG23	1.92	0.50
1:B:1039:MET:HG3	1:B:1580:LEU:HD11	1.93	0.50
1:D:505:LYS:HA	1:D:954:ARG:HD3	1.92	0.50
1:D:995:LEU:HD13	1:D:1674:VAL:HG22	1.93	0.50
2:E:1189:THR:O	2:E:1193:THR:OG1	2.28	0.50
2:L:1752:PHE:HB3	2:L:1755:ILE:HD13	1.92	0.50
1:F:950:THR:HA	1:F:953:VAL:HG12	1.93	0.50
2:H:1931:LEU:HD22	2:H:1935:GLU:HG2	1.92	0.50
1:I:881:ASN:HB3	1:I:944:ARG:HH22	1.75	0.50
1:I:1406:MET:HB3	1:I:1654:ILE:HG22	1.93	0.50
2:J:143:SER:OG	2:J:547:ILE:O	2.29	0.50
2:J:1177:SER:OG	2:J:1180:MET:SD	2.63	0.50
2:G:1032:ASP:OD2	2:G:1035:TRP:NE1	2.41	0.50
2:G:1189:THR:O	2:G:1193:THR:OG1	2.28	0.50
2:G:1752:PHE:HB3	2:G:1755:ILE:HD13	1.92	0.50
1:B:32:GLN:HA	1:B:35:PHE:CE1	2.47	0.50
1:B:881:ASN:HB3	1:B:944:ARG:HH22	1.75	0.50
1:B:1545:SER:O	1:B:1545:SER:OG	2.27	0.50
2:L:1322:PRO:HG2	2:L:1325:PHE:HB2	1.93	0.50
2:H:686:PRO:HB2	2:H:691:ALA:HB2	1.93	0.50
2:H:1752:PHE:HB3	2:H:1755:ILE:HD13	1.92	0.50
1:I:641:ARG:NH2	1:I:925:ASP:OD2	2.45	0.50
1:I:995:LEU:HD13	1:I:1674:VAL:HG22	1.93	0.50
2:J:892:ILE:O	2:J:896:ASN:ND2	2.45	0.50
2:G:1037:SER:HB2	2:G:1053:ILE:CG1	2.41	0.50
2:C:1931:LEU:HD22	2:C:1935:GLU:HG2	1.92	0.50
2:E:297:ARG:HG2	2:E:297:ARG:HH11	1.74	0.50
2:E:954:VAL:HG11	2:E:984:PHE:HE1	1.77	0.50
1:K:1773:VAL:HG22	1:K:1879:VAL:HG22	1.94	0.50
2:L:1142:LEU:O	2:L:1150:ARG:NH2	2.45	0.50
1:F:995:LEU:HD13	1:F:1674:VAL:HG22	1.93	0.50
1:I:29:ILE:HD11	2:J:1898:TYR:HE1	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:254:TRP:NE1	1:I:288:ASP:OD1	2.42	0.50
2:J:1309:GLU:O	2:J:1317:ARG:NH1	2.42	0.50
1:A:1017:ARG:NH1	1:A:1511:ASP:OD2	2.42	0.50
1:A:1406:MET:HB3	1:A:1654:ILE:HG22	1.93	0.50
1:A:1505:GLN:O	1:A:1509:GLY:N	2.43	0.50
2:G:1322:PRO:HG2	2:G:1325:PHE:HB2	1.93	0.50
1:B:400:ARG:NH1	1:B:1358:HIS:O	2.40	0.50
1:D:14:LEU:HD13	1:D:14:LEU:C	2.31	0.50
1:D:1773:VAL:HG22	1:D:1879:VAL:HG22	1.94	0.50
2:E:846:VAL:HG21	2:E:856:LYS:HD2	1.94	0.50
1:K:32:GLN:HA	1:K:35:PHE:CE1	2.47	0.50
1:K:641:ARG:NH2	1:K:925:ASP:OD2	2.45	0.50
2:L:954:VAL:HG11	2:L:984:PHE:HE1	1.77	0.50
2:J:1639:LYS:NZ	2:J:1654:GLU:OE1	2.44	0.50
1:B:364:GLU:OE1	1:K:364:GLU:OE1	2.29	0.50
1:B:995:LEU:HD13	1:B:1674:VAL:HG22	1.93	0.50
1:B:1773:VAL:HG22	1:B:1879:VAL:HG22	1.94	0.50
2:C:1775:GLN:OE1	2:C:1839:GLN:NE2	2.44	0.50
1:D:848:THR:HG23	1:I:844:LEU:HD23	1.92	0.50
1:D:1542:HIS:CB	1:D:1553:GLU:OE1	2.59	0.50
1:D:1673:TYR:CE1	1:D:1677:VAL:HG21	2.47	0.50
1:K:14:LEU:C	1:K:14:LEU:HD13	2.31	0.50
1:K:1673:TYR:CE1	1:K:1677:VAL:CG2	2.95	0.50
2:L:846:VAL:HG21	2:L:856:LYS:HD2	1.94	0.50
1:F:32:GLN:HA	1:F:35:PHE:CE1	2.47	0.50
1:F:1744:TYR:C	1:F:1747:ALA:CB	2.75	0.50
1:I:1542:HIS:CB	1:I:1553:GLU:OE1	2.59	0.50
1:A:1039:MET:HG3	1:A:1580:LEU:HD11	1.93	0.50
1:A:1744:TYR:C	1:A:1747:ALA:CB	2.75	0.50
2:G:686:PRO:HB2	2:G:691:ALA:HB2	1.93	0.50
2:E:65:LEU:HD11	2:E:88:LEU:HD23	1.94	0.50
2:E:686:PRO:HB2	2:E:691:ALA:HB2	1.93	0.50
1:K:995:LEU:HD13	1:K:1674:VAL:HG22	1.93	0.50
2:L:65:LEU:HD11	2:L:88:LEU:HD23	1.94	0.50
1:I:1673:TYR:CE1	1:I:1677:VAL:HG21	2.47	0.50
2:J:65:LEU:HD11	2:J:88:LEU:HD23	1.94	0.50
2:J:92:GLU:HA	2:J:96:LEU:HB2	1.94	0.50
1:A:32:GLN:HA	1:A:35:PHE:CE1	2.47	0.50
1:A:1542:HIS:CB	1:A:1553:GLU:OE1	2.59	0.50
2:G:92:GLU:HA	2:G:96:LEU:HB2	1.94	0.50
2:C:65:LEU:HD11	2:C:88:LEU:HD23	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1142:LEU:O	2:C:1150:ARG:NH2	2.45	0.50
1:D:1017:ARG:NH1	1:D:1511:ASP:OD2	2.42	0.50
2:E:1142:LEU:O	2:E:1150:ARG:NH2	2.45	0.50
1:K:1542:HIS:CB	1:K:1553:GLU:OE1	2.59	0.50
1:K:1673:TYR:CE1	1:K:1677:VAL:HG21	2.47	0.50
1:I:1751:GLU:HG3	1:I:1754:LYS:HE3	1.94	0.50
2:J:847:ARG:HG2	2:J:869:ASP:OD2	2.03	0.50
2:J:848:SER:HB3	2:J:854:ILE:HD11	1.93	0.50
1:B:1751:GLU:HG3	1:B:1754:LYS:HE3	1.94	0.50
2:C:217:GLU:OE2	2:C:221:ASN:ND2	2.37	0.50
2:C:892:ILE:O	2:C:896:ASN:ND2	2.45	0.50
1:D:1673:TYR:CE1	1:D:1677:VAL:CG2	2.95	0.50
1:K:471:THR:HG22	1:K:610:THR:HG21	1.92	0.50
1:F:505:LYS:HA	1:F:954:ARG:HD3	1.92	0.50
1:F:1542:HIS:CB	1:F:1553:GLU:OE1	2.59	0.50
1:I:950:THR:HA	1:I:953:VAL:HG12	1.93	0.50
1:I:1744:TYR:C	1:I:1747:ALA:CB	2.75	0.50
2:J:1314:ARG:HB2	2:J:1317:ARG:HD3	1.94	0.50
1:A:1578:LYS:HD2	1:A:1583:HIS:HA	1.94	0.49
1:A:1673:TYR:CE1	1:A:1677:VAL:HG21	2.47	0.49
1:A:1687:PHE:C	1:A:1687:PHE:CD2	2.86	0.49
1:B:641:ARG:NH2	1:B:925:ASP:OD2	2.45	0.49
1:B:1486:LEU:HD21	1:B:1761:LYS:HZ2	1.76	0.49
1:B:1542:HIS:CB	1:B:1553:GLU:OE1	2.59	0.49
1:K:1039:MET:HG3	1:K:1580:LEU:HD11	1.93	0.49
1:K:1406:MET:HB3	1:K:1654:ILE:HG22	1.93	0.49
2:L:1314:ARG:HB2	2:L:1317:ARG:HD3	1.94	0.49
1:F:641:ARG:NH2	1:F:925:ASP:OD2	2.45	0.49
1:F:1773:VAL:HG22	1:F:1879:VAL:HG22	1.94	0.49
2:H:846:VAL:HG21	2:H:856:LYS:HD2	1.94	0.49
2:H:1775:GLN:OE1	2:H:1839:GLN:NE2	2.44	0.49
2:J:1736:MET:HE3	2:J:1736:MET:N	2.26	0.49
1:A:1751:GLU:HG3	1:A:1754:LYS:HE3	1.94	0.49
1:B:1673:TYR:CE1	1:B:1677:VAL:CG2	2.95	0.49
1:B:1687:PHE:C	1:B:1687:PHE:CD2	2.86	0.49
2:C:92:GLU:HA	2:C:96:LEU:HB2	1.94	0.49
1:D:364:GLU:OE1	1:I:364:GLU:OE1	2.29	0.49
1:D:1687:PHE:C	1:D:1687:PHE:CD2	2.86	0.49
2:G:892:ILE:O	2:G:896:ASN:ND2	2.45	0.49
2:G:1314:ARG:HB2	2:G:1317:ARG:HD3	1.94	0.49
2:E:1639:LYS:NZ	2:E:1654:GLU:OE1	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:503:ASP:HB3	2:L:529:VAL:HA	1.94	0.49
2:H:92:GLU:HA	2:H:96:LEU:HB2	1.94	0.49
2:H:1177:SER:OG	2:H:1180:MET:SD	2.63	0.49
1:I:32:GLN:HA	1:I:35:PHE:CE1	2.47	0.49
2:J:1142:LEU:O	2:J:1150:ARG:NH2	2.45	0.49
1:A:641:ARG:NH2	1:A:925:ASP:OD2	2.45	0.49
1:A:1373:ARG:CZ	1:A:1550:ASP:HB2	2.43	0.49
2:G:954:VAL:HG11	2:G:984:PHE:HE1	1.77	0.49
2:G:1142:LEU:O	2:G:1150:ARG:NH2	2.45	0.49
2:C:1322:PRO:HG2	2:C:1325:PHE:HB2	1.93	0.49
1:D:1039:MET:HG3	1:D:1580:LEU:HD11	1.93	0.49
2:E:1314:ARG:HB2	2:E:1317:ARG:HD3	1.94	0.49
2:E:1537:ILE:HD12	2:E:1628:HIS:HD2	1.78	0.49
1:K:1505:GLN:O	1:K:1509:GLY:N	2.43	0.49
1:K:1687:PHE:C	1:K:1687:PHE:CD2	2.86	0.49
1:K:1751:GLU:HG3	1:K:1754:LYS:HE3	1.94	0.49
2:H:954:VAL:HG11	2:H:984:PHE:HE1	1.77	0.49
1:I:1578:LYS:HD2	1:I:1583:HIS:HA	1.94	0.49
1:A:1773:VAL:HG22	1:A:1879:VAL:HG22	1.94	0.49
2:G:65:LEU:HD11	2:G:88:LEU:HD23	1.94	0.49
2:G:1775:GLN:OE1	2:G:1839:GLN:NE2	2.44	0.49
1:B:1578:LYS:HD2	1:B:1583:HIS:HA	1.95	0.49
2:C:807:ILE:HG23	2:C:818:LYS:HB3	1.95	0.49
2:E:892:ILE:O	2:E:896:ASN:ND2	2.45	0.49
1:K:32:GLN:NE2	1:K:57:ALA:CA	2.76	0.49
1:F:1373:ARG:CZ	1:F:1550:ASP:HB2	2.43	0.49
1:F:1406:MET:HB3	1:F:1654:ILE:HG22	1.93	0.49
2:H:65:LEU:HD11	2:H:88:LEU:HD23	1.94	0.49
2:H:1142:LEU:O	2:H:1150:ARG:NH2	2.45	0.49
1:I:1373:ARG:CZ	1:I:1550:ASP:HB2	2.43	0.49
1:I:1673:TYR:CE1	1:I:1677:VAL:CG2	2.95	0.49
2:J:1267:TRP:NE1	2:J:1273:GLU:O	2.39	0.49
1:B:32:GLN:NE2	1:B:57:ALA:CA	2.76	0.49
2:C:846:VAL:HG21	2:C:856:LYS:HD2	1.94	0.49
2:C:1037:SER:OG	2:C:1053:ILE:CG1	2.61	0.49
1:D:1373:ARG:CZ	1:D:1550:ASP:HB2	2.43	0.49
2:E:1775:GLN:OE1	2:E:1839:GLN:NE2	2.44	0.49
1:K:413:LEU:HD12	1:K:439:ILE:HD13	1.95	0.49
1:K:950:THR:HA	1:K:953:VAL:HG12	1.93	0.49
1:F:1578:LYS:HD2	1:F:1583:HIS:HA	1.95	0.49
1:F:1751:GLU:HG3	1:F:1754:LYS:HE3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1322:PRO:HG2	2:H:1325:PHE:HB2	1.93	0.49
1:I:413:LEU:HD12	1:I:439:ILE:HD13	1.95	0.49
2:J:686:PRO:HB2	2:J:691:ALA:HB2	1.93	0.49
2:J:807:ILE:HG23	2:J:818:LYS:HB3	1.95	0.49
2:J:1736:MET:O	2:J:1751:ILE:HG13	2.13	0.49
1:A:32:GLN:NE2	1:A:57:ALA:CA	2.76	0.49
1:B:950:THR:HA	1:B:953:VAL:HG12	1.93	0.49
1:B:1673:TYR:CE1	1:B:1677:VAL:HG21	2.47	0.49
2:C:847:ARG:HG2	2:C:869:ASP:OD2	2.03	0.49
2:C:954:VAL:HG11	2:C:984:PHE:HE1	1.77	0.49
1:D:32:GLN:HA	1:D:35:PHE:CE1	2.47	0.49
1:D:950:THR:HA	1:D:953:VAL:HG12	1.93	0.49
1:D:1406:MET:HB3	1:D:1654:ILE:HG22	1.93	0.49
1:D:1751:GLU:HG3	1:D:1754:LYS:HE3	1.94	0.49
1:D:1775:LEU:HD23	1:D:1877:GLN:HB3	1.95	0.49
2:E:92:GLU:HA	2:E:96:LEU:HB2	1.94	0.49
1:K:688:ILE:HG13	1:K:875:THR:HG21	1.95	0.49
2:L:295:SER:O	2:L:298:LYS:CB	2.59	0.49
2:L:1309:GLU:O	2:L:1317:ARG:NH1	2.42	0.49
2:L:1639:LYS:NZ	2:L:1654:GLU:OE1	2.44	0.49
1:F:1017:ARG:NH1	1:F:1511:ASP:OD2	2.42	0.49
1:I:32:GLN:NE2	1:I:57:ALA:CA	2.76	0.49
2:J:503:ASP:HB3	2:J:529:VAL:HA	1.94	0.49
1:A:1673:TYR:CE1	1:A:1677:VAL:CG2	2.95	0.49
2:G:295:SER:O	2:G:298:LYS:CB	2.59	0.49
2:G:503:ASP:HB3	2:G:529:VAL:HA	1.94	0.49
2:C:848:SER:HB3	2:C:854:ILE:HD11	1.93	0.49
1:D:413:LEU:HD12	1:D:439:ILE:HD13	1.95	0.49
1:D:520:ARG:NH2	1:D:606:ASP:OD2	2.46	0.49
2:E:217:GLU:OE2	2:E:221:ASN:ND2	2.37	0.49
1:K:1775:LEU:HD23	1:K:1877:GLN:HB3	1.95	0.49
2:L:1048:VAL:O	2:L:1048:VAL:HG12	2.13	0.49
2:L:1537:ILE:HD12	2:L:1628:HIS:HD2	1.77	0.49
1:F:1673:TYR:CE1	1:F:1677:VAL:CG2	2.95	0.49
2:H:646:THR:OG1	2:H:677:GLN:OE1	2.28	0.49
2:H:892:ILE:O	2:H:896:ASN:ND2	2.45	0.49
2:H:1537:ILE:HD12	2:H:1628:HIS:HD2	1.77	0.49
2:H:1639:LYS:NZ	2:H:1654:GLU:OE1	2.44	0.49
1:I:1026:GLU:OE1	1:I:1594:ASN:ND2	2.40	0.49
1:I:1687:PHE:C	1:I:1687:PHE:CD2	2.86	0.49
1:I:1773:VAL:HG22	1:I:1879:VAL:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:846:VAL:HG21	2:G:856:LYS:HD2	1.94	0.49
2:G:1537:ILE:HD12	2:G:1628:HIS:HD2	1.77	0.49
1:B:413:LEU:HD12	1:B:439:ILE:HD13	1.95	0.49
1:D:32:GLN:NE2	1:D:57:ALA:CA	2.76	0.49
1:D:641:ARG:NH2	1:D:925:ASP:OD2	2.45	0.49
1:K:893:VAL:HG11	1:K:930:LEU:HD23	1.95	0.49
2:L:892:ILE:O	2:L:896:ASN:ND2	2.45	0.49
1:F:413:LEU:HD12	1:F:439:ILE:HD13	1.95	0.49
1:A:413:LEU:HD12	1:A:439:ILE:HD13	1.95	0.49
2:G:1736:MET:O	2:G:1751:ILE:HG13	2.13	0.49
2:C:503:ASP:HB3	2:C:529:VAL:HA	1.94	0.49
2:C:1314:ARG:HB2	2:C:1317:ARG:HD3	1.94	0.49
1:D:688:ILE:HG13	1:D:875:THR:HG21	1.95	0.49
2:L:1037:SER:OG	2:L:1053:ILE:CG1	2.61	0.49
2:J:372:ASN:HB3	2:J:515:LEU:HD21	1.95	0.49
2:J:846:VAL:HG21	2:J:856:LYS:HD2	1.94	0.49
1:A:520:ARG:NH2	1:A:606:ASP:OD2	2.46	0.48
2:G:807:ILE:HG23	2:G:818:LYS:HB3	1.95	0.48
1:B:1470:LEU:HD13	1:B:1489:ARG:HG2	1.95	0.48
1:D:781:LEU:HD12	1:D:784:ILE:HD12	1.95	0.48
1:K:520:ARG:NH2	1:K:606:ASP:OD2	2.46	0.48
1:K:1119:LYS:NZ	1:K:1337:GLU:OE2	2.46	0.48
1:F:1039:MET:HG3	1:F:1580:LEU:HD11	1.93	0.48
1:F:1673:TYR:CE1	1:F:1677:VAL:HG21	2.47	0.48
1:F:1687:PHE:C	1:F:1687:PHE:CD2	2.86	0.48
2:H:1037:SER:OG	2:H:1053:ILE:CG1	2.61	0.48
1:I:688:ILE:HG13	1:I:875:THR:HG21	1.95	0.48
1:A:893:VAL:HG11	1:A:930:LEU:HD23	1.95	0.48
2:C:1048:VAL:O	2:C:1048:VAL:HG12	2.13	0.48
2:C:1537:ILE:HD12	2:C:1628:HIS:HD2	1.77	0.48
2:E:372:ASN:HB3	2:E:515:LEU:HD21	1.95	0.48
1:K:1470:LEU:HD13	1:K:1489:ARG:HG2	1.95	0.48
1:K:1578:LYS:HD2	1:K:1583:HIS:HA	1.94	0.48
2:L:92:GLU:HA	2:L:96:LEU:HB2	1.94	0.48
2:L:686:PRO:HB2	2:L:691:ALA:HB2	1.93	0.48
1:F:32:GLN:NE2	1:F:57:ALA:CA	2.76	0.48
2:H:847:ARG:HG2	2:H:869:ASP:OD2	2.03	0.48
1:I:271:ASN:HB2	1:I:290:MET:HE1	1.94	0.48
2:J:1537:ILE:HD12	2:J:1628:HIS:HD2	1.78	0.48
1:A:1830:GLY:HA2	1:A:1831:GLY:HA2	1.62	0.48
2:C:143:SER:OG	2:C:547:ILE:O	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1119:LYS:NZ	1:D:1337:GLU:OE2	2.46	0.48
2:E:503:ASP:HB3	2:E:529:VAL:HA	1.94	0.48
2:L:1182:VAL:HG22	2:L:1197:LEU:HD23	1.95	0.48
2:L:1697:HIS:O	2:L:1701:THR:OG1	2.28	0.48
1:F:1505:GLN:O	1:F:1509:GLY:N	2.43	0.48
2:G:1737:ILE:CD1	2:G:1737:ILE:N	2.73	0.48
1:B:520:ARG:NH2	1:B:606:ASP:OD2	2.46	0.48
1:B:844:LEU:CD2	1:K:848:THR:HG23	2.43	0.48
1:B:1373:ARG:CZ	1:B:1550:ASP:HB2	2.43	0.48
2:C:1182:VAL:HG22	2:C:1197:LEU:HD23	1.95	0.48
1:D:848:THR:HG23	1:I:844:LEU:CD2	2.43	0.48
1:D:1026:GLU:OE1	1:D:1594:ASN:ND2	2.40	0.48
1:D:1470:LEU:HD13	1:D:1489:ARG:HG2	1.95	0.48
2:E:1736:MET:O	2:E:1751:ILE:HG13	2.13	0.48
2:L:807:ILE:HG23	2:L:818:LYS:HB3	1.95	0.48
2:L:1740:THR:O	2:L:1740:THR:OG1	2.31	0.48
1:F:781:LEU:HD12	1:F:784:ILE:HD12	1.95	0.48
1:F:1467:LEU:HD22	1:F:1757:GLU:OE2	2.14	0.48
2:H:1736:MET:O	2:H:1751:ILE:HG13	2.13	0.48
2:J:1037:SER:OG	2:J:1053:ILE:CG1	2.61	0.48
2:G:372:ASN:HB3	2:G:515:LEU:HD21	1.95	0.48
1:B:688:ILE:HG13	1:B:875:THR:HG21	1.94	0.48
2:C:1639:LYS:NZ	2:C:1654:GLU:OE1	2.44	0.48
1:D:18:LEU:HD13	2:E:1812:TYR:HE1	1.79	0.48
1:D:893:VAL:HG11	1:D:930:LEU:HD23	1.95	0.48
1:D:1030:TRP:O	1:D:1035:THR:OG1	2.31	0.48
1:K:18:LEU:HD13	2:L:1812:TYR:HE1	1.79	0.48
1:K:1373:ARG:CZ	1:K:1550:ASP:HB2	2.43	0.48
1:F:520:ARG:NH2	1:F:606:ASP:OD2	2.46	0.48
1:F:1470:LEU:HD13	1:F:1489:ARG:HG2	1.95	0.48
1:F:1775:LEU:HD23	1:F:1877:GLN:HB3	1.95	0.48
2:H:1767:GLU:OE2	2:H:1849:ARG:NE	2.36	0.48
2:J:596:GLY:N	2:J:618:GLU:OE1	2.46	0.48
2:J:1182:VAL:HG22	2:J:1197:LEU:HD23	1.96	0.48
1:A:688:ILE:HG13	1:A:875:THR:HG21	1.95	0.48
2:G:607:VAL:HG11	2:G:619:LEU:HD13	1.96	0.48
2:G:1048:VAL:O	2:G:1048:VAL:HG12	2.13	0.48
2:G:1182:VAL:HG22	2:G:1197:LEU:HD23	1.95	0.48
2:G:1309:GLU:O	2:G:1317:ARG:NH1	2.42	0.48
2:G:1639:LYS:NZ	2:G:1654:GLU:OE1	2.44	0.48
1:B:254:TRP:NE1	1:B:288:ASP:OD1	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1775:LEU:HD23	1:B:1877:GLN:HB3	1.95	0.48
2:C:686:PRO:HB2	2:C:691:ALA:HB2	1.93	0.48
2:C:1736:MET:O	2:C:1751:ILE:HG13	2.13	0.48
1:D:868:ILE:HB	1:D:925:ASP:HA	1.95	0.48
1:D:1173:LEU:HD13	1:F:1173:LEU:HD13	1.96	0.48
2:E:1048:VAL:O	2:E:1048:VAL:HG12	2.13	0.48
1:F:46:GLU:OE2	2:H:1667:THR:OG1	2.32	0.48
1:F:893:VAL:HG11	1:F:930:LEU:HD23	1.95	0.48
2:H:372:ASN:HB3	2:H:515:LEU:HD21	1.95	0.48
1:I:1470:LEU:HD13	1:I:1489:ARG:HG2	1.95	0.48
1:I:1486:LEU:HD21	1:I:1761:LYS:HZ2	1.78	0.48
2:J:1697:HIS:O	2:J:1701:THR:OG1	2.28	0.48
1:A:781:LEU:HD12	1:A:784:ILE:HD12	1.95	0.48
2:G:836:TYR:HD1	2:G:845:THR:HG21	1.55	0.48
1:B:1119:LYS:NZ	1:B:1337:GLU:OE2	2.46	0.48
1:B:1173:LEU:HD13	1:I:1173:LEU:HD13	1.96	0.48
2:C:277:LEU:HD21	2:C:468:LEU:HD11	1.96	0.48
2:C:372:ASN:HB3	2:C:515:LEU:HD21	1.95	0.48
2:C:1737:ILE:HG12	2:C:1748:THR:HG22	1.95	0.48
1:D:1578:LYS:HD2	1:D:1583:HIS:HA	1.94	0.48
1:K:868:ILE:HB	1:K:925:ASP:HA	1.95	0.48
1:K:1751:GLU:HG3	1:K:1754:LYS:HZ2	1.77	0.48
1:F:254:TRP:NE1	1:F:288:ASP:OD1	2.42	0.48
2:J:607:VAL:HG11	2:J:619:LEU:HD13	1.96	0.48
1:A:848:THR:HG23	1:F:844:LEU:CD2	2.43	0.48
1:A:1173:LEU:HD13	1:K:1173:LEU:HD13	1.96	0.48
1:A:1467:LEU:HD22	1:A:1757:GLU:OE2	2.14	0.48
1:A:1470:LEU:HD13	1:A:1489:ARG:HG2	1.95	0.48
1:B:1467:LEU:HD22	1:B:1757:GLU:OE2	2.14	0.48
1:D:1467:LEU:HD22	1:D:1757:GLU:OE2	2.14	0.48
2:L:1736:MET:O	2:L:1751:ILE:HG13	2.13	0.48
1:F:1751:GLU:HG3	1:F:1754:LYS:HZ2	1.73	0.48
2:H:1737:ILE:CD1	2:H:1737:ILE:N	2.73	0.48
1:I:18:LEU:HD13	2:J:1812:TYR:HE1	1.79	0.48
1:A:1486:LEU:HD21	1:A:1761:LYS:HZ2	1.78	0.48
1:B:893:VAL:HG11	1:B:930:LEU:HD23	1.95	0.48
1:D:848:THR:CG2	1:I:844:LEU:HD23	2.44	0.48
2:E:143:SER:OG	2:E:547:ILE:O	2.29	0.48
2:E:1037:SER:OG	2:E:1053:ILE:CG1	2.61	0.48
1:K:1484:GLU:OE2	1:K:1741:LYS:NZ	2.47	0.48
2:L:646:THR:OG1	2:L:677:GLN:OE1	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1314:ARG:HB2	2:H:1317:ARG:HD3	1.94	0.48
2:J:954:VAL:HG11	2:J:984:PHE:HE1	1.77	0.48
1:A:18:LEU:HD13	2:G:1812:TYR:HE1	1.79	0.48
1:A:868:ILE:HB	1:A:925:ASP:HA	1.95	0.48
2:E:807:ILE:HG23	2:E:818:LYS:HB3	1.95	0.48
1:K:781:LEU:HD12	1:K:784:ILE:HD12	1.95	0.48
2:H:249:TYR:HE2	2:H:260:PRO:HB3	1.79	0.48
2:H:807:ILE:HG23	2:H:818:LYS:HB3	1.95	0.48
1:I:1030:TRP:O	1:I:1035:THR:OG1	2.31	0.48
2:J:277:LEU:HD21	2:J:468:LEU:HD11	1.96	0.48
1:B:781:LEU:HD12	1:B:784:ILE:HD12	1.95	0.47
1:D:400:ARG:NH1	1:D:1358:HIS:O	2.40	0.47
1:K:1467:LEU:HD22	1:K:1757:GLU:OE2	2.14	0.47
2:H:490:TRP:HE1	2:H:516:THR:HG22	1.79	0.47
1:I:520:ARG:NH2	1:I:606:ASP:OD2	2.46	0.47
2:J:1048:VAL:O	2:J:1048:VAL:HG12	2.13	0.47
1:A:844:LEU:HD23	1:F:848:THR:CG2	2.44	0.47
2:G:490:TRP:HE1	2:G:516:THR:HG22	1.79	0.47
1:B:1030:TRP:O	1:B:1035:THR:OG1	2.31	0.47
1:A:1775:LEU:HD23	1:A:1877:GLN:HB3	1.95	0.47
2:G:847:ARG:HG2	2:G:869:ASP:OD2	2.03	0.47
1:B:18:LEU:HD13	2:C:1812:TYR:HE1	1.79	0.47
1:B:1484:GLU:OE2	1:B:1741:LYS:NZ	2.47	0.47
1:D:1505:GLN:O	1:D:1509:GLY:N	2.43	0.47
1:D:1744:TYR:C	1:D:1747:ALA:CB	2.75	0.47
2:E:249:TYR:HE2	2:E:260:PRO:HB3	1.79	0.47
2:L:277:LEU:HD21	2:L:468:LEU:HD11	1.96	0.47
1:F:1119:LYS:NZ	1:F:1337:GLU:OE2	2.46	0.47
2:H:217:GLU:OE2	2:H:221:ASN:ND2	2.37	0.47
2:H:503:ASP:HB3	2:H:529:VAL:HA	1.94	0.47
2:H:607:VAL:HG11	2:H:619:LEU:HD13	1.96	0.47
2:H:1048:VAL:HG12	2:H:1048:VAL:O	2.13	0.47
1:I:1119:LYS:NZ	1:I:1337:GLU:OE2	2.46	0.47
1:I:1775:LEU:HD23	1:I:1877:GLN:HB3	1.95	0.47
2:J:1737:ILE:HG12	2:J:1748:THR:HG22	1.95	0.47
2:J:1737:ILE:CD1	2:J:1737:ILE:N	2.73	0.47
1:A:844:LEU:CD2	1:F:848:THR:HG23	2.43	0.47
1:B:1744:TYR:C	1:B:1747:ALA:CB	2.75	0.47
2:E:234:ILE:HG22	2:E:307:GLY:HA2	1.96	0.47
1:K:539:SER:HB2	1:K:633:GLU:HA	1.97	0.47
1:K:1030:TRP:O	1:K:1035:THR:OG1	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:143:SER:OG	2:L:547:ILE:O	2.29	0.47
2:L:372:ASN:HB3	2:L:515:LEU:HD21	1.95	0.47
1:F:868:ILE:HB	1:F:925:ASP:HA	1.95	0.47
2:H:1737:ILE:HG12	2:H:1748:THR:HG22	1.95	0.47
1:I:781:LEU:HD12	1:I:784:ILE:HD12	1.95	0.47
1:I:1484:GLU:OE2	1:I:1741:LYS:NZ	2.47	0.47
2:J:646:THR:HB	2:J:677:GLN:CB	2.26	0.47
1:A:848:THR:CG2	1:F:844:LEU:HD23	2.44	0.47
1:B:868:ILE:HB	1:B:925:ASP:HA	1.95	0.47
2:E:553:ASN:O	2:E:556:LYS:NZ	2.39	0.47
2:L:607:VAL:HG11	2:L:619:LEU:HD13	1.96	0.47
1:F:688:ILE:HG13	1:F:875:THR:HG21	1.94	0.47
1:I:1467:LEU:HD22	1:I:1757:GLU:OE2	2.14	0.47
2:J:313:ALA:HB2	2:J:435:ALA:HB2	1.97	0.47
1:A:1010:GLU:HA	1:A:1664:ALA:HA	1.96	0.47
2:C:313:ALA:HB2	2:C:435:ALA:HB2	1.97	0.47
2:C:691:ALA:HA	2:C:694:TYR:HD2	1.80	0.47
2:E:736:ARG:NE	2:E:769:SER:O	2.48	0.47
2:L:490:TRP:HE1	2:L:516:THR:HG22	1.79	0.47
1:F:1030:TRP:O	1:F:1035:THR:OG1	2.31	0.47
1:F:1484:GLU:OE2	1:F:1741:LYS:NZ	2.47	0.47
1:A:1119:LYS:NZ	1:A:1337:GLU:OE2	2.46	0.47
1:A:1484:GLU:OE2	1:A:1741:LYS:NZ	2.47	0.47
2:G:249:TYR:HE2	2:G:260:PRO:HB3	1.79	0.47
2:G:736:ARG:NE	2:G:769:SER:O	2.48	0.47
2:C:596:GLY:N	2:C:618:GLU:OE1	2.46	0.47
2:C:607:VAL:HG11	2:C:619:LEU:HD13	1.96	0.47
2:C:1267:TRP:NE1	2:C:1273:GLU:O	2.39	0.47
1:D:1486:LEU:HD21	1:D:1761:LYS:HZ2	1.79	0.47
2:E:1737:ILE:CD1	2:E:1737:ILE:N	2.73	0.47
2:E:1908:ASP:HA	2:E:1911:THR:HG22	1.97	0.47
2:L:596:GLY:N	2:L:618:GLU:OE1	2.46	0.47
1:F:1010:GLU:HA	1:F:1664:ALA:HA	1.96	0.47
1:I:539:SER:HB2	1:I:633:GLU:HA	1.97	0.47
2:J:490:TRP:HE1	2:J:516:THR:HG22	1.79	0.47
2:J:587:ILE:HG13	2:J:589:ARG:H	1.80	0.47
2:G:313:ALA:HB2	2:G:435:ALA:HB2	1.97	0.47
2:G:587:ILE:HG13	2:G:589:ARG:H	1.80	0.47
1:B:18:LEU:HD13	2:C:1812:TYR:CE1	2.50	0.47
2:C:234:ILE:HG22	2:C:307:GLY:HA2	1.96	0.47
1:D:1271:GLN:HB2	1:D:1274:ILE:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1428:THR:OG1	1:D:1652:GLN:NE2	2.48	0.47
2:E:277:LEU:HD21	2:E:468:LEU:HD11	1.96	0.47
2:E:1697:HIS:O	2:E:1701:THR:OG1	2.28	0.47
2:E:1855:ILE:HD12	2:E:1907:LEU:HG	1.97	0.47
1:K:1010:GLU:HA	1:K:1664:ALA:HA	1.96	0.47
1:K:1428:THR:OG1	1:K:1652:GLN:NE2	2.48	0.47
2:L:1908:ASP:HA	2:L:1911:THR:HG22	1.97	0.47
2:H:234:ILE:HG22	2:H:307:GLY:HA2	1.96	0.47
2:H:587:ILE:HG13	2:H:589:ARG:H	1.80	0.47
2:H:1182:VAL:HG22	2:H:1197:LEU:HD23	1.95	0.47
2:H:1267:TRP:NE1	2:H:1273:GLU:O	2.39	0.47
2:H:1908:ASP:HA	2:H:1911:THR:HG22	1.97	0.47
1:I:893:VAL:HG11	1:I:930:LEU:HD23	1.95	0.47
2:J:249:TYR:HE2	2:J:260:PRO:HB3	1.79	0.47
1:A:1030:TRP:O	1:A:1035:THR:OG1	2.31	0.47
2:G:1037:SER:OG	2:G:1053:ILE:CG1	2.61	0.47
2:C:54:PRO:HG3	2:C:63:LYS:HG3	1.97	0.47
2:C:1691:TRP:O	2:C:1695:ASP:N	2.40	0.47
2:C:1908:ASP:HA	2:C:1911:THR:HG22	1.97	0.47
2:E:691:ALA:HA	2:E:694:TYR:HD2	1.80	0.47
2:E:1381:VAL:O	2:E:1422:THR:OG1	2.28	0.47
2:L:587:ILE:HG13	2:L:589:ARG:H	1.80	0.47
2:L:691:ALA:HA	2:L:694:TYR:HD2	1.80	0.47
2:L:736:ARG:NE	2:L:769:SER:O	2.48	0.47
2:L:1855:ILE:HD12	2:L:1907:LEU:HG	1.97	0.47
1:F:18:LEU:HD13	2:H:1812:TYR:HE1	1.79	0.47
1:F:1271:GLN:HB2	1:F:1274:ILE:HG23	1.97	0.47
2:H:691:ALA:HA	2:H:694:TYR:HD2	1.80	0.47
2:H:1855:ILE:HD12	2:H:1907:LEU:HG	1.97	0.47
2:J:1691:TRP:O	2:J:1695:ASP:N	2.40	0.47
2:G:1908:ASP:HA	2:G:1911:THR:HG22	1.97	0.47
1:B:401:THR:HG22	1:B:733:ILE:HG12	1.97	0.47
1:B:1792:THR:HG21	1:B:1838:GLU:HG2	1.97	0.47
2:C:490:TRP:HE1	2:C:516:THR:HG22	1.79	0.47
1:D:539:SER:HB2	1:D:633:GLU:HA	1.97	0.47
2:E:490:TRP:HE1	2:E:516:THR:HG22	1.79	0.47
2:E:596:GLY:HA3	2:E:650:ASN:HD22	1.80	0.47
1:K:18:LEU:HD13	2:L:1812:TYR:CE1	2.50	0.47
2:L:313:ALA:HB2	2:L:435:ALA:HB2	1.97	0.47
1:F:1226:SER:O	1:F:1226:SER:OG	2.32	0.47
2:G:277:LEU:HD21	2:G:468:LEU:HD11	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1740:THR:O	2:G:1740:THR:OG1	2.31	0.46
2:G:1767:GLU:OE2	2:G:1849:ARG:NE	2.36	0.46
2:G:1855:ILE:HD12	2:G:1907:LEU:HG	1.97	0.46
1:B:1010:GLU:HA	1:B:1664:ALA:HA	1.96	0.46
2:C:1422:THR:HG23	2:C:1474:PHE:HB2	1.97	0.46
1:D:18:LEU:HD13	2:E:1812:TYR:CE1	2.50	0.46
1:D:46:GLU:OE2	2:E:1667:THR:OG1	2.32	0.46
1:D:254:TRP:NE1	1:D:288:ASP:OD1	2.42	0.46
1:D:1484:GLU:OE2	1:D:1741:LYS:NZ	2.47	0.46
2:E:462:THR:HG21	2:E:488:VAL:HG22	1.98	0.46
1:K:1017:ARG:NH1	1:K:1511:ASP:OD2	2.42	0.46
1:K:1852:HIS:HA	1:K:1856:LYS:HE3	1.97	0.46
2:L:1037:SER:OG	2:L:1053:ILE:HD11	2.16	0.46
2:H:736:ARG:NE	2:H:769:SER:O	2.48	0.46
2:J:234:ILE:HG22	2:J:307:GLY:HA2	1.96	0.46
1:B:1852:HIS:HA	1:B:1856:LYS:HE3	1.97	0.46
1:D:1792:THR:HG21	1:D:1838:GLU:HG2	1.97	0.46
2:L:249:TYR:HE2	2:L:260:PRO:HB3	1.79	0.46
2:L:462:THR:HG21	2:L:488:VAL:HG22	1.98	0.46
2:L:596:GLY:HA3	2:L:650:ASN:HD22	1.81	0.46
2:L:1737:ILE:HG12	2:L:1748:THR:HG22	1.95	0.46
1:F:1792:THR:HG21	1:F:1838:GLU:HG2	1.97	0.46
1:I:868:ILE:HB	1:I:925:ASP:HA	1.95	0.46
1:I:1010:GLU:HA	1:I:1664:ALA:HA	1.96	0.46
2:J:691:ALA:HA	2:J:694:TYR:HD2	1.80	0.46
2:J:1037:SER:OG	2:J:1053:ILE:HD11	2.16	0.46
1:A:254:TRP:NE1	1:A:288:ASP:OD1	2.42	0.46
2:G:1037:SER:OG	2:G:1053:ILE:HD11	2.16	0.46
2:G:1691:TRP:O	2:G:1695:ASP:N	2.40	0.46
2:C:249:TYR:HE2	2:C:260:PRO:HB3	1.79	0.46
1:D:32:GLN:NE2	1:D:57:ALA:CB	2.78	0.46
2:E:864:LEU:HD22	2:E:898:ASP:HB2	1.97	0.46
1:F:18:LEU:HD13	2:H:1812:TYR:CE1	2.50	0.46
2:H:313:ALA:HB2	2:H:435:ALA:HB2	1.97	0.46
1:I:18:LEU:HD13	2:J:1812:TYR:CE1	2.50	0.46
1:I:1792:THR:HG21	1:I:1838:GLU:HG2	1.97	0.46
1:A:1428:THR:OG1	1:A:1652:GLN:NE2	2.48	0.46
2:G:462:THR:HG21	2:G:488:VAL:HG22	1.98	0.46
1:B:1226:SER:O	1:B:1226:SER:OG	2.32	0.46
2:C:587:ILE:HG13	2:C:589:ARG:H	1.80	0.46
2:C:835:THR:HG23	2:C:843:ILE:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1561:MET:N	1:D:1561:MET:HE3	2.31	0.46
2:E:1182:VAL:HG22	2:E:1197:LEU:HD23	1.96	0.46
1:K:254:TRP:NE1	1:K:288:ASP:OD1	2.42	0.46
2:L:234:ILE:HG22	2:L:307:GLY:HA2	1.96	0.46
2:L:864:LEU:HD22	2:L:898:ASP:HB2	1.98	0.46
1:F:32:GLN:NE2	1:F:57:ALA:CB	2.79	0.46
1:F:1428:THR:OG1	1:F:1652:GLN:NE2	2.48	0.46
2:H:462:THR:HG21	2:H:488:VAL:HG22	1.98	0.46
2:H:596:GLY:HA3	2:H:650:ASN:HD22	1.81	0.46
1:I:401:THR:HG22	1:I:733:ILE:HG12	1.97	0.46
2:J:736:ARG:NE	2:J:769:SER:O	2.48	0.46
1:A:1503:ALA:HA	1:A:1506:GLN:HE21	1.81	0.46
2:G:835:THR:HG23	2:G:843:ILE:O	2.16	0.46
2:G:860:ARG:NH2	2:G:1047:ASP:OD2	2.49	0.46
1:B:488:PRO:HG3	1:B:728:LYS:HG2	1.97	0.46
1:B:1428:THR:OG1	1:B:1652:GLN:NE2	2.48	0.46
2:C:462:THR:HG21	2:C:488:VAL:HG22	1.98	0.46
2:C:1638:ILE:HD13	2:C:1657:ILE:HD13	1.98	0.46
1:D:1852:HIS:HA	1:D:1856:LYS:HE3	1.97	0.46
2:E:313:ALA:HB2	2:E:435:ALA:HB2	1.97	0.46
2:L:1037:SER:CB	2:L:1053:ILE:CG1	2.92	0.46
2:L:1737:ILE:CD1	2:L:1737:ILE:N	2.73	0.46
1:F:678:VAL:HG22	1:F:767:ALA:HB3	1.98	0.46
2:J:835:THR:HG23	2:J:843:ILE:O	2.16	0.46
1:A:539:SER:HB2	1:A:633:GLU:HA	1.97	0.46
2:G:691:ALA:HA	2:G:694:TYR:HD2	1.80	0.46
2:G:1177:SER:OG	2:G:1180:MET:SD	2.63	0.46
1:D:678:VAL:HG22	1:D:767:ALA:HB3	1.98	0.46
2:E:1767:GLU:OE2	2:E:1849:ARG:NE	2.36	0.46
1:K:1503:ALA:HA	1:K:1506:GLN:HE21	1.81	0.46
2:L:245:GLN:HE21	2:L:506:PRO:HD3	1.81	0.46
2:L:1422:THR:HG23	2:L:1474:PHE:HB2	1.97	0.46
2:H:326:ASP:OD2	2:H:387:TYR:OH	2.33	0.46
2:H:900:GLN:HB3	2:H:1050:ARG:O	2.16	0.46
2:H:1697:HIS:O	2:H:1701:THR:OG1	2.28	0.46
2:J:295:SER:O	2:J:298:LYS:CB	2.59	0.46
2:J:1422:THR:HG23	2:J:1474:PHE:HB2	1.97	0.46
1:A:18:LEU:HD13	2:G:1812:TYR:CE1	2.50	0.46
1:A:1226:SER:O	1:A:1226:SER:OG	2.32	0.46
1:B:1017:ARG:NH1	1:B:1511:ASP:OD2	2.42	0.46
2:C:736:ARG:NE	2:C:769:SER:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1037:SER:OG	2:C:1053:ILE:HD11	2.16	0.46
2:C:1292:ILE:HD11	2:C:1366:LEU:HD23	1.98	0.46
2:C:1855:ILE:HD12	2:C:1907:LEU:HG	1.97	0.46
1:K:1271:GLN:HB2	1:K:1274:ILE:HG23	1.97	0.46
2:L:1292:ILE:HD11	2:L:1366:LEU:HD23	1.98	0.46
2:L:1638:ILE:HD13	2:L:1657:ILE:HD13	1.98	0.46
2:H:54:PRO:HG3	2:H:63:LYS:HG3	1.97	0.46
2:H:835:THR:HG23	2:H:843:ILE:O	2.16	0.46
2:H:1691:TRP:O	2:H:1695:ASP:N	2.40	0.46
2:J:716:VAL:HG11	2:J:730:LEU:HD13	1.98	0.46
2:J:860:ARG:NH2	2:J:1047:ASP:OD2	2.49	0.46
2:J:1638:ILE:HD13	2:J:1657:ILE:HD13	1.98	0.46
2:J:1855:ILE:HD12	2:J:1907:LEU:HG	1.97	0.46
2:J:1908:ASP:HA	2:J:1911:THR:HG22	1.97	0.46
1:A:401:THR:HG22	1:A:733:ILE:HG12	1.97	0.46
1:A:678:VAL:HG22	1:A:767:ALA:HB3	1.98	0.46
2:G:234:ILE:HG22	2:G:307:GLY:HA2	1.96	0.46
2:G:596:GLY:HA3	2:G:650:ASN:HD22	1.81	0.46
1:B:539:SER:HB2	1:B:633:GLU:HA	1.97	0.46
2:C:596:GLY:HA3	2:C:650:ASN:HD22	1.81	0.46
2:C:864:LEU:HD22	2:C:898:ASP:HB2	1.98	0.46
1:D:488:PRO:HG3	1:D:728:LYS:HG2	1.97	0.46
2:E:295:SER:O	2:E:298:LYS:CB	2.59	0.46
2:E:587:ILE:HG13	2:E:589:ARG:H	1.80	0.46
2:E:607:VAL:HG11	2:E:619:LEU:HD13	1.96	0.46
2:E:716:VAL:HG11	2:E:730:LEU:HD13	1.98	0.46
2:E:1037:SER:CB	2:E:1053:ILE:CG1	2.92	0.46
2:L:716:VAL:HG11	2:L:730:LEU:HD13	1.98	0.46
2:H:277:LEU:HD21	2:H:468:LEU:HD11	1.96	0.46
1:A:1792:THR:HG21	1:A:1838:GLU:HG2	1.97	0.46
1:A:1852:HIS:HA	1:A:1856:LYS:HE3	1.97	0.46
2:C:326:ASP:OD2	2:C:387:TYR:OH	2.33	0.46
1:D:401:THR:HG22	1:D:733:ILE:HG12	1.97	0.46
1:D:1010:GLU:HA	1:D:1664:ALA:HA	1.96	0.46
1:D:1545:SER:O	1:D:1545:SER:OG	2.27	0.46
2:E:646:THR:HB	2:E:677:GLN:CB	2.26	0.46
1:K:400:ARG:NH1	1:K:1358:HIS:O	2.40	0.46
2:H:143:SER:OG	2:H:547:ILE:O	2.29	0.46
2:H:259:THR:OG1	2:H:288:SER:HA	2.16	0.46
1:I:1428:THR:OG1	1:I:1652:GLN:NE2	2.48	0.46
2:J:245:GLN:HE21	2:J:506:PRO:HD3	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:462:THR:HG21	2:J:488:VAL:HG22	1.98	0.46
1:A:32:GLN:NE2	1:A:57:ALA:CB	2.79	0.46
2:G:1736:MET:HE2	2:G:1736:MET:CA	2.45	0.46
1:B:430:ARG:HG2	1:B:605:LEU:HD22	1.98	0.46
2:E:1037:SER:OG	2:E:1053:ILE:HD11	2.16	0.46
1:F:488:PRO:HG3	1:F:728:LYS:HG2	1.97	0.46
1:F:1303:GLY:HA2	1:F:1649:LYS:HZ1	1.81	0.46
2:J:1338:ILE:HG22	2:J:1390:VAL:HG11	1.98	0.46
1:A:430:ARG:HG2	1:A:605:LEU:HD22	1.98	0.45
1:A:1271:GLN:HB2	1:A:1274:ILE:HG23	1.97	0.45
2:G:54:PRO:HG3	2:G:63:LYS:HG3	1.97	0.45
1:B:937:LYS:HD2	1:K:855:SER:HB2	1.98	0.45
1:B:1503:ALA:HA	1:B:1506:GLN:HE21	1.81	0.45
2:C:646:THR:HB	2:C:677:GLN:CB	2.26	0.45
2:C:1740:THR:O	2:C:1740:THR:OG1	2.31	0.45
1:D:937:LYS:HD2	1:I:855:SER:HB2	1.98	0.45
2:E:54:PRO:HG3	2:E:63:LYS:HG3	1.97	0.45
2:E:860:ARG:NH2	2:E:1047:ASP:OD2	2.49	0.45
2:E:900:GLN:HB3	2:E:1050:ARG:O	2.16	0.45
2:L:835:THR:HG23	2:L:843:ILE:O	2.16	0.45
2:L:860:ARG:NH2	2:L:1047:ASP:OD2	2.49	0.45
2:L:1811:GLU:OE2	2:L:2010:TYR:OH	2.29	0.45
1:F:1852:HIS:HA	1:F:1856:LYS:HE3	1.97	0.45
1:I:678:VAL:HG22	1:I:767:ALA:HB3	1.98	0.45
1:I:1503:ALA:HA	1:I:1506:GLN:HE21	1.81	0.45
2:J:596:GLY:HA3	2:J:650:ASN:HD22	1.80	0.45
2:J:646:THR:OG1	2:J:677:GLN:OE1	2.28	0.45
2:G:646:THR:HB	2:G:677:GLN:CB	2.26	0.45
2:G:716:VAL:HG11	2:G:730:LEU:HD13	1.98	0.45
2:G:900:GLN:HB3	2:G:1050:ARG:O	2.16	0.45
1:B:32:GLN:NE2	1:B:57:ALA:CB	2.79	0.45
2:C:716:VAL:HG11	2:C:730:LEU:HD13	1.98	0.45
2:C:900:GLN:HB3	2:C:1050:ARG:O	2.16	0.45
1:D:431:GLU:O	1:D:435:GLU:N	2.49	0.45
1:D:844:LEU:HD23	1:I:848:THR:CG2	2.44	0.45
1:D:1503:ALA:HA	1:D:1506:GLN:HE21	1.81	0.45
2:E:259:THR:OG1	2:E:288:SER:HA	2.16	0.45
2:E:1338:ILE:HG22	2:E:1390:VAL:HG11	1.98	0.45
1:K:32:GLN:NE2	1:K:57:ALA:CB	2.79	0.45
1:K:401:THR:HG22	1:K:733:ILE:HG12	1.97	0.45
1:K:719:GLN:HG3	1:K:1612:ASP:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:54:PRO:HG3	2:L:63:LYS:HG3	1.97	0.45
2:L:259:THR:OG1	2:L:288:SER:HA	2.16	0.45
2:L:278:VAL:HB	2:L:479:ILE:HD13	1.99	0.45
2:H:1338:ILE:HG22	2:H:1390:VAL:HG11	1.98	0.45
1:I:402:PHE:HE1	1:I:1612:ASP:HB2	1.81	0.45
2:J:1292:ILE:HD11	2:J:1366:LEU:HD23	1.98	0.45
2:G:1195:VAL:HG13	2:G:1211:LEU:HB3	1.98	0.45
1:B:855:SER:HB2	1:K:937:LYS:HD2	1.98	0.45
2:E:1638:ILE:HD13	2:E:1657:ILE:HD13	1.98	0.45
1:F:719:GLN:HG3	1:F:1612:ASP:HA	1.99	0.45
2:H:808:ALA:HB3	2:H:811:VAL:HG13	1.98	0.45
2:H:864:LEU:HD22	2:H:898:ASP:HB2	1.98	0.45
2:H:1195:VAL:HG13	2:H:1211:LEU:HB3	1.99	0.45
2:H:1370:ASP:OD1	2:H:1370:ASP:N	2.50	0.45
1:I:488:PRO:HG3	1:I:728:LYS:HG2	1.97	0.45
2:J:54:PRO:HG3	2:J:63:LYS:HG3	1.97	0.45
1:A:855:SER:HB2	1:F:937:LYS:HD2	1.98	0.45
2:G:259:THR:OG1	2:G:288:SER:HA	2.16	0.45
2:G:1638:ILE:HD13	2:G:1657:ILE:HD13	1.98	0.45
1:B:402:PHE:HE1	1:B:1612:ASP:HB2	1.81	0.45
2:C:860:ARG:NH2	2:C:1047:ASP:OD2	2.49	0.45
2:C:1036:GLN:HB3	2:C:1051:THR:CG2	2.24	0.45
2:C:1850:SER:HB3	2:C:1973:SER:HB2	1.99	0.45
1:D:1226:SER:O	1:D:1226:SER:OG	2.32	0.45
1:D:1233:GLU:OE2	1:D:1680:ARG:NH1	2.50	0.45
2:E:326:ASP:OD2	2:E:387:TYR:OH	2.33	0.45
2:E:1292:ILE:HD11	2:E:1366:LEU:HD23	1.98	0.45
1:K:448:ILE:HD13	1:K:481:LYS:HG2	1.99	0.45
1:K:1792:THR:HG21	1:K:1838:GLU:HG2	1.97	0.45
2:L:1330:GLY:HA2	2:L:1374:THR:HG21	1.99	0.45
1:F:1486:LEU:HD21	1:F:1761:LYS:HZ2	1.81	0.45
2:H:245:GLN:HE21	2:H:506:PRO:HD3	1.81	0.45
1:I:400:ARG:NH1	1:I:1358:HIS:O	2.40	0.45
1:I:1107:GLU:OE1	1:I:1191:THR:OG1	2.29	0.45
2:G:245:GLN:HE21	2:G:506:PRO:HD3	1.81	0.45
2:C:259:THR:OG1	2:C:288:SER:HA	2.16	0.45
2:C:320:PRO:HA	2:C:321:PRO:HD3	1.89	0.45
2:C:1338:ILE:HG22	2:C:1390:VAL:HG11	1.98	0.45
2:E:1422:THR:HG23	2:E:1474:PHE:HB2	1.97	0.45
1:K:678:VAL:HG22	1:K:767:ALA:HB3	1.98	0.45
2:H:716:VAL:HG11	2:H:730:LEU:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1037:SER:OG	2:H:1053:ILE:HD11	2.16	0.45
2:H:1638:ILE:HD13	2:H:1657:ILE:HD13	1.98	0.45
2:J:278:VAL:HB	2:J:479:ILE:HD13	1.99	0.45
2:J:1850:SER:HB3	2:J:1973:SER:HB2	1.99	0.45
1:A:402:PHE:HE1	1:A:1612:ASP:HB2	1.81	0.45
1:A:1303:GLY:HA2	1:A:1649:LYS:HZ2	1.81	0.45
2:G:1338:ILE:HG22	2:G:1390:VAL:HG11	1.98	0.45
1:B:678:VAL:HG22	1:B:767:ALA:HB3	1.98	0.45
1:B:1107:GLU:OE1	1:B:1191:THR:OG1	2.29	0.45
2:C:245:GLN:HE21	2:C:506:PRO:HD3	1.81	0.45
2:E:808:ALA:HB3	2:E:811:VAL:HG13	1.98	0.45
2:E:835:THR:HG23	2:E:843:ILE:O	2.16	0.45
2:E:1330:GLY:HA2	2:E:1374:THR:HG21	1.99	0.45
1:K:1107:GLU:OE1	1:K:1191:THR:OG1	2.29	0.45
1:K:1233:GLU:OE2	1:K:1680:ARG:NH1	2.50	0.45
1:F:1830:GLY:HA2	1:F:1831:GLY:HA2	1.62	0.45
1:I:1226:SER:O	1:I:1226:SER:OG	2.32	0.45
2:J:259:THR:OG1	2:J:288:SER:HA	2.16	0.45
2:J:1800:ALA:O	2:J:2009:LYS:NZ	2.47	0.45
2:G:847:ARG:HG2	2:G:847:ARG:H	1.41	0.45
1:B:1830:GLY:HA2	1:B:1831:GLY:HA2	1.62	0.45
2:C:1195:VAL:HG13	2:C:1211:LEU:HB3	1.99	0.45
1:K:46:GLU:OE2	2:L:1667:THR:OG1	2.32	0.45
2:L:1850:SER:HB3	2:L:1973:SER:HB2	1.99	0.45
1:F:401:THR:HG22	1:F:733:ILE:HG12	1.97	0.45
1:F:539:SER:HB2	1:F:633:GLU:HA	1.97	0.45
1:A:488:PRO:HG3	1:A:728:LYS:HG2	1.97	0.45
2:G:176:LEU:HG	2:G:180:TYR:HD2	1.82	0.45
2:G:326:ASP:OD2	2:G:387:TYR:OH	2.33	0.45
2:G:1037:SER:CB	2:G:1053:ILE:CG1	2.92	0.45
1:D:1830:GLY:HA2	1:D:1831:GLY:HA2	1.62	0.45
2:E:731:GLN:HA	2:E:766:ILE:HB	1.99	0.45
2:L:731:GLN:HA	2:L:766:ILE:HB	1.99	0.45
2:L:1195:VAL:HG13	2:L:1211:LEU:HB3	1.98	0.45
1:F:1503:ALA:HA	1:F:1506:GLN:HE21	1.81	0.45
1:I:1271:GLN:HB2	1:I:1274:ILE:HG23	1.97	0.45
1:I:1852:HIS:HA	1:I:1856:LYS:HE3	1.97	0.45
2:J:176:LEU:HG	2:J:180:TYR:HD2	1.82	0.45
1:A:719:GLN:HG3	1:A:1612:ASP:HA	1.99	0.45
2:G:278:VAL:HB	2:G:479:ILE:HD13	1.99	0.45
2:G:1422:THR:HG23	2:G:1474:PHE:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2041:ILE:HD12	2:G:2041:ILE:HA	1.87	0.45
1:B:719:GLN:HG3	1:B:1612:ASP:HA	1.99	0.45
1:B:1271:GLN:HB2	1:B:1274:ILE:HG23	1.97	0.45
1:F:1026:GLU:OE1	1:F:1594:ASN:ND2	2.40	0.45
1:F:1107:GLU:OE1	1:F:1191:THR:OG1	2.29	0.45
2:H:176:LEU:HG	2:H:180:TYR:HD2	1.82	0.45
2:H:1422:THR:HG23	2:H:1474:PHE:HB2	1.97	0.45
2:H:1800:ALA:O	2:H:2009:LYS:NZ	2.48	0.45
1:I:1233:GLU:OE2	1:I:1680:ARG:NH1	2.50	0.45
2:G:808:ALA:HB3	2:G:811:VAL:HG13	1.98	0.45
2:G:1292:ILE:HD11	2:G:1366:LEU:HD23	1.98	0.45
2:G:1330:GLY:HA2	2:G:1374:THR:HG21	1.99	0.45
2:G:1789:PHE:CD2	2:G:1817:SER:HB3	2.52	0.45
1:B:1041:ALA:O	1:B:1630:THR:OG1	2.29	0.45
2:E:646:THR:OG1	2:E:677:GLN:OE1	2.28	0.45
2:E:1195:VAL:HG13	2:E:1211:LEU:HB3	1.99	0.45
2:E:1740:THR:O	2:E:1740:THR:OG1	2.31	0.45
1:K:488:PRO:HG3	1:K:728:LYS:HG2	1.97	0.45
1:F:717:TYR:CZ	1:F:721:ILE:HD11	2.52	0.45
2:H:860:ARG:NH2	2:H:1047:ASP:OD2	2.49	0.45
2:H:1086:LEU:HG	2:H:1092:ASP:HA	1.99	0.45
2:H:1292:ILE:HD11	2:H:1366:LEU:HD23	1.98	0.45
1:I:430:ARG:HG2	1:I:605:LEU:HD22	1.98	0.45
1:A:717:TYR:CZ	1:A:721:ILE:HD11	2.52	0.44
2:G:1086:LEU:HG	2:G:1092:ASP:HA	1.99	0.44
2:C:176:LEU:HG	2:C:180:TYR:HD2	1.82	0.44
1:D:448:ILE:HD13	1:D:481:LYS:HG2	1.99	0.44
1:F:1233:GLU:OE2	1:F:1680:ARG:NH1	2.50	0.44
1:F:1561:MET:N	1:F:1561:MET:HE3	2.32	0.44
2:H:553:ASN:O	2:H:556:LYS:NZ	2.39	0.44
2:H:1740:THR:O	2:H:1740:THR:OG1	2.31	0.44
1:I:32:GLN:NE2	1:I:57:ALA:CB	2.78	0.44
2:J:326:ASP:OD2	2:J:387:TYR:OH	2.33	0.44
2:J:864:LEU:HD22	2:J:898:ASP:HB2	1.97	0.44
1:B:16:GLU:CG	2:C:2038:ILE:HD11	2.46	0.44
2:C:604:PRO:HA	2:C:607:VAL:HG12	2.00	0.44
2:C:731:GLN:HA	2:C:766:ILE:HB	1.99	0.44
1:D:1020:VAL:HG11	1:D:1400:ILE:HG12	1.99	0.44
2:E:596:GLY:N	2:E:618:GLU:OE1	2.46	0.44
2:E:1782:THR:HG21	2:E:1831:VAL:HG21	2.00	0.44
2:L:176:LEU:HG	2:L:180:TYR:HD2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:900:GLN:HB3	2:L:1050:ARG:O	2.16	0.44
2:L:1338:ILE:HG22	2:L:1390:VAL:HG11	1.98	0.44
1:F:430:ARG:HG2	1:F:605:LEU:HD22	1.98	0.44
1:F:1097:ILE:O	1:F:1101:SER:OG	2.33	0.44
2:H:596:GLY:N	2:H:618:GLU:OE1	2.46	0.44
2:H:731:GLN:HA	2:H:766:ILE:HB	1.99	0.44
2:H:1789:PHE:CD2	2:H:1817:SER:HB3	2.52	0.44
1:B:431:GLU:O	1:B:435:GLU:N	2.49	0.44
2:C:1037:SER:CB	2:C:1053:ILE:CG1	2.92	0.44
1:D:47:ILE:HD12	2:E:1666:PHE:HE1	1.83	0.44
2:E:176:LEU:HG	2:E:180:TYR:HD2	1.82	0.44
2:E:278:VAL:HB	2:E:479:ILE:HD13	1.99	0.44
1:K:16:GLU:CG	2:L:2038:ILE:HD11	2.46	0.44
1:K:1486:LEU:HD21	1:K:1761:LYS:HZ2	1.81	0.44
1:K:1694:TYR:OH	2:L:1001:ASP:OD2	2.35	0.44
2:L:326:ASP:OD2	2:L:387:TYR:OH	2.33	0.44
2:L:1789:PHE:CD2	2:L:1817:SER:HB3	2.52	0.44
1:F:431:GLU:O	1:F:435:GLU:N	2.49	0.44
2:J:320:PRO:HA	2:J:321:PRO:HD3	1.89	0.44
2:J:604:PRO:HA	2:J:607:VAL:HG12	2.00	0.44
2:J:1789:PHE:CD2	2:J:1817:SER:HB3	2.52	0.44
2:G:1782:THR:HG21	2:G:1831:VAL:HG21	2.00	0.44
1:B:774:ILE:HD11	1:B:791:ALA:HB2	1.99	0.44
1:F:1303:GLY:H	1:F:1307:THR:HG22	1.83	0.44
1:I:448:ILE:HD13	1:I:481:LYS:HG2	1.99	0.44
1:I:1491:ARG:HA	1:I:1750:ILE:CD1	2.48	0.44
2:J:1370:ASP:N	2:J:1370:ASP:OD1	2.50	0.44
2:J:1739:GLU:H	2:J:1739:GLU:HG2	1.66	0.44
1:A:1373:ARG:HH21	1:A:1550:ASP:HB2	1.83	0.44
2:G:604:PRO:HA	2:G:607:VAL:HG12	2.00	0.44
2:G:864:LEU:HD22	2:G:898:ASP:HB2	1.98	0.44
2:G:1850:SER:HB3	2:G:1973:SER:HB2	1.99	0.44
1:D:1491:ARG:HA	1:D:1750:ILE:CD1	2.48	0.44
2:E:1810:GLY:HA2	2:E:1813:ALA:HB3	2.00	0.44
2:E:1850:SER:HB3	2:E:1973:SER:HB2	1.99	0.44
1:K:1020:VAL:HG11	1:K:1400:ILE:HG12	1.99	0.44
2:L:1800:ALA:O	2:L:2009:LYS:NZ	2.47	0.44
2:L:1866:PHE:HE2	2:L:1871:LEU:HD12	1.83	0.44
1:F:47:ILE:HD12	2:H:1666:PHE:HE1	1.83	0.44
2:H:919:TYR:HE1	2:H:995:LEU:HA	1.83	0.44
1:I:1020:VAL:HG11	1:I:1400:ILE:HG12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:1810:GLY:HA2	2:J:1813:ALA:HB3	2.00	0.44
2:G:919:TYR:HE1	2:G:995:LEU:HA	1.83	0.44
1:B:448:ILE:HD13	1:B:481:LYS:HG2	1.99	0.44
2:C:278:VAL:HB	2:C:479:ILE:HD13	1.99	0.44
2:C:1086:LEU:HG	2:C:1092:ASP:HA	1.99	0.44
2:C:1628:HIS:HA	2:C:1638:ILE:HG13	2.00	0.44
2:C:1849:ARG:HH11	2:C:1957:PRO:HG2	1.83	0.44
1:D:430:ARG:HG2	1:D:605:LEU:HD22	1.98	0.44
1:D:717:TYR:CZ	1:D:721:ILE:HD11	2.52	0.44
1:D:774:ILE:HD11	1:D:791:ALA:HB2	1.99	0.44
1:D:1303:GLY:H	1:D:1307:THR:HG22	1.83	0.44
2:E:245:GLN:HE21	2:E:506:PRO:HD3	1.81	0.44
2:E:287:ASP:HB3	2:E:288:SER:H	1.59	0.44
2:E:1737:ILE:HG12	2:E:1748:THR:HG22	1.95	0.44
2:E:1800:ALA:O	2:E:2009:LYS:NZ	2.47	0.44
2:E:1866:PHE:HE2	2:E:1871:LEU:HD12	1.83	0.44
1:K:47:ILE:HD12	2:L:1666:PHE:HE1	1.83	0.44
1:K:430:ARG:HG2	1:K:605:LEU:HD22	1.98	0.44
2:L:919:TYR:HE1	2:L:995:LEU:HA	1.83	0.44
1:F:774:ILE:HD11	1:F:791:ALA:HB2	1.99	0.44
1:F:1020:VAL:HG11	1:F:1400:ILE:HG12	1.99	0.44
1:F:1373:ARG:HH21	1:F:1550:ASP:HB2	1.83	0.44
1:F:1491:ARG:HA	1:F:1750:ILE:CD1	2.48	0.44
2:H:101:ILE:O	2:H:105:ALA:N	2.51	0.44
2:H:1782:THR:HG21	2:H:1831:VAL:HG21	2.00	0.44
1:I:774:ILE:HD11	1:I:791:ALA:HB2	1.99	0.44
1:I:1373:ARG:HH21	1:I:1550:ASP:HB2	1.83	0.44
1:I:1851:LEU:HD22	1:I:1855:ALA:HB1	2.00	0.44
1:A:1303:GLY:H	1:A:1307:THR:HG22	1.82	0.44
1:A:1491:ARG:HA	1:A:1750:ILE:CD1	2.48	0.44
2:G:1381:VAL:O	2:G:1422:THR:OG1	2.28	0.44
2:G:1810:GLY:HA2	2:G:1813:ALA:HB3	2.00	0.44
2:C:1697:HIS:O	2:C:1701:THR:OG1	2.28	0.44
1:D:402:PHE:HE1	1:D:1612:ASP:HB2	1.81	0.44
1:D:719:GLN:HG3	1:D:1612:ASP:HA	1.99	0.44
2:E:919:TYR:HE1	2:E:995:LEU:HA	1.83	0.44
2:E:1730:ARG:NH1	2:E:1759:SER:O	2.43	0.44
1:K:1106:ILE:HA	1:K:1188:GLN:NE2	2.33	0.44
2:L:1086:LEU:HG	2:L:1092:ASP:HA	1.99	0.44
2:L:1691:TRP:O	2:L:1695:ASP:N	2.40	0.44
2:H:1850:SER:HB3	2:H:1973:SER:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:719:GLN:HG3	1:I:1612:ASP:HA	1.99	0.44
1:I:1009:LEU:HG	1:I:1664:ALA:HB2	2.00	0.44
1:I:1303:GLY:H	1:I:1307:THR:HG22	1.83	0.44
2:J:1330:GLY:HA2	2:J:1374:THR:HG21	1.99	0.44
2:J:1628:HIS:HA	2:J:1638:ILE:HG13	2.00	0.44
1:A:448:ILE:HD13	1:A:481:LYS:HG2	1.99	0.44
1:A:1233:GLU:OE2	1:A:1680:ARG:NH1	2.50	0.44
2:G:731:GLN:HA	2:G:766:ILE:HB	1.99	0.44
1:B:717:TYR:CZ	1:B:721:ILE:HD11	2.52	0.44
1:B:1106:ILE:HA	1:B:1188:GLN:NE2	2.33	0.44
2:C:1789:PHE:CD2	2:C:1817:SER:HB3	2.52	0.44
2:E:641:ILE:HG12	2:E:645:SER:HB2	2.00	0.44
2:E:844:VAL:HB	2:E:845:THR:H	1.70	0.44
1:K:402:PHE:HE1	1:K:1612:ASP:HB2	1.81	0.44
2:L:264:ARG:NH1	2:L:284:ALA:O	2.51	0.44
2:L:808:ALA:HB3	2:L:811:VAL:HG13	1.98	0.44
2:L:1782:THR:HG21	2:L:1831:VAL:HG21	2.00	0.44
1:F:402:PHE:HE1	1:F:1612:ASP:HB2	1.81	0.44
1:F:448:ILE:HD13	1:F:481:LYS:HG2	1.99	0.44
2:J:900:GLN:HB3	2:J:1050:ARG:O	2.16	0.44
2:J:1086:LEU:HG	2:J:1092:ASP:HA	2.00	0.44
1:A:937:LYS:HD2	1:F:855:SER:HB2	1.98	0.44
1:A:1851:LEU:HD22	1:A:1855:ALA:HB1	2.00	0.44
2:G:101:ILE:O	2:G:105:ALA:N	2.51	0.44
2:G:596:GLY:N	2:G:618:GLU:OE1	2.46	0.44
2:C:264:ARG:NH1	2:C:284:ALA:O	2.51	0.44
2:C:844:VAL:HB	2:C:845:THR:H	1.70	0.44
2:C:1330:GLY:HA2	2:C:1374:THR:HG21	1.99	0.44
1:D:687:SER:HA	1:D:875:THR:HG22	2.00	0.44
2:E:1086:LEU:HG	2:E:1092:ASP:HA	2.00	0.44
2:E:1884:TRP:HB3	2:E:1906:ALA:HB2	2.00	0.44
2:L:604:PRO:HA	2:L:607:VAL:HG12	2.00	0.44
2:L:1810:GLY:HA2	2:L:1813:ALA:HB3	2.00	0.44
2:H:1330:GLY:HA2	2:H:1374:THR:HG21	1.99	0.44
2:H:1810:GLY:HA2	2:H:1813:ALA:HB3	2.00	0.44
1:I:13:LEU:HD21	2:J:2025:TYR:CE2	2.53	0.44
1:I:16:GLU:CG	2:J:2038:ILE:HD11	2.46	0.44
1:I:717:TYR:CZ	1:I:721:ILE:HD11	2.52	0.44
2:G:1800:ALA:O	2:G:2009:LYS:NZ	2.47	0.43
1:B:1020:VAL:HG11	1:B:1400:ILE:HG12	1.99	0.43
1:B:1397:GLY:O	1:B:1680:ARG:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1851:LEU:HD22	1:B:1855:ALA:HB1	2.00	0.43
2:C:1801:ASP:HA	2:C:2009:LYS:HD3	2.00	0.43
1:D:855:SER:HB2	1:I:937:LYS:HD2	1.98	0.43
1:K:1491:ARG:HA	1:K:1750:ILE:CD1	2.48	0.43
1:I:1830:GLY:HA2	1:I:1831:GLY:HA2	1.62	0.43
2:G:984:PHE:O	2:G:991:ARG:NH1	2.52	0.43
1:K:717:TYR:CZ	1:K:721:ILE:HD11	2.52	0.43
2:L:370:LEU:HD12	2:L:378:VAL:HG21	2.01	0.43
2:L:1665:VAL:HG12	2:L:1805:ALA:HB3	2.00	0.43
2:H:1665:VAL:HG12	2:H:1805:ALA:HB3	2.00	0.43
2:H:1884:TRP:HB3	2:H:1906:ALA:HB2	2.00	0.43
2:J:641:ILE:HG12	2:J:645:SER:HB2	2.00	0.43
2:G:534:ASP:HB2	2:G:543:PHE:CE1	2.53	0.43
1:B:1026:GLU:OE1	1:B:1594:ASN:ND2	2.40	0.43
1:B:1233:GLU:OE2	1:B:1680:ARG:NH1	2.50	0.43
2:C:919:TYR:HE1	2:C:995:LEU:HA	1.83	0.43
2:C:1665:VAL:HG12	2:C:1805:ALA:HB3	2.00	0.43
2:C:1810:GLY:HA2	2:C:1813:ALA:HB3	2.00	0.43
1:D:1851:LEU:HD22	1:D:1855:ALA:HB1	2.00	0.43
2:E:370:LEU:HD12	2:E:378:VAL:HG21	2.01	0.43
2:E:1370:ASP:N	2:E:1370:ASP:OD1	2.50	0.43
2:E:1665:VAL:HG12	2:E:1805:ALA:HB3	2.00	0.43
2:E:1789:PHE:CD2	2:E:1817:SER:HB3	2.52	0.43
2:L:641:ILE:HG12	2:L:645:SER:HB2	2.00	0.43
2:L:1849:ARG:HH11	2:L:1957:PRO:HG2	1.83	0.43
2:H:264:ARG:NH1	2:H:284:ALA:O	2.51	0.43
2:H:534:ASP:HB2	2:H:543:PHE:CE1	2.53	0.43
2:J:101:ILE:O	2:J:105:ALA:N	2.51	0.43
2:J:731:GLN:HA	2:J:766:ILE:HB	1.99	0.43
2:J:1782:THR:HG21	2:J:1831:VAL:HG21	2.00	0.43
1:A:13:LEU:HD21	2:G:2025:TYR:CE2	2.53	0.43
1:A:47:ILE:HD12	2:G:1666:PHE:HE1	1.83	0.43
1:A:1107:GLU:OE1	1:A:1191:THR:OG1	2.29	0.43
2:G:1665:VAL:HG12	2:G:1805:ALA:HB3	2.00	0.43
2:C:287:ASP:HB3	2:C:288:SER:H	1.59	0.43
2:C:808:ALA:HB3	2:C:811:VAL:HG13	1.98	0.43
1:D:1694:TYR:OH	2:E:1001:ASP:OD2	2.35	0.43
1:K:1421:PRO:HB2	1:K:1552:ASN:HD22	1.84	0.43
2:L:534:ASP:HB2	2:L:543:PHE:CE1	2.53	0.43
1:F:687:SER:HA	1:F:875:THR:HG22	2.00	0.43
2:H:1174:PHE:CD1	2:H:1197:LEU:HG	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:808:ALA:HB3	2:J:811:VAL:HG13	1.98	0.43
2:J:1665:VAL:HG12	2:J:1805:ALA:HB3	2.00	0.43
1:A:1020:VAL:HG11	1:A:1400:ILE:HG12	1.99	0.43
1:A:1744:TYR:HB2	1:K:1432:HIS:CE1	2.54	0.43
2:G:1866:PHE:HE2	2:G:1871:LEU:HD12	1.83	0.43
1:B:46:GLU:OE2	2:C:1667:THR:OG1	2.32	0.43
1:B:1744:TYR:HB2	1:I:1432:HIS:CE1	2.54	0.43
2:C:534:ASP:HB2	2:C:543:PHE:CE1	2.53	0.43
2:C:1370:ASP:OD1	2:C:1370:ASP:N	2.50	0.43
2:C:1782:THR:HG21	2:C:1831:VAL:HG21	2.00	0.43
2:E:264:ARG:NH1	2:E:284:ALA:O	2.51	0.43
1:K:1009:LEU:HG	1:K:1664:ALA:HB2	2.00	0.43
1:K:1397:GLY:O	1:K:1680:ARG:HG3	2.18	0.43
2:L:1174:PHE:CD1	2:L:1197:LEU:HG	2.54	0.43
2:L:1370:ASP:N	2:L:1370:ASP:OD1	2.50	0.43
2:L:1628:HIS:HA	2:L:1638:ILE:HG13	2.00	0.43
1:F:13:LEU:HD21	2:H:2025:TYR:CE2	2.53	0.43
2:J:919:TYR:HE1	2:J:995:LEU:HA	1.83	0.43
1:A:1421:PRO:HB2	1:A:1552:ASN:HD22	1.84	0.43
1:A:1694:TYR:OH	2:G:1001:ASP:OD2	2.35	0.43
2:G:1628:HIS:HA	2:G:1638:ILE:HG13	2.00	0.43
1:B:47:ILE:HD12	2:C:1666:PHE:HE1	1.83	0.43
1:B:1432:HIS:CE1	1:I:1744:TYR:HB2	2.54	0.43
1:B:1491:ARG:HA	1:B:1750:ILE:CD1	2.48	0.43
2:C:370:LEU:HD12	2:C:378:VAL:HG21	2.01	0.43
2:E:1174:PHE:CD1	2:E:1197:LEU:HG	2.54	0.43
1:K:1303:GLY:H	1:K:1307:THR:HG22	1.82	0.43
1:F:1421:PRO:HB2	1:F:1552:ASN:HD22	1.84	0.43
2:H:295:SER:O	2:H:298:LYS:CB	2.59	0.43
2:H:604:PRO:HA	2:H:607:VAL:HG12	2.00	0.43
2:H:984:PHE:O	2:H:991:ARG:NH1	2.52	0.43
2:H:1801:ASP:HA	2:H:2009:LYS:HD3	2.00	0.43
1:I:1220:VAL:HG21	1:I:1698:PHE:HD1	1.84	0.43
1:I:1694:TYR:OH	2:J:1001:ASP:OD2	2.35	0.43
2:J:109:LEU:HD22	2:J:114:THR:HG23	2.01	0.43
2:J:1849:ARG:HH11	2:J:1957:PRO:HG2	1.83	0.43
1:A:46:GLU:OE2	2:G:1667:THR:OG1	2.32	0.43
1:A:431:GLU:O	1:A:435:GLU:N	2.49	0.43
2:G:641:ILE:HG12	2:G:645:SER:HB2	2.00	0.43
2:C:109:LEU:HD22	2:C:114:THR:HG23	2.01	0.43
1:D:1106:ILE:HA	1:D:1188:GLN:NE2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1373:ARG:HH21	1:D:1550:ASP:HB2	1.83	0.43
2:E:604:PRO:HA	2:E:607:VAL:HG12	2.00	0.43
2:E:984:PHE:O	2:E:991:ARG:NH1	2.52	0.43
1:K:774:ILE:HD11	1:K:791:ALA:HB2	1.99	0.43
2:L:109:LEU:HD22	2:L:114:THR:HG23	2.01	0.43
2:H:278:VAL:HB	2:H:479:ILE:HD13	1.99	0.43
2:H:641:ILE:HG12	2:H:645:SER:HB2	2.00	0.43
2:H:1849:ARG:HH11	2:H:1957:PRO:HG2	1.83	0.43
1:I:171:THR:HG23	1:I:174:ASP:H	1.84	0.43
1:I:431:GLU:O	1:I:435:GLU:N	2.49	0.43
1:I:1106:ILE:HA	1:I:1188:GLN:NE2	2.33	0.43
1:I:1397:GLY:O	1:I:1680:ARG:HG3	2.18	0.43
2:J:1174:PHE:CD1	2:J:1197:LEU:HG	2.54	0.43
2:J:1195:VAL:HG13	2:J:1211:LEU:HB3	1.99	0.43
2:J:1767:GLU:OE2	2:J:1849:ARG:NE	2.36	0.43
1:A:1220:VAL:HG21	1:A:1698:PHE:HD1	1.84	0.43
2:G:109:LEU:HD22	2:G:114:THR:HG23	2.01	0.43
2:G:1174:PHE:CD1	2:G:1197:LEU:HG	2.54	0.43
2:G:1801:ASP:HA	2:G:2009:LYS:HD3	2.01	0.43
2:C:295:SER:O	2:C:298:LYS:CB	2.59	0.43
2:C:1866:PHE:HE2	2:C:1871:LEU:HD12	1.83	0.43
2:C:1890:ASN:HB2	2:C:1899:VAL:HB	2.01	0.43
1:D:1421:PRO:HB2	1:D:1552:ASN:HD22	1.84	0.43
2:E:1801:ASP:HA	2:E:2009:LYS:HD3	2.00	0.43
2:L:984:PHE:O	2:L:991:ARG:NH1	2.52	0.43
2:L:2041:ILE:HD12	2:L:2041:ILE:HA	1.87	0.43
2:H:370:LEU:HD12	2:H:378:VAL:HG21	2.01	0.43
1:I:1549:ASN:ND2	1:I:1549:ASN:C	2.73	0.43
2:J:534:ASP:HB2	2:J:543:PHE:CE1	2.54	0.43
1:A:774:ILE:HD11	1:A:791:ALA:HB2	1.99	0.43
1:A:1009:LEU:HG	1:A:1664:ALA:HB2	2.00	0.43
1:A:1432:HIS:CE1	1:K:1744:TYR:HB2	2.54	0.43
1:B:1303:GLY:H	1:B:1307:THR:HG22	1.83	0.43
1:D:1432:HIS:CE1	1:F:1744:TYR:HB2	2.54	0.43
2:E:1068:GLU:HA	2:E:1069:PRO:HD3	1.92	0.43
2:E:1890:ASN:HB2	2:E:1899:VAL:HB	2.01	0.43
2:L:1381:VAL:O	2:L:1422:THR:OG1	2.28	0.43
1:F:409:ALA:HB2	1:F:442:ARG:HE	1.84	0.43
1:F:1851:LEU:HD22	1:F:1855:ALA:HB1	2.00	0.43
2:H:1628:HIS:HA	2:H:1638:ILE:HG13	2.00	0.43
2:H:1866:PHE:HE2	2:H:1871:LEU:HD12	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:264:ARG:NH1	2:J:284:ALA:O	2.51	0.43
2:J:976:PRO:O	2:J:980:ILE:N	2.48	0.43
2:J:1884:TRP:HB3	2:J:1906:ALA:HB2	2.00	0.43
1:A:16:GLU:CG	2:G:2038:ILE:HD11	2.46	0.43
2:G:370:LEU:HD12	2:G:378:VAL:HG21	2.01	0.43
2:G:1370:ASP:N	2:G:1370:ASP:OD1	2.50	0.43
1:B:848:THR:CG2	1:K:844:LEU:HD23	2.44	0.43
1:B:1421:PRO:HB2	1:B:1552:ASN:HD22	1.84	0.43
1:D:13:LEU:HD21	2:E:2025:TYR:CE2	2.53	0.43
1:D:16:GLU:CG	2:E:2038:ILE:HD11	2.46	0.43
2:E:109:LEU:HD22	2:E:114:THR:HG23	2.01	0.43
2:E:283:ILE:O	2:E:286:THR:HG22	2.19	0.43
2:E:1628:HIS:HA	2:E:1638:ILE:HG13	2.00	0.43
1:K:770:PRO:HB2	1:K:799:ILE:HG12	2.01	0.43
2:L:158:ALA:HA	2:L:502:LEU:HB2	2.01	0.43
2:L:1801:ASP:HA	2:L:2009:LYS:HD3	2.01	0.43
2:L:1884:TRP:HB3	2:L:1906:ALA:HB2	2.00	0.43
1:F:17:LEU:HD23	2:H:2014:LEU:HD23	2.01	0.43
2:H:581:THR:H	2:H:584:SER:HG	1.64	0.43
1:I:687:SER:HA	1:I:875:THR:HG22	2.00	0.43
1:I:877:LEU:HD11	3:I:2001:NDP:C2D	2.47	0.43
1:I:1421:PRO:HB2	1:I:1552:ASN:HD22	1.84	0.43
1:A:877:LEU:HD11	3:A:2001:NDP:C2D	2.47	0.42
1:A:1279:PHE:HB2	1:A:1282:THR:HG23	2.01	0.42
2:G:264:ARG:NH1	2:G:284:ALA:O	2.51	0.42
2:G:290:GLU:N	2:G:290:GLU:CD	2.73	0.42
1:B:171:THR:HG23	1:B:174:ASP:H	1.84	0.42
2:C:158:ALA:HA	2:C:502:LEU:HB2	2.01	0.42
1:D:1009:LEU:HG	1:D:1664:ALA:HB2	2.00	0.42
1:D:1303:GLY:HA2	1:D:1649:LYS:HZ1	1.84	0.42
1:D:1744:TYR:HB2	1:F:1432:HIS:CE1	2.54	0.42
2:E:919:TYR:CE1	2:E:995:LEU:HA	2.54	0.42
1:K:13:LEU:HD21	2:L:2025:TYR:CE2	2.53	0.42
1:K:1851:LEU:HD22	1:K:1855:ALA:HB1	2.00	0.42
2:L:844:VAL:HB	2:L:845:THR:H	1.70	0.42
1:F:1009:LEU:HG	1:F:1664:ALA:HB2	2.00	0.42
1:F:1279:PHE:HB2	1:F:1282:THR:HG23	2.01	0.42
2:H:577:ILE:HB	2:H:1082:ILE:HD11	2.01	0.42
2:H:884:LEU:HD22	2:H:1021:LEU:HD12	2.01	0.42
2:H:1890:ASN:HB2	2:H:1899:VAL:HB	2.01	0.42
1:I:1017:ARG:NH1	1:I:1511:ASP:OD2	2.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:370:LEU:HD12	2:J:378:VAL:HG21	2.01	0.42
2:J:1801:ASP:HA	2:J:2009:LYS:HD3	2.00	0.42
2:J:1890:ASN:HB2	2:J:1899:VAL:HB	2.01	0.42
1:A:33:ASP:OD2	1:A:64:LYS:NZ	2.41	0.42
1:A:1549:ASN:ND2	1:A:1549:ASN:C	2.73	0.42
2:G:158:ALA:HA	2:G:502:LEU:HB2	2.01	0.42
2:G:646:THR:OG1	2:G:677:GLN:OE1	2.28	0.42
1:B:13:LEU:HD21	2:C:2025:TYR:CE2	2.53	0.42
1:B:770:PRO:HB2	1:B:799:ILE:HG12	2.01	0.42
1:B:1549:ASN:C	1:B:1549:ASN:ND2	2.73	0.42
2:C:641:ILE:HG12	2:C:645:SER:HB2	2.00	0.42
2:C:1174:PHE:CD1	2:C:1197:LEU:HG	2.54	0.42
2:C:1884:TRP:HB3	2:C:1906:ALA:HB2	2.00	0.42
1:D:981:GLU:HA	2:E:964:LEU:HA	2.01	0.42
1:D:1397:GLY:O	1:D:1680:ARG:HG3	2.18	0.42
2:E:184:VAL:HG12	2:E:188:ILE:HG12	2.01	0.42
2:E:884:LEU:HD22	2:E:1021:LEU:HD12	2.01	0.42
2:E:1561:ASN:HB3	2:E:1564:HIS:HD2	1.84	0.42
2:E:1849:ARG:HH11	2:E:1957:PRO:HG2	1.83	0.42
2:H:109:LEU:HD22	2:H:114:THR:HG23	2.01	0.42
2:H:158:ALA:HA	2:H:502:LEU:HB2	2.01	0.42
2:H:184:VAL:HG12	2:H:188:ILE:HG12	2.01	0.42
2:H:919:TYR:CE1	2:H:995:LEU:HA	2.54	0.42
1:I:46:GLU:OE2	2:J:1667:THR:OG1	2.32	0.42
1:I:47:ILE:HD12	2:J:1666:PHE:HE1	1.83	0.42
1:I:1279:PHE:HB2	1:I:1282:THR:HG23	2.01	0.42
2:G:1890:ASN:HB2	2:G:1899:VAL:HB	2.01	0.42
1:B:1009:LEU:HG	1:B:1664:ALA:HB2	2.00	0.42
1:B:1220:VAL:HG21	1:B:1698:PHE:HD1	1.84	0.42
2:C:184:VAL:HG12	2:C:188:ILE:HG12	2.01	0.42
2:C:884:LEU:HD22	2:C:1021:LEU:HD12	2.01	0.42
2:C:984:PHE:O	2:C:991:ARG:NH1	2.52	0.42
2:E:534:ASP:HB2	2:E:543:PHE:CE1	2.54	0.42
2:E:1386:THR:HG23	2:E:1411:PHE:HZ	1.84	0.42
1:K:1830:GLY:HA2	1:K:1831:GLY:HA2	1.62	0.42
2:L:1767:GLU:OE2	2:L:1849:ARG:NE	2.36	0.42
2:L:1890:ASN:HB2	2:L:1899:VAL:HB	2.01	0.42
1:F:1220:VAL:HG21	1:F:1698:PHE:HD1	1.84	0.42
2:J:884:LEU:HD22	2:J:1021:LEU:HD12	2.01	0.42
2:J:1386:THR:HG23	2:J:1411:PHE:HZ	1.84	0.42
2:J:1866:PHE:HE2	2:J:1871:LEU:HD12	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:LEU:HD23	2:G:2014:LEU:HD23	2.01	0.42
1:A:171:THR:HG23	1:A:174:ASP:H	1.84	0.42
1:A:1397:GLY:O	1:A:1680:ARG:HG3	2.18	0.42
2:G:184:VAL:HG12	2:G:188:ILE:HG12	2.01	0.42
2:G:919:TYR:CE1	2:G:995:LEU:HA	2.54	0.42
2:C:1730:ARG:NH1	2:C:1759:SER:O	2.43	0.42
2:C:2041:ILE:HD12	2:C:2041:ILE:HA	1.87	0.42
1:D:770:PRO:HB2	1:D:799:ILE:HG12	2.01	0.42
1:D:1279:PHE:HB2	1:D:1282:THR:HG23	2.01	0.42
2:L:184:VAL:HG12	2:L:188:ILE:HG12	2.01	0.42
2:L:283:ILE:O	2:L:286:THR:HG22	2.19	0.42
2:L:919:TYR:CE1	2:L:995:LEU:HA	2.54	0.42
2:L:1068:GLU:HA	2:L:1069:PRO:HD3	1.92	0.42
2:L:1730:ARG:NH1	2:L:1759:SER:O	2.43	0.42
1:F:171:THR:HG23	1:F:174:ASP:H	1.84	0.42
1:F:1001:VAL:HG11	1:F:1662:TYR:HB2	2.02	0.42
2:H:1310:ASP:OD1	2:H:1317:ARG:NH2	2.53	0.42
2:J:984:PHE:O	2:J:991:ARG:NH1	2.52	0.42
1:A:409:ALA:HB2	1:A:442:ARG:HE	1.84	0.42
1:A:687:SER:HA	1:A:875:THR:HG22	2.00	0.42
2:G:1737:ILE:HG12	2:G:1748:THR:HG22	1.95	0.42
2:G:1778:GLN:HA	2:G:1809:LEU:HD21	2.01	0.42
2:E:1485:CYS:HB3	2:E:1506:TYR:HB3	2.02	0.42
2:H:1068:GLU:HA	2:H:1069:PRO:HD3	1.92	0.42
1:I:35:PHE:HA	1:I:39:PHE:HD2	1.85	0.42
1:I:770:PRO:HB2	1:I:799:ILE:HG12	2.01	0.42
2:J:184:VAL:HG12	2:J:188:ILE:HG12	2.01	0.42
2:G:283:ILE:O	2:G:286:THR:HG22	2.19	0.42
2:G:577:ILE:HB	2:G:1082:ILE:HD11	2.01	0.42
2:G:1386:THR:HG23	2:G:1411:PHE:HZ	1.84	0.42
2:G:1849:ARG:HH11	2:G:1957:PRO:HG2	1.83	0.42
1:B:687:SER:HA	1:B:875:THR:HG22	2.00	0.42
1:B:1001:VAL:HG11	1:B:1662:TYR:HB2	2.02	0.42
1:D:171:THR:HG23	1:D:174:ASP:H	1.84	0.42
1:D:411:GLN:HE21	1:D:1629:LYS:HE2	1.85	0.42
2:E:528:ILE:HG21	2:E:547:ILE:HG13	2.02	0.42
1:K:17:LEU:HD23	2:L:2014:LEU:HD23	2.01	0.42
2:L:848:SER:HB3	2:L:854:ILE:HD12	2.00	0.42
1:F:35:PHE:HA	1:F:39:PHE:HD2	1.85	0.42
2:H:1037:SER:CB	2:H:1053:ILE:CG1	2.92	0.42
1:I:409:ALA:HB2	1:I:442:ARG:HE	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:283:ILE:O	2:J:286:THR:HG22	2.19	0.42
2:G:585:LYS:HG3	2:G:1106:GLU:HB2	2.02	0.42
2:G:1884:TRP:HB3	2:G:1906:ALA:HB2	2.00	0.42
2:C:528:ILE:HG21	2:C:547:ILE:HG13	2.02	0.42
2:C:848:SER:HB3	2:C:854:ILE:HD12	2.00	0.42
2:E:290:GLU:N	2:E:290:GLU:CD	2.73	0.42
2:E:1037:SER:N	2:E:1051:THR:HG21	2.35	0.42
2:E:1267:TRP:NE1	2:E:1273:GLU:O	2.39	0.42
2:L:1265:MET:HE2	2:L:1562:PRO:HG2	2.02	0.42
2:L:1485:CYS:HB3	2:L:1506:TYR:HB3	2.02	0.42
2:H:283:ILE:O	2:H:286:THR:HG22	2.19	0.42
2:H:290:GLU:N	2:H:290:GLU:CD	2.73	0.42
2:H:549:ASP:HB3	2:H:554:GLY:HA3	2.02	0.42
2:J:158:ALA:HA	2:J:502:LEU:HB2	2.01	0.42
2:J:1310:ASP:OD1	2:J:1317:ARG:NH2	2.53	0.42
2:J:1432:GLN:N	2:J:1525:SER:O	2.52	0.42
2:G:1739:GLU:H	2:G:1739:GLU:HG2	1.66	0.42
2:C:283:ILE:O	2:C:286:THR:HG22	2.19	0.42
2:C:1485:CYS:HB3	2:C:1506:TYR:HB3	2.02	0.42
1:K:768:ILE:HG12	1:K:770:PRO:HD3	2.02	0.42
1:K:1279:PHE:HB2	1:K:1282:THR:HG23	2.01	0.42
2:L:528:ILE:HG21	2:L:547:ILE:HG13	2.02	0.42
2:L:646:THR:HB	2:L:677:GLN:CB	2.26	0.42
2:L:1037:SER:N	2:L:1051:THR:HG21	2.35	0.42
2:H:528:ILE:HG21	2:H:547:ILE:HG13	2.02	0.42
2:H:646:THR:HB	2:H:677:GLN:CB	2.26	0.42
2:H:976:PRO:O	2:H:980:ILE:N	2.48	0.42
1:I:411:GLN:HE21	1:I:1629:LYS:HE2	1.85	0.42
1:I:745:VAL:HG23	1:I:802:MET:HG2	2.02	0.42
2:J:528:ILE:HG21	2:J:547:ILE:HG13	2.02	0.42
2:J:900:GLN:HE22	2:J:1033:SER:HB2	1.85	0.42
1:A:400:ARG:NH1	1:A:1358:HIS:O	2.40	0.42
2:G:1037:SER:N	2:G:1051:THR:HG21	2.35	0.42
1:B:409:ALA:HB2	1:B:442:ARG:HE	1.84	0.42
1:B:411:GLN:HE21	1:B:1629:LYS:HE2	1.85	0.42
2:C:1310:ASP:OD1	2:C:1317:ARG:NH2	2.53	0.42
1:D:409:ALA:HB2	1:D:442:ARG:HE	1.84	0.42
1:D:633:GLU:H	1:D:653:ARG:HH22	1.68	0.42
2:E:577:ILE:HB	2:E:1082:ILE:HD11	2.01	0.42
2:E:848:SER:HB3	2:E:854:ILE:HD12	2.00	0.42
2:E:1310:ASP:OD1	2:E:1317:ARG:NH2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:171:THR:HG23	1:K:174:ASP:H	1.84	0.42
1:K:1001:VAL:HG11	1:K:1662:TYR:HB2	2.02	0.42
2:L:1310:ASP:OD1	2:L:1317:ARG:NH2	2.53	0.42
1:F:1397:GLY:O	1:F:1680:ARG:HG3	2.18	0.42
1:F:1411:THR:HG22	1:F:1648:GLN:HG3	2.02	0.42
2:H:1376:ALA:HA	2:H:1394:GLY:HA2	2.02	0.42
2:H:1739:GLU:H	2:H:1739:GLU:HG2	1.66	0.42
2:J:714:SER:HA	2:J:717:ILE:HD12	2.02	0.42
2:J:1740:THR:O	2:J:1740:THR:OG1	2.31	0.42
2:J:1778:GLN:HA	2:J:1809:LEU:HD21	2.01	0.42
1:A:411:GLN:HE21	1:A:1629:LYS:HE2	1.85	0.42
1:A:1411:THR:HG22	1:A:1648:GLN:HG3	2.02	0.42
2:G:1217:ASN:HB3	2:G:1242:PHE:HB3	2.02	0.42
2:G:1859:PRO:HG3	2:G:1871:LEU:HD13	2.02	0.42
1:B:35:PHE:HA	1:B:39:PHE:HD2	1.85	0.42
1:B:1279:PHE:HB2	1:B:1282:THR:HG23	2.01	0.42
2:C:290:GLU:CD	2:C:290:GLU:N	2.73	0.42
2:C:1783:LEU:HD23	2:C:1783:LEU:HA	1.92	0.42
1:D:768:ILE:HG12	1:D:770:PRO:HD3	2.02	0.42
2:E:158:ALA:HA	2:E:502:LEU:HB2	2.01	0.42
2:E:1778:GLN:HA	2:E:1809:LEU:HD21	2.01	0.42
1:K:981:GLU:HA	2:L:964:LEU:HA	2.01	0.42
1:K:1549:ASN:ND2	1:K:1549:ASN:C	2.73	0.42
2:L:714:SER:HA	2:L:717:ILE:HD12	2.02	0.42
2:L:1386:THR:HG23	2:L:1411:PHE:HZ	1.84	0.42
2:L:1690:VAL:HG21	2:L:1787:ALA:HA	2.02	0.42
1:F:1649:LYS:HE3	1:F:1649:LYS:HB2	1.90	0.42
2:H:1386:THR:HG23	2:H:1411:PHE:HZ	1.84	0.42
2:H:1485:CYS:HB3	2:H:1506:TYR:HB3	2.02	0.42
1:I:1303:GLY:HA2	1:I:1649:LYS:HZ1	1.84	0.42
2:J:290:GLU:N	2:J:290:GLU:CD	2.73	0.42
2:J:1859:PRO:HG3	2:J:1871:LEU:HD13	2.02	0.42
1:A:1106:ILE:HA	1:A:1188:GLN:NE2	2.33	0.41
2:G:1376:ALA:HA	2:G:1394:GLY:HA2	2.02	0.41
1:B:17:LEU:HD23	2:C:2014:LEU:HD23	2.01	0.41
1:B:768:ILE:HG12	1:B:770:PRO:HD3	2.02	0.41
2:C:101:ILE:O	2:C:105:ALA:N	2.51	0.41
2:C:1386:THR:HG23	2:C:1411:PHE:HZ	1.84	0.41
2:C:1561:ASN:HB3	2:C:1564:HIS:HD2	1.85	0.41
1:D:35:PHE:HA	1:D:39:PHE:HD2	1.85	0.41
2:E:549:ASP:HB3	2:E:554:GLY:HA3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:714:SER:HA	2:E:717:ILE:HD12	2.02	0.41
2:E:741:HIS:HB3	2:E:853:PRO:HB2	2.02	0.41
2:E:900:GLN:HE22	2:E:1033:SER:HB2	1.85	0.41
1:K:35:PHE:HA	1:K:39:PHE:HD2	1.85	0.41
1:K:411:GLN:HE21	1:K:1629:LYS:HE2	1.85	0.41
1:K:687:SER:HA	1:K:875:THR:HG22	2.00	0.41
2:L:260:PRO:CD	2:L:289:TRP:CH2	3.03	0.41
2:L:298:LYS:HB3	2:L:450:PHE:HE1	1.85	0.41
2:L:884:LEU:HD22	2:L:1021:LEU:HD12	2.01	0.41
1:F:770:PRO:HB2	1:F:799:ILE:HG12	2.01	0.41
1:F:981:GLU:HA	2:H:964:LEU:HA	2.01	0.41
1:F:1106:ILE:HA	1:F:1188:GLN:NE2	2.33	0.41
1:F:1549:ASN:ND2	1:F:1549:ASN:C	2.73	0.41
2:H:585:LYS:HG3	2:H:1106:GLU:HB2	2.02	0.41
2:H:900:GLN:HE22	2:H:1033:SER:HB2	1.85	0.41
2:H:1037:SER:N	2:H:1051:THR:HG21	2.35	0.41
2:H:1432:GLN:N	2:H:1525:SER:O	2.52	0.41
2:J:43:GLU:HA	2:J:44:PRO:HD3	1.93	0.41
2:J:1561:ASN:HB3	2:J:1564:HIS:HD2	1.84	0.41
1:A:770:PRO:HB2	1:A:799:ILE:HG12	2.01	0.41
1:A:1112:ASN:HD22	1:A:1258:ARG:HH22	1.68	0.41
2:G:714:SER:HA	2:G:717:ILE:HD12	2.02	0.41
2:G:738:GLY:CA	2:G:1055:HIS:O	2.68	0.41
2:G:884:LEU:HD22	2:G:1021:LEU:HD12	2.01	0.41
2:G:976:PRO:O	2:G:980:ILE:N	2.48	0.41
2:G:1310:ASP:OD1	2:G:1317:ARG:NH2	2.53	0.41
2:G:1697:HIS:O	2:G:1701:THR:OG1	2.28	0.41
1:B:981:GLU:HA	2:C:964:LEU:HA	2.01	0.41
1:B:1107:GLU:HA	1:B:1108:PRO:HD3	1.92	0.41
2:C:549:ASP:HB3	2:C:554:GLY:HA3	2.02	0.41
2:C:919:TYR:CE1	2:C:995:LEU:HA	2.54	0.41
2:C:1265:MET:HE2	2:C:1562:PRO:HG2	2.02	0.41
2:C:1376:ALA:HA	2:C:1394:GLY:HA2	2.02	0.41
2:C:1690:VAL:HG21	2:C:1787:ALA:HA	2.02	0.41
2:C:1859:PRO:HG3	2:C:1871:LEU:HD13	2.03	0.41
1:D:1041:ALA:O	1:D:1630:THR:OG1	2.29	0.41
1:D:1112:ASN:HD22	1:D:1258:ARG:HH22	1.69	0.41
2:E:586:LEU:HD12	2:E:1108:PRO:HD3	2.03	0.41
1:K:633:GLU:H	1:K:653:ARG:HH22	1.68	0.41
2:G:1267:TRP:NE1	2:G:1273:GLU:O	2.39	0.41
1:B:1694:TYR:OH	2:C:1001:ASP:OD2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:745:VAL:HG23	1:D:802:MET:HG2	2.02	0.41
1:D:1549:ASN:ND2	1:D:1549:ASN:C	2.73	0.41
2:L:1561:ASN:HB3	2:L:1564:HIS:HD2	1.85	0.41
1:F:411:GLN:HE21	1:F:1629:LYS:HE2	1.85	0.41
1:F:1112:ASN:HD22	1:F:1258:ARG:HH22	1.69	0.41
2:H:738:GLY:CA	2:H:1055:HIS:O	2.68	0.41
2:H:848:SER:HB3	2:H:854:ILE:HD12	2.00	0.41
2:H:1778:GLN:HA	2:H:1809:LEU:HD21	2.01	0.41
2:J:549:ASP:HB3	2:J:554:GLY:HA3	2.02	0.41
2:J:1037:SER:N	2:J:1051:THR:HG21	2.35	0.41
1:A:745:VAL:HG23	1:A:802:MET:HG2	2.02	0.41
1:A:981:GLU:HA	2:G:964:LEU:HA	2.01	0.41
1:B:885:ALA:HA	1:B:888:ILE:HG22	2.03	0.41
2:C:260:PRO:CD	2:C:289:TRP:CH2	3.03	0.41
2:C:298:LYS:HB3	2:C:450:PHE:HE1	1.85	0.41
2:E:260:PRO:CD	2:E:289:TRP:CH2	3.03	0.41
1:K:1238:VAL:HG22	1:K:1392:LEU:HD11	2.02	0.41
1:F:768:ILE:HG12	1:F:770:PRO:HD3	2.02	0.41
1:I:885:ALA:HA	1:I:888:ILE:HG22	2.03	0.41
2:J:585:LYS:HG3	2:J:1106:GLU:HB2	2.02	0.41
2:J:919:TYR:CE1	2:J:995:LEU:HA	2.54	0.41
2:J:1736:MET:HE2	2:J:1736:MET:CA	2.42	0.41
1:A:885:ALA:HA	1:A:888:ILE:HG22	2.03	0.41
1:B:633:GLU:H	1:B:653:ARG:HH22	1.68	0.41
1:B:745:VAL:HG23	1:B:802:MET:HG2	2.02	0.41
2:C:577:ILE:HB	2:C:1082:ILE:HD11	2.01	0.41
2:C:900:GLN:HE22	2:C:1033:SER:HB2	1.85	0.41
2:C:1735:ALA:C	2:C:1736:MET:HE2	2.09	0.41
2:C:1778:GLN:HA	2:C:1809:LEU:HD21	2.01	0.41
2:C:1811:GLU:OE2	2:C:2010:TYR:OH	2.29	0.41
1:D:17:LEU:HD23	2:E:2014:LEU:HD23	2.01	0.41
1:D:1001:VAL:HG11	1:D:1662:TYR:HB2	2.02	0.41
2:E:658:MET:HG3	2:E:661:TRP:CZ2	2.56	0.41
1:K:409:ALA:HB2	1:K:442:ARG:HE	1.84	0.41
1:K:745:VAL:HG23	1:K:802:MET:HG2	2.02	0.41
1:K:1112:ASN:HD22	1:K:1258:ARG:HH22	1.68	0.41
1:K:1223:PHE:HA	1:K:1226:SER:HB3	2.03	0.41
2:L:1778:GLN:HA	2:L:1809:LEU:HD21	2.01	0.41
1:F:400:ARG:NH1	1:F:1358:HIS:O	2.40	0.41
2:H:1052:CYS:O	2:H:1052:CYS:SG	2.79	0.41
1:I:768:ILE:HG12	1:I:770:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:738:GLY:CA	2:J:1055:HIS:O	2.68	0.41
2:J:1217:ASN:HB3	2:J:1242:PHE:HB3	2.02	0.41
1:A:1001:VAL:HG11	1:A:1662:TYR:HB2	2.02	0.41
1:A:1238:VAL:HG22	1:A:1392:LEU:HD11	2.02	0.41
2:G:528:ILE:HG21	2:G:547:ILE:HG13	2.02	0.41
1:B:16:GLU:OE1	1:B:16:GLU:HA	2.21	0.41
1:B:18:LEU:O	1:B:21:GLN:HG3	2.21	0.41
2:C:915:ALA:HA	2:C:1000:ILE:HD11	2.03	0.41
2:C:1800:ALA:O	2:C:2009:LYS:NZ	2.48	0.41
1:D:1220:VAL:HG21	1:D:1698:PHE:HD1	1.84	0.41
1:D:1238:VAL:HG22	1:D:1392:LEU:HD11	2.02	0.41
2:E:585:LYS:HG3	2:E:1106:GLU:HB2	2.02	0.41
1:K:856:GLU:OE1	1:K:858:TRP:NE1	2.45	0.41
1:K:885:ALA:HA	1:K:888:ILE:HG22	2.03	0.41
2:L:327:SER:OG	2:L:333:GLY:O	2.32	0.41
2:L:577:ILE:HB	2:L:1082:ILE:HD11	2.01	0.41
2:L:1511:SER:OG	2:L:1512:HIS:N	2.54	0.41
2:L:1859:PRO:HG3	2:L:1871:LEU:HD13	2.02	0.41
2:H:658:MET:HG3	2:H:661:TRP:CZ2	2.56	0.41
2:H:741:HIS:HB3	2:H:853:PRO:HB2	2.02	0.41
1:I:981:GLU:HA	2:J:964:LEU:HA	2.01	0.41
1:I:1112:ASN:HD22	1:I:1258:ARG:HH22	1.69	0.41
2:J:577:ILE:HB	2:J:1082:ILE:HD11	2.01	0.41
2:J:1227:ARG:HD2	2:J:1565:VAL:HG11	2.02	0.41
2:J:1352:HIS:NE2	2:J:1354:SER:O	2.54	0.41
1:A:768:ILE:HG12	1:A:770:PRO:HD3	2.02	0.41
1:B:1223:PHE:HA	1:B:1226:SER:HB3	2.03	0.41
2:C:586:LEU:HD12	2:C:1108:PRO:HD3	2.03	0.41
2:C:738:GLY:CA	2:C:1055:HIS:O	2.68	0.41
1:D:1223:PHE:HA	1:D:1226:SER:HB3	2.03	0.41
1:D:1411:THR:HG22	1:D:1648:GLN:HG3	2.02	0.41
2:E:73:GLU:HA	2:E:74:PRO:HD3	1.89	0.41
2:E:581:THR:H	2:E:584:SER:HG	1.65	0.41
2:E:674:TYR:HA	2:E:675:PRO:HD3	1.90	0.41
2:E:807:ILE:HD13	2:E:807:ILE:HG21	1.88	0.41
2:E:1859:PRO:HG3	2:E:1871:LEU:HD13	2.02	0.41
1:K:1545:SER:O	1:K:1545:SER:OG	2.27	0.41
2:L:586:LEU:HD12	2:L:1108:PRO:HD3	2.03	0.41
2:L:915:ALA:HA	2:L:1000:ILE:HD11	2.03	0.41
1:F:18:LEU:O	1:F:21:GLN:HG3	2.21	0.41
2:H:726:PHE:HA	2:H:727:PRO:HD3	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1561:ASN:HB3	2:H:1564:HIS:HD2	1.85	0.41
1:I:17:LEU:HD23	2:J:2014:LEU:HD23	2.01	0.41
1:I:18:LEU:O	1:I:21:GLN:HG3	2.21	0.41
1:I:1238:VAL:HG22	1:I:1392:LEU:HD11	2.02	0.41
2:J:1170:ILE:O	2:J:1174:PHE:HD2	2.04	0.41
1:A:1082:GLU:HA	1:A:1083:PRO:HD3	1.94	0.41
1:A:1223:PHE:HA	1:A:1226:SER:HB3	2.03	0.41
1:B:1112:ASN:HD22	1:B:1258:ARG:HH22	1.69	0.41
2:C:714:SER:HA	2:C:717:ILE:HD12	2.02	0.41
2:C:1352:HIS:NE2	2:C:1354:SER:O	2.54	0.41
2:C:1737:ILE:HD13	2:C:1737:ILE:N	2.19	0.41
2:E:1052:CYS:O	2:E:1052:CYS:SG	2.79	0.41
2:E:1265:MET:HE2	2:E:1562:PRO:HG2	2.03	0.41
1:K:18:LEU:O	1:K:21:GLN:HG3	2.21	0.41
2:L:1217:ASN:HB3	2:L:1242:PHE:HB3	2.02	0.41
2:L:1376:ALA:HA	2:L:1394:GLY:HA2	2.02	0.41
2:H:586:LEU:HD12	2:H:1108:PRO:HD3	2.03	0.41
2:H:1227:ARG:HD2	2:H:1565:VAL:HG11	2.02	0.41
2:H:1783:LEU:HD23	2:H:1783:LEU:HA	1.92	0.41
1:I:16:GLU:HA	1:I:16:GLU:OE1	2.21	0.41
1:I:1411:THR:HG22	1:I:1648:GLN:HG3	2.02	0.41
1:A:35:PHE:HA	1:A:39:PHE:HD2	1.85	0.41
1:A:1423:LYS:NZ	1:K:1712:GLU:OE2	2.49	0.41
2:G:320:PRO:HA	2:G:321:PRO:HD3	1.89	0.41
2:G:586:LEU:HD12	2:G:1108:PRO:HD3	2.03	0.41
2:G:741:HIS:HB3	2:G:853:PRO:HB2	2.02	0.41
2:G:942:THR:HB	2:G:1012:GLN:HG3	2.03	0.41
2:G:1052:CYS:SG	2:G:1052:CYS:O	2.79	0.41
2:G:1170:ILE:O	2:G:1174:PHE:HD2	2.04	0.41
2:G:1511:SER:OG	2:G:1512:HIS:N	2.54	0.41
2:G:1561:ASN:HB3	2:G:1564:HIS:HD2	1.85	0.41
2:G:1690:VAL:HG21	2:G:1787:ALA:HA	2.02	0.41
1:B:14:LEU:HD13	1:B:14:LEU:O	2.21	0.41
1:B:1712:GLU:OE2	1:I:1423:LYS:NZ	2.49	0.41
1:B:1751:GLU:CB	1:B:1754:LYS:HE3	2.51	0.41
2:C:741:HIS:HE1	2:C:836:TYR:HE1	1.68	0.41
2:C:1037:SER:N	2:C:1051:THR:HG21	2.35	0.41
2:C:1511:SER:OG	2:C:1512:HIS:N	2.54	0.41
2:E:298:LYS:HB3	2:E:450:PHE:HE1	1.85	0.41
2:E:738:GLY:CA	2:E:1055:HIS:O	2.68	0.41
2:E:915:ALA:HA	2:E:1000:ILE:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1690:VAL:HG21	2:E:1787:ALA:HA	2.02	0.41
2:E:1916:PHE:O	2:E:1920:GLN:N	2.48	0.41
1:K:1220:VAL:HG21	1:K:1698:PHE:HD1	1.84	0.41
1:K:1649:LYS:HB2	1:K:1649:LYS:HE3	1.90	0.41
2:L:290:GLU:N	2:L:290:GLU:CD	2.73	0.41
2:L:900:GLN:HE22	2:L:1033:SER:HB2	1.85	0.41
2:L:942:THR:HB	2:L:1012:GLN:HG3	2.03	0.41
2:L:1739:GLU:H	2:L:1739:GLU:HG2	1.66	0.41
1:F:633:GLU:H	1:F:653:ARG:HH22	1.68	0.41
1:F:1223:PHE:HA	1:F:1226:SER:HB3	2.03	0.41
2:H:260:PRO:CD	2:H:289:TRP:CH2	3.03	0.41
2:H:942:THR:HB	2:H:1012:GLN:HG3	2.03	0.41
2:H:1170:ILE:O	2:H:1174:PHE:HD2	2.04	0.41
2:H:1217:ASN:HB3	2:H:1242:PHE:HB3	2.02	0.41
2:H:1690:VAL:HG21	2:H:1787:ALA:HA	2.02	0.41
2:H:1859:PRO:HG3	2:H:1871:LEU:HD13	2.03	0.41
1:I:1001:VAL:HG11	1:I:1662:TYR:HB2	2.02	0.41
1:I:1223:PHE:HA	1:I:1226:SER:HB3	2.03	0.41
2:J:260:PRO:HG2	2:J:289:TRP:CZ3	2.56	0.41
2:J:260:PRO:CD	2:J:289:TRP:CH2	3.03	0.41
2:J:741:HIS:HE1	2:J:836:TYR:HE1	1.68	0.41
2:J:848:SER:HB3	2:J:854:ILE:HD12	2.00	0.41
2:J:1485:CYS:HB3	2:J:1506:TYR:HB3	2.02	0.41
2:J:1702:TYR:O	2:J:1733:TYR:OH	2.30	0.41
1:A:14:LEU:HD13	1:A:14:LEU:O	2.21	0.41
2:G:260:PRO:HG2	2:G:289:TRP:CZ3	2.56	0.41
2:G:658:MET:HG3	2:G:661:TRP:CZ2	2.56	0.41
2:G:747:HIS:O	2:G:751:LEU:N	2.54	0.41
2:G:1068:GLU:HA	2:G:1069:PRO:HD3	1.92	0.41
2:C:43:GLU:HA	2:C:44:PRO:HD3	1.93	0.41
2:C:585:LYS:HG3	2:C:1106:GLU:HB2	2.02	0.41
2:C:942:THR:HB	2:C:1012:GLN:HG3	2.03	0.41
2:E:942:THR:HB	2:E:1012:GLN:HG3	2.03	0.41
1:K:14:LEU:HD13	1:K:14:LEU:O	2.21	0.41
1:K:371:LEU:HD23	1:K:371:LEU:HA	1.93	0.41
2:L:585:LYS:HG3	2:L:1106:GLU:HB2	2.02	0.41
2:L:741:HIS:HB3	2:L:853:PRO:HB2	2.02	0.41
2:J:581:THR:H	2:J:584:SER:HG	1.65	0.41
2:J:586:LEU:HD12	2:J:1108:PRO:HD3	2.03	0.41
2:J:691:ALA:HA	2:J:694:TYR:CD2	2.56	0.41
2:J:1511:SER:OG	2:J:1512:HIS:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1227:ARG:HD2	2:G:1565:VAL:HG11	2.02	0.40
2:G:1485:CYS:HB3	2:G:1506:TYR:HB3	2.02	0.40
1:B:1264:ARG:NH2	1:B:1271:GLN:O	2.54	0.40
2:C:646:THR:OG1	2:C:677:GLN:OE1	2.28	0.40
2:C:1170:ILE:O	2:C:1174:PHE:HD2	2.04	0.40
2:C:1217:ASN:HB3	2:C:1242:PHE:HB3	2.02	0.40
2:E:1737:ILE:HD13	2:E:1737:ILE:N	2.19	0.40
2:L:549:ASP:HB3	2:L:554:GLY:HA3	2.02	0.40
2:L:658:MET:HG3	2:L:661:TRP:CZ2	2.56	0.40
2:L:1227:ARG:HD2	2:L:1565:VAL:HG11	2.02	0.40
1:F:745:VAL:HG23	1:F:802:MET:HG2	2.02	0.40
1:F:1238:VAL:HG22	1:F:1392:LEU:HD11	2.02	0.40
2:J:915:ALA:HA	2:J:1000:ILE:HD11	2.03	0.40
2:J:1082:ILE:HD13	2:J:1082:ILE:HG21	1.91	0.40
2:J:1376:ALA:HA	2:J:1394:GLY:HA2	2.02	0.40
2:G:190:PHE:CZ	2:G:297:ARG:HD2	2.54	0.40
2:G:549:ASP:HB3	2:G:554:GLY:HA3	2.02	0.40
2:G:848:SER:HB3	2:G:854:ILE:HD12	2.00	0.40
2:G:900:GLN:HE22	2:G:1033:SER:HB2	1.85	0.40
2:G:1352:HIS:NE2	2:G:1354:SER:O	2.54	0.40
1:B:856:GLU:OE1	1:B:858:TRP:NE1	2.45	0.40
1:B:1553:GLU:HA	1:B:1556:THR:HG22	2.04	0.40
2:C:260:PRO:HG2	2:C:289:TRP:CZ3	2.56	0.40
2:C:741:HIS:HB3	2:C:853:PRO:HB2	2.02	0.40
2:C:1767:GLU:OE2	2:C:1849:ARG:NE	2.36	0.40
1:D:14:LEU:HD13	1:D:14:LEU:O	2.21	0.40
2:E:327:SER:OG	2:E:333:GLY:O	2.32	0.40
2:E:1227:ARG:HD2	2:E:1565:VAL:HG11	2.02	0.40
1:K:403:ASP:OD1	1:K:731:THR:OG1	2.30	0.40
1:K:1264:ARG:NH2	1:K:1271:GLN:O	2.54	0.40
2:L:381:GLY:H	2:L:386:LEU:HD11	1.87	0.40
2:L:1432:GLN:N	2:L:1525:SER:O	2.52	0.40
1:F:13:LEU:HG	2:H:2019:PHE:HE1	1.87	0.40
1:F:14:LEU:HD13	1:F:14:LEU:O	2.21	0.40
2:H:381:GLY:H	2:H:386:LEU:HD11	1.86	0.40
2:H:1730:ARG:NH1	2:H:1759:SER:O	2.43	0.40
2:J:404:GLN:HE22	2:J:413:LYS:HB2	1.87	0.40
2:J:741:HIS:HB3	2:J:853:PRO:HB2	2.02	0.40
1:A:18:LEU:O	1:A:21:GLN:HG3	2.21	0.40
1:A:498:GLY:HA2	1:A:873:ARG:HH22	1.86	0.40
1:A:1264:ARG:NH2	1:A:1271:GLN:O	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:73:GLU:HA	2:G:74:PRO:HD3	1.89	0.40
2:G:1265:MET:HE2	2:G:1562:PRO:HG2	2.02	0.40
1:B:1238:VAL:HG22	1:B:1392:LEU:HD11	2.02	0.40
1:B:1411:THR:HG22	1:B:1648:GLN:HG3	2.02	0.40
2:C:381:GLY:H	2:C:386:LEU:HD11	1.86	0.40
2:C:533:LEU:HB3	2:C:544:LYS:HB3	2.04	0.40
2:C:1052:CYS:SG	2:C:1052:CYS:O	2.79	0.40
2:C:1227:ARG:HD2	2:C:1565:VAL:HG11	2.02	0.40
1:D:2:LYS:HA	1:D:3:PRO:HD3	1.96	0.40
1:D:13:LEU:HG	2:E:2019:PHE:HE1	1.87	0.40
1:D:1521:PRO:O	1:D:1525:ALA:N	2.46	0.40
1:K:1411:THR:HG22	1:K:1648:GLN:HG3	2.02	0.40
1:F:885:ALA:HA	1:F:888:ILE:HG22	2.03	0.40
2:H:714:SER:HA	2:H:717:ILE:HD12	2.02	0.40
2:H:807:ILE:HG21	2:H:807:ILE:HD13	1.88	0.40
2:H:915:ALA:HA	2:H:1000:ILE:HD11	2.03	0.40
2:H:1849:ARG:HD3	2:H:1957:PRO:HB3	2.03	0.40
1:I:498:GLY:HA2	1:I:873:ARG:HH22	1.87	0.40
1:I:521:LYS:HB3	1:I:523:SER:H	1.87	0.40
1:I:1560:MET:HG3	1:I:1561:MET:HE3	2.04	0.40
1:I:1751:GLU:CB	1:I:1754:LYS:HE3	2.51	0.40
2:J:190:PHE:CZ	2:J:297:ARG:HD2	2.54	0.40
2:J:298:LYS:HB3	2:J:450:PHE:HE1	1.85	0.40
2:J:942:THR:HB	2:J:1012:GLN:HG3	2.03	0.40
1:A:1385:GLN:NE2	1:A:1594:ASN:OD1	2.52	0.40
1:A:1521:PRO:O	1:A:1525:ALA:N	2.46	0.40
2:G:298:LYS:HB3	2:G:450:PHE:HE1	1.85	0.40
2:G:1849:ARG:HD3	2:G:1957:PRO:HB3	2.03	0.40
1:B:1291:LEU:HB3	1:B:1292:ILE:H	1.68	0.40
1:D:521:LYS:HB3	1:D:523:SER:H	1.87	0.40
1:D:885:ALA:HA	1:D:888:ILE:HG22	2.03	0.40
1:D:1559:GLU:OE2	1:F:1716:LEU:HD11	2.22	0.40
1:D:1751:GLU:O	1:D:1754:LYS:CG	2.69	0.40
2:E:533:LEU:HB3	2:E:544:LYS:HB3	2.04	0.40
2:E:846:VAL:CG2	2:E:856:LYS:HD2	2.52	0.40
1:K:16:GLU:OE1	1:K:16:GLU:HA	2.21	0.40
1:K:1303:GLY:HA2	1:K:1649:LYS:NZ	2.37	0.40
1:K:1553:GLU:HA	1:K:1556:THR:HG22	2.04	0.40
1:K:1783:ASN:HB3	1:K:1786:PHE:HD2	1.86	0.40
2:L:1170:ILE:O	2:L:1174:PHE:HD2	2.04	0.40
2:L:1352:HIS:NE2	2:L:1354:SER:O	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:16:GLU:CG	2:H:2038:ILE:HD11	2.46	0.40
2:H:298:LYS:HB3	2:H:450:PHE:HE1	1.85	0.40
1:I:633:GLU:H	1:I:653:ARG:HH22	1.68	0.40
1:I:1264:ARG:NH2	1:I:1271:GLN:O	2.54	0.40
2:J:381:GLY:H	2:J:386:LEU:HD11	1.87	0.40
2:J:1381:VAL:O	2:J:1422:THR:OG1	2.28	0.40
2:J:1531:VAL:HG11	2:J:1795:LYS:HA	2.04	0.40
2:J:1737:ILE:HD13	2:J:1737:ILE:N	2.19	0.40
1:A:1157:ILE:HA	1:A:1158:PRO:HD3	1.93	0.40
1:A:1559:GLU:OE2	1:K:1716:LEU:HD11	2.22	0.40
2:G:260:PRO:CD	2:G:289:TRP:CH2	3.03	0.40
2:G:582:LYS:HD3	2:G:1108:PRO:HB3	2.04	0.40
2:G:691:ALA:HA	2:G:694:TYR:CD2	2.56	0.40
2:G:846:VAL:CG2	2:G:856:LYS:HD2	2.52	0.40
2:G:915:ALA:HA	2:G:1000:ILE:HD11	2.03	0.40
2:G:1201:VAL:HG11	2:G:1226:ASN:HB2	2.03	0.40
1:B:521:LYS:HB3	1:B:523:SER:H	1.87	0.40
2:C:404:GLN:HE22	2:C:413:LYS:HB2	1.87	0.40
1:D:18:LEU:O	1:D:21:GLN:HG3	2.21	0.40
1:D:1716:LEU:HD11	1:F:1559:GLU:OE2	2.22	0.40
2:E:1304:VAL:HA	2:E:1584:PHE:HE1	1.87	0.40
2:E:1739:GLU:H	2:E:1739:GLU:HG2	1.66	0.40
2:L:738:GLY:CA	2:L:1055:HIS:O	2.68	0.40
2:L:1052:CYS:O	2:L:1052:CYS:SG	2.79	0.40
1:F:16:GLU:OE1	1:F:16:GLU:HA	2.21	0.40
2:H:1352:HIS:NE2	2:H:1354:SER:O	2.54	0.40
1:I:1119:LYS:HE2	1:I:1341:PHE:CG	2.57	0.40
1:I:1491:ARG:CA	1:I:1750:ILE:CD1	2.96	0.40
2:J:846:VAL:CG2	2:J:856:LYS:HD2	2.52	0.40
2:J:1052:CYS:O	2:J:1052:CYS:SG	2.79	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1737/1887 (92%)	1650 (95%)	85 (5%)	2 (0%)	51	83
1	B	1737/1887 (92%)	1650 (95%)	85 (5%)	2 (0%)	51	83
1	D	1737/1887 (92%)	1650 (95%)	85 (5%)	2 (0%)	51	83
1	F	1737/1887 (92%)	1650 (95%)	85 (5%)	2 (0%)	51	83
1	I	1737/1887 (92%)	1650 (95%)	85 (5%)	2 (0%)	51	83
1	K	1737/1887 (92%)	1649 (95%)	85 (5%)	3 (0%)	47	79
2	C	2027/2051 (99%)	1899 (94%)	125 (6%)	3 (0%)	51	83
2	E	2027/2051 (99%)	1898 (94%)	126 (6%)	3 (0%)	51	83
2	G	2027/2051 (99%)	1898 (94%)	126 (6%)	3 (0%)	51	83
2	H	2027/2051 (99%)	1899 (94%)	125 (6%)	3 (0%)	51	83
2	J	2027/2051 (99%)	1898 (94%)	126 (6%)	3 (0%)	51	83
2	L	2027/2051 (99%)	1898 (94%)	126 (6%)	3 (0%)	51	83
All	All	22584/23628 (96%)	21289 (94%)	1264 (6%)	31 (0%)	54	83

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	1743	ASP
2	C	1743	ASP
2	E	1743	ASP
2	L	1743	ASP
2	H	1743	ASP
2	J	1743	ASP
1	K	329	GLU
2	G	287	ASP
2	C	287	ASP
2	E	287	ASP
2	L	287	ASP
2	H	287	ASP
2	J	287	ASP
1	A	1291	LEU
1	B	1291	LEU
1	D	1291	LEU
1	K	1291	LEU
1	F	1291	LEU
1	I	1291	LEU

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Mol	Chain	Res	Type
2	C	676	ILE
2	E	676	ILE
2	H	676	ILE
2	J	676	ILE
2	G	676	ILE
2	L	676	ILE
1	B	1292	ILE
1	D	1292	ILE
1	F	1292	ILE
1	I	1292	ILE
1	A	1292	ILE
1	K	1292	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1475/1565 (94%)	1455 (99%)	20 (1%)	67	86
1	B	1475/1565 (94%)	1455 (99%)	20 (1%)	67	86
1	D	1475/1565 (94%)	1455 (99%)	20 (1%)	67	86
1	F	1475/1565 (94%)	1455 (99%)	20 (1%)	67	86
1	I	1475/1565 (94%)	1455 (99%)	20 (1%)	67	86
1	K	1475/1565 (94%)	1455 (99%)	20 (1%)	67	86
2	C	1770/1789 (99%)	1739 (98%)	31 (2%)	59	82
2	E	1770/1789 (99%)	1739 (98%)	31 (2%)	59	82
2	G	1770/1789 (99%)	1739 (98%)	31 (2%)	59	82
2	H	1770/1789 (99%)	1739 (98%)	31 (2%)	59	82
2	J	1770/1789 (99%)	1739 (98%)	31 (2%)	59	82
2	L	1770/1789 (99%)	1739 (98%)	31 (2%)	59	82
All	All	19470/20124 (97%)	19164 (98%)	306 (2%)	64	84

All (306) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	356	ASN
1	A	407	ASN
1	A	427	ASN
1	A	457	ASN
1	A	536	THR
1	A	738	ASN
1	A	761	LEU
1	A	873	ARG
1	A	894	ARG
1	A	1064	ASN
1	A	1208	VAL
1	A	1283	MET
1	A	1288	ASN
1	A	1367	ARG
1	A	1411	THR
1	A	1430	ARG
1	A	1442	ASN
1	A	1546	THR
1	A	1549	ASN
1	A	1585	LYS
2	G	279	THR
2	G	288	SER
2	G	295	SER
2	G	376	ASN
2	G	485	ARG
2	G	553	ASN
2	G	572	ASN
2	G	669	LEU
2	G	676	ILE
2	G	679	LEU
2	G	680	THR
2	G	844	VAL
2	G	845	THR
2	G	847	ARG
2	G	936	ASN
2	G	1051	THR
2	G	1055	HIS
2	G	1164	MET
2	G	1355	ASN
2	G	1415	ASN
2	G	1737	ILE
2	G	1738	PHE
2	G	1739	GLU

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Mol	Chain	Res	Type
2	G	1740	THR
2	G	1743	ASP
2	G	1745	LYS
2	G	1746	LEU
2	G	1747	LYS
2	G	1748	THR
2	G	1749	GLU
2	G	1956	ARG
1	B	356	ASN
1	B	407	ASN
1	B	427	ASN
1	B	457	ASN
1	B	536	THR
1	B	738	ASN
1	B	761	LEU
1	B	873	ARG
1	B	894	ARG
1	B	1064	ASN
1	B	1208	VAL
1	B	1283	MET
1	B	1288	ASN
1	B	1367	ARG
1	B	1411	THR
1	B	1430	ARG
1	B	1442	ASN
1	B	1546	THR
1	B	1549	ASN
1	B	1585	LYS
2	C	279	THR
2	C	288	SER
2	C	295	SER
2	C	376	ASN
2	C	485	ARG
2	C	553	ASN
2	C	572	ASN
2	C	669	LEU
2	C	676	ILE
2	C	679	LEU
2	C	680	THR
2	C	844	VAL
2	C	845	THR
2	C	847	ARG

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Mol	Chain	Res	Type
2	C	936	ASN
2	C	1051	THR
2	C	1055	HIS
2	C	1164	MET
2	C	1355	ASN
2	C	1415	ASN
2	C	1737	ILE
2	C	1738	PHE
2	C	1739	GLU
2	C	1740	THR
2	C	1743	ASP
2	C	1745	LYS
2	C	1746	LEU
2	C	1747	LYS
2	C	1748	THR
2	C	1749	GLU
2	C	1956	ARG
1	D	356	ASN
1	D	407	ASN
1	D	427	ASN
1	D	457	ASN
1	D	536	THR
1	D	738	ASN
1	D	761	LEU
1	D	873	ARG
1	D	894	ARG
1	D	1064	ASN
1	D	1208	VAL
1	D	1283	MET
1	D	1288	ASN
1	D	1367	ARG
1	D	1411	THR
1	D	1430	ARG
1	D	1442	ASN
1	D	1546	THR
1	D	1549	ASN
1	D	1585	LYS
2	E	279	THR
2	E	288	SER
2	E	295	SER
2	E	376	ASN
2	E	485	ARG

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Mol	Chain	Res	Type
2	E	553	ASN
2	E	572	ASN
2	E	669	LEU
2	E	676	ILE
2	E	679	LEU
2	E	680	THR
2	E	844	VAL
2	E	845	THR
2	E	847	ARG
2	E	936	ASN
2	E	1051	THR
2	E	1055	HIS
2	E	1164	MET
2	E	1355	ASN
2	E	1415	ASN
2	E	1737	ILE
2	E	1738	PHE
2	E	1739	GLU
2	E	1740	THR
2	E	1743	ASP
2	E	1745	LYS
2	E	1746	LEU
2	E	1747	LYS
2	E	1748	THR
2	E	1749	GLU
2	E	1956	ARG
1	K	356	ASN
1	K	407	ASN
1	K	427	ASN
1	K	457	ASN
1	K	536	THR
1	K	738	ASN
1	K	761	LEU
1	K	873	ARG
1	K	894	ARG
1	K	1064	ASN
1	K	1208	VAL
1	K	1283	MET
1	K	1288	ASN
1	K	1367	ARG
1	K	1411	THR
1	K	1430	ARG

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Mol	Chain	Res	Type
1	K	1442	ASN
1	K	1546	THR
1	K	1549	ASN
1	K	1585	LYS
2	L	279	THR
2	L	288	SER
2	L	295	SER
2	L	376	ASN
2	L	485	ARG
2	L	553	ASN
2	L	572	ASN
2	L	669	LEU
2	L	676	ILE
2	L	679	LEU
2	L	680	THR
2	L	844	VAL
2	L	845	THR
2	L	847	ARG
2	L	936	ASN
2	L	1051	THR
2	L	1055	HIS
2	L	1164	MET
2	L	1355	ASN
2	L	1415	ASN
2	L	1737	ILE
2	L	1738	PHE
2	L	1739	GLU
2	L	1740	THR
2	L	1743	ASP
2	L	1745	LYS
2	L	1746	LEU
2	L	1747	LYS
2	L	1748	THR
2	L	1749	GLU
2	L	1956	ARG
1	F	356	ASN
1	F	407	ASN
1	F	427	ASN
1	F	457	ASN
1	F	536	THR
1	F	738	ASN
1	F	761	LEU

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Mol	Chain	Res	Type
1	F	873	ARG
1	F	894	ARG
1	F	1064	ASN
1	F	1208	VAL
1	F	1283	MET
1	F	1288	ASN
1	F	1367	ARG
1	F	1411	THR
1	F	1430	ARG
1	F	1442	ASN
1	F	1546	THR
1	F	1549	ASN
1	F	1585	LYS
2	H	279	THR
2	H	288	SER
2	H	295	SER
2	H	376	ASN
2	H	485	ARG
2	H	553	ASN
2	H	572	ASN
2	H	669	LEU
2	H	676	ILE
2	H	679	LEU
2	H	680	THR
2	H	844	VAL
2	H	845	THR
2	H	847	ARG
2	H	936	ASN
2	H	1051	THR
2	H	1055	HIS
2	H	1164	MET
2	H	1355	ASN
2	H	1415	ASN
2	H	1737	ILE
2	H	1738	PHE
2	H	1739	GLU
2	H	1740	THR
2	H	1743	ASP
2	H	1745	LYS
2	H	1746	LEU
2	H	1747	LYS
2	H	1748	THR

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Mol	Chain	Res	Type
2	H	1749	GLU
2	H	1956	ARG
1	I	356	ASN
1	I	407	ASN
1	I	427	ASN
1	I	457	ASN
1	I	536	THR
1	I	738	ASN
1	I	761	LEU
1	I	873	ARG
1	I	894	ARG
1	I	1064	ASN
1	I	1208	VAL
1	I	1283	MET
1	I	1288	ASN
1	I	1367	ARG
1	I	1411	THR
1	I	1430	ARG
1	I	1442	ASN
1	I	1546	THR
1	I	1549	ASN
1	I	1585	LYS
2	J	279	THR
2	J	288	SER
2	J	295	SER
2	J	376	ASN
2	J	485	ARG
2	J	553	ASN
2	J	572	ASN
2	J	669	LEU
2	J	676	ILE
2	J	679	LEU
2	J	680	THR
2	J	844	VAL
2	J	845	THR
2	J	847	ARG
2	J	936	ASN
2	J	1051	THR
2	J	1055	HIS
2	J	1164	MET
2	J	1355	ASN
2	J	1415	ASN

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Mol	Chain	Res	Type
2	J	1737	ILE
2	J	1738	PHE
2	J	1739	GLU
2	J	1740	THR
2	J	1743	ASP
2	J	1745	LYS
2	J	1746	LEU
2	J	1747	LYS
2	J	1748	THR
2	J	1749	GLU
2	J	1956	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (293) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	214	GLN
1	A	271	ASN
1	A	335	HIS
1	A	344	GLN
1	A	407	ASN
1	A	427	ASN
1	A	457	ASN
1	A	738	ASN
1	A	792	HIS
1	A	1064	ASN
1	A	1112	ASN
1	A	1123	GLN
1	A	1188	GLN
1	A	1239	HIS
1	A	1442	ASN
1	A	1506	GLN
1	A	1510	ASN
1	A	1549	ASN
1	A	1610	ASN
1	A	1652	GLN
1	A	1845	ASN
2	G	13	HIS
2	G	354	ASN
2	G	376	ASN
2	G	404	GLN
2	G	428	HIS

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Mol	Chain	Res	Type
2	G	440	ASN
2	G	553	ASN
2	G	572	ASN
2	G	612	ASN
2	G	747	HIS
2	G	936	ASN
2	G	993	GLN
2	G	1036	GLN
2	G	1049	GLN
2	G	1151	HIS
2	G	1202	GLN
2	G	1355	ASN
2	G	1415	ASN
2	G	1476	ASN
2	G	1564	HIS
2	G	1581	HIS
2	G	1628	HIS
2	G	1659	GLN
2	G	1928	GLN
2	G	1977	HIS
2	G	2000	ASN
1	B	32	GLN
1	B	214	GLN
1	B	271	ASN
1	B	335	HIS
1	B	344	GLN
1	B	356	ASN
1	B	407	ASN
1	B	427	ASN
1	B	457	ASN
1	B	738	ASN
1	B	792	HIS
1	B	1064	ASN
1	B	1112	ASN
1	B	1123	GLN
1	B	1188	GLN
1	B	1239	HIS
1	B	1442	ASN
1	B	1506	GLN
1	B	1510	ASN
1	B	1549	ASN
1	B	1610	ASN

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Mol	Chain	Res	Type
1	B	1652	GLN
1	B	1845	ASN
2	C	13	HIS
2	C	354	ASN
2	C	376	ASN
2	C	404	GLN
2	C	428	HIS
2	C	440	ASN
2	C	553	ASN
2	C	572	ASN
2	C	612	ASN
2	C	747	HIS
2	C	936	ASN
2	C	993	GLN
2	C	1036	GLN
2	C	1049	GLN
2	C	1151	HIS
2	C	1202	GLN
2	C	1355	ASN
2	C	1415	ASN
2	C	1476	ASN
2	C	1564	HIS
2	C	1581	HIS
2	C	1628	HIS
2	C	1659	GLN
2	C	1928	GLN
2	C	1977	HIS
2	C	2000	ASN
1	D	32	GLN
1	D	214	GLN
1	D	271	ASN
1	D	335	HIS
1	D	344	GLN
1	D	407	ASN
1	D	427	ASN
1	D	457	ASN
1	D	719	GLN
1	D	738	ASN
1	D	792	HIS
1	D	1064	ASN
1	D	1112	ASN
1	D	1123	GLN

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Mol	Chain	Res	Type
1	D	1188	GLN
1	D	1239	HIS
1	D	1442	ASN
1	D	1506	GLN
1	D	1510	ASN
1	D	1549	ASN
1	D	1552	ASN
1	D	1610	ASN
1	D	1652	GLN
1	D	1845	ASN
2	E	13	HIS
2	E	354	ASN
2	E	376	ASN
2	E	404	GLN
2	E	428	HIS
2	E	440	ASN
2	E	553	ASN
2	E	572	ASN
2	E	612	ASN
2	E	747	HIS
2	E	936	ASN
2	E	993	GLN
2	E	1036	GLN
2	E	1049	GLN
2	E	1151	HIS
2	E	1202	GLN
2	E	1355	ASN
2	E	1415	ASN
2	E	1476	ASN
2	E	1564	HIS
2	E	1581	HIS
2	E	1628	HIS
2	E	1659	GLN
2	E	1928	GLN
2	E	1977	HIS
2	E	2000	ASN
1	K	32	GLN
1	K	214	GLN
1	K	271	ASN
1	K	335	HIS
1	K	344	GLN
1	K	407	ASN

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Mol	Chain	Res	Type
1	K	427	ASN
1	K	457	ASN
1	K	719	GLN
1	K	738	ASN
1	K	792	HIS
1	K	1064	ASN
1	K	1112	ASN
1	K	1123	GLN
1	K	1188	GLN
1	K	1239	HIS
1	K	1442	ASN
1	K	1506	GLN
1	K	1510	ASN
1	K	1549	ASN
1	K	1610	ASN
1	K	1652	GLN
1	K	1845	ASN
2	L	13	HIS
2	L	354	ASN
2	L	376	ASN
2	L	428	HIS
2	L	440	ASN
2	L	553	ASN
2	L	572	ASN
2	L	612	ASN
2	L	747	HIS
2	L	936	ASN
2	L	993	GLN
2	L	1036	GLN
2	L	1049	GLN
2	L	1151	HIS
2	L	1202	GLN
2	L	1355	ASN
2	L	1415	ASN
2	L	1476	ASN
2	L	1564	HIS
2	L	1581	HIS
2	L	1628	HIS
2	L	1659	GLN
2	L	1928	GLN
2	L	1977	HIS
2	L	2000	ASN

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Mol	Chain	Res	Type
1	F	32	GLN
1	F	214	GLN
1	F	271	ASN
1	F	335	HIS
1	F	344	GLN
1	F	407	ASN
1	F	427	ASN
1	F	457	ASN
1	F	738	ASN
1	F	792	HIS
1	F	1064	ASN
1	F	1112	ASN
1	F	1123	GLN
1	F	1188	GLN
1	F	1239	HIS
1	F	1442	ASN
1	F	1506	GLN
1	F	1510	ASN
1	F	1549	ASN
1	F	1552	ASN
1	F	1610	ASN
1	F	1652	GLN
1	F	1845	ASN
2	H	13	HIS
2	H	354	ASN
2	H	376	ASN
2	H	404	GLN
2	H	428	HIS
2	H	440	ASN
2	H	553	ASN
2	H	572	ASN
2	H	612	ASN
2	H	747	HIS
2	H	936	ASN
2	H	993	GLN
2	H	1036	GLN
2	H	1049	GLN
2	H	1151	HIS
2	H	1202	GLN
2	H	1355	ASN
2	H	1415	ASN
2	H	1476	ASN

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Mol	Chain	Res	Type
2	H	1564	HIS
2	H	1581	HIS
2	H	1628	HIS
2	H	1659	GLN
2	H	1928	GLN
2	H	1977	HIS
2	H	2000	ASN
1	I	32	GLN
1	I	214	GLN
1	I	271	ASN
1	I	335	HIS
1	I	344	GLN
1	I	356	ASN
1	I	407	ASN
1	I	427	ASN
1	I	457	ASN
1	I	719	GLN
1	I	738	ASN
1	I	792	HIS
1	I	1064	ASN
1	I	1112	ASN
1	I	1123	GLN
1	I	1188	GLN
1	I	1239	HIS
1	I	1442	ASN
1	I	1506	GLN
1	I	1510	ASN
1	I	1549	ASN
1	I	1610	ASN
1	I	1652	GLN
2	J	13	HIS
2	J	354	ASN
2	J	376	ASN
2	J	404	GLN
2	J	428	HIS
2	J	440	ASN
2	J	553	ASN
2	J	572	ASN
2	J	612	ASN
2	J	747	HIS
2	J	936	ASN
2	J	993	GLN

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Mol	Chain	Res	Type
2	J	1036	GLN
2	J	1049	GLN
2	J	1151	HIS
2	J	1202	GLN
2	J	1355	ASN
2	J	1415	ASN
2	J	1476	ASN
2	J	1564	HIS
2	J	1581	HIS
2	J	1628	HIS
2	J	1659	GLN
2	J	1928	GLN
2	J	1977	HIS
2	J	2000	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	SEP	D	1440	1	8,9,10	1.45	1 (12%)	8,12,14	1.78	2 (25%)
1	SEP	A	1440	1	8,9,10	1.45	1 (12%)	8,12,14	1.78	2 (25%)
1	SEP	K	1440	1	8,9,10	1.45	1 (12%)	8,12,14	1.79	2 (25%)
1	SEP	I	1440	1	8,9,10	1.45	1 (12%)	8,12,14	1.79	2 (25%)
1	SEP	B	1440	1	8,9,10	1.46	1 (12%)	8,12,14	1.78	2 (25%)
1	SEP	F	1440	1	8,9,10	1.46	1 (12%)	8,12,14	1.79	2 (25%)

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
1	SEP	D	1440	1	-	2/5/8/10	-
1	SEP	A	1440	1	-	2/5/8/10	-
1	SEP	K	1440	1	-	0/5/8/10	-
1	SEP	I	1440	1	-	0/5/8/10	-
1	SEP	B	1440	1	-	2/5/8/10	-
1	SEP	F	1440	1	-	0/5/8/10	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	1440	SEP	P-O1P	3.19	1.60	1.50
1	A	1440	SEP	P-O1P	3.18	1.60	1.50
1	I	1440	SEP	P-O1P	3.18	1.60	1.50
1	B	1440	SEP	P-O1P	3.18	1.60	1.50
1	K	1440	SEP	P-O1P	3.18	1.60	1.50
1	D	1440	SEP	P-O1P	3.17	1.60	1.50

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1440	SEP	P-OG-CB	-3.53	108.58	118.30
1	K	1440	SEP	P-OG-CB	-3.53	108.58	118.30
1	B	1440	SEP	P-OG-CB	-3.53	108.58	118.30
1	F	1440	SEP	P-OG-CB	-3.53	108.58	118.30
1	D	1440	SEP	P-OG-CB	-3.52	108.60	118.30
1	I	1440	SEP	P-OG-CB	-3.52	108.60	118.30
1	D	1440	SEP	OG-CB-CA	2.53	110.61	108.14
1	I	1440	SEP	OG-CB-CA	2.53	110.61	108.14
1	B	1440	SEP	OG-CB-CA	2.52	110.60	108.14
1	F	1440	SEP	OG-CB-CA	2.52	110.60	108.14
1	A	1440	SEP	OG-CB-CA	2.51	110.59	108.14
1	K	1440	SEP	OG-CB-CA	2.51	110.59	108.14

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1440	SEP	CB-OG-P-O1P

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Mol	Chain	Res	Type	Atoms
1	B	1440	SEP	CB-OG-P-O1P
1	D	1440	SEP	CB-OG-P-O1P
1	A	1440	SEP	CB-OG-P-O3P
1	B	1440	SEP	CB-OG-P-O3P
1	D	1440	SEP	CB-OG-P-O3P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

12 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	$\#\|Z\|>2$
3	NDP	F	2001	-	45,52,52	1.29	5 (11%)	53,80,80	1.68	12 (22%)
3	NDP	I	2001	-	45,52,52	1.29	5 (11%)	53,80,80	1.69	12 (22%)
4	FMN	E	2101	-	33,33,33	1.13	3 (9%)	48,50,50	1.31	9 (18%)
3	NDP	D	2001	-	45,52,52	1.29	5 (11%)	53,80,80	1.69	12 (22%)
3	NDP	B	2001	-	45,52,52	1.29	5 (11%)	53,80,80	1.68	12 (22%)
4	FMN	H	2101	-	33,33,33	1.13	3 (9%)	48,50,50	1.30	9 (18%)
3	NDP	A	2001	-	45,52,52	1.29	5 (11%)	53,80,80	1.68	12 (22%)
4	FMN	C	2101	-	33,33,33	1.13	3 (9%)	48,50,50	1.30	9 (18%)
4	FMN	J	2101	-	33,33,33	1.13	3 (9%)	48,50,50	1.31	9 (18%)
4	FMN	L	2101	-	33,33,33	1.13	3 (9%)	48,50,50	1.31	8 (16%)
3	NDP	K	2001	-	45,52,52	1.29	5 (11%)	53,80,80	1.68	12 (22%)
4	FMN	G	2101	-	33,33,33	1.13	3 (9%)	48,50,50	1.31	8 (16%)

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
3	NDP	F	2001	-	-	12/30/77/77	0/5/5/5
3	NDP	I	2001	-	-	12/30/77/77	0/5/5/5
4	FMN	E	2101	-	-	5/18/18/18	0/3/3/3
3	NDP	D	2001	-	-	12/30/77/77	0/5/5/5
3	NDP	B	2001	-	-	12/30/77/77	0/5/5/5
4	FMN	H	2101	-	-	5/18/18/18	0/3/3/3
3	NDP	A	2001	-	-	12/30/77/77	0/5/5/5
4	FMN	C	2101	-	-	5/18/18/18	0/3/3/3
4	FMN	J	2101	-	-	5/18/18/18	0/3/3/3
4	FMN	L	2101	-	-	5/18/18/18	0/3/3/3
3	NDP	K	2001	-	-	12/30/77/77	0/5/5/5
4	FMN	G	2101	-	-	5/18/18/18	0/3/3/3

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	2101	FMN	C4A-N5	3.31	1.37	1.30
4	J	2101	FMN	C4A-N5	3.31	1.37	1.30
4	C	2101	FMN	C4A-N5	3.29	1.37	1.30
4	H	2101	FMN	C4A-N5	3.29	1.37	1.30
4	G	2101	FMN	C4A-N5	3.28	1.37	1.30
4	L	2101	FMN	C4A-N5	3.28	1.37	1.30
3	A	2001	NDP	O7N-C7N	-2.74	1.18	1.24
3	K	2001	NDP	O7N-C7N	-2.74	1.18	1.24
3	D	2001	NDP	O7N-C7N	-2.74	1.18	1.24
3	I	2001	NDP	O7N-C7N	-2.74	1.18	1.24
3	B	2001	NDP	O7N-C7N	-2.74	1.18	1.24
3	F	2001	NDP	O7N-C7N	-2.74	1.18	1.24
3	A	2001	NDP	C3B-C4B	-2.52	1.46	1.53
3	K	2001	NDP	C3B-C4B	-2.52	1.46	1.53
3	B	2001	NDP	C3B-C4B	-2.52	1.46	1.53
3	F	2001	NDP	C3B-C4B	-2.52	1.46	1.53
3	D	2001	NDP	C3B-C4B	-2.51	1.46	1.53
3	I	2001	NDP	C3B-C4B	-2.51	1.46	1.53
3	A	2001	NDP	O4D-C4D	-2.47	1.39	1.45
3	K	2001	NDP	O4D-C4D	-2.47	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2001	NDP	O4D-C4D	-2.46	1.39	1.45
3	F	2001	NDP	O4D-C4D	-2.46	1.39	1.45
3	D	2001	NDP	O4D-C4D	-2.44	1.39	1.45
3	I	2001	NDP	O4D-C4D	-2.44	1.39	1.45
3	B	2001	NDP	C5A-N7A	-2.23	1.31	1.39
3	F	2001	NDP	C5A-N7A	-2.23	1.31	1.39
3	A	2001	NDP	C5A-N7A	-2.23	1.31	1.39
3	K	2001	NDP	C5A-N7A	-2.23	1.31	1.39
3	D	2001	NDP	C5A-N7A	-2.23	1.31	1.39
3	I	2001	NDP	C5A-N7A	-2.23	1.31	1.39
4	E	2101	FMN	C10-N1	2.21	1.37	1.33
4	J	2101	FMN	C10-N1	2.21	1.37	1.33
4	G	2101	FMN	C10-N1	2.18	1.37	1.33
4	L	2101	FMN	C10-N1	2.18	1.37	1.33
4	C	2101	FMN	C10-N1	2.18	1.37	1.33
4	H	2101	FMN	C10-N1	2.18	1.37	1.33
3	D	2001	NDP	C6N-N1N	-2.18	1.31	1.37
3	I	2001	NDP	C6N-N1N	-2.18	1.31	1.37
3	A	2001	NDP	C6N-N1N	-2.16	1.31	1.37
3	K	2001	NDP	C6N-N1N	-2.16	1.31	1.37
3	B	2001	NDP	C6N-N1N	-2.16	1.31	1.37
3	F	2001	NDP	C6N-N1N	-2.16	1.31	1.37
4	C	2101	FMN	C4A-C10	-2.16	1.37	1.44
4	H	2101	FMN	C4A-C10	-2.16	1.37	1.44
4	E	2101	FMN	C4A-C10	-2.14	1.37	1.44
4	J	2101	FMN	C4A-C10	-2.14	1.37	1.44
4	G	2101	FMN	C4A-C10	-2.13	1.37	1.44
4	L	2101	FMN	C4A-C10	-2.13	1.37	1.44

All (124) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	2001	NDP	O4D-C4D-C5D	-4.20	95.54	109.37
3	I	2001	NDP	O4D-C4D-C5D	-4.20	95.54	109.37
3	A	2001	NDP	O4D-C4D-C5D	-4.20	95.56	109.37
3	K	2001	NDP	O4D-C4D-C5D	-4.20	95.56	109.37
3	B	2001	NDP	O4D-C4D-C5D	-4.19	95.58	109.37
3	F	2001	NDP	O4D-C4D-C5D	-4.19	95.58	109.37
3	D	2001	NDP	N3A-C2A-N1A	-4.07	122.31	128.68
3	I	2001	NDP	N3A-C2A-N1A	-4.07	122.31	128.68
3	A	2001	NDP	N3A-C2A-N1A	-4.06	122.33	128.68
3	K	2001	NDP	N3A-C2A-N1A	-4.06	122.33	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	2001	NDP	N3A-C2A-N1A	-4.06	122.33	128.68
3	F	2001	NDP	N3A-C2A-N1A	-4.06	122.33	128.68
3	A	2001	NDP	C5B-C4B-C3B	-3.89	100.60	115.18
3	K	2001	NDP	C5B-C4B-C3B	-3.89	100.60	115.18
3	B	2001	NDP	C5B-C4B-C3B	-3.89	100.61	115.18
3	F	2001	NDP	C5B-C4B-C3B	-3.89	100.61	115.18
3	D	2001	NDP	C5B-C4B-C3B	-3.89	100.62	115.18
3	I	2001	NDP	C5B-C4B-C3B	-3.89	100.62	115.18
4	G	2101	FMN	C4-N3-C2	-3.45	119.27	125.64
4	L	2101	FMN	C4-N3-C2	-3.45	119.27	125.64
4	C	2101	FMN	C4-N3-C2	-3.45	119.27	125.64
4	E	2101	FMN	C4-N3-C2	-3.45	119.28	125.64
4	J	2101	FMN	C4-N3-C2	-3.45	119.28	125.64
4	H	2101	FMN	C4-N3-C2	-3.43	119.31	125.64
3	A	2001	NDP	C4A-C5A-N7A	-3.31	105.95	109.40
3	K	2001	NDP	C4A-C5A-N7A	-3.31	105.95	109.40
3	D	2001	NDP	C4A-C5A-N7A	-3.30	105.96	109.40
3	I	2001	NDP	C4A-C5A-N7A	-3.30	105.96	109.40
3	B	2001	NDP	C4A-C5A-N7A	-3.29	105.97	109.40
3	F	2001	NDP	C4A-C5A-N7A	-3.29	105.97	109.40
3	B	2001	NDP	O2B-C2B-C1B	3.07	121.17	110.10
3	F	2001	NDP	O2B-C2B-C1B	3.07	121.17	110.10
3	D	2001	NDP	O2B-C2B-C1B	3.07	121.16	110.10
3	I	2001	NDP	O2B-C2B-C1B	3.07	121.16	110.10
3	A	2001	NDP	O2B-C2B-C1B	3.07	121.16	110.10
3	K	2001	NDP	O2B-C2B-C1B	3.07	121.16	110.10
4	G	2101	FMN	C4A-C4-N3	2.93	120.64	113.19
4	L	2101	FMN	C4A-C4-N3	2.93	120.64	113.19
4	E	2101	FMN	C4A-C4-N3	2.93	120.62	113.19
4	J	2101	FMN	C4A-C4-N3	2.93	120.62	113.19
3	B	2001	NDP	O3B-C3B-C2B	2.92	119.47	111.17
3	F	2001	NDP	O3B-C3B-C2B	2.92	119.47	111.17
3	D	2001	NDP	O3B-C3B-C2B	2.92	119.47	111.17
3	I	2001	NDP	O3B-C3B-C2B	2.92	119.47	111.17
4	C	2101	FMN	C4A-C4-N3	2.92	120.61	113.19
3	A	2001	NDP	O4D-C1D-N1N	-2.92	102.34	108.06
3	B	2001	NDP	O4D-C1D-N1N	-2.92	102.34	108.06
3	D	2001	NDP	O4D-C1D-N1N	-2.92	102.34	108.06
3	K	2001	NDP	O4D-C1D-N1N	-2.92	102.34	108.06
3	F	2001	NDP	O4D-C1D-N1N	-2.92	102.34	108.06
3	I	2001	NDP	O4D-C1D-N1N	-2.92	102.34	108.06
4	H	2101	FMN	C4A-C4-N3	2.92	120.61	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	2001	NDP	O3B-C3B-C2B	2.91	119.43	111.17
3	K	2001	NDP	O3B-C3B-C2B	2.91	119.43	111.17
4	G	2101	FMN	O4-C4-C4A	-2.73	119.36	126.60
4	L	2101	FMN	O4-C4-C4A	-2.73	119.36	126.60
3	A	2001	NDP	C1D-N1N-C2N	-2.73	116.57	121.11
3	K	2001	NDP	C1D-N1N-C2N	-2.73	116.57	121.11
3	B	2001	NDP	C1D-N1N-C2N	-2.73	116.57	121.11
3	F	2001	NDP	C1D-N1N-C2N	-2.73	116.57	121.11
3	D	2001	NDP	C1D-N1N-C2N	-2.72	116.58	121.11
3	I	2001	NDP	C1D-N1N-C2N	-2.72	116.58	121.11
4	E	2101	FMN	O4-C4-C4A	-2.72	119.40	126.60
4	J	2101	FMN	O4-C4-C4A	-2.72	119.40	126.60
4	C	2101	FMN	O4-C4-C4A	-2.71	119.41	126.60
4	H	2101	FMN	O4-C4-C4A	-2.71	119.41	126.60
4	E	2101	FMN	C4A-C10-N10	2.55	120.21	116.48
4	J	2101	FMN	C4A-C10-N10	2.55	120.21	116.48
4	C	2101	FMN	C4A-C10-N10	2.52	120.17	116.48
4	H	2101	FMN	C4A-C10-N10	2.52	120.17	116.48
4	G	2101	FMN	C4A-C10-N10	2.51	120.15	116.48
4	L	2101	FMN	C4A-C10-N10	2.51	120.15	116.48
4	E	2101	FMN	C4A-C10-N1	-2.35	119.27	124.73
4	J	2101	FMN	C4A-C10-N1	-2.35	119.27	124.73
3	D	2001	NDP	O2B-P2B-O1X	-2.34	100.34	109.39
3	I	2001	NDP	O2B-P2B-O1X	-2.34	100.34	109.39
3	A	2001	NDP	O2B-P2B-O1X	-2.34	100.35	109.39
3	K	2001	NDP	O2B-P2B-O1X	-2.34	100.35	109.39
3	B	2001	NDP	O2B-P2B-O1X	-2.34	100.36	109.39
3	F	2001	NDP	O2B-P2B-O1X	-2.34	100.36	109.39
4	G	2101	FMN	C4A-C10-N1	-2.34	119.30	124.73
4	L	2101	FMN	C4A-C10-N1	-2.34	119.30	124.73
4	C	2101	FMN	C4A-C10-N1	-2.33	119.33	124.73
4	H	2101	FMN	C4A-C10-N1	-2.33	119.33	124.73
3	A	2001	NDP	O2N-PN-O1N	2.32	123.70	112.24
3	K	2001	NDP	O2N-PN-O1N	2.32	123.70	112.24
3	B	2001	NDP	O2N-PN-O1N	2.32	123.69	112.24
3	F	2001	NDP	O2N-PN-O1N	2.32	123.69	112.24
3	D	2001	NDP	O2N-PN-O1N	2.31	123.68	112.24
3	I	2001	NDP	O2N-PN-O1N	2.31	123.68	112.24
3	A	2001	NDP	O3X-P2B-O2X	2.23	116.15	107.64
3	K	2001	NDP	O3X-P2B-O2X	2.23	116.15	107.64
4	G	2101	FMN	O4'-C4'-C5'	-2.23	104.91	109.92
4	L	2101	FMN	O4'-C4'-C5'	-2.23	104.91	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	2001	NDP	O3X-P2B-O2X	2.23	116.14	107.64
3	I	2001	NDP	O3X-P2B-O2X	2.23	116.14	107.64
4	C	2101	FMN	O4'-C4'-C5'	-2.22	104.92	109.92
4	H	2101	FMN	O4'-C4'-C5'	-2.22	104.92	109.92
3	B	2001	NDP	O3X-P2B-O2X	2.22	116.14	107.64
3	F	2001	NDP	O3X-P2B-O2X	2.22	116.14	107.64
4	E	2101	FMN	O4'-C4'-C5'	-2.22	104.93	109.92
4	J	2101	FMN	O4'-C4'-C5'	-2.22	104.93	109.92
4	G	2101	FMN	C9A-C5A-N5	-2.18	120.07	122.43
4	L	2101	FMN	C9A-C5A-N5	-2.18	120.07	122.43
3	D	2001	NDP	O3B-C3B-C4B	-2.17	104.79	111.05
3	I	2001	NDP	O3B-C3B-C4B	-2.17	104.79	111.05
3	A	2001	NDP	O3B-C3B-C4B	-2.16	104.79	111.05
3	K	2001	NDP	O3B-C3B-C4B	-2.16	104.79	111.05
3	B	2001	NDP	O3B-C3B-C4B	-2.16	104.81	111.05
3	F	2001	NDP	O3B-C3B-C4B	-2.16	104.81	111.05
4	E	2101	FMN	C9A-C5A-N5	-2.15	120.09	122.43
4	J	2101	FMN	C9A-C5A-N5	-2.15	120.09	122.43
4	C	2101	FMN	C9A-C5A-N5	-2.14	120.11	122.43
4	H	2101	FMN	C9A-C5A-N5	-2.14	120.11	122.43
4	G	2101	FMN	C5A-C9A-N10	2.08	120.10	117.95
4	L	2101	FMN	C5A-C9A-N10	2.08	120.10	117.95
4	E	2101	FMN	C5A-C9A-N10	2.05	120.07	117.95
4	J	2101	FMN	C5A-C9A-N10	2.05	120.07	117.95
4	C	2101	FMN	C5A-C9A-N10	2.05	120.07	117.95
4	H	2101	FMN	C5A-C9A-N10	2.05	120.07	117.95
4	E	2101	FMN	C4-C4A-C10	2.02	120.19	116.79
4	J	2101	FMN	C4-C4A-C10	2.02	120.19	116.79
4	C	2101	FMN	C4-C4A-C10	2.00	120.16	116.79
4	H	2101	FMN	C4-C4A-C10	2.00	120.16	116.79

There are no chirality outliers.

All (102) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2001	NDP	C5D-O5D-PN-O3
3	B	2001	NDP	C5D-O5D-PN-O3
3	D	2001	NDP	C5D-O5D-PN-O3
3	K	2001	NDP	C5D-O5D-PN-O3
3	F	2001	NDP	C5D-O5D-PN-O3
3	I	2001	NDP	C5D-O5D-PN-O3
4	G	2101	FMN	O3'-C3'-C4'-C5'

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Mol	Chain	Res	Type	Atoms
4	C	2101	FMN	O3'-C3'-C4'-C5'
4	E	2101	FMN	O3'-C3'-C4'-C5'
4	L	2101	FMN	O3'-C3'-C4'-C5'
4	H	2101	FMN	O3'-C3'-C4'-C5'
4	J	2101	FMN	O3'-C3'-C4'-C5'
3	A	2001	NDP	C1B-C2B-O2B-P2B
3	B	2001	NDP	C1B-C2B-O2B-P2B
3	D	2001	NDP	C1B-C2B-O2B-P2B
3	K	2001	NDP	C1B-C2B-O2B-P2B
3	F	2001	NDP	C1B-C2B-O2B-P2B
3	I	2001	NDP	C1B-C2B-O2B-P2B
4	G	2101	FMN	C2'-C3'-C4'-C5'
4	C	2101	FMN	C2'-C3'-C4'-C5'
4	E	2101	FMN	C2'-C3'-C4'-C5'
4	L	2101	FMN	C2'-C3'-C4'-C5'
4	H	2101	FMN	C2'-C3'-C4'-C5'
4	J	2101	FMN	C2'-C3'-C4'-C5'
4	G	2101	FMN	C2'-C3'-C4'-O4'
4	C	2101	FMN	C2'-C3'-C4'-O4'
4	E	2101	FMN	C2'-C3'-C4'-O4'
4	L	2101	FMN	C2'-C3'-C4'-O4'
4	H	2101	FMN	C2'-C3'-C4'-O4'
4	J	2101	FMN	C2'-C3'-C4'-O4'
4	G	2101	FMN	O3'-C3'-C4'-O4'
4	C	2101	FMN	O3'-C3'-C4'-O4'
4	E	2101	FMN	O3'-C3'-C4'-O4'
4	L	2101	FMN	O3'-C3'-C4'-O4'
4	H	2101	FMN	O3'-C3'-C4'-O4'
4	J	2101	FMN	O3'-C3'-C4'-O4'
3	A	2001	NDP	O4D-C4D-C5D-O5D
3	K	2001	NDP	O4D-C4D-C5D-O5D
3	A	2001	NDP	PN-O3-PA-O5B
3	B	2001	NDP	PN-O3-PA-O5B
3	D	2001	NDP	PN-O3-PA-O5B
3	K	2001	NDP	PN-O3-PA-O5B
3	F	2001	NDP	PN-O3-PA-O5B
3	I	2001	NDP	PN-O3-PA-O5B
3	B	2001	NDP	O4D-C4D-C5D-O5D
3	D	2001	NDP	O4D-C4D-C5D-O5D
3	F	2001	NDP	O4D-C4D-C5D-O5D
3	I	2001	NDP	O4D-C4D-C5D-O5D
3	A	2001	NDP	C2B-O2B-P2B-O1X

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Mol	Chain	Res	Type	Atoms
3	B	2001	NDP	C2B-O2B-P2B-O1X
3	D	2001	NDP	C2B-O2B-P2B-O1X
3	K	2001	NDP	C2B-O2B-P2B-O1X
3	F	2001	NDP	C2B-O2B-P2B-O1X
3	I	2001	NDP	C2B-O2B-P2B-O1X
4	G	2101	FMN	C4'-C5'-O5'-P
4	C	2101	FMN	C4'-C5'-O5'-P
4	E	2101	FMN	C4'-C5'-O5'-P
4	L	2101	FMN	C4'-C5'-O5'-P
4	H	2101	FMN	C4'-C5'-O5'-P
4	J	2101	FMN	C4'-C5'-O5'-P
3	A	2001	NDP	C5D-O5D-PN-O1N
3	B	2001	NDP	C5D-O5D-PN-O1N
3	D	2001	NDP	C5D-O5D-PN-O1N
3	K	2001	NDP	C5D-O5D-PN-O1N
3	F	2001	NDP	C5D-O5D-PN-O1N
3	I	2001	NDP	C5D-O5D-PN-O1N
3	A	2001	NDP	C2D-C1D-N1N-C6N
3	B	2001	NDP	C2D-C1D-N1N-C6N
3	D	2001	NDP	C2D-C1D-N1N-C6N
3	K	2001	NDP	C2D-C1D-N1N-C6N
3	F	2001	NDP	C2D-C1D-N1N-C6N
3	I	2001	NDP	C2D-C1D-N1N-C6N
3	A	2001	NDP	O4D-C1D-N1N-C6N
3	B	2001	NDP	O4D-C1D-N1N-C6N
3	D	2001	NDP	O4D-C1D-N1N-C6N
3	K	2001	NDP	O4D-C1D-N1N-C6N
3	F	2001	NDP	O4D-C1D-N1N-C6N
3	I	2001	NDP	O4D-C1D-N1N-C6N
3	A	2001	NDP	PA-O3-PN-O1N
3	B	2001	NDP	PA-O3-PN-O1N
3	D	2001	NDP	PA-O3-PN-O1N
3	K	2001	NDP	PA-O3-PN-O1N
3	F	2001	NDP	PA-O3-PN-O1N
3	I	2001	NDP	PA-O3-PN-O1N
3	A	2001	NDP	C3B-C2B-O2B-P2B
3	B	2001	NDP	C3B-C2B-O2B-P2B
3	D	2001	NDP	C3B-C2B-O2B-P2B
3	K	2001	NDP	C3B-C2B-O2B-P2B
3	F	2001	NDP	C3B-C2B-O2B-P2B
3	I	2001	NDP	C3B-C2B-O2B-P2B
3	A	2001	NDP	C2B-O2B-P2B-O3X

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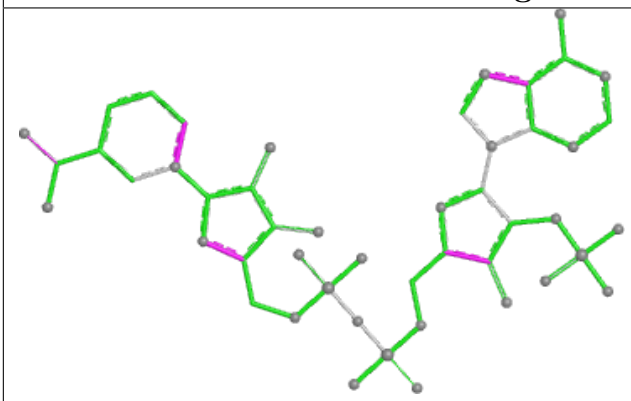
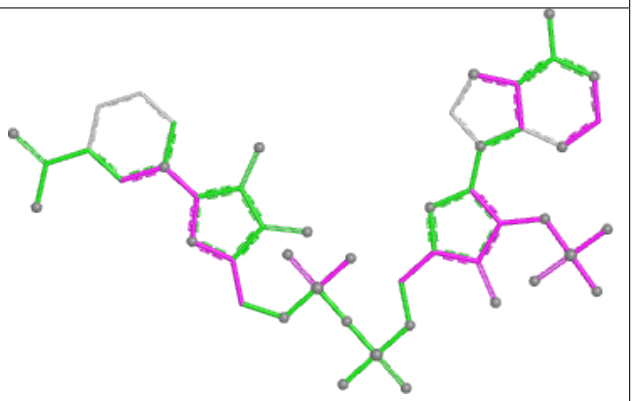
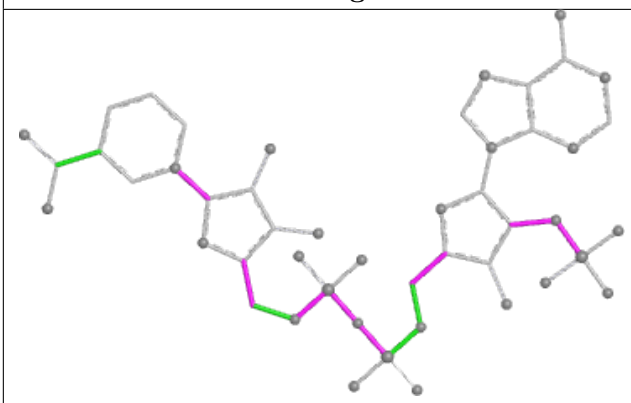
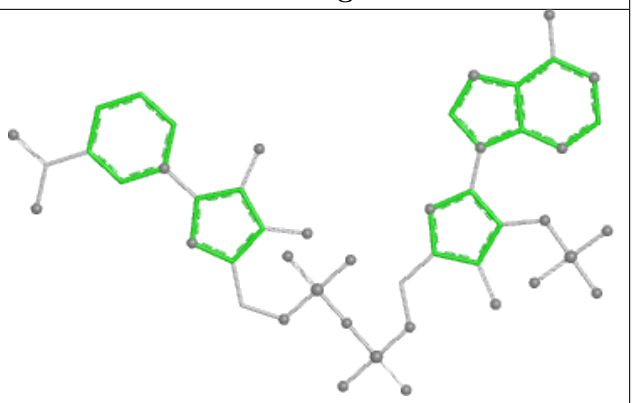
Mol	Chain	Res	Type	Atoms
3	B	2001	NDP	C2B-O2B-P2B-O3X
3	D	2001	NDP	C2B-O2B-P2B-O3X
3	K	2001	NDP	C2B-O2B-P2B-O3X
3	F	2001	NDP	C2B-O2B-P2B-O3X
3	I	2001	NDP	C2B-O2B-P2B-O3X
3	A	2001	NDP	O4B-C4B-C5B-O5B
3	B	2001	NDP	O4B-C4B-C5B-O5B
3	D	2001	NDP	O4B-C4B-C5B-O5B
3	K	2001	NDP	O4B-C4B-C5B-O5B
3	F	2001	NDP	O4B-C4B-C5B-O5B
3	I	2001	NDP	O4B-C4B-C5B-O5B

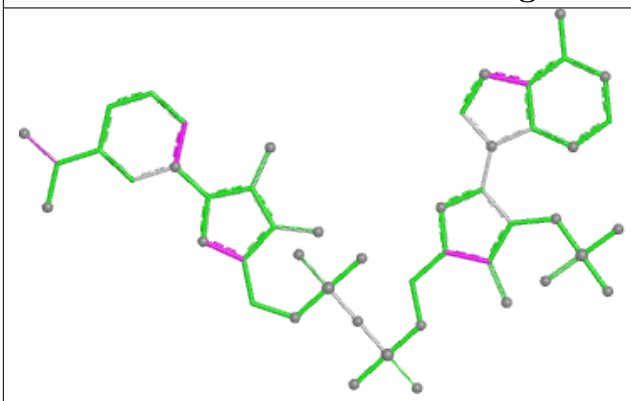
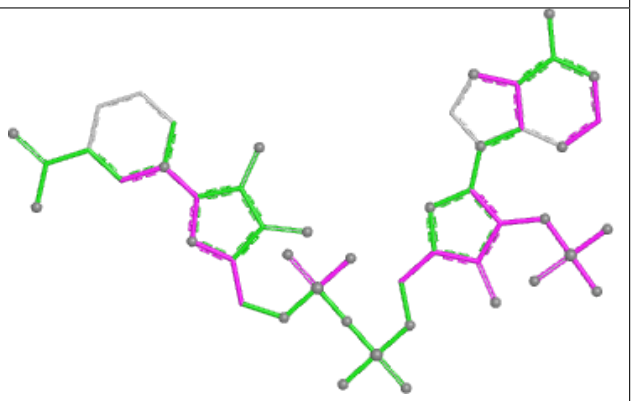
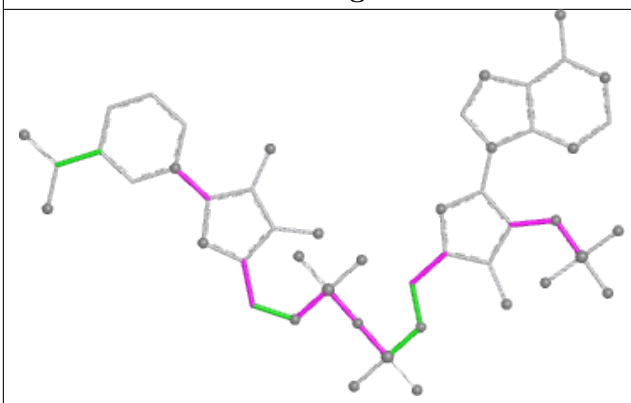
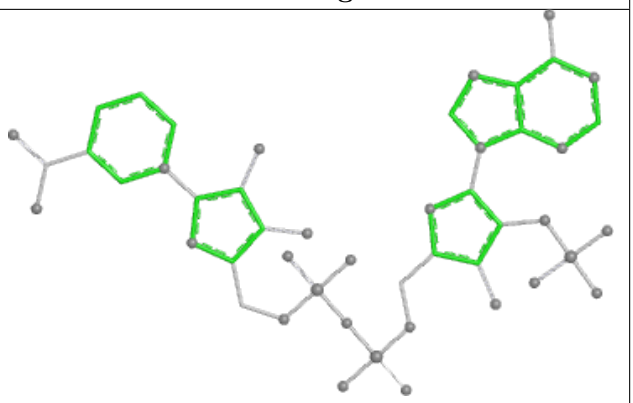
There are no ring outliers.

6 monomers are involved in 44 short contacts:

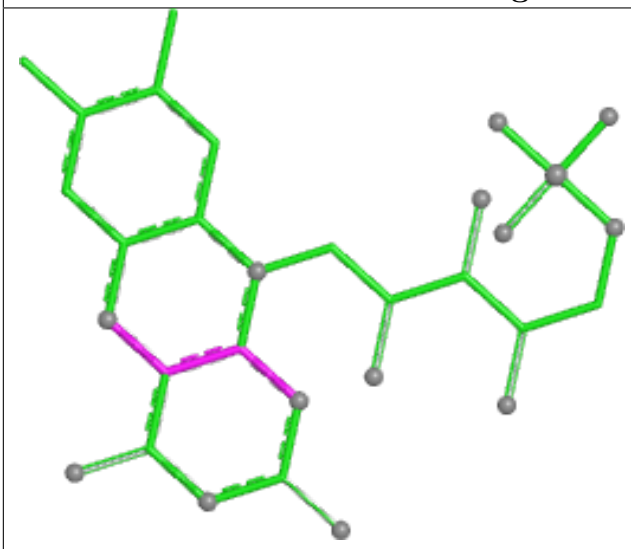
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	2001	NDP	7	0
3	I	2001	NDP	8	0
3	D	2001	NDP	7	0
3	B	2001	NDP	7	0
3	A	2001	NDP	8	0
3	K	2001	NDP	7	0

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.

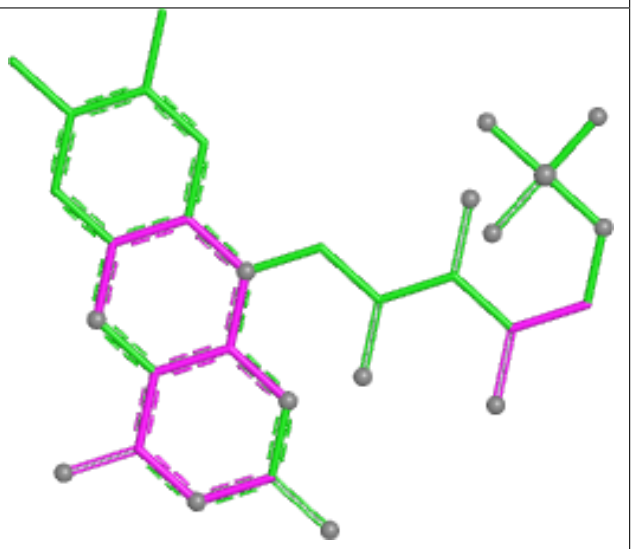
Ligand NDP F 2001	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand NDP I 2001	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

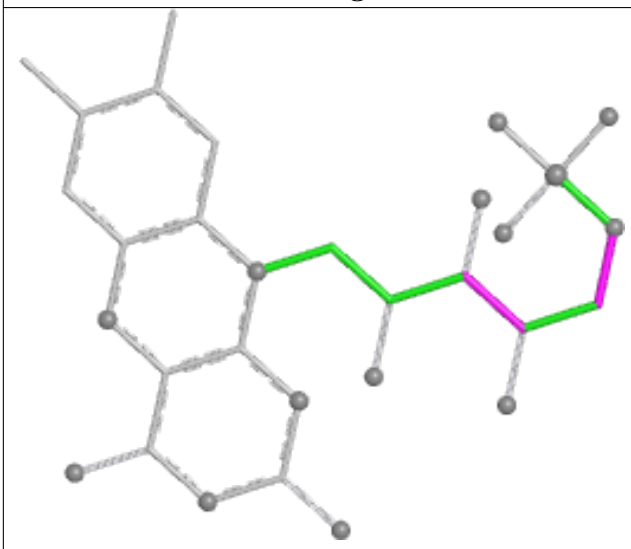
Ligand FMN E 2101



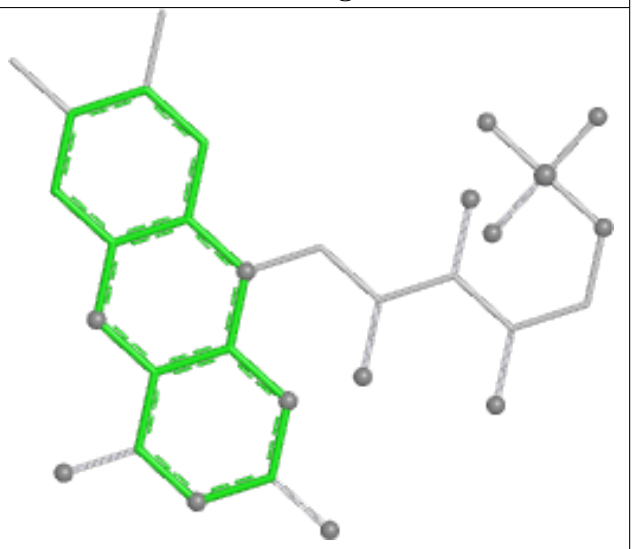
Bond lengths



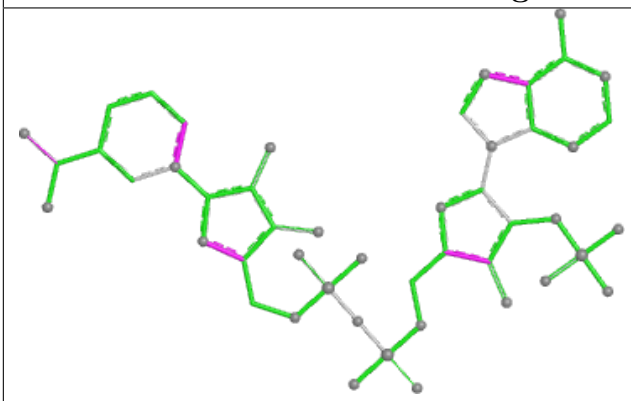
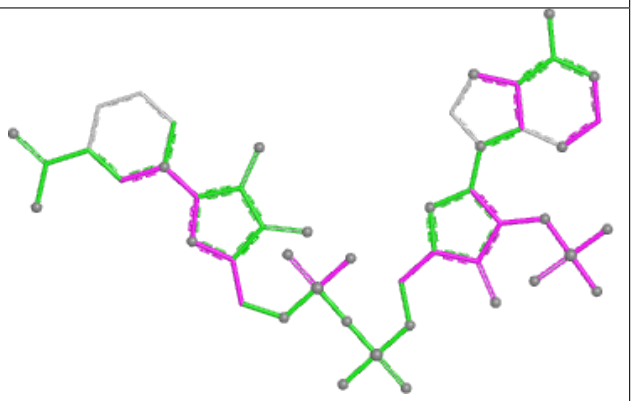
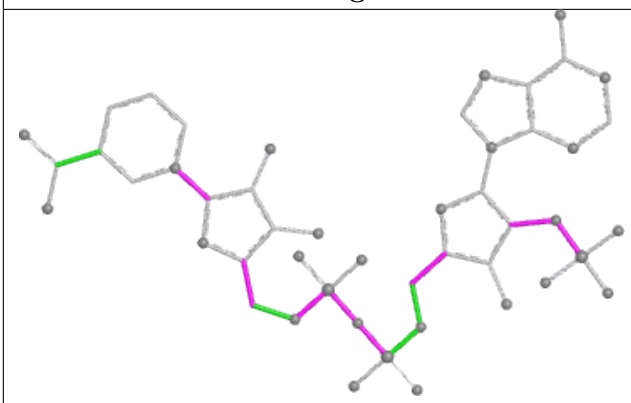
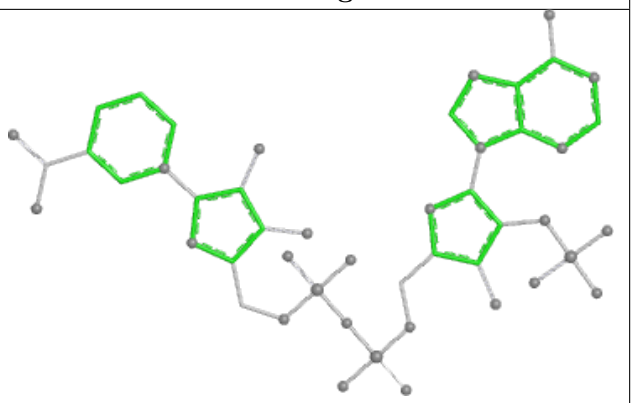
Bond angles

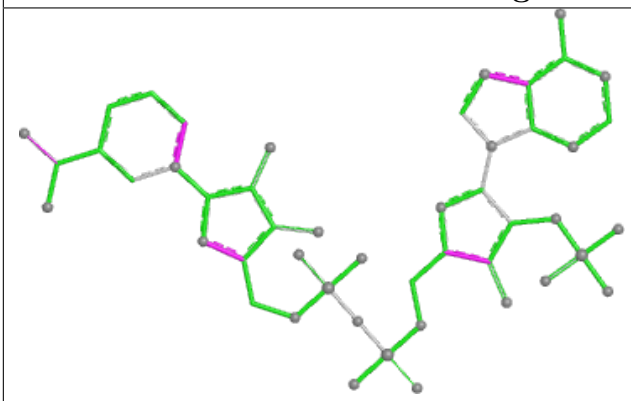
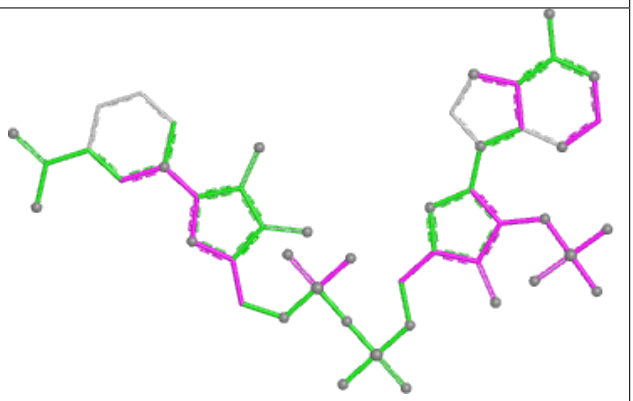
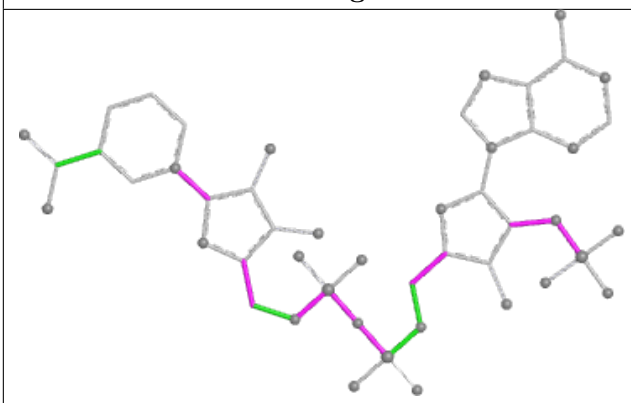
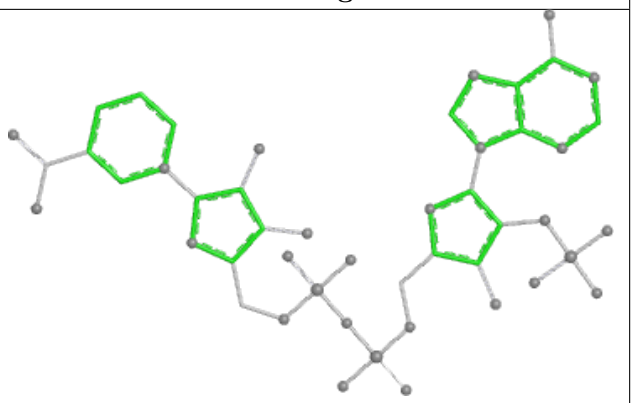


Torsions

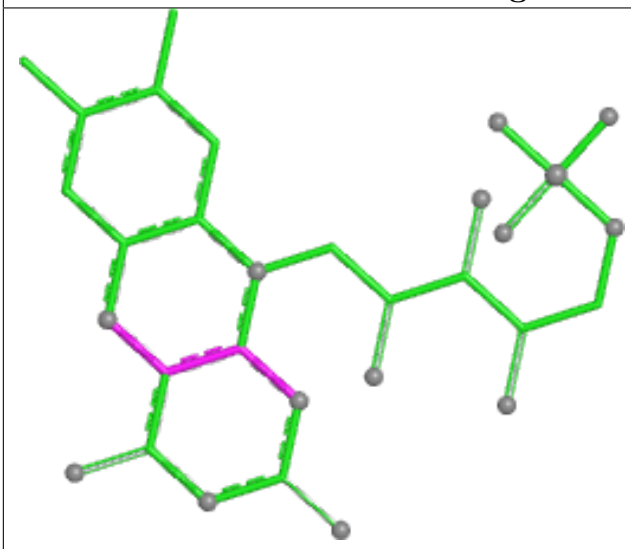


Rings

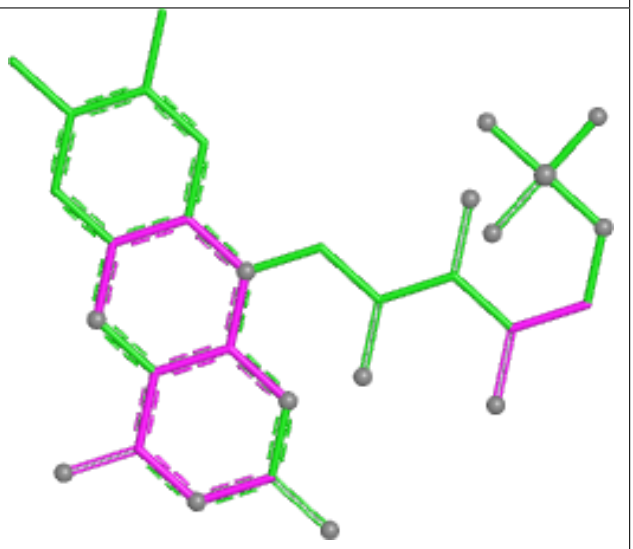
Ligand NDP D 2001	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NDP B 2001	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

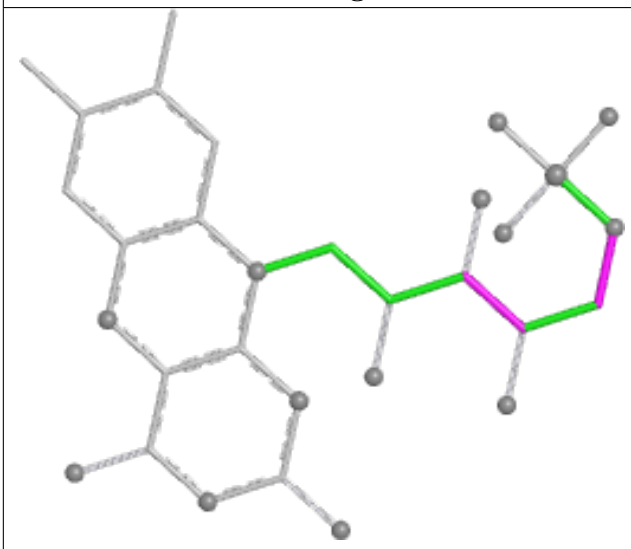
Ligand FMN H 2101



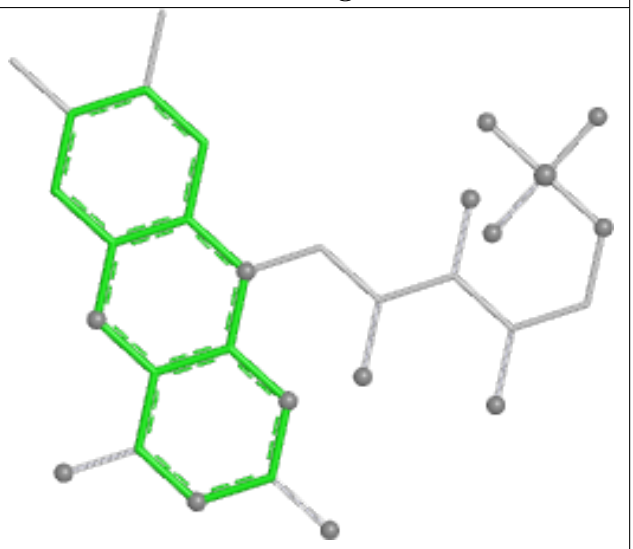
Bond lengths



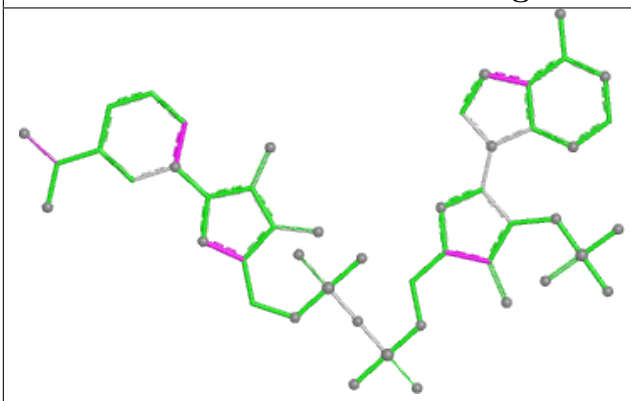
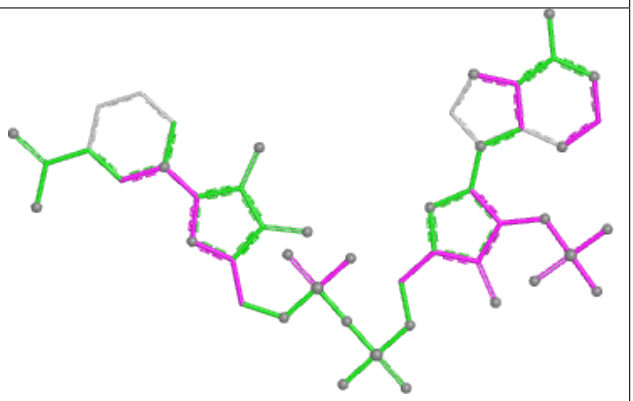
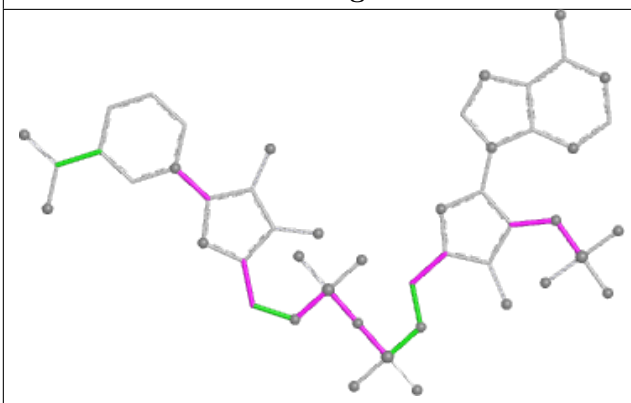
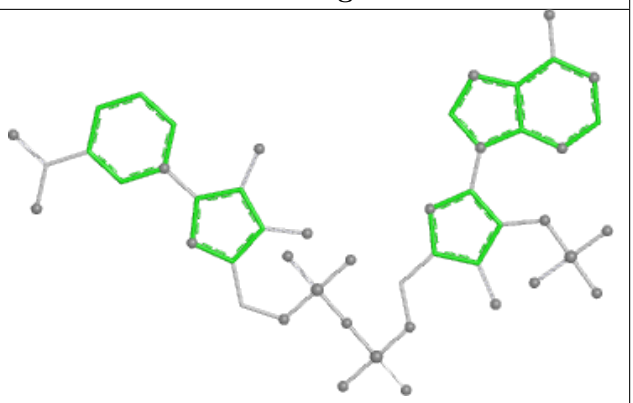
Bond angles



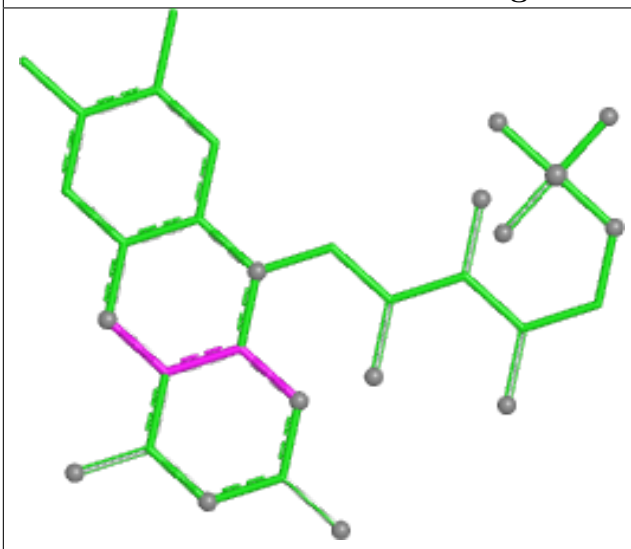
Torsions



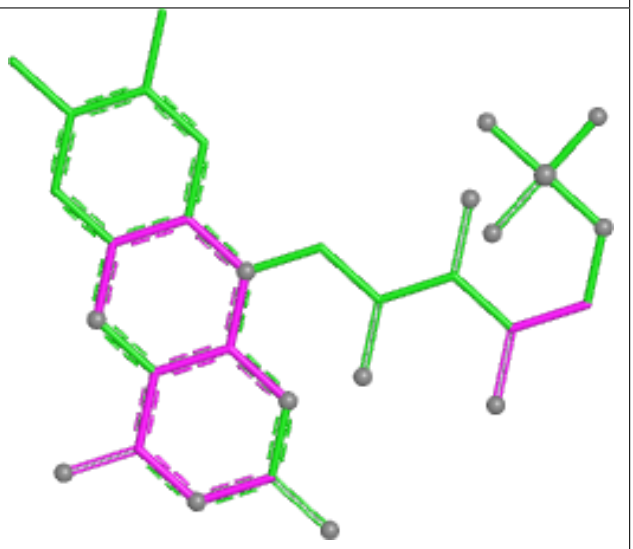
Rings

Ligand NDP A 2001	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

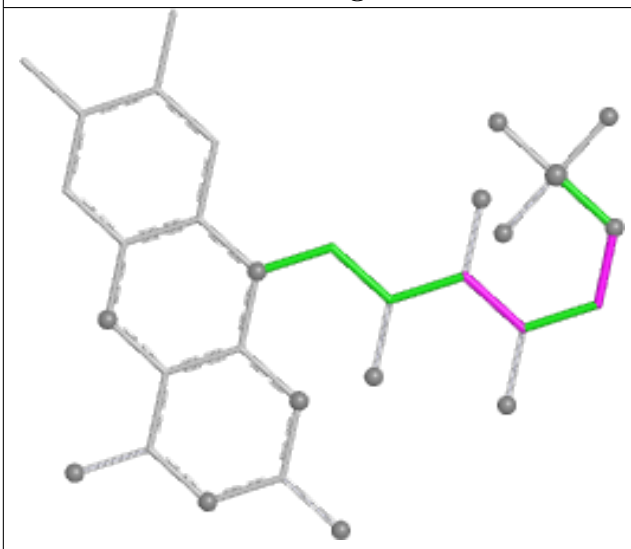
Ligand FMN C 2101



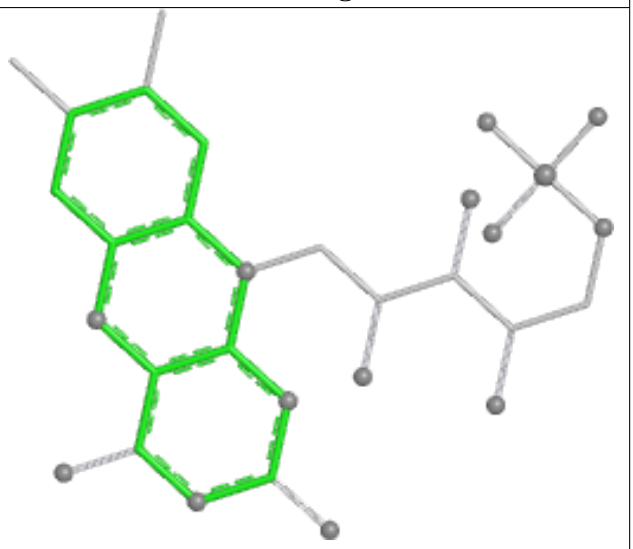
Bond lengths



Bond angles

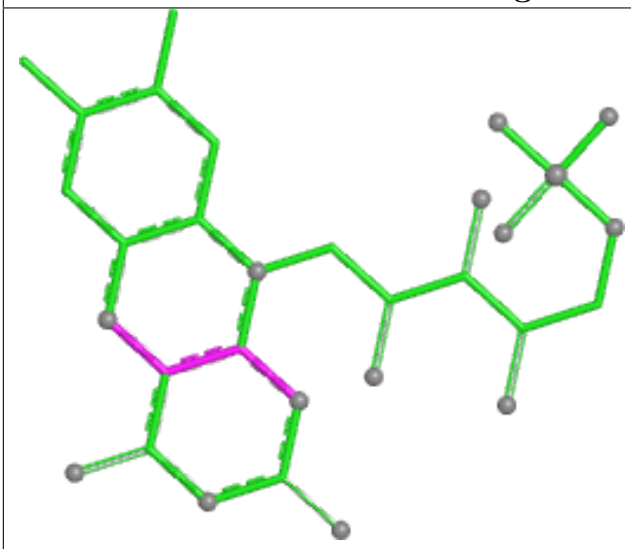


Torsions

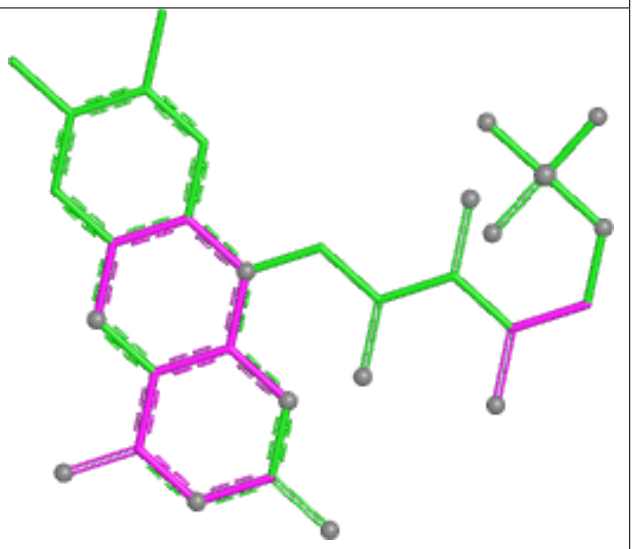


Rings

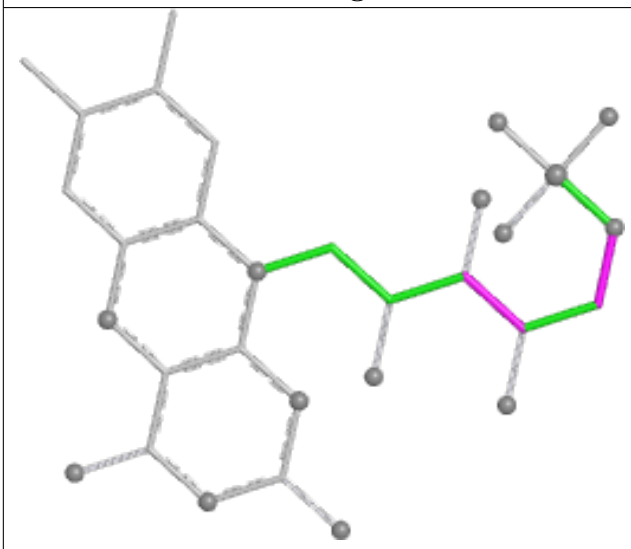
Ligand FMN J 2101



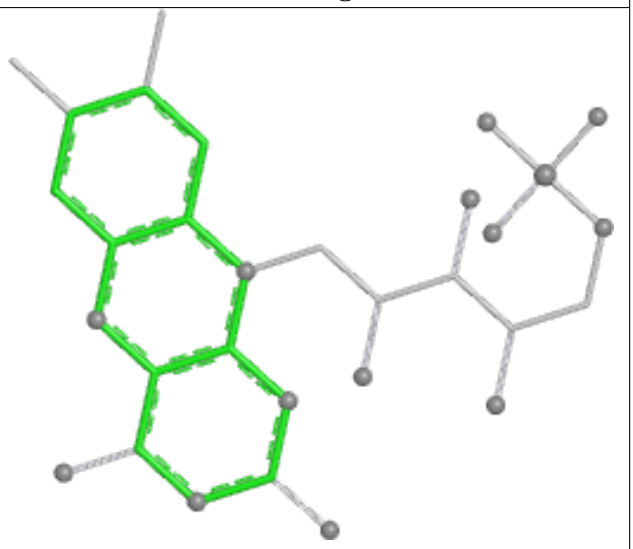
Bond lengths



Bond angles

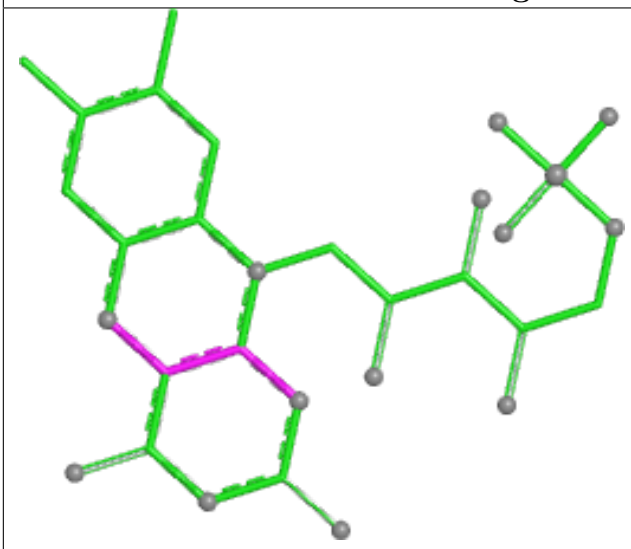


Torsions

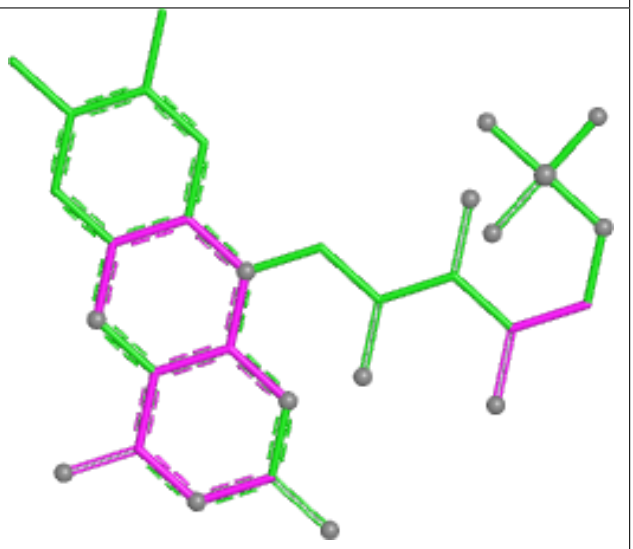


Rings

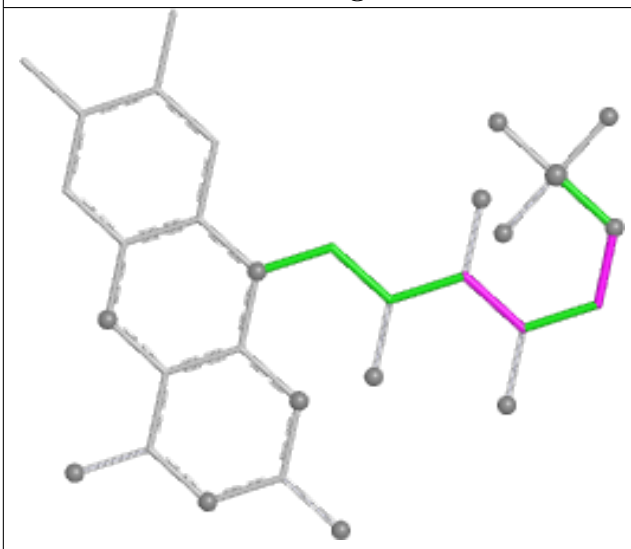
Ligand FMN L 2101



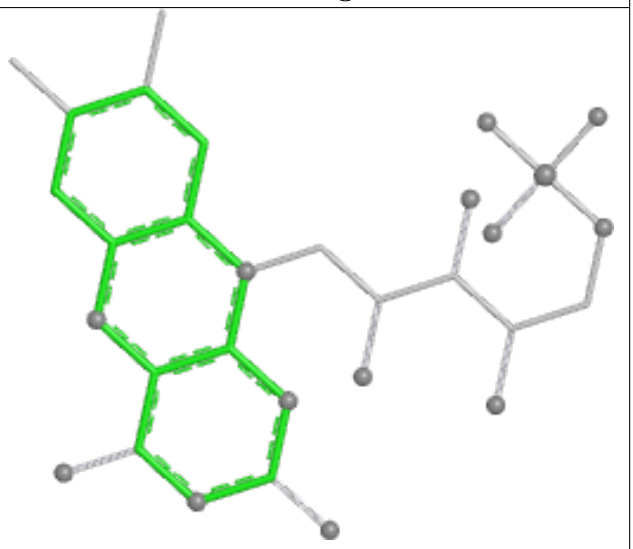
Bond lengths



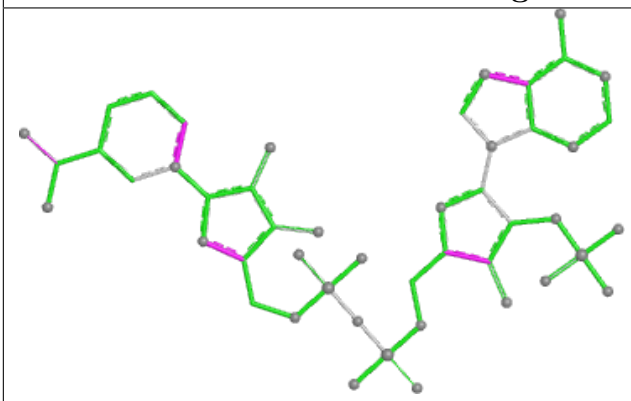
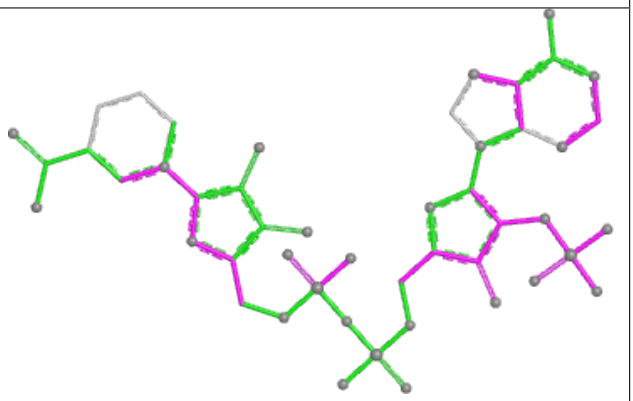
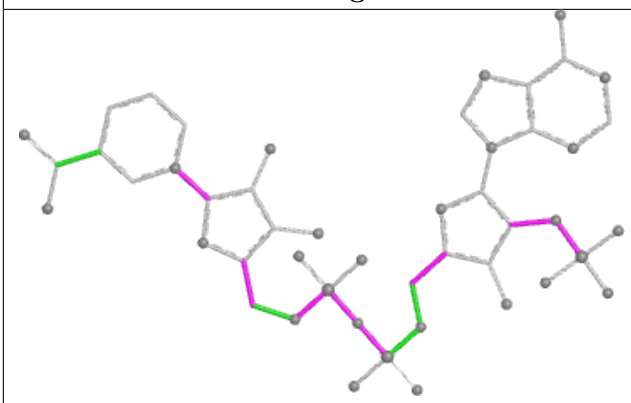
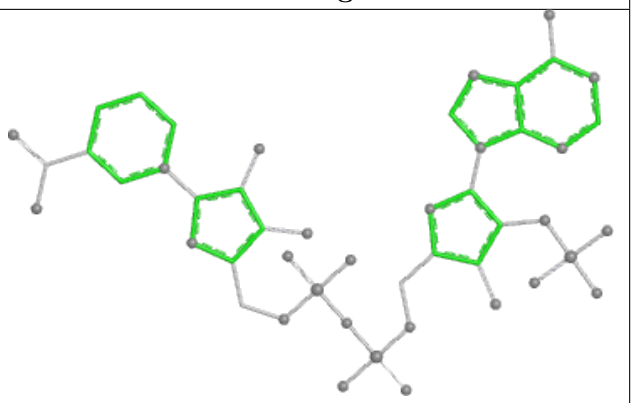
Bond angles



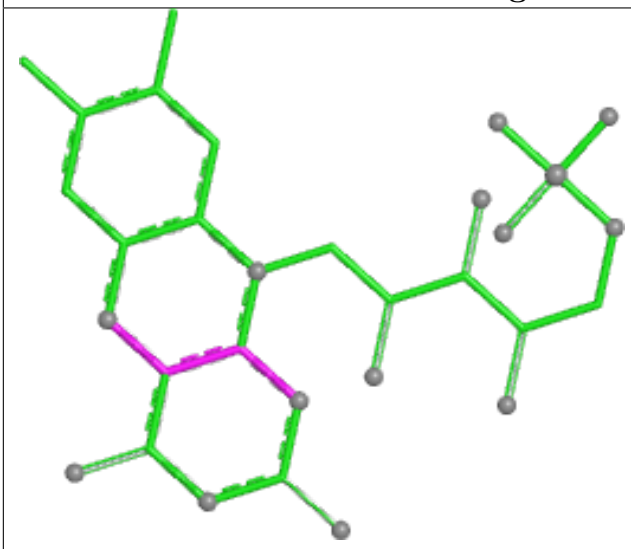
Torsions



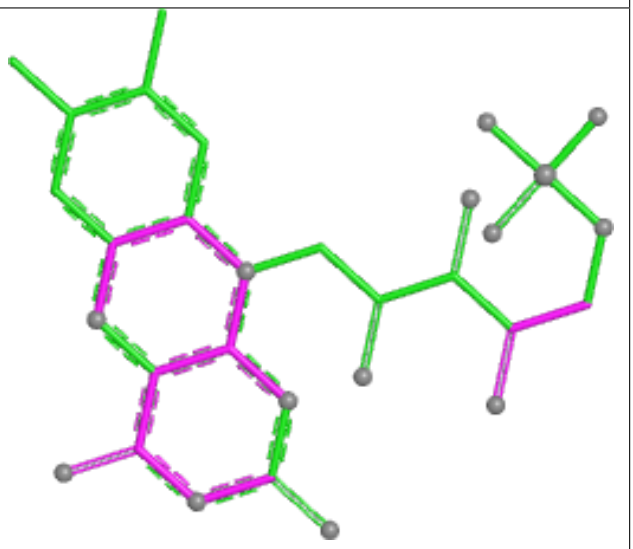
Rings

Ligand NDP K 2001	
 Bond lengths	 Bond angles
 Torsions	 Rings

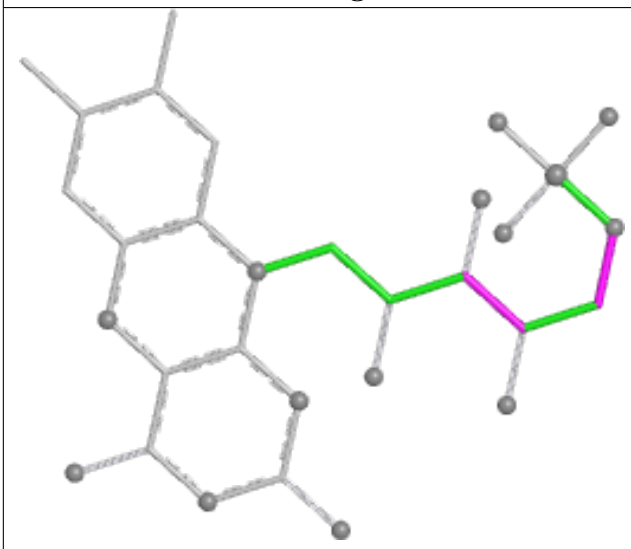
Ligand FMN G 2101



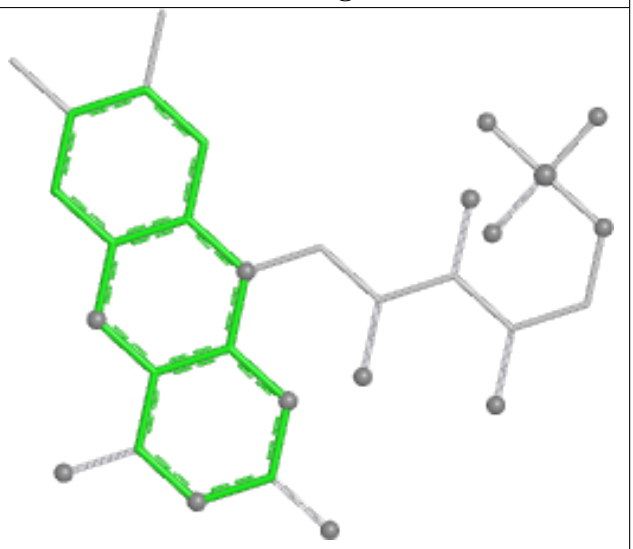
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

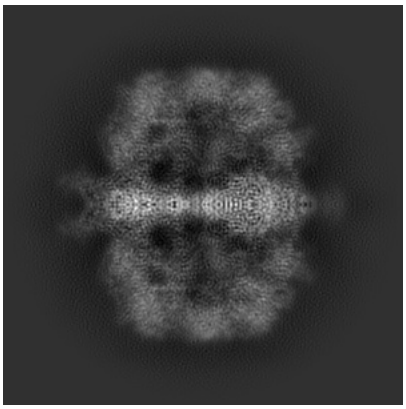
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10420. These allow visual inspection of the internal detail of the map and identification of artifacts.

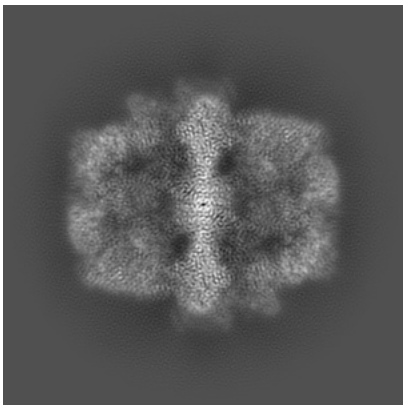
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

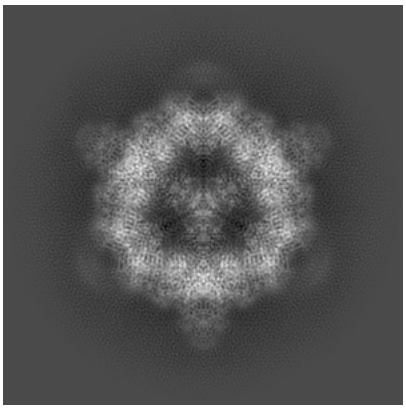
6.1.1 Primary map



X

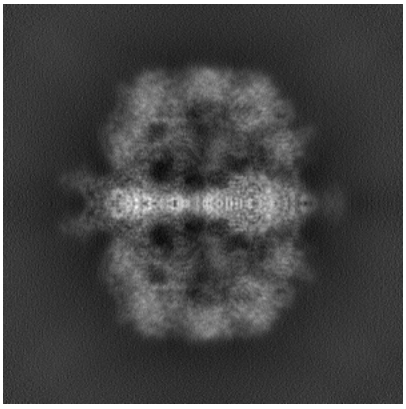


Y

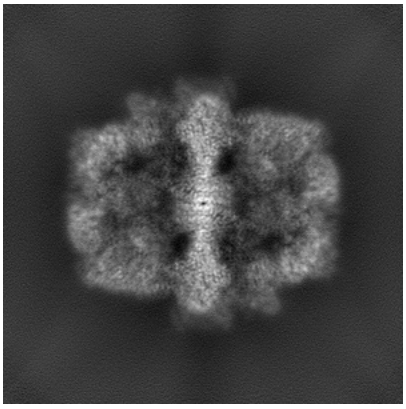


Z

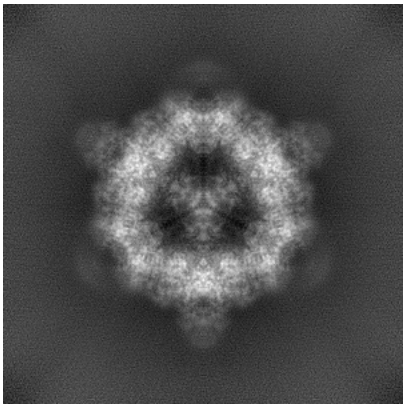
6.1.2 Raw map



X



Y

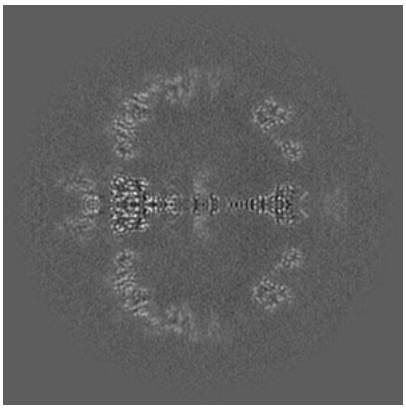


Z

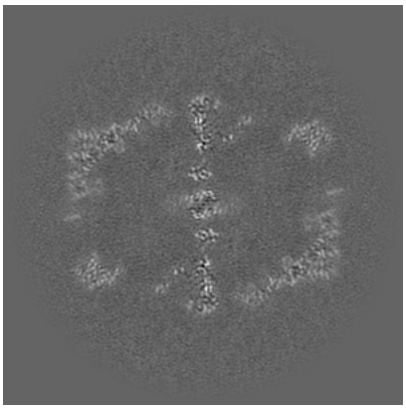
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

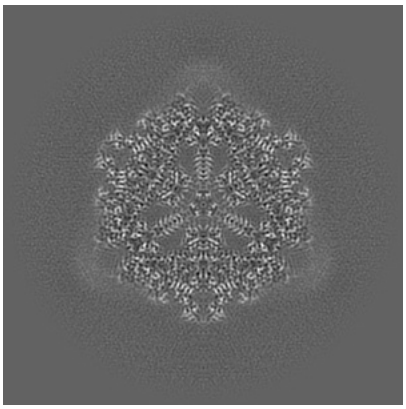
6.2.1 Primary map



X Index: 240

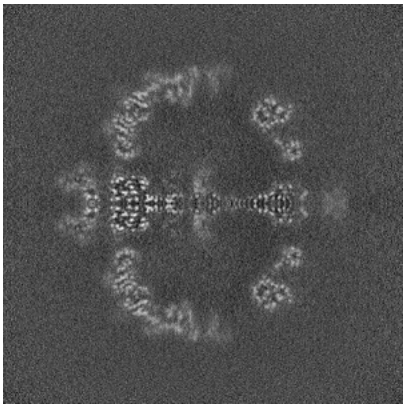


Y Index: 240

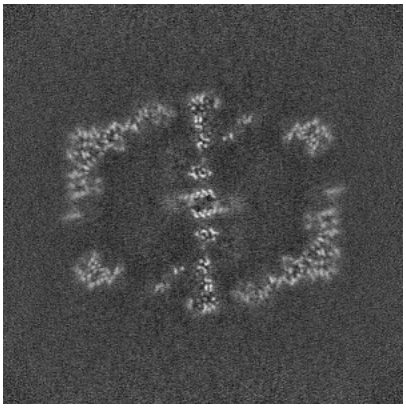


Z Index: 240

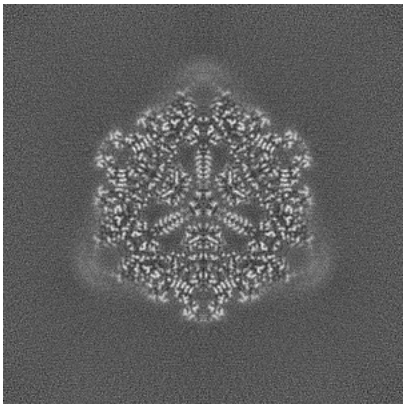
6.2.2 Raw map



X Index: 240



Y Index: 240

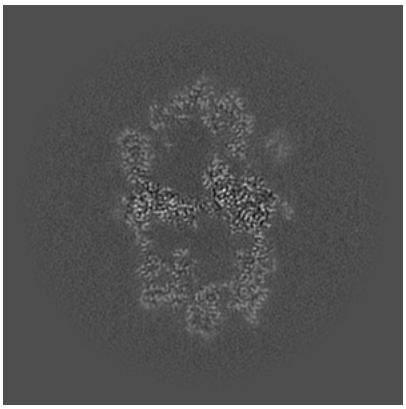


Z Index: 240

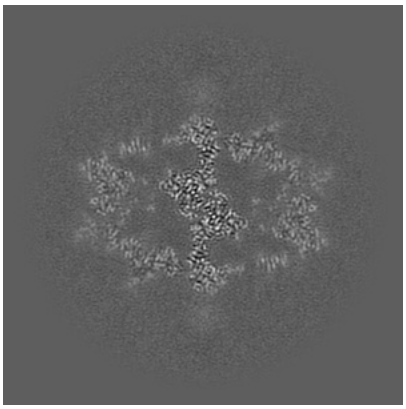
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

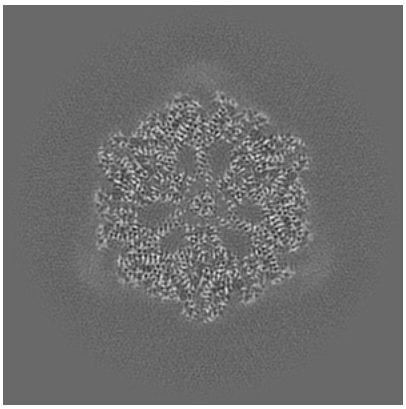
6.3.1 Primary map



X Index: 319

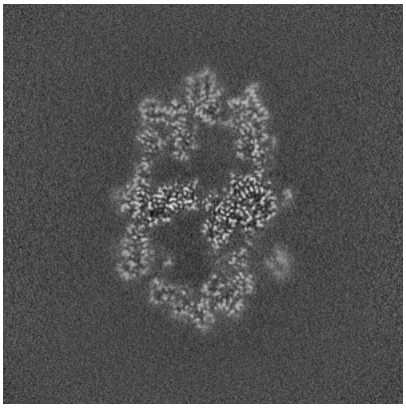


Y Index: 161

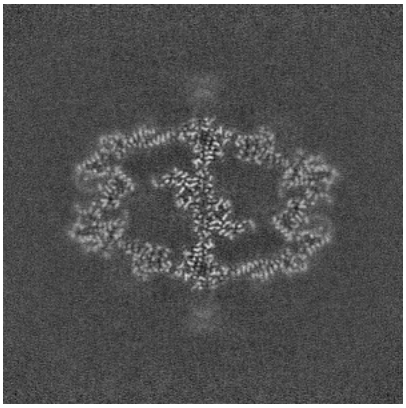


Z Index: 236

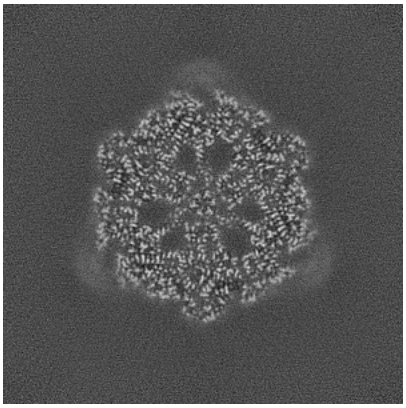
6.3.2 Raw map



X Index: 160



Y Index: 169

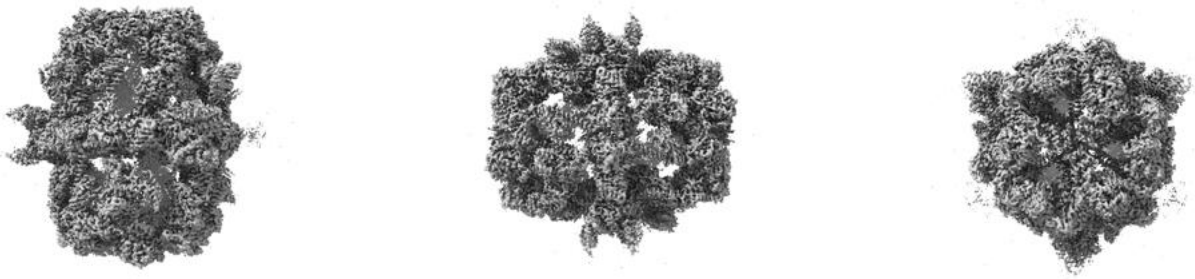


Z Index: 235

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

6.4 Orthogonal surface views (i)

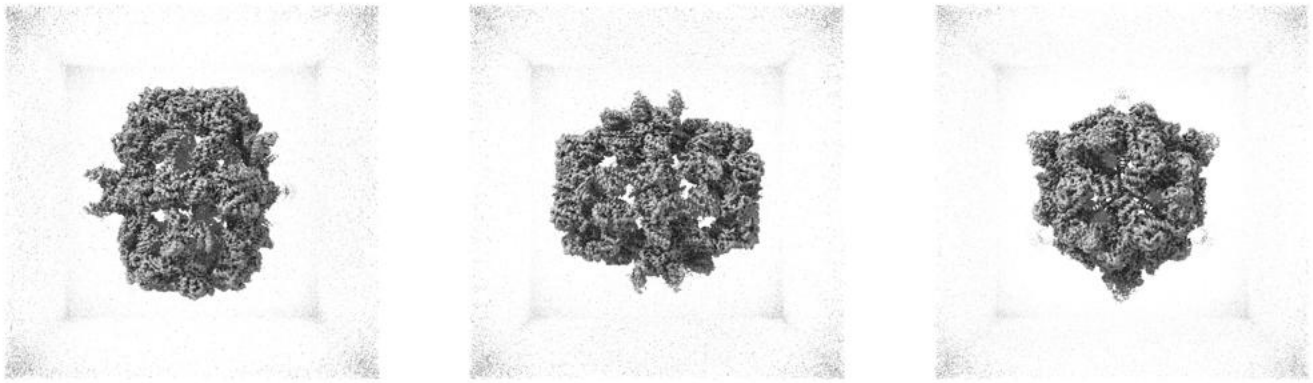
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

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

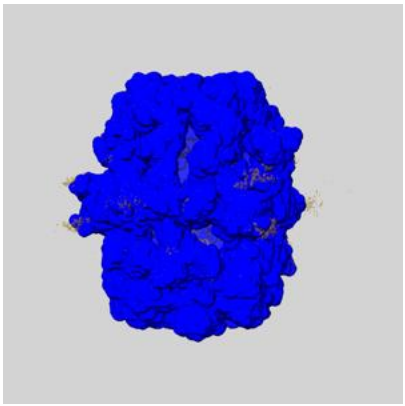
6.5 Mask visualisation

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

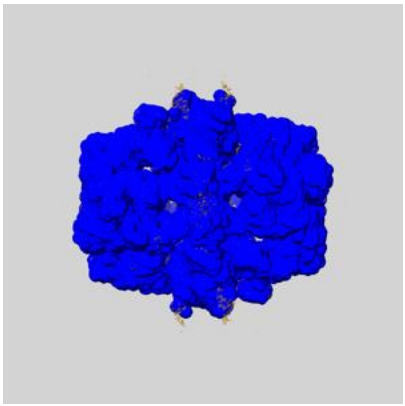
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

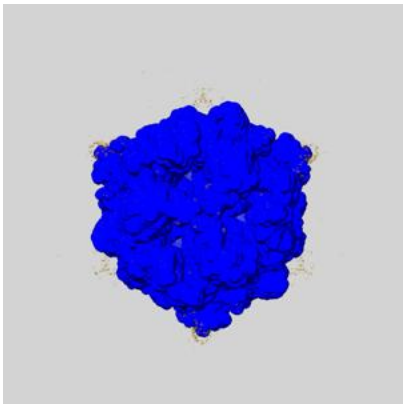
6.5.1 emd_10420_msk_1.map



X



Y

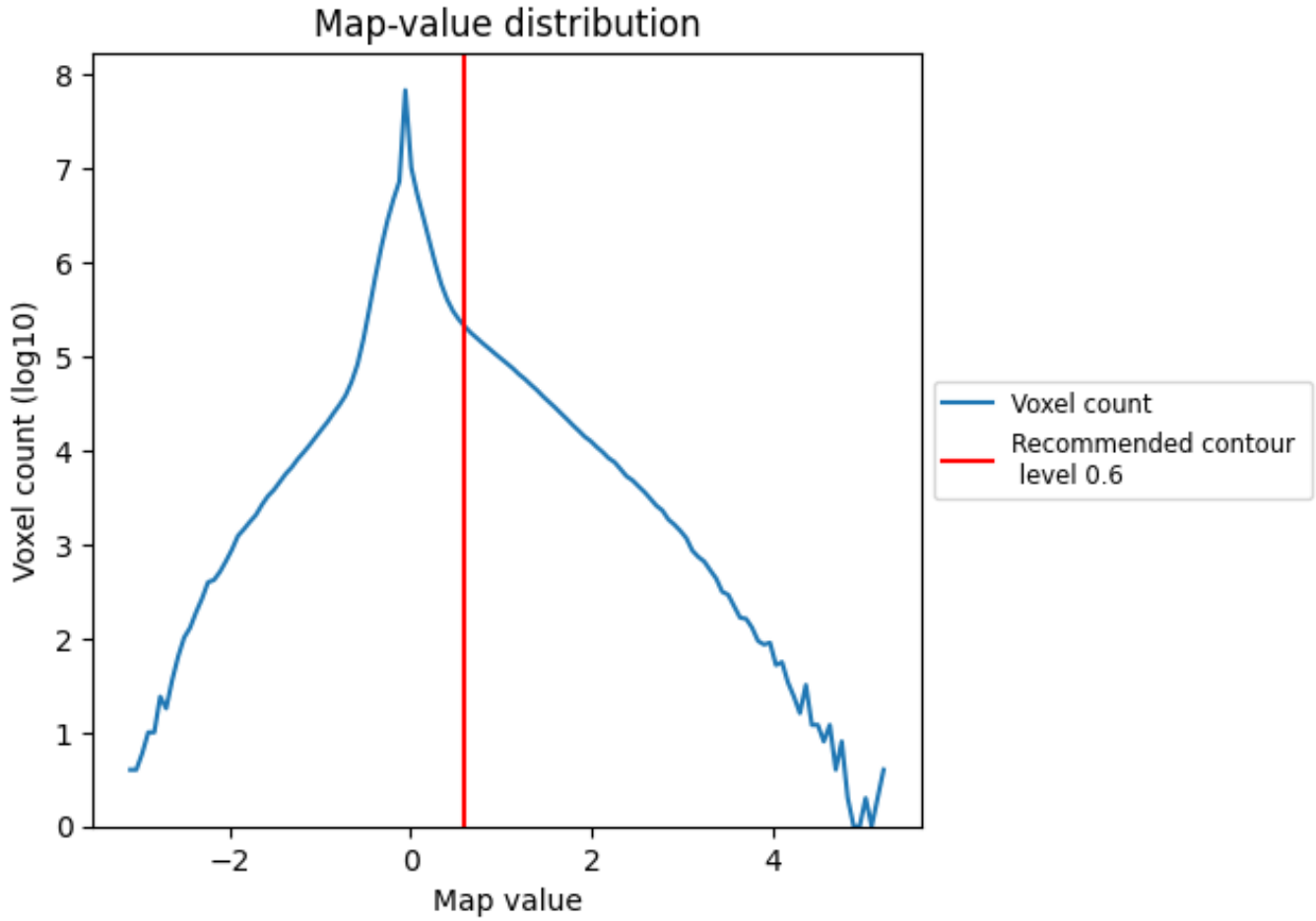


Z

7 Map analysis

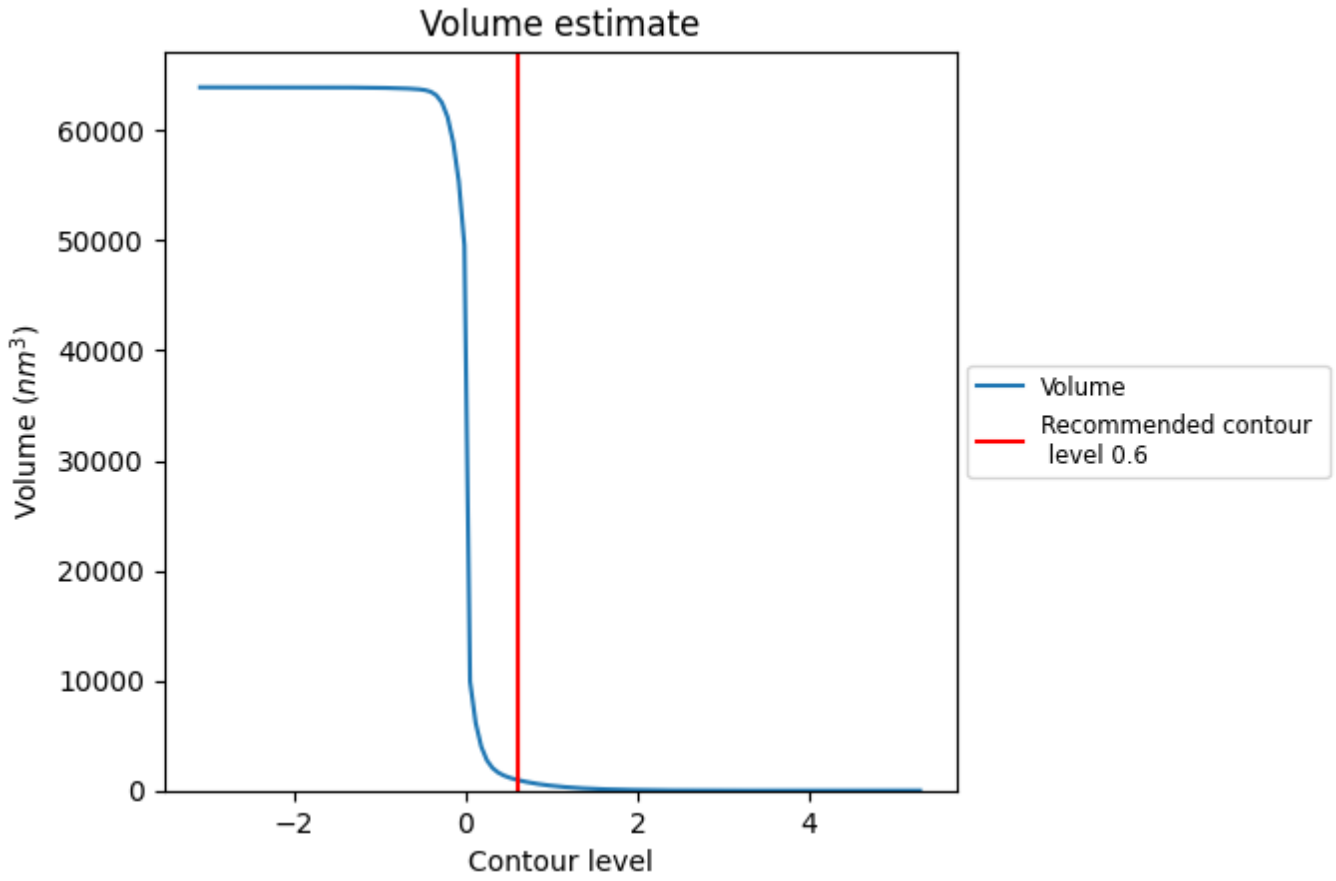
This section contains the results of statistical analysis of the map.

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.

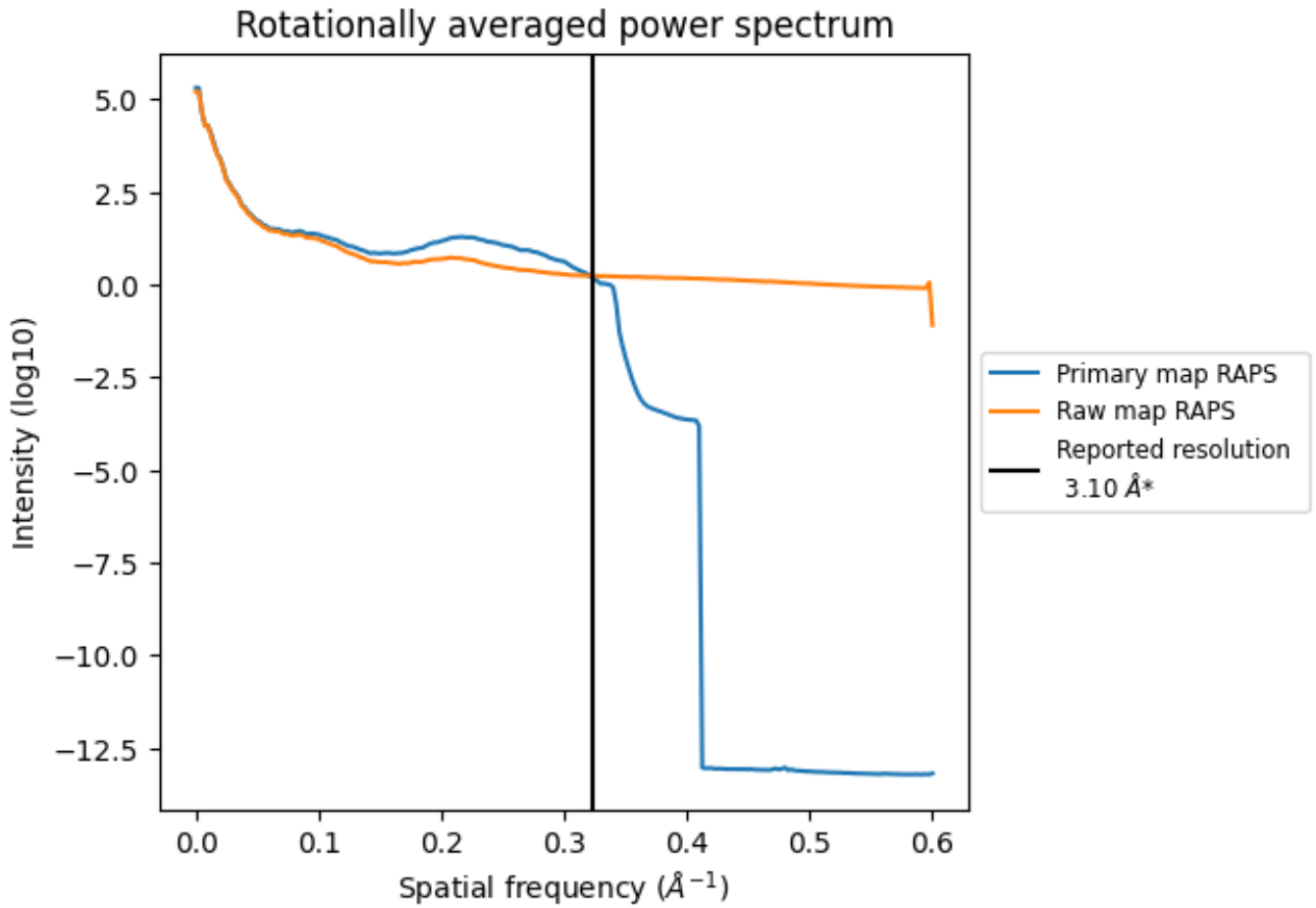
7.2 Volume estimate



The volume at the recommended contour level is 970 nm^3; this corresponds to an approximate mass of 876 kDa.

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

7.3 Rotationally averaged power spectrum (i)

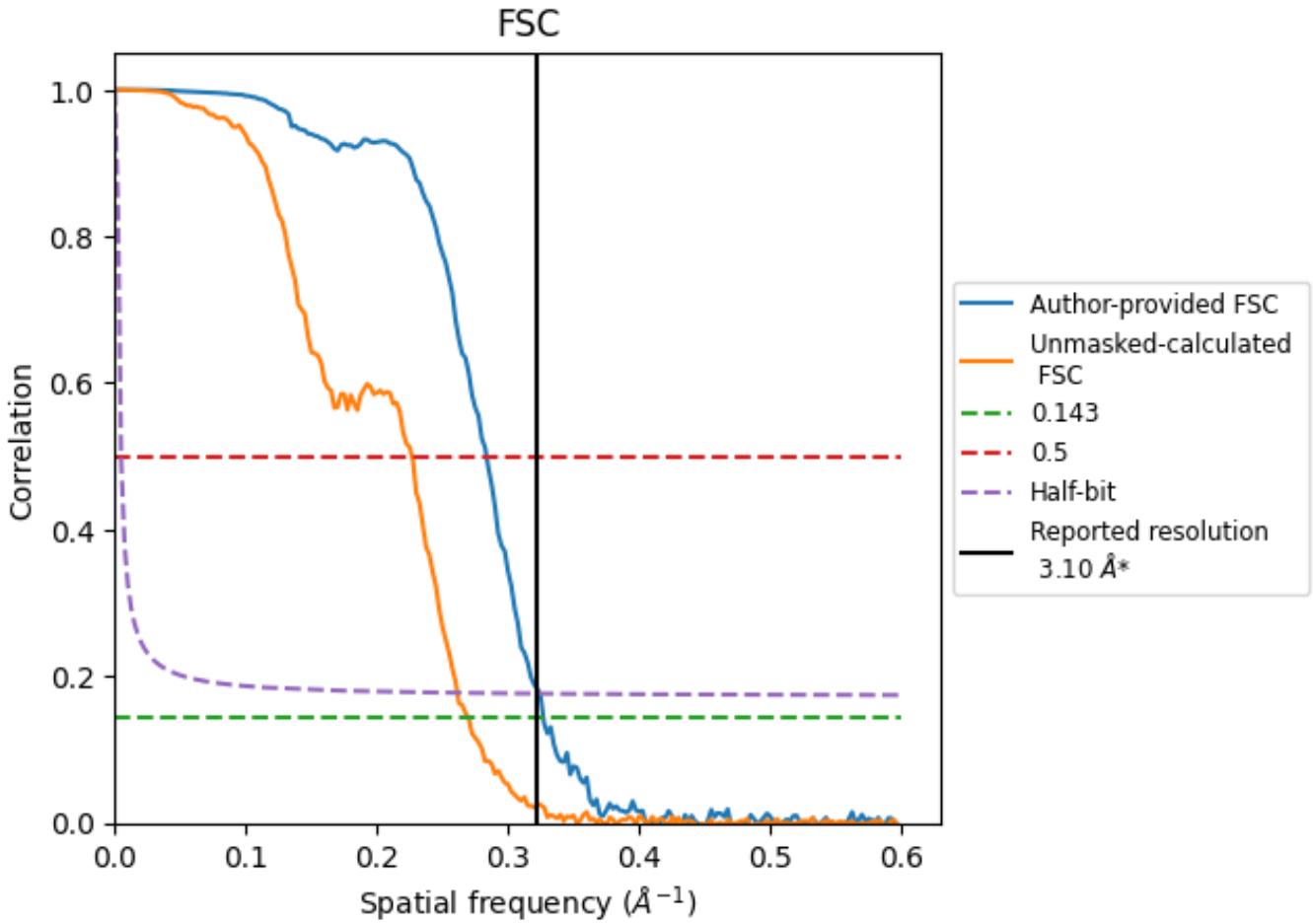


*Reported resolution corresponds to spatial frequency of 0.323 $Å^{-1}$

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 0.323 Å^{-1}

8.2 Resolution estimates (i)

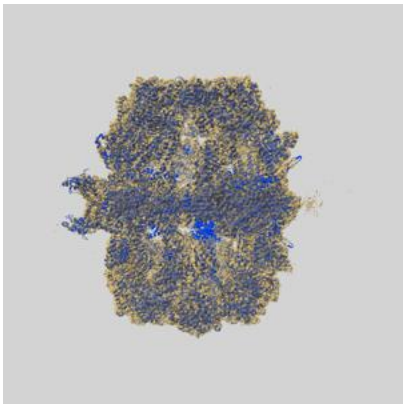
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.06	3.52	3.09
Unmasked-calculated*	3.70	4.41	3.83

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.70 differs from the reported value 3.1 by more than 10 %

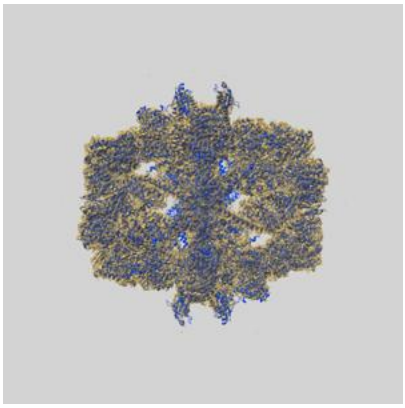
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10420 and PDB model 6TA1. Per-residue inclusion information can be found in section 3 on page 7.

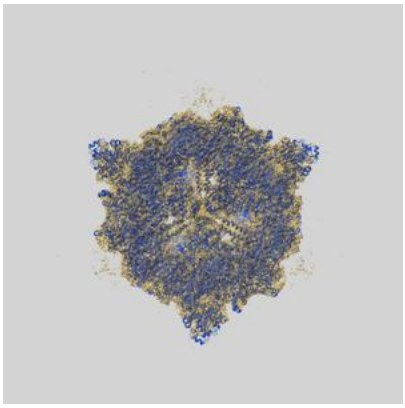
9.1 Map-model overlay



X



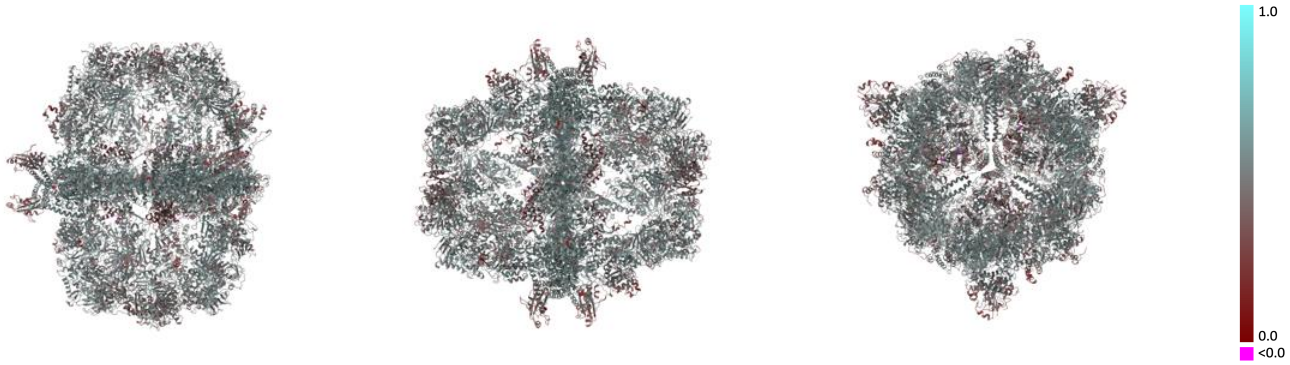
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

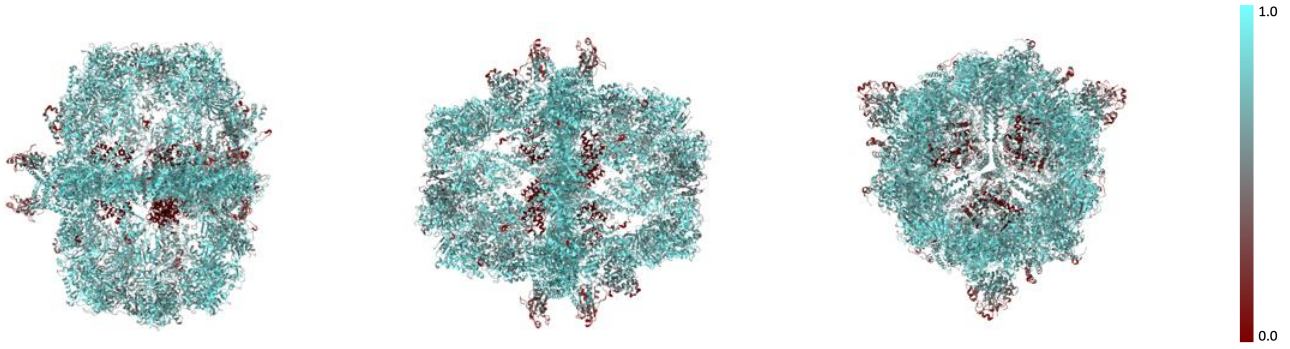
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

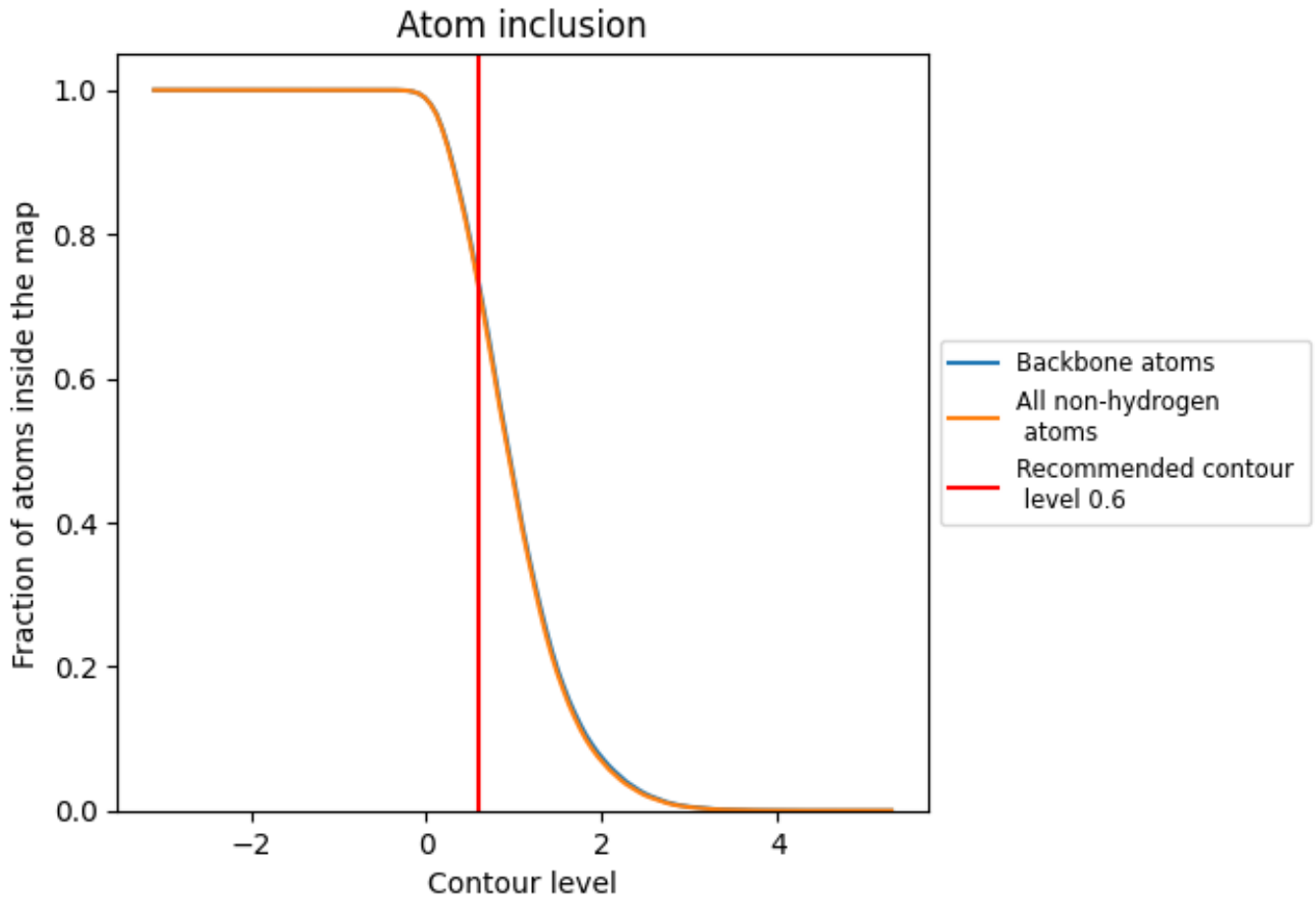
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.6).

9.4 Atom inclusion (i)



At the recommended contour level, 73% of all backbone atoms, 72% 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 (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7223	0.4880
A	0.7174	0.4960
B	0.7146	0.4950
C	0.7343	0.4810
D	0.7149	0.4950
E	0.7334	0.4810
F	0.7146	0.4950
G	0.7345	0.4820
H	0.7343	0.4810
I	0.7149	0.4950
J	0.7334	0.4810
K	0.7174	0.4960
L	0.7345	0.4820