Full wwPDB EM Validation Report ⓘ

May 18, 2024 – 02:57 pm BST

PDB ID	:	6RW8
EMDB ID	:	EMD-10034
Title	:	Cryo-EM structure of Xenorhabdus nematophila XptA1
Authors	:	Roderer, D.; Leidreiter, F.; Gatsogiannis, C.; Meusch, D.; Benz, R.; Raunser, S.
Deposited on	:	2019-06-04
Resolution	:	2.84 Å(reported)
Based on initial model	:	1VW1

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:

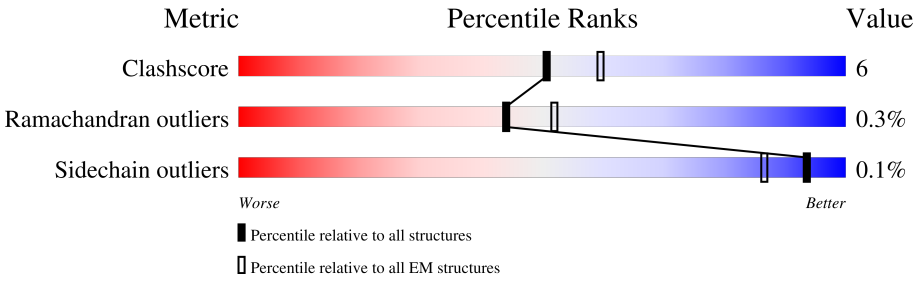
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance

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

The reported resolution of this entry is 2.84 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	77% 16% 7%
1	B	2523	76% 16% 7%
1	C	2523	77% 15% 7%
1	D	2523	77% 16% 7%
1	E	2523	77% 16% 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).

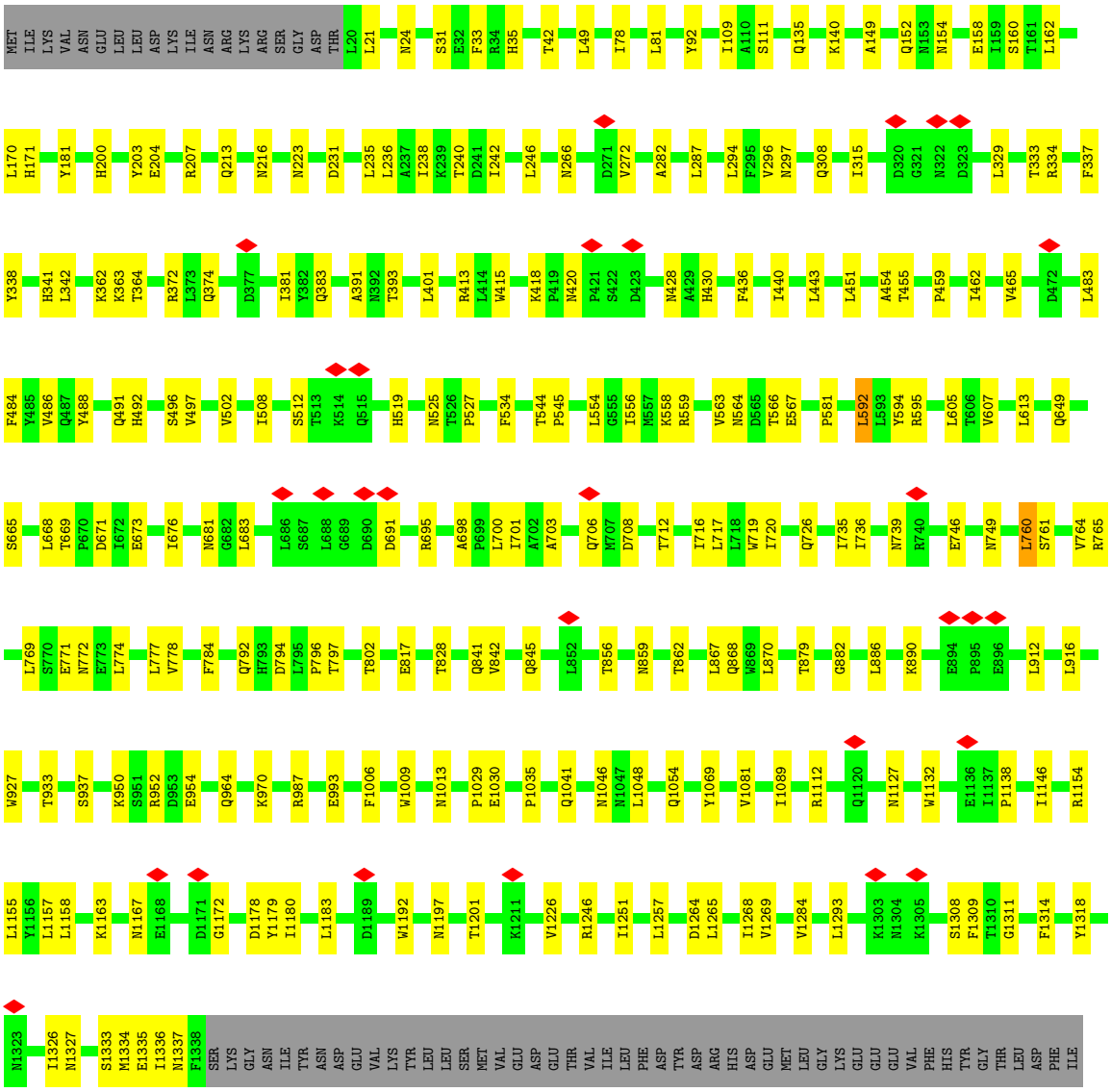
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2337	Total	C	N	O	S	0	0
			18700	11894	3132	3607	67		
1	B	2337	Total	C	N	O	S	0	0
			18700	11894	3132	3607	67		
1	C	2337	Total	C	N	O	S	0	0
			18700	11894	3132	3607	67		
1	D	2337	Total	C	N	O	S	0	0
			18700	11894	3132	3607	67		
1	E	2337	Total	C	N	O	S	0	0
		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

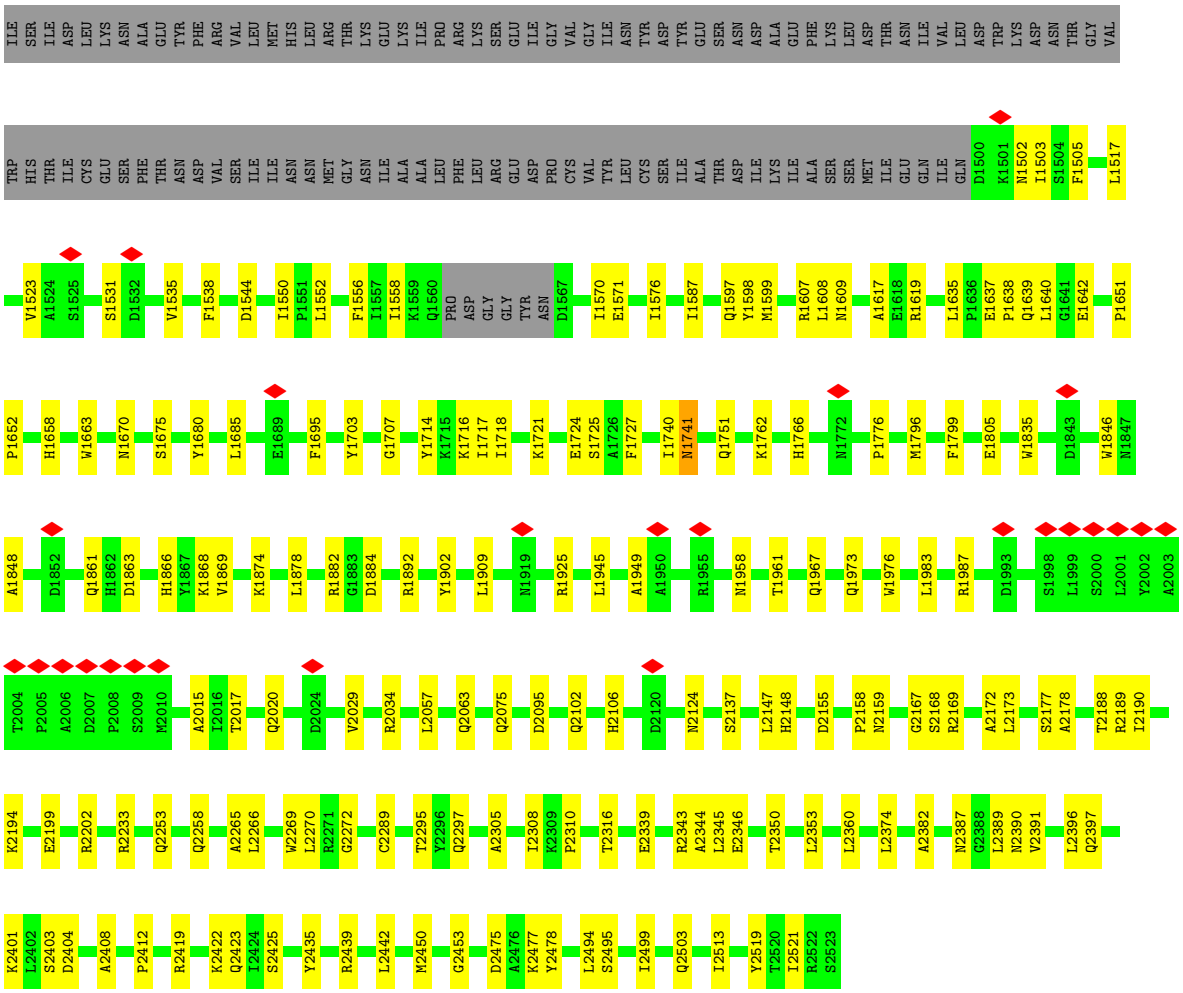
3 Residue-property plots (i)

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)

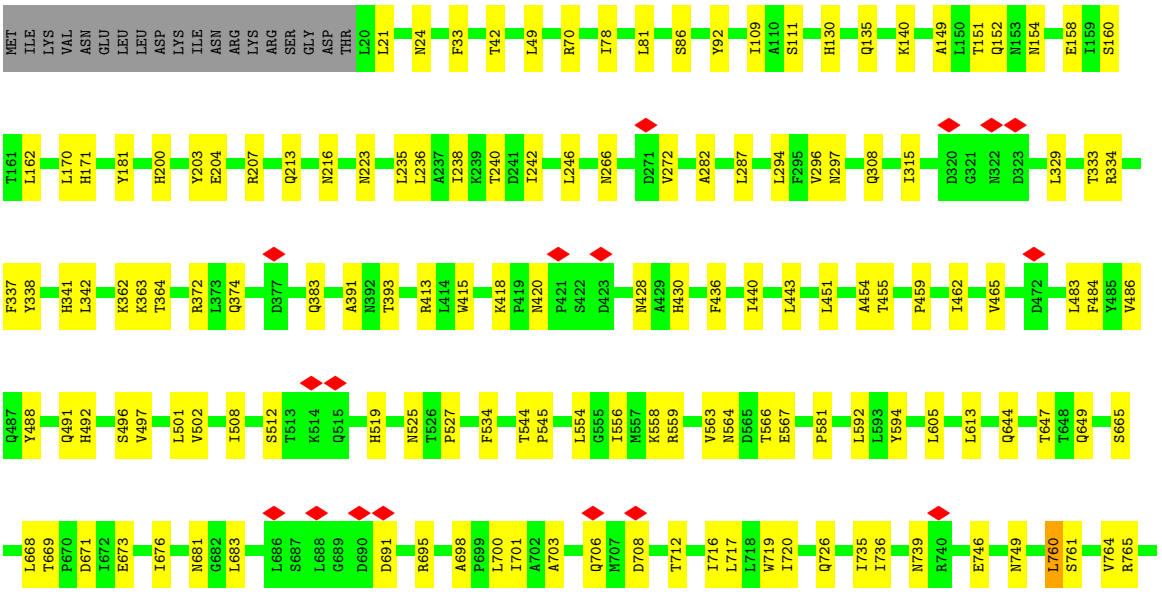
Chain A:

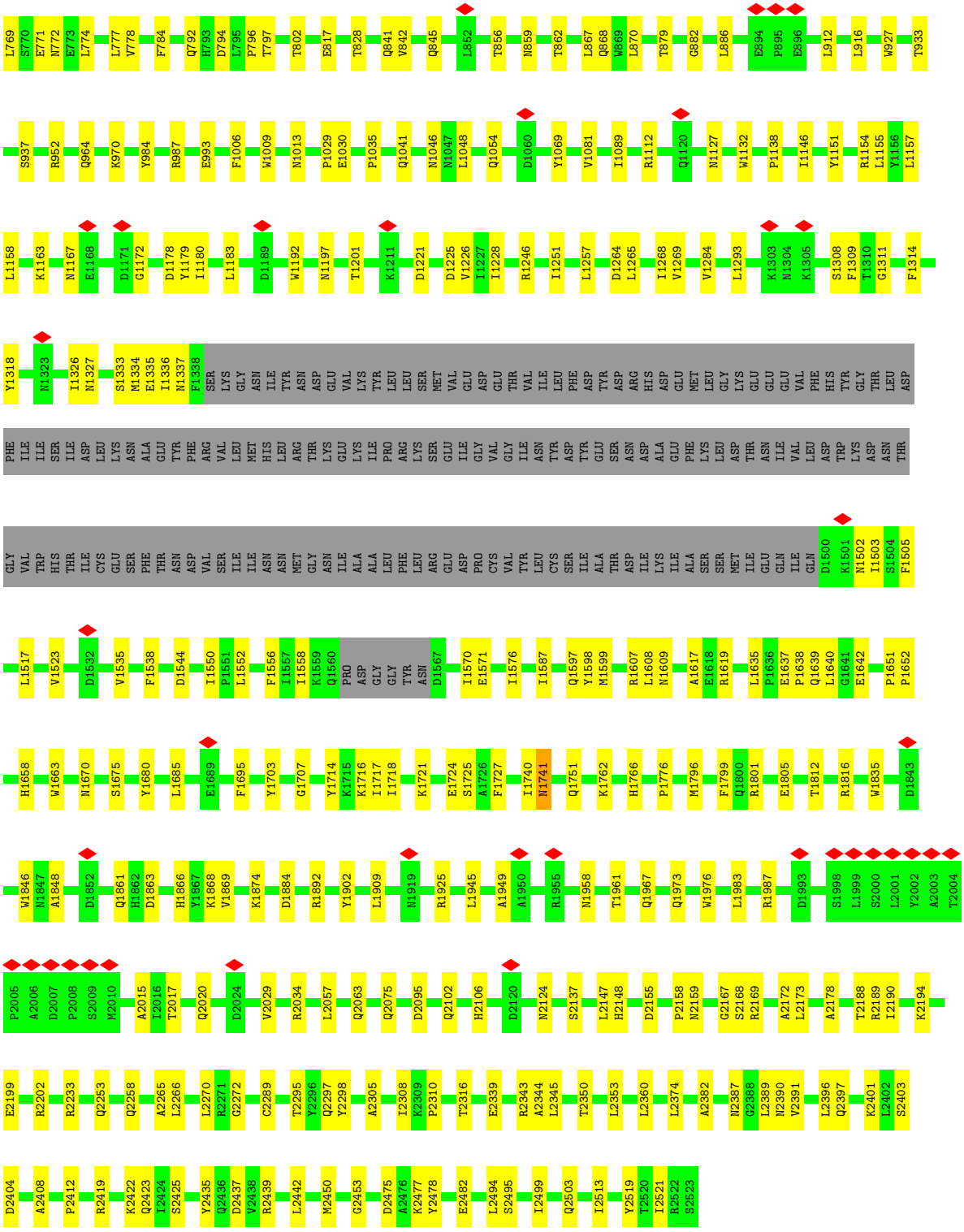




• Molecule 1: A component of insecticidal toxin complex (Tc)

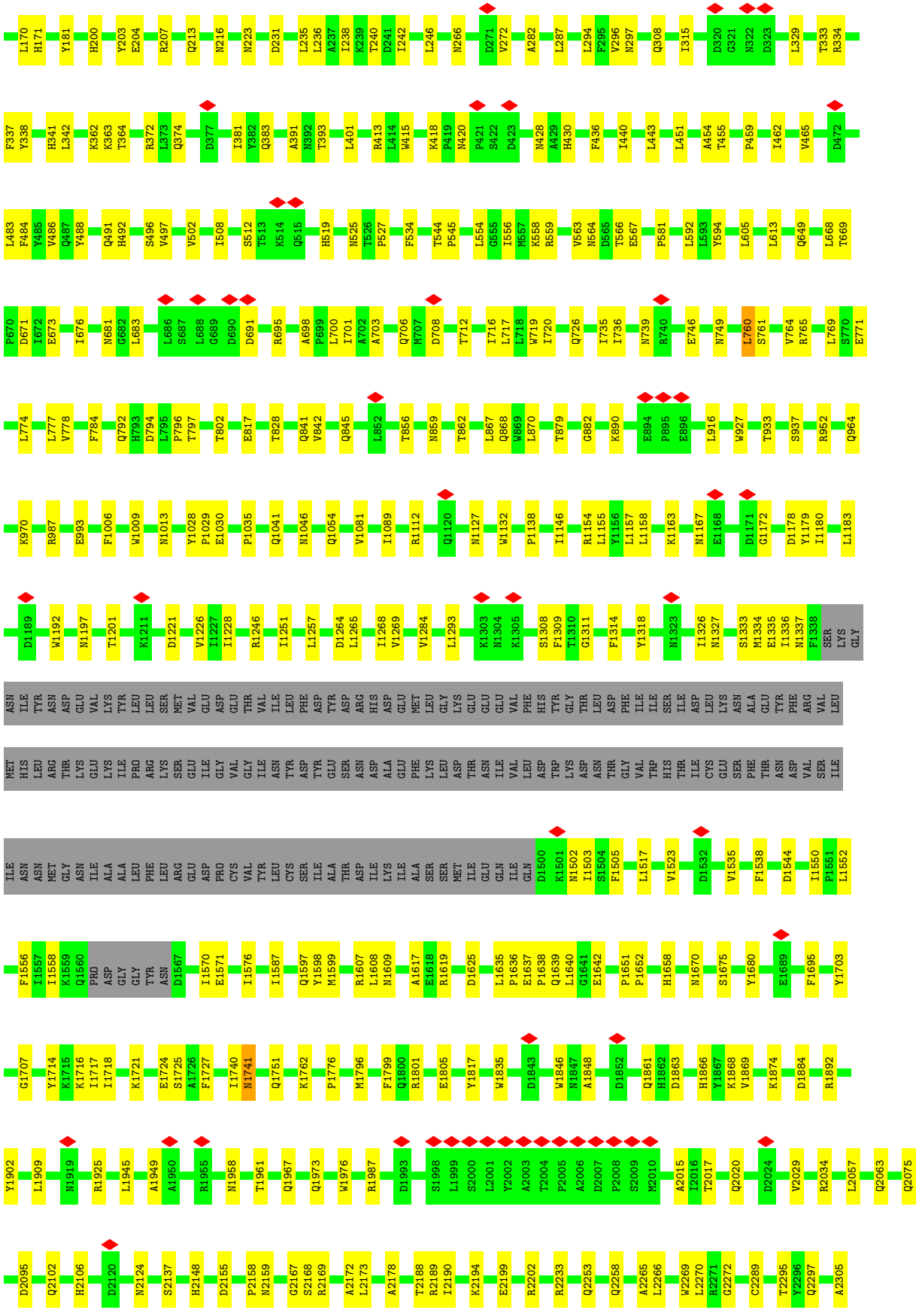
Chain B:

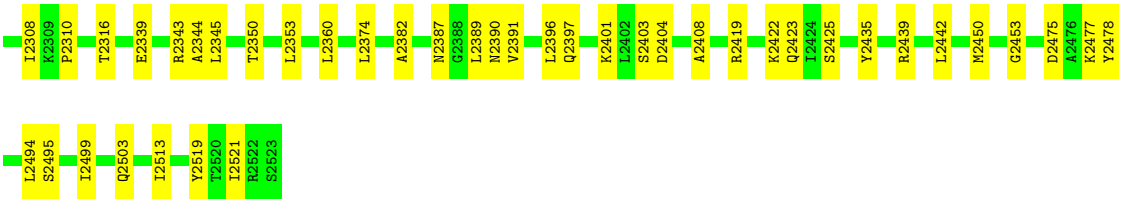




• Molecule 1: A component of insecticidal toxin complex (Tc)

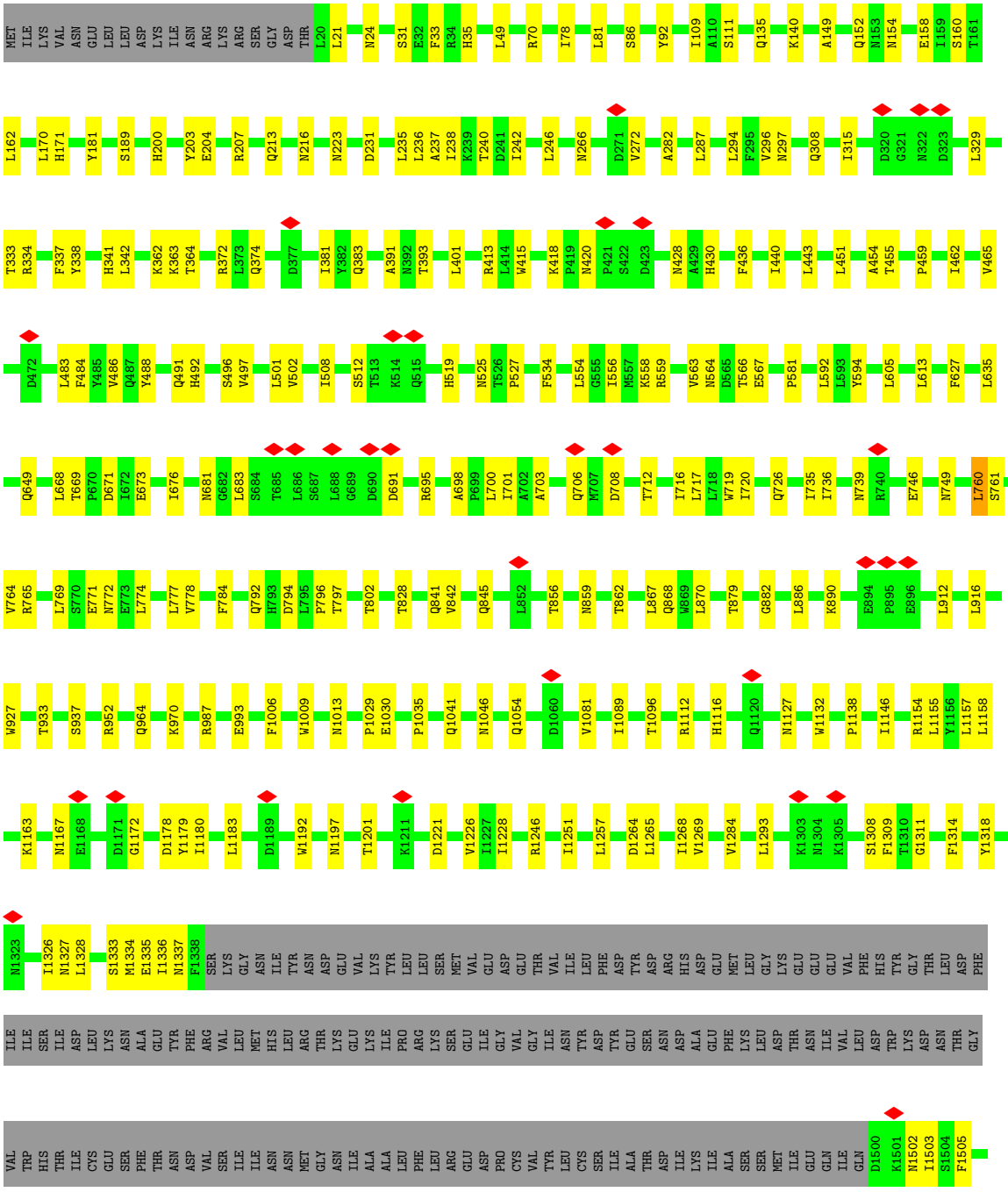
Chain C:

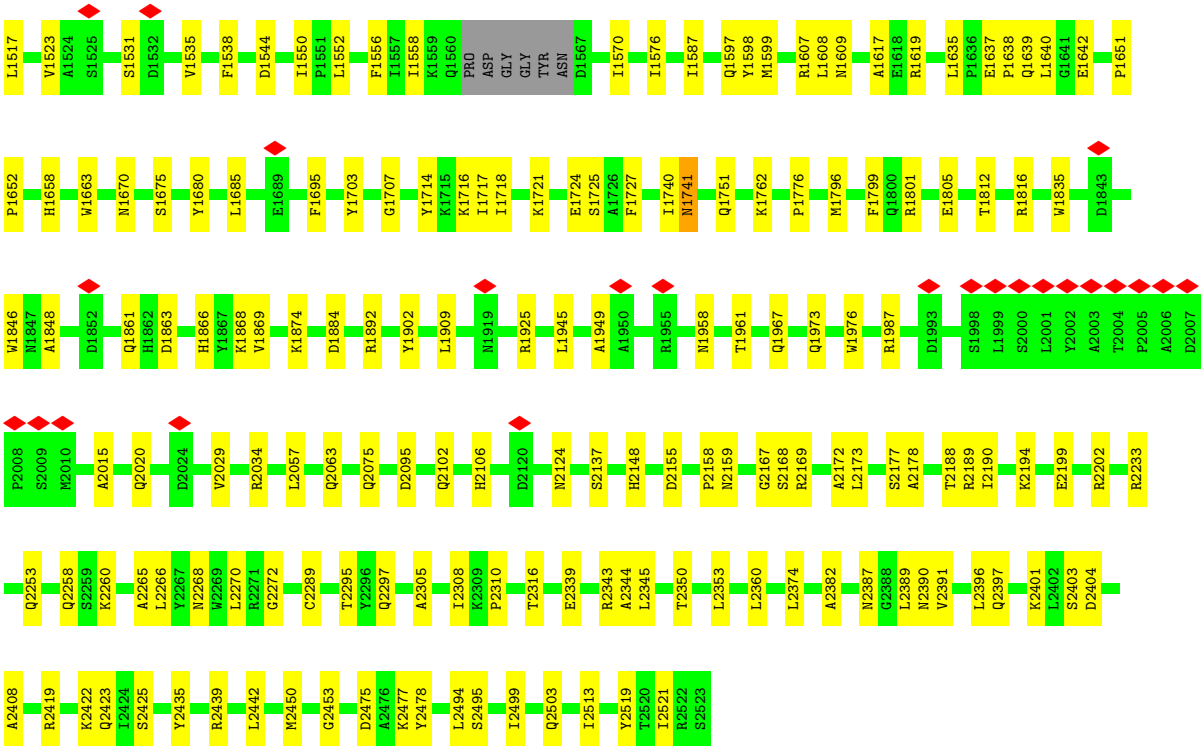

L170 H171 Y181 H200 Y203 E204 R207 Q213 N216 N223 D231 L235 L236 A237 I238 K239 T240 D241 I242 L246 N266 D271 V272 A282 L287 L294 F295 V296 N297 Q308 I315 D320 G321 N322 D323 L329 T333 R334
F337 Y338 H341 L342 K362 K363 T364 R372 L373 Q374 D377 I381 Y382 Q383 A391 N392 T393 L401 R413 L414 W415 K418 P419 N420 P421 S422 D423 N428 A429 H430 F436 I440 L443 L451 A454 T455 P459 I462 V465 D472
L483 F484 Y485 V486 Q487 Y488 Q491 H492 S496 V497 V502 I508 S512 T513 K514 Q515 H519 N525 T526 P527 F534 T544 P545 L554 G555 I556 K557 K558 R559 V563 N564 D565 T566 E567 P581 L592 L593 Y594 L605 L613 Q649 L668 T669
P670 D671 I672 E673 I676 N681 G682 L683 L686 S687 L688 G689 D690 D691 R695 A698 P699 L700 I701 A702 A703 Q706 M707 D708 T712 I716 L717 L718 W719 I720 Q726 I735 I736 N739 R740 E746 N749 L760 S761 V764 R765 L769 S770 E771
L774 L777 V778 F784 Q792 H793 D794 L795 P796 T797 T802 E817 T828 Q841 V842 Q845 L852 T856 N859 T862 L867 Q868 W869 L870 T879 G882 K890 E894 P895 E896 L916 W927 T933 S937 R952 Q964
K970 R987 E993 F1006 W1009 N1013 Y1028 P1029 E1030 P1035 Q1041 N1046 Q1054 V1081 I1089 R1112 Q1120 N1127 W1132 P1138 I1146 R1154 L1155 Y1156 L1157 L1158 K1163 N1167 E1168 D1171 G1172 D1178 Y1179 I1180 L1183
D1189 W1192 N1197 T1201 K1211 D1221 V1226 I1227 I1228 R1246 I1251 L1257 D1264 L1265 I1268 V1269 V1284 L1293 K1303 N1304 K1305 S1308 F1309 T1310 G1311 F1314 Y1318 N1323 I1326 N1327 S1333 M1334 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 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 L1517 V1523 D1532 V1535 F1538 D1544 I1550 P1551 L1552
F1556 I1557 I1558 K1559 Q1560 PRO ASP GLY GLY TYR ASN D1567 I1570 E1571 I1576 I1587 Q1597 Y1598 M1599 R1607 L1608 N1609 A1617 E1618 R1619 D1625 L1635 P1636 E1637 P1638 Q1639 L1640 G1641 E1642 P1651 P1652 H1658 N1670 S1675 Y1680 E1689 F1695 Y1703
G1707 Y1714 K1715 K1716 I1717 I1718 K1721 E1724 S1725 A1726 F1727 I1740 N1741 Q1751 K1762 P1776 M1796 F1799 Q1800 R1801 E1805 Y1817 W1835 D1843 W1846 N1847 A1848 D1852 Q1861 H1862 D1863 H1866 Y1867 K1868 V1869 K1874 D1884 R1892
Y1902 L1909 N1919 R1925 L1945 A1949 A1950 R1955 N1958 T1961 Q1967 Q1973 W1976 R1987 D1993 S1998 L1999 S2000 L2001 Y2002 A2003 T2004 P2005 A2006 D2007 P2008 S2009 M2010 A2015 I2016 T2017 Q2020 D2024 V2029 R2034 L2067 Q2063 Q2075
D2095 Q2102 H2106 D2120 N2124 S2137 H2148 D2155 P2158 N2159 G2167 S2168 R2169 A2172 L2173 A2178 T2188 R2189 I2190 K2194 E2199 R2202 R2233 Q2253 Q2258 A2265 L2266 W2269 L2270 R2271 G2272 C2289 T2295 Y2296 Q2297 A2305



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

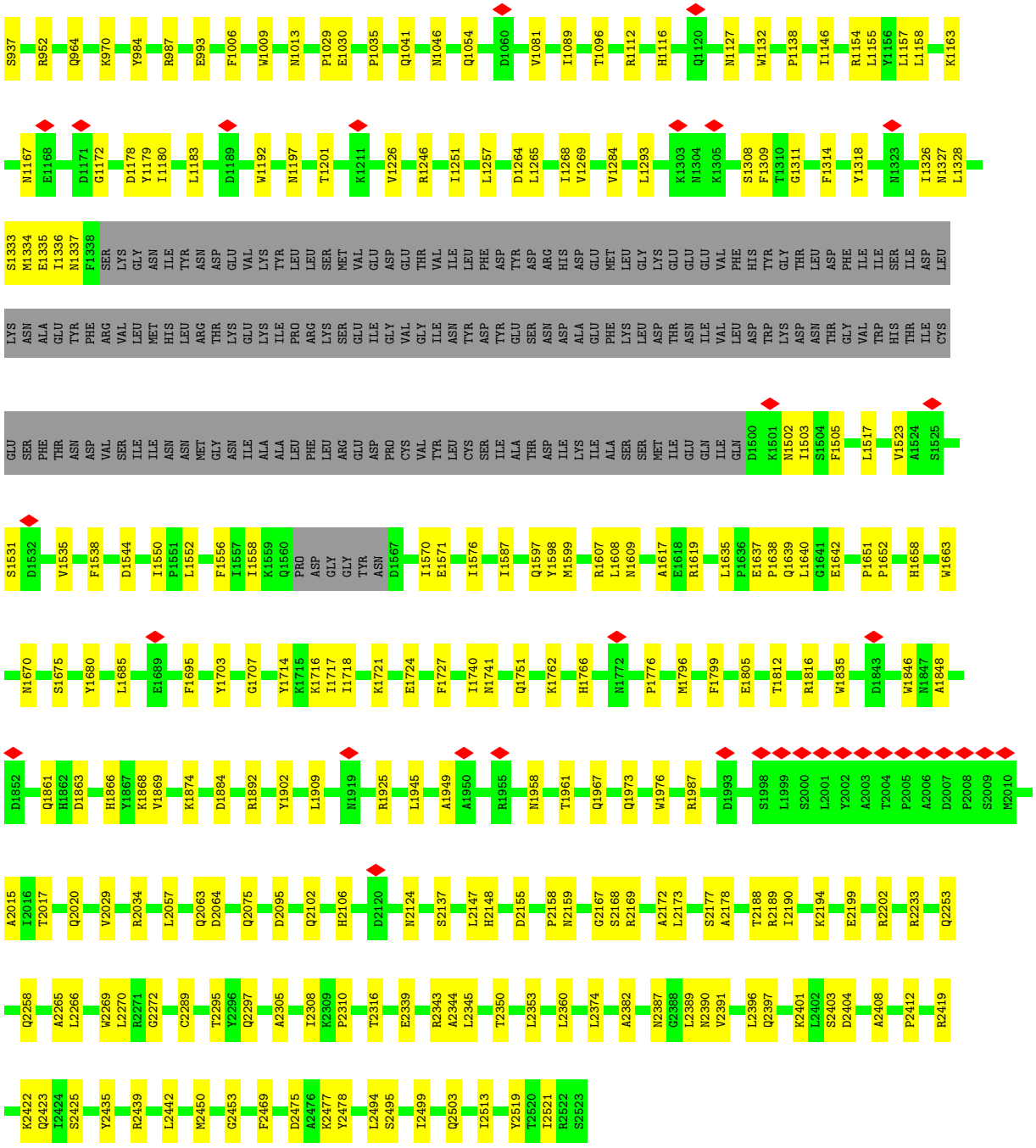
Chain D:





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

Chain E:


S937 R952 Q964 K970 Y984 R987 E993 F1006 W1009 N1013 P1029 E1030 P1035 Q1041 N1046 Q1054 D1060 V1081 I1089 T1096 R1112 H1116 Q1120 N1127 W1132 P1138 I1146 R1154 L1155 Y1156 L1157 L1158 K1163
N1167 E1168 D1171 G1172 D1178 Y1179 I1180 L1183 D1189 W1192 N1197 T1201 K1211 V1226 R1246 I1251 L1257 D1264 L1265 I1268 V1269 V1284 L1293 K1303 N1304 K1305 S1308 F1309 T1310 G1311 F1314 Y1318 N1323 I1326 N1327 L1328
S1333 M1334 E1335 I1336 N1337 F1338 SER LYS GLY ASN ILE TYR ASN ASP GLU VAL LYS TYR LEU LEU SER MET VAL GLU ASP GLU 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 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 L1517 V1523 A1524 S1525
S1531 D1532 V1535 F1538 D1544 I1550 P1551 L1552 F1556 I1557 I1558 K1559 Q1560 PRO ASP GLY GLY TYR ASN D1567 I1570 E1571 I1576 I1587 Q1597 Y1598 M1599 R1607 L1608 N1609 A1617 E1618 R1619 L1635 P1636 E1637 P1638 Q1639 L1640 G1641 E1642 P1651 P1652 H1658 W1663
N1670 S1675 Y1680 L1685 E1689 F1695 Y1703 G1707 Y1714 K1715 K1716 I1717 I1718 K1721 E1724 F1727 I1740 N1741 Q1751 K1762 H1766 N1772 P1776 M1796 F1799 E1805 T1812 R1816 W1835 D1843 W1846 N1847 A1848
D1852 Q1861 H1862 D1863 H1866 Y1867 K1868 V1869 K1874 D1884 R1892 Y1902 L1909 N1919 R1925 L1945 A1949 A1950 R1955 N1958 T1961 Q1967 Q1973 W1976 R1987 D1993 S1998 L1999 S2000 L2001 Y2002 A2003 T2004 P2005 A2006 D2007 P2008 S2009 M2010
A2015 I2016 T2017 Q2020 V2029 R2034 L2057 Q2063 D2064 Q2075 D2095 Q2102 H2106 D2120 N2124 S2137 L2147 H2148 D2155 P2158 N2159 G2167 S2168 R2169 A2172 L2173 S2177 A2178 T2188 R2189 I2190 K2194 E2199 R2202 R2233 Q2253
Q2258 A2265 L2266 W2269 L2270 R2271 G2272 C2289 T2295 Y2296 Q2297 A2305 I2308 K2309 P2310 T2316 E2339 R2343 A2344 L2345 T2350 L2353 L2360 L2374 A2382 N2387 G2388 L2389 N2390 V2391 L2396 Q2397 K2401 L2402 S2403 D2404 A2408 P2412 R2419
K2422 Q2423 I2424 S2425 Y2435 R2439 L2442 M2450 G2453 F2469 D2475 A2476 K2477 Y2478 L2494 S2495 I2499 Q2503 I2513 Y2519 I2520 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	218992	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.130	Depositor
Minimum map value	-0.040	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.028	Depositor
Map size (Å)	456.0, 456.0, 456.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.14, 1.14, 1.14	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	0.36	0/19100	0.60	3/25936 (0.0%)
1	B	0.36	0/19100	0.60	3/25936 (0.0%)
1	C	0.36	0/19100	0.60	3/25936 (0.0%)
1	D	0.36	0/19100	0.60	3/25936 (0.0%)
1	E	0.36	0/19100	0.60	3/25936 (0.0%)
All	All	0.36	0/95500	0.60	15/129680 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	3
1	C	0	3
1	D	0	3
1	E	0	3
All	All	0	15

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	668	LEU	C-N-CA	10.59	148.18	121.70
1	B	668	LEU	C-N-CA	10.58	148.16	121.70
1	C	668	LEU	C-N-CA	10.58	148.15	121.70
1	D	668	LEU	C-N-CA	10.58	148.15	121.70
1	E	668	LEU	C-N-CA	10.58	148.14	121.70
1	B	760	LEU	CB-CG-CD2	-6.37	100.17	111.00
1	C	760	LEU	CB-CG-CD2	-6.37	100.17	111.00
1	D	760	LEU	CB-CG-CD2	-6.34	100.23	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	760	LEU	CB-CG-CD2	-6.33	100.24	111.00
1	E	760	LEU	CB-CG-CD2	-6.32	100.26	111.00
1	B	592	LEU	CA-CB-CG	5.96	129.00	115.30
1	C	592	LEU	CA-CB-CG	5.96	129.00	115.30
1	E	592	LEU	CA-CB-CG	5.95	128.99	115.30
1	D	592	LEU	CA-CB-CG	5.95	128.97	115.30
1	A	592	LEU	CA-CB-CG	5.93	128.95	115.30

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1741	ASN	Peptide
1	A	2344	ALA	Peptide
1	A	2450	MET	Peptide
1	B	1741	ASN	Peptide
1	B	2344	ALA	Peptide
1	B	2450	MET	Peptide
1	C	1741	ASN	Peptide
1	C	2344	ALA	Peptide
1	C	2450	MET	Peptide
1	D	1741	ASN	Peptide
1	D	2344	ALA	Peptide
1	D	2450	MET	Peptide
1	E	1741	ASN	Peptide
1	E	2344	ALA	Peptide
1	E	2450	MET	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	18399	248	0
1	B	18700	0	18399	253	0
1	C	18700	0	18399	240	0
1	D	18700	0	18399	246	0
1	E	18700	0	18399	246	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	93500	0	91995	1099	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 (1099) 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:E:1598:TYR:HB3	1:E:1640:LEU:HD22	1.73	0.70
1:A:1598:TYR:HB3	1:A:1640:LEU:HD22	1.73	0.70
1:C:525:ASN:HD21	1:C:534:PHE:H	1.40	0.70
1:D:525:ASN:HD21	1:D:534:PHE:H	1.39	0.70
1:B:1598:TYR:HB3	1:B:1640:LEU:HD22	1.73	0.69
1:D:1598:TYR:HB3	1:D:1640:LEU:HD22	1.73	0.69
1:B:525:ASN:HD21	1:B:534:PHE:H	1.39	0.69
1:C:374:GLN:HE21	1:C:413:ARG:HD2	1.58	0.69
1:D:374:GLN:HE21	1:D:413:ARG:HD2	1.59	0.68
1:C:1598:TYR:HB3	1:C:1640:LEU:HD22	1.73	0.68
1:E:525:ASN:HD21	1:E:534:PHE:H	1.39	0.68
1:A:525:ASN:HD21	1:A:534:PHE:H	1.39	0.68
1:B:374:GLN:HE21	1:B:413:ARG:HD2	1.58	0.68
1:E:374:GLN:HE21	1:E:413:ARG:HD2	1.58	0.67
1:B:2194:LYS:HD2	1:D:1054:GLN:HE21	1.60	0.67
1:A:374:GLN:HE21	1:A:413:ARG:HD2	1.58	0.66
1:A:2194:LYS:HD2	1:C:1054:GLN:HE21	1.60	0.66
1:C:2194:LYS:HD2	1:E:1054:GLN:HE21	1.60	0.66
1:A:1054:GLN:HE21	1:D:2194:LYS:HD2	1.59	0.65
1:D:216:ASN:HD22	1:D:491:GLN:HE21	1.44	0.65
1:B:372:ARG:HB2	1:B:415:TRP:HB2	1.79	0.65
1:B:1054:GLN:HE21	1:E:2194:LYS:HD2	1.62	0.65
1:E:372:ARG:HB2	1:E:415:TRP:HB2	1.79	0.65
1:C:216:ASN:HD22	1:C:491:GLN:HE21	1.44	0.64
1:A:216:ASN:HD22	1:A:491:GLN:HE21	1.44	0.64
1:A:372:ARG:HB2	1:A:415:TRP:HB2	1.79	0.64
1:D:372:ARG:HB2	1:D:415:TRP:HB2	1.79	0.64
1:C:372:ARG:HB2	1:C:415:TRP:HB2	1.79	0.64
1:E:216:ASN:HD22	1:E:491:GLN:HE21	1.44	0.64
1:B:216:ASN:HD22	1:B:491:GLN:HE21	1.44	0.63
1:E:1607:ARG:NH2	1:E:1638:PRO:O	2.32	0.62
1:A:1607:ARG:NH2	1:A:1638:PRO:O	2.32	0.62
1:D:761:SER:OG	1:D:765:ARG:NH2	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:761:SER:OG	1:E:765:ARG:NH2	2.33	0.62
1:B:1607:ARG:NH2	1:B:1638:PRO:O	2.32	0.62
1:E:2020:GLN:H	1:E:2316:THR:HG22	1.64	0.62
1:A:761:SER:OG	1:A:765:ARG:NH2	2.33	0.62
1:A:2020:GLN:H	1:A:2316:THR:HG22	1.64	0.62
1:C:761:SER:OG	1:C:765:ARG:NH2	2.33	0.62
1:C:1607:ARG:NH2	1:C:1638:PRO:O	2.32	0.62
1:D:2020:GLN:H	1:D:2316:THR:HG22	1.64	0.62
1:D:2396:LEU:HB2	1:D:2499:ILE:HD12	1.82	0.61
1:A:1724:GLU:HG2	1:A:1762:LYS:HD2	1.83	0.61
1:B:761:SER:OG	1:B:765:ARG:NH2	2.33	0.61
1:C:2020:GLN:H	1:C:2316:THR:HG22	1.64	0.61
1:A:2258:GLN:HB3	1:B:2015:ALA:HB2	1.82	0.61
1:D:1607:ARG:NH2	1:D:1638:PRO:O	2.32	0.61
1:A:337:PHE:HB3	1:A:341:HIS:HD2	1.65	0.61
1:D:2270:LEU:HD21	1:E:2057:LEU:HD11	1.82	0.61
1:B:1724:GLU:HG2	1:B:1762:LYS:HD2	1.83	0.61
1:E:337:PHE:HB3	1:E:341:HIS:HD2	1.66	0.61
1:E:2396:LEU:HB2	1:E:2499:ILE:HD12	1.82	0.61
1:B:2020:GLN:H	1:B:2316:THR:HG22	1.64	0.61
1:B:2258:GLN:HB3	1:C:2015:ALA:HB2	1.83	0.61
1:E:1724:GLU:HG2	1:E:1762:LYS:HD2	1.83	0.61
1:D:1724:GLU:HG2	1:D:1762:LYS:HD2	1.82	0.61
1:C:2258:GLN:HB3	1:D:2015:ALA:HB2	1.81	0.61
1:C:2396:LEU:HB2	1:C:2499:ILE:HD12	1.82	0.61
1:C:1724:GLU:HG2	1:C:1762:LYS:HD2	1.83	0.61
1:A:1505:PHE:HB3	1:A:1517:LEU:HB2	1.83	0.60
1:C:337:PHE:HB3	1:C:341:HIS:HD2	1.65	0.60
1:E:1505:PHE:HB3	1:E:1517:LEU:HB2	1.83	0.60
1:D:337:PHE:HB3	1:D:341:HIS:HD2	1.65	0.60
1:C:1505:PHE:HB3	1:C:1517:LEU:HB2	1.83	0.60
1:A:2396:LEU:HB2	1:A:2499:ILE:HD12	1.82	0.60
1:D:1607:ARG:HE	1:D:1640:LEU:HD21	1.67	0.60
1:E:1607:ARG:HE	1:E:1640:LEU:HD21	1.67	0.60
1:C:342:LEU:HA	1:C:362:LYS:H	1.67	0.60
1:C:1556:PHE:HB2	1:C:1570:ILE:HB	1.84	0.59
1:B:337:PHE:HB3	1:B:341:HIS:HD2	1.65	0.59
1:B:1505:PHE:HB3	1:B:1517:LEU:HB2	1.83	0.59
1:B:1607:ARG:HE	1:B:1640:LEU:HD21	1.67	0.59
1:A:1607:ARG:HE	1:A:1640:LEU:HD21	1.67	0.59
1:D:342:LEU:HA	1:D:362:LYS:H	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1505:PHE:HB3	1:D:1517:LEU:HB2	1.83	0.59
1:E:342:LEU:HA	1:E:362:LYS:H	1.67	0.59
1:A:342:LEU:HA	1:A:362:LYS:H	1.67	0.59
1:B:2396:LEU:HB2	1:B:2499:ILE:HD12	1.82	0.59
1:C:1607:ARG:HE	1:C:1640:LEU:HD21	1.67	0.59
1:A:1556:PHE:HB2	1:A:1570:ILE:HB	1.84	0.59
1:A:2015:ALA:HB2	1:E:2258:GLN:HB3	1.83	0.59
1:B:342:LEU:HA	1:B:362:LYS:H	1.67	0.59
1:E:1556:PHE:HB2	1:E:1570:ILE:HB	1.84	0.59
1:B:2034:ARG:NH1	1:B:2475:ASP:O	2.36	0.59
1:D:1335:GLU:HG2	1:D:1535:VAL:HG22	1.85	0.59
1:D:2258:GLN:HB3	1:E:2015:ALA:HB2	1.84	0.59
1:A:2034:ARG:NH1	1:A:2475:ASP:O	2.36	0.59
1:B:534:PHE:HB2	1:B:556:ILE:HD13	1.85	0.59
1:B:364:THR:H	1:B:391:ALA:HB2	1.68	0.58
1:C:2034:ARG:NH1	1:C:2475:ASP:O	2.36	0.58
1:E:2034:ARG:NH1	1:E:2475:ASP:O	2.36	0.58
1:A:1246:ARG:HD2	1:A:1269:VAL:HG21	1.86	0.58
1:A:1335:GLU:HG2	1:A:1535:VAL:HG22	1.85	0.58
1:B:1246:ARG:HD2	1:B:1269:VAL:HG21	1.86	0.58
1:E:364:THR:H	1:E:391:ALA:HB2	1.68	0.58
1:A:534:PHE:HB2	1:A:556:ILE:HD13	1.85	0.58
1:B:1335:GLU:HG2	1:B:1535:VAL:HG22	1.85	0.58
1:A:2423:GLN:HE22	1:A:2425:SER:HB3	1.69	0.58
1:C:534:PHE:HB2	1:C:556:ILE:HD13	1.85	0.58
1:B:2423:GLN:HE22	1:B:2425:SER:HB3	1.69	0.58
1:A:987:ARG:NH1	1:A:993:GLU:OE2	2.37	0.58
1:B:987:ARG:NH1	1:B:993:GLU:OE2	2.37	0.58
1:B:1556:PHE:HB2	1:B:1570:ILE:HB	1.84	0.58
1:D:364:THR:H	1:D:391:ALA:HB2	1.68	0.58
1:D:1556:PHE:HB2	1:D:1570:ILE:HB	1.84	0.58
1:A:1703:TYR:HB3	1:A:1707:GLY:HA2	1.86	0.58
1:C:364:THR:H	1:C:391:ALA:HB2	1.68	0.58
1:C:1246:ARG:HD2	1:C:1269:VAL:HG21	1.86	0.58
1:E:1335:GLU:HG2	1:E:1535:VAL:HG22	1.85	0.58
1:A:364:THR:H	1:A:391:ALA:HB2	1.68	0.58
1:E:987:ARG:NH1	1:E:993:GLU:OE2	2.37	0.58
1:E:1246:ARG:HD2	1:E:1269:VAL:HG21	1.86	0.58
1:E:2423:GLN:HE22	1:E:2425:SER:HB3	1.69	0.58
1:C:1703:TYR:HB3	1:C:1707:GLY:HA2	1.86	0.58
1:D:706:GLN:HE22	1:E:2265:ALA:HA	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:987:ARG:NH1	1:D:993:GLU:OE2	2.37	0.58
1:D:2034:ARG:NH1	1:D:2475:ASP:O	2.36	0.58
1:B:1703:TYR:HB3	1:B:1707:GLY:HA2	1.86	0.57
1:C:1335:GLU:HG2	1:C:1535:VAL:HG22	1.85	0.57
1:C:2423:GLN:HE22	1:C:2425:SER:HB3	1.69	0.57
1:D:1703:TYR:HB3	1:D:1707:GLY:HA2	1.86	0.57
1:E:1703:TYR:HB3	1:E:1707:GLY:HA2	1.86	0.57
1:D:1246:ARG:HD2	1:D:1269:VAL:HG21	1.86	0.57
1:E:534:PHE:HB2	1:E:556:ILE:HD13	1.85	0.57
1:B:1327:ASN:ND2	1:B:1544:ASP:OD1	2.37	0.57
1:D:296:VAL:HG13	1:D:315:ILE:HD11	1.86	0.57
1:D:2423:GLN:HE22	1:D:2425:SER:HB3	1.69	0.57
1:E:1639:GLN:NE2	1:E:1642:GLU:O	2.38	0.57
1:A:158:GLU:OE2	1:B:1892:ARG:NH2	2.37	0.57
1:A:2265:ALA:HA	1:E:706:GLN:HE22	1.69	0.57
1:C:1639:GLN:NE2	1:C:1642:GLU:O	2.38	0.57
1:A:828:THR:HG22	1:A:856:THR:HG22	1.87	0.57
1:D:242:ILE:HA	1:D:246:LEU:HD23	1.87	0.57
1:C:987:ARG:NH1	1:C:993:GLU:OE2	2.37	0.57
1:D:534:PHE:HB2	1:D:556:ILE:HD13	1.85	0.57
1:D:2360:LEU:HD11	1:D:2387:ASN:HB3	1.87	0.57
1:A:2057:LEU:HD11	1:E:2270:LEU:HD21	1.87	0.57
1:B:828:THR:HG22	1:B:856:THR:HG22	1.87	0.57
1:B:2270:LEU:HD21	1:C:2057:LEU:HD11	1.85	0.57
1:C:242:ILE:HA	1:C:246:LEU:HD23	1.87	0.57
1:C:333:THR:HB	1:C:430:HIS:HB3	1.87	0.57
1:A:1639:GLN:NE2	1:A:1642:GLU:O	2.38	0.57
1:B:160:SER:HA	1:B:970:LYS:HA	1.87	0.57
1:C:296:VAL:HG13	1:C:315:ILE:HD11	1.86	0.57
1:D:158:GLU:OE2	1:E:1892:ARG:NH2	2.38	0.57
1:D:333:THR:HB	1:D:430:HIS:HB3	1.87	0.57
1:D:1639:GLN:NE2	1:D:1642:GLU:O	2.38	0.57
1:A:296:VAL:HG13	1:A:315:ILE:HD11	1.86	0.56
1:A:1892:ARG:NH2	1:E:158:GLU:OE2	2.38	0.56
1:B:296:VAL:HG13	1:B:315:ILE:HD11	1.86	0.56
1:B:1639:GLN:NE2	1:B:1642:GLU:O	2.38	0.56
1:C:1607:ARG:NH1	1:C:1637:GLU:OE1	2.38	0.56
1:E:1607:ARG:NH1	1:E:1637:GLU:OE1	2.38	0.56
1:D:1670:ASN:ND2	1:D:1675:SER:OG	2.39	0.56
1:E:1327:ASN:ND2	1:E:1544:ASP:OD1	2.37	0.56
1:C:1670:ASN:ND2	1:C:1675:SER:OG	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:649:GLN:NE2	1:D:802:THR:OG1	2.39	0.56
1:D:828:THR:HG22	1:D:856:THR:HG22	1.87	0.56
1:E:649:GLN:NE2	1:E:802:THR:OG1	2.39	0.56
1:A:242:ILE:HA	1:A:246:LEU:HD23	1.87	0.56
1:B:333:THR:HB	1:B:430:HIS:HB3	1.87	0.56
1:D:1607:ARG:NH1	1:D:1637:GLU:OE1	2.38	0.56
1:E:1670:ASN:ND2	1:E:1675:SER:OG	2.39	0.56
1:E:242:ILE:HA	1:E:246:LEU:HD23	1.86	0.56
1:E:333:THR:HB	1:E:430:HIS:HB3	1.87	0.56
1:A:160:SER:HA	1:A:970:LYS:HA	1.87	0.56
1:A:333:THR:HB	1:A:430:HIS:HB3	1.87	0.56
1:B:706:GLN:HE22	1:C:2265:ALA:HA	1.71	0.56
1:E:2442:LEU:HD12	1:E:2494:LEU:HD12	1.88	0.56
1:B:242:ILE:HA	1:B:246:LEU:HD23	1.86	0.56
1:B:649:GLN:NE2	1:B:802:THR:OG1	2.39	0.56
1:A:649:GLN:NE2	1:A:802:THR:OG1	2.39	0.56
1:A:2442:LEU:HD12	1:A:2494:LEU:HD12	1.88	0.56
1:B:2360:LEU:HD11	1:B:2387:ASN:HB3	1.87	0.56
1:B:2442:LEU:HD12	1:B:2494:LEU:HD12	1.88	0.56
1:C:649:GLN:NE2	1:C:802:THR:OG1	2.39	0.56
1:C:2442:LEU:HD12	1:C:2494:LEU:HD12	1.88	0.56
1:D:160:SER:HA	1:D:970:LYS:HA	1.87	0.56
1:E:296:VAL:HG13	1:E:315:ILE:HD11	1.86	0.56
1:A:1607:ARG:NH1	1:A:1637:GLU:OE1	2.38	0.56
1:B:158:GLU:OE2	1:C:1892:ARG:NH2	2.38	0.56
1:B:1607:ARG:NH1	1:B:1637:GLU:OE1	2.38	0.56
1:C:2360:LEU:HD11	1:C:2387:ASN:HB3	1.87	0.56
1:E:160:SER:HA	1:E:970:LYS:HA	1.87	0.56
1:B:1009:TRP:HA	1:B:1013:ASN:HB2	1.88	0.56
1:C:564:ASN:H	1:C:567:GLU:HB3	1.71	0.56
1:C:558:LYS:HA	1:C:563:VAL:HG12	1.88	0.55
1:C:2345:LEU:HB2	1:C:2521:ILE:HB	1.88	0.55
1:D:213:GLN:HE21	1:D:916:LEU:HD23	1.71	0.55
1:A:1670:ASN:ND2	1:A:1675:SER:OG	2.38	0.55
1:C:158:GLU:OE2	1:D:1892:ARG:NH2	2.39	0.55
1:C:706:GLN:HE22	1:D:2265:ALA:HA	1.71	0.55
1:C:1009:TRP:HA	1:C:1013:ASN:HB2	1.89	0.55
1:D:2442:LEU:HD12	1:D:2494:LEU:HD12	1.88	0.55
1:E:828:THR:HG22	1:E:856:THR:HG22	1.87	0.55
1:B:558:LYS:HA	1:B:563:VAL:HG12	1.88	0.55
1:B:719:TRP:HD1	1:B:778:VAL:HG22	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1670:ASN:ND2	1:B:1675:SER:OG	2.38	0.55
1:B:2345:LEU:HB2	1:B:2521:ILE:HB	1.88	0.55
1:D:558:LYS:HA	1:D:563:VAL:HG12	1.88	0.55
1:D:1009:TRP:HA	1:D:1013:ASN:HB2	1.88	0.55
1:D:2345:LEU:HB2	1:D:2521:ILE:HB	1.88	0.55
1:E:558:LYS:HA	1:E:563:VAL:HG12	1.88	0.55
1:A:558:LYS:HA	1:A:563:VAL:HG12	1.88	0.55
1:A:564:ASN:H	1:A:567:GLU:HB3	1.71	0.55
1:A:2345:LEU:HB2	1:A:2521:ILE:HB	1.88	0.55
1:A:2360:LEU:HD11	1:A:2387:ASN:HB3	1.87	0.55
1:C:828:THR:HG22	1:C:856:THR:HG22	1.87	0.55
1:A:605:LEU:HD21	1:A:613:LEU:HD13	1.89	0.55
1:A:1009:TRP:HA	1:A:1013:ASN:HB2	1.88	0.55
1:C:605:LEU:HD21	1:C:613:LEU:HD13	1.89	0.55
1:C:2270:LEU:HD21	1:D:2057:LEU:HD11	1.87	0.55
1:E:564:ASN:H	1:E:567:GLU:HB3	1.71	0.55
1:B:2266:LEU:O	1:B:2270:LEU:HB2	2.07	0.55
1:C:160:SER:HA	1:C:970:LYS:HA	1.87	0.55
1:C:213:GLN:HE21	1:C:916:LEU:HD23	1.71	0.55
1:D:2034:ARG:NH1	1:D:2477:LYS:O	2.40	0.55
1:D:564:ASN:H	1:D:567:GLU:HB3	1.71	0.55
1:D:605:LEU:HD21	1:D:613:LEU:HD13	1.89	0.55
1:D:2266:LEU:O	1:D:2270:LEU:HB2	2.07	0.55
1:E:605:LEU:HD21	1:E:613:LEU:HD13	1.89	0.55
1:C:2169:ARG:HG3	1:C:2172:ALA:HB2	1.89	0.55
1:D:1246:ARG:HG3	1:D:1265:LEU:HD21	1.89	0.55
1:B:605:LEU:HD21	1:B:613:LEU:HD13	1.89	0.55
1:D:2169:ARG:HG3	1:D:2172:ALA:HB2	1.89	0.55
1:E:213:GLN:HE21	1:E:916:LEU:HD23	1.71	0.55
1:A:2169:ARG:HG3	1:A:2172:ALA:HB2	1.89	0.55
1:A:2270:LEU:HD21	1:B:2057:LEU:HD11	1.87	0.55
1:B:564:ASN:H	1:B:567:GLU:HB3	1.71	0.55
1:B:1251:ILE:HG22	1:B:1257:LEU:HA	1.89	0.55
1:B:2169:ARG:HG3	1:B:2172:ALA:HB2	1.89	0.55
1:D:111:SER:OG	1:D:1967:GLN:OE1	2.22	0.55
1:E:719:TRP:HD1	1:E:778:VAL:HG22	1.72	0.55
1:E:1009:TRP:HA	1:E:1013:ASN:HB2	1.89	0.55
1:E:2034:ARG:NH1	1:E:2477:LYS:O	2.40	0.55
1:E:2169:ARG:HG3	1:E:2172:ALA:HB2	1.89	0.55
1:B:213:GLN:HE21	1:B:916:LEU:HD23	1.71	0.54
1:B:1246:ARG:HG3	1:B:1265:LEU:HD21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:719:TRP:HD1	1:C:778:VAL:HG22	1.72	0.54
1:C:1251:ILE:HG22	1:C:1257:LEU:HA	1.89	0.54
1:D:1251:ILE:HG22	1:D:1257:LEU:HA	1.89	0.54
1:E:2360:LEU:HD11	1:E:2387:ASN:HB3	1.87	0.54
1:B:1703:TYR:O	1:B:1751:GLN:NE2	2.36	0.54
1:E:2345:LEU:HB2	1:E:2521:ILE:HB	1.88	0.54
1:C:2034:ARG:NH1	1:C:2477:LYS:O	2.40	0.54
1:A:2435:TYR:HB3	1:B:2350:THR:HG21	1.89	0.54
1:C:2266:LEU:O	1:C:2270:LEU:HB2	2.07	0.54
1:A:1327:ASN:ND2	1:A:1544:ASP:OD1	2.37	0.54
1:D:1327:ASN:ND2	1:D:1544:ASP:OD1	2.37	0.54
1:A:213:GLN:HE21	1:A:916:LEU:HD23	1.71	0.54
1:A:1251:ILE:HG22	1:A:1257:LEU:HA	1.89	0.54
1:A:2266:LEU:O	1:A:2270:LEU:HB2	2.07	0.54
1:C:1246:ARG:HG3	1:C:1265:LEU:HD21	1.89	0.54
1:A:719:TRP:HD1	1:A:778:VAL:HG22	1.72	0.54
1:C:1703:TYR:O	1:C:1751:GLN:NE2	2.36	0.54
1:A:964:GLN:OE1	1:B:1987:ARG:NH1	2.41	0.54
1:D:236:LEU:HB2	1:D:484:PHE:HB2	1.90	0.54
1:D:719:TRP:HD1	1:D:778:VAL:HG22	1.72	0.54
1:E:1251:ILE:HG22	1:E:1257:LEU:HA	1.90	0.54
1:A:1246:ARG:HG3	1:A:1265:LEU:HD21	1.89	0.54
1:B:794:ASP:HB3	1:B:796:PRO:HD2	1.90	0.54
1:C:794:ASP:HB3	1:C:796:PRO:HD2	1.90	0.54
1:A:706:GLN:HE22	1:B:2265:ALA:HA	1.72	0.54
1:A:2350:THR:HG21	1:E:2435:TYR:HB3	1.89	0.54
1:C:701:ILE:HD13	1:C:717:LEU:HD21	1.90	0.54
1:D:1167:ASN:ND2	1:D:1172:GLY:O	2.41	0.54
1:E:1167:ASN:ND2	1:E:1172:GLY:O	2.41	0.54
1:A:236:LEU:HB2	1:A:484:PHE:HB2	1.90	0.53
1:E:2266:LEU:O	1:E:2270:LEU:HB2	2.07	0.53
1:A:701:ILE:HD13	1:A:717:LEU:HD21	1.91	0.53
1:A:1167:ASN:ND2	1:A:1172:GLY:O	2.41	0.53
1:B:2034:ARG:NH1	1:B:2477:LYS:O	2.40	0.53
1:A:1503:ILE:HG22	1:A:1558:ILE:HA	1.91	0.53
1:C:735:ILE:O	1:C:739:ASN:ND2	2.42	0.53
1:D:964:GLN:OE1	1:E:1987:ARG:NH1	2.41	0.53
1:C:1167:ASN:ND2	1:C:1172:GLY:O	2.41	0.53
1:A:2034:ARG:NH1	1:A:2477:LYS:O	2.40	0.53
1:C:111:SER:OG	1:C:1967:GLN:OE1	2.22	0.53
1:B:964:GLN:OE1	1:C:1987:ARG:NH1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1318:TYR:HB2	1:B:1326:ILE:HD11	1.91	0.53
1:D:701:ILE:HD13	1:D:717:LEU:HD21	1.91	0.53
1:D:1503:ILE:HG22	1:D:1558:ILE:HA	1.91	0.53
1:D:1703:TYR:O	1:D:1751:GLN:NE2	2.36	0.53
1:A:1987:ARG:NH1	1:E:964:GLN:OE1	2.41	0.53
1:C:1327:ASN:ND2	1:C:1544:ASP:OD1	2.37	0.53
1:D:1318:TYR:HB2	1:D:1326:ILE:HD11	1.91	0.53
1:A:716:ILE:HG23	1:A:760:LEU:HD13	1.91	0.53
1:A:735:ILE:O	1:A:739:ASN:ND2	2.42	0.53
1:A:2029:VAL:HG11	1:B:2339:GLU:HG2	1.91	0.53
1:B:716:ILE:HG23	1:B:760:LEU:HD13	1.91	0.53
1:B:735:ILE:O	1:B:739:ASN:ND2	2.42	0.53
1:C:964:GLN:OE1	1:D:1987:ARG:NH1	2.42	0.53
1:D:794:ASP:HB3	1:D:796:PRO:HD2	1.90	0.53
1:E:1503:ILE:HG22	1:E:1558:ILE:HA	1.91	0.53
1:A:794:ASP:HB3	1:A:796:PRO:HD2	1.90	0.53
1:C:1158:LEU:HD21	1:C:1183:LEU:HD12	1.91	0.53
1:D:716:ILE:HG23	1:D:760:LEU:HD13	1.91	0.53
1:D:735:ILE:O	1:D:739:ASN:ND2	2.42	0.53
1:A:1311:GLY:HA2	1:A:1334:MET:HA	1.91	0.52
1:B:1503:ILE:HG22	1:B:1558:ILE:HA	1.91	0.52
1:D:1158:LEU:HD21	1:D:1183:LEU:HD12	1.91	0.52
1:C:2029:VAL:HG11	1:D:2339:GLU:HG2	1.91	0.52
1:E:701:ILE:HD13	1:E:717:LEU:HD21	1.90	0.52
1:E:716:ILE:HG23	1:E:760:LEU:HD13	1.91	0.52
1:C:2435:TYR:HB3	1:D:2350:THR:HG21	1.90	0.52
1:D:135:GLN:HA	1:D:140:LYS:HD3	1.92	0.52
1:D:2029:VAL:HG11	1:E:2339:GLU:HG2	1.90	0.52
1:E:1246:ARG:HG3	1:E:1265:LEU:HD21	1.89	0.52
1:E:111:SER:OG	1:E:1967:GLN:OE1	2.22	0.52
1:E:135:GLN:HA	1:E:140:LYS:HD3	1.92	0.52
1:A:135:GLN:HA	1:A:140:LYS:HD3	1.92	0.52
1:B:1158:LEU:HD21	1:B:1183:LEU:HD12	1.91	0.52
1:E:236:LEU:HB2	1:E:484:PHE:HB2	1.90	0.52
1:D:937:SER:OG	1:D:952:ARG:NH1	2.43	0.52
1:E:735:ILE:O	1:E:739:ASN:ND2	2.42	0.52
1:B:393:THR:OG1	1:C:1925:ARG:NH2	2.43	0.52
1:B:2435:TYR:HB3	1:C:2350:THR:HG21	1.90	0.52
1:D:240:THR:OG1	1:D:454:ALA:O	2.28	0.52
1:E:937:SER:OG	1:E:952:ARG:NH1	2.42	0.52
1:E:1680:TYR:OH	1:E:1695:PHE:O	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:LEU:HB2	1:B:484:PHE:HB2	1.91	0.52
1:B:937:SER:OG	1:B:952:ARG:NH1	2.42	0.52
1:C:236:LEU:HB2	1:C:484:PHE:HB2	1.90	0.52
1:B:2029:VAL:HG11	1:C:2339:GLU:HG2	1.90	0.52
1:B:701:ILE:HD13	1:B:717:LEU:HD21	1.91	0.52
1:B:2102:GLN:O	1:B:2106:HIS:ND1	2.43	0.52
1:C:240:THR:OG1	1:C:454:ALA:O	2.28	0.52
1:E:794:ASP:HB3	1:E:796:PRO:HD2	1.90	0.52
1:E:1651:PRO:HG2	1:E:1658:HIS:HE1	1.75	0.52
1:A:937:SER:OG	1:A:952:ARG:NH1	2.42	0.51
1:C:170:LEU:HD13	1:C:181:TYR:HE1	1.75	0.51
1:C:1318:TYR:HB2	1:C:1326:ILE:HD11	1.91	0.51
1:C:1651:PRO:HG2	1:C:1658:HIS:HE1	1.75	0.51
1:A:726:GLN:OE1	1:A:749:ASN:ND2	2.42	0.51
1:A:1318:TYR:HB2	1:A:1326:ILE:HD11	1.91	0.51
1:A:1805:GLU:OE2	1:D:2202:ARG:NH2	2.42	0.51
1:C:135:GLN:HA	1:C:140:LYS:HD3	1.92	0.51
1:C:937:SER:OG	1:C:952:ARG:NH1	2.43	0.51
1:D:451:LEU:HD13	1:D:462:ILE:HD11	1.93	0.51
1:A:170:LEU:HD13	1:A:181:TYR:HE1	1.75	0.51
1:A:1651:PRO:HG2	1:A:1658:HIS:HE1	1.75	0.51
1:A:2102:GLN:O	1:A:2106:HIS:ND1	2.43	0.51
1:B:1167:ASN:ND2	1:B:1172:GLY:O	2.41	0.51
1:B:2202:ARG:NH2	1:D:1805:GLU:OE2	2.43	0.51
1:C:716:ILE:HG23	1:C:760:LEU:HD13	1.91	0.51
1:C:2408:ALA:O	1:C:2419:ARG:NH1	2.44	0.51
1:A:451:LEU:HD13	1:A:462:ILE:HD11	1.93	0.51
1:B:170:LEU:HD13	1:B:181:TYR:HE1	1.75	0.51
1:B:1651:PRO:HG2	1:B:1658:HIS:HE1	1.75	0.51
1:B:2408:ALA:O	1:B:2419:ARG:NH1	2.44	0.51
1:E:170:LEU:HD13	1:E:181:TYR:HE1	1.75	0.51
1:E:867:LEU:HD23	1:E:870:LEU:HD12	1.93	0.51
1:E:1158:LEU:HD21	1:E:1183:LEU:HD12	1.91	0.51
1:A:769:LEU:HD13	1:A:774:LEU:HD13	1.93	0.51
1:B:2295:THR:HG1	1:B:2478:TYR:HH	1.57	0.51
1:D:726:GLN:OE1	1:D:749:ASN:ND2	2.42	0.51
1:E:451:LEU:HD13	1:E:462:ILE:HD11	1.93	0.51
1:A:2408:ALA:O	1:A:2419:ARG:NH1	2.44	0.51
1:B:1311:GLY:HA2	1:B:1334:MET:HA	1.91	0.51
1:C:2102:GLN:O	1:C:2106:HIS:ND1	2.43	0.51
1:E:1318:TYR:HB2	1:E:1326:ILE:HD11	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1158:LEU:HD21	1:A:1183:LEU:HD12	1.91	0.51
1:A:2202:ARG:NH2	1:C:1805:GLU:OE2	2.43	0.51
1:C:451:LEU:HD13	1:C:462:ILE:HD11	1.93	0.51
1:C:1680:TYR:OH	1:C:1695:PHE:O	2.25	0.51
1:D:170:LEU:HD13	1:D:181:TYR:HE1	1.75	0.51
1:A:712:THR:HG22	1:A:771:GLU:HB2	1.93	0.51
1:A:2272:GLY:HA3	1:E:703:ALA:HB2	1.92	0.51
1:D:1651:PRO:HG2	1:D:1658:HIS:HE1	1.75	0.51
1:D:2295:THR:OG1	1:D:2478:TYR:OH	2.27	0.51
1:B:78:ILE:HD13	1:B:81:LEU:HD22	1.93	0.51
1:B:135:GLN:HA	1:B:140:LYS:HD3	1.92	0.51
1:C:712:THR:HG22	1:C:771:GLU:HB2	1.93	0.51
1:C:1503:ILE:HG22	1:C:1558:ILE:HA	1.91	0.51
1:C:2095:ASP:OD1	1:C:2233:ARG:NH1	2.44	0.51
1:E:1311:GLY:HA2	1:E:1334:MET:HA	1.92	0.51
1:A:2063:GLN:NE2	1:E:708:ASP:OD1	2.44	0.51
1:A:2095:ASP:OD1	1:A:2233:ARG:NH1	2.44	0.51
1:B:712:THR:HG22	1:B:771:GLU:HB2	1.93	0.51
1:D:712:THR:HG22	1:D:771:GLU:HB2	1.93	0.51
1:D:1311:GLY:HA2	1:D:1334:MET:HA	1.92	0.51
1:D:2199:GLU:OE1	1:E:2124:ASN:ND2	2.43	0.51
1:D:2408:ALA:O	1:D:2419:ARG:NH1	2.44	0.51
1:D:2435:TYR:HB3	1:E:2350:THR:HG21	1.93	0.51
1:A:1835:TRP:CZ2	1:A:1868:LYS:HG3	2.46	0.50
1:C:726:GLN:OE1	1:C:749:ASN:ND2	2.42	0.50
1:D:78:ILE:HD13	1:D:81:LEU:HD22	1.93	0.50
1:D:708:ASP:OD1	1:E:2063:GLN:NE2	2.45	0.50
1:D:1835:TRP:CZ2	1:D:1868:LYS:HG3	2.46	0.50
1:E:792:GLN:HB2	1:E:797:THR:HG21	1.94	0.50
1:A:240:THR:OG1	1:A:454:ALA:O	2.28	0.50
1:A:393:THR:OG1	1:B:1925:ARG:NH2	2.44	0.50
1:B:451:LEU:HD13	1:B:462:ILE:HD11	1.93	0.50
1:C:1311:GLY:HA2	1:C:1334:MET:HA	1.92	0.50
1:A:488:TYR:O	1:A:492:HIS:CB	2.60	0.50
1:E:2102:GLN:O	1:E:2106:HIS:ND1	2.43	0.50
1:A:297:ASN:ND2	1:A:308:GLN:O	2.43	0.50
1:B:488:TYR:O	1:B:492:HIS:CB	2.60	0.50
1:B:792:GLN:HB2	1:B:797:THR:HG21	1.94	0.50
1:B:1127:ASN:ND2	1:B:1848:ALA:O	2.41	0.50
1:B:1835:TRP:CZ2	1:B:1868:LYS:HG3	2.46	0.50
1:B:2295:THR:OG1	1:B:2478:TYR:OH	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2095:ASP:OD1	1:E:2233:ARG:NH1	2.44	0.50
1:B:726:GLN:OE1	1:B:749:ASN:ND2	2.42	0.50
1:C:78:ILE:HD13	1:C:81:LEU:HD22	1.93	0.50
1:C:1835:TRP:CZ2	1:C:1868:LYS:HG3	2.46	0.50
1:E:1308:SER:OG	1:E:1337:ASN:OD1	2.30	0.50
1:E:2408:ALA:O	1:E:2419:ARG:NH1	2.44	0.50
1:A:1308:SER:OG	1:A:1337:ASN:OD1	2.30	0.50
1:A:1680:TYR:OH	1:A:1695:PHE:O	2.26	0.50
1:A:2295:THR:OG1	1:A:2478:TYR:OH	2.27	0.50
1:C:488:TYR:O	1:C:492:HIS:CB	2.60	0.50
1:C:769:LEU:HD13	1:C:774:LEU:HD13	1.93	0.50
1:C:2401:LYS:HE2	1:C:2403:SER:HB3	1.94	0.50
1:E:1835:TRP:CZ2	1:E:1868:LYS:HG3	2.46	0.50
1:A:111:SER:OG	1:A:1967:GLN:OE1	2.22	0.50
1:B:1805:GLU:OE2	1:E:2202:ARG:NH2	2.45	0.50
1:B:2095:ASP:OD1	1:B:2233:ARG:NH1	2.44	0.50
1:B:2401:LYS:HE2	1:B:2403:SER:HB3	1.94	0.50
1:D:769:LEU:HD13	1:D:774:LEU:HD13	1.93	0.50
1:D:867:LEU:HD23	1:D:870:LEU:HD12	1.93	0.50
1:A:78:ILE:HD13	1:A:81:LEU:HD22	1.93	0.50
1:A:1138:PRO:HB2	1:D:2173:LEU:HB3	1.93	0.50
1:A:2401:LYS:HE2	1:A:2403:SER:HB3	1.94	0.50
1:D:393:THR:OG1	1:E:1925:ARG:NH2	2.45	0.50
1:E:78:ILE:HD13	1:E:81:LEU:HD22	1.92	0.50
1:E:488:TYR:O	1:E:492:HIS:CB	2.60	0.50
1:E:712:THR:HG22	1:E:771:GLU:HB2	1.93	0.50
1:B:111:SER:OG	1:B:1967:GLN:OE1	2.22	0.50
1:B:769:LEU:HD13	1:B:774:LEU:HD13	1.93	0.50
1:B:1089:ILE:HD11	1:B:1293:LEU:HD12	1.94	0.50
1:C:1155:LEU:HD22	1:C:1192:TRP:HH2	1.77	0.50
1:D:297:ASN:ND2	1:D:308:GLN:O	2.43	0.50
1:D:1680:TYR:OH	1:D:1695:PHE:O	2.25	0.50
1:E:769:LEU:HD13	1:E:774:LEU:HD13	1.93	0.50
1:C:867:LEU:HD23	1:C:870:LEU:HD12	1.93	0.49
1:C:1308:SER:OG	1:C:1337:ASN:OD1	2.30	0.49
1:D:2253:GLN:HE21	1:E:2075:GLN:NE2	2.09	0.49
1:E:1089:ILE:HD11	1:E:1293:LEU:HD12	1.94	0.49
1:A:867:LEU:HD23	1:A:870:LEU:HD12	1.93	0.49
1:C:1035:PRO:HB3	1:C:1796:MET:HB3	1.94	0.49
1:A:1925:ARG:NH2	1:E:393:THR:OG1	2.44	0.49
1:A:2339:GLU:HG2	1:E:2029:VAL:HG11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:669:THR:HG22	1:C:671:ASP:H	1.78	0.49
1:C:792:GLN:HB2	1:C:797:THR:HG21	1.94	0.49
1:C:1127:ASN:ND2	1:C:1848:ALA:O	2.41	0.49
1:D:716:ILE:HD11	1:D:764:VAL:HG21	1.94	0.49
1:A:1035:PRO:HB3	1:A:1796:MET:HB3	1.94	0.49
1:B:1155:LEU:HD22	1:B:1192:TRP:HH2	1.77	0.49
1:C:1089:ILE:HD11	1:C:1293:LEU:HD12	1.94	0.49
1:C:2297:GLN:NE2	1:C:2305:ALA:O	2.39	0.49
1:D:1714:TYR:H	1:D:1718:ILE:HG22	1.77	0.49
1:E:669:THR:HG22	1:E:671:ASP:H	1.78	0.49
1:A:2253:GLN:HE21	1:B:2075:GLN:NE2	2.10	0.49
1:B:240:THR:OG1	1:B:454:ALA:O	2.28	0.49
1:B:867:LEU:HD23	1:B:870:LEU:HD12	1.93	0.49
1:D:1035:PRO:HB3	1:D:1796:MET:HB3	1.94	0.49
1:D:2095:ASP:OD1	1:D:2233:ARG:NH1	2.44	0.49
1:E:297:ASN:ND2	1:E:308:GLN:O	2.44	0.49
1:A:669:THR:HG22	1:A:671:ASP:H	1.78	0.49
1:A:1703:TYR:O	1:A:1751:GLN:NE2	2.36	0.49
1:B:1035:PRO:HB3	1:B:1796:MET:HB3	1.94	0.49
1:B:2253:GLN:HE21	1:C:2075:GLN:NE2	2.10	0.49
1:D:2297:GLN:NE2	1:D:2305:ALA:O	2.39	0.49
1:A:1155:LEU:HD22	1:A:1192:TRP:HH2	1.77	0.49
1:B:42:THR:OG1	1:B:1571:GLU:OE2	2.31	0.49
1:B:708:ASP:OD1	1:C:2063:GLN:NE2	2.46	0.49
1:C:393:THR:OG1	1:D:1925:ARG:NH2	2.45	0.49
1:C:708:ASP:OD1	1:D:2063:GLN:NE2	2.46	0.49
1:D:1958:ASN:O	1:D:1961:THR:OG1	2.31	0.49
1:E:240:THR:OG1	1:E:454:ALA:O	2.28	0.49
1:A:792:GLN:HB2	1:A:797:THR:HG21	1.94	0.49
1:B:1308:SER:OG	1:B:1337:ASN:OD1	2.30	0.49
1:B:1958:ASN:O	1:B:1961:THR:OG1	2.31	0.49
1:C:2253:GLN:HE21	1:D:2075:GLN:NE2	2.11	0.49
1:D:240:THR:HG21	1:D:455:THR:HG22	1.95	0.49
1:D:488:TYR:O	1:D:492:HIS:CB	2.60	0.49
1:D:2102:GLN:O	1:D:2106:HIS:ND1	2.43	0.49
1:E:1958:ASN:O	1:E:1961:THR:OG1	2.31	0.49
1:C:2202:ARG:NH2	1:E:1805:GLU:OE2	2.45	0.49
1:D:2353:LEU:HD12	1:D:2513:ILE:HB	1.95	0.49
1:E:1714:TYR:H	1:E:1718:ILE:HG22	1.77	0.49
1:E:2401:LYS:HE2	1:E:2403:SER:HB3	1.94	0.49
1:A:1089:ILE:HD11	1:A:1293:LEU:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:ARG:NH2	1:B:512:SER:OG	2.46	0.49
1:B:2353:LEU:HD12	1:B:2513:ILE:HB	1.95	0.49
1:C:240:THR:HG21	1:C:455:THR:HG22	1.95	0.49
1:C:2353:LEU:HD12	1:C:2513:ILE:HB	1.95	0.49
1:E:42:THR:OG1	1:E:1571:GLU:OE2	2.31	0.49
1:E:726:GLN:OE1	1:E:749:ASN:ND2	2.42	0.49
1:C:2173:LEU:HB3	1:E:1138:PRO:HB2	1.94	0.48
1:D:1155:LEU:HD22	1:D:1192:TRP:HH2	1.77	0.48
1:A:2199:GLU:OE1	1:B:2124:ASN:ND2	2.45	0.48
1:C:297:ASN:ND2	1:C:308:GLN:O	2.43	0.48
1:C:703:ALA:HB2	1:D:2272:GLY:HA3	1.95	0.48
1:D:792:GLN:HB2	1:D:797:THR:HG21	1.94	0.48
1:D:2401:LYS:HE2	1:D:2403:SER:HB3	1.94	0.48
1:B:716:ILE:HD11	1:B:764:VAL:HG21	1.94	0.48
1:B:1680:TYR:OH	1:B:1695:PHE:O	2.25	0.48
1:D:669:THR:HG22	1:D:671:ASP:H	1.78	0.48
1:D:1308:SER:OG	1:D:1337:ASN:OD1	2.30	0.48
1:A:1127:ASN:ND2	1:A:1848:ALA:O	2.41	0.48
1:A:1884:ASP:OD1	1:A:1902:TYR:OH	2.31	0.48
1:A:2173:LEU:HB3	1:C:1138:PRO:HB2	1.94	0.48
1:B:1138:PRO:HB2	1:E:2173:LEU:HB3	1.95	0.48
1:B:1884:ASP:OD1	1:B:1902:TYR:OH	2.31	0.48
1:E:334:ARG:NH2	1:E:512:SER:OG	2.46	0.48
1:A:716:ILE:HD11	1:A:764:VAL:HG21	1.94	0.48
1:A:1958:ASN:O	1:A:1961:THR:OG1	2.31	0.48
1:A:2353:LEU:HD12	1:A:2513:ILE:HB	1.95	0.48
1:E:1035:PRO:HB3	1:E:1796:MET:HB3	1.94	0.48
1:A:334:ARG:NH2	1:A:512:SER:OG	2.46	0.48
1:B:669:THR:HG22	1:B:671:ASP:H	1.77	0.48
1:B:691:ASP:O	1:B:695:ARG:NH2	2.47	0.48
1:C:334:ARG:NH2	1:C:512:SER:OG	2.46	0.48
1:D:879:THR:HG23	1:D:882:GLY:H	1.79	0.48
1:E:1155:LEU:HD22	1:E:1192:TRP:HH2	1.77	0.48
1:D:691:ASP:O	1:D:695:ARG:NH2	2.47	0.48
1:D:1089:ILE:HD11	1:D:1293:LEU:HD12	1.94	0.48
1:E:2297:GLN:NE2	1:E:2305:ALA:O	2.39	0.48
1:E:2353:LEU:HD12	1:E:2513:ILE:HB	1.95	0.48
1:A:708:ASP:OD1	1:B:2063:GLN:NE2	2.47	0.48
1:B:2173:LEU:HB3	1:D:1138:PRO:HB2	1.95	0.48
1:C:462:ILE:HA	1:C:465:VAL:HG22	1.95	0.48
1:C:777:LEU:HD22	1:C:784:PHE:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1030:GLU:HG2	1:C:1869:VAL:HB	1.96	0.48
1:C:1884:ASP:OD1	1:C:1902:TYR:OH	2.31	0.48
1:E:691:ASP:O	1:E:695:ARG:NH2	2.47	0.48
1:A:240:THR:HG21	1:A:455:THR:HG22	1.95	0.48
1:C:673:GLU:HA	1:C:676:ILE:HD12	1.96	0.48
1:D:334:ARG:NH2	1:D:512:SER:OG	2.46	0.48
1:D:1314:PHE:HE2	1:D:1333:SER:HB3	1.79	0.48
1:E:1703:TYR:O	1:E:1751:GLN:NE2	2.36	0.48
1:B:240:THR:HG21	1:B:455:THR:HG22	1.95	0.47
1:B:1029:PRO:HD2	1:B:1866:HIS:CD2	2.49	0.47
1:B:1714:TYR:H	1:B:1718:ILE:HG22	1.77	0.47
1:C:691:ASP:O	1:C:695:ARG:NH2	2.47	0.47
1:D:777:LEU:HD22	1:D:784:PHE:HB2	1.96	0.47
1:D:1029:PRO:HD2	1:D:1866:HIS:CD2	2.49	0.47
1:A:691:ASP:O	1:A:695:ARG:NH2	2.47	0.47
1:A:777:LEU:HD22	1:A:784:PHE:HB2	1.96	0.47
1:A:1714:TYR:H	1:A:1718:ILE:HG22	1.77	0.47
1:A:2422:LYS:H	1:A:2519:TYR:HA	1.80	0.47
1:B:777:LEU:HD22	1:B:784:PHE:HB2	1.96	0.47
1:D:1030:GLU:HG2	1:D:1869:VAL:HB	1.96	0.47
1:E:462:ILE:HA	1:E:465:VAL:HG22	1.95	0.47
1:E:716:ILE:HD11	1:E:764:VAL:HG21	1.94	0.47
1:E:777:LEU:HD22	1:E:784:PHE:HB2	1.96	0.47
1:E:1799:PHE:CE2	1:E:1874:LYS:HB3	2.50	0.47
1:A:1030:GLU:HG2	1:A:1869:VAL:HB	1.96	0.47
1:B:1030:GLU:HG2	1:B:1869:VAL:HB	1.96	0.47
1:C:841:GLN:O	1:C:845:GLN:HB2	2.15	0.47
1:C:1799:PHE:CE2	1:C:1874:LYS:HB3	2.50	0.47
1:D:2189:ARG:HD2	1:E:2190:ILE:HD12	1.97	0.47
1:E:1030:GLU:HG2	1:E:1869:VAL:HB	1.96	0.47
1:A:703:ALA:HB2	1:B:2272:GLY:HA3	1.95	0.47
1:B:879:THR:HG23	1:B:882:GLY:H	1.79	0.47
1:C:1714:TYR:H	1:C:1718:ILE:HG22	1.77	0.47
1:D:673:GLU:HA	1:D:676:ILE:HD12	1.96	0.47
1:D:1550:ILE:HB	1:D:1576:ILE:HB	1.97	0.47
1:E:240:THR:HG21	1:E:455:THR:HG22	1.95	0.47
1:A:462:ILE:HA	1:A:465:VAL:HG22	1.95	0.47
1:A:879:THR:HG23	1:A:882:GLY:H	1.79	0.47
1:A:1799:PHE:CE2	1:A:1874:LYS:HB3	2.50	0.47
1:A:2124:ASN:ND2	1:E:2199:GLU:OE1	2.47	0.47
1:B:462:ILE:HA	1:B:465:VAL:HG22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:703:ALA:HB2	1:C:2272:GLY:HA3	1.96	0.47
1:B:1264:ASP:O	1:B:1268:ILE:HB	2.15	0.47
1:C:716:ILE:HD11	1:C:764:VAL:HG21	1.94	0.47
1:D:462:ILE:HA	1:D:465:VAL:HG22	1.95	0.47
1:E:673:GLU:HA	1:E:676:ILE:HD12	1.96	0.47
1:A:1309:PHE:HD1	1:A:1336:ILE:HG12	1.80	0.47
1:A:1550:ILE:HB	1:A:1576:ILE:HB	1.97	0.47
1:B:736:ILE:HG23	1:B:746:GLU:HG2	1.97	0.47
1:B:2422:LYS:H	1:B:2519:TYR:HA	1.79	0.47
1:D:1652:PRO:O	1:D:1658:HIS:NE2	2.48	0.47
1:D:1799:PHE:CE2	1:D:1874:LYS:HB3	2.50	0.47
1:A:683:LEU:HD12	1:A:700:LEU:HD12	1.97	0.47
1:B:717:LEU:HA	1:B:720:ILE:HG22	1.97	0.47
1:B:1799:PHE:CE2	1:B:1874:LYS:HB3	2.50	0.47
1:C:1029:PRO:HD2	1:C:1866:HIS:CD2	2.49	0.47
1:C:1314:PHE:HE2	1:C:1333:SER:HB3	1.79	0.47
1:C:1652:PRO:O	1:C:1658:HIS:NE2	2.48	0.47
1:D:2387:ASN:ND2	1:D:2404:ASP:OD2	2.40	0.47
1:E:92:TYR:HA	1:E:1945:LEU:HD11	1.97	0.47
1:E:736:ILE:HG23	1:E:746:GLU:HG2	1.97	0.47
1:E:2422:LYS:H	1:E:2519:TYR:HA	1.79	0.47
1:C:717:LEU:HA	1:C:720:ILE:HG22	1.97	0.47
1:C:1309:PHE:HD1	1:C:1336:ILE:HG12	1.80	0.47
1:C:2295:THR:HG1	1:C:2478:TYR:HH	1.58	0.47
1:D:736:ILE:HG23	1:D:746:GLU:HG2	1.97	0.47
1:D:841:GLN:O	1:D:845:GLN:HB2	2.15	0.47
1:E:1264:ASP:O	1:E:1268:ILE:HB	2.15	0.47
1:E:1884:ASP:OD1	1:E:1902:TYR:OH	2.31	0.47
1:E:2387:ASN:ND2	1:E:2404:ASP:OD2	2.40	0.47
1:A:736:ILE:HG23	1:A:746:GLU:HG2	1.97	0.47
1:A:1029:PRO:HD2	1:A:1866:HIS:CD2	2.49	0.47
1:B:841:GLN:O	1:B:845:GLN:HB2	2.15	0.47
1:C:1081:VAL:O	1:C:1597:GLN:NE2	2.48	0.47
1:D:683:LEU:HD12	1:D:700:LEU:HD12	1.97	0.47
1:E:879:THR:HG23	1:E:882:GLY:H	1.79	0.47
1:E:1309:PHE:HD1	1:E:1336:ILE:HG12	1.80	0.47
1:A:92:TYR:HA	1:A:1945:LEU:HD11	1.97	0.47
1:A:673:GLU:HA	1:A:676:ILE:HD12	1.96	0.47
1:A:1284:VAL:HB	1:A:1587:ILE:HB	1.97	0.47
1:B:1550:ILE:HB	1:B:1576:ILE:HB	1.97	0.47
1:C:1958:ASN:O	1:C:1961:THR:OG1	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:223:ASN:HD22	1:E:868:GLN:HG2	1.80	0.47
1:E:1607:ARG:HB2	1:E:1640:LEU:HD11	1.97	0.47
1:A:496:SER:OG	1:A:497:VAL:N	2.48	0.46
1:B:223:ASN:HD22	1:B:868:GLN:HG2	1.80	0.46
1:B:683:LEU:HD12	1:B:700:LEU:HD12	1.97	0.46
1:C:683:LEU:HD12	1:C:700:LEU:HD12	1.97	0.46
1:C:879:THR:HG23	1:C:882:GLY:H	1.79	0.46
1:C:1264:ASP:O	1:C:1268:ILE:HB	2.15	0.46
1:D:717:LEU:HA	1:D:720:ILE:HG22	1.97	0.46
1:D:1607:ARG:HB2	1:D:1640:LEU:HD11	1.97	0.46
1:A:2189:ARG:HD2	1:B:2190:ILE:HD12	1.97	0.46
1:B:92:TYR:HA	1:B:1945:LEU:HD11	1.97	0.46
1:B:1006:PHE:HA	1:B:1009:TRP:HB2	1.97	0.46
1:B:1314:PHE:HE2	1:B:1333:SER:HB3	1.79	0.46
1:C:496:SER:OG	1:C:497:VAL:N	2.48	0.46
1:C:736:ILE:HG23	1:C:746:GLU:HG2	1.97	0.46
1:C:1284:VAL:HB	1:C:1587:ILE:HB	1.97	0.46
1:A:1264:ASP:O	1:A:1268:ILE:HB	2.15	0.46
1:A:1652:PRO:O	1:A:1658:HIS:NE2	2.48	0.46
1:B:1284:VAL:HB	1:B:1587:ILE:HB	1.97	0.46
1:B:1727:PHE:HB3	1:B:1740:ILE:HD12	1.98	0.46
1:C:42:THR:OG1	1:C:1571:GLU:OE2	2.31	0.46
1:C:508:ILE:HG23	1:C:519:HIS:HD2	1.80	0.46
1:D:1284:VAL:HB	1:D:1587:ILE:HB	1.97	0.46
1:E:1284:VAL:HB	1:E:1587:ILE:HB	1.98	0.46
1:E:1314:PHE:HE2	1:E:1333:SER:HB3	1.79	0.46
1:E:1550:ILE:HB	1:E:1576:ILE:HB	1.97	0.46
1:A:81:LEU:HD12	1:A:1835:TRP:HZ2	1.81	0.46
1:B:1607:ARG:HB2	1:B:1640:LEU:HD11	1.97	0.46
1:C:81:LEU:HD12	1:C:1835:TRP:HZ2	1.81	0.46
1:C:1006:PHE:HA	1:C:1009:TRP:HB2	1.97	0.46
1:E:717:LEU:HA	1:E:720:ILE:HG22	1.97	0.46
1:E:1652:PRO:O	1:E:1658:HIS:NE2	2.48	0.46
1:E:1721:LYS:H	1:E:1724:GLU:HB2	1.81	0.46
1:A:665:SER:OG	1:B:817:GLU:OE2	2.25	0.46
1:A:1314:PHE:HE2	1:A:1333:SER:HB3	1.79	0.46
1:A:1721:LYS:H	1:A:1724:GLU:HB2	1.81	0.46
1:B:673:GLU:HA	1:B:676:ILE:HD12	1.96	0.46
1:D:1884:ASP:OD1	1:D:1902:TYR:OH	2.31	0.46
1:B:1652:PRO:O	1:B:1658:HIS:NE2	2.48	0.46
1:C:223:ASN:HD22	1:C:868:GLN:HG2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2387:ASN:ND2	1:C:2404:ASP:OD2	2.40	0.46
1:D:1180:ILE:HD11	1:D:1197:ASN:HB3	1.98	0.46
1:E:683:LEU:HD12	1:E:700:LEU:HD12	1.97	0.46
1:E:1029:PRO:HD2	1:E:1866:HIS:CD2	2.49	0.46
1:E:1727:PHE:HB3	1:E:1740:ILE:HD12	1.98	0.46
1:A:223:ASN:HD22	1:A:868:GLN:HG2	1.80	0.46
1:A:1727:PHE:HB3	1:A:1740:ILE:HD12	1.98	0.46
1:C:1607:ARG:HB2	1:C:1640:LEU:HD11	1.97	0.46
1:D:508:ILE:HG23	1:D:519:HIS:HD2	1.80	0.46
1:E:496:SER:OG	1:E:497:VAL:N	2.48	0.46
1:E:841:GLN:O	1:E:845:GLN:HB2	2.15	0.46
1:A:841:GLN:O	1:A:845:GLN:HB2	2.15	0.46
1:A:1006:PHE:HA	1:A:1009:TRP:HB2	1.97	0.46
1:A:1081:VAL:O	1:A:1597:GLN:NE2	2.48	0.46
1:B:508:ILE:HG23	1:B:519:HIS:HD2	1.80	0.46
1:B:1180:ILE:HD11	1:B:1197:ASN:HB3	1.98	0.46
1:B:1309:PHE:HD1	1:B:1336:ILE:HG12	1.80	0.46
1:B:2188:THR:HG23	1:C:2137:SER:HB2	1.98	0.46
1:C:2422:LYS:H	1:C:2519:TYR:HA	1.80	0.46
1:D:496:SER:OG	1:D:497:VAL:N	2.48	0.46
1:D:1264:ASP:O	1:D:1268:ILE:HB	2.15	0.46
1:D:1721:LYS:H	1:D:1724:GLU:HB2	1.81	0.46
1:A:842:VAL:HG23	1:E:566:THR:HG21	1.98	0.46
1:A:1523:VAL:HG22	1:A:1538:PHE:HA	1.98	0.46
1:A:2075:GLN:NE2	1:E:2253:GLN:HE21	2.14	0.46
1:A:2382:ALA:HB3	1:A:2389:LEU:HB2	1.98	0.46
1:B:2178:ALA:HB1	1:C:2148:HIS:CE1	2.51	0.46
1:C:1721:LYS:H	1:C:1724:GLU:HB2	1.81	0.46
1:C:1727:PHE:HB3	1:C:1740:ILE:HD12	1.98	0.46
1:D:92:TYR:HA	1:D:1945:LEU:HD11	1.97	0.46
1:D:282:ALA:HA	1:D:287:LEU:HB2	1.97	0.46
1:D:2422:LYS:H	1:D:2519:TYR:HA	1.80	0.46
1:A:2137:SER:HB2	1:E:2188:THR:HG23	1.98	0.46
1:B:282:ALA:HA	1:B:287:LEU:HB2	1.97	0.46
1:B:496:SER:OG	1:B:497:VAL:N	2.48	0.46
1:B:2199:GLU:OE1	1:C:2124:ASN:ND2	2.46	0.46
1:A:508:ILE:HG23	1:A:519:HIS:HD2	1.80	0.45
1:A:817:GLU:OE2	1:E:665:SER:OG	2.22	0.45
1:B:297:ASN:ND2	1:B:308:GLN:O	2.43	0.45
1:B:1721:LYS:H	1:B:1724:GLU:HB2	1.81	0.45
1:C:1550:ILE:HB	1:C:1576:ILE:HB	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:223:ASN:HD22	1:D:868:GLN:HG2	1.80	0.45
1:E:2382:ALA:HB3	1:E:2389:LEU:HB2	1.98	0.45
1:A:282:ALA:HA	1:A:287:LEU:HB2	1.97	0.45
1:A:1607:ARG:HB2	1:A:1640:LEU:HD11	1.97	0.45
1:A:2148:HIS:CE1	1:E:2178:ALA:HB1	2.51	0.45
1:B:2189:ARG:HD2	1:C:2190:ILE:HD12	1.98	0.45
1:B:2382:ALA:HB3	1:B:2389:LEU:HB2	1.98	0.45
1:D:554:LEU:HD23	1:D:558:LYS:HE2	1.99	0.45
1:D:1006:PHE:HA	1:D:1009:TRP:HB2	1.97	0.45
1:D:1081:VAL:O	1:D:1597:GLN:NE2	2.48	0.45
1:E:508:ILE:HG23	1:E:519:HIS:HD2	1.80	0.45
1:B:1523:VAL:HG22	1:B:1538:PHE:HA	1.98	0.45
1:C:1863:ASP:OD1	1:C:1863:ASP:N	2.50	0.45
1:D:81:LEU:HD12	1:D:1835:TRP:HZ2	1.81	0.45
1:E:200:HIS:HB3	1:E:203:TYR:HB3	1.99	0.45
1:E:282:ALA:HA	1:E:287:LEU:HB2	1.98	0.45
1:A:42:THR:OG1	1:A:1571:GLU:OE2	2.31	0.45
1:A:1531:SER:OG	1:B:1766:HIS:NE2	2.36	0.45
1:A:1766:HIS:NE2	1:E:1531:SER:OG	2.36	0.45
1:C:372:ARG:HG2	1:C:383:GLN:HG3	1.99	0.45
1:D:2382:ALA:HB3	1:D:2389:LEU:HB2	1.98	0.45
1:E:372:ARG:HG2	1:E:383:GLN:HG3	1.99	0.45
1:B:200:HIS:HB3	1:B:203:TYR:HB3	1.98	0.45
1:C:92:TYR:HA	1:C:1945:LEU:HD11	1.97	0.45
1:A:717:LEU:HA	1:A:720:ILE:HG22	1.97	0.45
1:B:1597:GLN:HB3	1:B:1609:ASN:HB2	1.99	0.45
1:B:2387:ASN:ND2	1:B:2404:ASP:OD2	2.40	0.45
1:C:200:HIS:HB3	1:C:203:TYR:HB3	1.99	0.45
1:C:282:ALA:HA	1:C:287:LEU:HB2	1.97	0.45
1:D:2188:THR:HG23	1:E:2137:SER:HB2	1.99	0.45
1:E:81:LEU:HD12	1:E:1835:TRP:HZ2	1.81	0.45
1:E:1523:VAL:HG22	1:E:1538:PHE:HA	1.98	0.45
1:A:1863:ASP:OD1	1:A:1863:ASP:N	2.50	0.45
1:B:1799:PHE:HE2	1:B:1874:LYS:HB3	1.82	0.45
1:C:109:ILE:H	1:C:152:GLN:HE22	1.65	0.45
1:C:488:TYR:O	1:C:492:HIS:HB2	2.17	0.45
1:D:1309:PHE:HD1	1:D:1336:ILE:HG12	1.80	0.45
1:E:1006:PHE:HA	1:E:1009:TRP:HB2	1.97	0.45
1:A:2190:ILE:HD12	1:E:2189:ARG:HD2	1.99	0.45
1:B:81:LEU:HD12	1:B:1835:TRP:HZ2	1.81	0.45
1:B:554:LEU:HD23	1:B:558:LYS:HE2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1973:GLN:HA	1:B:1976:TRP:HD1	1.82	0.45
1:C:1523:VAL:HG22	1:C:1538:PHE:HA	1.98	0.45
1:D:1863:ASP:OD1	1:D:1863:ASP:N	2.50	0.45
1:D:2158:PRO:HA	1:D:2168:SER:HB3	1.99	0.45
1:D:2167:GLY:HA2	1:E:2159:ASN:HB3	1.99	0.45
1:A:488:TYR:O	1:A:492:HIS:HB2	2.17	0.45
1:A:1597:GLN:HB3	1:A:1609:ASN:HB2	1.99	0.45
1:C:2188:THR:HG23	1:D:2137:SER:HB2	1.99	0.45
1:C:2382:ALA:HB3	1:C:2389:LEU:HB2	1.99	0.45
1:D:1727:PHE:HB3	1:D:1740:ILE:HD12	1.98	0.45
1:E:2295:THR:OG1	1:E:2478:TYR:OH	2.27	0.45
1:A:2397:GLN:HA	1:A:2495:SER:HA	1.99	0.45
1:B:488:TYR:O	1:B:492:HIS:HB2	2.17	0.45
1:C:1799:PHE:HE2	1:C:1874:LYS:HB3	1.82	0.45
1:E:2158:PRO:HA	1:E:2168:SER:HB3	1.99	0.45
1:C:2178:ALA:HB1	1:D:2148:HIS:CE1	2.52	0.44
1:D:203:TYR:OH	1:D:237:ALA:O	2.30	0.44
1:E:109:ILE:H	1:E:152:GLN:HE22	1.65	0.44
1:E:1180:ILE:HD11	1:E:1197:ASN:HB3	1.98	0.44
1:E:1597:GLN:HB3	1:E:1609:ASN:HB2	1.99	0.44
1:A:1180:ILE:HD11	1:A:1197:ASN:HB3	1.98	0.44
1:A:1973:GLN:HA	1:A:1976:TRP:HD1	1.82	0.44
1:C:525:ASN:ND2	1:C:534:PHE:H	2.12	0.44
1:C:681:ASN:ND2	1:E:2310:PRO:O	2.50	0.44
1:C:2158:PRO:HA	1:C:2168:SER:HB3	1.99	0.44
1:D:33:PHE:HZ	1:D:49:LEU:HD23	1.83	0.44
1:E:488:TYR:O	1:E:492:HIS:HB2	2.17	0.44
1:E:1799:PHE:HE2	1:E:1874:LYS:HB3	1.82	0.44
1:E:2397:GLN:HA	1:E:2495:SER:HA	1.99	0.44
1:A:2188:THR:HG23	1:B:2137:SER:HB2	1.99	0.44
1:C:1041:GLN:NE2	1:C:1046:ASN:OD1	2.51	0.44
1:C:1180:ILE:HD11	1:C:1197:ASN:HB3	1.98	0.44
1:C:1597:GLN:HB3	1:C:1609:ASN:HB2	1.99	0.44
1:C:1625:ASP:OD1	1:C:1817:TYR:OH	2.26	0.44
1:C:2189:ARG:HD2	1:D:2190:ILE:HD12	2.00	0.44
1:D:1973:GLN:HA	1:D:1976:TRP:HD1	1.82	0.44
1:E:698:ALA:HA	1:E:701:ILE:HG22	2.00	0.44
1:A:33:PHE:HZ	1:A:49:LEU:HD23	1.83	0.44
1:A:372:ARG:HG2	1:A:383:GLN:HG3	1.99	0.44
1:A:1909:LEU:HB3	1:A:1976:TRP:CH2	2.53	0.44
1:B:1151:TYR:OH	1:B:1225:ASP:O	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:200:HIS:HB3	1:D:203:TYR:HB3	1.98	0.44
1:D:525:ASN:ND2	1:D:534:PHE:H	2.12	0.44
1:E:1041:GLN:NE2	1:E:1046:ASN:OD1	2.51	0.44
1:A:200:HIS:HB3	1:A:203:TYR:HB3	1.99	0.44
1:A:701:ILE:HG21	1:A:717:LEU:HD11	2.00	0.44
1:A:1550:ILE:HG22	1:A:1552:LEU:HG	2.00	0.44
1:A:1799:PHE:HE2	1:A:1874:LYS:HB3	1.82	0.44
1:A:2178:ALA:HB1	1:B:2148:HIS:CE1	2.53	0.44
1:C:1973:GLN:HA	1:C:1976:TRP:HD1	1.82	0.44
1:D:698:ALA:HA	1:D:701:ILE:HG22	2.00	0.44
1:E:1550:ILE:HG22	1:E:1552:LEU:HG	2.00	0.44
1:A:1163:LYS:HB2	1:A:1178:ASP:HB2	1.99	0.44
1:A:1846:TRP:HB3	1:A:1861:GLN:HB3	2.00	0.44
1:A:2297:GLN:NE2	1:A:2305:ALA:O	2.39	0.44
1:C:1909:LEU:HB3	1:C:1976:TRP:CH2	2.53	0.44
1:D:703:ALA:HB2	1:E:2272:GLY:HA3	1.98	0.44
1:D:1041:GLN:NE2	1:D:1046:ASN:OD1	2.51	0.44
1:D:1909:LEU:HB3	1:D:1976:TRP:CH2	2.53	0.44
1:E:1846:TRP:HB3	1:E:1861:GLN:HB3	2.00	0.44
1:E:1973:GLN:HA	1:E:1976:TRP:HD1	1.82	0.44
1:A:554:LEU:HD23	1:A:558:LYS:HE2	1.99	0.44
1:A:1041:GLN:NE2	1:A:1046:ASN:OD1	2.51	0.44
1:B:1863:ASP:N	1:B:1863:ASP:OD1	2.50	0.44
1:D:109:ILE:H	1:D:152:GLN:HE22	1.65	0.44
1:D:1523:VAL:HG22	1:D:1538:PHE:HA	1.98	0.44
1:D:1597:GLN:HB3	1:D:1609:ASN:HB2	1.99	0.44
1:D:1846:TRP:HB3	1:D:1861:GLN:HB3	2.00	0.44
1:A:2269:TRP:HA	1:E:703:ALA:HB1	2.00	0.44
1:B:372:ARG:HG2	1:B:383:GLN:HG3	1.99	0.44
1:B:1550:ILE:HG22	1:B:1552:LEU:HG	2.00	0.44
1:B:1846:TRP:HB3	1:B:1861:GLN:HB3	2.00	0.44
1:B:2397:GLN:HA	1:B:2495:SER:HA	2.00	0.44
1:C:33:PHE:HZ	1:C:49:LEU:HD23	1.83	0.44
1:C:554:LEU:HD23	1:C:558:LYS:HE2	1.99	0.44
1:D:1550:ILE:HG22	1:D:1552:LEU:HG	2.00	0.44
1:D:2178:ALA:HB1	1:E:2148:HIS:CE1	2.53	0.44
1:E:554:LEU:HD23	1:E:558:LYS:HE2	1.99	0.44
1:E:701:ILE:HG21	1:E:717:LEU:HD11	2.00	0.44
1:E:1863:ASP:N	1:E:1863:ASP:OD1	2.50	0.44
1:A:149:ALA:O	1:A:154:ASN:ND2	2.44	0.44
1:B:701:ILE:HG21	1:B:717:LEU:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1163:LYS:HB2	1:C:1178:ASP:HB2	1.99	0.44
1:D:1163:LYS:HB2	1:D:1178:ASP:HB2	1.99	0.44
1:D:2289:CYS:HB3	1:D:2308:ILE:HD13	2.00	0.44
1:E:436:PHE:HB3	1:E:440:ILE:HG23	2.00	0.44
1:A:698:ALA:HA	1:A:701:ILE:HG22	1.99	0.43
1:D:436:PHE:HB3	1:D:440:ILE:HG23	2.00	0.43
1:D:488:TYR:O	1:D:492:HIS:HB2	2.17	0.43
1:D:2397:GLN:HA	1:D:2495:SER:HA	2.00	0.43
1:A:2158:PRO:HA	1:A:2168:SER:HB3	1.99	0.43
1:A:2167:GLY:HA2	1:B:2159:ASN:HB3	1.99	0.43
1:B:1041:GLN:NE2	1:B:1046:ASN:OD1	2.51	0.43
1:B:2297:GLN:NE2	1:B:2305:ALA:O	2.39	0.43
1:C:701:ILE:HG21	1:C:717:LEU:HD11	2.00	0.43
1:D:372:ARG:HG2	1:D:383:GLN:HG3	1.99	0.43
1:D:1799:PHE:HE2	1:D:1874:LYS:HB3	1.82	0.43
1:E:1127:ASN:ND2	1:E:1848:ALA:O	2.41	0.43
1:A:436:PHE:HB3	1:A:440:ILE:HG23	2.00	0.43
1:A:1146:ILE:HD11	1:A:1157:LEU:HD21	2.01	0.43
1:B:33:PHE:HZ	1:B:49:LEU:HD23	1.83	0.43
1:B:2158:PRO:HA	1:B:2168:SER:HB3	1.99	0.43
1:B:2167:GLY:HA2	1:C:2159:ASN:HB3	2.00	0.43
1:B:2289:CYS:HB3	1:B:2308:ILE:HD13	2.00	0.43
1:B:2310:PRO:O	1:E:681:ASN:ND2	2.52	0.43
1:E:1096:THR:OG1	1:E:1116:HIS:NE2	2.41	0.43
1:E:1909:LEU:HB3	1:E:1976:TRP:CH2	2.53	0.43
1:C:2199:GLU:OE1	1:D:2124:ASN:ND2	2.46	0.43
1:D:701:ILE:HG21	1:D:717:LEU:HD11	2.00	0.43
1:D:1599:MET:HB2	1:D:1608:LEU:HD11	2.01	0.43
1:A:2017:THR:O	1:E:772:ASN:ND2	2.50	0.43
1:B:1163:LYS:HB2	1:B:1178:ASP:HB2	1.99	0.43
1:D:1531:SER:OG	1:E:1766:HIS:NE2	2.37	0.43
1:E:1163:LYS:HB2	1:E:1178:ASP:HB2	1.99	0.43
1:A:2159:ASN:HB3	1:E:2167:GLY:HA2	2.01	0.43
1:B:698:ALA:HA	1:B:701:ILE:HG22	2.00	0.43
1:B:1081:VAL:O	1:B:1597:GLN:NE2	2.48	0.43
1:B:1909:LEU:HB3	1:B:1976:TRP:CH2	2.53	0.43
1:C:1179:TYR:HB2	1:C:1201:THR:HA	2.01	0.43
1:D:334:ARG:HG3	1:D:338:TYR:CG	2.54	0.43
1:D:566:THR:HG21	1:E:842:VAL:HG23	2.01	0.43
1:E:33:PHE:HZ	1:E:49:LEU:HD23	1.83	0.43
1:E:1146:ILE:HD11	1:E:1157:LEU:HD21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:HIS:HD2	1:E:363:LYS:HE2	1.84	0.43
1:C:1550:ILE:HG22	1:C:1552:LEU:HG	2.00	0.43
1:C:1846:TRP:HB3	1:C:1861:GLN:HB3	2.00	0.43
1:C:2397:GLN:HA	1:C:2495:SER:HA	2.00	0.43
1:D:235:LEU:HD23	1:D:238:ILE:HD12	2.01	0.43
1:E:235:LEU:HD23	1:E:238:ILE:HD12	2.01	0.43
1:A:31:SER:O	1:A:35:HIS:ND1	2.41	0.43
1:A:235:LEU:HD23	1:A:238:ILE:HD12	2.01	0.43
1:B:109:ILE:H	1:B:152:GLN:HE22	1.65	0.43
1:C:334:ARG:HG3	1:C:338:TYR:CG	2.54	0.43
1:D:1179:TYR:HB2	1:D:1201:THR:HA	2.01	0.43
1:A:109:ILE:H	1:A:152:GLN:HE22	1.65	0.43
1:A:2289:CYS:HB3	1:A:2308:ILE:HD13	2.00	0.43
1:B:1146:ILE:HD11	1:B:1157:LEU:HD21	2.01	0.43
1:C:698:ALA:HA	1:C:701:ILE:HG22	2.00	0.43
1:E:334:ARG:HG3	1:E:338:TYR:CG	2.54	0.43
1:A:334:ARG:HG3	1:A:338:TYR:CG	2.54	0.43
1:A:1617:ALA:HB2	1:E:1154:ARG:HH21	1.84	0.43
1:A:2346:GLU:HB3	1:E:2469:PHE:CE2	2.54	0.43
1:B:235:LEU:HD23	1:B:238:ILE:HD12	2.01	0.43
1:B:334:ARG:HG3	1:B:338:TYR:CG	2.54	0.43
1:B:566:THR:HG21	1:C:842:VAL:HG23	2.01	0.43
1:B:859:ASN:HB3	1:B:862:THR:HG22	2.01	0.43
1:C:235:LEU:HD23	1:C:238:ILE:HD12	2.01	0.43
1:C:1028:TYR:OH	1:C:1967:GLN:O	2.31	0.43
1:C:2289:CYS:HB3	1:C:2308:ILE:HD13	2.00	0.43
1:D:563:VAL:HG22	1:D:567:GLU:HB3	2.01	0.43
1:E:21:LEU:H	1:E:24:ASN:HD22	1.67	0.43
1:E:1599:MET:HB2	1:E:1608:LEU:HD11	2.01	0.43
1:B:130:HIS:ND1	1:B:984:TYR:OH	2.37	0.42
1:B:527:PRO:O	1:B:559:ARG:NH1	2.52	0.42
1:B:665:SER:OG	1:C:817:GLU:OE2	2.25	0.42
1:C:1154:ARG:HH21	1:D:1617:ALA:HB2	1.83	0.42
1:C:2167:GLY:HA2	1:D:2159:ASN:HB3	2.01	0.42
1:D:266:ASN:HD22	1:D:443:LEU:HD22	1.84	0.42
1:B:1179:TYR:HB2	1:B:1201:THR:HA	2.01	0.42
1:C:527:PRO:O	1:C:559:ARG:NH1	2.52	0.42
1:D:859:ASN:HB3	1:D:862:THR:HG22	2.00	0.42
1:E:413:ARG:HG3	1:E:428:ASN:HB3	2.02	0.42
1:E:2289:CYS:HB3	1:E:2308:ILE:HD13	2.00	0.42
1:A:607:VAL:H	1:A:607:VAL:HG22	1.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:ASN:HD22	1:B:443:LEU:HD22	1.84	0.42
1:B:436:PHE:HB3	1:B:440:ILE:HG23	2.00	0.42
1:E:162:LEU:HD11	1:E:933:THR:HG21	2.02	0.42
1:E:527:PRO:O	1:E:559:ARG:NH1	2.52	0.42
1:A:413:ARG:HG3	1:A:428:ASN:HB3	2.02	0.42
1:A:563:VAL:HG22	1:A:567:GLU:HB3	2.01	0.42
1:B:162:LEU:HD11	1:B:933:THR:HG21	2.02	0.42
1:C:21:LEU:H	1:C:24:ASN:HD22	1.67	0.42
1:C:1599:MET:HB2	1:C:1608:LEU:HD11	2.01	0.42
1:E:1179:TYR:HB2	1:E:1201:THR:HA	2.01	0.42
1:A:859:ASN:HB3	1:A:862:THR:HG22	2.01	0.42
1:C:544:THR:HA	1:C:545:PRO:HD3	1.89	0.42
1:E:563:VAL:HG22	1:E:567:GLU:HB3	2.01	0.42
1:A:266:ASN:HD22	1:A:443:LEU:HD22	1.84	0.42
1:A:527:PRO:O	1:A:559:ARG:NH1	2.52	0.42
1:B:703:ALA:HB1	1:C:2269:TRP:HA	2.02	0.42
1:C:266:ASN:HD22	1:C:443:LEU:HD22	1.85	0.42
1:C:413:ARG:HG3	1:C:428:ASN:HB3	2.01	0.42
1:C:859:ASN:HB3	1:C:862:THR:HG22	2.01	0.42
1:D:149:ALA:O	1:D:154:ASN:ND2	2.44	0.42
1:D:703:ALA:HB1	1:E:2269:TRP:HA	2.02	0.42
1:D:1096:THR:OG1	1:D:1116:HIS:NE2	2.41	0.42
1:D:1127:ASN:ND2	1:D:1848:ALA:O	2.41	0.42
1:D:1146:ILE:HD11	1:D:1157:LEU:HD21	2.01	0.42
1:E:859:ASN:HB3	1:E:862:THR:HG22	2.01	0.42
1:A:2387:ASN:ND2	1:A:2404:ASP:OD2	2.40	0.42
1:C:162:LEU:HD11	1:C:933:THR:HG21	2.02	0.42
1:C:436:PHE:HB3	1:C:440:ILE:HG23	2.00	0.42
1:D:502:VAL:HG11	1:D:594:TYR:HD2	1.85	0.42
1:E:1112:ARG:HD2	1:E:1132:TRP:CE2	2.55	0.42
1:A:1599:MET:HB2	1:A:1608:LEU:HD11	2.01	0.42
1:A:2310:PRO:O	1:D:681:ASN:ND2	2.52	0.42
1:B:21:LEU:H	1:B:24:ASN:HD22	1.67	0.42
1:B:363:LYS:HE2	1:C:171:HIS:HD2	1.84	0.42
1:B:483:LEU:HA	1:B:486:VAL:HG22	2.02	0.42
1:B:1179:TYR:H	1:B:1201:THR:HB	1.85	0.42
1:C:315:ILE:HG22	1:C:329:LEU:HB2	2.02	0.42
1:C:502:VAL:HG11	1:C:594:TYR:HD2	1.85	0.42
1:C:1716:LYS:HG2	1:C:1717:ILE:H	1.85	0.42
1:D:363:LYS:HE2	1:E:171:HIS:HD2	1.85	0.42
1:E:31:SER:O	1:E:35:HIS:ND1	2.41	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:GLU:HB3	1:A:927:TRP:HZ3	1.85	0.42
1:A:483:LEU:HA	1:A:486:VAL:HG22	2.02	0.42
1:A:1716:LYS:HG2	1:A:1717:ILE:H	1.85	0.42
1:A:1983:LEU:HD23	1:A:1983:LEU:HA	1.92	0.42
1:B:2298:TYR:OH	1:B:2482:GLU:O	2.32	0.42
1:C:563:VAL:HG22	1:C:567:GLU:HB3	2.01	0.42
1:C:1146:ILE:HD11	1:C:1157:LEU:HD21	2.01	0.42
1:D:162:LEU:HD11	1:D:933:THR:HG21	2.02	0.42
1:A:1179:TYR:H	1:A:1201:THR:HB	1.85	0.41
1:E:502:VAL:HG11	1:E:594:TYR:HD2	1.85	0.41
1:B:681:ASN:ND2	1:D:2310:PRO:O	2.53	0.41
1:B:760:LEU:HA	1:B:760:LEU:HD23	1.88	0.41
1:C:2374:LEU:HD23	1:C:2391:VAL:HG23	2.02	0.41
1:D:1112:ARG:HD2	1:D:1132:TRP:CE2	2.55	0.41
1:E:204:GLU:HB3	1:E:927:TRP:HZ3	1.85	0.41
1:E:1716:LYS:HG2	1:E:1717:ILE:H	1.85	0.41
1:A:21:LEU:H	1:A:24:ASN:HD22	1.67	0.41
1:B:203:TYR:CZ	1:B:207:ARG:HD2	2.55	0.41
1:B:413:ARG:HG3	1:B:428:ASN:HB3	2.01	0.41
1:B:886:LEU:HD11	1:B:912:LEU:HD21	2.03	0.41
1:B:952:ARG:HH21	1:B:964:GLN:HG2	1.85	0.41
1:B:1599:MET:HB2	1:B:1608:LEU:HD11	2.01	0.41
1:C:1112:ARG:HD2	1:C:1132:TRP:CE2	2.55	0.41
1:D:315:ILE:HG22	1:D:329:LEU:HB2	2.02	0.41
1:D:1179:TYR:H	1:D:1201:THR:HB	1.85	0.41
1:E:1081:VAL:O	1:E:1597:GLN:NE2	2.48	0.41
1:A:162:LEU:HD11	1:A:933:THR:HG21	2.02	0.41
1:A:2439:ARG:N	1:A:2503:GLN:HE22	2.19	0.41
1:B:149:ALA:O	1:B:154:ASN:ND2	2.44	0.41
1:B:2437:ASP:OD2	1:C:2350:THR:N	2.45	0.41
1:C:483:LEU:HA	1:C:486:VAL:HG22	2.02	0.41
1:D:294:LEU:HB3	1:D:459:PRO:HG2	2.03	0.41
1:D:527:PRO:O	1:D:559:ARG:NH1	2.52	0.41
1:D:1716:LYS:HG2	1:D:1717:ILE:H	1.85	0.41
1:D:2374:LEU:HD23	1:D:2391:VAL:HG23	2.02	0.41
1:E:886:LEU:HD11	1:E:912:LEU:HD21	2.03	0.41
1:E:2374:LEU:HD23	1:E:2391:VAL:HG23	2.02	0.41
1:E:2439:ARG:N	1:E:2503:GLN:HE22	2.19	0.41
1:A:1179:TYR:HB2	1:A:1201:THR:HA	2.01	0.41
1:A:2155:ASP:OD2	1:A:2169:ARG:NH2	2.54	0.41
1:B:294:LEU:HB3	1:B:459:PRO:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2412:PRO:O	1:B:2419:ARG:NH2	2.54	0.41
1:C:566:THR:HG21	1:D:842:VAL:HG23	2.02	0.41
1:C:2155:ASP:OD2	1:C:2169:ARG:NH2	2.54	0.41
1:D:31:SER:O	1:D:35:HIS:ND1	2.41	0.41
1:D:1154:ARG:HH21	1:E:1617:ALA:HB2	1.85	0.41
1:E:952:ARG:HH21	1:E:964:GLN:HG2	1.85	0.41
1:E:1179:TYR:H	1:E:1201:THR:HB	1.85	0.41
1:A:566:THR:HG21	1:B:842:VAL:HG23	2.02	0.41
1:B:1112:ARG:HD2	1:B:1132:TRP:CE2	2.55	0.41
1:C:1619:ARG:HH21	1:C:1635:LEU:HD21	1.85	0.41
1:D:952:ARG:HH21	1:D:964:GLN:HG2	1.85	0.41
1:D:2260:LYS:HE3	1:E:2064:ASP:HB3	2.03	0.41
1:E:2155:ASP:OD2	1:E:2169:ARG:NH2	2.54	0.41
1:A:502:VAL:HG11	1:A:594:TYR:HD2	1.85	0.41
1:A:1112:ARG:HD2	1:A:1132:TRP:CE2	2.55	0.41
1:B:315:ILE:HG22	1:B:329:LEU:HB2	2.02	0.41
1:B:502:VAL:HG11	1:B:594:TYR:HD2	1.85	0.41
1:C:294:LEU:HB3	1:C:459:PRO:HG2	2.03	0.41
1:C:1179:TYR:H	1:C:1201:THR:HB	1.85	0.41
1:E:130:HIS:ND1	1:E:984:TYR:OH	2.37	0.41
1:A:950:LYS:N	1:A:954:GLU:OE1	2.44	0.41
1:A:2412:PRO:O	1:A:2419:ARG:NH2	2.54	0.41
1:B:772:ASN:ND2	1:C:2017:THR:O	2.53	0.41
1:B:1716:LYS:HG2	1:B:1717:ILE:H	1.85	0.41
1:B:1801:ARG:HA	1:B:1801:ARG:HD2	1.88	0.41
1:B:2155:ASP:OD2	1:B:2169:ARG:NH2	2.54	0.41
1:C:2439:ARG:N	1:C:2503:GLN:HE22	2.19	0.41
1:D:413:ARG:HG3	1:D:428:ASN:HB3	2.01	0.41
1:D:2063:GLN:HE21	1:D:2268:ASN:ND2	2.19	0.41
1:D:2439:ARG:N	1:D:2503:GLN:HE22	2.19	0.41
1:E:545:PRO:HB3	1:E:565:ASP:HB3	2.03	0.41
1:A:203:TYR:CZ	1:A:207:ARG:HD2	2.56	0.41
1:A:294:LEU:HB3	1:A:459:PRO:HG2	2.03	0.41
1:A:681:ASN:ND2	1:C:2310:PRO:O	2.53	0.41
1:A:772:ASN:ND2	1:B:2017:THR:O	2.54	0.41
1:A:952:ARG:HH21	1:A:964:GLN:HG2	1.86	0.41
1:A:1663:TRP:HA	1:A:1685:LEU:H	1.86	0.41
1:B:151:THR:HG23	1:B:154:ASN:H	1.86	0.41
1:B:563:VAL:HG22	1:B:567:GLU:HB3	2.01	0.41
1:B:1154:ARG:HH21	1:C:1617:ALA:HB2	1.84	0.41
1:B:2439:ARG:N	1:B:2503:GLN:HE22	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:203:TYR:CZ	1:C:207:ARG:HD2	2.56	0.41
1:C:952:ARG:HH21	1:C:964:GLN:HG2	1.86	0.41
1:D:70:ARG:HD2	1:D:86:SER:HB3	2.03	0.41
1:D:1318:TYR:HB3	1:D:1328:LEU:HD23	2.03	0.41
1:D:1619:ARG:HH21	1:D:1635:LEU:HD21	1.86	0.41
1:D:2177:SER:HB3	1:E:2147:LEU:HD21	2.03	0.41
1:E:203:TYR:CZ	1:E:207:ARG:HD2	2.56	0.41
1:E:266:ASN:HD22	1:E:443:LEU:HD22	1.85	0.41
1:E:483:LEU:HA	1:E:486:VAL:HG22	2.02	0.41
1:A:315:ILE:HG22	1:A:329:LEU:HB2	2.02	0.41
1:B:1663:TRP:HA	1:B:1685:LEU:H	1.86	0.41
1:C:151:THR:HG23	1:C:154:ASN:H	1.86	0.41
1:C:1221:ASP:HB2	1:C:1228:ILE:HD11	2.03	0.41
1:C:1725:SER:O	1:C:1741:ASN:ND2	2.54	0.41
1:D:204:GLU:HB3	1:D:927:TRP:HZ3	1.85	0.41
1:D:231:ASP:HB2	1:D:890:LYS:HG3	2.03	0.41
1:D:1221:ASP:HB2	1:D:1228:ILE:HD11	2.03	0.41
1:E:294:LEU:HB3	1:E:459:PRO:HG2	2.03	0.41
1:E:1619:ARG:HH21	1:E:1635:LEU:HD21	1.86	0.41
1:E:1663:TRP:HA	1:E:1685:LEU:H	1.86	0.41
1:E:1812:THR:O	1:E:1816:ARG:HG2	2.21	0.41
1:E:2412:PRO:O	1:E:2419:ARG:NH2	2.54	0.41
1:A:381:ILE:HD13	1:A:401:LEU:HD21	2.03	0.40
1:A:1725:SER:O	1:A:1741:ASN:ND2	2.54	0.40
1:B:70:ARG:HD2	1:B:86:SER:HB3	2.03	0.40
1:B:204:GLU:HB3	1:B:927:TRP:HZ3	1.85	0.40
1:B:223:ASN:HB3	1:B:868:GLN:HB3	2.03	0.40
1:B:1048:LEU:HD12	1:B:1069:TYR:HB2	2.03	0.40
1:B:1812:THR:O	1:B:1816:ARG:HG2	2.21	0.40
1:B:2374:LEU:HD23	1:B:2391:VAL:HG23	2.02	0.40
1:D:483:LEU:HA	1:D:486:VAL:HG22	2.02	0.40
1:D:1812:THR:O	1:D:1816:ARG:HG2	2.21	0.40
1:E:381:ILE:HD13	1:E:401:LEU:HD21	2.03	0.40
1:E:1318:TYR:HB3	1:E:1328:LEU:HD23	2.03	0.40
1:A:231:ASP:HB2	1:A:890:LYS:HG3	2.04	0.40
1:A:1154:ARG:HH21	1:B:1617:ALA:HB2	1.85	0.40
1:B:501:LEU:HD23	1:B:501:LEU:HA	1.83	0.40
1:B:525:ASN:ND2	1:B:534:PHE:H	2.12	0.40
1:B:1619:ARG:HH21	1:B:1635:LEU:HD21	1.86	0.40
1:B:1725:SER:O	1:B:1741:ASN:ND2	2.54	0.40
1:C:231:ASP:HB2	1:C:890:LYS:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:363:LYS:HE2	1:D:171:HIS:HD2	1.87	0.40
1:C:418:LYS:HE2	1:C:420:ASN:HB3	2.03	0.40
1:C:1801:ARG:HA	1:C:1801:ARG:HD2	1.88	0.40
1:D:21:LEU:H	1:D:24:ASN:HD22	1.67	0.40
1:D:381:ILE:HD13	1:D:401:LEU:HD21	2.03	0.40
1:D:886:LEU:HD11	1:D:912:LEU:HD21	2.03	0.40
1:D:1725:SER:O	1:D:1741:ASN:ND2	2.54	0.40
1:D:2155:ASP:OD2	1:D:2169:ARG:NH2	2.54	0.40
1:E:70:ARG:HD2	1:E:86:SER:HB3	2.03	0.40
1:A:363:LYS:HE2	1:B:171:HIS:HD2	1.86	0.40
1:A:418:LYS:HE2	1:A:420:ASN:HB3	2.03	0.40
1:A:544:THR:HA	1:A:545:PRO:HD3	1.89	0.40
1:A:886:LEU:HD11	1:A:912:LEU:HD21	2.03	0.40
1:A:2147:LEU:HD21	1:E:2177:SER:HB3	2.03	0.40
1:C:204:GLU:HB3	1:C:927:TRP:HZ3	1.85	0.40
1:D:189:SER:HB2	1:D:200:HIS:HD1	1.87	0.40
1:D:501:LEU:HD23	1:D:501:LEU:HA	1.83	0.40
1:E:231:ASP:HB2	1:E:890:LYS:HG3	2.03	0.40
1:E:644:GLN:HA	1:E:647:THR:HG22	2.04	0.40
1:A:592:LEU:HA	1:A:595:ARG:HB2	2.04	0.40
1:A:1048:LEU:HD12	1:A:1069:TYR:HB2	2.03	0.40
1:A:2374:LEU:HD23	1:A:2391:VAL:HG23	2.02	0.40
1:B:1983:LEU:HD23	1:B:1983:LEU:HA	1.91	0.40
1:C:31:SER:O	1:C:35:HIS:ND1	2.41	0.40
1:C:106:PRO:HG3	1:C:1967:GLN:HE21	1.87	0.40
1:C:381:ILE:HD13	1:C:401:LEU:HD21	2.04	0.40
1:A:1619:ARG:HH21	1:A:1635:LEU:HD21	1.86	0.40
1:A:1878:LEU:O	1:A:1882:ARG:HG2	2.21	0.40
1:A:2177:SER:HB3	1:B:2147:LEU:HD21	2.03	0.40
1:B:418:LYS:HE2	1:B:420:ASN:HB3	2.03	0.40
1:B:544:THR:HA	1:B:545:PRO:HD3	1.89	0.40
1:B:644:GLN:HA	1:B:647:THR:HG22	2.04	0.40
1:B:1221:ASP:HB2	1:B:1228:ILE:HD11	2.03	0.40
1:C:1635:LEU:HA	1:C:1636:PRO:HD3	1.95	0.40
1:D:203:TYR:CZ	1:D:207:ARG:HD2	2.55	0.40
1:D:418:LYS:HE2	1:D:420:ASN:HB3	2.03	0.40
1:D:627:PHE:HE2	1:D:635:LEU:HD13	1.87	0.40
1:D:772:ASN:ND2	1:E:2017:THR:O	2.51	0.40
1:D:1663:TRP:HA	1:D:1685:LEU:H	1.86	0.40
1:D:1801:ARG:HD2	1:D:1801:ARG:HA	1.88	0.40
1:E:592:LEU:HA	1:E:595:ARG:HB2	2.04	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%)	2162 (93%)	162 (7%)	7 (0%)	41	61
1	B	2331/2523 (92%)	2162 (93%)	162 (7%)	7 (0%)	41	61
1	C	2331/2523 (92%)	2162 (93%)	162 (7%)	7 (0%)	41	61
1	D	2331/2523 (92%)	2162 (93%)	162 (7%)	7 (0%)	41	61
1	E	2331/2523 (92%)	2162 (93%)	162 (7%)	7 (0%)	41	61
All	All	11655/12615 (92%)	10810 (93%)	810 (7%)	35 (0%)	44	61

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1949	ALA
1	A	2453	GLY
1	B	1949	ALA
1	B	2453	GLY
1	C	1949	ALA
1	C	2453	GLY
1	D	1949	ALA
1	D	2453	GLY
1	E	1949	ALA
1	E	2453	GLY
1	A	1502	ASN
1	B	1502	ASN
1	C	1502	ASN
1	D	1502	ASN
1	E	1502	ASN
1	A	581	PRO
1	A	2343	ARG
1	B	2343	ARG

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Mol	Chain	Res	Type
1	C	581	PRO
1	C	2343	ARG
1	D	581	PRO
1	D	2343	ARG
1	E	581	PRO
1	E	2343	ARG
1	B	581	PRO
1	A	272	VAL
1	B	272	VAL
1	C	272	VAL
1	D	272	VAL
1	E	272	VAL
1	A	1776	PRO
1	B	1776	PRO
1	C	1776	PRO
1	D	1776	PRO
1	E	1776	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%)	2047 (100%)	2 (0%)	93 97
1	B	2049/2222 (92%)	2047 (100%)	2 (0%)	93 97
1	C	2049/2222 (92%)	2047 (100%)	2 (0%)	93 97
1	D	2049/2222 (92%)	2047 (100%)	2 (0%)	93 97
1	E	2049/2222 (92%)	2047 (100%)	2 (0%)	93 97
All	All	10245/11110 (92%)	10235 (100%)	10 (0%)	93 97

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1226	VAL
1	A	2390	ASN

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Mol	Chain	Res	Type
1	B	1226	VAL
1	B	2390	ASN
1	C	1226	VAL
1	C	2390	ASN
1	D	1226	VAL
1	D	2390	ASN
1	E	1226	VAL
1	E	2390	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (170) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	GLN
1	A	171	HIS
1	A	213	GLN
1	A	216	ASN
1	A	223	ASN
1	A	341	HIS
1	A	343	ASN
1	A	374	GLN
1	A	392	ASN
1	A	394	HIS
1	A	519	HIS
1	A	525	ASN
1	A	649	GLN
1	A	706	GLN
1	A	793	HIS
1	A	845	GLN
1	A	1041	GLN
1	A	1046	ASN
1	A	1054	GLN
1	A	1068	ASN
1	A	1121	HIS
1	A	1197	ASN
1	A	1634	ASN
1	A	1670	ASN
1	A	1800	GLN
1	A	1866	HIS
1	A	2063	GLN
1	A	2075	GLN
1	A	2306	HIS
1	A	2314	HIS

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Mol	Chain	Res	Type
1	A	2390	ASN
1	A	2503	GLN
1	A	2516	HIS
1	B	55	GLN
1	B	152	GLN
1	B	171	HIS
1	B	213	GLN
1	B	216	ASN
1	B	223	ASN
1	B	341	HIS
1	B	343	ASN
1	B	374	GLN
1	B	392	ASN
1	B	394	HIS
1	B	519	HIS
1	B	525	ASN
1	B	649	GLN
1	B	706	GLN
1	B	793	HIS
1	B	845	GLN
1	B	1041	GLN
1	B	1046	ASN
1	B	1051	GLN
1	B	1054	GLN
1	B	1121	HIS
1	B	1197	ASN
1	B	1634	ASN
1	B	1670	ASN
1	B	1800	GLN
1	B	1866	HIS
1	B	2063	GLN
1	B	2075	GLN
1	B	2306	HIS
1	B	2314	HIS
1	B	2390	ASN
1	B	2503	GLN
1	B	2516	HIS
1	C	55	GLN
1	C	74	GLN
1	C	152	GLN
1	C	171	HIS
1	C	213	GLN

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Mol	Chain	Res	Type
1	C	216	ASN
1	C	223	ASN
1	C	306	ASN
1	C	341	HIS
1	C	343	ASN
1	C	374	GLN
1	C	392	ASN
1	C	394	HIS
1	C	519	HIS
1	C	525	ASN
1	C	649	GLN
1	C	706	GLN
1	C	793	HIS
1	C	845	GLN
1	C	1041	GLN
1	C	1046	ASN
1	C	1051	GLN
1	C	1054	GLN
1	C	1121	HIS
1	C	1197	ASN
1	C	1634	ASN
1	C	1670	ASN
1	C	1800	GLN
1	C	1866	HIS
1	C	2063	GLN
1	C	2075	GLN
1	C	2306	HIS
1	C	2314	HIS
1	C	2390	ASN
1	C	2503	GLN
1	C	2516	HIS
1	D	55	GLN
1	D	152	GLN
1	D	171	HIS
1	D	213	GLN
1	D	216	ASN
1	D	223	ASN
1	D	341	HIS
1	D	343	ASN
1	D	374	GLN
1	D	392	ASN
1	D	394	HIS

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Mol	Chain	Res	Type
1	D	519	HIS
1	D	525	ASN
1	D	649	GLN
1	D	706	GLN
1	D	793	HIS
1	D	845	GLN
1	D	1041	GLN
1	D	1046	ASN
1	D	1051	GLN
1	D	1054	GLN
1	D	1121	HIS
1	D	1197	ASN
1	D	1634	ASN
1	D	1670	ASN
1	D	1800	GLN
1	D	1866	HIS
1	D	2063	GLN
1	D	2075	GLN
1	D	2306	HIS
1	D	2314	HIS
1	D	2390	ASN
1	D	2503	GLN
1	D	2516	HIS
1	E	55	GLN
1	E	152	GLN
1	E	171	HIS
1	E	213	GLN
1	E	216	ASN
1	E	223	ASN
1	E	341	HIS
1	E	343	ASN
1	E	374	GLN
1	E	392	ASN
1	E	394	HIS
1	E	519	HIS
1	E	525	ASN
1	E	649	GLN
1	E	706	GLN
1	E	793	HIS
1	E	845	GLN
1	E	1041	GLN
1	E	1051	GLN

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Mol	Chain	Res	Type
1	E	1054	GLN
1	E	1121	HIS
1	E	1197	ASN
1	E	1634	ASN
1	E	1670	ASN
1	E	1800	GLN
1	E	1866	HIS
1	E	2063	GLN
1	E	2075	GLN
1	E	2306	HIS
1	E	2314	HIS
1	E	2390	ASN
1	E	2503	GLN
1	E	2516	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

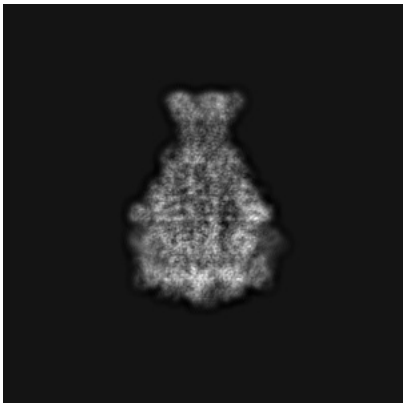
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10034. These allow visual inspection of the internal detail of the map and identification of artifacts.

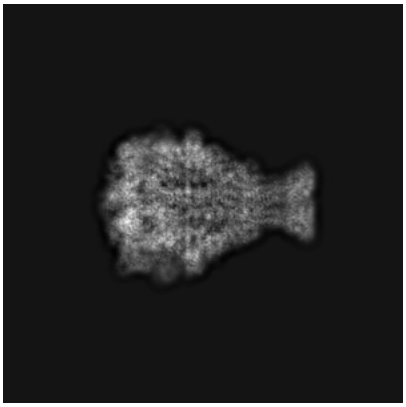
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

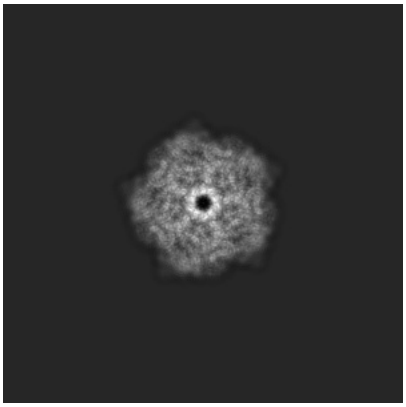
6.1.1 Primary map



X



Y

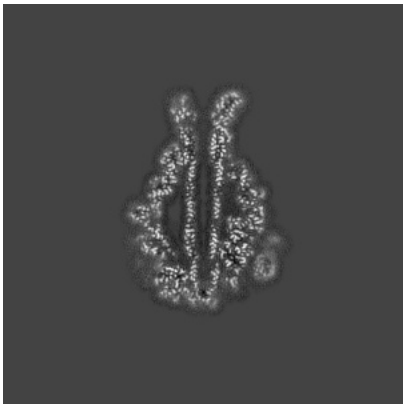


Z

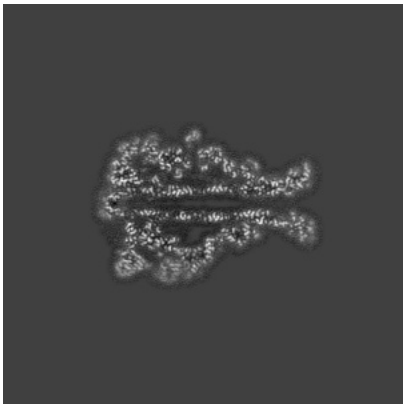
The images above show the map projected in three orthogonal directions.

6.2 Central slices

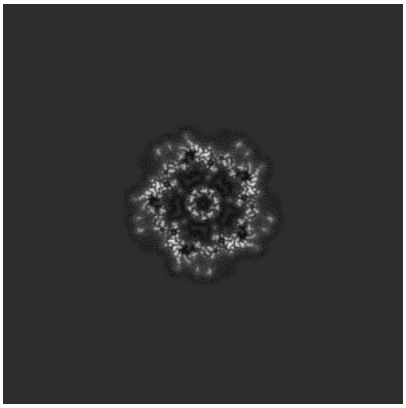
6.2.1 Primary map



X Index: 200



Y Index: 200



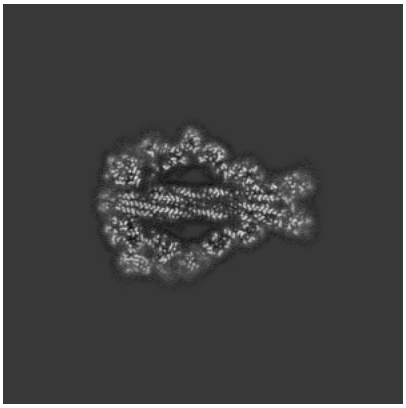
Z Index: 200

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

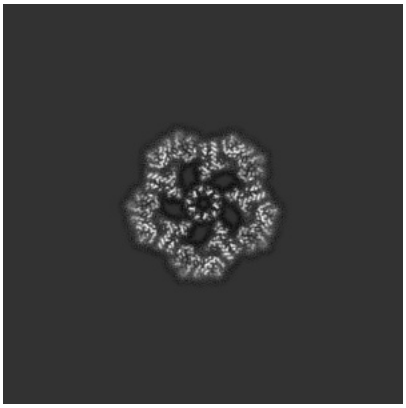
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 211



Y Index: 191

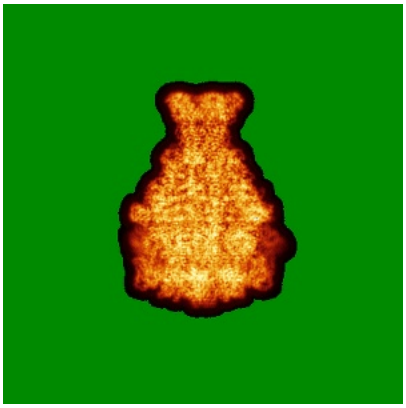


Z Index: 184

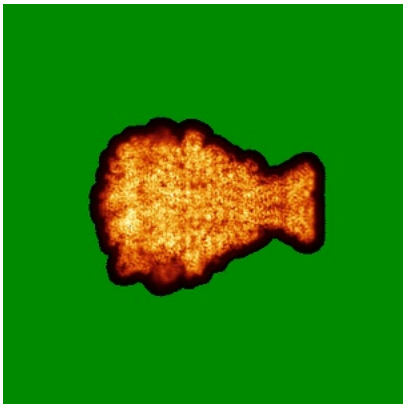
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

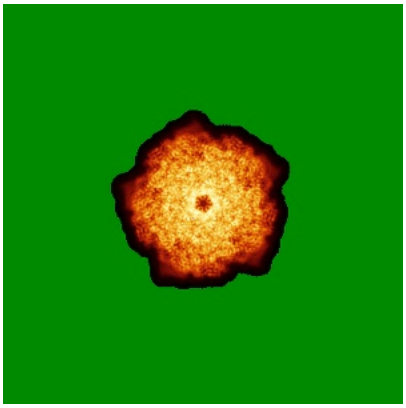
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.028. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

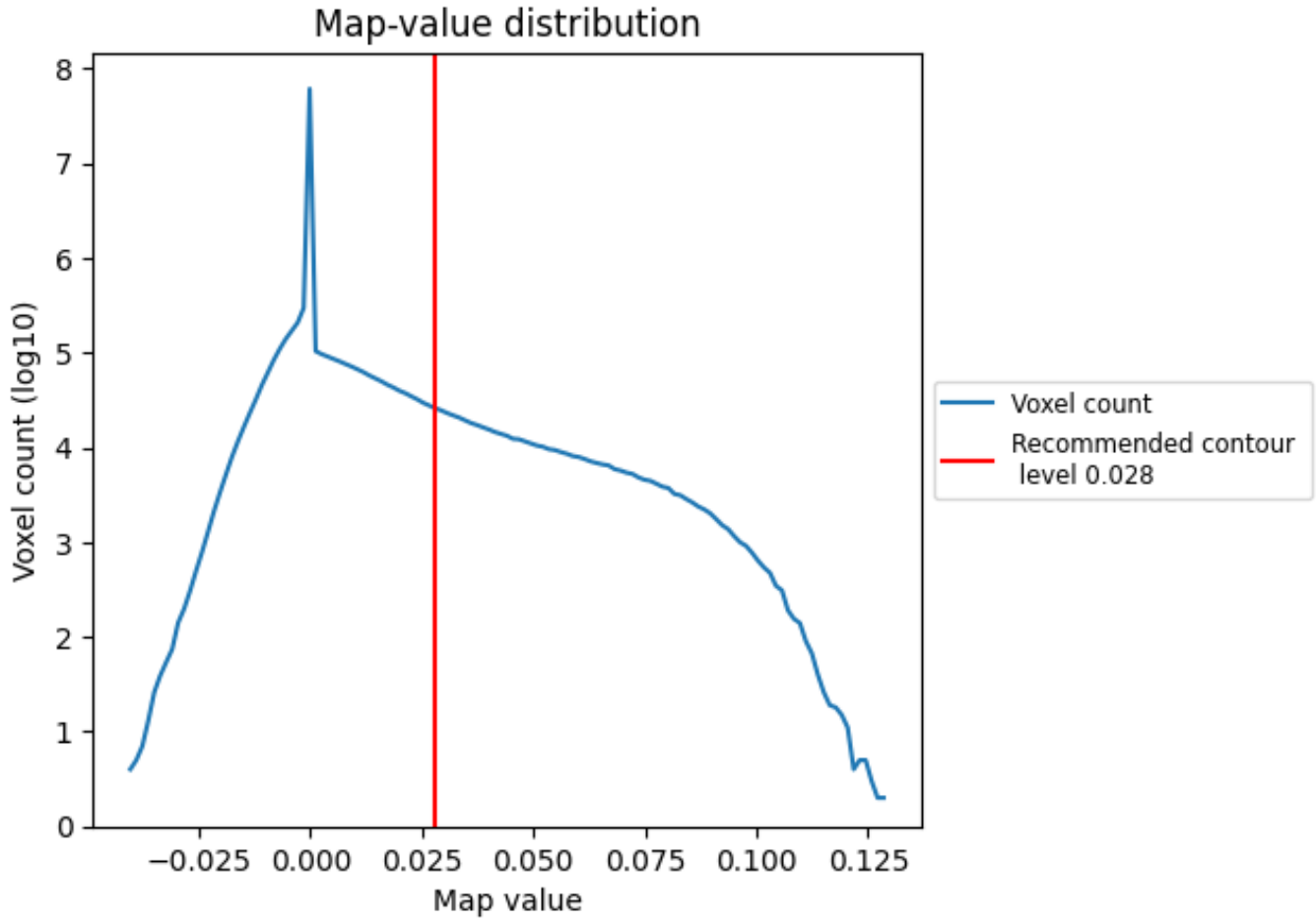
6.6 Mask visualisation (i)

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

7 Map analysis

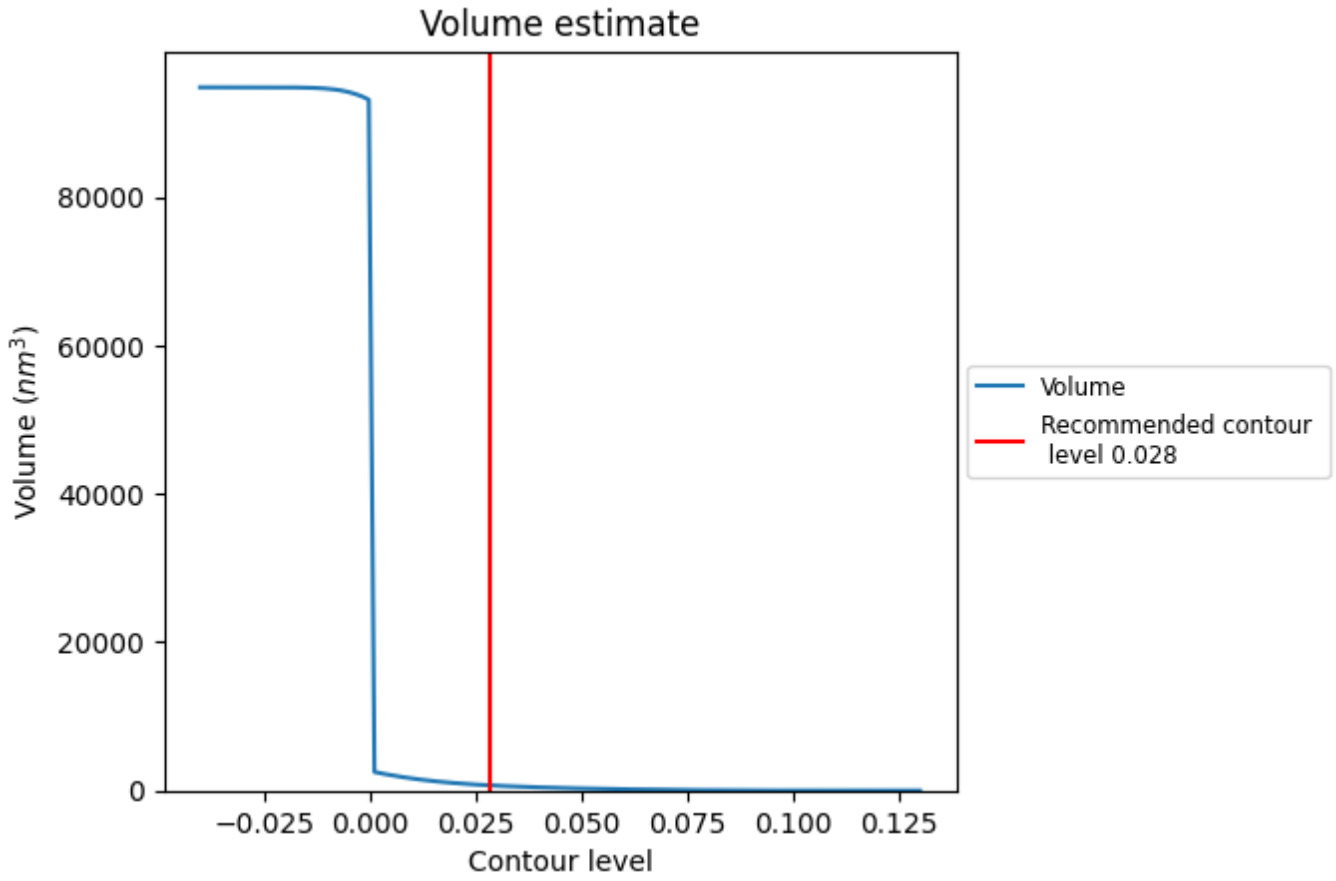
This section contains the results of statistical analysis of the map.

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.

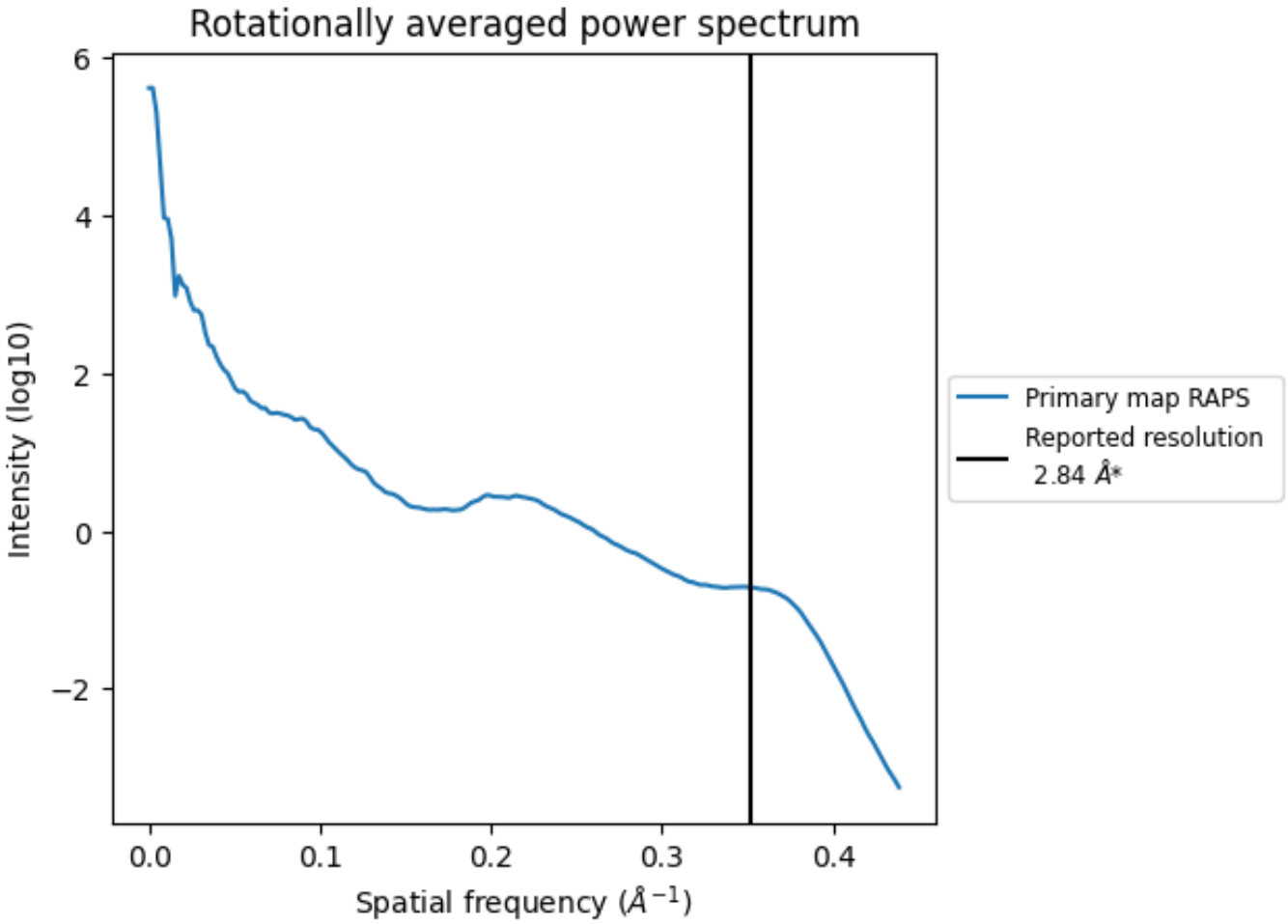
7.2 Volume estimate



The volume at the recommended contour level is 708 nm^3; this corresponds to an approximate mass of 639 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 0.352 $Å^{-1}$

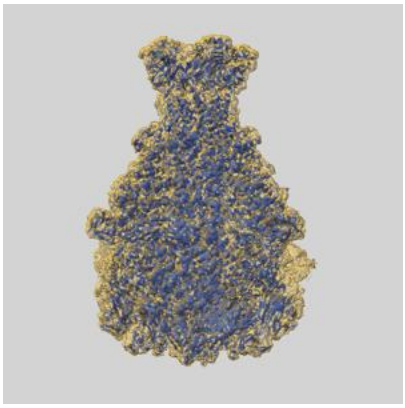
8 Fourier-Shell correlation

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

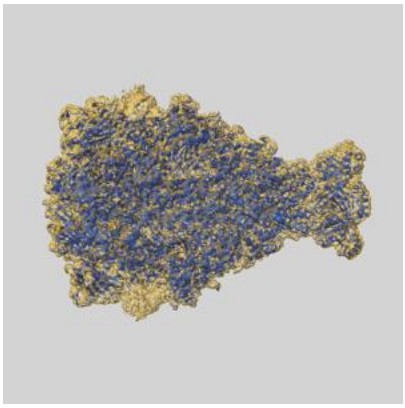
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10034 and PDB model 6RW8. Per-residue inclusion information can be found in section 3 on page 4.

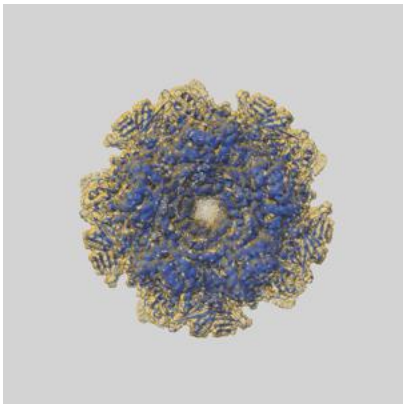
9.1 Map-model overlay



X



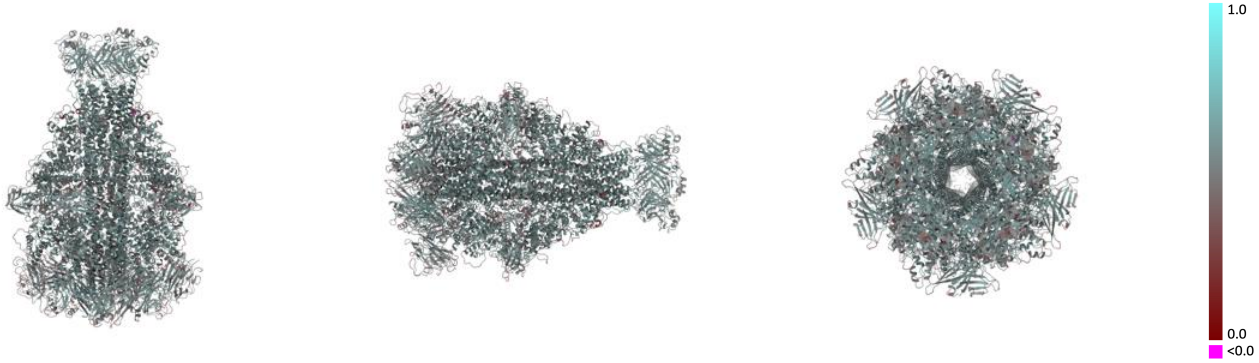
Y



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.

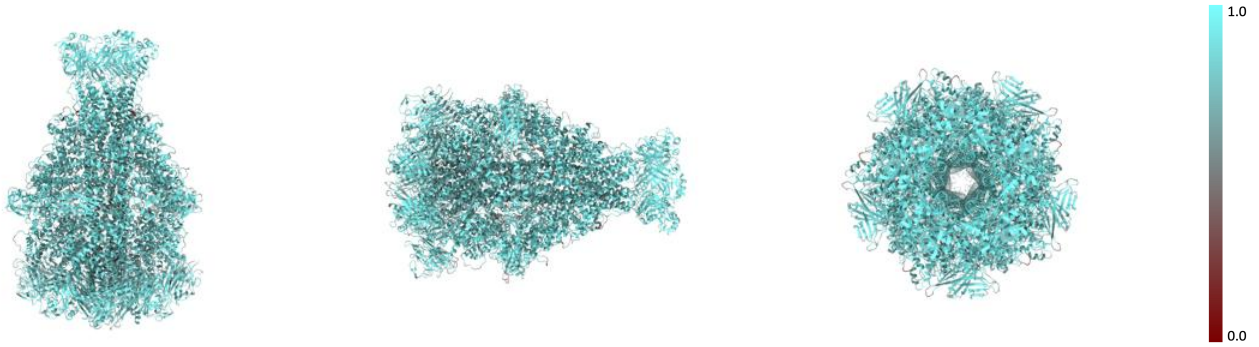
9.2 Q-score mapped to coordinate model



X Y Z

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

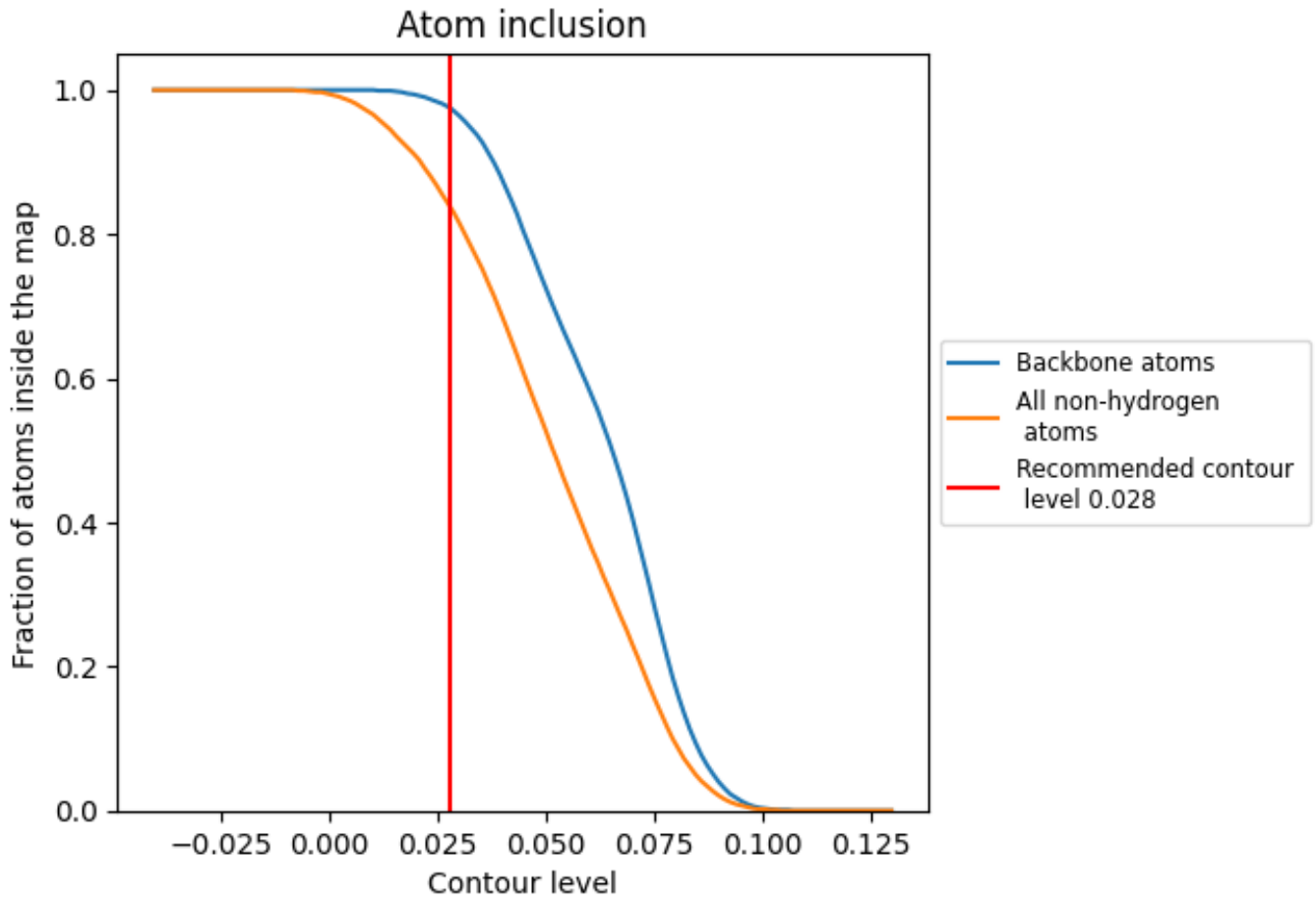
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.028).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 84% 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	0.8380	0.5250
A	0.8380	0.5250
B	0.8380	0.5240
C	0.8390	0.5250
D	0.8380	0.5250
E	0.8370	0.5250