Full wwPDB EM Validation Report ⓘ

Dec 17, 2022 – 05:13 pm GMT

PDB ID	:	6YEY
EMDB ID	:	EMD-10797
Title	:	Xenorhabdus nematophila XptA1 in complex with porcine mucosa heparin
Authors	:	Roderer, D.; Broecker, F.; Sitsel, O.; Kaplonek, P.; Leidreiter, F.; Seeberger, P.H.; Raunser, S.
Deposited on	:	2020-03-25
Resolution	:	3.70 Å(reported)
Based on initial model	:	6RW8

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:

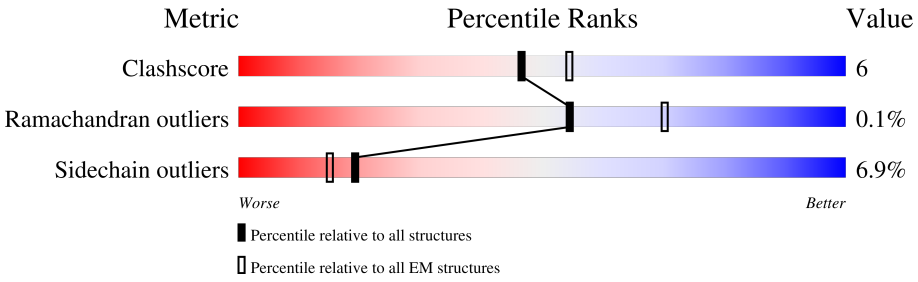
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 3.70 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	2523	73% 18% • 7%
1	B	2523	73% 18% • 7%
1	C	2523	72% 19% • 7%
1	D	2523	72% 19% • 7%
1	E	2523	73% 19% • 7%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 93500 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called A component of insecticidal toxin complex (Tc).

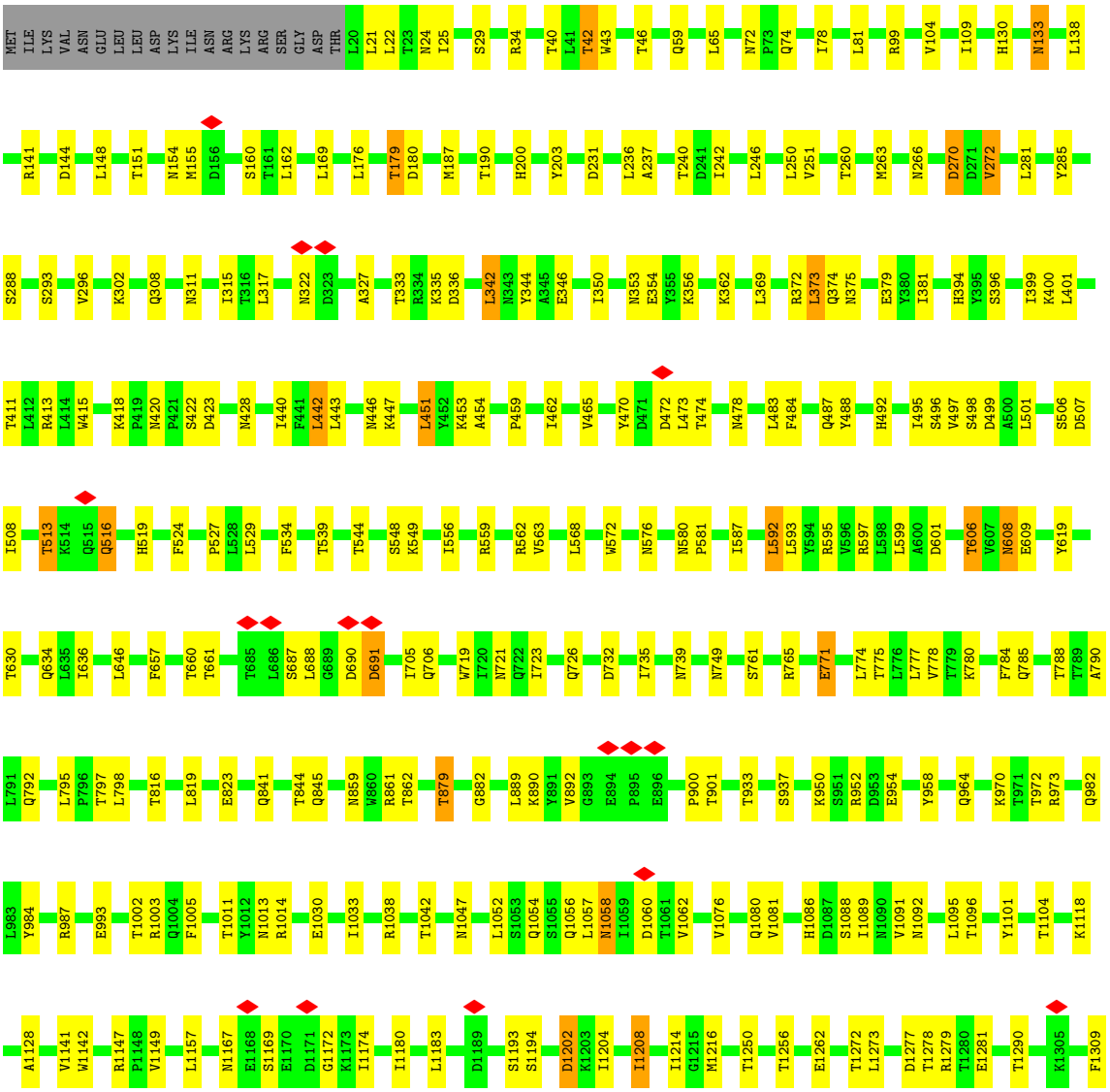
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2337	Total	C	N	O	S	0	0
			18700	11894	3132	3607	67		
1	B	2337	Total	C	N	O	S	0	0
			18700	11894	3132	3607	67		
1	C	2337	Total	C	N	O	S	0	0
			18700	11894	3132	3607	67		
1	D	2337	Total	C	N	O	S	0	0
			18700	11894	3132	3607	67		
1	E	2337	Total	C	N	O	S	0	0
			18700	11894	3132	3607	67		

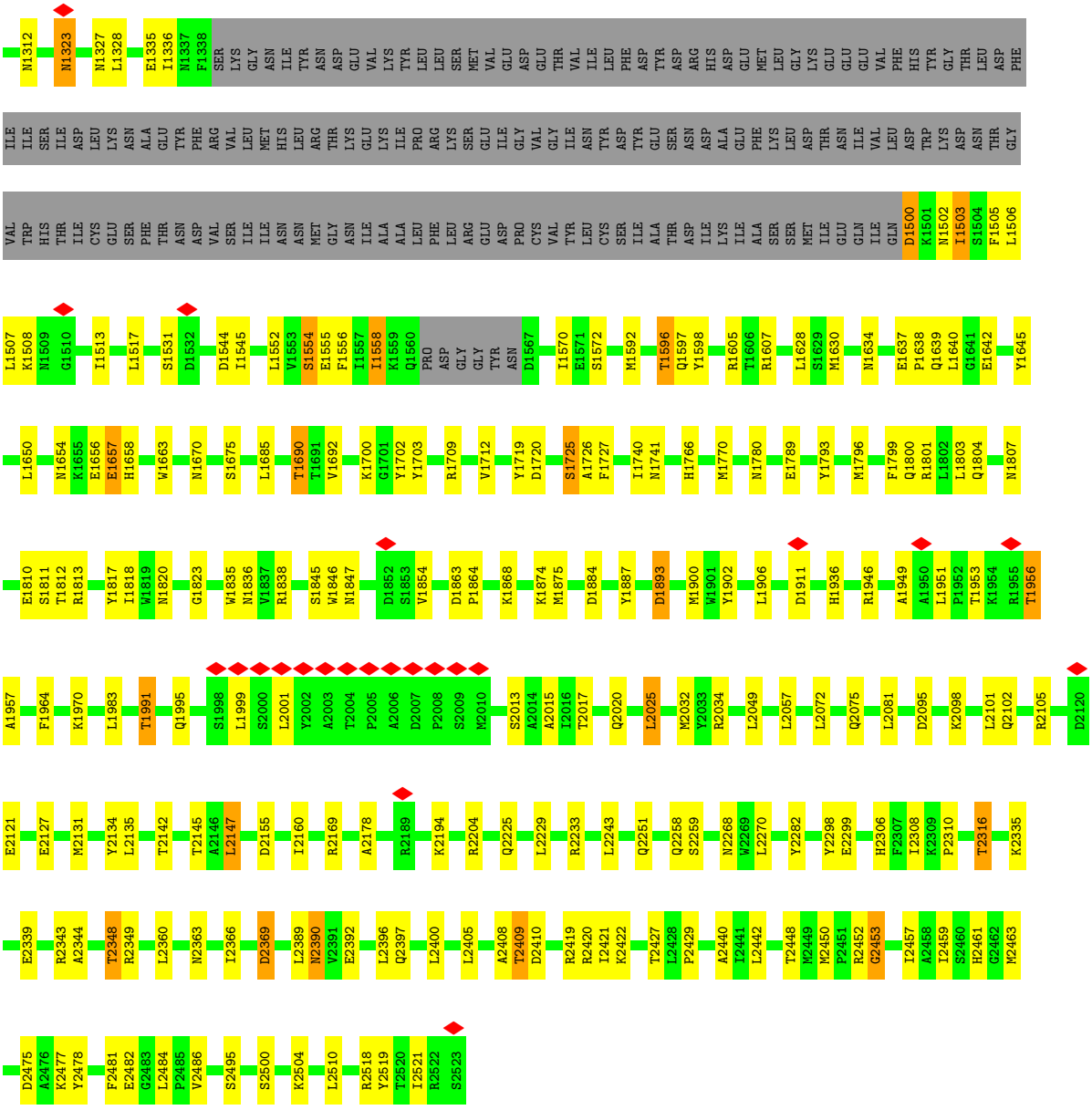
3 Residue-property plots (i)

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: A component of insecticidal toxin complex (Tc)

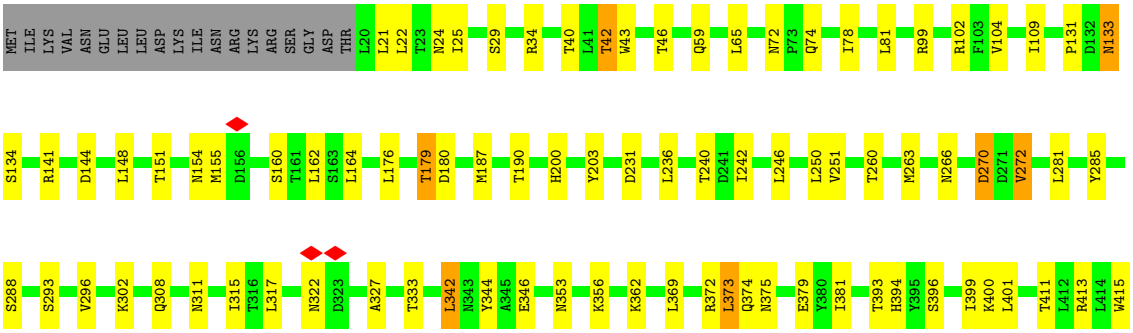
Chain A:

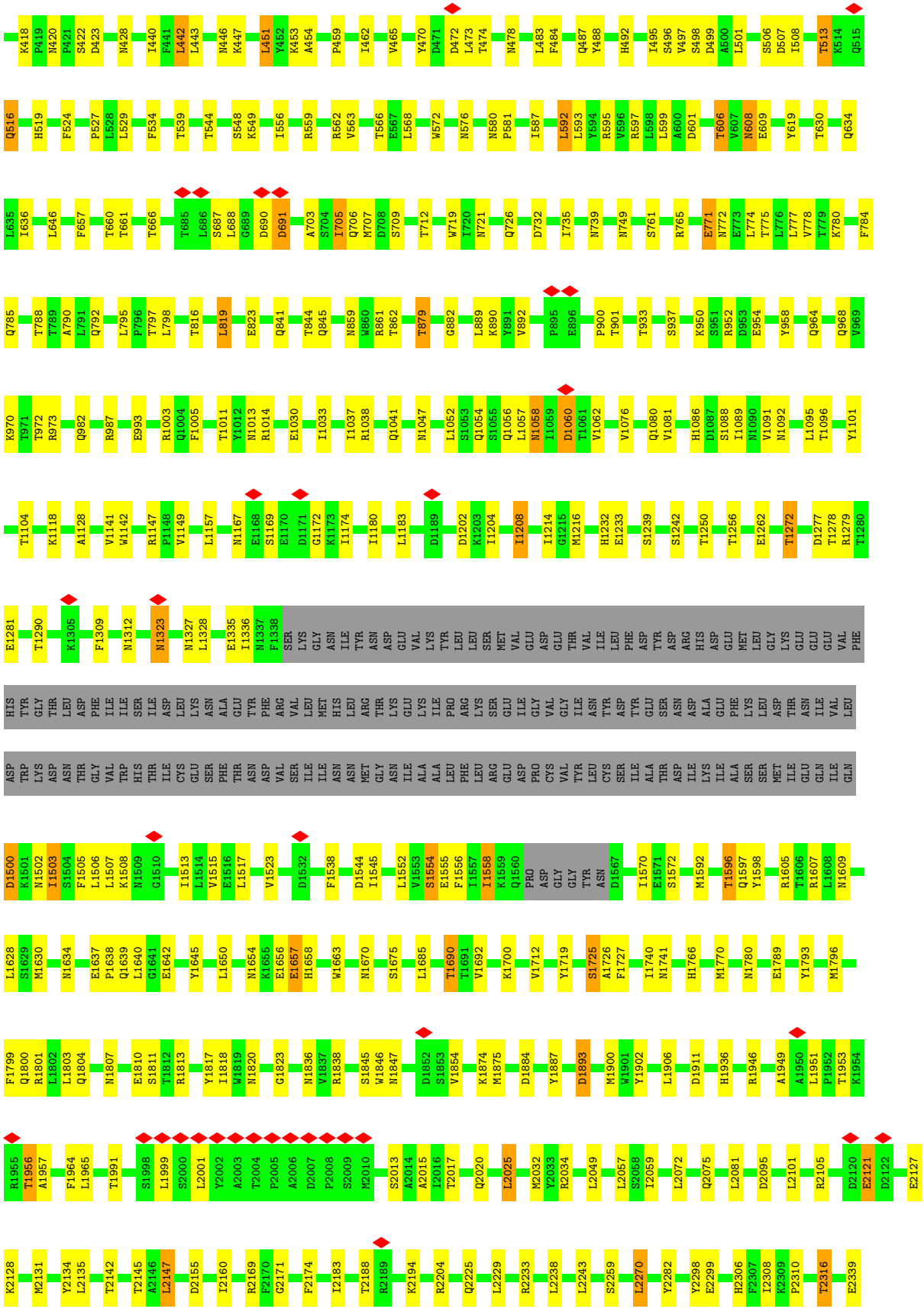


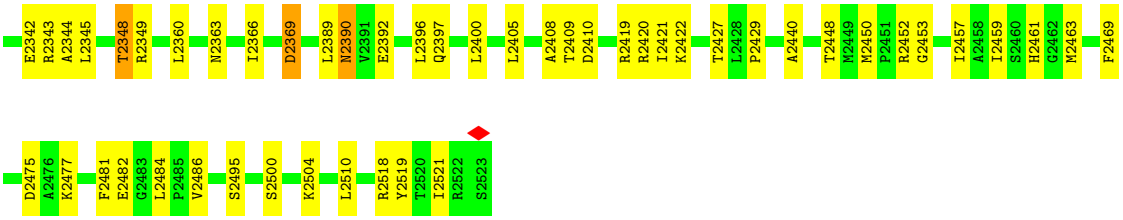


• Molecule 1: A component of insecticidal toxin complex (Tc)

Chain B:

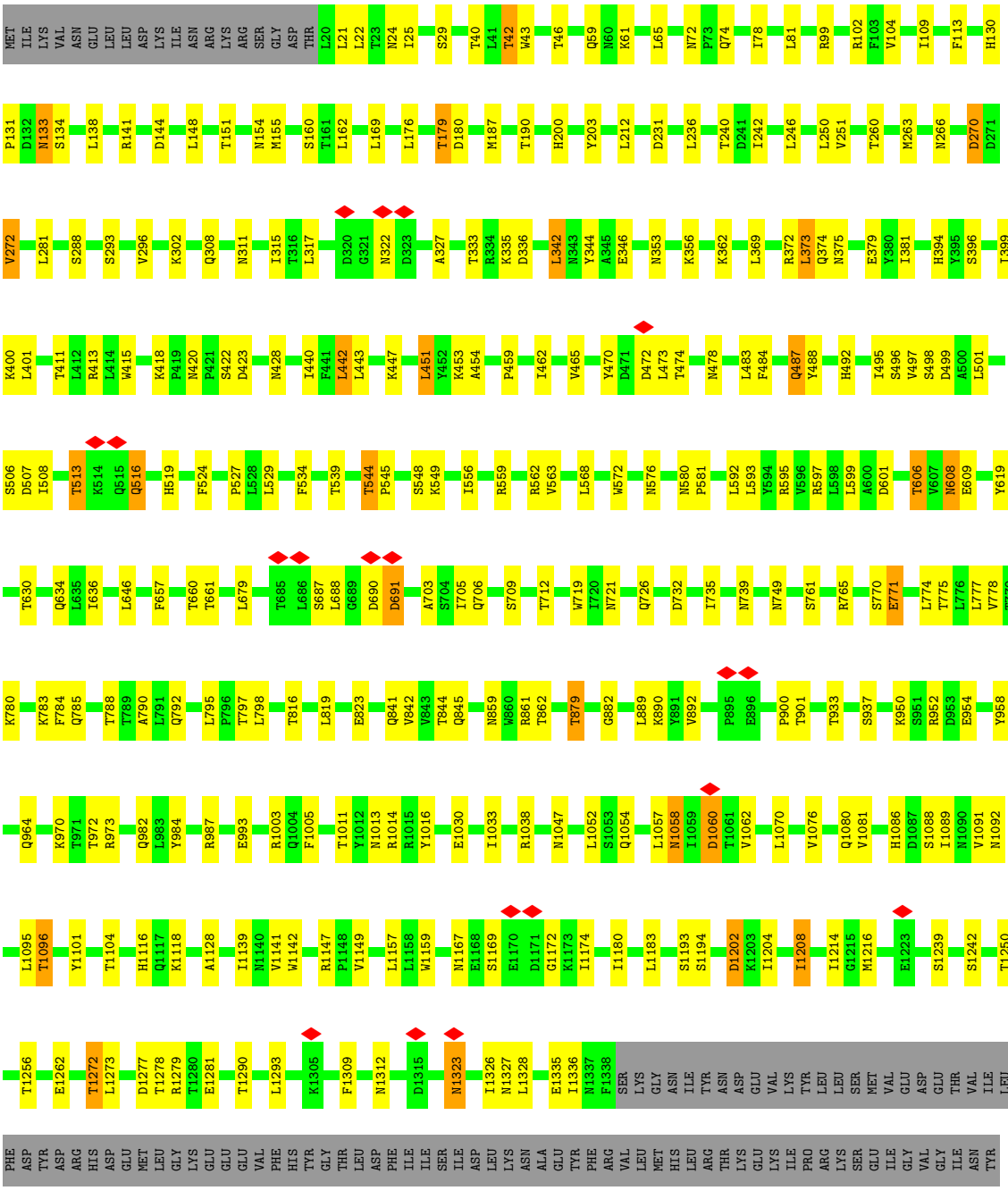


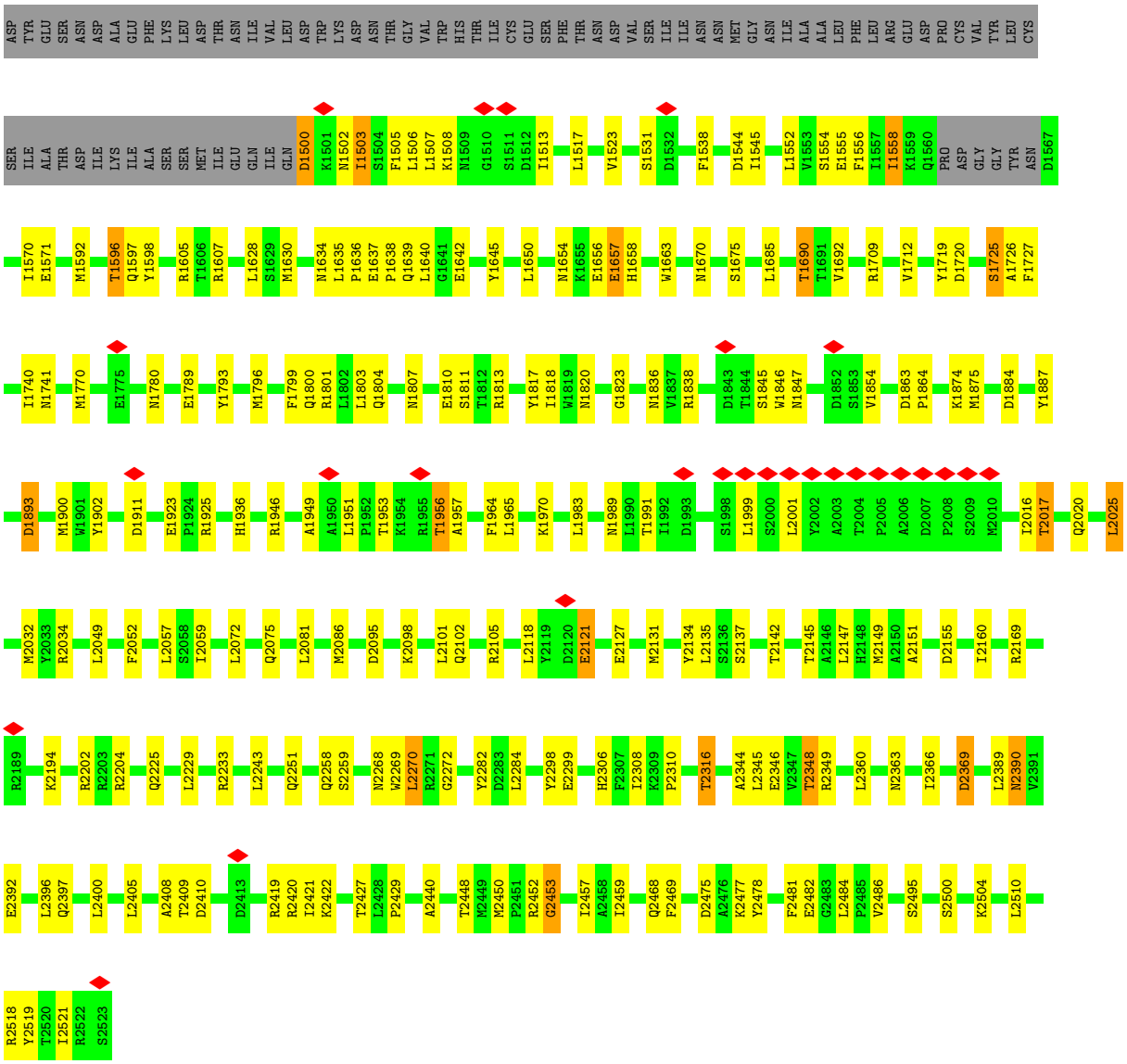

K418 P419 N420 P421 S422 D423 N428 I440 F441 L442 L443 N446 K447 L451 Y452 K453 A454 P459 I462 V465 Y470 D471 D472 L473 T474 N478 L483 F484 Q487 Y488 H492 I495 S496 V497 S498 D499 A500 L501 S506 D507 I508 T513 K514 Q515
Q516 H519 F524 P527 L528 L529 F534 T539 T544 S548 K549 I556 R559 R562 V563 T566 E567 L568 W572 N576 N580 P581 I587 L592 L593 Y594 R595 V596 R597 L598 L599 A600 D601 T606 V607 N608 E609 Y619 T630 Q634
L635 I636 L646 F657 T660 T661 T666 T685 L686 S687 I688 G689 D690 D691 A703 S704 T705 Q706 M707 D708 S709 T712 W719 T720 N721 Q726 D732 I735 N739 N749 S761 R765 E771 N772 E773 L774 T775 L776 L777 V778 T779 K780 F784
Q785 T788 T789 A790 L791 Q792 L795 P796 T797 L798 T816 L819 E823 Q841 T844 Q845 N859 V860 R861 T862 T879 G882 L889 K890 Y891 V892 P895 E896 P900 T901 T933 S937 K950 S951 R952 D953 E954 Y958 Q964 Q968 V969
K970 T971 T972 R973 Q982 R987 E993 R1003 Q1004 F1005 T1011 Y1012 N1013 R1014 E1030 I1033 I1037 R1038 Q1041 N1047 L1052 S1053 Q1054 S1055 Q1056 L1057 N1058 I1059 D1060 T1061 V1062 V1076 Q1080 V1081 H1086 D1087 S1088 I1089 N1090 V1091 N1092 L1095 T1096 Y1101
T1104 K1118 A1128 V1141 W1142 R1147 P1148 V1149 L1157 N1167 E1168 S1169 E1170 D1171 G1172 K1173 I1174 I1180 L1183 D1189 D1202 K1203 I1204 I1208 I1214 G1215 M1216 H1232 E1233 S1239 S1242 T1250 T1256 E1262 T1272 D1277 T1278 R1279 T1280
E1281 T1290 K1305 F1309 N1312 N1323 N1327 L1328 E1335 I1336 N1337 F1338 SER LYS GLY ASN ILE TYR ASN ASP GLU VAL LYS TYR LEU LEU SER MET VAL GLU ASP GLU THR VAL ILE LEU PHE ASP TYR ASP ARG HIS ASP GLU MET LEU GLY LYS GLU GLU GLU VAL PHE
HIS TYR GLY THR LEU ASP PHE ILE ILE SER ILE ASP LEU LYS ASN ALA GLU TYR PHE ARG VAL LEU MET HIS LEU ARG THR LYS GLU LYS ILE PRO ARG LYS SER GLU ILE GLY VAL GLY ILE ASN TYR ASP TYR GLU SER ASN ASP ALA GLU PHE LYS LEU ASP THR ASN ILE ILE VAL LEU
ASP TRP LYS ASP ASN THR GLY VAL TRP HIS THR ILE CYS GLU SER PHE THR ASN ASP VAL SER ILE ILE ASN ASN MET GLY ASN ILE ALA ALA LEU PHE LEU ARG GLU ASP PRO CYS VAL TYR LEU CYS SER ILE ALA THR ASP ILE LYS ILE ALA ALA SER SER MET ILE GLU GLN ILE GLN
D1500 K1501 N1502 I1503 S1504 F1505 L1506 L1507 K1508 N1509 G1510 I1513 L1514 V1515 E1516 L1517 V1523 D1532 F1538 D1544 I1545 L1552 V1553 S1554 E1555 F1556 I1557 T1558 K1559 Q1560 PRO ASP GLY GLY TYR ASN D1567 I1570 E1571 S1572 M1592 T1596 Q1597 Y1598 R1605 T1606 R1607 L1608 N1609
L1628 S1629 M1630 N1634 E1637 P1638 Q1639 L1640 G1641 E1642 Y1645 L1650 N1654 K1665 E1656 E1657 H1658 W1663 N1670 S1675 L1685 T1690 T1691 V1692 K1700 V1712 Y1719 S1725 A1726 F1727 I1740 N1741 H1766 M1770 N1780 E1789 Y1793 M1796
F1799 Q1800 R1801 L1802 L1803 Q1804 N1807 E1810 S1811 T1812 R1813 Y1817 I1818 W1819 N1820 G1823 N1836 V1837 R1838 S1845 W1846 N1847 D1852 S1853 V1854 K1874 M1875 D1884 D1893 Y1887 M1900 W1901 Y1902 L1906 D1911 H1936 R1946 A1949 A1950 L1951 P1952 T1953 K1954
R1955 T1956 A1957 F1964 L1965 T1991 S1998 L1999 S2000 L2001 Y2002 A2003 T2004 P2005 A2006 D2007 P2008 S2009 M2010 S2013 A2014 A2015 I2016 T2017 Q2020 L2025 M2032 Y2033 R2034 L2049 L2057 S2058 I2059 L2072 Q2075 L2081 D2095 L2101 R2105 D2120 E2121 D2122 E2127
K2128 M2131 Y2134 L2135 T2142 T2145 A2146 L2147 D2155 I2160 R2169 F2170 G2171 F2174 I2183 T2188 R2189 K2194 R2204 Q2225 L2229 R2233 L2238 L2243 S2259 L2270 Y2282 Y2298 E2299 H2306 F2307 I2308 K2309 P2310 T2316 E2339



• Molecule 1: A component of insecticidal toxin complex (Tc)

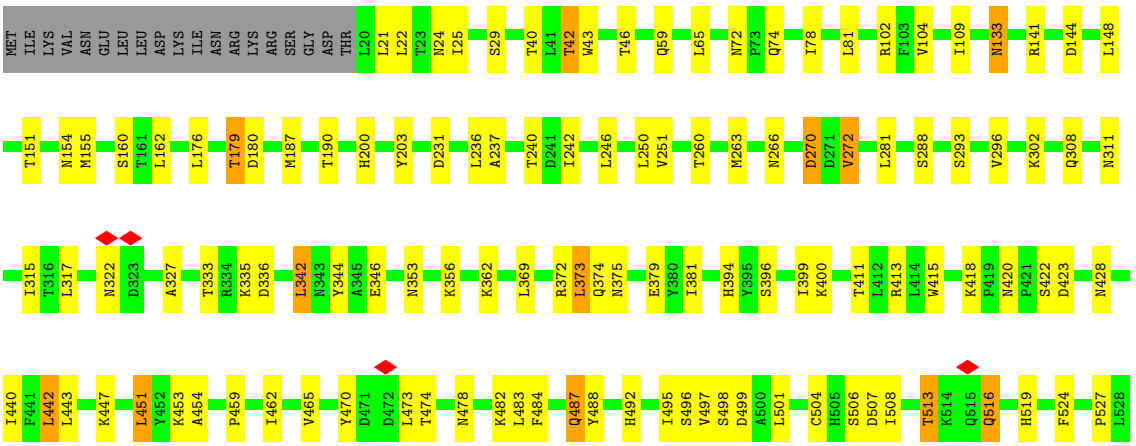
Chain C:

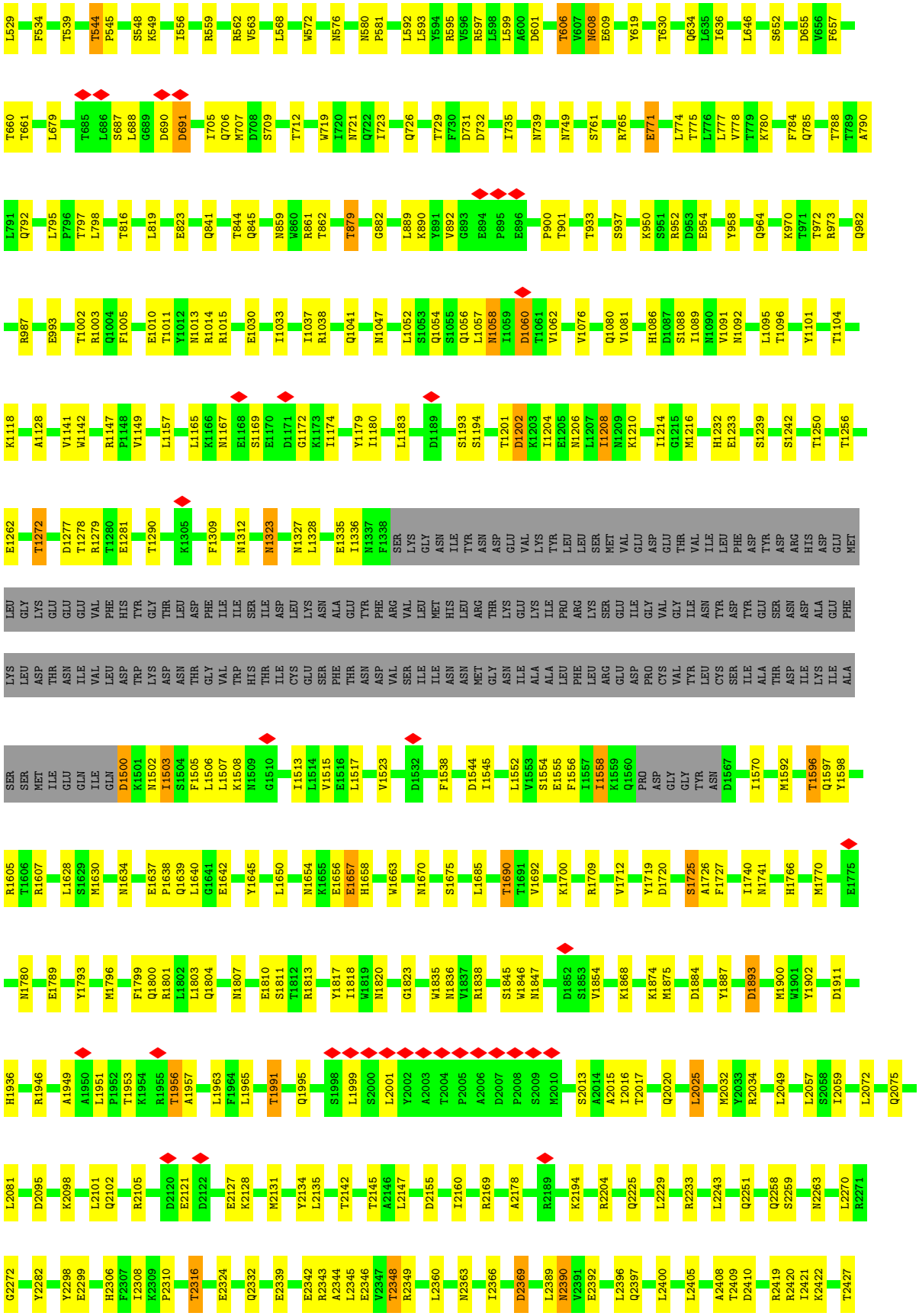




• Molecule 1: A component of insecticidal toxin complex (Tc)

Chain D:

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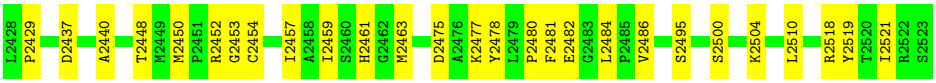
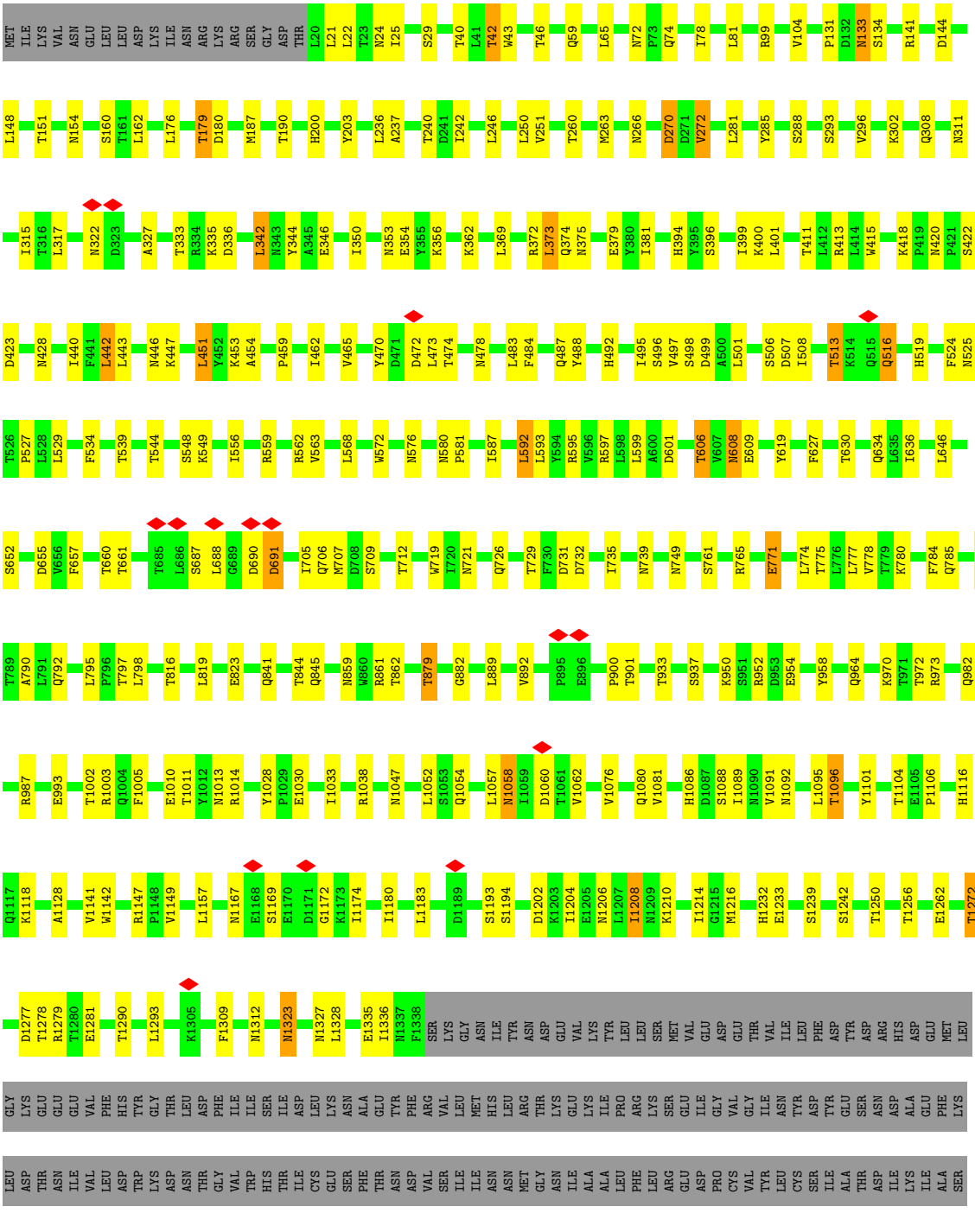
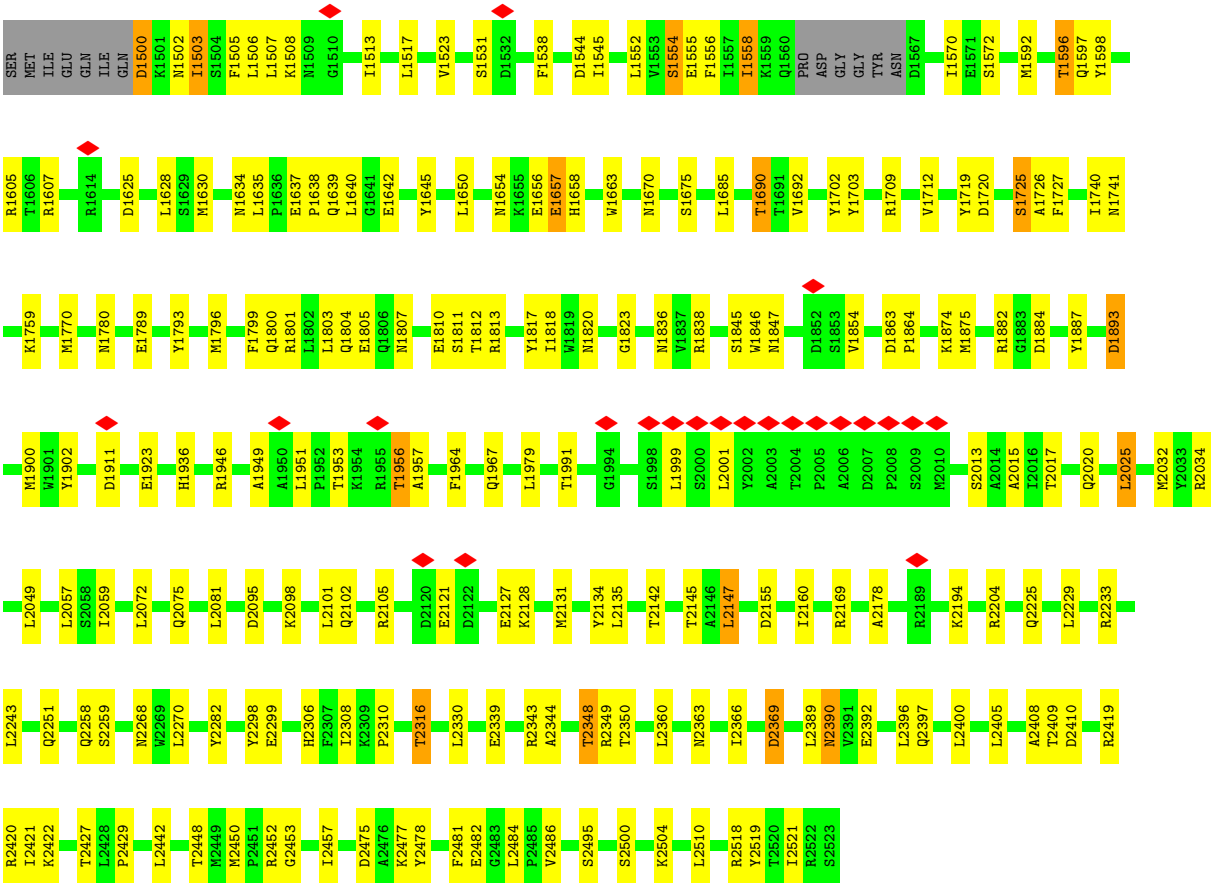
T660 T661 L679 T685 L686 S687 L688 G689 D690 D691 I705 Q706 M707 D708 S709 T712 W719 I720 N721 Q722 I723 Q726 T729 F730 D731 D732 I735 N739 N749 S761 R765 E771 L774 T775 L776 L777 V778 T779 K780 F784 Q785 T788 T789 A790
L791 Q792 L795 P796 T797 L798 T816 L819 E823 Q841 T844 Q845 N859 W860 R861 T862 T879 G882 L889 K890 Y891 V892 G893 E894 P895 E896 P900 T901 T933 S937 K950 S951 R952 D953 E954 Y958 Q964 K970 T971 T972 R973 Q982
R987 E993 T1002 R1003 Q1004 F1005 E1010 T1011 Y1012 N1013 R1014 R1015 E1030 I1033 I1037 R1038 Q1041 N1047 L1052 S1053 Q1054 S1055 Q1056 L1057 N1058 I1059 D1060 T1061 V1062 V1076 Q1080 V1081 H1086 D1087 S1088 I1089 N1090 V1091 N1092 L1095 T1096 Y1101 T1104
K1118 A1128 V1141 W1142 R1147 P1148 V1149 L1157 L1165 K1166 N1167 E1168 S1169 E1170 D1171 G1172 K1173 I1174 Y1179 I1180 L1183 D1189 S1193 S1194 T1201 D1202 K1203 I1204 E1205 N1206 L1207 I1208 N1209 K1210 I1214 G1215 M1216 H1232 E1233 S1239 S1242 T1250 T1256
E1262 T1272 D1277 T1278 R1279 T1280 E1281 T1290 K1305 F1309 N1312 N1323 N1327 L1328 E1335 I1336 N1337 F1338 SER LYS GLY ASN ILE TYR ASN ASP GLU VAL LYS TYR LEU LEU SER MET VAL GLU ASP GLU THR VAL ILE LEU PHE ASP TYR ASP ARG HIS ASP GLU MET
LEU GLY LYS GLU GLU VAL PHE HIS TYR GLY THR LEU ASP PHE ILE ILE SER ILE ASP LEU LYS ASN ALA GLU TYR PHE ARG VAL LEU MET HIS LEU ARG THR LYS GLU LYS ILE PRO ARG LYS SER GLU ILE GLY VAL GLY ILE ASN TYR ASP TYR GLU SER ASN ASP ALA GLU PHE
LYS LEU ASP THR ASN ILE VAL LEU ASP TRP LYS ASP ASN THR GLY VAL TRP HIS THR ILE CYS GLU SER PHE THR ASN ASP VAL SER ILE ILE ASN ASN MET GLY ASN ILE ALA ALA LEU PHE LEU ARG GLU ASP PRO CYS VAL TYR LEU CYS SER ILE ALA THR ASP ILE LYS ILE ALA
SER SER MET ILE GLU GLN ILE GLN D1500 K1501 N1502 I1503 S1504 F1505 L1506 L1507 K1508 N1509 G1510 I1513 L1514 V1515 E1516 L1517 V1523 D1532 F1538 D1544 I1545 L1552 V1553 S1554 E1555 F1556 I1557 I1558 K1559 Q1560 PRO ASP GLY GLY TYR ASN D1567 I1570 M1592 T1596 Q1597 Y1598
R1605 T1606 R1607 L1628 S1629 M1630 N1634 E1637 P1638 Q1639 L1640 G1641 E1642 Y1645 L1650 N1654 K1655 E1656 E1657 H1658 W1663 N1670 S1675 L1685 T1690 T1691 V1692 K1700 R1709 V1712 Y1719 D1720 S1725 A1726 F1727 I1740 N1741 H1766 M1770 E1775
N1780 E1789 Y1793 M1796 F1799 Q1800 R1801 L1802 L1803 Q1804 N1807 E1810 S1811 T1812 R1813 Y1817 I1818 W1819 N1820 G1823 W1835 N1836 V1837 R1838 S1845 W1846 N1847 D1852 S1853 V1854 K1868 K1874 M1875 D1884 Y1887 D1893 M1900 W1901 Y1902 D1911
H1936 R1946 A1949 A1950 L1951 P1952 T1953 K1954 R1955 T1956 A1957 L1963 F1964 L1965 T1991 Q1995 S1998 L1999 S2000 L2001 Y2002 A2003 T2004 P2005 A2006 D2007 P2008 S2009 M2010 S2013 A2014 A2015 I2016 T2017 Q2020 L2025 M2032 Y2033 R2034 L2049 L2057 S2058 I2059 L2072 Q2075
L2081 D2095 K2098 L2101 Q2102 R2105 D2120 E2121 D2122 E2127 K2128 M2131 Y2134 L2135 T2142 T2145 A2146 L2147 D2155 I2160 R2169 A2178 R2189 K2194 R2204 Q2225 L2229 R2233 L2243 Q2251 Q2258 S2259 N2263 L2270 R2271
G2272 Y2282 Y2298 E2299 H2306 F2307 I2308 K2309 P2310 T2316 E2324 Q2332 E2339 E2342 R2343 A2344 L2345 E2346 V2347 T2348 R2349 L2360 N2363 I2366 D2369 L2389 N2390 V2391 E2392 L2396 Q2397 L2400 L2405 A2408 T2409 D2410 R2419 R2420 I2421 K2422 T2427



• Molecule 1: A component of insecticidal toxin complex (Tc)

Chain E:

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R1605 T1606 R1607 R1614 D1625 L1628 S1629 M1630 N1634 L1635 P1636 E1637 P1638 Q1639 L1640 G1641 E1642 Y1645 L1650 N1654 K1655 E1656 E1657 H1658 W1663 N1670 S1675 L1685 T1690 T1691 V1692 Y1702 Y1703 R1709 V1712 Y1719 D1720 S1725 A1726 F1727 I1740 N1741
K1759 M1770 N1780 E1789 Y1793 M1796 F1799 Q1800 R1801 L1802 L1803 Q1804 E1805 Q1806 N1807 E1810 S1811 T1812 R1813 Y1817 I1818 W1819 N1820 G1823 N1836 V1837 R1838 S1845 W1846 N1847 D1852 S1853 V1854 D1863 P1864 K1874 M1875 R1882 G1883 D1884 Y1887 D1893
M1900 W1901 Y1902 D1911 E1923 H1936 R1946 A1949 A1950 L1951 P1952 T1953 K1954 R1955 T1956 A1957 F1964 Q1967 L1979 T1991 G1994 S1998 L1999 S2000 L2001 Y2002 A2003 T2004 P2005 A2006 D2007 P2008 S2009 M2010 S2013 A2014 A2015 I2016 T2017 Q2020 L2025 M2032 Y2033 R2034
L2049 L2057 S2058 I2059 L2072 Q2075 L2081 D2095 K2098 L2101 Q2102 R2105 D2120 E2121 D2122 E2127 K2128 M2131 Y2134 L2135 T2142 T2145 A2146 L2147 D2155 I2160 R2169 A2178 R2189 K2194 R2204 Q2225 L2229 R2233
L2243 Q2251 Q2258 S2259 N2268 W2269 L2270 Y2282 Y2298 E2299 H2306 F2307 I2308 K2309 P2310 T2316 L2330 E2339 R2343 A2344 T2348 R2349 T2350 L2360 N2363 I2366 D2369 L2389 W2390 V2391 E2392 L2396 Q2397 L2400 L2405 A2408 T2409 D2410 R2419
R2420 I2421 K2422 T2427 L2428 P2429 L2442 T2448 M2449 M2450 P2451 R2452 G2453 I2457 D2475 A2476 K2477 Y2478 F2481 E2482 G2483 L2484 P2485 V2486 S2495 S2500 K2504 L2510 R2518 Y2519 T2520 I2521 R2522 S2523

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	172596	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	52	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	0.111	Depositor
Minimum map value	-0.060	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.028	Depositor
Map size (Å)	484.0, 484.0, 484.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.21, 1.21, 1.21	Depositor

5 Model quality

5.1 Standard geometry

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	0.34	0/19100	0.50	0/25936
1	B	0.34	0/19100	0.50	0/25936
1	C	0.34	0/19100	0.50	0/25936
1	D	0.34	0/19100	0.50	0/25936
1	E	0.34	0/19100	0.50	0/25936
All	All	0.34	0/95500	0.50	0/129680

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	2
1	D	0	2
1	E	0	2
All	All	0	10

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1558	ILE	Peptide
1	A	2344	ALA	Peptide
1	B	1558	ILE	Peptide
1	B	2344	ALA	Peptide
1	C	1558	ILE	Peptide

Continued on next page...

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Mol	Chain	Res	Type	Group
1	C	2344	ALA	Peptide
1	D	1558	ILE	Peptide
1	D	2344	ALA	Peptide
1	E	1558	ILE	Peptide
1	E	2344	ALA	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	18700	0	18400	247	0
1	B	18700	0	18400	247	0
1	C	18700	0	18400	266	0
1	D	18700	0	18400	251	0
1	E	18700	0	18400	250	0
All	All	93500	0	92000	1200	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 6.

All (1200) 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:B:236:LEU:HB2	1:B:484:PHE:HB2	1.74	0.70
1:A:236:LEU:HB2	1:A:484:PHE:HB2	1.74	0.70
1:C:236:LEU:HB2	1:C:484:PHE:HB2	1.74	0.70
1:D:236:LEU:HB2	1:D:484:PHE:HB2	1.74	0.69
1:E:236:LEU:HB2	1:E:484:PHE:HB2	1.74	0.69
1:C:2258:GLN:HB3	1:D:2015:ALA:HB2	1.76	0.67
1:C:2194:LYS:HD2	1:E:1054:GLN:HE21	1.60	0.67
1:D:1663:TRP:HA	1:D:1685:LEU:H	1.62	0.65
1:E:1663:TRP:HA	1:E:1685:LEU:H	1.62	0.65
1:C:1607:ARG:HE	1:C:1640:LEU:HD21	1.63	0.64
1:E:1607:ARG:HE	1:E:1640:LEU:HD21	1.63	0.64
1:A:1663:TRP:HA	1:A:1685:LEU:H	1.62	0.64
1:B:1663:TRP:HA	1:B:1685:LEU:H	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1663:TRP:HA	1:C:1685:LEU:H	1.62	0.63
1:D:1607:ARG:HE	1:D:1640:LEU:HD21	1.63	0.63
1:B:1607:ARG:HE	1:B:1640:LEU:HD21	1.63	0.63
1:E:534:PHE:HB2	1:E:556:ILE:HD13	1.81	0.62
1:A:1607:ARG:HE	1:A:1640:LEU:HD21	1.63	0.62
1:D:534:PHE:HB2	1:D:556:ILE:HD13	1.81	0.62
1:A:1500:ASP:OD1	1:A:1500:ASP:N	2.33	0.62
1:A:534:PHE:HB2	1:A:556:ILE:HD13	1.81	0.62
1:B:1500:ASP:OD1	1:B:1500:ASP:N	2.33	0.61
1:E:1598:TYR:HB3	1:E:1640:LEU:HD22	1.82	0.61
1:A:151:THR:HG23	1:A:154:ASN:H	1.66	0.61
1:B:534:PHE:HB2	1:B:556:ILE:HD13	1.81	0.61
1:B:1500:ASP:HB2	1:B:1502:ASN:H	1.66	0.61
1:C:1598:TYR:HB3	1:C:1640:LEU:HD22	1.82	0.61
1:A:1598:TYR:HB3	1:A:1640:LEU:HD22	1.83	0.61
1:D:151:THR:HG23	1:D:154:ASN:H	1.66	0.61
1:C:374:GLN:HE21	1:C:413:ARG:HD2	1.66	0.61
1:C:1052:LEU:HD11	1:C:1062:VAL:HG23	1.83	0.61
1:C:1500:ASP:HB2	1:C:1502:ASN:H	1.66	0.61
1:C:534:PHE:HB2	1:C:556:ILE:HD13	1.81	0.61
1:D:242:ILE:HA	1:D:246:LEU:HD23	1.83	0.61
1:E:1500:ASP:HB2	1:E:1502:ASN:H	1.66	0.61
1:C:1500:ASP:N	1:C:1500:ASP:OD1	2.33	0.61
1:C:242:ILE:HA	1:C:246:LEU:HD23	1.83	0.60
1:D:1500:ASP:OD1	1:D:1500:ASP:N	2.33	0.60
1:A:374:GLN:HE21	1:A:413:ARG:HD2	1.66	0.60
1:C:151:THR:HG23	1:C:154:ASN:H	1.65	0.60
1:D:1052:LEU:HD11	1:D:1062:VAL:HG23	1.83	0.60
1:A:771:GLU:HA	1:A:774:LEU:HB3	1.84	0.60
1:B:374:GLN:HE21	1:B:413:ARG:HD2	1.66	0.60
1:B:1598:TYR:HB3	1:B:1640:LEU:HD22	1.82	0.60
1:D:1500:ASP:HB2	1:D:1502:ASN:H	1.66	0.60
1:B:1052:LEU:HD11	1:B:1062:VAL:HG23	1.83	0.60
1:E:242:ILE:HA	1:E:246:LEU:HD23	1.83	0.60
1:B:242:ILE:HA	1:B:246:LEU:HD23	1.83	0.60
1:E:151:THR:HG23	1:E:154:ASN:H	1.66	0.60
1:E:374:GLN:HE21	1:E:413:ARG:HD2	1.66	0.60
1:B:151:THR:HG23	1:B:154:ASN:H	1.66	0.60
1:D:374:GLN:HE21	1:D:413:ARG:HD2	1.66	0.60
1:D:1598:TYR:HB3	1:D:1640:LEU:HD22	1.82	0.60
1:B:1005:PHE:O	1:B:1013:ASN:ND2	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:889:LEU:HD22	1:D:900:PRO:HB3	1.84	0.60
1:E:1500:ASP:N	1:E:1500:ASP:OD1	2.33	0.60
1:A:242:ILE:HA	1:A:246:LEU:HD23	1.83	0.60
1:A:1500:ASP:HB2	1:A:1502:ASN:H	1.66	0.59
1:B:1505:PHE:HB3	1:B:1517:LEU:HB2	1.84	0.59
1:A:889:LEU:HD22	1:A:900:PRO:HB3	1.84	0.59
1:C:2284:LEU:HD11	1:D:2332:GLN:HG3	1.84	0.59
1:E:1005:PHE:O	1:E:1013:ASN:ND2	2.35	0.59
1:A:1766:HIS:HE2	1:E:1531:SER:HG	1.50	0.59
1:B:777:LEU:HD22	1:B:784:PHE:HB2	1.85	0.59
1:C:889:LEU:HD22	1:C:900:PRO:HB3	1.84	0.59
1:E:1052:LEU:HD11	1:E:1062:VAL:HG23	1.83	0.59
1:A:1505:PHE:HB3	1:A:1517:LEU:HB2	1.84	0.59
1:C:771:GLU:HA	1:C:774:LEU:HB3	1.84	0.59
1:C:1654:ASN:OD1	1:C:1658:HIS:NE2	2.36	0.59
1:D:1820:ASN:ND2	1:D:1823:GLY:O	2.36	0.59
1:E:777:LEU:HD22	1:E:784:PHE:HB2	1.85	0.59
1:A:1052:LEU:HD11	1:A:1062:VAL:HG23	1.83	0.59
1:D:771:GLU:HA	1:D:774:LEU:HB3	1.84	0.59
1:E:889:LEU:HD22	1:E:900:PRO:HB3	1.84	0.59
1:C:657:PHE:O	1:C:661:THR:HB	2.03	0.59
1:E:1820:ASN:ND2	1:E:1823:GLY:O	2.36	0.59
1:A:1005:PHE:O	1:A:1013:ASN:ND2	2.35	0.59
1:A:1820:ASN:ND2	1:A:1823:GLY:O	2.36	0.59
1:A:657:PHE:O	1:A:661:THR:HB	2.03	0.58
1:B:937:SER:OG	1:B:952:ARG:NH1	2.36	0.58
1:C:1505:PHE:HB3	1:C:1517:LEU:HB2	1.84	0.58
1:B:771:GLU:HA	1:B:774:LEU:HB3	1.84	0.58
1:B:1820:ASN:ND2	1:B:1823:GLY:O	2.36	0.58
1:E:771:GLU:HA	1:E:774:LEU:HB3	1.84	0.58
1:E:1505:PHE:HB3	1:E:1517:LEU:HB2	1.84	0.58
1:C:1820:ASN:ND2	1:C:1823:GLY:O	2.36	0.58
1:E:657:PHE:O	1:E:661:THR:HB	2.03	0.58
1:A:937:SER:OG	1:A:952:ARG:NH1	2.36	0.58
1:A:1650:LEU:HB2	1:A:1690:THR:HG23	1.86	0.58
1:A:1654:ASN:OD1	1:A:1658:HIS:NE2	2.35	0.58
1:A:2194:LYS:HD2	1:C:1054:GLN:HE21	1.68	0.58
1:B:599:LEU:HD21	1:B:636:ILE:HG12	1.86	0.58
1:D:1650:LEU:HB2	1:D:1690:THR:HG23	1.86	0.58
1:D:1654:ASN:OD1	1:D:1658:HIS:NE2	2.36	0.58
1:C:599:LEU:HD21	1:C:636:ILE:HG12	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1005:PHE:O	1:C:1013:ASN:ND2	2.35	0.58
1:D:657:PHE:O	1:D:661:THR:HB	2.03	0.58
1:D:777:LEU:HD22	1:D:784:PHE:HB2	1.85	0.58
1:A:599:LEU:HD21	1:A:636:ILE:HG12	1.86	0.58
1:E:1654:ASN:OD1	1:E:1658:HIS:NE2	2.35	0.58
1:A:2348:THR:HB	1:A:2518:ARG:HG2	1.86	0.58
1:D:1505:PHE:HB3	1:D:1517:LEU:HB2	1.84	0.58
1:E:2348:THR:HB	1:E:2518:ARG:HG2	1.86	0.58
1:A:777:LEU:HD22	1:A:784:PHE:HB2	1.85	0.57
1:B:889:LEU:HD22	1:B:900:PRO:HB3	1.84	0.57
1:B:2348:THR:HB	1:B:2518:ARG:HG2	1.86	0.57
1:C:2348:THR:HB	1:C:2518:ARG:HG2	1.86	0.57
1:D:1556:PHE:HB2	1:D:1570:ILE:HB	1.86	0.57
1:B:657:PHE:O	1:B:661:THR:HB	2.03	0.57
1:D:599:LEU:HD21	1:D:636:ILE:HG12	1.86	0.57
1:D:1323:ASN:OD1	1:D:1323:ASN:N	2.38	0.57
1:D:1725:SER:OG	1:D:1726:ALA:N	2.38	0.57
1:E:302:LYS:HG3	1:E:308:GLN:HE21	1.70	0.57
1:E:1645:TYR:HB2	1:E:1770:MET:HB2	1.87	0.57
1:A:1531:SER:HG	1:B:1766:HIS:HE2	1.51	0.57
1:C:777:LEU:HD22	1:C:784:PHE:HB2	1.85	0.57
1:C:937:SER:OG	1:C:952:ARG:NH1	2.37	0.57
1:D:1005:PHE:O	1:D:1013:ASN:ND2	2.35	0.57
1:A:59:GLN:OE1	1:A:1946:ARG:NH2	2.38	0.57
1:D:2348:THR:HB	1:D:2518:ARG:HG2	1.86	0.57
1:E:353:ASN:O	1:E:400:LYS:NZ	2.38	0.57
1:A:1323:ASN:OD1	1:A:1323:ASN:N	2.38	0.57
1:B:1645:TYR:HB2	1:B:1770:MET:HB2	1.87	0.57
1:C:302:LYS:HG3	1:C:308:GLN:HE21	1.70	0.57
1:E:937:SER:OG	1:E:952:ARG:NH1	2.37	0.57
1:A:353:ASN:O	1:A:400:LYS:NZ	2.38	0.57
1:B:353:ASN:O	1:B:400:LYS:NZ	2.38	0.57
1:C:1323:ASN:OD1	1:C:1323:ASN:N	2.38	0.57
1:C:1810:GLU:OE1	1:C:1813:ARG:NH1	2.38	0.57
1:D:353:ASN:O	1:D:400:LYS:NZ	2.38	0.57
1:D:937:SER:OG	1:D:952:ARG:NH1	2.36	0.57
1:E:1556:PHE:HB2	1:E:1570:ILE:HB	1.86	0.57
1:B:1810:GLU:OE1	1:B:1813:ARG:NH1	2.38	0.57
1:C:1650:LEU:HB2	1:C:1690:THR:HG23	1.86	0.57
1:D:1810:GLU:OE1	1:D:1813:ARG:NH1	2.38	0.57
1:C:1556:PHE:HB2	1:C:1570:ILE:HB	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1650:LEU:HB2	1:E:1690:THR:HG23	1.86	0.57
1:B:1650:LEU:HB2	1:B:1690:THR:HG23	1.86	0.57
1:E:1810:GLU:OE1	1:E:1813:ARG:NH1	2.38	0.57
1:A:1810:GLU:OE1	1:A:1813:ARG:NH1	2.38	0.56
1:B:59:GLN:OE1	1:B:1946:ARG:NH2	2.38	0.56
1:B:1556:PHE:HB2	1:B:1570:ILE:HB	1.86	0.56
1:B:1654:ASN:OD1	1:B:1658:HIS:NE2	2.36	0.56
1:D:22:LEU:HD23	1:D:25:ILE:HD12	1.87	0.56
1:A:1556:PHE:HB2	1:A:1570:ILE:HB	1.86	0.56
1:A:1725:SER:OG	1:A:1726:ALA:N	2.38	0.56
1:C:22:LEU:HD23	1:C:25:ILE:HD12	1.87	0.56
1:C:1645:TYR:HB2	1:C:1770:MET:HB2	1.87	0.56
1:E:599:LEU:HD21	1:E:636:ILE:HG12	1.86	0.56
1:B:608:ASN:OD1	1:B:608:ASN:N	2.39	0.56
1:C:726:GLN:OE1	1:C:749:ASN:ND2	2.37	0.56
1:D:719:TRP:HD1	1:D:778:VAL:HG22	1.70	0.56
1:E:1725:SER:OG	1:E:1726:ALA:N	2.38	0.56
1:A:302:LYS:HG3	1:A:308:GLN:HE21	1.69	0.56
1:B:302:LYS:HG3	1:B:308:GLN:HE21	1.69	0.56
1:A:719:TRP:HD1	1:A:778:VAL:HG22	1.70	0.56
1:A:1645:TYR:HB2	1:A:1770:MET:HB2	1.87	0.56
1:B:719:TRP:HD1	1:B:778:VAL:HG22	1.70	0.56
1:B:1323:ASN:N	1:B:1323:ASN:OD1	2.38	0.56
1:D:726:GLN:OE1	1:D:749:ASN:ND2	2.37	0.56
1:A:133:ASN:OD1	1:A:133:ASN:N	2.39	0.56
1:A:2390:ASN:ND2	1:A:2392:GLU:OE2	2.39	0.56
1:E:1323:ASN:N	1:E:1323:ASN:OD1	2.38	0.56
1:D:302:LYS:HG3	1:D:308:GLN:HE21	1.70	0.56
1:E:608:ASN:N	1:E:608:ASN:OD1	2.39	0.56
1:C:353:ASN:O	1:C:400:LYS:NZ	2.38	0.56
1:C:719:TRP:HD1	1:C:778:VAL:HG22	1.70	0.56
1:C:2390:ASN:ND2	1:C:2392:GLU:OE2	2.39	0.56
1:D:133:ASN:OD1	1:D:133:ASN:N	2.39	0.56
1:D:1645:TYR:HB2	1:D:1770:MET:HB2	1.87	0.56
1:D:496:SER:OG	1:D:497:VAL:N	2.39	0.56
1:A:496:SER:OG	1:A:497:VAL:N	2.39	0.55
1:C:59:GLN:OE1	1:C:1946:ARG:NH2	2.38	0.55
1:E:719:TRP:HD1	1:E:778:VAL:HG22	1.70	0.55
1:A:22:LEU:HD23	1:A:25:ILE:HD12	1.87	0.55
1:A:1057:LEU:O	1:A:1807:ASN:ND2	2.40	0.55
1:B:22:LEU:HD23	1:B:25:ILE:HD12	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:ASN:N	1:B:133:ASN:OD1	2.39	0.55
1:B:1327:ASN:ND2	1:B:1544:ASP:OD1	2.39	0.55
1:D:1057:LEU:O	1:D:1807:ASN:ND2	2.40	0.55
1:D:2478:TYR:O	1:E:2343:ARG:NH2	2.39	0.55
1:B:1057:LEU:O	1:B:1807:ASN:ND2	2.40	0.55
1:B:1607:ARG:NH2	1:B:1638:PRO:O	2.40	0.55
1:B:2390:ASN:ND2	1:B:2392:GLU:OE2	2.39	0.55
1:C:879:THR:HG23	1:C:882:GLY:H	1.72	0.55
1:D:735:ILE:O	1:D:739:ASN:ND2	2.39	0.55
1:D:879:THR:HG23	1:D:882:GLY:H	1.72	0.55
1:A:1607:ARG:NH2	1:A:1638:PRO:O	2.40	0.55
1:B:566:THR:HG21	1:C:842:VAL:HG23	1.88	0.55
1:C:1607:ARG:NH2	1:C:1638:PRO:O	2.40	0.55
1:D:608:ASN:OD1	1:D:608:ASN:N	2.39	0.55
1:E:22:LEU:HD23	1:E:25:ILE:HD12	1.87	0.55
1:B:703:ALA:HB2	1:C:2272:GLY:HA3	1.88	0.55
1:C:608:ASN:N	1:C:608:ASN:OD1	2.39	0.55
1:E:2390:ASN:ND2	1:E:2392:GLU:OE2	2.39	0.55
1:C:133:ASN:OD1	1:C:133:ASN:N	2.39	0.55
1:D:1607:ARG:NH2	1:D:1638:PRO:O	2.40	0.55
1:D:2390:ASN:ND2	1:D:2392:GLU:OE2	2.39	0.55
1:E:133:ASN:N	1:E:133:ASN:OD1	2.39	0.55
1:A:508:ILE:HG23	1:A:519:HIS:HD2	1.72	0.55
1:B:726:GLN:OE1	1:B:749:ASN:ND2	2.37	0.55
1:E:496:SER:OG	1:E:497:VAL:N	2.39	0.55
1:A:2408:ALA:O	1:A:2419:ARG:NH1	2.40	0.55
1:B:879:THR:HG23	1:B:882:GLY:H	1.72	0.55
1:B:2408:ALA:O	1:B:2419:ARG:NH1	2.40	0.54
1:C:1057:LEU:O	1:C:1807:ASN:ND2	2.40	0.54
1:E:1607:ARG:NH2	1:E:1638:PRO:O	2.40	0.54
1:E:2095:ASP:OD1	1:E:2233:ARG:NH1	2.41	0.54
1:A:726:GLN:OE1	1:A:749:ASN:ND2	2.37	0.54
1:A:1312:ASN:ND2	1:A:1335:GLU:OE2	2.39	0.54
1:A:2095:ASP:OD1	1:A:2233:ARG:NH1	2.41	0.54
1:C:496:SER:OG	1:C:497:VAL:N	2.39	0.54
1:D:2408:ALA:O	1:D:2419:ARG:NH1	2.40	0.54
1:C:2408:ALA:O	1:C:2419:ARG:NH1	2.40	0.54
1:D:59:GLN:OE1	1:D:1946:ARG:NH2	2.38	0.54
1:D:2400:LEU:HD11	1:D:2405:LEU:HD21	1.90	0.54
1:E:1327:ASN:ND2	1:E:1544:ASP:OD1	2.39	0.54
1:E:1813:ARG:NH2	1:E:1817:TYR:OH	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:496:SER:OG	1:B:497:VAL:N	2.39	0.54
1:E:879:THR:HG23	1:E:882:GLY:H	1.72	0.54
1:A:608:ASN:OD1	1:A:608:ASN:N	2.39	0.54
1:A:879:THR:HG23	1:A:882:GLY:H	1.72	0.54
1:D:1813:ARG:NH2	1:D:1817:TYR:OH	2.41	0.54
1:D:2095:ASP:OD1	1:D:2233:ARG:NH1	2.41	0.54
1:E:508:ILE:HG23	1:E:519:HIS:HD2	1.73	0.54
1:A:1607:ARG:NH1	1:A:1637:GLU:OE1	2.41	0.54
1:A:2034:ARG:NH1	1:A:2475:ASP:O	2.41	0.54
1:B:1607:ARG:NH1	1:B:1637:GLU:OE1	2.41	0.54
1:D:1607:ARG:NH1	1:D:1637:GLU:OE1	2.41	0.54
1:E:1057:LEU:O	1:E:1807:ASN:ND2	2.40	0.54
1:A:1327:ASN:ND2	1:A:1544:ASP:OD1	2.39	0.54
1:A:1813:ARG:NH2	1:A:1817:TYR:OH	2.41	0.54
1:B:1725:SER:OG	1:B:1726:ALA:N	2.38	0.54
1:C:270:ASP:N	1:C:270:ASP:OD1	2.41	0.54
1:C:2400:LEU:HD11	1:C:2405:LEU:HD21	1.90	0.54
1:E:270:ASP:N	1:E:270:ASP:OD1	2.41	0.54
1:E:706:GLN:O	1:E:765:ARG:NH2	2.41	0.54
1:E:735:ILE:O	1:E:739:ASN:ND2	2.39	0.54
1:E:2400:LEU:HD11	1:E:2405:LEU:HD21	1.90	0.54
1:C:2452:ARG:NH1	1:D:2339:GLU:O	2.32	0.54
1:D:572:TRP:O	1:D:576:ASN:ND2	2.41	0.54
1:E:2408:ALA:O	1:E:2419:ARG:NH1	2.40	0.54
1:B:706:GLN:O	1:B:765:ARG:NH2	2.41	0.54
1:C:1081:VAL:O	1:C:1597:GLN:NE2	2.41	0.54
1:C:2095:ASP:OD1	1:C:2233:ARG:NH1	2.41	0.54
1:D:687:SER:OG	1:D:688:LEU:N	2.41	0.54
1:D:706:GLN:O	1:D:765:ARG:NH2	2.41	0.54
1:E:726:GLN:OE1	1:E:749:ASN:ND2	2.37	0.54
1:A:488:TYR:O	1:A:492:HIS:HB2	2.09	0.53
1:A:2400:LEU:HD11	1:A:2405:LEU:HD21	1.90	0.53
1:A:2478:TYR:O	1:B:2343:ARG:NH2	2.41	0.53
1:B:508:ILE:HG23	1:B:519:HIS:HD2	1.72	0.53
1:B:2095:ASP:OD1	1:B:2233:ARG:NH1	2.41	0.53
1:C:1725:SER:OG	1:C:1726:ALA:N	2.38	0.53
1:D:488:TYR:O	1:D:492:HIS:HB2	2.09	0.53
1:E:572:TRP:O	1:E:576:ASN:ND2	2.41	0.53
1:A:735:ILE:O	1:A:739:ASN:ND2	2.39	0.53
1:C:1607:ARG:NH1	1:C:1637:GLU:OE1	2.41	0.53
1:D:2427:THR:HG22	1:D:2429:PRO:HD3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:59:GLN:OE1	1:E:1946:ARG:NH2	2.38	0.53
1:E:2034:ARG:NH1	1:E:2475:ASP:O	2.41	0.53
1:E:2427:THR:HG22	1:E:2429:PRO:HD3	1.91	0.53
1:A:1081:VAL:O	1:A:1597:GLN:NE2	2.41	0.53
1:C:508:ILE:HG23	1:C:519:HIS:HD2	1.72	0.53
1:C:1813:ARG:NH2	1:C:1817:TYR:OH	2.41	0.53
1:C:2251:GLN:NE2	1:D:2013:SER:OG	2.33	0.53
1:D:508:ILE:HG23	1:D:519:HIS:HD2	1.73	0.53
1:D:2034:ARG:NH1	1:D:2475:ASP:O	2.41	0.53
1:E:1607:ARG:NH1	1:E:1637:GLU:OE1	2.41	0.53
1:A:1639:GLN:NE2	1:A:1642:GLU:O	2.42	0.53
1:B:2034:ARG:NH1	1:B:2475:ASP:O	2.41	0.53
1:B:2400:LEU:HD11	1:B:2405:LEU:HD21	1.90	0.53
1:C:2034:ARG:NH1	1:C:2475:ASP:O	2.41	0.53
1:A:687:SER:OG	1:A:688:LEU:N	2.41	0.53
1:C:488:TYR:O	1:C:492:HIS:HB2	2.09	0.53
1:C:1725:SER:O	1:C:1741:ASN:ND2	2.42	0.53
1:B:1508:LYS:HG2	1:B:1513:ILE:HA	1.91	0.53
1:C:572:TRP:O	1:C:576:ASN:ND2	2.41	0.53
1:C:1639:GLN:NE2	1:C:1642:GLU:O	2.42	0.53
1:E:687:SER:OG	1:E:688:LEU:N	2.41	0.53
1:A:572:TRP:O	1:A:576:ASN:ND2	2.41	0.53
1:B:488:TYR:O	1:B:492:HIS:HB2	2.09	0.53
1:B:524:PHE:O	1:B:559:ARG:NH2	2.41	0.53
1:D:1725:SER:O	1:D:1741:ASN:ND2	2.42	0.53
1:C:687:SER:OG	1:C:688:LEU:N	2.41	0.53
1:E:524:PHE:O	1:E:559:ARG:NH2	2.42	0.53
1:E:1725:SER:O	1:E:1741:ASN:ND2	2.42	0.53
1:A:1725:SER:O	1:A:1741:ASN:ND2	2.42	0.53
1:B:1639:GLN:NE2	1:B:1642:GLU:O	2.42	0.53
1:B:1813:ARG:NH2	1:B:1817:TYR:OH	2.41	0.53
1:C:1327:ASN:ND2	1:C:1544:ASP:OD1	2.39	0.53
1:D:1327:ASN:ND2	1:D:1544:ASP:OD1	2.39	0.53
1:E:1639:GLN:NE2	1:E:1642:GLU:O	2.42	0.53
1:A:293:SER:O	1:A:311:ASN:ND2	2.43	0.52
1:A:524:PHE:O	1:A:559:ARG:NH2	2.41	0.52
1:B:580:ASN:OD1	1:B:580:ASN:N	2.42	0.52
1:B:2427:THR:HG22	1:B:2429:PRO:HD3	1.91	0.52
1:C:342:LEU:HA	1:C:362:LYS:H	1.75	0.52
1:D:270:ASP:OD1	1:D:270:ASP:N	2.41	0.52
1:D:524:PHE:O	1:D:559:ARG:NH2	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1639:GLN:NE2	1:D:1642:GLU:O	2.42	0.52
1:D:1801:ARG:NH1	1:D:1804:GLN:OE1	2.42	0.52
1:E:488:TYR:O	1:E:492:HIS:HB2	2.09	0.52
1:A:270:ASP:OD1	1:A:270:ASP:N	2.41	0.52
1:A:342:LEU:HA	1:A:362:LYS:H	1.74	0.52
1:A:1508:LYS:HG2	1:A:1513:ILE:HA	1.91	0.52
1:C:524:PHE:O	1:C:559:ARG:NH2	2.41	0.52
1:C:1508:LYS:HG2	1:C:1513:ILE:HA	1.91	0.52
1:E:1801:ARG:NH1	1:E:1804:GLN:OE1	2.42	0.52
1:A:2427:THR:HG22	1:A:2429:PRO:HD3	1.91	0.52
1:C:2453:GLY:H	1:D:2342:GLU:HB2	1.74	0.52
1:B:293:SER:O	1:B:311:ASN:ND2	2.43	0.52
1:B:687:SER:OG	1:B:688:LEU:N	2.41	0.52
1:C:706:GLN:O	1:C:765:ARG:NH2	2.41	0.52
1:D:580:ASN:OD1	1:D:580:ASN:N	2.43	0.52
1:D:1508:LYS:HG2	1:D:1513:ILE:HA	1.91	0.52
1:E:1312:ASN:ND2	1:E:1335:GLU:OE2	2.39	0.52
1:B:572:TRP:O	1:B:576:ASN:ND2	2.41	0.52
1:B:1801:ARG:NH1	1:B:1804:GLN:OE1	2.42	0.52
1:C:293:SER:O	1:C:311:ASN:ND2	2.43	0.52
1:E:2500:SER:HA	1:E:2504:LYS:HD2	1.92	0.52
1:A:372:ARG:HB2	1:A:415:TRP:HB2	1.92	0.52
1:A:780:LYS:NZ	1:A:823:GLU:OE1	2.43	0.52
1:A:1605:ARG:NH1	1:A:1640:LEU:O	2.43	0.52
1:B:707:MET:O	1:C:2268:ASN:ND2	2.42	0.52
1:C:792:GLN:HB2	1:C:797:THR:HG21	1.92	0.52
1:D:792:GLN:HB2	1:D:797:THR:HG21	1.92	0.52
1:E:179:THR:OG1	1:E:180:ASP:N	2.43	0.52
1:A:580:ASN:OD1	1:A:580:ASN:N	2.42	0.52
1:B:1605:ARG:NH1	1:B:1640:LEU:O	2.43	0.52
1:E:1508:LYS:HG2	1:E:1513:ILE:HA	1.91	0.52
1:B:1725:SER:O	1:B:1741:ASN:ND2	2.42	0.52
1:C:1592:MET:HB2	1:C:1596:THR:HG23	1.92	0.52
1:C:1801:ARG:NH1	1:C:1804:GLN:OE1	2.42	0.52
1:A:250:LEU:HD23	1:A:447:LYS:HB2	1.92	0.52
1:A:1801:ARG:NH1	1:A:1804:GLN:OE1	2.42	0.52
1:B:735:ILE:O	1:B:739:ASN:ND2	2.39	0.52
1:D:1278:THR:OG1	1:D:1279:ARG:N	2.43	0.52
1:E:293:SER:O	1:E:311:ASN:ND2	2.43	0.52
1:E:1605:ARG:NH1	1:E:1640:LEU:O	2.43	0.52
1:A:1167:ASN:ND2	1:A:1169:SER:OG	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1670:ASN:ND2	1:A:1675:SER:OG	2.43	0.52
1:B:792:GLN:HB2	1:B:797:THR:HG21	1.92	0.52
1:C:580:ASN:N	1:C:580:ASN:OD1	2.42	0.52
1:C:2427:THR:HG22	1:C:2429:PRO:HD3	1.91	0.52
1:E:250:LEU:HD23	1:E:447:LYS:HB2	1.92	0.52
1:E:527:PRO:O	1:E:559:ARG:NH1	2.43	0.52
1:E:1780:ASN:ND2	1:E:1845:SER:O	2.43	0.52
1:B:179:THR:OG1	1:B:180:ASP:N	2.43	0.51
1:C:1780:ASN:ND2	1:C:1845:SER:O	2.43	0.51
1:D:293:SER:O	1:D:311:ASN:ND2	2.43	0.51
1:D:690:ASP:OD1	1:D:721:ASN:ND2	2.44	0.51
1:D:780:LYS:NZ	1:D:823:GLU:OE1	2.43	0.51
1:E:580:ASN:N	1:E:580:ASN:OD1	2.43	0.51
1:A:690:ASP:OD1	1:A:721:ASN:ND2	2.44	0.51
1:A:2020:GLN:H	1:A:2316:THR:HG22	1.76	0.51
1:B:1278:THR:OG1	1:B:1279:ARG:N	2.43	0.51
1:C:1167:ASN:ND2	1:C:1169:SER:OG	2.43	0.51
1:D:179:THR:OG1	1:D:180:ASP:N	2.43	0.51
1:D:1670:ASN:ND2	1:D:1675:SER:OG	2.43	0.51
1:D:2500:SER:HA	1:D:2504:LYS:HD2	1.92	0.51
1:E:792:GLN:HB2	1:E:797:THR:HG21	1.92	0.51
1:B:1670:ASN:ND2	1:B:1675:SER:OG	2.43	0.51
1:C:2468:GLN:NE2	1:D:2346:GLU:OE1	2.43	0.51
1:D:1592:MET:HB2	1:D:1596:THR:HG23	1.92	0.51
1:D:1605:ARG:NH1	1:D:1640:LEU:O	2.43	0.51
1:D:1846:TRP:HE3	1:D:1847:ASN:HB2	1.75	0.51
1:A:179:THR:OG1	1:A:180:ASP:N	2.43	0.51
1:B:160:SER:HA	1:B:970:LYS:HA	1.92	0.51
1:C:1670:ASN:ND2	1:C:1675:SER:OG	2.43	0.51
1:D:1167:ASN:ND2	1:D:1169:SER:OG	2.43	0.51
1:B:342:LEU:HA	1:B:362:LYS:H	1.74	0.51
1:B:372:ARG:HB2	1:B:415:TRP:HB2	1.92	0.51
1:B:780:LYS:NZ	1:B:823:GLU:OE1	2.43	0.51
1:B:1167:ASN:ND2	1:B:1169:SER:OG	2.43	0.51
1:C:1278:THR:OG1	1:C:1279:ARG:N	2.43	0.51
1:C:1628:LEU:O	1:C:1836:ASN:ND2	2.44	0.51
1:D:1081:VAL:O	1:D:1597:GLN:NE2	2.41	0.51
1:E:372:ARG:HB2	1:E:415:TRP:HB2	1.92	0.51
1:E:1278:THR:OG1	1:E:1279:ARG:N	2.43	0.51
1:B:250:LEU:HD23	1:B:447:LYS:HB2	1.92	0.51
1:B:1081:VAL:O	1:B:1597:GLN:NE2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1628:LEU:O	1:E:1836:ASN:ND2	2.44	0.51
1:E:1670:ASN:ND2	1:E:1675:SER:OG	2.43	0.51
1:A:527:PRO:O	1:A:559:ARG:NH1	2.43	0.51
1:A:792:GLN:HB2	1:A:797:THR:HG21	1.92	0.51
1:A:1628:LEU:O	1:A:1836:ASN:ND2	2.44	0.51
1:A:2155:ASP:OD2	1:A:2169:ARG:NH2	2.44	0.51
1:B:1592:MET:HB2	1:B:1596:THR:HG23	1.92	0.51
1:C:179:THR:OG1	1:C:180:ASP:N	2.43	0.51
1:C:250:LEU:HD23	1:C:447:LYS:HB2	1.92	0.51
1:C:1605:ARG:NH1	1:C:1640:LEU:O	2.43	0.51
1:C:1800:GLN:HE21	1:C:1804:GLN:HE21	1.59	0.51
1:D:342:LEU:HA	1:D:362:LYS:H	1.74	0.51
1:D:372:ARG:HB2	1:D:415:TRP:HB2	1.92	0.51
1:D:1780:ASN:ND2	1:D:1845:SER:O	2.43	0.51
1:E:160:SER:HA	1:E:970:LYS:HA	1.92	0.51
1:E:342:LEU:HA	1:E:362:LYS:H	1.74	0.51
1:E:2020:GLN:H	1:E:2316:THR:HG22	1.76	0.51
1:B:270:ASP:OD1	1:B:270:ASP:N	2.41	0.51
1:B:1628:LEU:O	1:B:1836:ASN:ND2	2.44	0.51
1:B:1846:TRP:HE3	1:B:1847:ASN:HB2	1.75	0.51
1:C:735:ILE:O	1:C:739:ASN:ND2	2.39	0.51
1:D:160:SER:HA	1:D:970:LYS:HA	1.92	0.51
1:B:1780:ASN:ND2	1:B:1845:SER:O	2.43	0.51
1:C:527:PRO:O	1:C:559:ARG:NH1	2.43	0.51
1:D:2020:GLN:H	1:D:2316:THR:HG22	1.75	0.51
1:E:780:LYS:NZ	1:E:823:GLU:OE1	2.43	0.51
1:E:2155:ASP:OD2	1:E:2169:ARG:NH2	2.44	0.51
1:A:160:SER:HA	1:A:970:LYS:HA	1.92	0.51
1:A:706:GLN:O	1:A:765:ARG:NH2	2.41	0.51
1:A:1780:ASN:ND2	1:A:1845:SER:O	2.43	0.51
1:B:690:ASP:OD1	1:B:721:ASN:ND2	2.44	0.51
1:B:1086:HIS:NE2	1:B:1091:VAL:O	2.44	0.51
1:C:372:ARG:HB2	1:C:415:TRP:HB2	1.92	0.51
1:D:1800:GLN:HE21	1:D:1804:GLN:HE21	1.59	0.51
1:A:2500:SER:HA	1:A:2504:LYS:HD2	1.92	0.50
1:B:527:PRO:O	1:B:559:ARG:NH1	2.43	0.50
1:B:2020:GLN:H	1:B:2316:THR:HG22	1.75	0.50
1:C:1846:TRP:HE3	1:C:1847:ASN:HB2	1.75	0.50
1:E:1167:ASN:ND2	1:E:1169:SER:OG	2.43	0.50
1:A:1088:SER:OG	1:A:1089:ILE:N	2.45	0.50
1:B:1800:GLN:HE21	1:B:1804:GLN:HE21	1.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2155:ASP:OD2	1:B:2169:ARG:NH2	2.44	0.50
1:C:690:ASP:OD1	1:C:721:ASN:ND2	2.44	0.50
1:C:2020:GLN:H	1:C:2316:THR:HG22	1.76	0.50
1:D:250:LEU:HD23	1:D:447:LYS:HB2	1.92	0.50
1:D:527:PRO:O	1:D:559:ARG:NH1	2.43	0.50
1:D:1086:HIS:NE2	1:D:1091:VAL:O	2.44	0.50
1:E:1592:MET:HB2	1:E:1596:THR:HG23	1.92	0.50
1:A:1086:HIS:NE2	1:A:1091:VAL:O	2.44	0.50
1:B:2500:SER:HA	1:B:2504:LYS:HD2	1.92	0.50
1:C:160:SER:HA	1:C:970:LYS:HA	1.92	0.50
1:C:619:TYR:OH	1:C:634:GLN:NE2	2.45	0.50
1:C:2500:SER:HA	1:C:2504:LYS:HD2	1.92	0.50
1:D:2389:LEU:HD23	1:D:2396:LEU:HD11	1.94	0.50
1:A:1592:MET:HB2	1:A:1596:THR:HG23	1.92	0.50
1:E:690:ASP:OD1	1:E:721:ASN:ND2	2.44	0.50
1:A:1846:TRP:HE3	1:A:1847:ASN:HB2	1.75	0.50
1:D:1628:LEU:O	1:D:1836:ASN:ND2	2.44	0.50
1:C:1088:SER:OG	1:C:1089:ILE:N	2.45	0.50
1:A:1278:THR:OG1	1:A:1279:ARG:N	2.43	0.50
1:E:1086:HIS:NE2	1:E:1091:VAL:O	2.44	0.50
1:E:1846:TRP:HE3	1:E:1847:ASN:HB2	1.75	0.50
1:B:1088:SER:OG	1:B:1089:ILE:N	2.45	0.50
1:B:2422:LYS:H	1:B:2519:TYR:HA	1.77	0.50
1:C:1086:HIS:NE2	1:C:1091:VAL:O	2.44	0.50
1:C:2422:LYS:H	1:C:2519:TYR:HA	1.77	0.50
1:E:859:ASN:HB3	1:E:862:THR:HG22	1.94	0.50
1:A:506:SER:O	1:A:595:ARG:NH1	2.45	0.50
1:A:859:ASN:HB3	1:A:862:THR:HG22	1.94	0.50
1:A:2032:MET:HG2	1:A:2452:ARG:HG3	1.94	0.50
1:B:43:TRP:HA	1:B:46:THR:HB	1.94	0.50
1:D:1088:SER:OG	1:D:1089:ILE:N	2.45	0.50
1:E:2389:LEU:HD23	1:E:2396:LEU:HD11	1.94	0.50
1:A:2422:LYS:H	1:A:2519:TYR:HA	1.77	0.49
1:D:2032:MET:HG2	1:D:2452:ARG:HG3	1.94	0.49
1:E:1088:SER:OG	1:E:1089:ILE:N	2.45	0.49
1:B:859:ASN:HB3	1:B:862:THR:HG22	1.94	0.49
1:D:43:TRP:HA	1:D:46:THR:HB	1.95	0.49
1:C:43:TRP:HA	1:C:46:THR:HB	1.94	0.49
1:C:2149:MET:HB3	1:E:1106:PRO:HG2	1.95	0.49
1:D:859:ASN:HB3	1:D:862:THR:HG22	1.94	0.49
1:D:2155:ASP:OD2	1:D:2169:ARG:NH2	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:43:TRP:HA	1:E:46:THR:HB	1.94	0.49
1:A:43:TRP:HA	1:A:46:THR:HB	1.94	0.49
1:A:1630:MET:O	1:A:1634:ASN:ND2	2.45	0.49
1:B:21:LEU:H	1:B:24:ASN:HD22	1.61	0.49
1:B:1630:MET:O	1:B:1634:ASN:ND2	2.45	0.49
1:C:845:GLN:OE1	1:C:879:THR:OG1	2.31	0.49
1:C:1167:ASN:ND2	1:C:1172:GLY:O	2.46	0.49
1:C:1503:ILE:HG22	1:C:1558:ILE:HG12	1.95	0.49
1:D:619:TYR:OH	1:D:634:GLN:NE2	2.45	0.49
1:E:1800:GLN:HE21	1:E:1804:GLN:HE21	1.59	0.49
1:B:1167:ASN:ND2	1:B:1172:GLY:O	2.46	0.49
1:B:2349:ARG:NH1	1:B:2410:ASP:OD2	2.46	0.49
1:D:2422:LYS:H	1:D:2519:TYR:HA	1.77	0.49
1:E:1081:VAL:O	1:E:1597:GLN:NE2	2.41	0.49
1:A:1800:GLN:HE21	1:A:1804:GLN:HE21	1.59	0.49
1:A:2349:ARG:NH1	1:A:2410:ASP:OD2	2.46	0.49
1:B:1503:ILE:HG22	1:B:1558:ILE:HG12	1.95	0.49
1:D:482:LYS:NZ	1:D:504:CYS:O	2.40	0.49
1:D:1503:ILE:HG22	1:D:1558:ILE:HG12	1.95	0.49
1:D:2349:ARG:NH1	1:D:2410:ASP:OD2	2.46	0.49
1:E:1503:ILE:HG22	1:E:1558:ILE:HG12	1.95	0.49
1:A:21:LEU:H	1:A:24:ASN:HD22	1.61	0.49
1:A:317:LEU:HA	1:A:327:ALA:HA	1.95	0.49
1:B:459:PRO:HA	1:B:462:ILE:HG22	1.95	0.49
1:B:2032:MET:HG2	1:B:2452:ARG:HG3	1.94	0.49
1:C:1506:LEU:HB3	1:C:1555:GLU:HB2	1.95	0.49
1:C:2155:ASP:OD2	1:C:2169:ARG:NH2	2.44	0.49
1:D:1167:ASN:ND2	1:D:1172:GLY:O	2.46	0.49
1:E:21:LEU:H	1:E:24:ASN:HD22	1.61	0.49
1:E:72:ASN:ND2	1:E:74:GLN:OE1	2.43	0.49
1:E:1167:ASN:ND2	1:E:1172:GLY:O	2.46	0.49
1:E:2422:LYS:H	1:E:2519:TYR:HA	1.77	0.49
1:A:459:PRO:HA	1:A:462:ILE:HG22	1.95	0.49
1:C:506:SER:O	1:C:595:ARG:NH1	2.45	0.49
1:B:2469:PHE:CZ	1:C:2346:GLU:HB3	2.47	0.49
1:C:780:LYS:NZ	1:C:823:GLU:OE1	2.43	0.49
1:C:859:ASN:HB3	1:C:862:THR:HG22	1.94	0.49
1:C:1312:ASN:ND2	1:C:1335:GLU:OE2	2.39	0.49
1:C:2032:MET:HG2	1:C:2452:ARG:HG3	1.94	0.49
1:E:506:SER:O	1:E:595:ARG:NH1	2.45	0.49
1:B:845:GLN:OE1	1:B:879:THR:OG1	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2389:LEU:HD23	1:B:2396:LEU:HD11	1.94	0.48
1:D:2421:ILE:HD12	1:D:2484:LEU:HB3	1.95	0.48
1:A:1503:ILE:HG22	1:A:1558:ILE:HG12	1.95	0.48
1:A:2421:ILE:HD12	1:A:2484:LEU:HB3	1.95	0.48
1:B:1506:LEU:HB3	1:B:1555:GLU:HB2	1.95	0.48
1:C:21:LEU:H	1:C:24:ASN:HD22	1.61	0.48
1:D:506:SER:O	1:D:595:ARG:NH1	2.45	0.48
1:E:506:SER:OG	1:E:507:ASP:N	2.47	0.48
1:E:619:TYR:OH	1:E:634:GLN:NE2	2.45	0.48
1:E:1506:LEU:HB3	1:E:1555:GLU:HB2	1.95	0.48
1:A:1167:ASN:ND2	1:A:1172:GLY:O	2.46	0.48
1:B:2421:ILE:HD12	1:B:2484:LEU:HB3	1.95	0.48
1:C:1202:ASP:OD1	1:C:1202:ASP:N	2.37	0.48
1:C:2389:LEU:HD23	1:C:2396:LEU:HD11	1.94	0.48
1:D:375:ASN:OD1	1:D:375:ASN:N	2.47	0.48
1:D:422:SER:OG	1:D:423:ASP:N	2.46	0.48
1:E:1147:ARG:NH1	1:E:1216:MET:O	2.46	0.48
1:A:619:TYR:OH	1:A:634:GLN:NE2	2.45	0.48
1:A:2389:LEU:HD23	1:A:2396:LEU:HD11	1.94	0.48
1:D:21:LEU:H	1:D:24:ASN:HD22	1.61	0.48
1:E:317:LEU:HA	1:E:327:ALA:HA	1.95	0.48
1:B:506:SER:O	1:B:595:ARG:NH1	2.45	0.48
1:D:506:SER:OG	1:D:507:ASP:N	2.47	0.48
1:D:1147:ARG:NH1	1:D:1216:MET:O	2.46	0.48
1:A:952:ARG:HH21	1:A:964:GLN:HG2	1.79	0.48
1:A:1147:ARG:NH1	1:A:1216:MET:O	2.47	0.48
1:A:2343:ARG:NH2	1:E:2478:TYR:O	2.46	0.48
1:B:506:SER:OG	1:B:507:ASP:N	2.47	0.48
1:B:952:ARG:HH21	1:B:964:GLN:HG2	1.79	0.48
1:C:506:SER:OG	1:C:507:ASP:N	2.47	0.48
1:E:2349:ARG:NH1	1:E:2410:ASP:OD2	2.46	0.48
1:A:950:LYS:N	1:A:954:GLU:OE1	2.42	0.48
1:B:317:LEU:HA	1:B:327:ALA:HA	1.95	0.48
1:B:1147:ARG:NH1	1:B:1216:MET:O	2.47	0.48
1:C:1272:THR:O	1:C:1272:THR:OG1	2.30	0.48
1:C:459:PRO:HA	1:C:462:ILE:HG22	1.95	0.48
1:C:1630:MET:O	1:C:1634:ASN:ND2	2.45	0.48
1:E:2032:MET:HG2	1:E:2452:ARG:HG3	1.94	0.48
1:C:1147:ARG:NH1	1:C:1216:MET:O	2.47	0.48
1:D:72:ASN:ND2	1:D:74:GLN:OE1	2.43	0.48
1:E:2421:ILE:HD12	1:E:2484:LEU:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:ASN:OD1	1:A:375:ASN:N	2.47	0.48
1:A:1167:ASN:HB3	1:A:1174:ILE:H	1.78	0.48
1:B:72:ASN:ND2	1:B:74:GLN:OE1	2.43	0.48
1:C:952:ARG:HH21	1:C:964:GLN:HG2	1.79	0.48
1:D:459:PRO:HA	1:D:462:ILE:HG22	1.95	0.48
1:D:845:GLN:OE1	1:D:879:THR:OG1	2.30	0.48
1:E:1167:ASN:HB3	1:E:1174:ILE:H	1.78	0.48
1:E:459:PRO:HA	1:E:462:ILE:HG22	1.95	0.47
1:A:987:ARG:NH1	1:A:993:GLU:OE2	2.47	0.47
1:B:1278:THR:HG23	1:B:1281:GLU:H	1.80	0.47
1:C:2421:ILE:HD12	1:C:2484:LEU:HB3	1.95	0.47
1:E:2072:LEU:HA	1:E:2075:GLN:HE21	1.79	0.47
1:A:1709:ARG:NE	1:A:1720:ASP:OD2	2.40	0.47
1:B:987:ARG:NH1	1:B:993:GLU:OE2	2.48	0.47
1:C:2202:ARG:NH2	1:E:1805:GLU:OE1	2.47	0.47
1:C:2349:ARG:NH1	1:C:2410:ASP:OD2	2.46	0.47
1:D:495:ILE:HB	1:D:499:ASP:HB3	1.97	0.47
1:A:1278:THR:HG23	1:A:1281:GLU:H	1.80	0.47
1:A:1506:LEU:HB3	1:A:1555:GLU:HB2	1.95	0.47
1:C:1167:ASN:HB3	1:C:1174:ILE:H	1.78	0.47
1:D:952:ARG:HH21	1:D:964:GLN:HG2	1.79	0.47
1:E:987:ARG:NH1	1:E:993:GLU:OE2	2.47	0.47
1:E:1206:ASN:O	1:E:1210:LYS:NZ	2.37	0.47
1:B:495:ILE:HB	1:B:499:ASP:HB3	1.97	0.47
1:C:495:ILE:HB	1:C:499:ASP:HB3	1.97	0.47
1:C:606:THR:OG1	1:C:609:GLU:OE2	2.31	0.47
1:C:1278:THR:HG23	1:C:1281:GLU:H	1.80	0.47
1:D:317:LEU:HA	1:D:327:ALA:HA	1.95	0.47
1:D:1312:ASN:ND2	1:D:1335:GLU:OE2	2.39	0.47
1:E:952:ARG:HH21	1:E:964:GLN:HG2	1.79	0.47
1:A:373:LEU:O	1:A:381:ILE:N	2.47	0.47
1:B:422:SER:OG	1:B:423:ASP:N	2.47	0.47
1:B:619:TYR:OH	1:B:634:GLN:NE2	2.45	0.47
1:B:1727:PHE:H	1:B:1741:ASN:HD22	1.63	0.47
1:C:2072:LEU:HA	1:C:2075:GLN:HE21	1.80	0.47
1:D:987:ARG:NH1	1:D:993:GLU:OE2	2.47	0.47
1:A:130:HIS:HD1	1:A:984:TYR:HH	1.60	0.47
1:A:506:SER:OG	1:A:507:ASP:N	2.47	0.47
1:B:42:THR:O	1:B:42:THR:OG1	2.33	0.47
1:B:2072:LEU:HA	1:B:2075:GLN:HE21	1.79	0.47
1:B:2127:GLU:OE1	1:B:2204:ARG:NH2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:317:LEU:HA	1:C:327:ALA:HA	1.95	0.47
1:C:2127:GLU:OE1	1:C:2204:ARG:NH2	2.48	0.47
1:C:2298:TYR:OH	1:C:2482:GLU:O	2.33	0.47
1:D:1272:THR:O	1:D:1272:THR:OG1	2.30	0.47
1:D:1506:LEU:HB3	1:D:1555:GLU:HB2	1.95	0.47
1:E:495:ILE:HB	1:E:499:ASP:HB3	1.97	0.47
1:E:562:ARG:NH1	1:E:601:ASP:OD2	2.48	0.47
1:A:42:THR:O	1:A:42:THR:OG1	2.33	0.47
1:C:375:ASN:OD1	1:C:375:ASN:N	2.47	0.47
1:A:462:ILE:HA	1:A:465:VAL:HG22	1.97	0.47
1:A:495:ILE:HB	1:A:499:ASP:HB3	1.97	0.47
1:A:1727:PHE:H	1:A:1741:ASN:HD22	1.63	0.47
1:A:2127:GLU:OE1	1:A:2204:ARG:NH2	2.48	0.47
1:B:373:LEU:O	1:B:381:ILE:N	2.47	0.47
1:C:1727:PHE:H	1:C:1741:ASN:HD22	1.63	0.47
1:E:1596:THR:OG1	1:E:1597:GLN:N	2.48	0.47
1:A:99:ARG:NH1	1:A:1964:PHE:O	2.47	0.47
1:A:562:ARG:NH1	1:A:601:ASP:OD2	2.48	0.47
1:A:1596:THR:OG1	1:A:1597:GLN:N	2.48	0.47
1:A:2049:LEU:HD11	1:A:2282:TYR:HA	1.97	0.47
1:B:462:ILE:HA	1:B:465:VAL:HG22	1.97	0.47
1:B:1956:THR:OG1	1:B:1957:ALA:N	2.48	0.47
1:C:987:ARG:NH1	1:C:993:GLU:OE2	2.47	0.47
1:C:2299:GLU:O	1:C:2420:ARG:NH1	2.48	0.47
1:D:606:THR:OG1	1:D:609:GLU:OE2	2.31	0.47
1:D:2072:LEU:HA	1:D:2075:GLN:HE21	1.79	0.47
1:E:1956:THR:OG1	1:E:1957:ALA:N	2.48	0.47
1:A:2409:THR:O	1:A:2409:THR:OG1	2.33	0.46
1:B:1167:ASN:HB3	1:B:1174:ILE:H	1.78	0.46
1:C:770:SER:HB3	1:D:2016:ILE:HG13	1.97	0.46
1:D:1167:ASN:HB3	1:D:1174:ILE:H	1.79	0.46
1:D:2049:LEU:HD11	1:D:2282:TYR:HA	1.97	0.46
1:D:2299:GLU:O	1:D:2420:ARG:NH1	2.48	0.46
1:A:2072:LEU:HA	1:A:2075:GLN:HE21	1.79	0.46
1:B:968:GLN:HB3	1:C:1989:ASN:HD22	1.80	0.46
1:B:1312:ASN:ND2	1:B:1335:GLU:OE2	2.39	0.46
1:C:562:ARG:NH1	1:C:601:ASP:OD2	2.48	0.46
1:E:1278:THR:HG23	1:E:1281:GLU:H	1.80	0.46
1:A:2251:GLN:NE2	1:B:2013:SER:OG	2.41	0.46
1:C:373:LEU:O	1:C:381:ILE:N	2.47	0.46
1:C:703:ALA:HB2	1:D:2272:GLY:HA3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1038:ARG:NH2	1:D:1789:GLU:OE2	2.49	0.46
1:D:2025:LEU:HD13	1:D:2310:PRO:HA	1.97	0.46
1:E:296:VAL:HG13	1:E:315:ILE:HD11	1.98	0.46
1:E:375:ASN:OD1	1:E:375:ASN:N	2.47	0.46
1:E:1038:ARG:NH2	1:E:1789:GLU:OE2	2.49	0.46
1:A:2025:LEU:HD13	1:A:2310:PRO:HA	1.97	0.46
1:B:562:ARG:NH1	1:B:601:ASP:OD2	2.48	0.46
1:D:950:LYS:N	1:D:954:GLU:OE1	2.42	0.46
1:D:1956:THR:OG1	1:D:1957:ALA:N	2.48	0.46
1:B:1058:ASN:OD1	1:B:1058:ASN:N	2.49	0.46
1:B:1789:GLU:HA	1:B:1793:TYR:HB2	1.98	0.46
1:B:2049:LEU:HD11	1:B:2282:TYR:HA	1.97	0.46
1:C:470:TYR:OH	1:C:478:ASN:ND2	2.49	0.46
1:C:1596:THR:OG1	1:C:1597:GLN:N	2.48	0.46
1:E:422:SER:OG	1:E:423:ASP:N	2.46	0.46
1:E:845:GLN:OE1	1:E:879:THR:OG1	2.30	0.46
1:E:2299:GLU:O	1:E:2420:ARG:NH1	2.48	0.46
1:A:296:VAL:HG13	1:A:315:ILE:HD11	1.98	0.46
1:B:296:VAL:HG13	1:B:315:ILE:HD11	1.98	0.46
1:C:1239:SER:OG	1:C:1242:SER:OG	2.33	0.46
1:D:1596:THR:OG1	1:D:1597:GLN:N	2.48	0.46
1:D:1630:MET:O	1:D:1634:ASN:ND2	2.45	0.46
1:A:470:TYR:OH	1:A:478:ASN:ND2	2.49	0.46
1:B:1142:TRP:HH2	1:B:1214:ILE:HD12	1.81	0.46
1:B:2025:LEU:HD13	1:B:2310:PRO:HA	1.97	0.46
1:D:296:VAL:HG13	1:D:315:ILE:HD11	1.98	0.46
1:D:1278:THR:HG23	1:D:1281:GLU:H	1.79	0.46
1:E:1554:SER:OG	1:E:1572:SER:O	2.32	0.46
1:B:950:LYS:N	1:B:954:GLU:OE1	2.42	0.46
1:B:1554:SER:OG	1:B:1572:SER:O	2.32	0.46
1:C:841:GLN:HA	1:C:844:THR:HG22	1.98	0.46
1:D:562:ARG:NH1	1:D:601:ASP:OD2	2.48	0.46
1:D:2127:GLU:OE1	1:D:2204:ARG:NH2	2.48	0.46
1:D:2298:TYR:OH	1:D:2482:GLU:O	2.33	0.46
1:A:2299:GLU:O	1:A:2420:ARG:NH1	2.48	0.46
1:C:462:ILE:HA	1:C:465:VAL:HG22	1.97	0.46
1:D:42:THR:O	1:D:42:THR:OG1	2.33	0.46
1:E:42:THR:O	1:E:42:THR:OG1	2.33	0.46
1:E:462:ILE:HA	1:E:465:VAL:HG22	1.97	0.46
1:E:950:LYS:N	1:E:954:GLU:OE1	2.42	0.46
1:A:1789:GLU:HA	1:A:1793:TYR:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:841:GLN:HA	1:B:844:THR:HG22	1.98	0.46
1:B:1596:THR:OG1	1:B:1597:GLN:N	2.48	0.46
1:B:2299:GLU:O	1:B:2420:ARG:NH1	2.48	0.46
1:C:487:GLN:HE21	1:C:487:GLN:HB3	1.55	0.46
1:C:1038:ARG:NH2	1:C:1789:GLU:OE2	2.49	0.46
1:C:1789:GLU:HA	1:C:1793:TYR:HB2	1.97	0.46
1:D:462:ILE:HA	1:D:465:VAL:HG22	1.97	0.46
1:D:470:TYR:OH	1:D:478:ASN:ND2	2.49	0.46
1:D:841:GLN:HA	1:D:844:THR:HG22	1.98	0.46
1:D:1142:TRP:HH2	1:D:1214:ILE:HD12	1.81	0.46
1:A:1142:TRP:HH2	1:A:1214:ILE:HD12	1.81	0.45
1:B:2298:TYR:OH	1:B:2482:GLU:O	2.33	0.45
1:B:2369:ASP:OD1	1:B:2369:ASP:N	2.50	0.45
1:A:1956:THR:OG1	1:A:1957:ALA:N	2.48	0.45
1:B:375:ASN:OD1	1:B:375:ASN:N	2.47	0.45
1:B:2174:PHE:HB2	1:C:2151:ALA:HB2	1.97	0.45
1:C:422:SER:OG	1:C:423:ASP:N	2.46	0.45
1:C:788:THR:HG22	1:C:790:ALA:H	1.81	0.45
1:C:2049:LEU:HD11	1:C:2282:TYR:HA	1.97	0.45
1:C:2052:PHE:CE1	1:D:2324:GLU:HG3	2.51	0.45
1:D:1080:GLN:NE2	1:D:1101:TYR:OH	2.50	0.45
1:A:788:THR:HG22	1:A:790:ALA:H	1.82	0.45
1:B:568:LEU:HD11	1:B:593:LEU:HD21	1.98	0.45
1:C:1956:THR:OG1	1:C:1957:ALA:N	2.48	0.45
1:A:29:SER:HB3	1:A:1003:ARG:HG2	1.99	0.45
1:A:568:LEU:HD11	1:A:593:LEU:HD21	1.98	0.45
1:B:29:SER:HB3	1:B:1003:ARG:HG2	1.99	0.45
1:B:1080:GLN:NE2	1:B:1101:TYR:OH	2.50	0.45
1:B:1118:LYS:HB2	1:B:1128:ALA:HB2	1.98	0.45
1:D:1058:ASN:OD1	1:D:1058:ASN:N	2.49	0.45
1:E:470:TYR:OH	1:E:478:ASN:ND2	2.49	0.45
1:E:841:GLN:HA	1:E:844:THR:HG22	1.98	0.45
1:A:418:LYS:HE2	1:A:420:ASN:HB3	1.98	0.45
1:A:2298:TYR:OH	1:A:2482:GLU:O	2.33	0.45
1:A:2397:GLN:HA	1:A:2495:SER:HA	1.99	0.45
1:C:418:LYS:HE2	1:C:420:ASN:HB3	1.98	0.45
1:C:1142:TRP:HH2	1:C:1214:ILE:HD12	1.81	0.45
1:C:2025:LEU:HD13	1:C:2310:PRO:HA	1.97	0.45
1:E:29:SER:HB3	1:E:1003:ARG:HG2	1.99	0.45
1:A:841:GLN:HA	1:A:844:THR:HG22	1.98	0.45
1:A:1038:ARG:NH2	1:A:1789:GLU:OE2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1232:HIS:ND1	1:B:1233:GLU:O	2.41	0.45
1:C:296:VAL:HG13	1:C:315:ILE:HD11	1.98	0.45
1:D:2369:ASP:OD1	1:D:2369:ASP:N	2.50	0.45
1:D:2437:ASP:OD2	1:E:2350:THR:N	2.45	0.45
1:E:513:THR:OG1	1:E:516:GLN:NE2	2.50	0.45
1:E:1727:PHE:H	1:E:1741:ASN:HD22	1.63	0.45
1:A:513:THR:OG1	1:A:516:GLN:NE2	2.50	0.45
1:A:2034:ARG:NH1	1:A:2477:LYS:O	2.50	0.45
1:B:788:THR:HG22	1:B:790:ALA:H	1.81	0.45
1:C:568:LEU:HD11	1:C:593:LEU:HD21	1.98	0.45
1:C:1801:ARG:HD2	1:C:1801:ARG:HA	1.73	0.45
1:D:418:LYS:HE2	1:D:420:ASN:HB3	1.98	0.45
1:D:788:THR:HG22	1:D:790:ALA:H	1.81	0.45
1:D:1118:LYS:HB2	1:D:1128:ALA:HB2	1.98	0.45
1:D:2034:ARG:NH1	1:D:2477:LYS:O	2.50	0.45
1:E:1657:GLU:OE2	1:E:1719:TYR:OH	2.35	0.45
1:E:2049:LEU:HD11	1:E:2282:TYR:HA	1.97	0.45
1:E:2127:GLU:OE1	1:E:2204:ARG:NH2	2.48	0.45
1:E:2397:GLN:HA	1:E:2495:SER:HA	1.99	0.45
1:B:99:ARG:NH1	1:B:1964:PHE:O	2.48	0.45
1:B:470:TYR:OH	1:B:478:ASN:ND2	2.49	0.45
1:B:513:THR:OG1	1:B:516:GLN:NE2	2.50	0.45
1:B:1038:ARG:NH2	1:B:1789:GLU:OE2	2.49	0.45
1:B:1657:GLU:OE2	1:B:1719:TYR:OH	2.35	0.45
1:C:42:THR:O	1:C:42:THR:OG1	2.33	0.45
1:D:263:MET:HA	1:D:443:LEU:HD21	1.99	0.45
1:D:513:THR:OG1	1:D:516:GLN:NE2	2.50	0.45
1:D:1727:PHE:H	1:D:1741:ASN:HD22	1.63	0.45
1:E:1058:ASN:OD1	1:E:1058:ASN:N	2.49	0.45
1:E:1142:TRP:HH2	1:E:1214:ILE:HD12	1.81	0.45
1:E:1893:ASP:OD1	1:E:1893:ASP:N	2.50	0.45
1:E:2025:LEU:HD13	1:E:2310:PRO:HA	1.97	0.45
1:E:2298:TYR:OH	1:E:2482:GLU:O	2.33	0.45
1:E:2369:ASP:OD1	1:E:2369:ASP:N	2.50	0.45
1:A:498:SER:HA	1:A:501:LEU:HD12	1.99	0.45
1:A:1042:THR:OG1	1:A:1789:GLU:OE1	2.31	0.45
1:A:1054:GLN:HE21	1:D:2194:LYS:HD2	1.82	0.45
1:B:1700:LYS:HE3	1:B:1700:LYS:HB3	1.90	0.45
1:B:2034:ARG:NH1	1:B:2477:LYS:O	2.50	0.45
1:B:2397:GLN:HA	1:B:2495:SER:HA	1.99	0.45
1:C:29:SER:HB3	1:C:1003:ARG:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:498:SER:HA	1:C:501:LEU:HD12	1.99	0.45
1:D:568:LEU:HD11	1:D:593:LEU:HD21	1.98	0.45
1:C:513:THR:OG1	1:C:516:GLN:NE2	2.50	0.45
1:C:1118:LYS:HB2	1:C:1128:ALA:HB2	1.98	0.45
1:D:1010:GLU:OE2	1:E:1812:THR:OG1	2.30	0.45
1:D:1789:GLU:HA	1:D:1793:TYR:HB2	1.98	0.45
1:E:263:MET:HA	1:E:443:LEU:HD21	1.99	0.45
1:E:1118:LYS:HB2	1:E:1128:ALA:HB2	1.98	0.45
1:A:413:ARG:HG3	1:A:428:ASN:HB3	1.99	0.44
1:B:606:THR:OG1	1:B:609:GLU:OE2	2.31	0.44
1:B:772:ASN:ND2	1:C:2017:THR:O	2.50	0.44
1:C:1080:GLN:NE2	1:C:1101:TYR:OH	2.50	0.44
1:D:373:LEU:O	1:D:381:ILE:N	2.47	0.44
1:E:568:LEU:HD11	1:E:593:LEU:HD21	1.98	0.44
1:E:1080:GLN:NE2	1:E:1101:TYR:OH	2.50	0.44
1:E:1630:MET:O	1:E:1634:ASN:ND2	2.45	0.44
1:A:1202:ASP:OD1	1:A:1202:ASP:N	2.37	0.44
1:C:1893:ASP:OD1	1:C:1893:ASP:N	2.50	0.44
1:D:29:SER:HB3	1:D:1003:ARG:HG2	1.99	0.44
1:D:1893:ASP:N	1:D:1893:ASP:OD1	2.50	0.44
1:E:78:ILE:HD13	1:E:81:LEU:HD22	2.00	0.44
1:E:418:LYS:HE2	1:E:420:ASN:HB3	1.98	0.44
1:E:2134:TYR:HB3	1:E:2194:LYS:HB2	1.99	0.44
1:A:845:GLN:OE1	1:A:879:THR:OG1	2.31	0.44
1:A:1554:SER:OG	1:A:1572:SER:O	2.32	0.44
1:B:413:ARG:HG3	1:B:428:ASN:HB3	1.99	0.44
1:B:1239:SER:OG	1:B:1242:SER:OG	2.33	0.44
1:D:413:ARG:HG3	1:D:428:ASN:HB3	1.99	0.44
1:D:2397:GLN:HA	1:D:2495:SER:HA	1.99	0.44
1:E:413:ARG:HG3	1:E:428:ASN:HB3	2.00	0.44
1:E:788:THR:HG22	1:E:790:ALA:H	1.82	0.44
1:E:1789:GLU:HA	1:E:1793:TYR:HB2	1.97	0.44
1:A:1080:GLN:NE2	1:A:1101:TYR:OH	2.50	0.44
1:A:1893:ASP:N	1:A:1893:ASP:OD1	2.50	0.44
1:B:418:LYS:HE2	1:B:420:ASN:HB3	1.98	0.44
1:B:2171:GLY:N	1:C:2155:ASP:OD1	2.43	0.44
1:C:2059:ILE:HD13	1:C:2059:ILE:HA	1.84	0.44
1:D:498:SER:HA	1:D:501:LEU:HD12	1.99	0.44
1:E:1709:ARG:NE	1:E:1720:ASP:OD2	2.40	0.44
1:E:2034:ARG:NH1	1:E:2477:LYS:O	2.50	0.44
1:A:78:ILE:HD13	1:A:81:LEU:HD22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1058:ASN:N	1:A:1058:ASN:OD1	2.49	0.44
1:A:1118:LYS:HB2	1:A:1128:ALA:HB2	1.98	0.44
1:A:2369:ASP:N	1:A:2369:ASP:OD1	2.50	0.44
1:C:78:ILE:HD13	1:C:81:LEU:HD22	2.00	0.44
1:D:1801:ARG:HD2	1:D:1801:ARG:HA	1.73	0.44
1:A:200:HIS:HB3	1:A:203:TYR:HB3	1.99	0.44
1:A:1799:PHE:HE2	1:A:1874:LYS:HB3	1.83	0.44
1:C:2369:ASP:N	1:C:2369:ASP:OD1	2.50	0.44
1:E:1336:ILE:HD11	1:E:1503:ILE:HG21	2.00	0.44
1:E:1799:PHE:HE2	1:E:1874:LYS:HB3	1.83	0.44
1:A:451:LEU:HD22	1:A:462:ILE:HD12	2.00	0.44
1:C:72:ASN:ND2	1:C:74:GLN:OE1	2.43	0.44
1:C:263:MET:HA	1:C:443:LEU:HD21	1.99	0.44
1:A:1906:LEU:HD23	1:A:1906:LEU:HA	1.86	0.44
1:C:1058:ASN:OD1	1:C:1058:ASN:N	2.49	0.44
1:C:1293:LEU:HD23	1:C:1293:LEU:HA	1.88	0.44
1:C:2397:GLN:HA	1:C:2495:SER:HA	1.99	0.44
1:D:1799:PHE:HE2	1:D:1874:LYS:HB3	1.83	0.44
1:E:1293:LEU:HD23	1:E:1293:LEU:HA	1.87	0.44
1:A:263:MET:HA	1:A:443:LEU:HD21	1.99	0.44
1:A:606:THR:OG1	1:A:609:GLU:OE2	2.31	0.44
1:A:1002:THR:O	1:A:1002:THR:OG1	2.31	0.44
1:A:1531:SER:OG	1:B:1766:HIS:NE2	2.40	0.44
1:B:78:ILE:HD13	1:B:81:LEU:HD22	2.00	0.44
1:B:200:HIS:HB3	1:B:203:TYR:HB3	2.00	0.44
1:C:950:LYS:N	1:C:954:GLU:OE1	2.42	0.44
1:D:200:HIS:HB3	1:D:203:TYR:HB3	1.99	0.44
1:A:422:SER:OG	1:A:423:ASP:N	2.46	0.43
1:A:1657:GLU:OE2	1:A:1719:TYR:OH	2.35	0.43
1:B:2134:TYR:HB3	1:B:2194:LYS:HB2	1.99	0.43
1:B:2194:LYS:HD2	1:D:1054:GLN:HE21	1.83	0.43
1:C:2034:ARG:NH1	1:C:2477:LYS:O	2.50	0.43
1:A:597:ARG:NE	1:A:601:ASP:OD2	2.51	0.43
1:B:263:MET:HA	1:B:443:LEU:HD21	1.99	0.43
1:C:141:ARG:NH1	1:C:958:TYR:O	2.51	0.43
1:C:2478:TYR:O	1:D:2343:ARG:NH2	2.50	0.43
1:D:597:ARG:NE	1:D:601:ASP:OD2	2.51	0.43
1:E:729:THR:OG1	1:E:731:ASP:O	2.35	0.43
1:A:401:LEU:HD23	1:A:401:LEU:HA	1.84	0.43
1:B:498:SER:HA	1:B:501:LEU:HD12	1.99	0.43
1:C:413:ARG:HG3	1:C:428:ASN:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1709:ARG:NE	1:C:1720:ASP:OD2	2.40	0.43
1:C:2348:THR:HA	1:C:2518:ARG:HA	2.01	0.43
1:D:1709:ARG:NE	1:D:1720:ASP:OD2	2.40	0.43
1:D:2059:ILE:HD13	1:D:2059:ILE:HA	1.84	0.43
1:D:2345:LEU:HD23	1:D:2345:LEU:HA	1.84	0.43
1:E:141:ARG:NH1	1:E:958:TYR:O	2.51	0.43
1:E:498:SER:HA	1:E:501:LEU:HD12	1.99	0.43
1:A:2013:SER:OG	1:E:2251:GLN:NE2	2.43	0.43
1:B:1336:ILE:HD11	1:B:1503:ILE:HG21	2.00	0.43
1:B:1893:ASP:OD1	1:B:1893:ASP:N	2.50	0.43
1:D:1336:ILE:HD11	1:D:1503:ILE:HG21	2.00	0.43
1:D:2251:GLN:NE2	1:E:2013:SER:OG	2.40	0.43
1:E:451:LEU:HD22	1:E:462:ILE:HD12	2.00	0.43
1:A:2134:TYR:HB3	1:A:2194:LYS:HB2	1.99	0.43
1:B:1799:PHE:HE2	1:B:1874:LYS:HB3	1.83	0.43
1:C:200:HIS:HB3	1:C:203:TYR:HB3	2.00	0.43
1:C:597:ARG:NE	1:C:601:ASP:OD2	2.51	0.43
1:C:1336:ILE:HD11	1:C:1503:ILE:HG21	2.00	0.43
1:C:1531:SER:OG	1:D:1766:HIS:NE2	2.48	0.43
1:C:2134:TYR:HB3	1:C:2194:LYS:HB2	1.99	0.43
1:E:99:ARG:NH1	1:E:1964:PHE:O	2.48	0.43
1:E:285:TYR:OH	1:E:446:ASN:OD1	2.37	0.43
1:A:1336:ILE:HD11	1:A:1503:ILE:HG21	2.00	0.43
1:A:1863:ASP:HA	1:A:1864:PRO:HD3	1.83	0.43
1:B:141:ARG:NH1	1:B:958:TYR:O	2.51	0.43
1:B:597:ARG:NE	1:B:601:ASP:OD2	2.51	0.43
1:B:2348:THR:HA	1:B:2518:ARG:HA	2.01	0.43
1:C:138:LEU:HD23	1:C:138:LEU:HA	1.90	0.43
1:D:78:ILE:HD13	1:D:81:LEU:HD22	2.00	0.43
1:D:141:ARG:NH1	1:D:958:TYR:O	2.51	0.43
1:E:203:TYR:OH	1:E:237:ALA:O	2.30	0.43
1:E:1002:THR:O	1:E:1002:THR:OG1	2.31	0.43
1:E:1923:GLU:H	1:E:1923:GLU:HG3	1.65	0.43
1:E:2059:ILE:HD13	1:E:2059:ILE:HA	1.84	0.43
1:E:2348:THR:HA	1:E:2518:ARG:HA	2.01	0.43
1:B:1056:GLN:HB3	1:E:2128:LYS:HE3	2.00	0.43
1:B:2128:LYS:HE3	1:D:1056:GLN:HB3	2.01	0.43
1:B:2345:LEU:HD23	1:B:2345:LEU:HA	1.84	0.43
1:C:1799:PHE:HE2	1:C:1874:LYS:HB3	1.83	0.43
1:D:1657:GLU:OE2	1:D:1719:TYR:OH	2.35	0.43
1:E:597:ARG:NE	1:E:601:ASP:OD2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:ASN:ND2	1:A:74:GLN:OE1	2.43	0.43
1:A:1991:THR:OG1	1:A:1995:GLN:O	2.34	0.43
1:B:1801:ARG:HD2	1:B:1801:ARG:HA	1.73	0.43
1:C:272:VAL:HG12	1:C:442:LEU:HD12	2.01	0.43
1:C:1326:ILE:HD12	1:C:1326:ILE:HA	1.88	0.43
1:D:723:ILE:HD13	1:D:723:ILE:HA	1.87	0.43
1:D:2134:TYR:HB3	1:D:2194:LYS:HB2	1.99	0.43
1:E:1654:ASN:H	1:E:1658:HIS:CD2	2.37	0.43
1:A:335:LYS:HB3	1:A:336:ASP:H	1.74	0.43
1:A:1056:GLN:HB3	1:D:2128:LYS:HE3	2.00	0.43
1:A:2034:ARG:NH2	1:A:2482:GLU:OE2	2.52	0.43
1:A:2258:GLN:HB3	1:B:2015:ALA:HB2	2.00	0.43
1:B:982:GLN:NE2	1:B:1014:ARG:O	2.52	0.43
1:B:1204:ILE:O	1:B:1208:ILE:HB	2.19	0.43
1:C:99:ARG:NH1	1:C:1964:PHE:O	2.47	0.43
1:E:2101:LEU:HD12	1:E:2101:LEU:HA	1.92	0.43
1:A:1884:ASP:OD1	1:A:1902:TYR:OH	2.37	0.43
1:B:691:ASP:OD1	1:B:691:ASP:N	2.52	0.43
1:B:2101:LEU:HD21	1:B:2225:GLN:HB3	2.01	0.43
1:C:401:LEU:HD23	1:C:401:LEU:HA	1.84	0.43
1:C:2101:LEU:HD21	1:C:2225:GLN:HB3	2.01	0.43
1:C:2270:LEU:HD12	1:C:2270:LEU:HA	1.90	0.43
1:D:203:TYR:OH	1:D:237:ALA:O	2.30	0.43
1:D:982:GLN:NE2	1:D:1014:ARG:O	2.52	0.43
1:E:200:HIS:HB3	1:E:203:TYR:HB3	2.00	0.43
1:E:1204:ILE:O	1:E:1208:ILE:HB	2.19	0.43
1:E:1232:HIS:ND1	1:E:1233:GLU:O	2.41	0.43
1:A:141:ARG:NH1	1:A:958:TYR:O	2.51	0.42
1:B:451:LEU:HD22	1:B:462:ILE:HD12	2.00	0.42
1:B:1054:GLN:HE21	1:E:2194:LYS:HD2	1.84	0.42
1:C:982:GLN:NE2	1:C:1014:ARG:O	2.52	0.42
1:C:1204:ILE:O	1:C:1208:ILE:HB	2.19	0.42
1:E:606:THR:OG1	1:E:609:GLU:OE2	2.31	0.42
1:E:2034:ARG:NH2	1:E:2482:GLU:OE2	2.52	0.42
1:B:266:ASN:HD22	1:B:443:LEU:HD22	1.84	0.42
1:C:266:ASN:HD22	1:C:443:LEU:HD22	1.84	0.42
1:C:709:SER:O	1:C:712:THR:OG1	2.31	0.42
1:D:451:LEU:HD22	1:D:462:ILE:HD12	2.00	0.42
1:E:250:LEU:HD22	1:E:451:LEU:HD12	2.02	0.42
1:E:1239:SER:HG	1:E:1242:SER:HG	1.56	0.42
1:A:761:SER:OG	1:A:765:ARG:NH2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1654:ASN:H	1:A:1658:HIS:CD2	2.37	0.42
1:A:2101:LEU:HD21	1:A:2225:GLN:HB3	2.01	0.42
1:A:2178:ALA:HB2	1:B:2147:LEU:HB3	2.02	0.42
1:B:761:SER:OG	1:B:765:ARG:NH2	2.52	0.42
1:B:1272:THR:O	1:B:1272:THR:OG1	2.30	0.42
1:B:2034:ARG:NH2	1:B:2482:GLU:OE2	2.52	0.42
1:B:2059:ILE:HD13	1:B:2059:ILE:HA	1.84	0.42
1:C:2034:ARG:NH2	1:C:2482:GLU:OE2	2.52	0.42
1:D:1507:LEU:HD11	1:D:1552:LEU:HD13	2.01	0.42
1:D:2034:ARG:NH2	1:D:2482:GLU:OE2	2.52	0.42
1:A:34:ARG:HA	1:A:34:ARG:HD2	1.85	0.42
1:A:982:GLN:NE2	1:A:1014:ARG:O	2.52	0.42
1:A:2348:THR:HA	1:A:2518:ARG:HA	2.01	0.42
1:B:344:TYR:HD2	1:B:346:GLU:HG3	1.85	0.42
1:B:1884:ASP:OD1	1:B:1902:TYR:OH	2.37	0.42
1:D:1654:ASN:H	1:D:1658:HIS:CD2	2.37	0.42
1:E:373:LEU:O	1:E:381:ILE:N	2.47	0.42
1:E:982:GLN:NE2	1:E:1014:ARG:O	2.52	0.42
1:E:1635:LEU:HD23	1:E:1635:LEU:HA	1.93	0.42
1:A:169:LEU:HD23	1:A:169:LEU:HA	1.91	0.42
1:A:2306:HIS:NE2	1:A:2308:ILE:O	2.53	0.42
1:B:272:VAL:HG12	1:B:442:LEU:HD12	2.01	0.42
1:B:356:LYS:HE2	1:B:396:SER:HB2	2.01	0.42
1:B:2188:THR:HG23	1:C:2137:SER:HB2	2.01	0.42
1:C:335:LYS:HB3	1:C:336:ASP:H	1.74	0.42
1:C:1096:THR:HG1	1:C:1116:HIS:HE2	1.61	0.42
1:D:2178:ALA:HB2	1:E:2147:LEU:HB3	2.02	0.42
1:E:272:VAL:HG12	1:E:442:LEU:HD12	2.01	0.42
1:E:2306:HIS:NE2	1:E:2308:ILE:O	2.53	0.42
1:A:1309:PHE:HD1	1:A:1336:ILE:HG12	1.85	0.42
1:C:1273:LEU:HD23	1:C:1273:LEU:HA	1.90	0.42
1:C:1884:ASP:OD1	1:C:1902:TYR:OH	2.37	0.42
1:C:1970:LYS:HB3	1:C:1970:LYS:HE3	1.86	0.42
1:D:250:LEU:HD22	1:D:451:LEU:HD12	2.02	0.42
1:D:266:ASN:HD22	1:D:443:LEU:HD22	1.84	0.42
1:D:487:GLN:HE21	1:D:487:GLN:HB3	1.55	0.42
1:D:729:THR:OG1	1:D:731:ASP:O	2.35	0.42
1:D:761:SER:OG	1:D:765:ARG:NH2	2.52	0.42
1:D:1206:ASN:O	1:D:1210:LYS:NZ	2.37	0.42
1:E:401:LEU:HD23	1:E:401:LEU:HA	1.84	0.42
1:B:666:THR:O	1:B:666:THR:OG1	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2270:LEU:HD12	1:B:2270:LEU:HA	1.91	0.42
1:C:2469:PHE:CZ	1:D:2518:ARG:HB3	2.55	0.42
1:D:1193:SER:OG	1:D:1194:SER:N	2.53	0.42
1:D:2306:HIS:NE2	1:D:2308:ILE:O	2.53	0.42
1:D:2348:THR:HA	1:D:2518:ARG:HA	2.01	0.42
1:E:1625:ASP:OD1	1:E:1817:TYR:OH	2.33	0.42
1:A:162:LEU:HD11	1:A:933:THR:HG21	2.02	0.42
1:B:1507:LEU:HD11	1:B:1552:LEU:HD13	2.01	0.42
1:B:1654:ASN:H	1:B:1658:HIS:CD2	2.37	0.42
1:D:544:THR:HA	1:D:545:PRO:HD3	1.91	0.42
1:D:1204:ILE:O	1:D:1208:ILE:HB	2.19	0.42
1:E:356:LYS:HE2	1:E:396:SER:HB2	2.01	0.42
1:E:1309:PHE:HD1	1:E:1336:ILE:HG12	1.85	0.42
1:A:691:ASP:OD1	1:A:691:ASP:N	2.52	0.42
1:A:1983:LEU:HD23	1:A:1983:LEU:HA	1.87	0.42
1:B:548:SER:OG	1:B:549:LYS:N	2.53	0.42
1:C:344:TYR:HD2	1:C:346:GLU:HG3	1.85	0.42
1:C:451:LEU:HD22	1:C:462:ILE:HD12	2.00	0.42
1:C:1983:LEU:HD23	1:C:1983:LEU:HA	1.87	0.42
1:D:2452:ARG:NH1	1:E:2339:GLU:O	2.49	0.42
1:E:240:THR:OG1	1:E:454:ALA:O	2.38	0.42
1:A:356:LYS:HE2	1:A:396:SER:HB2	2.01	0.42
1:A:723:ILE:HD13	1:A:723:ILE:HA	1.87	0.42
1:A:1204:ILE:O	1:A:1208:ILE:HB	2.19	0.42
1:B:393:THR:OG1	1:C:1925:ARG:NH2	2.52	0.42
1:C:1309:PHE:HD1	1:C:1336:ILE:HG12	1.85	0.42
1:C:1657:GLU:OE2	1:C:1719:TYR:OH	2.35	0.42
1:D:785:GLN:HG2	1:D:861:ARG:HB2	2.02	0.42
1:D:1015:ARG:HH22	1:E:1882:ARG:HH21	1.67	0.42
1:E:162:LEU:HD11	1:E:933:THR:HG21	2.02	0.42
1:E:709:SER:O	1:E:712:THR:OG1	2.31	0.42
1:A:240:THR:OG1	1:A:454:ALA:O	2.38	0.41
1:A:344:TYR:HD2	1:A:346:GLU:HG3	1.85	0.41
1:C:548:SER:OG	1:C:549:LYS:N	2.53	0.41
1:C:691:ASP:OD1	1:C:691:ASP:N	2.52	0.41
1:C:1654:ASN:H	1:C:1658:HIS:CD2	2.37	0.41
1:C:1863:ASP:HA	1:C:1864:PRO:HD3	1.83	0.41
1:D:691:ASP:OD1	1:D:691:ASP:N	2.52	0.41
1:E:266:ASN:HD22	1:E:443:LEU:HD22	1.84	0.41
1:E:1507:LEU:HD11	1:E:1552:LEU:HD13	2.01	0.41
1:A:138:LEU:HD23	1:A:138:LEU:HA	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:ASN:HD22	1:A:443:LEU:HD22	1.84	0.41
1:B:285:TYR:OH	1:B:446:ASN:OD1	2.37	0.41
1:B:2440:ALA:HB3	1:B:2459:ILE:HB	2.03	0.41
1:C:109:ILE:HD13	1:C:155:MET:HB2	2.02	0.41
1:C:785:GLN:HG2	1:C:861:ARG:HB2	2.02	0.41
1:C:1507:LEU:HD11	1:C:1552:LEU:HD13	2.01	0.41
1:D:1060:ASP:OD1	1:D:1060:ASP:N	2.53	0.41
1:D:1232:HIS:ND1	1:D:1233:GLU:O	2.41	0.41
1:D:1523:VAL:HG22	1:D:1538:PHE:HA	2.02	0.41
1:D:1884:ASP:OD1	1:D:1902:TYR:OH	2.37	0.41
1:D:2457:ILE:HG23	1:D:2481:PHE:HE2	1.85	0.41
1:E:344:TYR:HD2	1:E:346:GLU:HG3	1.85	0.41
1:E:652:SER:N	1:E:655:ASP:OD2	2.50	0.41
1:A:203:TYR:OH	1:A:237:ALA:O	2.30	0.41
1:A:2452:ARG:NH1	1:B:2339:GLU:O	2.47	0.41
1:B:250:LEU:HD22	1:B:451:LEU:HD12	2.02	0.41
1:B:1309:PHE:HD1	1:B:1336:ILE:HG12	1.85	0.41
1:B:2306:HIS:NE2	1:B:2308:ILE:O	2.53	0.41
1:B:2459:ILE:HD13	1:B:2459:ILE:HA	1.90	0.41
1:C:130:HIS:HD1	1:C:984:TYR:HH	1.64	0.41
1:C:356:LYS:HE2	1:C:396:SER:HB2	2.01	0.41
1:C:2345:LEU:HD23	1:C:2345:LEU:HA	1.84	0.41
1:D:272:VAL:HG12	1:D:442:LEU:HD12	2.01	0.41
1:D:599:LEU:HD23	1:D:599:LEU:HA	1.91	0.41
1:D:652:SER:N	1:D:655:ASP:OD2	2.50	0.41
1:D:1239:SER:OG	1:D:1242:SER:OG	2.33	0.41
1:D:2101:LEU:HD21	1:D:2225:GLN:HB3	2.01	0.41
1:E:691:ASP:OD1	1:E:691:ASP:N	2.52	0.41
1:E:1096:THR:HG1	1:E:1116:HIS:HE2	1.62	0.41
1:E:1884:ASP:OD1	1:E:1902:TYR:OH	2.37	0.41
1:E:2101:LEU:HD21	1:E:2225:GLN:HB3	2.01	0.41
1:E:2330:LEU:HD23	1:E:2330:LEU:HA	1.92	0.41
1:E:2457:ILE:HG23	1:E:2481:PHE:HE2	1.85	0.41
1:A:1193:SER:OG	1:A:1194:SER:N	2.53	0.41
1:A:2452:ARG:HB3	1:A:2453:GLY:H	1.69	0.41
1:B:102:ARG:HH22	1:B:1965:LEU:HD11	1.86	0.41
1:B:109:ILE:HD13	1:B:155:MET:HB2	2.02	0.41
1:B:162:LEU:HD11	1:B:933:THR:HG21	2.02	0.41
1:B:240:THR:OG1	1:B:454:ALA:O	2.38	0.41
1:B:2419:ARG:HG2	1:B:2521:ILE:HG23	2.03	0.41
1:C:761:SER:OG	1:C:765:ARG:NH2	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1060:ASP:OD1	1:C:1060:ASP:N	2.53	0.41
1:C:2121:GLU:H	1:C:2121:GLU:HG3	1.74	0.41
1:C:2306:HIS:NE2	1:C:2308:ILE:O	2.53	0.41
1:C:2440:ALA:HB3	1:C:2459:ILE:HB	2.03	0.41
1:D:356:LYS:HE2	1:D:396:SER:HB2	2.01	0.41
1:D:707:MET:O	1:E:2268:ASN:ND2	2.53	0.41
1:D:1700:LYS:HE3	1:D:1700:LYS:HB3	1.90	0.41
1:D:1991:THR:OG1	1:D:1995:GLN:O	2.34	0.41
1:E:1523:VAL:HG22	1:E:1538:PHE:HA	2.02	0.41
1:A:592:LEU:HA	1:A:595:ARG:HB2	2.03	0.41
1:A:2457:ILE:HG23	1:A:2481:PHE:HE2	1.85	0.41
1:B:703:ALA:HB1	1:C:2269:TRP:HA	2.02	0.41
1:B:785:GLN:HG2	1:B:861:ARG:HB2	2.03	0.41
1:B:2121:GLU:H	1:B:2121:GLU:HG3	1.74	0.41
1:C:250:LEU:HD22	1:C:451:LEU:HD12	2.02	0.41
1:C:2419:ARG:HG2	1:C:2521:ILE:HG23	2.03	0.41
1:D:548:SER:OG	1:D:549:LYS:N	2.53	0.41
1:E:548:SER:OG	1:E:549:LYS:N	2.53	0.41
1:E:1193:SER:OG	1:E:1194:SER:N	2.53	0.41
1:E:2098:LYS:HE2	1:E:2102:GLN:HE21	1.86	0.41
1:A:272:VAL:HG12	1:A:442:LEU:HD12	2.01	0.41
1:A:508:ILE:HB	1:A:587:ILE:HD11	2.03	0.41
1:A:972:THR:OG1	1:A:973:ARG:N	2.54	0.41
1:A:1507:LEU:HD11	1:A:1552:LEU:HD13	2.02	0.41
1:B:401:LEU:HD23	1:B:401:LEU:HA	1.84	0.41
1:B:2457:ILE:HG23	1:B:2481:PHE:HE2	1.85	0.41
1:C:544:THR:HA	1:C:545:PRO:HD3	1.91	0.41
1:C:1070:LEU:HD23	1:C:1070:LEU:HA	1.92	0.41
1:C:2098:LYS:HE2	1:C:2102:GLN:HE21	1.86	0.41
1:D:1165:LEU:HD23	1:D:1165:LEU:HA	1.92	0.41
1:D:2098:LYS:HE2	1:D:2102:GLN:HE21	1.86	0.41
1:D:2419:ARG:HG2	1:D:2521:ILE:HG23	2.03	0.41
1:E:131:PRO:HG2	1:E:134:SER:HB2	2.03	0.41
1:E:972:THR:OG1	1:E:973:ARG:N	2.54	0.41
1:E:1028:TYR:OH	1:E:1967:GLN:O	2.28	0.41
1:E:1272:THR:O	1:E:1272:THR:OG1	2.30	0.41
1:A:2419:ARG:HG2	1:A:2521:ILE:HG23	2.03	0.41
1:B:131:PRO:HG2	1:B:134:SER:HB2	2.03	0.41
1:B:231:ASP:HB2	1:B:890:LYS:HE2	2.03	0.41
1:B:819:LEU:HD12	1:C:2016:ILE:HG21	2.03	0.41
1:B:1037:ILE:HA	1:B:1041:GLN:HE22	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1906:LEU:HD23	1:B:1906:LEU:HA	1.86	0.41
1:B:2238:LEU:HD23	1:C:2086:MET:HA	2.02	0.41
1:C:1523:VAL:HG22	1:C:1538:PHE:HA	2.02	0.41
1:D:162:LEU:HD11	1:D:933:THR:HG21	2.02	0.41
1:D:2258:GLN:HB3	1:E:2015:ALA:HB2	2.02	0.41
1:E:472:ASP:OD1	1:E:472:ASP:N	2.54	0.41
1:E:761:SER:OG	1:E:765:ARG:NH2	2.52	0.41
1:A:231:ASP:HB2	1:A:890:LYS:HE2	2.03	0.41
1:A:350:ILE:HB	1:A:354:GLU:HG2	2.03	0.41
1:A:381:ILE:HG21	1:A:399:ILE:HG23	2.03	0.41
1:A:472:ASP:OD1	1:A:472:ASP:N	2.54	0.41
1:A:548:SER:OG	1:A:549:LYS:N	2.53	0.41
1:A:785:GLN:HG2	1:A:861:ARG:HB2	2.02	0.41
1:A:2015:ALA:HB2	1:E:2258:GLN:HB3	2.02	0.41
1:A:2098:LYS:HE2	1:A:2102:GLN:HE21	1.86	0.41
1:A:2440:ALA:HB3	1:A:2459:ILE:HB	2.02	0.41
1:B:972:THR:OG1	1:B:973:ARG:N	2.54	0.41
1:C:231:ASP:HB2	1:C:890:LYS:HE2	2.03	0.41
1:D:344:TYR:HD2	1:D:346:GLU:HG3	1.85	0.41
1:E:335:LYS:HB3	1:E:336:ASP:H	1.74	0.41
1:E:785:GLN:HG2	1:E:861:ARG:HB2	2.03	0.41
1:E:2419:ARG:HG2	1:E:2521:ILE:HG23	2.03	0.41
1:A:1812:THR:OG1	1:E:1010:GLU:OE2	2.32	0.41
1:A:2268:ASN:ND2	1:E:707:MET:O	2.54	0.41
1:A:2339:GLU:O	1:E:2452:ARG:NH1	2.51	0.41
1:B:472:ASP:N	1:B:472:ASP:OD1	2.54	0.41
1:B:599:LEU:HD23	1:B:599:LEU:HA	1.90	0.41
1:B:1060:ASP:OD1	1:B:1060:ASP:N	2.53	0.41
1:B:1507:LEU:HB3	1:B:1515:VAL:HB	2.03	0.41
1:C:169:LEU:HD23	1:C:169:LEU:HA	1.91	0.41
1:C:212:LEU:HD23	1:C:212:LEU:HA	1.95	0.41
1:C:783:LYS:HA	1:C:783:LYS:HD3	1.90	0.41
1:C:2101:LEU:HD12	1:C:2101:LEU:HA	1.92	0.41
1:C:2457:ILE:HG23	1:C:2481:PHE:HE2	1.85	0.41
1:C:2459:ILE:HD13	1:C:2459:ILE:HA	1.90	0.41
1:D:109:ILE:HD13	1:D:155:MET:HB2	2.02	0.41
1:D:373:LEU:HD13	1:D:399:ILE:HD11	2.03	0.41
1:D:1037:ILE:HA	1:D:1041:GLN:HE22	1.86	0.41
1:D:1202:ASP:OD1	1:D:1202:ASP:N	2.37	0.41
1:D:1309:PHE:HD1	1:D:1336:ILE:HG12	1.85	0.41
1:D:1963:LEU:HD23	1:D:1963:LEU:HA	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:508:ILE:HB	1:E:587:ILE:HD11	2.03	0.41
1:E:1759:LYS:HA	1:E:1759:LYS:HD3	1.93	0.41
1:A:373:LEU:HD13	1:A:399:ILE:HD11	2.03	0.41
1:A:1273:LEU:HD23	1:A:1273:LEU:HA	1.90	0.41
1:A:1700:LYS:HE3	1:A:1700:LYS:HB3	1.90	0.41
1:A:2147:LEU:HB3	1:E:2178:ALA:HB2	2.03	0.41
1:B:34:ARG:HA	1:B:34:ARG:HD2	1.85	0.41
1:B:373:LEU:HD13	1:B:399:ILE:HD11	2.03	0.41
1:B:785:GLN:HA	1:B:859:ASN:HD21	1.86	0.41
1:C:102:ARG:HH22	1:C:1965:LEU:HD11	1.86	0.41
1:C:131:PRO:HG2	1:C:134:SER:HB2	2.03	0.41
1:C:1863:ASP:OD1	1:C:1863:ASP:N	2.54	0.41
1:C:1923:GLU:H	1:C:1923:GLU:HG3	1.65	0.41
1:C:2118:LEU:HD23	1:C:2118:LEU:HA	1.90	0.41
1:C:2194:LYS:HD2	1:E:1054:GLN:NE2	2.32	0.41
1:D:335:LYS:HB3	1:D:336:ASP:H	1.74	0.41
1:D:381:ILE:HG21	1:D:399:ILE:HG23	2.03	0.41
1:D:679:LEU:HD12	1:D:679:LEU:HA	1.90	0.41
1:E:350:ILE:HB	1:E:354:GLU:HG2	2.03	0.41
1:E:373:LEU:HD13	1:E:399:ILE:HD11	2.03	0.41
1:E:592:LEU:HA	1:E:595:ARG:HB2	2.03	0.41
1:E:1863:ASP:HA	1:E:1864:PRO:HD3	1.83	0.41
1:A:1863:ASP:N	1:A:1863:ASP:OD1	2.54	0.40
1:A:2335:LYS:HE2	1:A:2335:LYS:HB3	1.98	0.40
1:A:2442:LEU:HB3	1:A:2457:ILE:HG12	2.03	0.40
1:B:705:ILE:H	1:B:705:ILE:HG12	1.69	0.40
1:B:1523:VAL:HG22	1:B:1538:PHE:HA	2.02	0.40
1:C:472:ASP:N	1:C:472:ASP:OD1	2.54	0.40
1:C:679:LEU:HD12	1:C:679:LEU:HA	1.91	0.40
1:C:1193:SER:OG	1:C:1194:SER:N	2.53	0.40
1:D:102:ARG:HH22	1:D:1965:LEU:HD11	1.86	0.40
1:D:240:THR:OG1	1:D:454:ALA:O	2.38	0.40
1:D:709:SER:O	1:D:712:THR:OG1	2.31	0.40
1:D:2440:ALA:HB3	1:D:2459:ILE:HB	2.02	0.40
1:E:1946:ARG:H	1:E:1946:ARG:HG2	1.75	0.40
1:A:109:ILE:HD13	1:A:155:MET:HB2	2.02	0.40
1:A:250:LEU:HD22	1:A:451:LEU:HD12	2.02	0.40
1:A:285:TYR:OH	1:A:446:ASN:OD1	2.37	0.40
1:A:1702:TYR:HB3	1:A:1703:TYR:HD1	1.87	0.40
1:A:1970:LYS:HE3	1:A:1970:LYS:HB3	1.86	0.40
1:B:164:LEU:HD23	1:B:164:LEU:HA	1.95	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:592:LEU:HA	1:B:595:ARG:HB2	2.03	0.40
1:B:2461:HIS:CE1	1:B:2463:MET:HB3	2.57	0.40
1:C:42:THR:OG1	1:C:1571:GLU:OE2	2.38	0.40
1:C:240:THR:OG1	1:C:454:ALA:O	2.38	0.40
1:C:373:LEU:HD13	1:C:399:ILE:HD11	2.03	0.40
1:C:972:THR:OG1	1:C:973:ARG:N	2.54	0.40
1:D:1835:TRP:CZ2	1:D:1868:LYS:HG3	2.56	0.40
1:D:2263:ASN:OD1	1:D:2263:ASN:N	2.54	0.40
1:E:1702:TYR:HB3	1:E:1703:TYR:HD1	1.86	0.40
1:B:508:ILE:HB	1:B:587:ILE:HD11	2.03	0.40
1:B:2183:ILE:HD12	1:B:2183:ILE:HA	1.92	0.40
1:C:162:LEU:HD11	1:C:933:THR:HG21	2.02	0.40
1:C:785:GLN:HA	1:C:859:ASN:HD21	1.87	0.40
1:C:1139:ILE:HG23	1:C:1159:TRP:CE2	2.57	0.40
1:C:2452:ARG:HB3	1:C:2453:GLY:H	1.69	0.40
1:D:231:ASP:HB2	1:D:890:LYS:HE2	2.03	0.40
1:D:1002:THR:O	1:D:1002:THR:OG1	2.31	0.40
1:D:2454:CYS:HB3	1:D:2480:PRO:HA	2.04	0.40
1:A:2461:HIS:CE1	1:A:2463:MET:HB3	2.57	0.40
1:C:61:LYS:HE3	1:C:61:LYS:HB3	1.93	0.40
1:C:113:PHE:O	1:C:1016:TYR:OH	2.34	0.40
1:D:972:THR:OG1	1:D:973:ARG:N	2.54	0.40
1:D:1507:LEU:HB3	1:D:1515:VAL:HB	2.03	0.40
1:E:381:ILE:HG21	1:E:399:ILE:HG23	2.03	0.40
1:E:2442:LEU:HB3	1:E:2457:ILE:HG12	2.03	0.40
1:A:236:LEU:HD13	1:A:484:PHE:HA	2.04	0.40
1:A:785:GLN:HA	1:A:859:ASN:HD21	1.87	0.40
1:A:1835:TRP:CZ2	1:A:1868:LYS:HG3	2.56	0.40
1:A:1946:ARG:H	1:A:1946:ARG:HG2	1.74	0.40
1:A:2453:GLY:H	1:B:2342:GLU:HB2	1.87	0.40
1:B:709:SER:O	1:B:712:THR:OG1	2.31	0.40
1:B:1597:GLN:HB3	1:B:1609:ASN:HB2	2.04	0.40
1:C:1635:LEU:HA	1:C:1636:PRO:HD3	1.93	0.40
1:D:1179:TYR:H	1:D:1201:THR:HB	1.87	0.40
1:D:2461:HIS:CE1	1:D:2463:MET:HB3	2.57	0.40
1:E:236:LEU:HD13	1:E:484:PHE:HA	2.04	0.40
1:E:525:ASN:HD22	1:E:525:ASN:HA	1.72	0.40
1:E:627:PHE:HD1	1:E:627:PHE:HA	1.77	0.40
1:E:1979:LEU:HA	1:E:1979:LEU:HD23	1.90	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	2331/2523 (92%)	2158 (93%)	170 (7%)	3 (0%)	51	83
1	B	2331/2523 (92%)	2158 (93%)	170 (7%)	3 (0%)	51	83
1	C	2331/2523 (92%)	2160 (93%)	168 (7%)	3 (0%)	51	83
1	D	2331/2523 (92%)	2159 (93%)	169 (7%)	3 (0%)	51	83
1	E	2331/2523 (92%)	2160 (93%)	168 (7%)	3 (0%)	51	83
All	All	11655/12615 (92%)	10795 (93%)	845 (7%)	15 (0%)	54	83

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1949	ALA
1	C	1949	ALA
1	D	1949	ALA
1	A	2453	GLY
1	B	1949	ALA
1	B	2453	GLY
1	C	2453	GLY
1	D	2453	GLY
1	E	1949	ALA
1	E	2453	GLY
1	A	581	PRO
1	B	581	PRO
1	C	581	PRO
1	D	581	PRO
1	E	581	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	2049/2222 (92%)	1908 (93%)	141 (7%)	15 46
1	B	2049/2222 (92%)	1908 (93%)	141 (7%)	15 46
1	C	2049/2222 (92%)	1908 (93%)	141 (7%)	15 46
1	D	2049/2222 (92%)	1908 (93%)	141 (7%)	15 46
1	E	2049/2222 (92%)	1908 (93%)	141 (7%)	15 46
All	All	10245/11110 (92%)	9540 (93%)	705 (7%)	19 46

All (705) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	THR
1	A	42	THR
1	A	65	LEU
1	A	104	VAL
1	A	133	ASN
1	A	144	ASP
1	A	148	LEU
1	A	176	LEU
1	A	179	THR
1	A	187	MET
1	A	190	THR
1	A	251	VAL
1	A	260	THR
1	A	270	ASP
1	A	272	VAL
1	A	281	LEU
1	A	288	SER
1	A	322	ASN
1	A	333	THR
1	A	342	LEU
1	A	369	LEU
1	A	373	LEU
1	A	379	GLU
1	A	394	HIS
1	A	411	THR
1	A	440	ILE
1	A	442	LEU
1	A	451	LEU

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Mol	Chain	Res	Type
1	A	453	LYS
1	A	473	LEU
1	A	474	THR
1	A	483	LEU
1	A	487	GLN
1	A	513	THR
1	A	516	GLN
1	A	529	LEU
1	A	539	THR
1	A	544	THR
1	A	563	VAL
1	A	592	LEU
1	A	606	THR
1	A	608	ASN
1	A	630	THR
1	A	646	LEU
1	A	660	THR
1	A	691	ASP
1	A	705	ILE
1	A	732	ASP
1	A	771	GLU
1	A	775	THR
1	A	795	LEU
1	A	798	LEU
1	A	816	THR
1	A	819	LEU
1	A	879	THR
1	A	892	VAL
1	A	901	THR
1	A	1011	THR
1	A	1030	GLU
1	A	1033	ILE
1	A	1047	ASN
1	A	1058	ASN
1	A	1060	ASP
1	A	1076	VAL
1	A	1092	ASN
1	A	1095	LEU
1	A	1096	THR
1	A	1104	THR
1	A	1141	VAL
1	A	1149	VAL

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Mol	Chain	Res	Type
1	A	1157	LEU
1	A	1180	ILE
1	A	1183	LEU
1	A	1202	ASP
1	A	1208	ILE
1	A	1250	THR
1	A	1256	THR
1	A	1262	GLU
1	A	1272	THR
1	A	1277	ASP
1	A	1290	THR
1	A	1323	ASN
1	A	1328	LEU
1	A	1500	ASP
1	A	1503	ILE
1	A	1545	ILE
1	A	1554	SER
1	A	1596	THR
1	A	1656	GLU
1	A	1657	GLU
1	A	1690	THR
1	A	1692	VAL
1	A	1712	VAL
1	A	1725	SER
1	A	1740	ILE
1	A	1796	MET
1	A	1803	LEU
1	A	1811	SER
1	A	1818	ILE
1	A	1838	ARG
1	A	1854	VAL
1	A	1875	MET
1	A	1887	TYR
1	A	1893	ASP
1	A	1900	MET
1	A	1911	ASP
1	A	1936	HIS
1	A	1951	LEU
1	A	1953	THR
1	A	1956	THR
1	A	1991	THR
1	A	1999	LEU

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Mol	Chain	Res	Type
1	A	2001	LEU
1	A	2017	THR
1	A	2025	LEU
1	A	2057	LEU
1	A	2081	LEU
1	A	2105	ARG
1	A	2121	GLU
1	A	2131	MET
1	A	2135	LEU
1	A	2142	THR
1	A	2145	THR
1	A	2147	LEU
1	A	2160	ILE
1	A	2229	LEU
1	A	2243	LEU
1	A	2259	SER
1	A	2270	LEU
1	A	2316	THR
1	A	2348	THR
1	A	2360	LEU
1	A	2363	ASN
1	A	2366	ILE
1	A	2369	ASP
1	A	2390	ASN
1	A	2409	THR
1	A	2448	THR
1	A	2450	MET
1	A	2486	VAL
1	A	2510	LEU
1	B	40	THR
1	B	42	THR
1	B	65	LEU
1	B	104	VAL
1	B	133	ASN
1	B	144	ASP
1	B	148	LEU
1	B	176	LEU
1	B	179	THR
1	B	187	MET
1	B	190	THR
1	B	251	VAL
1	B	260	THR

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Mol	Chain	Res	Type
1	B	270	ASP
1	B	272	VAL
1	B	281	LEU
1	B	288	SER
1	B	322	ASN
1	B	333	THR
1	B	342	LEU
1	B	369	LEU
1	B	373	LEU
1	B	379	GLU
1	B	394	HIS
1	B	411	THR
1	B	440	ILE
1	B	442	LEU
1	B	451	LEU
1	B	453	LYS
1	B	473	LEU
1	B	474	THR
1	B	483	LEU
1	B	487	GLN
1	B	513	THR
1	B	516	GLN
1	B	529	LEU
1	B	539	THR
1	B	544	THR
1	B	563	VAL
1	B	592	LEU
1	B	606	THR
1	B	608	ASN
1	B	630	THR
1	B	646	LEU
1	B	660	THR
1	B	691	ASP
1	B	705	ILE
1	B	732	ASP
1	B	771	GLU
1	B	775	THR
1	B	795	LEU
1	B	798	LEU
1	B	816	THR
1	B	819	LEU
1	B	879	THR

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Mol	Chain	Res	Type
1	B	892	VAL
1	B	901	THR
1	B	1011	THR
1	B	1030	GLU
1	B	1033	ILE
1	B	1047	ASN
1	B	1058	ASN
1	B	1060	ASP
1	B	1076	VAL
1	B	1092	ASN
1	B	1095	LEU
1	B	1096	THR
1	B	1104	THR
1	B	1141	VAL
1	B	1149	VAL
1	B	1157	LEU
1	B	1180	ILE
1	B	1183	LEU
1	B	1202	ASP
1	B	1208	ILE
1	B	1250	THR
1	B	1256	THR
1	B	1262	GLU
1	B	1272	THR
1	B	1277	ASP
1	B	1290	THR
1	B	1323	ASN
1	B	1328	LEU
1	B	1500	ASP
1	B	1503	ILE
1	B	1545	ILE
1	B	1554	SER
1	B	1596	THR
1	B	1656	GLU
1	B	1657	GLU
1	B	1690	THR
1	B	1692	VAL
1	B	1712	VAL
1	B	1725	SER
1	B	1740	ILE
1	B	1796	MET
1	B	1803	LEU

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Mol	Chain	Res	Type
1	B	1811	SER
1	B	1818	ILE
1	B	1838	ARG
1	B	1854	VAL
1	B	1875	MET
1	B	1887	TYR
1	B	1893	ASP
1	B	1900	MET
1	B	1911	ASP
1	B	1936	HIS
1	B	1951	LEU
1	B	1953	THR
1	B	1956	THR
1	B	1991	THR
1	B	1999	LEU
1	B	2001	LEU
1	B	2017	THR
1	B	2025	LEU
1	B	2057	LEU
1	B	2081	LEU
1	B	2105	ARG
1	B	2121	GLU
1	B	2131	MET
1	B	2135	LEU
1	B	2142	THR
1	B	2145	THR
1	B	2147	LEU
1	B	2160	ILE
1	B	2229	LEU
1	B	2243	LEU
1	B	2259	SER
1	B	2270	LEU
1	B	2316	THR
1	B	2348	THR
1	B	2360	LEU
1	B	2363	ASN
1	B	2366	ILE
1	B	2369	ASP
1	B	2390	ASN
1	B	2409	THR
1	B	2448	THR
1	B	2450	MET

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Mol	Chain	Res	Type
1	B	2486	VAL
1	B	2510	LEU
1	C	40	THR
1	C	42	THR
1	C	65	LEU
1	C	104	VAL
1	C	133	ASN
1	C	144	ASP
1	C	148	LEU
1	C	176	LEU
1	C	179	THR
1	C	187	MET
1	C	190	THR
1	C	251	VAL
1	C	260	THR
1	C	270	ASP
1	C	272	VAL
1	C	281	LEU
1	C	288	SER
1	C	322	ASN
1	C	333	THR
1	C	342	LEU
1	C	369	LEU
1	C	373	LEU
1	C	379	GLU
1	C	394	HIS
1	C	411	THR
1	C	440	ILE
1	C	442	LEU
1	C	451	LEU
1	C	453	LYS
1	C	473	LEU
1	C	474	THR
1	C	483	LEU
1	C	487	GLN
1	C	513	THR
1	C	516	GLN
1	C	529	LEU
1	C	539	THR
1	C	544	THR
1	C	563	VAL
1	C	592	LEU

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Mol	Chain	Res	Type
1	C	606	THR
1	C	608	ASN
1	C	630	THR
1	C	646	LEU
1	C	660	THR
1	C	691	ASP
1	C	705	ILE
1	C	732	ASP
1	C	771	GLU
1	C	775	THR
1	C	795	LEU
1	C	798	LEU
1	C	816	THR
1	C	819	LEU
1	C	879	THR
1	C	892	VAL
1	C	901	THR
1	C	1011	THR
1	C	1030	GLU
1	C	1033	ILE
1	C	1047	ASN
1	C	1058	ASN
1	C	1060	ASP
1	C	1076	VAL
1	C	1092	ASN
1	C	1095	LEU
1	C	1096	THR
1	C	1104	THR
1	C	1141	VAL
1	C	1149	VAL
1	C	1157	LEU
1	C	1180	ILE
1	C	1183	LEU
1	C	1202	ASP
1	C	1208	ILE
1	C	1250	THR
1	C	1256	THR
1	C	1262	GLU
1	C	1272	THR
1	C	1277	ASP
1	C	1290	THR
1	C	1323	ASN

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Mol	Chain	Res	Type
1	C	1328	LEU
1	C	1500	ASP
1	C	1503	ILE
1	C	1545	ILE
1	C	1554	SER
1	C	1596	THR
1	C	1656	GLU
1	C	1657	GLU
1	C	1690	THR
1	C	1692	VAL
1	C	1712	VAL
1	C	1725	SER
1	C	1740	ILE
1	C	1796	MET
1	C	1803	LEU
1	C	1811	SER
1	C	1818	ILE
1	C	1838	ARG
1	C	1854	VAL
1	C	1875	MET
1	C	1887	TYR
1	C	1893	ASP
1	C	1900	MET
1	C	1911	ASP
1	C	1936	HIS
1	C	1951	LEU
1	C	1953	THR
1	C	1956	THR
1	C	1991	THR
1	C	1999	LEU
1	C	2001	LEU
1	C	2017	THR
1	C	2025	LEU
1	C	2057	LEU
1	C	2081	LEU
1	C	2105	ARG
1	C	2121	GLU
1	C	2131	MET
1	C	2135	LEU
1	C	2142	THR
1	C	2145	THR
1	C	2147	LEU

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Mol	Chain	Res	Type
1	C	2160	ILE
1	C	2229	LEU
1	C	2243	LEU
1	C	2259	SER
1	C	2270	LEU
1	C	2316	THR
1	C	2348	THR
1	C	2360	LEU
1	C	2363	ASN
1	C	2366	ILE
1	C	2369	ASP
1	C	2390	ASN
1	C	2409	THR
1	C	2448	THR
1	C	2450	MET
1	C	2486	VAL
1	C	2510	LEU
1	D	40	THR
1	D	42	THR
1	D	65	LEU
1	D	104	VAL
1	D	133	ASN
1	D	144	ASP
1	D	148	LEU
1	D	176	LEU
1	D	179	THR
1	D	187	MET
1	D	190	THR
1	D	251	VAL
1	D	260	THR
1	D	270	ASP
1	D	272	VAL
1	D	281	LEU
1	D	288	SER
1	D	322	ASN
1	D	333	THR
1	D	342	LEU
1	D	369	LEU
1	D	373	LEU
1	D	379	GLU
1	D	394	HIS
1	D	411	THR

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Mol	Chain	Res	Type
1	D	440	ILE
1	D	442	LEU
1	D	451	LEU
1	D	453	LYS
1	D	473	LEU
1	D	474	THR
1	D	483	LEU
1	D	487	GLN
1	D	513	THR
1	D	516	GLN
1	D	529	LEU
1	D	539	THR
1	D	544	THR
1	D	563	VAL
1	D	592	LEU
1	D	606	THR
1	D	608	ASN
1	D	630	THR
1	D	646	LEU
1	D	660	THR
1	D	691	ASP
1	D	705	ILE
1	D	732	ASP
1	D	771	GLU
1	D	775	THR
1	D	795	LEU
1	D	798	LEU
1	D	816	THR
1	D	819	LEU
1	D	879	THR
1	D	892	VAL
1	D	901	THR
1	D	1011	THR
1	D	1030	GLU
1	D	1033	ILE
1	D	1047	ASN
1	D	1058	ASN
1	D	1060	ASP
1	D	1076	VAL
1	D	1092	ASN
1	D	1095	LEU
1	D	1096	THR

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Mol	Chain	Res	Type
1	D	1104	THR
1	D	1141	VAL
1	D	1149	VAL
1	D	1157	LEU
1	D	1180	ILE
1	D	1183	LEU
1	D	1202	ASP
1	D	1208	ILE
1	D	1250	THR
1	D	1256	THR
1	D	1262	GLU
1	D	1272	THR
1	D	1277	ASP
1	D	1290	THR
1	D	1323	ASN
1	D	1328	LEU
1	D	1500	ASP
1	D	1503	ILE
1	D	1545	ILE
1	D	1554	SER
1	D	1596	THR
1	D	1656	GLU
1	D	1657	GLU
1	D	1690	THR
1	D	1692	VAL
1	D	1712	VAL
1	D	1725	SER
1	D	1740	ILE
1	D	1796	MET
1	D	1803	LEU
1	D	1811	SER
1	D	1818	ILE
1	D	1838	ARG
1	D	1854	VAL
1	D	1875	MET
1	D	1887	TYR
1	D	1893	ASP
1	D	1900	MET
1	D	1911	ASP
1	D	1936	HIS
1	D	1951	LEU
1	D	1953	THR

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Mol	Chain	Res	Type
1	D	1956	THR
1	D	1991	THR
1	D	1999	LEU
1	D	2001	LEU
1	D	2017	THR
1	D	2025	LEU
1	D	2057	LEU
1	D	2081	LEU
1	D	2105	ARG
1	D	2121	GLU
1	D	2131	MET
1	D	2135	LEU
1	D	2142	THR
1	D	2145	THR
1	D	2147	LEU
1	D	2160	ILE
1	D	2229	LEU
1	D	2243	LEU
1	D	2259	SER
1	D	2270	LEU
1	D	2316	THR
1	D	2348	THR
1	D	2360	LEU
1	D	2363	ASN
1	D	2366	ILE
1	D	2369	ASP
1	D	2390	ASN
1	D	2409	THR
1	D	2448	THR
1	D	2450	MET
1	D	2486	VAL
1	D	2510	LEU
1	E	40	THR
1	E	42	THR
1	E	65	LEU
1	E	104	VAL
1	E	133	ASN
1	E	144	ASP
1	E	148	LEU
1	E	176	LEU
1	E	179	THR
1	E	187	MET

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Mol	Chain	Res	Type
1	E	190	THR
1	E	251	VAL
1	E	260	THR
1	E	270	ASP
1	E	272	VAL
1	E	281	LEU
1	E	288	SER
1	E	322	ASN
1	E	333	THR
1	E	342	LEU
1	E	369	LEU
1	E	373	LEU
1	E	379	GLU
1	E	394	HIS
1	E	411	THR
1	E	440	ILE
1	E	442	LEU
1	E	451	LEU
1	E	453	LYS
1	E	473	LEU
1	E	474	THR
1	E	483	LEU
1	E	487	GLN
1	E	513	THR
1	E	516	GLN
1	E	529	LEU
1	E	539	THR
1	E	544	THR
1	E	563	VAL
1	E	592	LEU
1	E	606	THR
1	E	608	ASN
1	E	630	THR
1	E	646	LEU
1	E	660	THR
1	E	691	ASP
1	E	705	ILE
1	E	732	ASP
1	E	771	GLU
1	E	775	THR
1	E	795	LEU
1	E	798	LEU

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Mol	Chain	Res	Type
1	E	816	THR
1	E	819	LEU
1	E	879	THR
1	E	892	VAL
1	E	901	THR
1	E	1011	THR
1	E	1030	GLU
1	E	1033	ILE
1	E	1047	ASN
1	E	1058	ASN
1	E	1060	ASP
1	E	1076	VAL
1	E	1092	ASN
1	E	1095	LEU
1	E	1096	THR
1	E	1104	THR
1	E	1141	VAL
1	E	1149	VAL
1	E	1157	LEU
1	E	1180	ILE
1	E	1183	LEU
1	E	1202	ASP
1	E	1208	ILE
1	E	1250	THR
1	E	1256	THR
1	E	1262	GLU
1	E	1272	THR
1	E	1277	ASP
1	E	1290	THR
1	E	1323	ASN
1	E	1328	LEU
1	E	1500	ASP
1	E	1503	ILE
1	E	1545	ILE
1	E	1554	SER
1	E	1596	THR
1	E	1656	GLU
1	E	1657	GLU
1	E	1690	THR
1	E	1692	VAL
1	E	1712	VAL
1	E	1725	SER

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Mol	Chain	Res	Type
1	E	1740	ILE
1	E	1796	MET
1	E	1803	LEU
1	E	1811	SER
1	E	1818	ILE
1	E	1838	ARG
1	E	1854	VAL
1	E	1875	MET
1	E	1887	TYR
1	E	1893	ASP
1	E	1900	MET
1	E	1911	ASP
1	E	1936	HIS
1	E	1951	LEU
1	E	1953	THR
1	E	1956	THR
1	E	1991	THR
1	E	1999	LEU
1	E	2001	LEU
1	E	2017	THR
1	E	2025	LEU
1	E	2057	LEU
1	E	2081	LEU
1	E	2105	ARG
1	E	2121	GLU
1	E	2131	MET
1	E	2135	LEU
1	E	2142	THR
1	E	2145	THR
1	E	2147	LEU
1	E	2160	ILE
1	E	2229	LEU
1	E	2243	LEU
1	E	2259	SER
1	E	2270	LEU
1	E	2316	THR
1	E	2348	THR
1	E	2360	LEU
1	E	2363	ASN
1	E	2366	ILE
1	E	2369	ASP
1	E	2390	ASN

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Mol	Chain	Res	Type
1	E	2409	THR
1	E	2448	THR
1	E	2450	MET
1	E	2486	VAL
1	E	2510	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (203) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	55	GLN
1	A	139	ASN
1	A	171	HIS
1	A	172	ASN
1	A	200	HIS
1	A	213	GLN
1	A	216	ASN
1	A	311	ASN
1	A	341	HIS
1	A	374	GLN
1	A	478	ASN
1	A	516	GLN
1	A	519	HIS
1	A	551	HIS
1	A	634	GLN
1	A	681	ASN
1	A	706	GLN
1	A	722	GLN
1	A	766	ASN
1	A	1041	GLN
1	A	1054	GLN
1	A	1056	GLN
1	A	1080	GLN
1	A	1167	ASN
1	A	1197	ASN
1	A	1206	ASN
1	A	1502	ASN
1	A	1522	HIS
1	A	1670	ASN
1	A	1741	ASN
1	A	1800	GLN
1	A	1807	ASN

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Mol	Chain	Res	Type
1	A	1939	GLN
1	A	2075	GLN
1	A	2159	ASN
1	A	2239	GLN
1	A	2251	GLN
1	A	2314	HIS
1	A	2390	ASN
1	A	2516	HIS
1	B	24	ASN
1	B	55	GLN
1	B	139	ASN
1	B	171	HIS
1	B	172	ASN
1	B	200	HIS
1	B	213	GLN
1	B	216	ASN
1	B	311	ASN
1	B	341	HIS
1	B	374	GLN
1	B	478	ASN
1	B	516	GLN
1	B	519	HIS
1	B	551	HIS
1	B	634	GLN
1	B	681	ASN
1	B	706	GLN
1	B	722	GLN
1	B	766	ASN
1	B	919	GLN
1	B	1041	GLN
1	B	1054	GLN
1	B	1056	GLN
1	B	1080	GLN
1	B	1167	ASN
1	B	1197	ASN
1	B	1206	ASN
1	B	1502	ASN
1	B	1522	HIS
1	B	1670	ASN
1	B	1741	ASN
1	B	1800	GLN
1	B	1939	GLN

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Mol	Chain	Res	Type
1	B	2075	GLN
1	B	2159	ASN
1	B	2239	GLN
1	B	2390	ASN
1	B	2468	GLN
1	B	2516	HIS
1	C	24	ASN
1	C	55	GLN
1	C	139	ASN
1	C	171	HIS
1	C	172	ASN
1	C	200	HIS
1	C	213	GLN
1	C	216	ASN
1	C	311	ASN
1	C	341	HIS
1	C	374	GLN
1	C	478	ASN
1	C	487	GLN
1	C	516	GLN
1	C	519	HIS
1	C	551	HIS
1	C	634	GLN
1	C	681	ASN
1	C	706	GLN
1	C	722	GLN
1	C	766	ASN
1	C	1041	GLN
1	C	1054	GLN
1	C	1056	GLN
1	C	1080	GLN
1	C	1167	ASN
1	C	1197	ASN
1	C	1206	ASN
1	C	1502	ASN
1	C	1522	HIS
1	C	1670	ASN
1	C	1741	ASN
1	C	1800	GLN
1	C	1939	GLN
1	C	2159	ASN
1	C	2239	GLN

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Mol	Chain	Res	Type
1	C	2251	GLN
1	C	2314	HIS
1	C	2390	ASN
1	C	2468	GLN
1	C	2470	GLN
1	C	2516	HIS
1	D	24	ASN
1	D	55	GLN
1	D	139	ASN
1	D	172	ASN
1	D	200	HIS
1	D	213	GLN
1	D	216	ASN
1	D	311	ASN
1	D	341	HIS
1	D	374	GLN
1	D	478	ASN
1	D	516	GLN
1	D	519	HIS
1	D	551	HIS
1	D	634	GLN
1	D	681	ASN
1	D	706	GLN
1	D	722	GLN
1	D	766	ASN
1	D	919	GLN
1	D	1041	GLN
1	D	1054	GLN
1	D	1056	GLN
1	D	1080	GLN
1	D	1167	ASN
1	D	1197	ASN
1	D	1206	ASN
1	D	1502	ASN
1	D	1522	HIS
1	D	1670	ASN
1	D	1741	ASN
1	D	1800	GLN
1	D	1807	ASN
1	D	1939	GLN
1	D	2075	GLN
1	D	2159	ASN

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Mol	Chain	Res	Type
1	D	2239	GLN
1	D	2251	GLN
1	D	2390	ASN
1	D	2516	HIS
1	E	24	ASN
1	E	55	GLN
1	E	139	ASN
1	E	171	HIS
1	E	172	ASN
1	E	200	HIS
1	E	213	GLN
1	E	216	ASN
1	E	311	ASN
1	E	341	HIS
1	E	374	GLN
1	E	478	ASN
1	E	516	GLN
1	E	519	HIS
1	E	551	HIS
1	E	634	GLN
1	E	681	ASN
1	E	706	GLN
1	E	722	GLN
1	E	766	ASN
1	E	1041	GLN
1	E	1054	GLN
1	E	1056	GLN
1	E	1080	GLN
1	E	1167	ASN
1	E	1197	ASN
1	E	1206	ASN
1	E	1502	ASN
1	E	1522	HIS
1	E	1670	ASN
1	E	1741	ASN
1	E	1800	GLN
1	E	1939	GLN
1	E	2075	GLN
1	E	2102	GLN
1	E	2159	ASN
1	E	2239	GLN
1	E	2251	GLN

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Mol	Chain	Res	Type
1	E	2390	ASN
1	E	2516	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

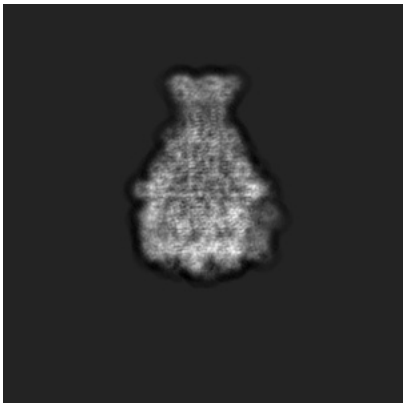
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10797. These allow visual inspection of the internal detail of the map and identification of artifacts.

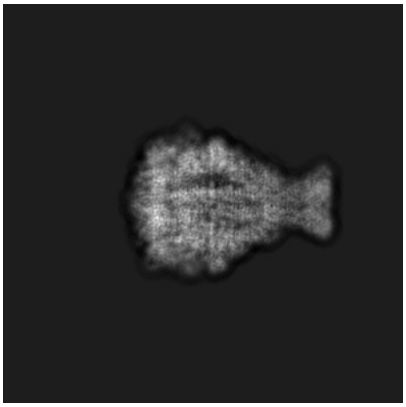
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

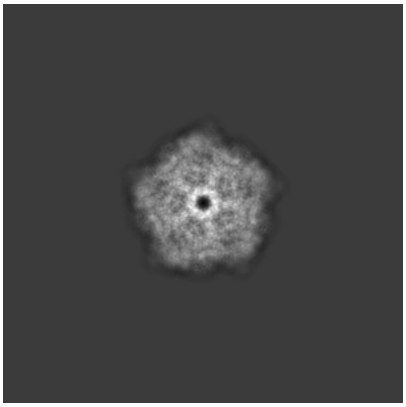
6.1.1 Primary map



X



Y

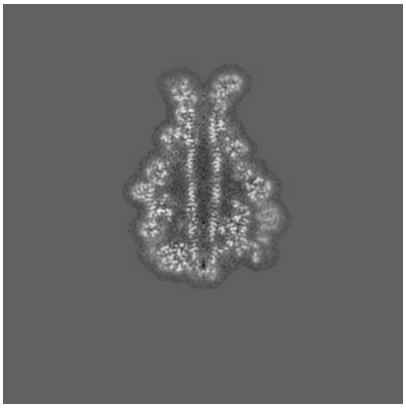


Z

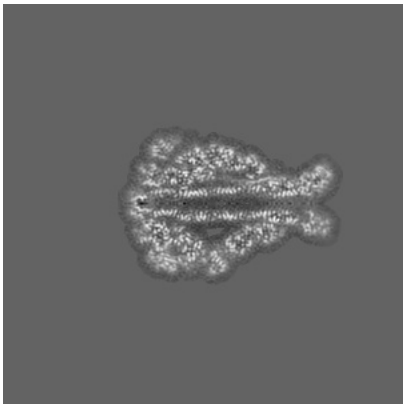
The images above show the map projected in three orthogonal directions.

6.2 Central slices

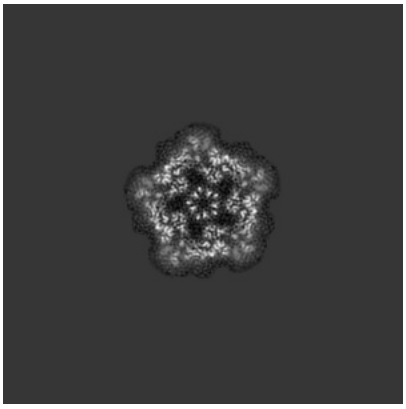
6.2.1 Primary map



X Index: 200



Y Index: 200

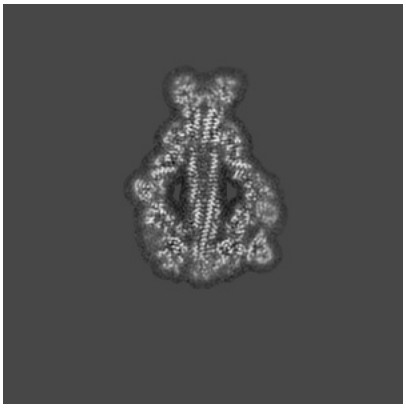


Z Index: 200

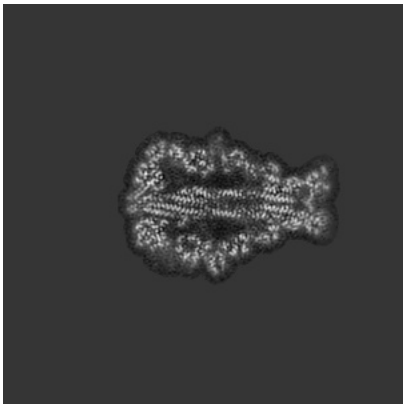
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

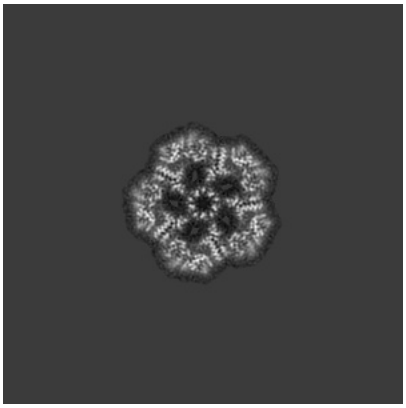
6.3.1 Primary map



X Index: 192



Y Index: 192



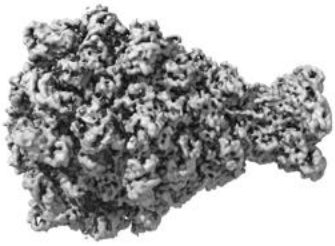
Z Index: 208

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 0.028. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

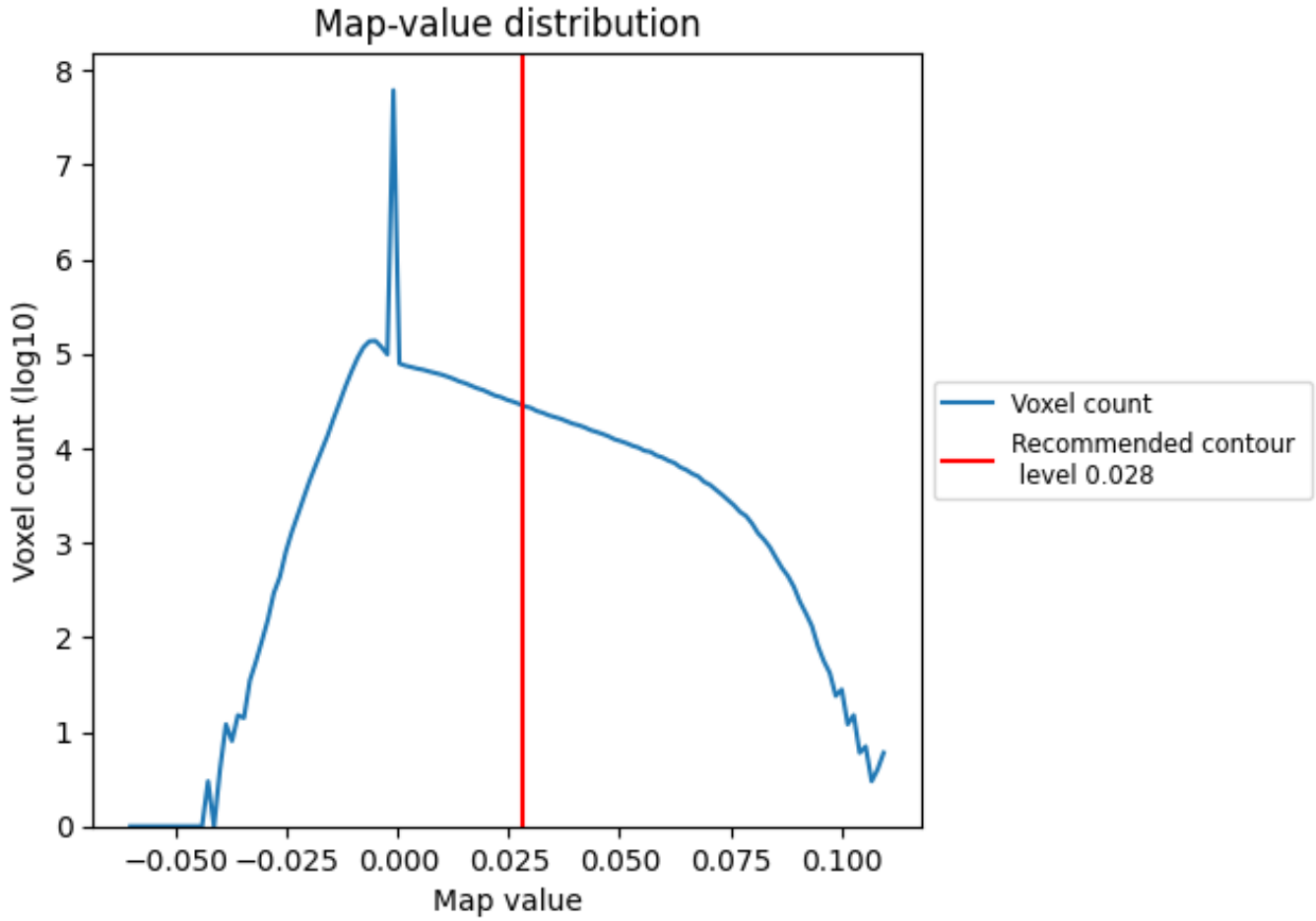
6.5 Mask visualisation (i)

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

7 Map analysis

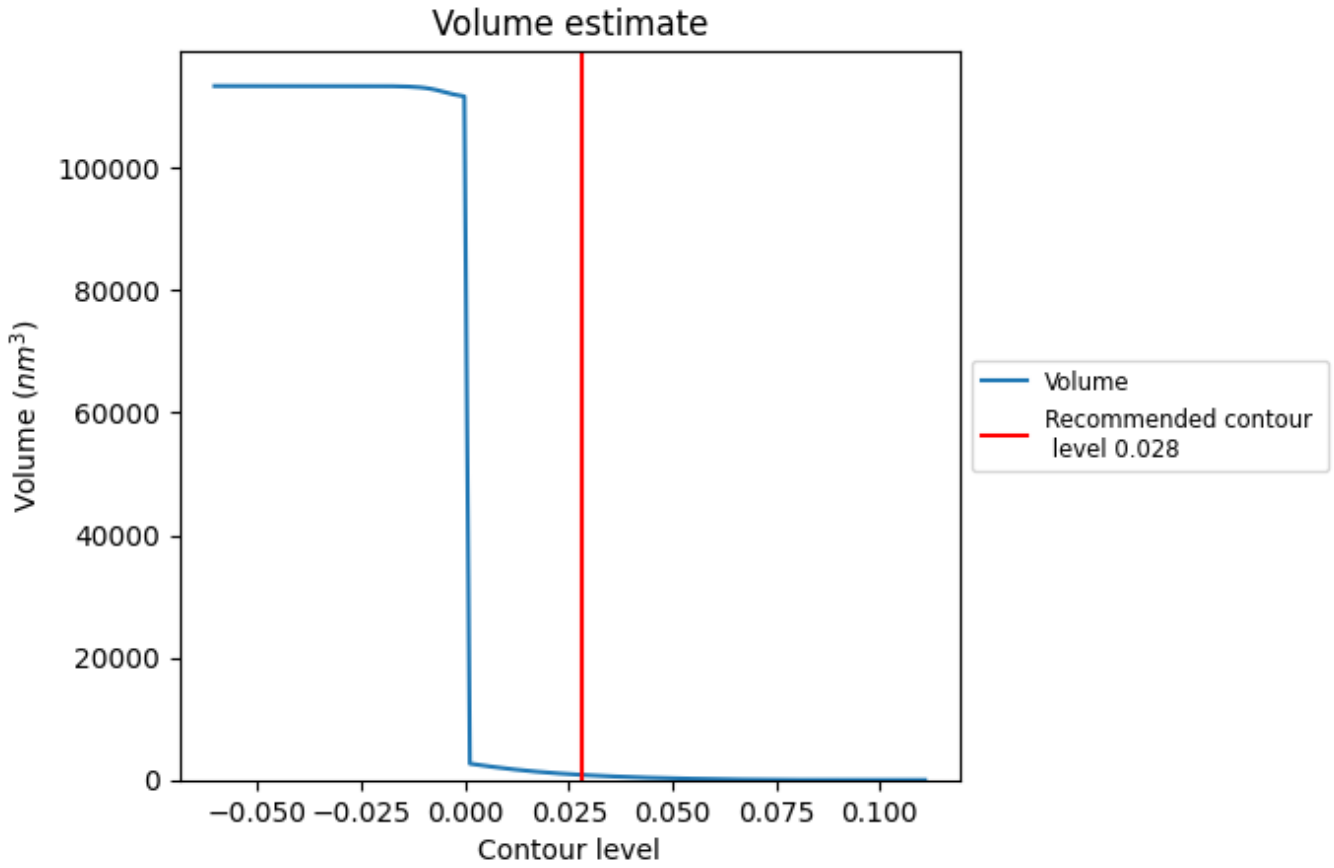
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

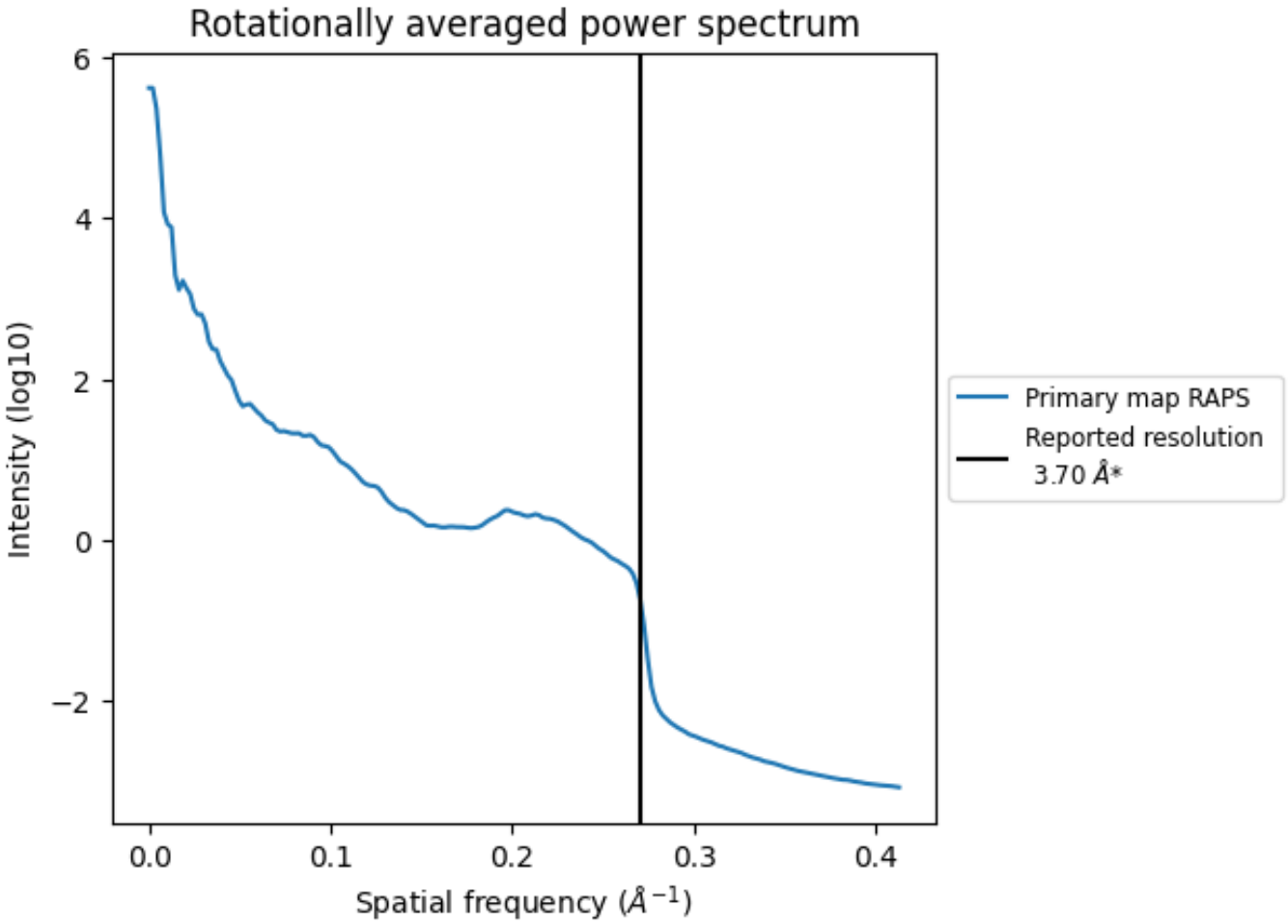
7.2 Volume estimate



The volume at the recommended contour level is 836 nm^3; this corresponds to an approximate mass of 755 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 0.270 $Å^{-1}$

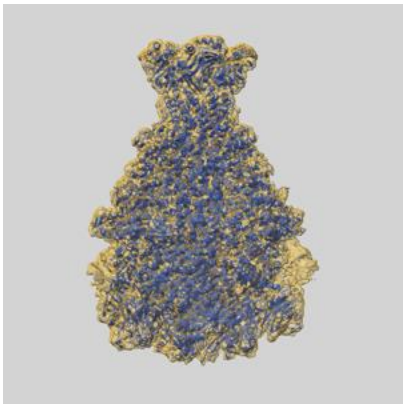
8 Fourier-Shell correlation (i)

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

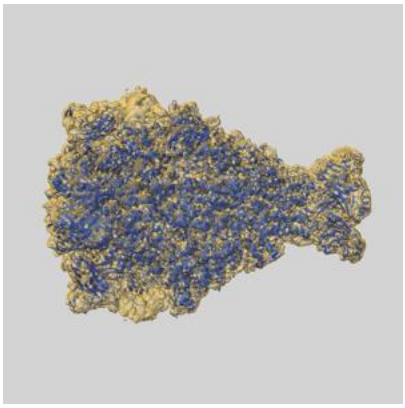
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10797 and PDB model 6YEY. Per-residue inclusion information can be found in section 3 on page 4.

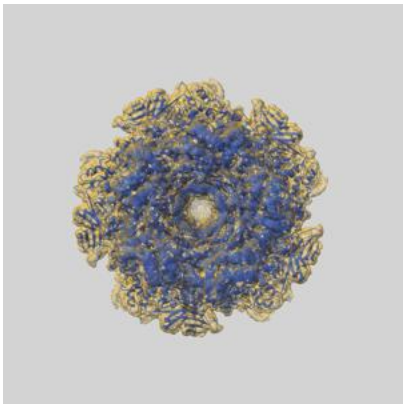
9.1 Map-model overlay



X



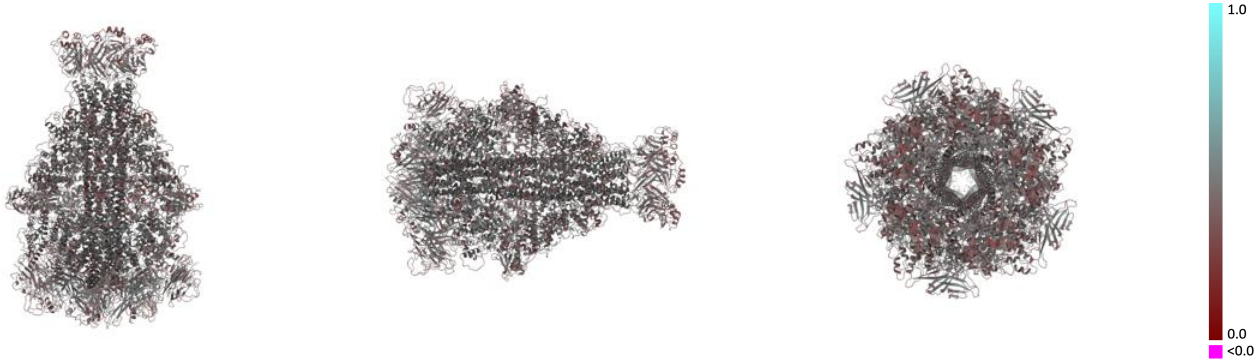
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.028 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.

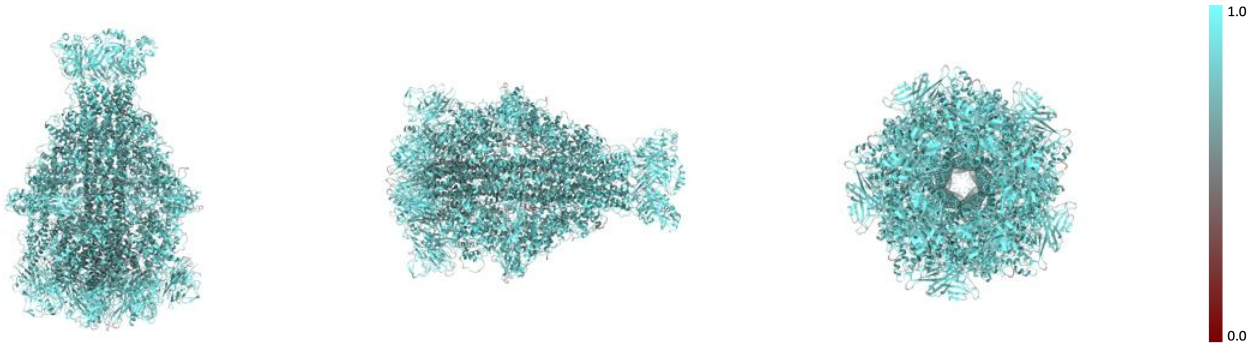
9.2 Q-score mapped to coordinate model (i)



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.

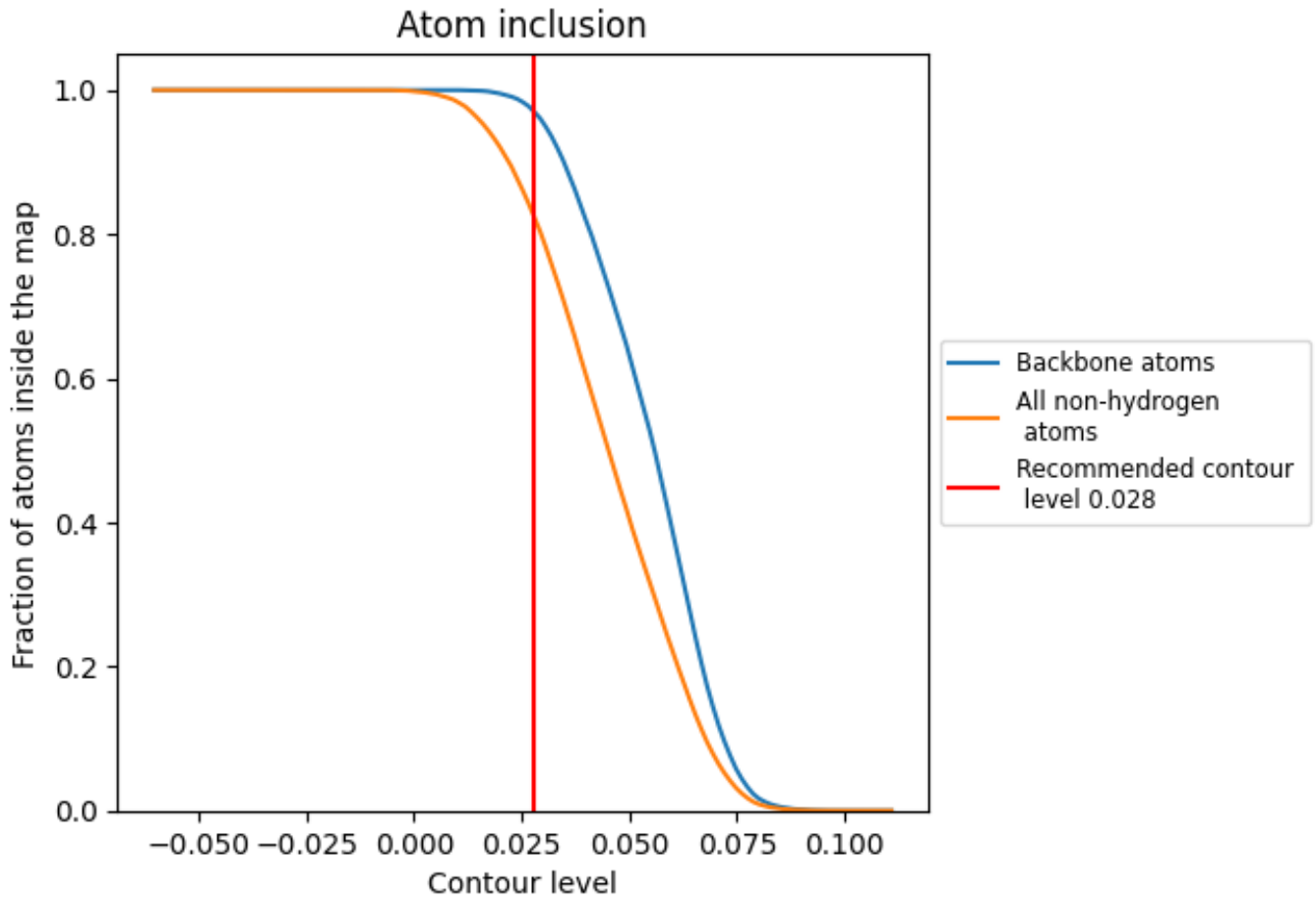
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.028).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 82% 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 (0.028) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8227	0.4340
A	0.8246	0.4360
B	0.8241	0.4360
C	0.8152	0.4230
D	0.8244	0.4370
E	0.8255	0.4360