Full wwPDB EM Validation Report ⓘ

Mar 18, 2023 – 07:23 am GMT

PDB ID	:	8ATO
EMDB ID	:	EMD-15654
Title	:	Structure of the giant inhibitor of apoptosis, BIRC6 bound to the regulator SMAC
Authors	:	Dietz, L.; Elliott, P.R.
Deposited on	:	2022-08-23
Resolution	:	3.00 Å(reported)

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

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

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

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

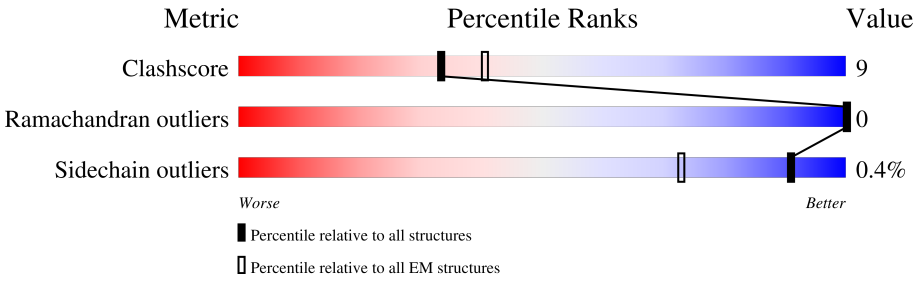
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

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 3.00 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	4859	20% 47% 12% 41%
1	B	4859	17% 45% 14% 40%
2	C	184	68% 61% 20% • 18%
2	D	184	71% 70% 11% 18%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 46909 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 Baculoviral IAP repeat-containing protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2871	Total 22195	C 14154	N 3782	O 4102	S 157	0	0
1	B	2892	Total 22348	C 14249	N 3807	O 4135	S 157	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q9NR09
A	0	PRO	-	expression tag	UNP Q9NR09
B	-1	GLY	-	expression tag	UNP Q9NR09
B	0	PRO	-	expression tag	UNP Q9NR09

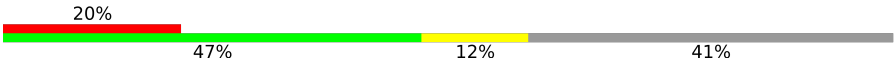
- Molecule 2 is a protein called Diablo IAP-binding mitochondrial protein.

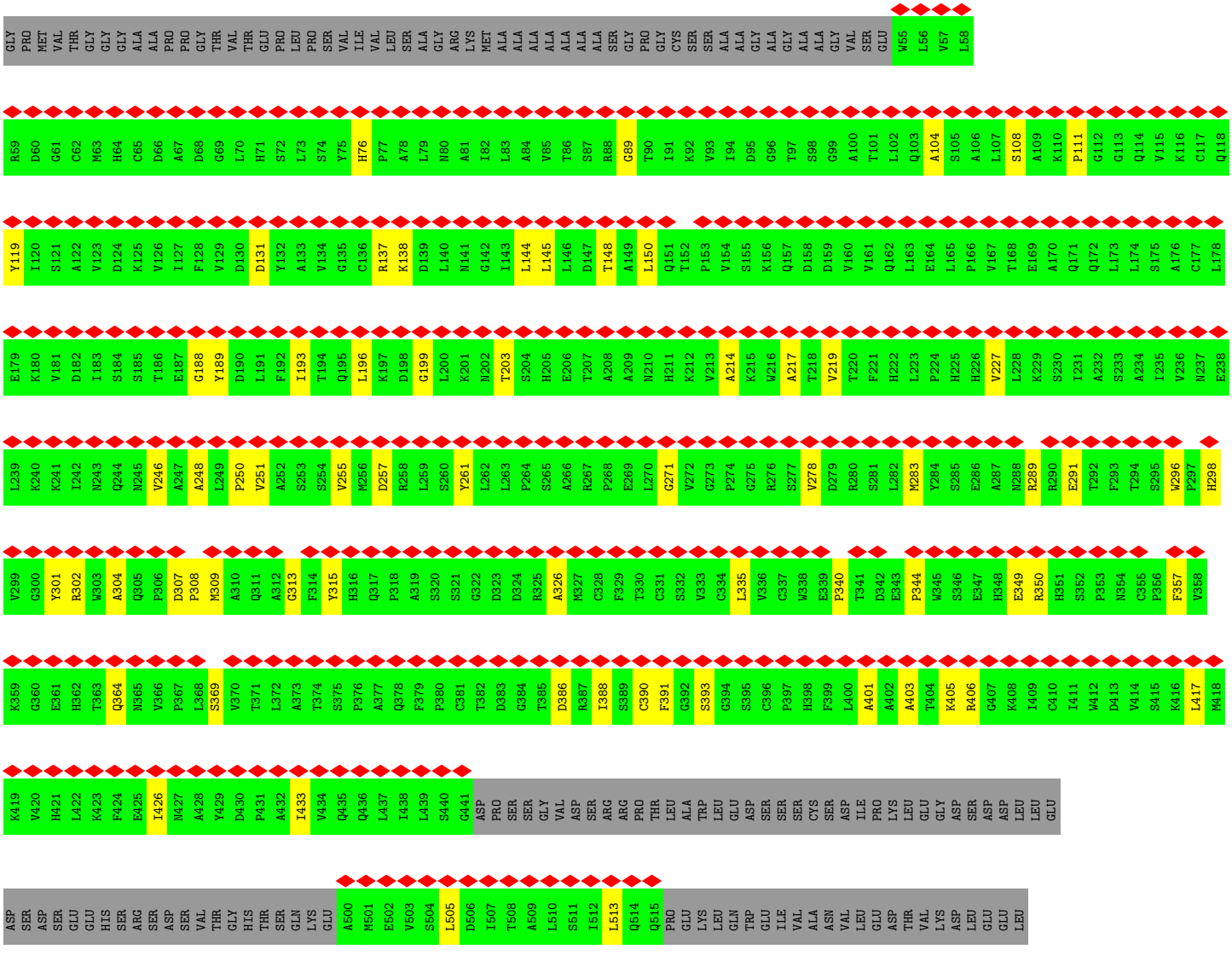
Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	150	Total 1183	C 739	N 198	O 241	S 5	0	0
2	D	150	Total 1183	C 739	N 198	O 241	S 5	0	0

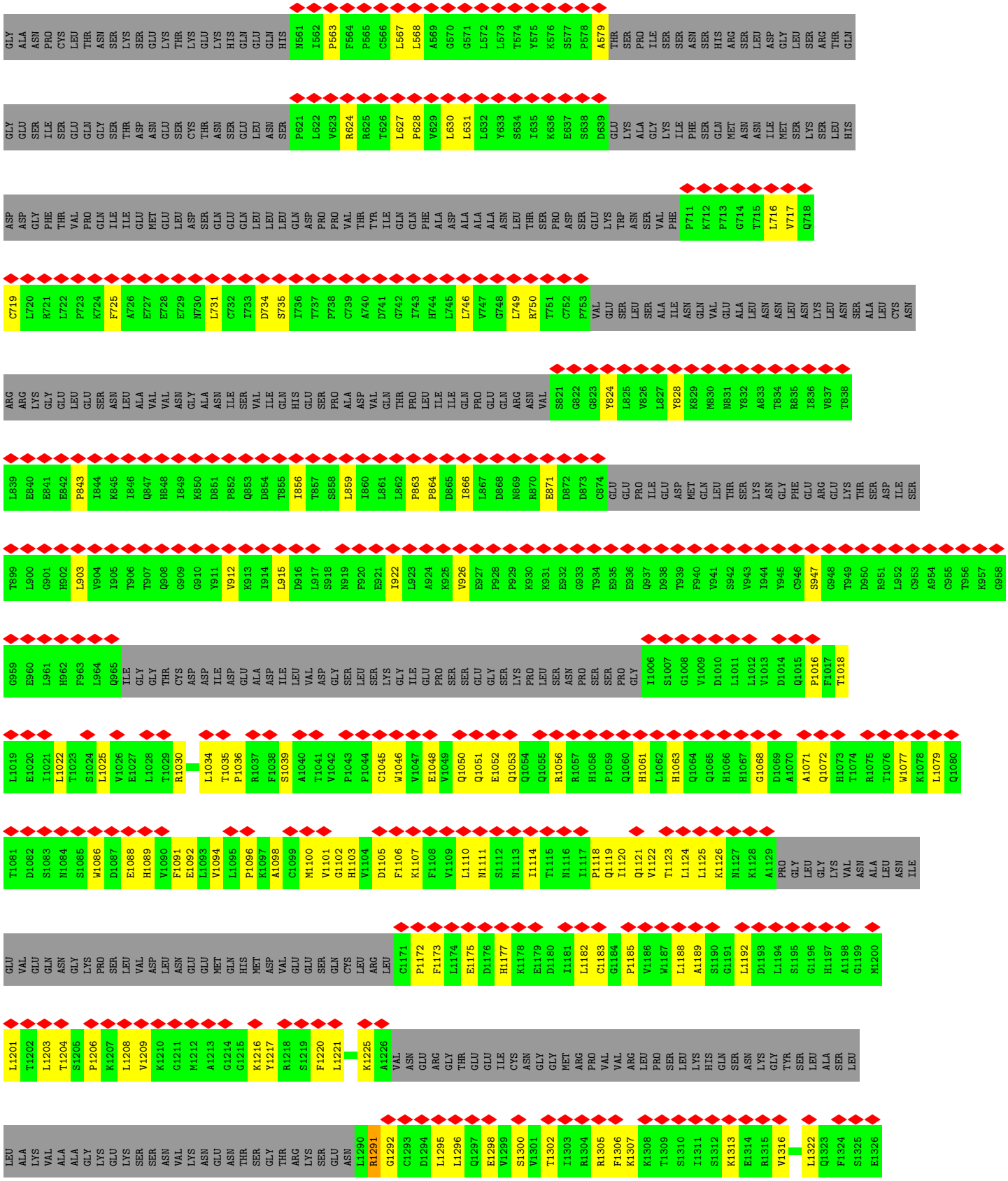
3 Residue-property plots (i)

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: Baculoviral IAP repeat-containing protein 6

Chain A: 

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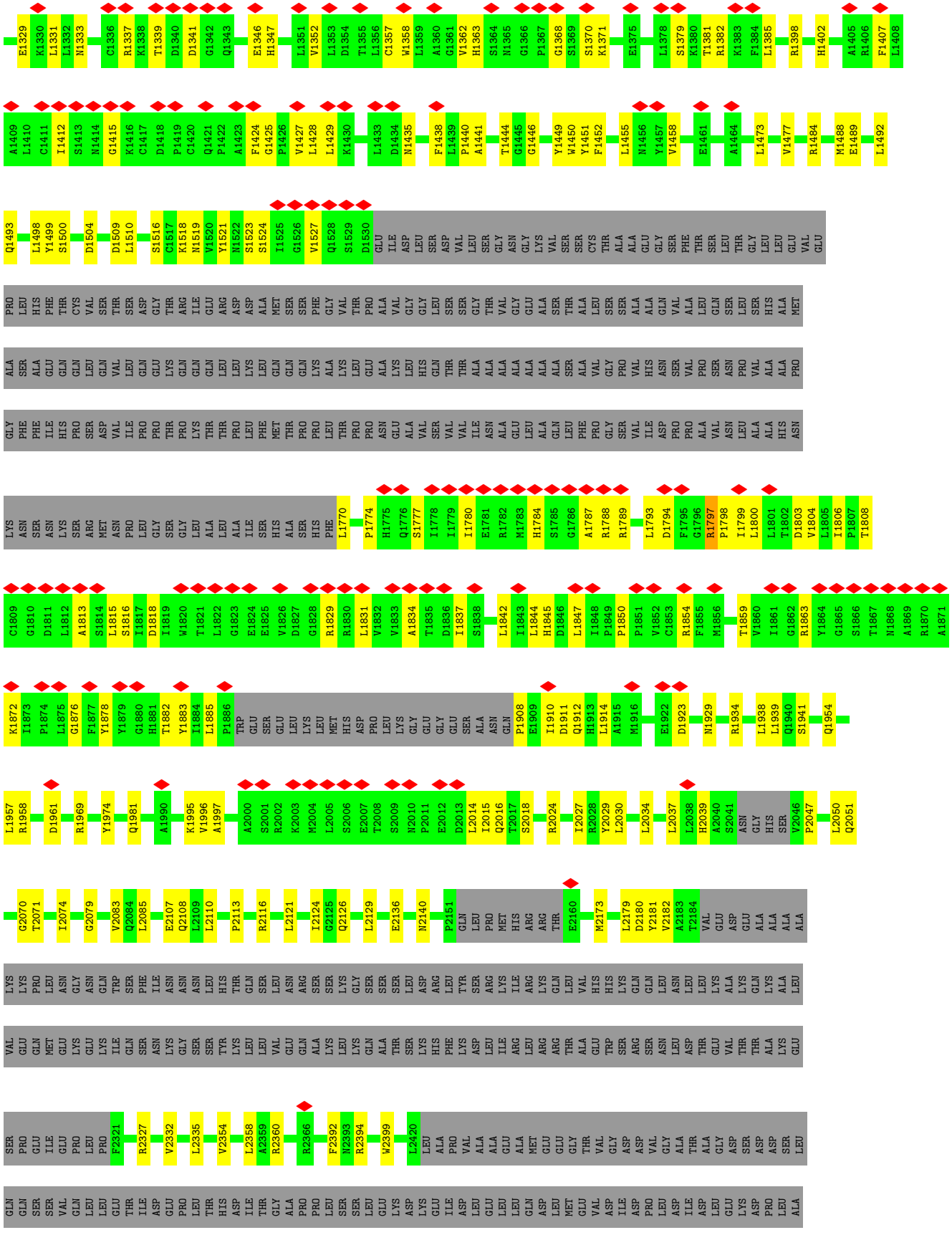
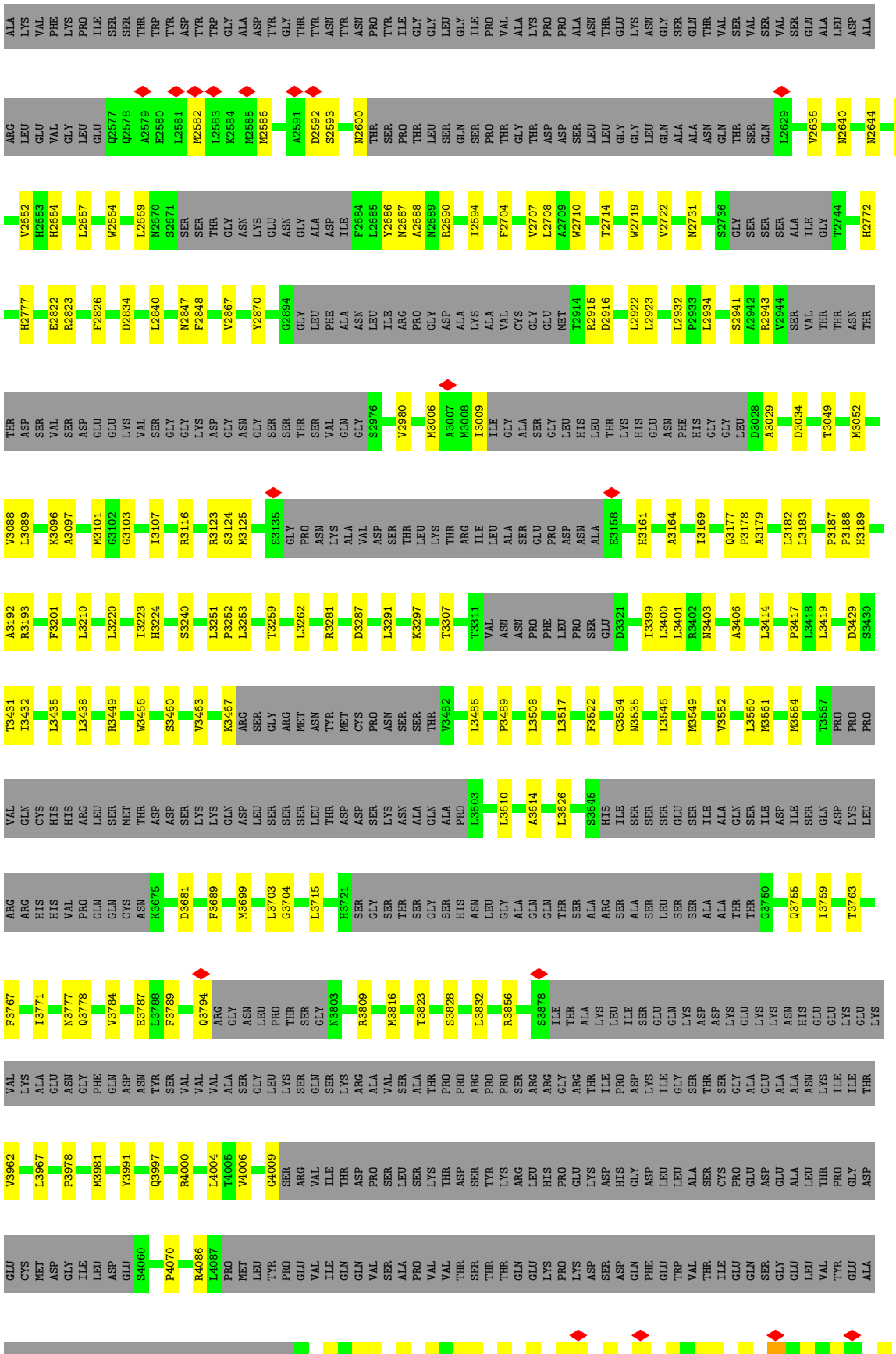
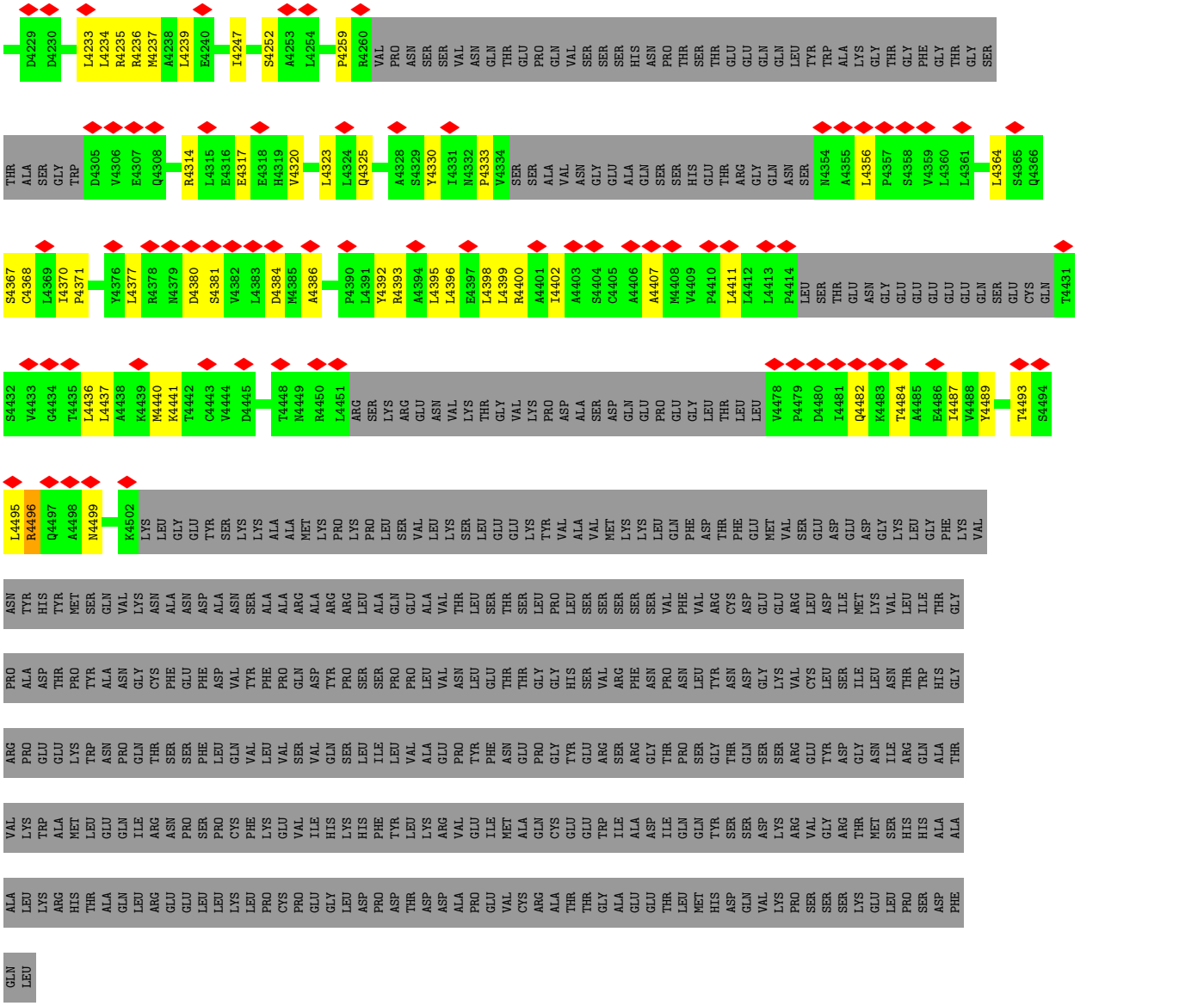
N561 I562 P563 F564 P565 C566 L567 L568 A569 G570 G571 L572 L573 T574 Y575 K576 S577 P578 A579
THR SER PRO ILE SER SER ASN SER HIS ARG SER LEU ASP GLY LEU SER ARG THR GLN
GLY GLU SER ILE SER GLU GLN GLY SER THR ASP ASN GLU SER CYS THR ASN SER GLU LEU ASN SER
P621 L622 V623 R624 R625 T626 L627 P628 V629 L630 L631 L632 Y633 S634 I635 K636 E637 S638 D639
GLU LYS ALA GLY LYS ILE PHE SER GLN MET ASN ASN ILE MET SER LYS SER LEU HIS
ASP ASP GLY PHE THR VAL PRO GLN ILE ILE GLU MET GLU LEU ASP SER GLN GLU GLN LEU LEU LEU GLN
ASP PRO PRO VAL THR TYR ILE GLN GLN PHE ALA ASP ALA ALA ALA ASN LEU THR SER PRO ASP SER GLU LYS TRP ASN SER VAL PHE
P711 K712 P713 G714 T715 L716 V717 Q718
C719 L720 R721 L722 P723 K724 F725 A726 E727 E728 E729 N730 L731 C732 I733 D734 S735 I736 T737 P738 C739 A740 D741 G742 I743 H744 L745 L746 V747 G748 L749 R750 T751 C752 F753
VAL GLU SER LEU SER ALA ILE ASN GLN VAL GLU ALA LEU ASN ASN LEU ASN LYS LEU ASN SER ALA LEU CYS ASN
ARG ARG LYS GLY GLU LEU GLU SER ASN LEU ALA VAL VAL ASN GLY ALA ASN ILE SER VAL ILE GLN HIS GLU SER PRO ALA ASP VAL GLN THR PRO LEU ILE ILE GLN PRO GLU GLN ARG ASN VAL
S821 G822 G823 Y824 L825 V826 L827 Y828 K829 M830 N831 Y832 A833 T834 R835 I836 V837 T838
L839 E840 E841 E842 P843 I844 K845 I846 Q847 H848 I849 K850 D851 P852 Q853 D854 T855 I856 T857 S858 L859 I860 L861 L862 P863 P864 D865 I866 L867 D868 N869 R870 E871 D872 D873 C874
GLU GLU PRO ILE GLU ASP MET GLN LEU THR SER LYS ASN GLY PHE GLU ARG GLU LYS THR SER ASP ILE SER
T899 L900 G901 H902 L903 V904 I905 T906 T907 Q908 G909 G910 Y911 V912 K913 I914 L915 D916 L917 S918 N919 F920 E921 I922 L923 A924 K925 V926 E927 P928 P929 K930 K931 E932 G933 T934 E935 E936 Q937 D938 T939 F940 V941 S942 V943 I944 Y945 C946 S947 G948 T949 D950 R951 L952 C953 A954 C955 T956 K957 G958
G959 E960 L961 H962 F963 L964 Q965 ILE GLY GLY THR CYS ASP ASP ILE ASP GLU ALA ASP ILE LEU LEU VAL ASP GLY SER LEU SER LYS GLY ILE GLU PRO SER SER GLU GLY SER LYS PRO LEU SER ASN PRO SER SER PRO GLY
I1006 S1007 G1008 V1009 D1010 L1011 L1012 V1013 D1014 Q1015 P1016 F1017 T1018
L1019 E1020 I1021 L1022 T1023 S1024 L1025 V1026 E1027 L1028 T1029 R1030 L1034 T1035 P1036 R1037 F1038 S1039 A1040 T1041 V1042 P1043 P1044 C1045 W1046 V1047 E1048 V1049 Q1050 Q1051 E1052 Q1053 Q1054 Q1055 R1056 R1057 H1058 P1059 Q1060 H1061 L1062 H1063 Q1064 Q1065 H1066 H1067 G1068 D1069 A1070 A1071 Q1072 H1073 T1074 R1075 T1076 W1077 K1078 L1079 Q1080
T1081 D1082 S1083 N1084 S1085 W1086 D1087 E1088 H1089 V1090 F1091 E1092 L1093 V1094 L1095 P1096 K1097 A1098 C1099 M1100 V1101 G1102 H1103 V1104 D1105 F1106 K1107 F1108 V1109 L1110 N1111 S1112 N1113 I1114 T1115 N1116 I1117 P1118 Q1119 I1120 Q1121 V1122 T1123 L1124 L1125 K1126 N1127 K1128 A1129
PRO GLY LEU GLY LYS VAL ASN ALA LEU ASN ILE
GLU VAL GLU GLN ASN GLY LYS PRO SER LEU VAL ASP LEU ASN GLU GLU MET GLN HIS MET ASP VAL GLU GLU SER GLN CYS LEU ARG LEU
C1171 P1172 F1173 L1174 E1175 D1176 H1177 K1178 E1179 D1180 I1181 L1182 C1183 G1184 P1185 V1186 W1187 L1188 A1189 S1190 G1191 L1192 D1193 L1194 S1195 G1196 H1197 A1198 G1199 M1200
L1201 T1202 L1203 T1204 S1205 P1206 K1207 L1208 V1209 K1210 G1211 M1212 A1213 G1214 G1215 K1216 Y1217 R1218 S1219 F1220 L1221 K1225 A1226
VAL ASN GLU ARG GLY THR GLU GLU ILE CYS ASN GLY GLY MET ARG PRO VAL VAL ARG LEU PRO SER LEU LYS HIS GLN SER ASN LYS GLY TYR SER LEU ALA SER LEU
LEU ALA LYS VAL ALA ALA GLY LYS GLU LYS SER SER ASN VAL LYS ASN GLU ASN THR SER GLY THR ARG LYS SER GLU ASN
L1290 R1291 G1292 C1293 D1294 L1295 L1296 Q1297 E1298 V1299 S1300 V1301 T1302 I1303 R1304 R1305 F1306 K1307 K1308 T1309 S1310 I1311 S1312 K1313 E1314 R1315 V1316 L1322 Q1323 F1324 S1325 E1326

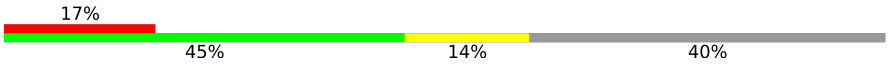


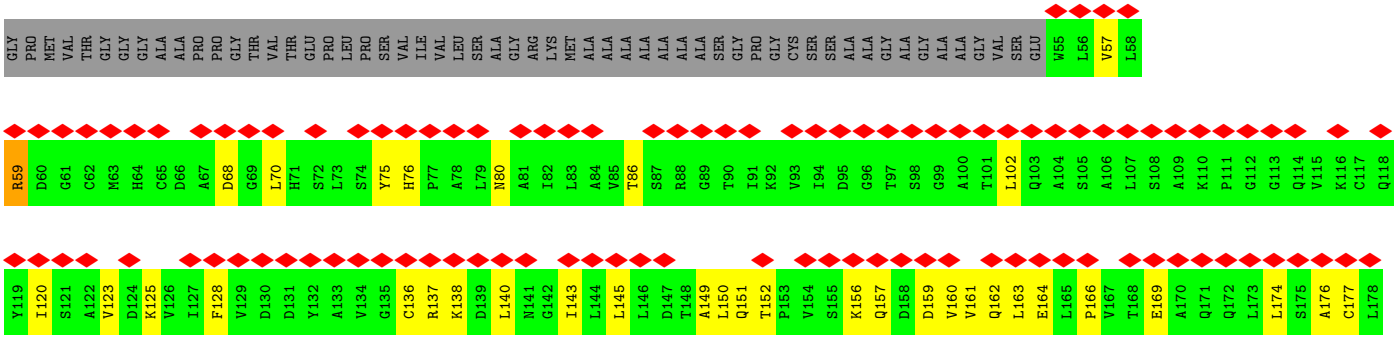


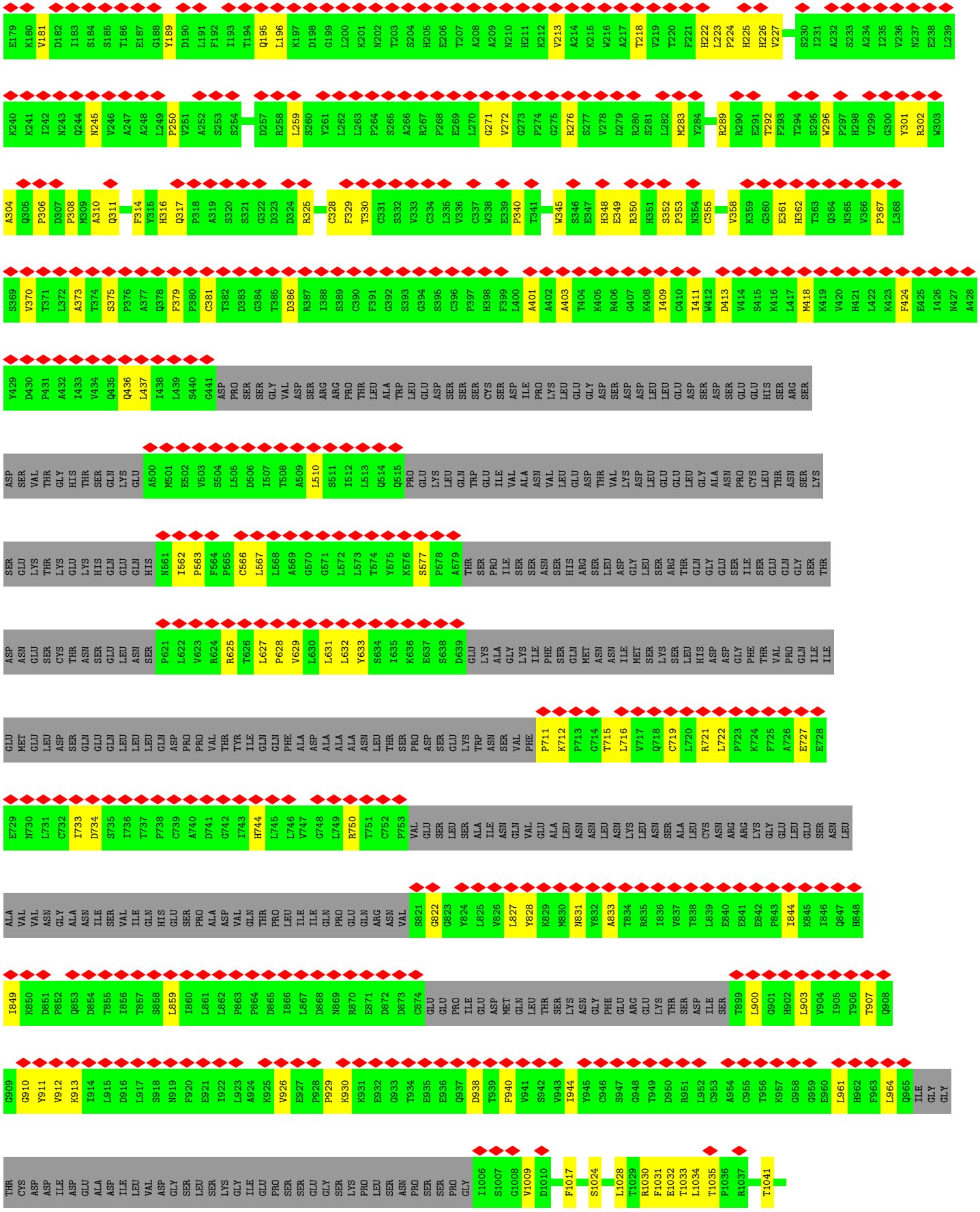


• Molecule 1: Baculoviral IAP repeat-containing protein 6

Chain B:



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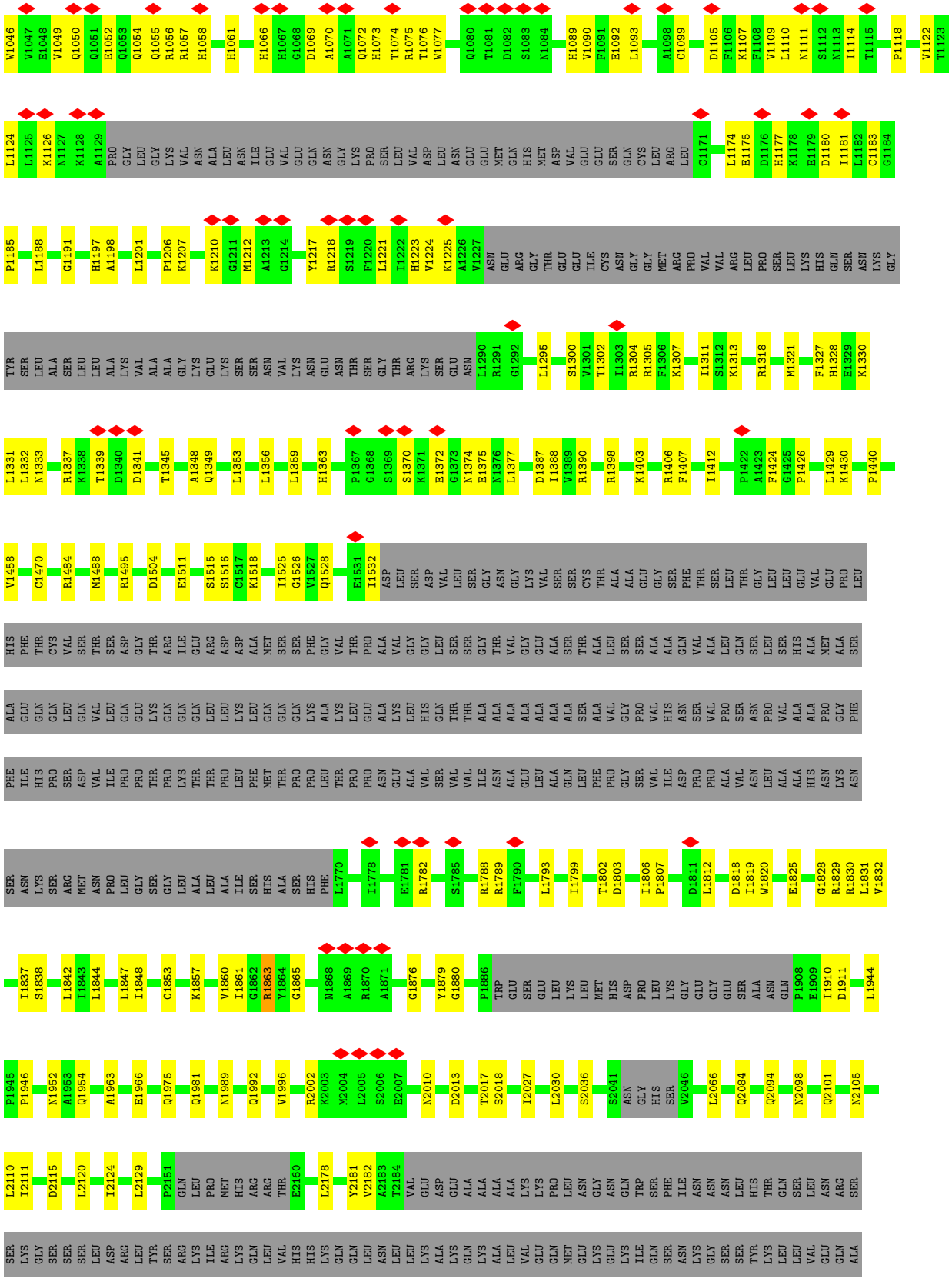
K240 K241 I242 N243 Q244 N245 V246 A247 A248 L249 P250 V251 A252 S253 S254 D257 R258 L259 S260 Y261 L262 L263 P264 S265 A266 R267 P268 E269 L270 G271 V272 G273 P274 G275 R276 S277 V278 D279 R280 S281 L282 M283 Y284 R289 R290 E291 T292 F293 T294 S295 W296 P297 H298 V299 G300 Y301 R302 W303
A304 Q305 P306 D307 P308 M309 A310 Q311 F314 Y315 H316 Q317 P318 A319 S320 S321 G322 D323 D324 R325 C328 F329 T330 C331 S332 V333 C334 L335 V336 C337 W338 E339 P340 T341 W345 S346 E347 H348 E349 R350 H351 S352 P353 N354 C355 V358 K359 G360 E361 H362 T363 Q364 N365 V366 P367 L368
S369 V370 T371 L372 A373 T374 S375 P376 A377 Q378 F379 P380 C381 T382 D383 G384 T385 D386 R387 I388 S389 C390 F391 G392 S393 G394 S395 C396 P397 H398 F399 L400 A401 A402 A403 T404 K405 R406 C407 K408 I409 C410 I411 W412 D413 V414 S415 K416 L417 M418 K419 V420 H421 L422 K423 F424 E425 I426 N427 A428
Y429 D430 P431 A432 I433 V434 Q435 Q436 L437 I438 L439 S440 G441 ASP PRO SER SER GLY VAL ASP SER ARG ARG PRO THR LEU ALA TRP LEU GLU ASP SER SER SER CYS SER ASP ILE PRO LYS LEU GLU GLY ASP SER ASP ASP LEU LEU GLU ASP SER ASP SER GLU GLU HIS SER ARG SER
ASP SER VAL THR GLY HIS THR SER GLN LYS GLU A500 N501 E502 V503 S504 L505 D506 I507 T508 A509 L510 S511 I512 L513 Q514 Q515 PRO GLU LYS LEU GLN TRP GLU ILE VAL ALA ASN VAL LEU GLU ASP THR VAL LYS ASP LEU GLU GLU LEU GLY ALA ASN PRO CYS LEU THR ASN SER LYS
SER GLU LYS THR LYS GLU LYS HIS GLN GLU GLN HIS N561 I562 P563 F564 P565 C566 L567 L568 A569 G570 G571 L572 L573 T574 Y575 K576 S577 P578 A579 THR SER PRO ILE SER SER ASN SER HIS ARG SER LEU ASP GLY LEU SER ARG THR GLN GLY GLU SER ILE SER GLU GLN GLY SER THR
ASP ASN GLU SER CYS THR ASN SER GLU LEU ASN SER P621 L622 V623 R624 R625 T626 L627 P628 V629 L630 L631 L632 Y633 S634 I635 K636 E637 S638 D639 GLU LYS ALA GLY LYS ILE PHE SER GLN MET ASN ASN ILE MET SER LYS SER LEU HIS ASP ASP GLY PHE THR VAL PRO GLN ILE ILE
GLU MET GLU LEU ASP SER GLN GLU GLN LEU LEU LEU GLN ASP PRO PRO VAL THR TYR ILE GLN GLN PHE ALA ASP ALA ALA ALA ASN LEU THR SER PRO ASP SER GLU LYS TRP ASN SER VAL PHE P711 K712 P713 G714 T715 L716 V717 Q718 C719 L720 R721 L722 P723 K724 F725 A726 E727 E728
E729 N730 L731 C732 I733 D734 S735 I736 T737 P738 C739 A740 D741 G742 I743 H744 L745 L746 V747 G748 L749 R750 T751 C752 P753 VAL GLU SER LEU SER ALA ILE ASN GLN VAL GLU ALA LEU ASN ASN LEU ASN LYS LEU ASN SER ALA LEU CYS ASN ARG ARG LYS GLY GLU LEU GLU SER ASN LEU
ALA VAL VAL ASN GLY ALA ASN ILE SER VAL ILE GLN HIS GLU SER PRO ALA ASP VAL GLN THR PRO LEU ILE ILE GLN PRO GLU GLN ARG ASN VAL S821 G822 G823 Y824 L825 V826 L827 Y828 K829 M830 N831 Y832 A833 T834 R835 I836 V837 T838 L839 E840 E841 E842 P843 I844 K845 I846 Q847 H848
I849 K850 D851 P852 Q853 D854 T855 I856 T857 S858 L859 I860 L861 L862 P863 P864 D865 I866 L867 D868 N869 R870 E871 D872 D873 C874 GLU GLU PRO ILE GLU ASP MET GLN LEU THR SER LYS ASN GLY PHE GLU ARG GLU LYS THR SER ASP ILE SER T899 L900 G901 H902 L903 V904 I905 T906 T907 Q908
G909 G910 Y911 V912 K913 I914 L915 D916 L917 S918 N919 F920 E921 I922 L923 A924 K925 V926 E927 P928 P929 K930 K931 E932 G933 T934 E935 E936 Q937 D938 T939 F940 V941 S942 V943 I944 Y945 C946 S947 G948 T949 D950 R951 L952 C953 A954 C955 T956 K957 G958 G959 E960 L961 H962 F963 L964 Q965 ILE GLY GLY
THR CYS ASP ASP ILE ASP GLU ALA ASP ILE LEU VAL ASP GLY SER LEU SER LYS GLY ILE GLU PRO SER SER GLU GLY SER LYS PRO LEU SER ASN PRO SER SER PRO GLY I1006 S1007 G1008 V1009 D1010 F1017 S1024 L1028 T1029 R1030 F1031 E1032 T1033 L1034 T1035 P1036 R1037 T1041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L1124 L1125 K1126 N1127 K1128 A1129 PRO GLY LEU GLY LYS VAL ASN ALA LEU ASN ILE GLU VAL VAL GLU GLN ASN GLY LYS PRO SER LEU VAL ASP LEU ASN GLU GLU MET GLN HIS MET ASP VAL GLU GLU SER GLN CYS LEU ARG LEU C1171 L1174 E1175 D1176 H1177 K1178 E1179 D1180 I1181 L1182 C1183 G1184
P1185 L1188 G1191 H1197 A1198 L1201 P1206 K1207 K1210 G1211 M1212 A1213 G1214 Y1217 R1218 S1219 F1220 L1221 I1222 H1223 V1224 K1225 A1226 V1227 ASN GLU ARG GLY THR GLU GLU ILE CYS ASN GLY GLY MET ARG PRO VAL VAL ARG LEU PRO SER LEU LYS HIS GLN SER ASN LYS GLY
TYR SER LEU ALA SER LEU LEU ALA LYS VAL ALA ALA GLY LYS GLU LYS SER SER ASN VAL LYS ASN GLU GLU ASN THR SER GLY THR ARG LYS SER GLU ASN L1290 R1291 G1292 L1295 S1300 V1301 T1302 I1303 R1304 R1305 F1306 K1307 I1311 S1312 K1313 R1318 M1321 F1327 H1328 E1329 K1330
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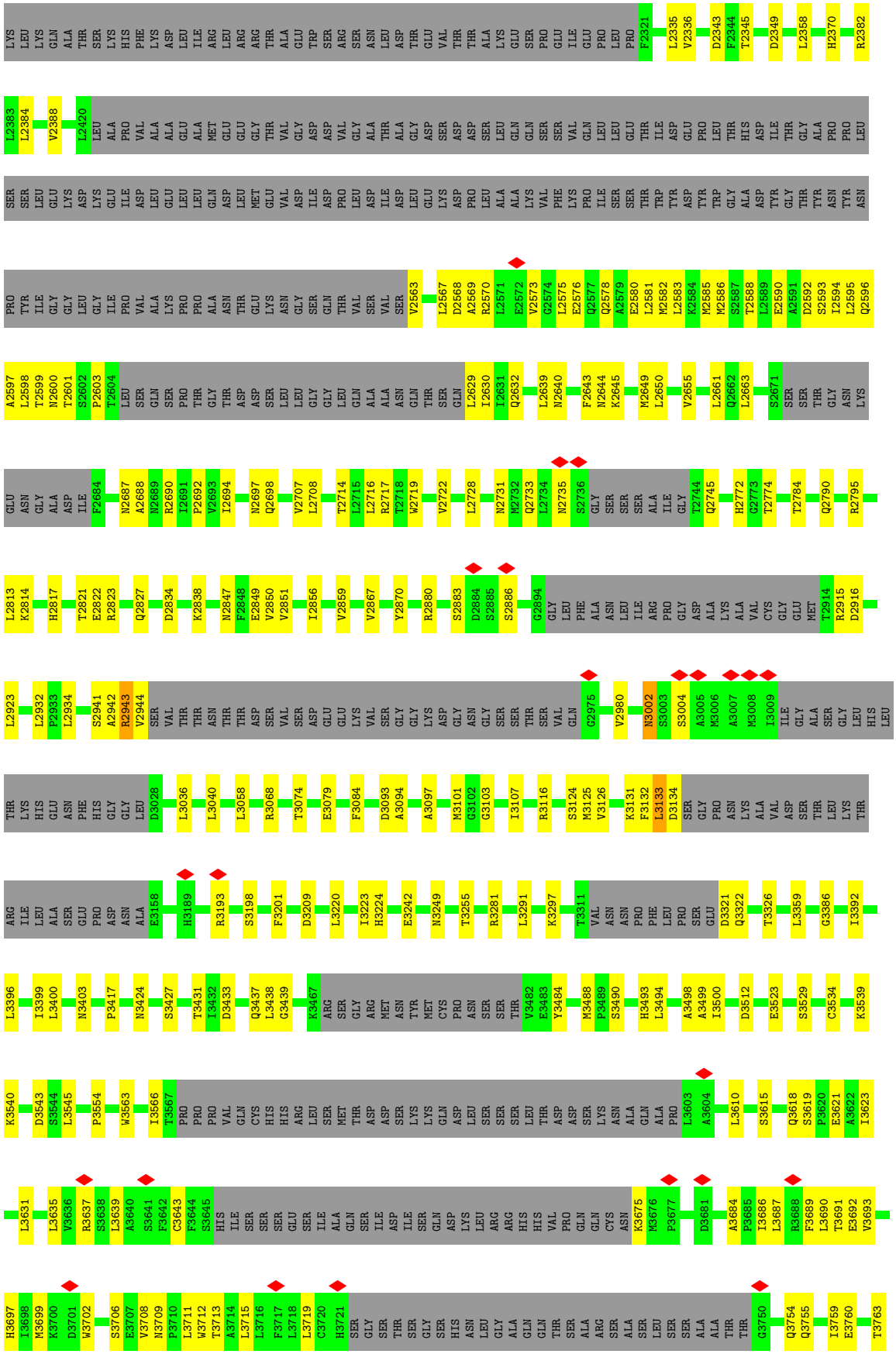
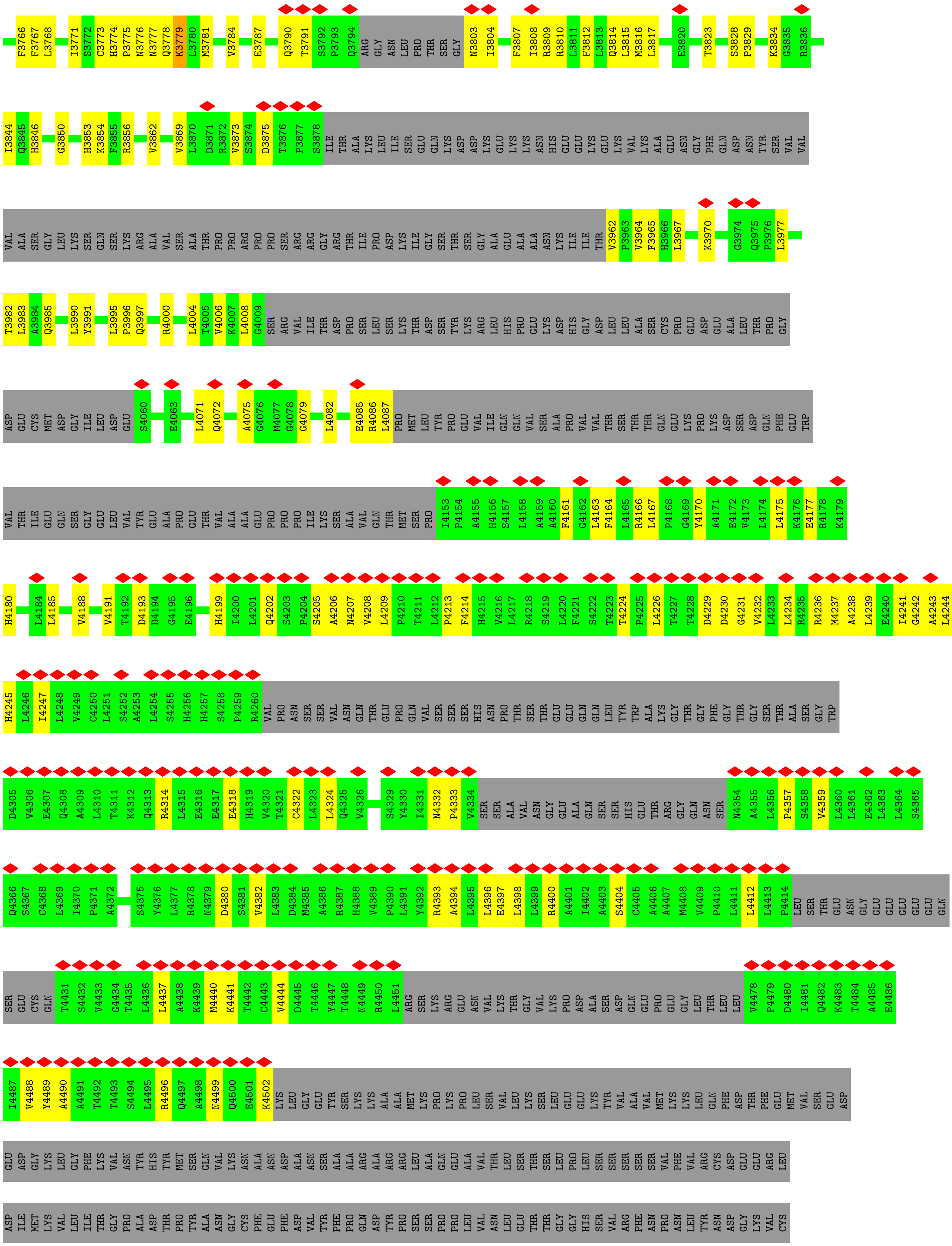
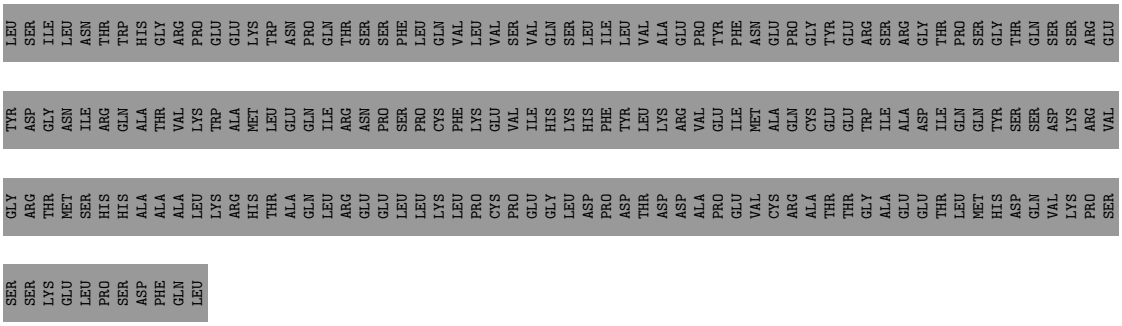
V1458 C1470 R1484 M1488 R1495 D1504 E1511 S1515 S1516 C1517 K1518 I1525 G1526 V1527 Q1528 E1531 I1532 ASP LEU SER ASP VAL LEU LEU SER GLY ASN GLY LYS VAL SER SER CYS THR ALA ALA GLU GLY SER PHE THR SER LEU LEU THR GLY LEU LEU GLU VAL GLU PRO LEU
HIS PHE THR CYS VAL SER THR SER ASP GLY THR ARG ILE GLU ARG ASP ASP ALA MET SER SER PHE GLY VAL THR PRO ALA VAL GLY GLY LEU SER SER GLY THR VAL GLY GLU ALA SER THR ALA LEU SER SER ALA ALA GLN VAL ALA LEU GLN SER LEU SER HIS ALA MET ALA SER
ALA GLU GLN GLN LEU GLU LYS GLN GLN LEU LYS LEU GLN GLN GLN LYS ALA LYS LEU GLU ALA LYS LEU HIS GLN THR THR ALA ALA ALA ALA ALA ALA ALA SER ALA VAL GLY PRO VAL HIS ASN SER VAL PRO SER ASN PRO VAL ALA ALA ALA PRO GLY PHE
PHE ILE HIS PRO SER ASP VAL ILE PRO PRO THR PRO LYS THR THR PRO LEU PHE MET THR PRO PRO LEU THR PRO PRO ASN GLU ALA VAL SER VAL VAL ILE ASN ALA GLU LEU ALA GLN LEU PHE PRO GLY SER VAL ILE ASP PRO PRO ALA VAL ASN LEU ALA ALA HIS ASN LYS ASN
SER ASN LYS SER ARG MET ASN PRO LEU GLY SER GLY LEU ALA ALA LEU ILE SER HIS ALA SER HIS PHE L1770 I1778 E1781 R1782 S1785 R1788 R1789 F1790 L1793 I1799 T1802 D1803 I1806 P1807 D1811 L1812 D1818 I1819 W1820 E1825 G1828 R1829 R1830 L1831 V1832
I1837 S1838 L1842 I1843 L1844 L1847 I1848 C1853 K1857 V1860 I1861 G1862 R1863 Y1864 G1865 N1868 A1869 R1870 A1871 G1876 Y1879 G1880 P1886 TRP GLU SER GLU LEU LYS LEU MET HIS ASP PRO LEU LYS GLY GLU GLY GLU SER ALA ASN GLN P1908 E1909 I1910 D1911 L1944
P1945 P1946 N1952 A1953 Q1954 A1963 E1966 Q1975 Q1981 N1989 Q1992 V1996 R2002 K2003 M2004 L2005 S2006 E2007 N2010 D2013 T2017 S2018 I2027 L2030 S2036 S2041 ASN GLY HIS SER V2046 L2066 Q2084 Q2094 N2098 Q2101 N2105
L2110 I2111 D2115 L2120 I2124 L2129 P2151 GLN LEU PRO MET HIS ARG ARG THR E2160 L2178 Y2181 Y2182 A2183 T2184 VAL GLU ASP GLU ALA ALA ALA ALA LYS LYS PRO LEU ASN GLY ASN GLN TRP SER PHE ILE ASN ASN ASN LEU HIS THR GLN SER LEU ASN ARG SER
SER LYS GLY SER SER LEU ASP ARG LEU TYR SER ARG LYS ILE ARG LYS GLN LEU VAL HIS HIS LYS GLN GLN LEU LEU ASN LYS GLN LYS ALA LYS LEU VAL GLU GLN MET GLU LYS GLU LYS ILE GLN SER ASN LYS GLY SER SER TYR LYS LEU LEU VAL GLU GLN ALA

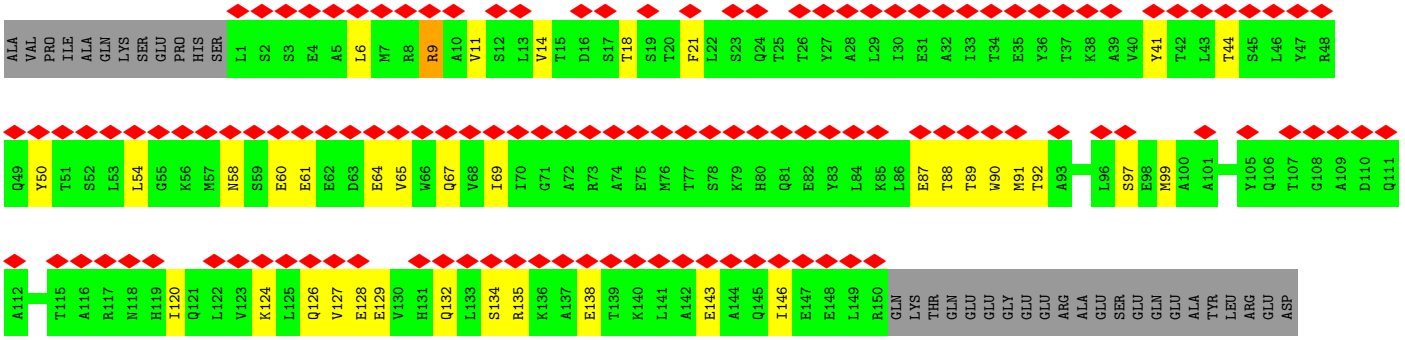



F3766 F3767 L3768 I3771 S3772 C3773 H3774 P3775 N3776 N3777 Q3778 K3779 L3780 M3781 V3784 E3787 Q3790 T3791 S3792 P3793 Q3794 ARG GLY ASN LEU PRO THR SER GLY N3803 I3804 F3807 I3808 R3809 R3810 L3811 F3812 L3813 Q3814 L3815 M3816 L3817 E3820 T3823 S3828 P3829 K3834 G3835 R3836
I3844 Q3845 H3846 G3850 H3853 K3854 F3855 R3856 V3862 V3869 L3870 D3871 R3872 V3873 S3874 D3875 T3876 P3877 S3878 ILE THR ALA LYS LEU ILE SER GLU GLN LYS ASP ASP LYS GLU LYS LYS ASN HIS GLU GLU LYS GLU LYS VAL LYS ALA GLU ASN GLY PHE GLN ASP ASN TYR SER VAL VAL
VAL ALA SER GLY LEU LYS SER GLN SER LYS ARG ALA VAL SER ALA THR PRO PRO ARG PRO PRO SER ARG ARG GLY ARG THR ILE PRO ASP LYS ILE GLY SER THR SER GLY ALA GLU ALA ALA ASN LYS ILE ILE THR V3962 P3963 V3964 F3965 H3966 L3967 K3970 G3974 Q3975 P3976 L3977
T3982 L3983 A3984 Q3985 L3990 Y3991 L3995 P3996 Q3997 R4000 L4004 T4005 V4006 K4007 L4008 G4009 SER ARG VAL ILE THR ASP PRO SER LEU SER LYS THR ASP SER TYR LYS ARG LEU HIS PRO GLU LYS ASP HIS GLY ASP LEU LEU ALA SER CYS PRO GLU ASP GLU ALA LEU THR PRO GLY
ASP GLU CYS MET ASP GLY ILE LEU ASP GLU S4060 E4063 L4071 Q4072 A4075 G4076 M4077 G4078 G4079 L4082 E4085 R4086 L4087 PRO MET LEU TYR PRO GLU VAL ILE GLN GLN VAL SER ALA PRO VAL VAL THR SER THR THR GLN GLU LYS PRO LYS ASP SER ASP GLN PHE GLU TRP
VAL THR ILE GLU GLN SER GLY GLU LEU VAL TYR GLU ALA PRO GLU THR VAL ALA ALA GLU PRO PRO PRO ILE LYS SER ALA VAL GLN THR MET SER PRO I4153 P4154 A4155 H4156 S4157 L4158 A4159 A4160 F4161 G4162 L4163 F4164 L4165 R4166 L4167 P4168 G4169 Y4170 A4171 E4172 V4173 L4174 L4175 K4176 E4177 R4178 K4179
H4180 L4184 L4185 V4188 V4191 T4192 D4193 D4194 G4195 E4196 H4199 I4200 L4201 Q4202 S4203 P4204 S4205 A4206 N4207 V4208 L4209 P4210 T4211 L4212 P4213 F4214 H4215 V4216 L4217 R4218 S4219 L4220 F4221 S4222 T4223 T4224 P4225 L4226 T4227 T4228 D4229 D4230 G4231 V4232 L4233 L4234 R4235 R4236 M4237 A4238 L4239 E4240 I4241 G4242 A4243 L4244
H4245 L4246 I4247 L4248 V4249 C4250 L4251 S4252 A4253 L4254 S4255 H4256 H4257 S4258 P4259 R4260 VAL PRO ASN SER SER VAL ASN GLN THR GLU PRO GLN VAL SER SER SER HIS ASN PRO THR SER THR GLU GLU GLN GLN LEU TYR TRP ALA LYS GLY THR GLY PHE GLY THR GLY SER THR ALA SER GLY TRP
D4305 V4306 E4307 Q4308 A4309 L4310 T4311 K4312 Q4313 R4314 L4315 E4316 E4317 E4318 H4319 V4320 T4321 C4322 L4323 L4324 Q4325 V4326 S4329 Y4330 I4331 N4332 P4333 V4334 SER SER ALA VAL ASN GLY GLU ALA GLN SER SER HIS GLU THR ARG GLY GLN ASN SER N4354 A4355 L4356 P4357 S4358 V4359 L4360 L4361 E4362 L4363 L4364 S4365
Q4366 S4367 C4368 L4369 I4370 P4371 A4372 S4375 Y4376 L4377 R4378 N4379 D4380 S4381 V4382 L4383 D4384 M4385 A4386 R4387 H4388 V4389 P4390 L4391 Y4392 R4393 A4394 L4395 L4396 E4397 L4398 L4399 R4400 A4401 I4402 A4403 S4404 C4405 A4406 A4407 M4408 V4409 P4410 L4411 L4412 L4413 P4414 LEU SER THR GLU ASN GLY GLU GLU GLU GLU GLN
SER GLU CYS GLN T4431 S4432 V4433 G4434 T4435 L4436 L4437 A4438 K4439 M4440 K4441 T4442 C4443 V4444 D4445 T4446 Y4447 T4448 N4449 R4450 L4451 ARG SER LYS ARG GLU ASN VAL LYS THR GLY VAL LYS PRO ASP ALA SER ASP GLN GLU PRO GLU GLY LEU THR LEU LEU V4478 P4479 D4480 I4481 Q4482 K4483 T4484 A4485 E4486
I4487 V4488 Y4489 A4490 A4491 T4492 T4493 S4494 L4495 R4496 Q4497 A4498 N4499 Q4500 E4501 K4502 LYS LEU GLY GLU TYR SER LYS LYS ALA ALA MET LYS PRO LYS PRO LEU SER VAL LEU LYS SER LEU GLU GLU LYS TYR VAL ALA VAL MET LYS LYS LEU GLN PHE ASP THR PHE GLU MET VAL SER GLU ASP
GLU ASP GLY LYS LEU GLY PHE LYS VAL ASN TYR HIS TYR MET SER GLN VAL LYS ASN ALA ASN ASP ALA ASN SER ALA ALA ALA ARG ALA ARG ARG LEU ALA GLN GLU ALA VAL THR LEU SER THR SER LEU PRO LEU SER SER SER SER VAL PHE VAL ARG CYS ASP GLU GLU ARG LEU
ASP ILE MET LYS VAL LEU ILE THR GLY PRO ALA ASP THR PRO TYR ALA ASN GLY CYS PHE GLU PHE ASP VAL TYR PHE PRO GLN ASP TYR PRO SER SER PRO PRO LEU VAL ASN LEU GLU THR THR GLY GLY HIS SER VAL ARG PHE ASN PRO ASN LEU TYR ASN ASP GLY LYS VAL CYS



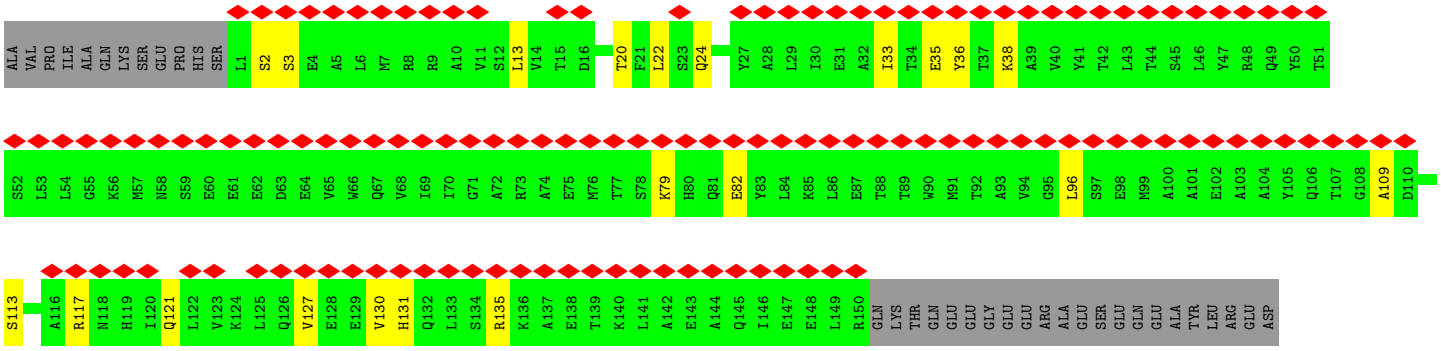
• Molecule 2: Diablo IAP-binding mitochondrial protein

Chain C:



• Molecule 2: Diablo IAP-binding mitochondrial protein

Chain D:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	36872	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 ($e^-/Å^2$)	47.27	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.429	Depositor
Minimum map value	-0.750	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.070	Depositor
Recommended contour level	0.144	Depositor
Map size (Å)	248.7, 248.7, 248.7	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.829, 0.829, 0.829	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	0.24	0/22620	0.47	0/30734
1	B	0.24	0/22774	0.47	0/30945
2	C	0.23	0/1197	0.46	0/1620
2	D	0.24	0/1197	0.44	0/1620
All	All	0.24	0/47788	0.47	0/64919

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	22195	0	22593	384	0
1	B	22348	0	22749	463	0
2	C	1183	0	1185	23	0
2	D	1183	0	1185	15	0
All	All	46909	0	47712	860	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 9.

All (860) 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:1818:ASP:HB2	1:B:1857:LYS:HB3	1.62	0.81
1:B:1032:GLU:HB3	1:B:1307:LYS:HG3	1.66	0.76
1:A:1052:GLU:OE1	1:A:1056:ARG:NH1	2.17	0.76
1:A:1103:HIS:O	1:A:1305:ARG:NH2	2.18	0.76
1:A:1806:ILE:HG12	1:A:1876:GLY:HA3	1.68	0.75
1:B:1035:THR:H	1:B:1305:ARG:HH21	1.35	0.75
1:B:4397:GLU:HG3	1:B:4400:ARG:HH12	1.51	0.74
1:B:2733:GLN:HE22	1:B:2735:ASN:HB2	1.52	0.74
1:A:4356:LEU:HB3	1:A:4407:ALA:HB1	1.70	0.74
1:B:1526:GLY:O	1:B:1528:GLN:NE2	2.21	0.73
1:B:3834:LYS:HG3	1:B:3875:ASP:HB3	1.69	0.73
1:A:4396:LEU:HD21	1:A:4489:TYR:HD1	1.53	0.73
1:B:1812:LEU:HD11	1:B:1860:VAL:HB	1.72	0.72
1:A:302:ARG:H	1:A:340:PRO:HB3	1.54	0.72
1:B:3534:CYS:HA	1:B:3539:LYS:HD3	1.73	0.71
1:B:4214:PHE:HB2	1:B:4322:CYS:HB3	1.70	0.71
1:B:349:GLU:HG2	1:B:353:PRO:HA	1.71	0.71
1:A:4247:ILE:HG23	1:A:4323:LEU:HD11	1.71	0.71
1:B:3116:ARG:HD3	1:B:3417:PRO:HA	1.72	0.70
1:B:3490:SER:HB3	1:B:3493:HIS:HD2	1.56	0.70
1:B:910:GLY:HA2	1:B:940:PHE:H	1.56	0.70
1:B:2847:ASN:HB3	1:B:2849:GLU:HG2	1.73	0.70
1:B:4238:ALA:HB1	1:B:4244:LEU:HD23	1.74	0.70
1:A:4364:LEU:HD12	1:A:4411:LEU:HD22	1.74	0.70
1:A:1816:SER:HG	1:A:1859:THR:HG1	1.34	0.69
1:A:4381:SER:HB2	1:A:4384:ASP:HB2	1.74	0.69
1:B:4400:ARG:HH21	1:B:4488:VAL:HG11	1.57	0.69
1:B:1504:ASP:O	1:B:1981:GLN:NE2	2.25	0.69
1:A:1440:PRO:HG2	1:A:2015:ILE:HG22	1.74	0.69
1:A:4441:LYS:HG3	1:A:4493:THR:HG21	1.75	0.68
1:B:4324:LEU:HD13	1:B:4398:LEU:HB2	1.76	0.68
1:A:1092:GLU:HB2	1:A:1220:PHE:HB3	1.74	0.68
1:A:2934:LEU:HA	1:A:2941:SER:HA	1.75	0.68
1:B:2094:GLN:NE2	1:B:2098:ASN:OD1	2.26	0.68
1:A:326:ALA:HB3	1:A:335:LEU:HB2	1.75	0.68
1:B:4239:LEU:HD21	1:B:4359:VAL:HB	1.76	0.68
1:B:929:PRO:HG2	1:B:938:ASP:HB3	1.76	0.67
1:B:59:ARG:HH11	1:B:929:PRO:HA	1.58	0.67
1:B:317:GLN:HB3	1:B:325:ARG:HE	1.60	0.67
1:A:1806:ILE:HB	1:A:1842:LEU:HD21	1.77	0.67
1:A:513:LEU:H	1:A:567:LEU:HD11	1.59	0.66
1:B:350:ARG:HD2	1:B:1788:ARG:HE	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:734:ASP:HB2	1:B:750:ARG:HH21	1.60	0.66
1:A:4437:LEU:HD13	1:A:4496:ARG:HE	1.60	0.66
1:B:195:GLN:NE2	1:B:222:HIS:O	2.28	0.66
1:A:1118:PRO:HB3	1:A:1292:GLY:HA3	1.76	0.65
1:B:1041:THR:HG22	1:B:1092:GLU:HB3	1.77	0.65
1:A:3828:SER:HB3	1:A:4006:VAL:HB	1.77	0.65
1:B:1034:LEU:HA	1:B:1305:ARG:HE	1.61	0.65
2:C:132:GLN:HA	2:C:135:ARG:HG2	1.78	0.65
1:B:3002:ASN:O	1:B:3002:ASN:ND2	2.27	0.65
1:A:3240:SER:HB3	1:A:3281:ARG:HB2	1.78	0.65
1:B:3002:ASN:C	1:B:3002:ASN:HD22	1.99	0.65
1:A:2688:ALA:O	1:A:2731:ASN:ND2	2.24	0.65
1:B:1033:THR:HG23	1:B:1304:ARG:HG2	1.78	0.65
1:B:3697:HIS:NE2	1:B:3997:GLN:O	2.28	0.65
1:A:563:PRO:HB2	1:A:717:VAL:HG22	1.76	0.65
1:A:1504:ASP:O	1:A:1981:GLN:NE2	2.30	0.65
1:A:1101:VAL:HG22	1:A:1216:LYS:HE3	1.79	0.64
1:B:1345:THR:HG23	1:B:1348:ALA:H	1.63	0.64
1:B:3699:MET:HA	1:B:3702:TRP:HB3	1.79	0.64
1:A:1382:ARG:HG2	1:A:1427:VAL:HG11	1.79	0.64
1:B:349:GLU:OE1	1:B:1057:ARG:NH1	2.30	0.64
1:B:3767:PHE:HB3	1:B:3815:LEU:HD12	1.80	0.64
1:A:1061:HIS:HD2	1:A:1071:ALA:HB3	1.62	0.64
1:A:863:PRO:HD2	1:A:866:ILE:HD12	1.80	0.63
1:B:1109:VAL:HA	1:B:1198:ALA:HA	1.80	0.63
1:B:328:CYS:SG	1:B:329:PHE:N	2.71	0.63
1:B:4242:GLY:HA2	1:B:4245:HIS:HB3	1.79	0.63
1:A:1107:LYS:HB2	1:A:1300:SER:HB2	1.81	0.63
1:A:1333:ASN:OD1	1:A:1337:ARG:NH2	2.31	0.63
1:A:1500:SER:OG	1:A:1974:TYR:OH	2.16	0.63
1:A:1046:TRP:HB3	1:A:1077:TRP:HB3	1.80	0.63
1:B:128:PHE:HB3	1:B:150:LEU:HD22	1.81	0.63
1:B:1107:LYS:HE3	1:B:1300:SER:HB3	1.80	0.63
1:B:1054:GLN:NE2	1:B:1074:THR:O	2.32	0.63
1:B:1484:ARG:NH1	1:B:2018:SER:O	2.31	0.63
1:A:2915:ARG:HH11	1:B:2772:HIS:HB2	1.63	0.62
1:A:3116:ARG:HD3	1:A:3417:PRO:HA	1.79	0.62
2:D:35:GLU:HA	2:D:38:LYS:HG2	1.81	0.62
1:A:2107:GLU:HG3	1:B:3488:MET:HE1	1.81	0.62
1:B:1177:HIS:HB3	1:B:1180:ASP:HB2	1.81	0.62
1:A:1111:ASN:H	1:A:1114:ILE:HD12	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3681:ASP:OD1	1:A:3755:GLN:NE2	2.33	0.62
1:A:4396:LEU:HD23	1:A:4399:LEU:HD21	1.81	0.62
1:B:2645:LYS:NZ	1:B:2649:MET:SD	2.73	0.62
1:B:510:LEU:HD11	1:B:567:LEU:HD11	1.82	0.61
1:B:1831:LEU:HD12	1:B:1832:VAL:HG12	1.82	0.61
1:B:3803:ASN:HA	1:B:4087:LEU:HA	1.82	0.61
1:A:716:LEU:HD21	1:A:719:CYS:HB2	1.81	0.61
1:A:3809:ARG:NH2	1:A:4189:LEU:O	2.33	0.61
1:B:2735:ASN:OD1	1:B:2745:GLN:NE2	2.34	0.61
1:B:2714:THR:OG1	1:B:2719:TRP:NE1	2.34	0.61
1:A:1381:THR:O	1:A:1385:LEU:N	2.34	0.61
1:B:2598:LEU:HD12	1:B:2599:THR:HG23	1.82	0.61
1:B:2790:GLN:HG3	1:B:2838:LYS:HE3	1.82	0.61
1:A:1126:LYS:HD3	1:A:1217:TYR:HB3	1.81	0.61
1:A:3429:ASP:HA	1:A:3432:ILE:HD12	1.83	0.61
1:B:1030:ARG:HE	1:B:1031:PHE:H	1.47	0.61
1:B:1174:LEU:HA	1:B:1181:ILE:HD11	1.83	0.61
1:A:1206:PRO:HA	1:A:1209:VAL:HB	1.83	0.61
1:A:4495:LEU:O	1:A:4499:ASN:ND2	2.34	0.61
1:A:196:LEU:HA	1:A:219:VAL:HG21	1.83	0.61
1:A:2136:GLU:O	1:A:2140:ASN:ND2	2.33	0.61
1:B:245:ASN:ND2	1:B:361:GLU:OE1	2.34	0.61
1:A:1346:GLU:HB2	1:A:1997:ALA:HA	1.83	0.60
1:B:3816:MET:HE3	1:B:4071:LEU:HD13	1.83	0.60
1:B:3967:LEU:HD12	1:B:4004:LEU:HB3	1.82	0.60
2:D:117:ARG:HH21	2:D:121:GLN:HB3	1.66	0.60
1:B:3834:LYS:HE2	1:B:3875:ASP:HA	1.83	0.60
1:A:1524:SER:HA	1:A:1774:PRO:HG3	1.83	0.60
1:A:3789:PHE:O	1:A:4086:ARG:NH2	2.34	0.60
1:B:2582:MET:HA	1:B:2585:MET:HB3	1.84	0.60
1:B:3787:GLU:O	1:B:3791:THR:OG1	2.12	0.60
1:B:3543:ASP:HB3	1:B:3615:SER:HB2	1.84	0.60
1:A:2664:TRP:HE1	1:A:2694:ILE:HB	1.67	0.59
1:B:1946:PRO:O	1:B:1952:ASN:ND2	2.35	0.59
1:B:2822:GLU:O	1:B:2827:GLN:NE2	2.35	0.59
1:A:912:VAL:HB	1:A:926:VAL:HB	1.84	0.59
1:A:3220:LEU:HD21	1:A:3223:ILE:HD11	1.84	0.59
1:B:2567:LEU:HD13	1:B:2581:LEU:HD22	1.84	0.59
1:A:1106:PHE:HB3	1:A:1201:LEU:HB2	1.84	0.59
1:B:3816:MET:HE1	1:B:4071:LEU:HA	1.84	0.59
1:A:1797:ARG:NH1	1:A:1798:PRO:O	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2714:THR:OG1	1:A:2719:TRP:NE1	2.32	0.59
1:B:1412:ILE:HD13	1:B:1424:PHE:HB3	1.85	0.59
1:B:1844:LEU:HB3	1:B:1847:LEU:HD21	1.83	0.59
1:B:1028:LEU:HD12	1:B:1318:ARG:HG3	1.85	0.59
1:A:3522:PHE:HD1	1:A:3549:MET:HE2	1.66	0.59
1:A:3193:ARG:NH1	2:D:24:GLN:OE1	2.36	0.59
1:B:4499:ASN:HA	1:B:4502:LYS:HB3	1.85	0.59
1:B:3637:ARG:HG2	1:B:3675:LYS:HE3	1.85	0.58
1:A:1292:GLY:HA2	1:A:1295:LEU:HD12	1.85	0.58
1:B:3790:GLN:HE22	1:B:4082:LEU:HD13	1.68	0.58
1:A:1063:HIS:O	1:A:1829:ARG:N	2.36	0.58
1:B:859:LEU:HD12	1:B:903:LEU:HD11	1.86	0.58
1:A:1794:ASP:HB2	1:A:1854:ARG:HH12	1.69	0.58
1:A:2636:VAL:O	1:A:2640:ASN:ND2	2.37	0.58
1:B:577:SER:OG	1:B:625:ARG:NH1	2.36	0.58
1:B:4393:ARG:HA	1:B:4396:LEU:HD12	1.85	0.58
1:B:4437:LEU:O	1:B:4489:TYR:OH	2.21	0.58
1:B:3715:LEU:HD13	1:B:3763:THR:HG22	1.85	0.58
1:B:3990:LEU:HD12	1:B:3995:LEU:HD22	1.85	0.58
1:A:349:GLU:HB2	1:A:1056:ARG:HG2	1.86	0.57
1:A:1473:LEU:HD22	1:A:2030:LEU:HD13	1.85	0.57
1:B:59:ARG:HH12	1:B:930:LYS:HG2	1.69	0.57
1:A:1122:VAL:HG11	1:A:1203:LEU:HD13	1.84	0.57
1:A:3823:THR:OG1	1:A:4000:ARG:O	2.20	0.57
2:D:127:VAL:HA	2:D:130:VAL:HG12	1.86	0.57
1:A:119:TYR:OH	1:A:947:SER:OG	2.22	0.57
1:A:1398:ARG:NH1	1:A:1803:ASP:OD2	2.37	0.57
1:A:2071:THR:HG22	1:A:2074:ILE:HG12	1.87	0.57
1:A:3771:ILE:HG23	1:A:3778:GLN:HG2	1.85	0.57
1:B:176:ALA:O	1:B:181:VAL:N	2.36	0.57
1:A:1086:TRP:NE1	1:A:1088:GLU:O	2.38	0.57
1:A:4165:LEU:HA	1:A:4170:TYR:HD2	1.70	0.57
1:A:2707:VAL:HA	1:A:2710:TRP:NE1	2.20	0.57
1:B:1398:ARG:NH1	1:B:1516:SER:O	2.37	0.57
1:A:1173:PHE:HZ	1:A:1221:LEU:HD22	1.70	0.57
1:A:2394:ARG:NH1	1:B:3074:THR:O	2.38	0.57
1:B:2650:LEU:HB3	1:B:2707:VAL:HG21	1.87	0.57
1:B:3201:PHE:HE2	1:B:3291:LEU:HG	1.70	0.57
1:A:1804:VAL:H	1:A:1844:LEU:HB3	1.69	0.57
1:A:2669:LEU:HD22	1:A:2690:ARG:HD3	1.86	0.57
1:A:2916:ASP:OD2	1:B:2774:THR:OG1	2.23	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:PRO:HA	1:B:218:THR:HA	1.86	0.57
1:A:137:ARG:HD2	1:A:145:LEU:HD12	1.87	0.56
1:A:1441:ALA:HB2	1:A:2014:LEU:HD21	1.86	0.56
1:A:4206:ALA:HA	1:A:4209:LEU:HD23	1.86	0.56
1:B:3494:LEU:HD22	1:B:3545:LEU:HD11	1.87	0.56
1:A:426:ILE:HD13	1:A:505:LEU:HD23	1.87	0.56
1:A:1182:LEU:HD13	1:A:1208:LEU:HD13	1.87	0.56
1:A:1435:ASN:HA	1:A:1438:PHE:HD2	1.70	0.56
1:A:1780:ILE:HB	1:A:1789:ARG:HG2	1.85	0.56
1:A:3794:GLN:O	1:A:4086:ARG:NH1	2.39	0.56
1:B:822:GLY:N	1:B:849:ILE:O	2.34	0.56
1:B:1032:GLU:OE2	1:B:1305:ARG:NH1	2.38	0.56
1:A:1521:TYR:OH	1:A:1770:LEU:O	2.23	0.56
1:A:1818:ASP:HA	1:A:1831:LEU:H	1.69	0.56
1:B:1009:VAL:HG21	1:B:1313:LYS:HD2	1.86	0.56
1:A:1527:VAL:HA	1:A:1793:LEU:HD13	1.87	0.56
1:B:160:VAL:HA	1:B:224:PRO:HA	1.88	0.56
1:B:2592:ASP:OD1	1:B:2593:SER:N	2.38	0.56
1:B:1126:LYS:HE2	1:B:1207:LYS:HB2	1.88	0.56
1:A:1121:GLN:HG2	1:A:1185:PRO:HB3	1.88	0.56
1:A:1123:THR:HG23	1:A:1183:CYS:H	1.71	0.56
1:B:1356:LEU:HB3	1:B:1407:PHE:CE1	2.40	0.56
1:B:3823:THR:OG1	1:B:4000:ARG:O	2.24	0.56
1:B:628:PRO:HB2	1:B:722:LEU:HD12	1.86	0.56
1:A:199:GLY:HA3	1:A:219:VAL:HG22	1.88	0.55
1:B:151:GLN:HE22	1:B:162:GLN:H	1.54	0.55
1:B:1403:LYS:HE3	1:B:1848:ILE:HD11	1.87	0.55
1:B:1333:ASN:O	1:B:1337:ARG:HG2	2.06	0.55
1:B:4226:LEU:H	1:B:4333:PRO:HB3	1.72	0.55
1:A:1050:GLN:HB2	1:A:1053:GLN:HG3	1.88	0.55
1:B:272:VAL:HA	1:B:292:THR:HG22	1.88	0.55
1:B:301:TYR:HB2	1:B:304:ALA:HB3	1.89	0.55
1:B:3124:SER:OG	1:B:3125:MET:N	2.39	0.55
1:B:3639:LEU:O	1:B:3643:CYS:N	2.40	0.55
1:A:2649:MET:HG2	1:A:2654:HIS:HB2	1.89	0.55
1:A:2772:HIS:HB2	1:B:2915:ARG:HH11	1.70	0.55
1:A:4393:ARG:HH22	1:A:4400:ARG:HH22	1.55	0.55
1:B:716:LEU:HD21	1:B:719:CYS:HB2	1.89	0.55
1:B:1017:PHE:HE2	1:B:1330:LYS:HB3	1.71	0.55
1:B:3810:ARG:HE	1:B:3814:GLN:HE22	1.54	0.55
1:A:1329:GLU:O	1:A:1333:ASN:ND2	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2640:ASN:O	1:A:2644:ASN:ND2	2.40	0.55
1:A:4386:ALA:O	1:A:4482:GLN:NE2	2.39	0.55
1:B:177:CYS:SG	1:B:189:TYR:OH	2.56	0.55
1:B:224:PRO:HG2	1:B:227:VAL:HB	1.89	0.55
1:B:1332:LEU:HD12	1:B:1388:ILE:HD11	1.89	0.55
1:B:1525:ILE:HG12	1:B:1793:LEU:HD13	1.89	0.55
1:B:4244:LEU:HD22	1:B:4247:ILE:HD12	1.88	0.55
1:A:289:ARG:NE	1:A:313:GLY:O	2.40	0.55
1:A:391:PHE:HB3	1:A:405:LYS:HE2	1.89	0.54
1:A:3438:LEU:O	1:A:3449:ARG:NH1	2.36	0.54
1:A:3534:CYS:SG	1:A:3535:ASN:N	2.80	0.54
1:A:3978:PRO:HG2	1:A:3981:MET:HB2	1.89	0.54
1:B:401:ALA:HA	1:B:411:ILE:HA	1.88	0.54
1:B:2583:LEU:HD23	1:B:2586:MET:HG3	1.89	0.54
1:B:3829:PRO:HA	1:B:3854:LYS:HE3	1.88	0.54
1:A:2180:ASP:OD1	1:A:2360:ARG:NH1	2.39	0.54
1:B:3093:ASP:OD1	1:B:3094:ALA:N	2.40	0.54
1:B:3635:LEU:HD21	1:B:3711:LEU:HD21	1.88	0.54
1:A:4236:ARG:O	1:A:4239:LEU:N	2.40	0.54
1:B:283:MET:O	1:B:289:ARG:NH1	2.41	0.54
2:C:90:TRP:CD1	2:C:127:VAL:HG21	2.42	0.54
1:A:203:THR:HG21	1:A:214:ALA:HB2	1.88	0.54
1:A:1908:PRO:HB3	1:A:1912:GLN:HE21	1.71	0.54
1:B:1363:HIS:ND1	1:B:1374:ASN:OD1	2.28	0.54
1:B:2596:GLN:HA	1:B:2600:ASN:HB3	1.90	0.54
1:B:3804:ILE:HB	1:B:3808:ILE:HG21	1.90	0.54
1:A:2708:LEU:HD21	1:A:2722:VAL:HG21	1.90	0.54
1:B:3817:LEU:HD21	1:B:4185:LEU:HD23	1.88	0.54
1:A:1509:ASP:OD1	1:A:1510:LEU:N	2.41	0.54
1:B:3554:PRO:HG3	1:B:3621:GLU:HG3	1.89	0.54
1:B:4237:MET:O	1:B:4241:ILE:HG12	2.07	0.54
1:A:104:ALA:H	1:A:217:ALA:HB2	1.72	0.54
1:A:301:TYR:HB2	1:A:304:ALA:HB3	1.89	0.53
1:A:1815:LEU:HB3	1:A:1834:ALA:HB3	1.90	0.53
1:A:1929:ASN:HB3	1:B:3810:ARG:NH1	2.22	0.53
1:B:1802:THR:HG22	1:B:1880:GLY:HA2	1.90	0.53
1:A:1402:HIS:HB2	1:A:1450:TRP:CH2	2.43	0.53
1:B:1820:TRP:HB3	1:B:1828:GLY:HA2	1.91	0.53
1:B:2731:ASN:OD1	1:B:2795:ARG:NH2	2.41	0.53
1:A:2070:GLY:HA3	1:A:2074:ILE:HD11	1.91	0.53
1:B:2640:ASN:O	1:B:2644:ASN:ND2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1051:GLN:HG3	1:A:1072:GLN:HB3	1.90	0.53
1:B:102:LEU:HB3	1:B:213:VAL:HA	1.91	0.53
1:B:2036:SER:HB2	1:B:2594:ILE:HD11	1.90	0.53
1:B:3768:LEU:HD13	1:B:3771:ILE:HD11	1.91	0.53
1:B:4082:LEU:O	1:B:4086:ARG:HG2	2.08	0.53
1:A:76:HIS:CE1	1:A:144:LEU:HB2	2.43	0.53
1:B:120:ILE:HB	1:B:123:VAL:HG22	1.90	0.53
1:B:3359:LEU:HD12	1:B:3396:LEU:HD13	1.91	0.53
1:A:119:TYR:HE2	1:A:947:SER:H	1.54	0.53
1:A:3610:LEU:HD12	1:A:3689:PHE:CG	2.43	0.53
1:A:3224:HIS:HB2	1:A:3297:LYS:HB2	1.90	0.53
1:B:712:LYS:O	1:B:715:THR:OG1	2.25	0.53
1:B:2583:LEU:HA	1:B:2586:MET:HG2	1.91	0.53
1:B:2688:ALA:O	1:B:2731:ASN:ND2	2.42	0.53
1:A:289:ARG:HG2	1:A:315:TYR:HB3	1.90	0.52
1:A:731:LEU:HD13	1:A:749:LEU:HD13	1.91	0.52
1:A:4177:GLU:OE1	1:A:4180:HIS:HB2	2.09	0.52
1:A:1061:HIS:ND1	1:A:1072:GLN:OE1	2.41	0.52
1:A:1339:THR:OG1	1:A:1341:ASP:OD1	2.26	0.52
1:A:4220:LEU:HD21	1:A:4234:LEU:HD11	1.92	0.52
1:B:1058:HIS:CD2	1:B:1061:HIS:HB2	2.45	0.52
1:B:1093:LEU:O	1:B:1217:TYR:OH	2.16	0.52
1:A:1800:LEU:HG	1:A:1850:PRO:HB2	1.92	0.52
1:B:3242:GLU:OE2	1:B:3281:ARG:NH1	2.42	0.52
1:B:4163:LEU:HA	1:B:4166:ARG:HD2	1.91	0.52
1:B:4177:GLU:OE2	1:B:4180:HIS:N	2.35	0.52
1:A:1086:TRP:HD1	1:A:1088:GLU:H	1.57	0.52
1:A:1954:GLN:OE1	1:A:1958:ARG:NH2	2.40	0.52
1:B:1331:LEU:HB3	1:B:1356:LEU:HD11	1.91	0.52
1:B:2697:ASN:OD1	1:B:2698:GLN:N	2.43	0.52
1:B:3774:HIS:HA	1:B:3997:GLN:NE2	2.24	0.52
1:A:350:ARG:HD2	1:A:1787:ALA:HA	1.91	0.52
1:A:1450:TRP:HZ2	1:A:1845:HIS:CE1	2.27	0.52
1:B:2639:LEU:HD22	1:B:2643:PHE:HE2	1.74	0.52
1:A:2657:LEU:HD11	1:A:2704:PHE:HE1	1.75	0.52
1:A:4226:LEU:H	1:A:4333:PRO:HB3	1.75	0.52
1:B:3812:PHE:CE1	1:B:3816:MET:HG2	2.45	0.52
1:B:145:LEU:HB2	1:B:149:ALA:HB2	1.92	0.52
1:B:4224:THR:HG21	1:B:4234:LEU:HD13	1.92	0.52
1:A:1094:VAL:HB	1:A:1220:PHE:CD1	2.44	0.52
1:A:119:TYR:HH	1:A:947:SER:HG	1.54	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2332:VAL:HG13	1:A:2358:LEU:HD11	1.91	0.52
1:A:3560:LEU:O	1:A:3564:MET:HG2	2.10	0.52
1:B:57:VAL:HG13	1:B:964:LEU:HD21	1.91	0.52
2:D:109:ALA:O	2:D:113:SER:OG	2.28	0.52
1:A:1182:LEU:HB3	1:A:1208:LEU:HB2	1.90	0.51
1:A:4436:LEU:HD23	1:A:4440:MET:HE1	1.91	0.51
1:B:2384:LEU:HD22	1:B:2663:LEU:HD21	1.92	0.51
1:A:2582:MET:O	1:A:2586:MET:HG2	2.11	0.51
1:A:1957:LEU:HB3	1:A:1958:ARG:HD3	1.93	0.51
1:A:3006:MET:SD	1:A:3009:ILE:HA	2.51	0.51
1:B:367:PRO:HD2	1:B:370:VAL:HB	1.92	0.51
1:B:3774:HIS:ND1	1:B:3777:ASN:OD1	2.44	0.51
2:C:6:LEU:O	2:C:9:ARG:HD3	2.10	0.51
1:A:568:LEU:HD12	1:A:630:LEU:HD21	1.92	0.51
1:B:1188:LEU:HD12	1:B:1201:LEU:HD11	1.92	0.51
1:B:2582:MET:O	1:B:2586:MET:N	2.40	0.51
1:A:1098:ALA:HA	1:A:1216:LYS:HB2	1.91	0.51
1:A:2024:ARG:HA	1:A:2027:ILE:HG12	1.91	0.51
1:B:3689:PHE:O	1:B:3693:VAL:HG23	2.10	0.51
1:B:3856:ARG:NH1	1:B:3873:VAL:O	2.44	0.51
2:C:126:GLN:O	2:C:129:GLU:HG2	2.11	0.51
1:B:1406:ARG:NH1	1:B:2576:GLU:OE1	2.43	0.51
1:A:390:CYS:N	1:A:405:LYS:HZ3	2.09	0.51
1:B:2692:PRO:HG3	1:B:2728:LEU:HB3	1.93	0.51
1:A:131:ASP:O	1:A:406:ARG:NH2	2.43	0.51
1:A:2687:ASN:HB3	1:A:2690:ARG:HG3	1.93	0.51
1:A:2826:PHE:O	1:A:2915:ARG:NH2	2.42	0.51
1:A:3816:MET:HG3	1:A:4070:PRO:HB2	1.93	0.51
1:B:721:ARG:NH2	1:B:727:GLU:OE1	2.37	0.51
1:B:1111:ASN:ND2	1:B:1295:LEU:O	2.42	0.51
1:B:4206:ALA:HA	1:B:4209:LEU:HG	1.92	0.51
1:A:393:SER:HA	1:A:401:ALA:HB3	1.92	0.50
1:B:1049:VAL:N	1:B:1076:THR:O	2.35	0.50
1:B:1831:LEU:O	1:B:2569:ALA:N	2.28	0.50
1:B:1105:ASP:HB2	1:B:1302:THR:HB	1.92	0.50
1:B:1118:PRO:HG3	1:B:1295:LEU:HD22	1.92	0.50
1:B:3774:HIS:HA	1:B:3997:GLN:HE22	1.74	0.50
1:A:76:HIS:HE1	1:A:144:LEU:HB2	1.75	0.50
1:A:1105:ASP:HB2	1:A:1302:THR:HB	1.93	0.50
1:A:1914:LEU:HD21	1:A:1995:LYS:HB2	1.94	0.50
1:B:3433:ASP:OD2	1:B:3853:HIS:ND1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3499:ALA:HB1	1:B:3850:GLY:HA2	1.93	0.50
1:A:1051:GLN:HG2	1:A:1072:GLN:HE21	1.75	0.50
1:A:1845:HIS:HB3	1:A:1847:LEU:HG	1.93	0.50
1:B:250:PRO:HD3	1:B:362:HIS:HB3	1.93	0.50
1:B:345:TRP:HZ3	1:B:358:VAL:HA	1.75	0.50
1:B:3498:ALA:HB2	1:B:3545:LEU:HD23	1.93	0.50
1:A:4236:ARG:O	1:A:4239:LEU:HG	2.12	0.50
1:B:2084:GLN:HG2	1:B:2603:PRO:HG3	1.92	0.50
1:B:3862:VAL:HA	1:B:3983:LEU:HD12	1.92	0.50
1:B:4324:LEU:HD11	1:B:4394:ALA:HB1	1.94	0.50
1:A:1398:ARG:HB2	1:A:1519:ASN:HD21	1.77	0.50
1:B:1046:TRP:HB3	1:B:1077:TRP:HB3	1.94	0.50
1:B:1863:ARG:HD3	1:B:1865:GLY:H	1.77	0.50
1:A:1086:TRP:HD1	1:A:1088:GLU:N	2.09	0.50
1:A:1777:SER:HB2	1:A:1872:LYS:HE3	1.94	0.50
1:B:174:LEU:HB2	1:B:196:LEU:HD21	1.93	0.50
1:B:1073:HIS:HB3	1:B:1302:THR:HG23	1.92	0.50
1:B:3812:PHE:O	1:B:3816:MET:HB3	2.11	0.50
1:A:4194:ASP:OD1	1:A:4198:SER:N	2.39	0.50
1:B:2582:MET:O	1:B:2586:MET:HG2	2.12	0.50
1:B:3400:LEU:HD22	1:B:3431:THR:HG23	1.93	0.50
1:B:4207:ASN:OD1	1:B:4208:VAL:HG23	2.11	0.50
2:D:22:LEU:HB2	2:D:96:LEU:HD23	1.93	0.50
1:B:1030:ARG:HH22	1:B:2573:VAL:HG23	1.75	0.50
1:A:1313:LYS:HB2	1:A:1316:VAL:HB	1.92	0.49
1:A:1934:ARG:HH21	1:A:1938:LEU:HD13	1.76	0.49
1:A:4395:LEU:HD12	1:A:4398:LEU:HD11	1.93	0.49
1:B:68:ASP:HB2	1:B:86:THR:HB	1.94	0.49
1:B:1844:LEU:HD23	1:B:1847:LEU:HD21	1.94	0.49
1:B:3209:ASP:OD1	1:B:3209:ASP:N	2.43	0.49
1:A:1110:LEU:HD13	1:A:1114:ILE:HG21	1.94	0.49
1:A:3456:TRP:CZ2	1:A:3489:PRO:HB3	2.47	0.49
2:D:2:SER:OG	2:D:3:SER:N	2.45	0.49
1:A:856:ILE:HD13	1:A:903:LEU:HD11	1.93	0.49
1:A:3614:ALA:HB2	1:A:3689:PHE:CD1	2.48	0.49
1:A:3967:LEU:HD23	1:A:4004:LEU:HD22	1.95	0.49
1:B:145:LEU:HD22	1:B:164:GLU:HB3	1.93	0.49
1:B:722:LEU:HD13	1:B:733:ILE:HD12	1.94	0.49
1:A:391:PHE:HB2	1:A:403:ALA:HB3	1.93	0.49
1:B:1090:VAL:HG13	1:B:1221:LEU:HD12	1.94	0.49
1:B:1212:MET:HG3	1:B:1218:ARG:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1819:ILE:O	1:B:1829:ARG:N	2.44	0.49
1:B:57:VAL:HB	1:B:926:VAL:HG22	1.94	0.49
1:B:296:TRP:HE3	1:B:316:HIS:CD2	2.31	0.49
1:B:302:ARG:H	1:B:340:PRO:HB3	1.76	0.49
1:B:2335:LEU:HB3	1:B:2358:LEU:HD12	1.94	0.49
2:C:41:TYR:HA	2:C:44:THR:HG22	1.93	0.49
1:A:1938:LEU:O	1:A:1941:SER:OG	2.21	0.49
1:B:3713:THR:HG22	1:B:3784:VAL:HG13	1.95	0.49
1:B:3754:GLN:NE2	1:B:3755:GLN:HG3	2.28	0.49
1:B:4180:HIS:CD2	1:B:4205:SER:HB3	2.48	0.49
1:A:1412:ILE:HG23	1:A:1424:PHE:CE1	2.48	0.48
1:B:1525:ILE:HD11	1:B:1793:LEU:HB3	1.95	0.48
1:B:1782:ARG:NE	1:B:1789:ARG:HH22	2.11	0.48
1:A:1425:GLY:O	1:A:1428:LEU:HG	2.13	0.48
1:A:1938:LEU:HD21	1:A:1969:ARG:HG2	1.96	0.48
1:A:3401:LEU:HD21	1:A:3435:LEU:HD11	1.95	0.48
1:B:1110:LEU:HD23	1:B:1114:ILE:HG21	1.94	0.48
1:A:2121:LEU:O	1:A:2124:ILE:HG22	2.14	0.48
2:C:87:GLU:O	2:C:91:MET:HG2	2.13	0.48
1:A:386:ASP:HB2	1:A:406:ARG:HA	1.96	0.48
1:A:2173:MET:CE	1:B:3126:VAL:HG22	2.43	0.48
1:A:3177:GLN:HG2	1:A:3178:PRO:HD2	1.95	0.48
1:B:1911:ASP:N	1:B:1911:ASP:OD1	2.46	0.48
1:B:4238:ALA:HA	1:B:4243:ALA:HB3	1.94	0.48
1:A:1455:LEU:HD13	1:A:1458:VAL:HG21	1.96	0.48
1:A:1788:ARG:HH21	1:A:1859:THR:HB	1.78	0.48
1:A:3097:ALA:O	1:A:3101:MET:HG3	2.14	0.48
1:A:3189:HIS:HB3	1:A:3192:ALA:HB2	1.95	0.48
1:B:566:CYS:HB3	1:B:632:LEU:HD23	1.94	0.48
1:B:1028:LEU:O	1:B:1318:ARG:NH2	2.46	0.48
1:B:1532:ILE:HG23	1:B:1782:ARG:HH12	1.79	0.48
1:B:2735:ASN:HD21	1:B:2745:GLN:HB2	1.79	0.48
1:B:3869:VAL:O	1:B:3873:VAL:HG12	2.13	0.48
1:A:3201:PHE:HE2	1:A:3291:LEU:HB2	1.79	0.48
1:A:4395:LEU:HA	1:A:4398:LEU:HG	1.95	0.48
1:B:4207:ASN:OD1	1:B:4208:VAL:N	2.47	0.48
1:A:349:GLU:HB2	1:A:1056:ARG:HE	1.79	0.48
1:A:2173:MET:HE2	1:B:3126:VAL:HG22	1.96	0.48
1:B:1799:ILE:N	1:B:1853:CYS:O	2.34	0.48
1:B:3512:ASP:OD1	1:B:3512:ASP:N	2.43	0.48
1:A:1961:ASP:OD1	1:A:1961:ASP:N	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:436:GLN:HB3	1:B:721:ARG:HD3	1.94	0.47
1:B:3995:LEU:HD12	1:B:3996:PRO:HD2	1.96	0.47
1:B:140:LEU:O	1:B:143:ILE:HG12	2.14	0.47
1:A:1048:GLU:HA	1:A:1077:TRP:HA	1.97	0.47
1:B:411:ILE:HD11	1:B:424:PHE:HD1	1.79	0.47
1:B:4085:GLU:HG3	1:B:4166:ARG:NH1	2.29	0.47
1:B:4167:LEU:HD22	1:B:4170:TYR:HB2	1.97	0.47
1:A:2079:GLY:O	1:A:2083:VAL:HG23	2.14	0.47
1:A:3251:LEU:HD23	1:B:2717:ARG:HE	1.80	0.47
1:B:225:HIS:CD2	1:B:259:LEU:HD22	2.49	0.47
1:B:4244:LEU:HA	1:B:4247:ILE:HB	1.96	0.47
2:C:50:TYR:HD1	2:C:69:ILE:HD13	1.79	0.47
1:A:188:GLY:HA3	1:A:227:VAL:HG13	1.97	0.47
1:A:1493:GLN:HG2	1:A:1499:TYR:HA	1.96	0.47
1:A:1784:HIS:HB2	1:A:1787:ALA:HB2	1.96	0.47
1:A:2652:VAL:HG13	1:A:2654:HIS:ND1	2.30	0.47
1:A:2654:HIS:CG	1:B:3068:ARG:HD2	2.50	0.47
1:A:3832:LEU:O	1:A:3856:ARG:NH2	2.48	0.47
1:A:283:MET:CE	1:A:289:ARG:HG3	2.44	0.47
1:A:3088:VAL:HG12	1:A:3089:LEU:HD12	1.94	0.47
1:A:4218:ARG:NH1	1:A:4222:SER:HB2	2.30	0.47
1:B:75:TYR:HB2	1:B:944:ILE:HG12	1.96	0.47
1:B:330:THR:OG1	1:B:355:CYS:SG	2.52	0.47
1:B:411:ILE:HD11	1:B:424:PHE:CD1	2.49	0.47
1:B:3719:LEU:HD11	1:B:3760:GLU:HB3	1.97	0.47
1:B:3773:CYS:HB2	1:B:3991:TYR:OH	2.15	0.47
1:A:1206:PRO:HG2	1:A:1370:SER:OG	2.15	0.47
1:A:1368:GLY:HA2	1:A:1371:LYS:HB2	1.96	0.47
1:A:3179:ALA:HB1	1:A:3182:LEU:HD12	1.97	0.47
1:B:1359:LEU:HD22	1:B:1377:LEU:HD13	1.97	0.47
1:B:2850:VAL:HG12	1:B:2942:ALA:HA	1.96	0.47
1:A:3259:THR:HA	1:A:3262:LEU:HD12	1.97	0.47
1:B:1111:ASN:HB2	1:B:1114:ILE:HG13	1.96	0.47
1:B:3689:PHE:O	1:B:3692:GLU:HG3	2.15	0.47
1:A:1022:LEU:HD23	1:A:1025:LEU:HD12	1.97	0.47
1:A:4218:ARG:CZ	1:A:4325:GLN:HE22	2.28	0.47
1:B:3490:SER:HB3	1:B:3493:HIS:CD2	2.45	0.47
1:B:4072:GLN:HG3	1:B:4175:LEU:HB3	1.95	0.47
1:A:2870:TYR:OH	1:A:2916:ASP:OD1	2.24	0.47
1:A:3429:ASP:OD1	1:A:3429:ASP:N	2.48	0.47
1:B:1058:HIS:HE1	1:B:1830:ARG:HD2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3058:LEU:HD12	1:B:3101:MET:HE2	1.97	0.47
1:B:2590:GLU:O	1:B:2594:ILE:HG12	2.15	0.46
1:B:3220:LEU:HD21	1:B:3223:ILE:HD11	1.96	0.46
1:B:4332:ASN:ND2	1:B:4404:SER:OG	2.49	0.46
1:A:1092:GLU:HB2	1:A:1220:PHE:CB	2.44	0.46
1:A:1188:LEU:HA	1:A:1201:LEU:HD21	1.97	0.46
1:A:1415:GLY:HA3	1:A:1424:PHE:HE2	1.79	0.46
1:B:306:PRO:O	1:B:310:ALA:CB	2.63	0.46
1:A:138:LYS:HG2	1:A:369:SER:HB2	1.96	0.46
1:A:1331:LEU:HD11	1:A:1352:VAL:HG23	1.98	0.46
1:A:2050:LEU:HG	1:A:2085:LEU:HD11	1.97	0.46
1:A:4377:LEU:HD22	1:A:4440:MET:HE3	1.96	0.46
1:B:1782:ARG:HG3	1:B:1789:ARG:HH22	1.80	0.46
2:C:99:MET:SD	2:D:20:THR:HG23	2.55	0.46
2:C:128:GLU:O	2:C:132:GLN:HB2	2.14	0.46
1:A:1938:LEU:HD11	1:A:1969:ARG:HE	1.81	0.46
1:A:3517:LEU:HD22	1:A:3552:VAL:HG11	1.97	0.46
1:A:4252:SER:HB2	1:A:4368:CYS:SG	2.56	0.46
1:B:1812:LEU:O	1:B:1838:SER:OG	2.33	0.46
1:B:744:HIS:ND1	1:B:828:TYR:O	2.42	0.46
1:B:3712:TRP:HB2	1:B:3784:VAL:HG11	1.98	0.46
2:C:58:ASN:ND2	2:C:60:GLU:OE2	2.49	0.46
1:A:433:ILE:HD11	1:A:631:LEU:HD11	1.97	0.46
1:B:70:LEU:HD12	1:B:961:LEU:HD21	1.98	0.46
1:B:1066:HIS:NE2	1:B:1825:GLU:O	2.46	0.46
1:A:250:PRO:HG3	1:A:364:GLN:H	1.81	0.46
1:A:3784:VAL:O	1:A:3787:GLU:HG3	2.15	0.46
1:B:349:GLU:HB2	1:B:1056:ARG:NH2	2.30	0.46
1:B:403:ALA:HB2	1:B:409:ILE:HG23	1.98	0.46
1:B:1863:ARG:HD3	1:B:1865:GLY:N	2.31	0.46
1:B:2349:ASP:N	1:B:2349:ASP:OD1	2.47	0.46
1:B:3610:LEU:HD11	1:B:3686:ILE:HD13	1.98	0.46
1:B:3759:ILE:O	1:B:3763:THR:HG23	2.16	0.46
1:A:2034:LEU:HD12	1:A:2037:LEU:HD11	1.98	0.46
1:B:413:ASP:O	1:B:418:MET:HA	2.16	0.46
1:B:2595:LEU:O	1:B:2599:THR:OG1	2.33	0.46
1:A:3123:ARG:O	1:B:1954:GLN:NE2	2.49	0.46
1:A:296:TRP:NE1	1:A:298:HIS:HB2	2.31	0.45
1:A:1172:PRO:HG2	1:A:1175:GLU:HB2	1.98	0.45
1:A:1452:PHE:CD2	1:A:2029:TYR:HB3	2.52	0.45
1:A:2179:LEU:HA	1:A:2182:VAL:HG12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2932:LEU:O	1:A:2980:VAL:HG23	2.17	0.45
1:A:4384:ASP:OD2	1:A:4392:TYR:OH	2.30	0.45
1:B:1110:LEU:N	1:B:1197:HIS:O	2.47	0.45
1:B:4180:HIS:HE1	1:B:4208:VAL:HB	1.81	0.45
1:A:4317:GLU:HA	1:A:4320:VAL:HG22	1.99	0.45
1:B:3193:ARG:NE	2:C:91:MET:SD	2.86	0.45
1:B:3566:ILE:HG21	1:B:3631:LEU:HD21	1.98	0.45
1:B:4314:ARG:HE	1:B:4318:GLU:HG3	1.80	0.45
1:A:1189:ALA:HA	1:A:1192:LEU:HB2	1.99	0.45
1:B:2575:LEU:O	1:B:2578:GLN:NE2	2.50	0.45
1:B:4229:ASP:N	1:B:4229:ASP:OD1	2.49	0.45
1:A:1425:GLY:O	1:A:1429:LEU:HD23	2.16	0.45
1:B:163:LEU:HD11	1:B:259:LEU:HD21	1.99	0.45
1:B:1174:LEU:HD21	1:B:1225:LYS:HD3	1.99	0.45
1:B:2817:HIS:HB2	1:B:2859:VAL:HG22	1.98	0.45
1:B:2851:VAL:HG13	1:B:2856:ILE:HD11	1.99	0.45
1:A:1125:LEU:HD23	1:A:1177:HIS:CD2	2.51	0.45
1:A:2686:TYR:CE2	1:B:3249:ASN:HB3	2.50	0.45
1:B:1057:ARG:HH22	1:B:1861:ILE:HG21	1.81	0.45
1:B:1110:LEU:HB3	1:B:1114:ILE:HD12	1.98	0.45
1:B:3427:SER:HB3	1:B:3493:HIS:CD2	2.51	0.45
1:A:1489:GLU:HA	1:A:1492:LEU:HG	1.98	0.45
1:A:1516:SER:HB2	1:A:1518:LYS:NZ	2.32	0.45
1:A:3161:HIS:CE1	1:A:3307:THR:HA	2.51	0.45
1:A:3715:LEU:HD21	1:A:3763:THR:HG22	1.97	0.45
1:B:2932:LEU:O	1:B:2980:VAL:HG23	2.17	0.45
1:B:3097:ALA:O	1:B:3101:MET:HG3	2.15	0.45
1:B:3708:VAL:HA	1:B:3711:LEU:HD23	1.99	0.45
1:B:4180:HIS:CE1	1:B:4208:VAL:HB	2.51	0.45
1:A:3049:THR:HG23	1:A:3052:MET:H	1.80	0.45
2:C:18:THR:HA	2:C:21:PHE:HB3	1.98	0.45
1:A:915:LEU:HG	1:A:922:ILE:HA	1.99	0.45
1:A:1910:ILE:HG22	1:A:1911:ASP:H	1.82	0.45
1:A:3400:LEU:HD22	1:A:3431:THR:HG23	1.99	0.45
1:B:348:HIS:O	1:B:352:SER:N	2.48	0.45
1:B:1070:ALA:HA	1:B:1073:HIS:HB2	1.98	0.45
1:B:2178:LEU:O	1:B:2182:VAL:HG23	2.17	0.45
1:B:3712:TRP:HD1	1:B:3767:PHE:CE1	2.35	0.45
1:A:89:GLY:HA3	1:A:150:LEU:HD11	1.99	0.45
1:B:151:GLN:NE2	1:B:162:GLN:OE1	2.50	0.45
1:B:627:LEU:HG	1:B:629:VAL:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:631:LEU:HB3	1:B:633:TYR:CE2	2.51	0.45
1:B:1191:GLY:HA3	1:B:1201:LEU:HD23	1.99	0.45
1:B:2129:LEU:HD21	1:B:2182:VAL:HG22	1.98	0.45
1:B:3775:PRO:HA	1:B:3778:GLN:HG2	1.99	0.45
1:A:246:VAL:HG23	1:A:248:ALA:H	1.82	0.45
1:A:2129:LEU:HD22	1:A:2181:TYR:HD2	1.81	0.45
1:A:4218:ARG:HG3	1:A:4325:GLN:OE1	2.17	0.45
1:B:308:PRO:O	1:B:311:GLN:HG3	2.17	0.45
1:A:734:ASP:HB3	1:A:750:ARG:HD3	1.99	0.44
1:A:1498:LEU:HD13	1:A:1974:TYR:CD2	2.52	0.44
1:A:4386:ALA:HA	1:A:4482:GLN:HE21	1.82	0.44
1:B:1488:MET:HE3	1:B:1488:MET:HA	1.98	0.44
1:B:2593:SER:O	1:B:2597:ALA:N	2.49	0.44
2:D:127:VAL:O	2:D:131:HIS:ND1	2.39	0.44
2:D:131:HIS:O	2:D:135:ARG:HG2	2.18	0.44
1:A:2173:MET:HE1	1:B:3126:VAL:HA	1.98	0.44
1:A:3699:MET:O	1:A:3703:LEU:N	2.42	0.44
1:B:1387:ASP:OD1	1:B:1390:ARG:NH2	2.33	0.44
1:B:1440:PRO:O	1:B:2018:SER:OG	2.30	0.44
1:B:4191:VAL:HG12	1:B:4193:ASP:H	1.81	0.44
2:C:143:GLU:HA	2:C:146:ILE:HG12	1.98	0.44
1:A:4314:ARG:O	1:A:4317:GLU:HG3	2.18	0.44
1:A:4380:ASP:OD1	1:A:4380:ASP:N	2.51	0.44
1:B:1024:SER:HB3	1:B:1311:ILE:HD11	1.99	0.44
1:B:1034:LEU:HD11	1:B:1099:CYS:SG	2.57	0.44
1:A:1100:MET:SD	1:A:1209:VAL:HG13	2.57	0.44
1:A:1102:GLY:HA2	1:A:1306:PHE:CE2	2.53	0.44
1:B:1177:HIS:O	1:B:1181:ILE:HG13	2.17	0.44
1:B:2013:ASP:O	1:B:2017:THR:OG1	2.28	0.44
1:B:2600:ASN:OD1	1:B:2601:THR:N	2.51	0.44
1:B:3386:GLY:HA2	1:B:3392:ILE:HG22	1.99	0.44
1:B:3982:THR:N	1:B:3985:GLN:OE1	2.50	0.44
1:A:1347:HIS:CD2	1:A:1885:LEU:HD22	2.51	0.44
1:A:4236:ARG:HA	1:A:4239:LEU:HG	2.00	0.44
1:B:2943:ARG:HD3	1:B:2944:VAL:N	2.33	0.44
1:A:1923:ASP:HA	1:B:3809:ARG:NH2	2.33	0.44
1:A:3614:ALA:HB2	1:A:3689:PHE:HD1	1.82	0.44
1:A:4186:ARG:NE	1:A:4193:ASP:O	2.35	0.44
1:B:125:LYS:HD3	1:B:138:LYS:HG3	2.00	0.44
1:B:137:ARG:NE	1:B:375:SER:O	2.51	0.44
1:A:108:SER:HB2	1:A:111:PRO:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1119:GLN:HE22	1:A:1291:ARG:HG3	1.83	0.44
1:A:1402:HIS:HB2	1:A:1450:TRP:CZ2	2.52	0.44
1:A:2834:ASP:OD1	1:A:2834:ASP:N	2.49	0.44
1:A:3096:LYS:HE3	1:A:3096:LYS:HB2	1.84	0.44
1:A:4218:ARG:HH12	1:A:4222:SER:HB2	1.82	0.44
1:B:1863:ARG:HH11	1:B:1865:GLY:H	1.65	0.44
1:B:3399:ILE:HA	1:B:3403:ASN:O	2.18	0.44
1:B:3790:GLN:HE22	1:B:4082:LEU:HB2	1.83	0.44
1:A:357:PHE:HB3	1:A:1056:ARG:HH12	1.83	0.44
1:B:2834:ASP:OD1	1:B:2834:ASP:N	2.51	0.44
1:B:3322:GLN:O	1:B:3326:THR:OG1	2.33	0.44
2:C:65:VAL:O	2:C:69:ILE:HG13	2.18	0.44
2:C:88:THR:HG22	2:D:13:LEU:HD11	2.00	0.44
2:C:97:SER:HB3	2:C:120:ILE:HB	1.99	0.44
1:A:307:ASP:HB3	1:A:308:PRO:HD3	1.98	0.44
1:A:2335:LEU:HD22	1:A:2354:VAL:HG13	1.99	0.44
1:B:1089:HIS:O	1:B:1223:HIS:ND1	2.51	0.44
1:B:2120:LEU:O	1:B:2124:ILE:HG12	2.18	0.44
1:B:2821:THR:HG23	1:B:2823:ARG:H	1.82	0.44
1:B:3209:ASP:HB3	1:B:3281:ARG:HG2	1.99	0.44
1:A:1035:THR:OG1	1:A:1036:PRO:HD3	2.17	0.43
1:A:1346:GLU:HG3	1:A:1996:VAL:HG13	1.98	0.43
1:A:1523:SER:N	1:A:1878:TYR:O	2.51	0.43
1:A:4163:LEU:HD23	1:A:4166:ARG:HH22	1.82	0.43
1:B:1034:LEU:HD13	1:B:1305:ARG:HE	1.82	0.43
1:B:2129:LEU:HD22	1:B:2181:TYR:HD2	1.83	0.43
1:B:2563:VAL:HG11	1:B:2588:THR:HG22	1.99	0.43
1:B:3967:LEU:HB2	1:B:3977:LEU:HB2	1.99	0.43
1:B:4079:GLY:O	1:B:4082:LEU:HG	2.17	0.43
1:A:1120:ILE:HD12	1:A:1188:LEU:HB2	1.99	0.43
1:A:3169:ILE:HD11	1:A:3210:LEU:HD22	2.00	0.43
1:B:3691:THR:HG23	1:B:3766:PHE:HA	2.00	0.43
1:B:4397:GLU:HG3	1:B:4400:ARG:NH1	2.26	0.43
1:B:1122:VAL:HG22	1:B:1224:VAL:HG23	1.99	0.43
1:B:1812:LEU:HD23	1:B:1837:ILE:HG21	2.00	0.43
1:B:3687:LEU:HD12	1:B:3690:LEU:HD11	2.01	0.43
1:A:2108:GLN:OE1	1:A:2110:LEU:N	2.45	0.43
1:A:4484:THR:HA	1:A:4487:ILE:HG22	2.00	0.43
1:B:152:THR:HB	1:B:379:PHE:HZ	1.84	0.43
1:B:306:PRO:O	1:B:310:ALA:HB2	2.19	0.43
1:B:1206:PRO:HG2	1:B:1370:SER:OG	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3004:SER:HA	1:B:3079:GLU:HG2	1.99	0.43
1:B:3529:SER:O	1:B:3539:LYS:NZ	2.38	0.43
1:A:1225:LYS:HB3	1:A:1291:ARG:CZ	2.47	0.43
1:A:1451:TYR:O	1:A:1455:LEU:HD23	2.19	0.43
1:A:2777:HIS:ND1	1:B:3255:THR:OG1	2.48	0.43
1:B:1207:LYS:HA	1:B:1210:LYS:HE2	2.01	0.43
1:B:4229:ASP:HA	1:B:4232:VAL:HG12	2.00	0.43
1:B:4230:ASP:OD1	1:B:4231:GLY:N	2.52	0.43
1:A:1094:VAL:HG13	1:A:1124:LEU:HD11	1.99	0.43
1:A:1110:LEU:HD21	1:A:1296:LEU:HD23	2.01	0.43
1:A:1484:ARG:NH1	1:A:2018:SER:O	2.41	0.43
1:A:2867:VAL:HG11	1:A:2923:LEU:HD11	2.01	0.43
1:A:3399:ILE:HA	1:A:3403:ASN:O	2.18	0.43
1:A:3991:TYR:CE1	1:A:3997:GLN:HA	2.54	0.43
1:B:345:TRP:CZ3	1:B:358:VAL:HA	2.54	0.43
1:B:912:VAL:HG23	1:B:940:PHE:CD2	2.53	0.43
1:B:1124:LEU:H	1:B:1185:PRO:HB3	1.82	0.43
1:B:2880:ARG:NH1	1:B:2886:SER:O	2.47	0.43
2:C:60:GLU:HG2	2:C:61:GLU:N	2.34	0.43
1:A:291:GLU:HG2	1:A:417:LEU:HD22	2.00	0.43
1:A:1789:ARG:HD2	1:A:1789:ARG:HA	1.77	0.43
1:A:3401:LEU:HD13	1:A:3456:TRP:CD2	2.54	0.43
1:B:157:GLN:HG3	1:B:226:HIS:HB3	1.99	0.43
1:B:166:PRO:HG2	1:B:169:GLU:HG3	2.00	0.43
1:B:1033:THR:HA	1:B:1304:ARG:HG2	2.00	0.43
1:B:2388:VAL:HG12	1:B:2655:VAL:HB	1.99	0.43
1:A:3463:VAL:HG21	1:A:3486:LEU:HB3	2.01	0.43
1:A:3561:MET:HE1	1:A:3626:LEU:HA	2.00	0.43
1:A:4233:LEU:O	1:A:4237:MET:HE2	2.19	0.43
1:A:4259:PRO:HA	1:A:4367:SER:O	2.19	0.43
1:B:1076:THR:HG22	1:B:1300:SER:HB2	2.01	0.43
1:B:2370:HIS:CE1	1:B:2632:GLN:HE21	2.36	0.43
1:B:3439:GLY:HA3	1:B:3500:ILE:HD13	2.00	0.43
2:C:134:SER:OG	2:C:138:GLU:OE2	2.37	0.43
1:A:271:GLY:HA3	1:A:278:VAL:HG22	2.01	0.43
1:A:388:ILE:HA	1:A:405:LYS:HD2	2.01	0.43
1:A:579:ALA:HB2	1:A:624:ARG:H	1.84	0.43
1:A:1089:HIS:HB3	1:A:1091:PHE:CZ	2.54	0.43
1:A:1347:HIS:CE1	1:A:1883:TYR:HH	2.37	0.43
1:A:1934:ARG:HD2	1:A:1934:ARG:HA	1.84	0.43
1:A:2039:HIS:NE2	1:A:2600:ASN:O	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2392:PHE:HB3	1:A:2399:TRP:CD1	2.53	0.43
1:A:3508:LEU:HD23	1:A:3508:LEU:H	1.84	0.43
1:B:136:CYS:SG	1:B:418:MET:HB3	2.58	0.43
1:B:1363:HIS:O	1:B:1374:ASN:ND2	2.37	0.43
1:B:1532:ILE:HG12	1:B:1782:ARG:HH12	1.84	0.43
1:B:3103:GLY:O	1:B:3107:ILE:HG23	2.19	0.43
1:B:2568:ASP:OD2	1:B:2570:ARG:NH1	2.51	0.43
1:B:3778:GLN:O	1:B:3781:MET:HG2	2.19	0.43
1:B:4199:HIS:ND1	1:B:4202:GLN:OE1	2.47	0.43
1:A:1322:LEU:HD23	1:A:1363:HIS:CE1	2.54	0.42
1:A:1357:CYS:HA	1:A:1407:PHE:HD1	1.83	0.42
1:A:2360:ARG:HA	1:A:2360:ARG:HD3	1.89	0.42
1:A:3029:ALA:HA	1:A:3034:ASP:HB3	2.00	0.42
1:A:3962:VAL:N	1:A:4009:GLY:O	2.52	0.42
1:B:156:LYS:HB2	1:B:159:ASP:CG	2.40	0.42
1:B:2934:LEU:HA	1:B:2941:SER:HA	2.00	0.42
1:B:2934:LEU:HD23	1:B:2934:LEU:H	1.84	0.42
1:B:3132:PHE:O	1:B:3133:LEU:C	2.57	0.42
1:B:3224:HIS:HB2	1:B:3297:LYS:HB2	2.00	0.42
1:A:1357:CYS:SG	1:A:1407:PHE:HB2	2.59	0.42
1:A:1473:LEU:O	1:A:1477:VAL:HG12	2.19	0.42
1:B:929:PRO:HG3	1:B:940:PHE:CE1	2.55	0.42
1:B:1050:GLN:HE22	1:B:1052:GLU:HB2	1.83	0.42
1:B:1372:GLU:O	1:B:1375:GLU:HG2	2.19	0.42
1:B:2115:ASP:OD1	1:B:2115:ASP:N	2.51	0.42
1:B:3424:ASN:HD22	1:B:3484:TYR:HB3	1.85	0.42
1:A:1034:LEU:HG	1:A:1036:PRO:HD2	2.00	0.42
1:A:1061:HIS:HE1	1:A:1068:GLY:HA2	1.83	0.42
1:A:1923:ASP:HA	1:B:3809:ARG:HH22	1.84	0.42
1:A:4370:ILE:HB	1:A:4371:PRO:HD3	2.02	0.42
1:B:271:GLY:HA2	1:B:276:ARG:HB3	2.01	0.42
1:B:1328:HIS:O	1:B:1332:LEU:HD23	2.19	0.42
2:D:79:LYS:HA	2:D:82:GLU:HG2	2.02	0.42
1:A:1799:ILE:HG12	1:A:1882:THR:HG22	2.01	0.42
1:B:1495:ARG:HD3	1:B:1944:LEU:HD13	1.99	0.42
1:A:309:MET:HA	1:A:344:PRO:HG2	2.01	0.42
1:A:1039:SER:H	1:A:1096:PRO:HG2	1.84	0.42
1:A:2592:ASP:OD1	1:A:2593:SER:N	2.52	0.42
1:A:3124:SER:OG	1:A:3125:MET:N	2.48	0.42
1:B:314:PHE:HE1	1:B:328:CYS:HB2	1.84	0.42
1:B:831:ASN:OD1	1:B:833:ALA:N	2.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2336:VAL:CG1	1:B:2358:LEU:HD11	2.50	0.42
1:B:2814:LYS:HE3	1:B:2814:LYS:HB2	1.83	0.42
1:A:1045:CYS:O	1:A:1079:LEU:HD12	2.19	0.42
1:A:3460:SER:HB2	1:A:3489:PRO:HG3	2.02	0.42
1:B:381:CYS:SG	1:B:386:ASP:HB2	2.60	0.42
1:B:437:LEU:HD21	1:B:627:LEU:HD13	2.01	0.42
1:B:744:HIS:CD2	1:B:900:LEU:HB2	2.54	0.42
1:B:827:LEU:HB3	1:B:844:ILE:HB	2.01	0.42
1:B:2343:ASP:OD1	1:B:2345:THR:OG1	2.36	0.42
1:A:89:GLY:HA3	1:A:150:LEU:HD21	2.02	0.42
1:A:2083:VAL:CG2	1:A:2124:ILE:HG13	2.50	0.42
1:B:1069:ASP:O	1:B:1073:HIS:N	2.52	0.42
1:B:1174:LEU:HD12	1:B:1175:GLU:HG2	2.02	0.42
1:B:1803:ASP:HB3	1:B:1879:TYR:HB2	2.01	0.42
1:B:2716:LEU:HA	1:B:2716:LEU:HD12	1.78	0.42
1:B:2867:VAL:HG21	1:B:2923:LEU:HD11	2.01	0.42
1:B:4161:PHE:HZ	1:B:4213:PRO:HA	1.85	0.42
1:B:4412:LEU:HB3	1:B:4496:ARG:NH2	2.35	0.42
1:A:746:LEU:HD11	1:A:859:LEU:HD11	2.02	0.42
1:A:864:PRO:O	1:A:871:GLU:HB3	2.20	0.42
1:B:161:VAL:HG11	1:B:225:HIS:HB2	2.02	0.42
1:B:2643:PHE:CE2	1:B:2694:ILE:HD13	2.55	0.42
1:B:2870:TYR:OH	1:B:2916:ASP:OD1	2.25	0.42
1:B:3523:GLU:HG2	1:B:3563:TRP:CH2	2.55	0.42
1:A:250:PRO:HG3	1:A:364:GLN:N	2.35	0.42
1:A:2129:LEU:HD21	1:A:2182:VAL:HB	2.01	0.42
1:A:3704:GLY:HA3	1:A:3777:ASN:HD21	1.85	0.42
1:B:76:HIS:O	1:B:80:ASN:N	2.53	0.42
1:B:138:LYS:H	1:B:373:ALA:HA	1.85	0.42
1:B:1910:ILE:HD12	1:B:1910:ILE:H	1.84	0.42
1:B:2687:ASN:HB3	1:B:2690:ARG:HG2	2.01	0.42
1:A:627:LEU:HD12	1:A:628:PRO:HD2	2.02	0.42
1:A:3103:GLY:O	1:A:3107:ILE:HG23	2.20	0.42
1:A:3287:ASP:O	1:B:2883:SER:OG	2.38	0.42
1:B:1055:GLN:OE1	1:B:1058:HIS:HD2	2.03	0.42
1:B:1863:ARG:NH1	1:B:1865:GLY:H	2.18	0.42
1:B:3776:ASN:OD1	1:B:3779:LYS:HE3	2.20	0.42
1:A:734:ASP:OD1	1:A:735:SER:N	2.53	0.41
1:A:1016:PRO:HB2	1:A:1018:THR:HG23	2.01	0.41
1:A:1813:ALA:N	1:A:1863:ARG:HE	2.18	0.41
1:A:2051:GLN:N	1:A:2051:GLN:OE1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3755:GLN:O	1:A:3759:ILE:HG12	2.20	0.41
1:B:345:TRP:HB3	1:B:1056:ARG:NH1	2.35	0.41
1:B:562:ILE:N	1:B:563:PRO:HA	2.35	0.41
1:B:1349:GLN:O	1:B:1353:LEU:HD23	2.20	0.41
1:B:3040:LEU:HD23	1:B:3040:LEU:HA	1.86	0.41
1:B:4380:ASP:HB2	1:B:4440:MET:HG3	2.02	0.41
1:B:4441:LYS:HZ1	1:B:4490:ALA:HA	1.85	0.41
1:A:2113:PRO:HB3	1:A:2116:ARG:NH2	2.35	0.41
1:A:3210:LEU:HD23	1:A:3210:LEU:HA	1.89	0.41
1:B:1072:GLN:O	1:B:1075:ARG:HG2	2.19	0.41
1:B:1426:PRO:HB2	1:B:1430:LYS:NZ	2.35	0.41
1:B:3198:SER:HA	1:B:3291:LEU:O	2.20	0.41
1:B:3706:SER:HA	1:B:3709:ASN:ND2	2.35	0.41
1:B:3759:ILE:HD13	1:B:3759:ILE:HA	1.90	0.41
1:B:4382:VAL:HG12	1:B:4444:VAL:HG12	2.01	0.41
1:A:513:LEU:N	1:A:567:LEU:HD11	2.32	0.41
1:B:1066:HIS:CE1	1:B:1825:GLU:HB3	2.55	0.41
1:B:2567:LEU:HD11	1:B:2580:GLU:HG3	2.01	0.41
1:B:3618:GLN:HB2	1:B:3846:HIS:HE2	1.85	0.41
1:A:1446:GLY:O	1:A:1449:TYR:HB3	2.20	0.41
1:B:1470:CYS:HA	1:B:2030:LEU:HD11	2.01	0.41
1:B:2101:GLN:O	1:B:2105:ASN:HB2	2.20	0.41
1:A:251:VAL:O	1:A:255:VAL:HG23	2.20	0.41
1:A:1046:TRP:HZ3	1:A:1298:GLU:HA	1.85	0.41
1:A:1488:MET:HE2	1:A:1488:MET:HB2	1.79	0.41
1:A:2126:GLN:HG2	1:A:2181:TYR:CG	2.55	0.41
1:A:3187:PRO:HA	1:A:3188:PRO:HD3	1.98	0.41
1:A:3767:PHE:O	1:A:3771:ILE:HG12	2.21	0.41
1:A:4235:ARG:HD3	1:A:4330:TYR:CE1	2.55	0.41
1:B:1126:LYS:HD2	1:B:1183:CYS:HA	2.02	0.41
1:B:1511:GLU:HA	1:B:1515:SER:O	2.21	0.41
1:B:2027:ILE:HG21	1:B:2066:LEU:HD11	2.02	0.41
1:B:3767:PHE:O	1:B:3771:ILE:HG12	2.20	0.41
1:B:4185:LEU:HA	1:B:4188:VAL:HG22	2.02	0.41
2:D:79:LYS:HD3	2:D:82:GLU:OE2	2.20	0.41
1:A:1322:LEU:HD23	1:A:1363:HIS:HE1	1.86	0.41
1:A:1484:ARG:NH2	1:A:2016:GLN:O	2.53	0.41
1:A:3406:ALA:HB2	1:A:3419:LEU:HD12	2.03	0.41
1:B:907:THR:OG1	1:B:911:TYR:O	2.26	0.41
1:B:3396:LEU:HA	1:B:3399:ILE:HG12	2.02	0.41
1:B:3433:ASP:O	1:B:3437:GLN:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4236:ARG:HH11	1:B:4357:PRO:HG3	1.85	0.41
2:C:11:VAL:HA	2:C:14:VAL:HB	2.01	0.41
1:A:283:MET:O	1:A:283:MET:HG3	2.21	0.41
1:A:1358:TRP:O	1:A:1362:VAL:HG23	2.21	0.41
1:A:1808:THR:OG1	1:A:1837:ILE:O	2.29	0.41
1:A:4399:LEU:HA	1:A:4402:ILE:HG22	2.03	0.41
1:B:195:GLN:HB2	1:B:223:LEU:HD11	2.02	0.41
1:B:2010:ASN:N	1:B:2010:ASN:OD1	2.54	0.41
1:B:3719:LEU:HD22	1:B:3807:PHE:CD2	2.56	0.41
1:B:3962:VAL:HG12	1:B:3964:VAL:HG13	2.02	0.41
1:B:4161:PHE:HA	1:B:4164:PHE:HB2	2.01	0.41
1:A:1444:THR:OG1	1:A:1518:LYS:HD2	2.21	0.41
1:A:1488:MET:SD	1:A:1939:LEU:HD23	2.61	0.41
1:B:1321:MET:HG3	1:B:1327:PHE:HE2	1.86	0.41
1:B:2629:LEU:HB3	1:B:2630:ILE:H	1.59	0.41
1:B:2823:ARG:HD3	1:B:2823:ARG:HA	1.92	0.41
1:B:3709:ASN:HA	1:B:3712:TRP:CZ3	2.55	0.41
1:B:3965:PHE:HA	1:B:4008:LEU:HA	2.02	0.41
2:D:33:ILE:O	2:D:36:TYR:HB3	2.21	0.41
1:A:145:LEU:HD13	1:A:148:THR:HG21	2.03	0.41
1:A:189:TYR:CE1	1:A:193:ILE:HG13	2.56	0.41
1:A:257:ASP:O	1:A:261:TYR:HB2	2.20	0.41
1:A:725:PHE:HB2	1:A:824:TYR:CE2	2.55	0.41
1:A:1103:HIS:ND1	1:A:1204:THR:HG21	2.36	0.41
1:A:1379:SER:HA	1:A:1382:ARG:HH11	1.85	0.41
1:A:2923:LEU:HD23	1:A:2923:LEU:HA	1.89	0.41
1:A:3164:ALA:HB1	1:A:3183:LEU:HD22	2.02	0.41
1:B:711:PRO:HB2	1:B:712:LYS:H	1.57	0.41
1:B:1518:LYS:HG3	1:B:1989:ASN:ND2	2.36	0.41
1:B:1807:PRO:HD3	1:B:1876:GLY:HA2	2.02	0.41
1:B:2110:LEU:HD12	1:B:2111:ILE:H	1.86	0.41
1:B:2661:LEU:HD23	1:B:2661:LEU:HA	1.88	0.41
1:B:2813:LEU:HD12	1:B:2851:VAL:HG21	2.03	0.41
1:B:3828:SER:HB3	1:B:4006:VAL:HG13	2.03	0.41
1:B:4075:ALA:HB3	1:B:4175:LEU:HD11	2.03	0.41
1:A:2113:PRO:HB3	1:A:2116:ARG:HH21	1.86	0.41
1:B:301:TYR:HB3	1:B:340:PRO:HA	2.03	0.41
1:B:907:THR:HG21	1:B:913:LYS:HD2	2.02	0.41
1:B:1109:VAL:HG23	1:B:1198:ALA:HB2	2.03	0.41
1:B:1806:ILE:HB	1:B:1842:LEU:HD21	2.03	0.41
1:B:2110:LEU:HD12	1:B:2111:ILE:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3396:LEU:HD23	1:B:3438:LEU:HD11	2.02	0.41
1:B:3684:ALA:HB2	1:B:3759:ILE:HD13	2.03	0.41
1:A:828:TYR:CE1	1:A:843:PRO:HB3	2.56	0.40
1:A:2822:GLU:HG3	1:A:2823:ARG:HG2	2.03	0.40
1:A:2840:LEU:HD11	1:A:2922:LEU:HD23	2.03	0.40
1:A:3253:LEU:HD12	1:B:2717:ARG:HD2	2.02	0.40
1:A:3414:LEU:O	1:B:2382:ARG:NH1	2.52	0.40
1:B:1429:LEU:HD13	1:B:1458:VAL:O	2.21	0.40
1:B:2708:LEU:HD21	1:B:2722:VAL:HG21	2.02	0.40
1:B:3540:LYS:HD2	1:B:3844:ILE:HG21	2.01	0.40
1:A:1061:HIS:CG	1:A:1072:GLN:HG3	2.56	0.40
1:A:4165:LEU:HA	1:A:4170:TYR:CD2	2.54	0.40
1:B:1105:ASP:OD2	1:B:1304:ARG:NH2	2.54	0.40
1:B:1339:THR:OG1	1:B:1341:ASP:OD1	2.24	0.40
1:B:1963:ALA:O	1:B:1966:GLU:HG2	2.22	0.40
1:B:1992:GLN:O	1:B:1996:VAL:HG23	2.21	0.40
1:B:2923:LEU:HD21	1:B:3036:LEU:HG	2.04	0.40
1:B:3321:ASP:OD1	1:B:3321:ASP:N	2.55	0.40
2:C:64:GLU:O	2:C:67:GLN:HG2	2.21	0.40
2:C:89:THR:HA	2:C:92:THR:HG22	2.03	0.40
1:A:1446:GLY:O	1:A:1450:TRP:CE3	2.74	0.40
1:A:3252:PRO:HD3	1:B:2784:THR:HG21	2.02	0.40
1:A:3546:LEU:HD23	1:A:3546:LEU:HA	1.96	0.40
1:A:4235:ARG:NH2	1:A:4330:TYR:O	2.54	0.40
2:C:54:LEU:HD23	2:C:54:LEU:HA	1.93	0.40
1:A:4211:THR:HG22	1:A:4215:HIS:HB2	2.02	0.40
1:A:1030:ARG:HG3	1:A:1307:LYS:HD3	2.04	0.40
1:A:1126:LYS:O	1:A:1177:HIS:ND1	2.54	0.40
1:A:2047:PRO:O	1:A:2051:GLN:NE2	2.38	0.40
1:A:2586:MET:HB3	1:A:2586:MET:HE3	1.91	0.40
1:A:2772:HIS:HB2	1:B:2915:ARG:NH1	2.34	0.40
1:A:2847:ASN:OD1	1:A:2848:PHE:N	2.55	0.40
1:A:4209:LEU:HA	1:A:4212:LEU:HD23	2.03	0.40
1:B:1124:LEU:HA	1:B:1181:ILE:HG21	2.04	0.40
1:B:1789:ARG:HB2	1:B:1860:VAL:HG22	2.04	0.40
1:B:3040:LEU:HB3	1:B:3084:PHE:CE1	2.56	0.40
1:B:3619:SER:O	1:B:3623:ILE:HG12	2.21	0.40
2:C:90:TRP:HZ2	2:C:124:LYS:HA	1.86	0.40
2:D:127:VAL:HB	2:D:131:HIS:CE1	2.57	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	2799/4859 (58%)	2712 (97%)	87 (3%)	0	100	100
1	B	2820/4859 (58%)	2741 (97%)	79 (3%)	0	100	100
2	C	148/184 (80%)	146 (99%)	2 (1%)	0	100	100
2	D	148/184 (80%)	147 (99%)	1 (1%)	0	100	100
All	All	5915/10086 (59%)	5746 (97%)	169 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	2517/4217 (60%)	2509 (100%)	8 (0%)	92	97
1	B	2534/4217 (60%)	2523 (100%)	11 (0%)	91	97
2	C	128/157 (82%)	127 (99%)	1 (1%)	81	93
2	D	128/157 (82%)	128 (100%)	0	100	100
All	All	5307/8748 (61%)	5287 (100%)	20 (0%)	91	97

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1291	ARG
1	A	1797	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2327	ARG
1	A	2943	ARG
1	A	3467	LYS
1	A	4179	LYS
1	A	4218	ARG
1	A	4496	ARG
1	B	59	ARG
1	B	1863	ARG
1	B	1975	GLN
1	B	2002	ARG
1	B	2943	ARG
1	B	3002	ASN
1	B	3131	LYS
1	B	3133	LEU
1	B	3134	ASP
1	B	3779	LYS
1	B	3970	LYS
2	C	9	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1072	GLN
1	A	1365	ASN
1	A	1925	GLN
1	A	1929	ASN
1	A	3161	HIS
1	A	4202	GLN
1	B	151	GLN
1	B	1058	HIS
1	B	2370	HIS
1	B	2735	ASN
1	B	2745	GLN
1	B	3493	HIS
1	B	3790	GLN
1	B	3997	GLN

5.3.3 RNA

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.

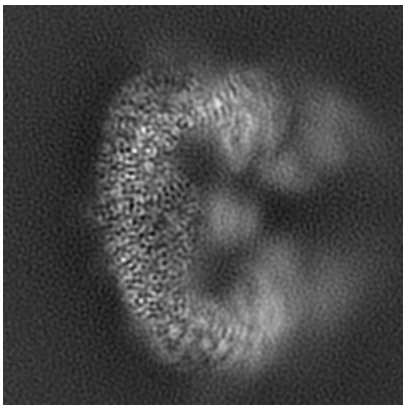
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-15654. These allow visual inspection of the internal detail of the map and identification of artifacts.

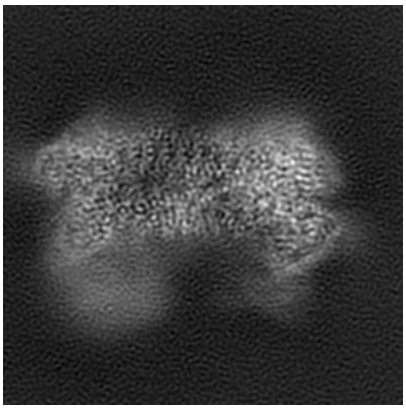
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

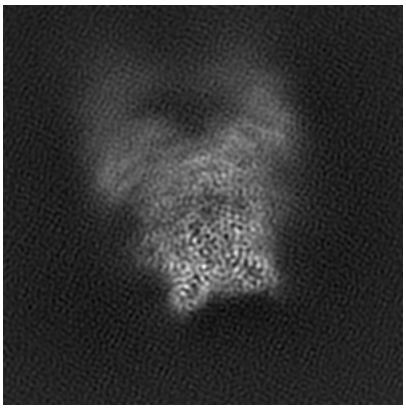
6.1.1 Primary map



X

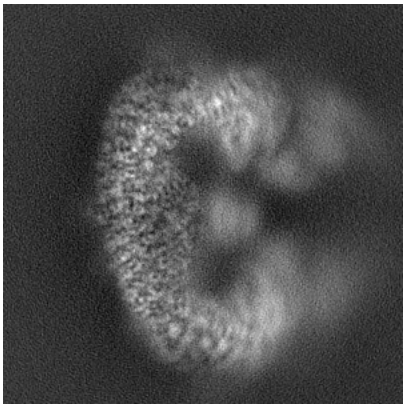


Y

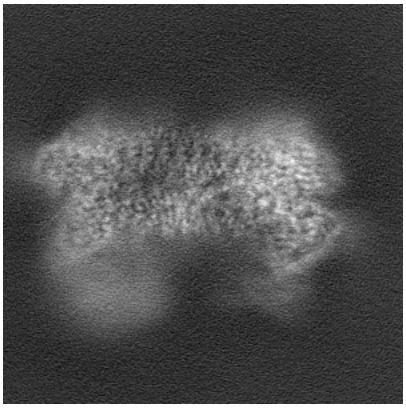


Z

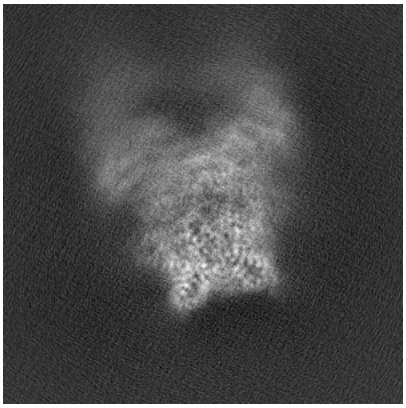
6.1.2 Raw map



X



Y

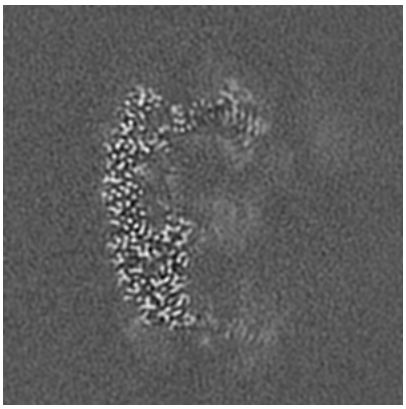


Z

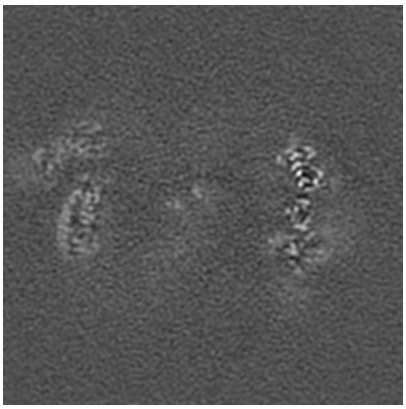
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

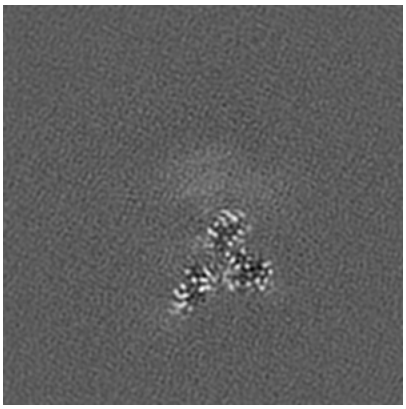
6.2.1 Primary map



X Index: 150

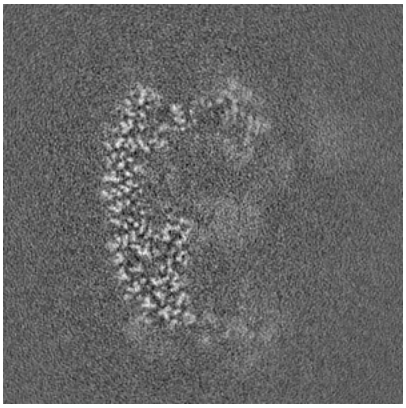


Y Index: 150

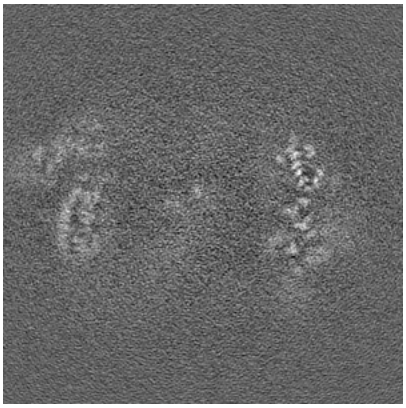


Z Index: 150

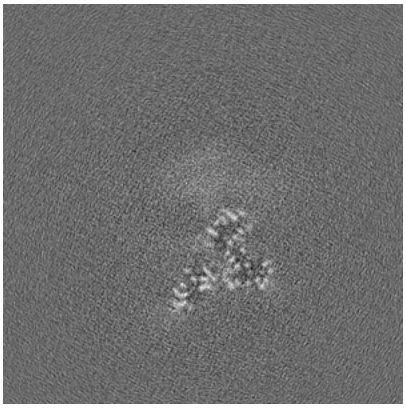
6.2.2 Raw map



X Index: 150



Y Index: 150

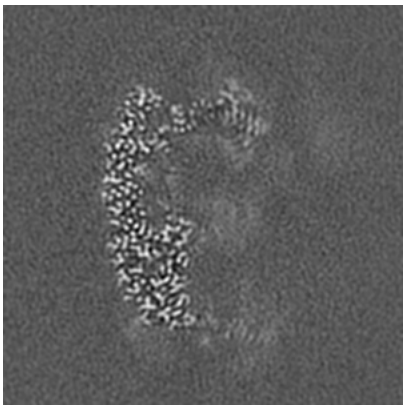


Z Index: 150

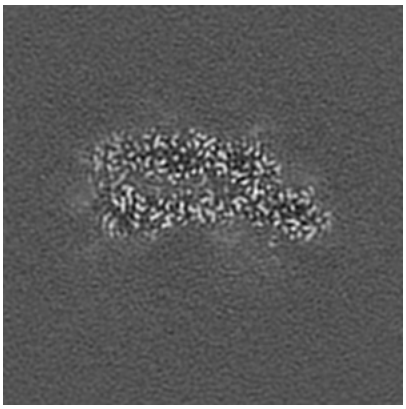
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

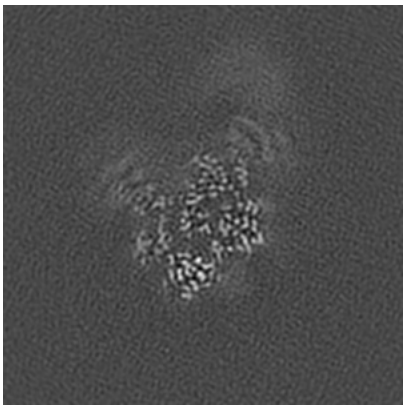
6.3.1 Primary map



X Index: 150

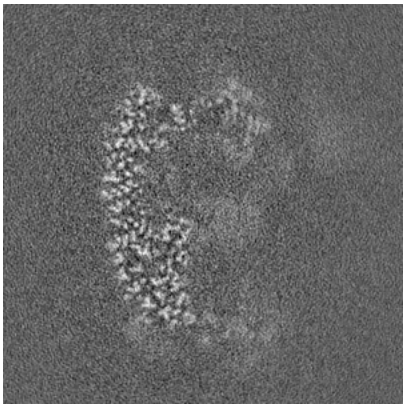


Y Index: 99

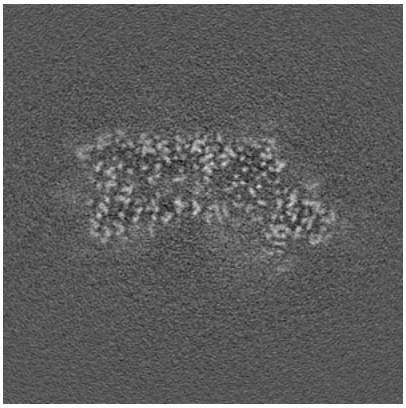


Z Index: 217

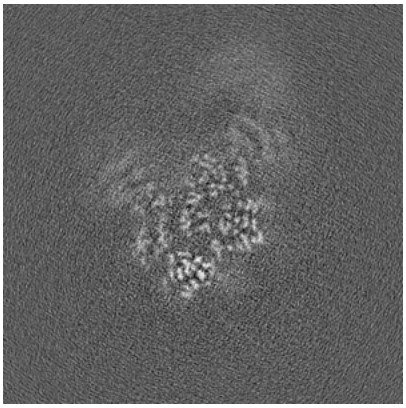
6.3.2 Raw map



X Index: 150



Y Index: 104



Z Index: 217

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

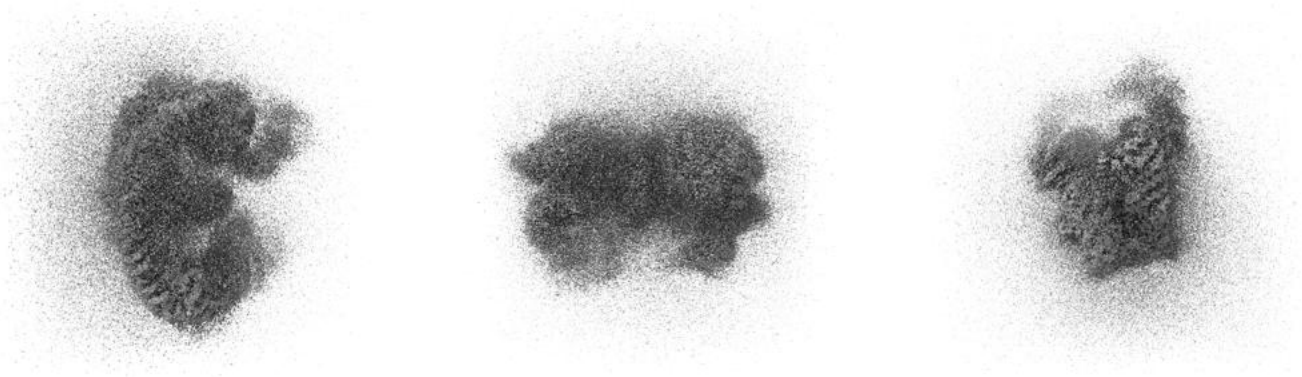
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.144. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

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

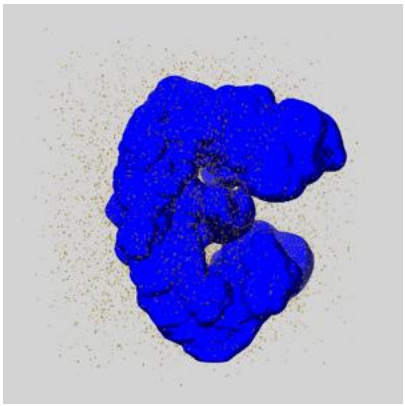
6.5 Mask visualisation

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

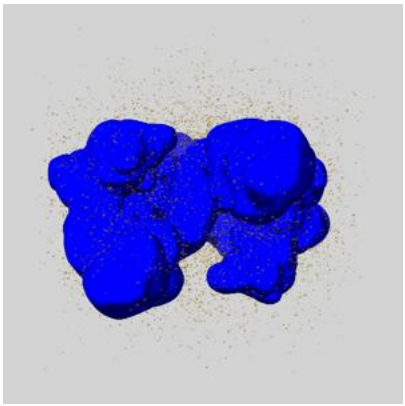
A mask typically either:

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

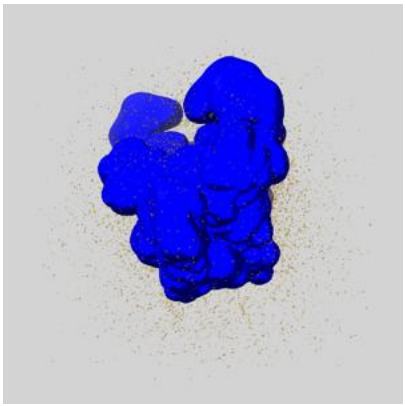
6.5.1 emd_15654_msk_1.map



X



Y

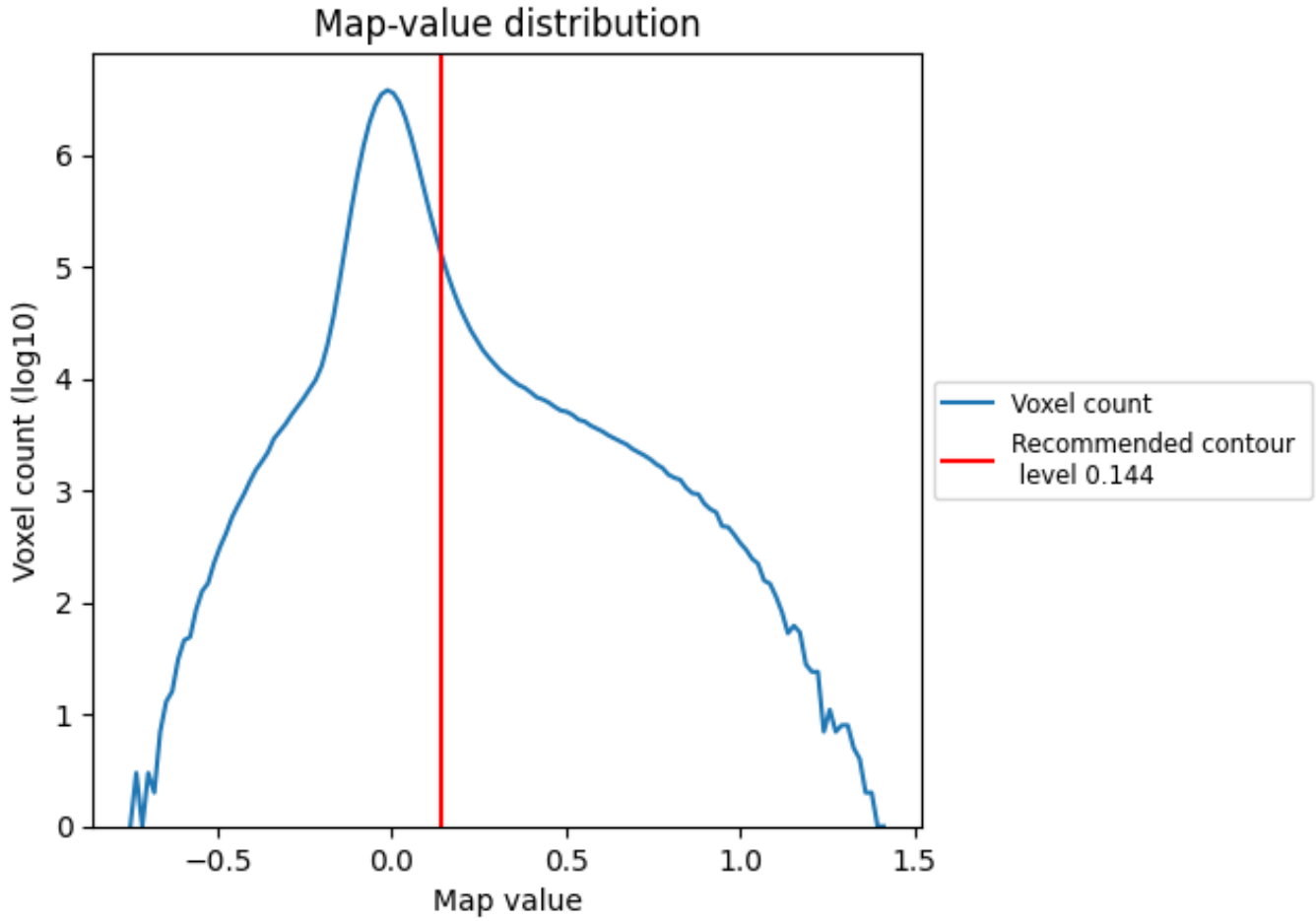


Z

7 Map analysis

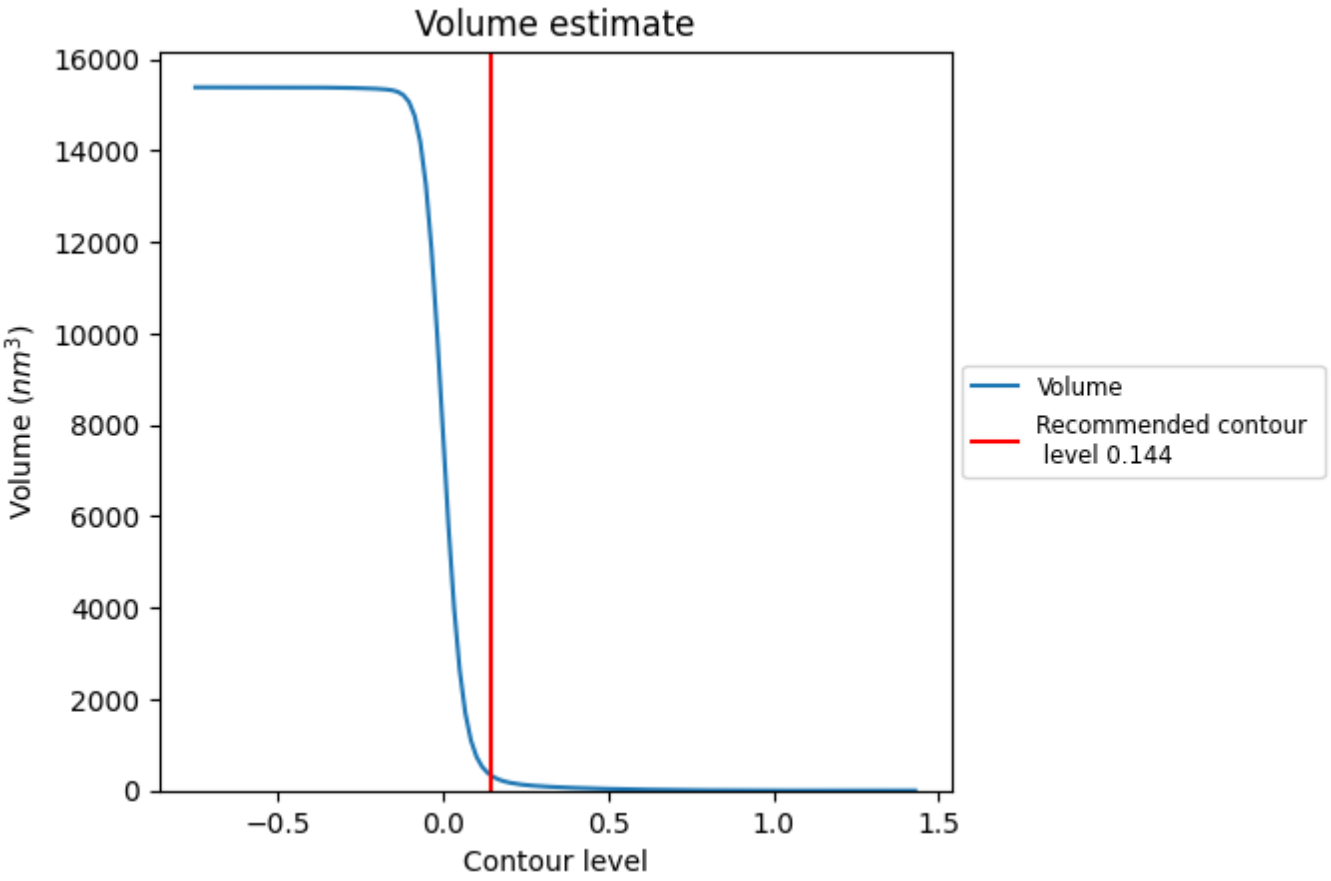
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

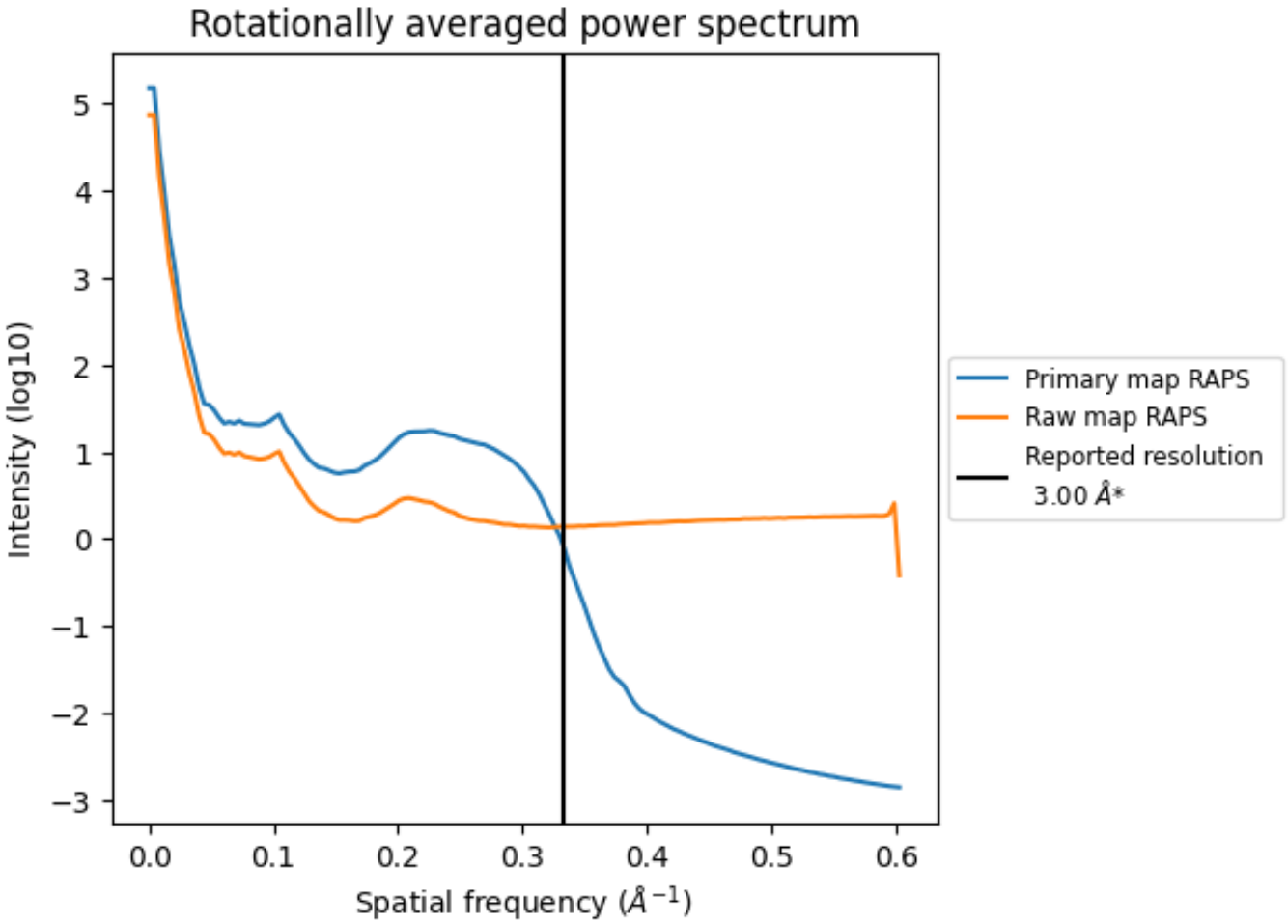
7.2 Volume estimate (i)



The volume at the recommended contour level is 339 nm^3; this corresponds to an approximate mass of 307 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)

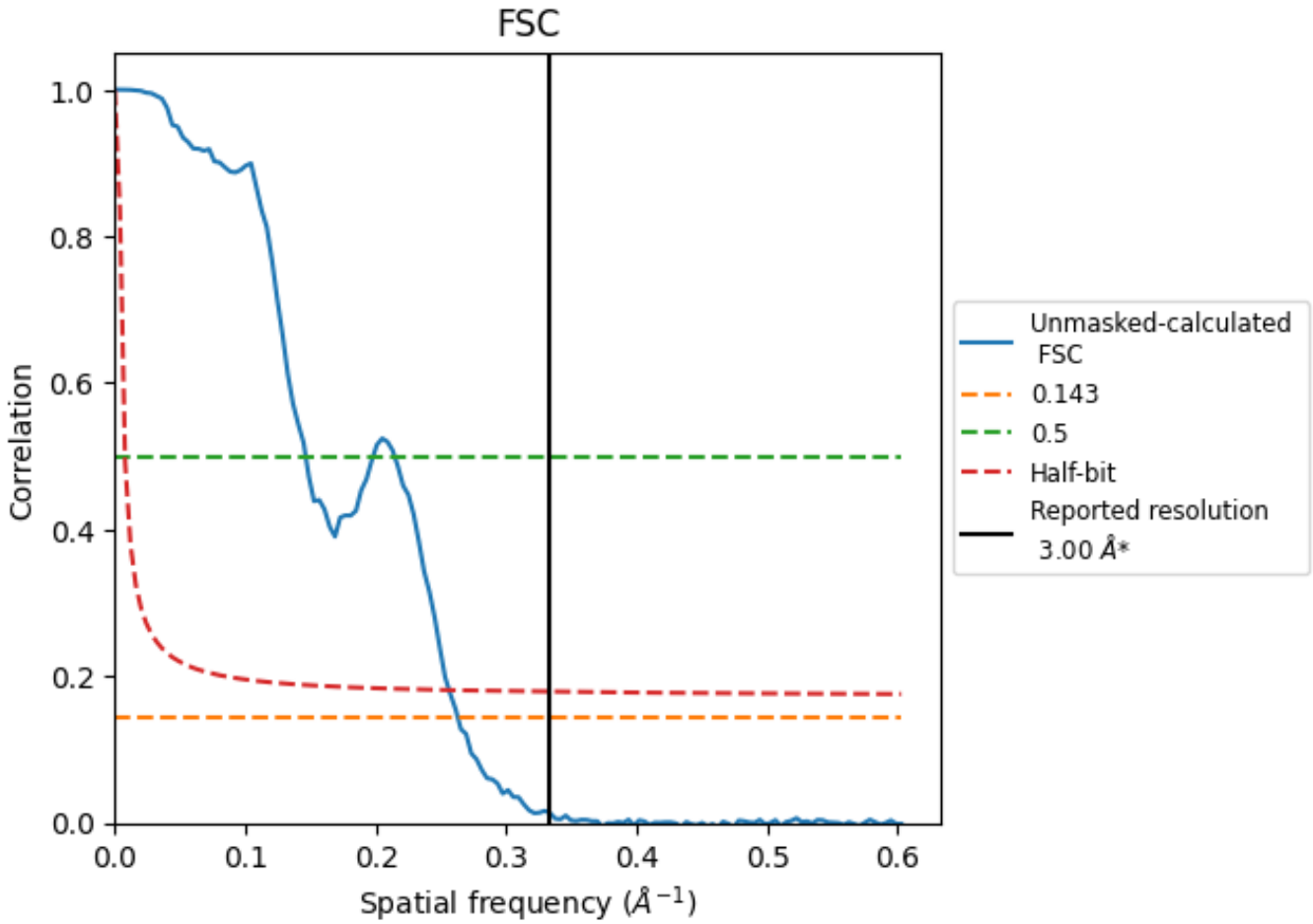


*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

8.2 Resolution estimates (i)

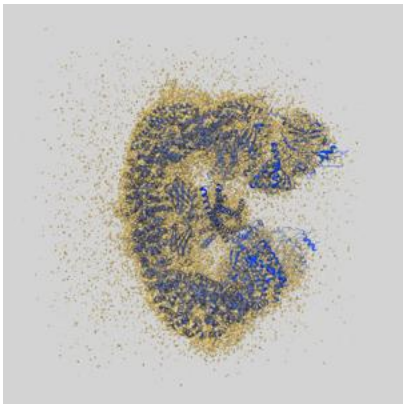
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.80	6.83	3.90

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.80 differs from the reported value 3.0 by more than 10 %

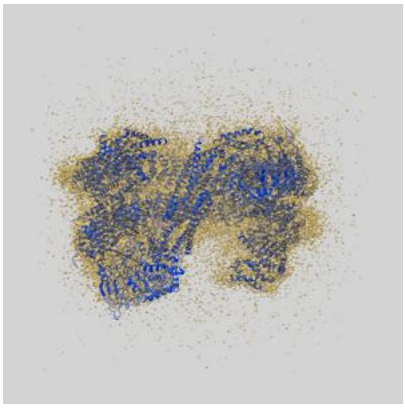
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-15654 and PDB model 8ATO. Per-residue inclusion information can be found in section 3 on page 4.

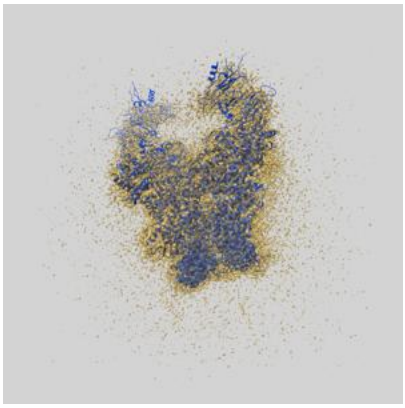
9.1 Map-model overlay



X



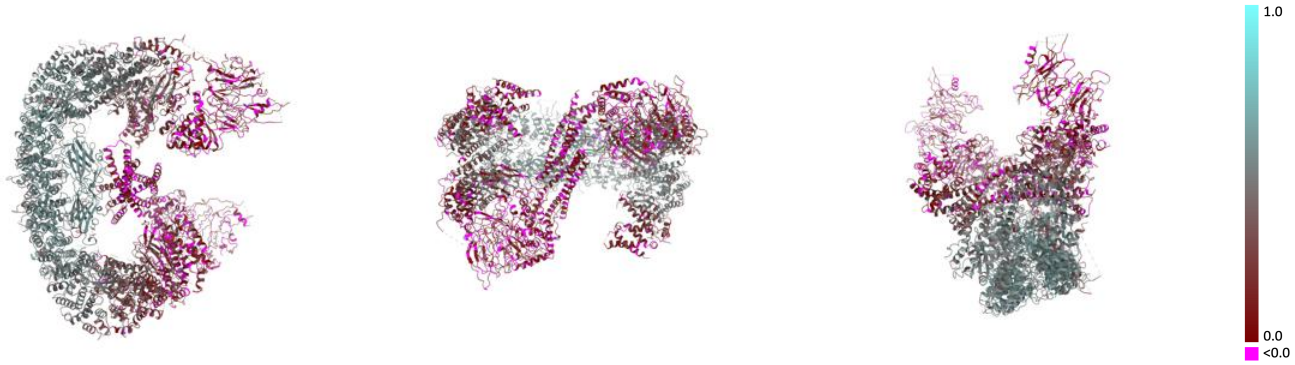
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.144 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.

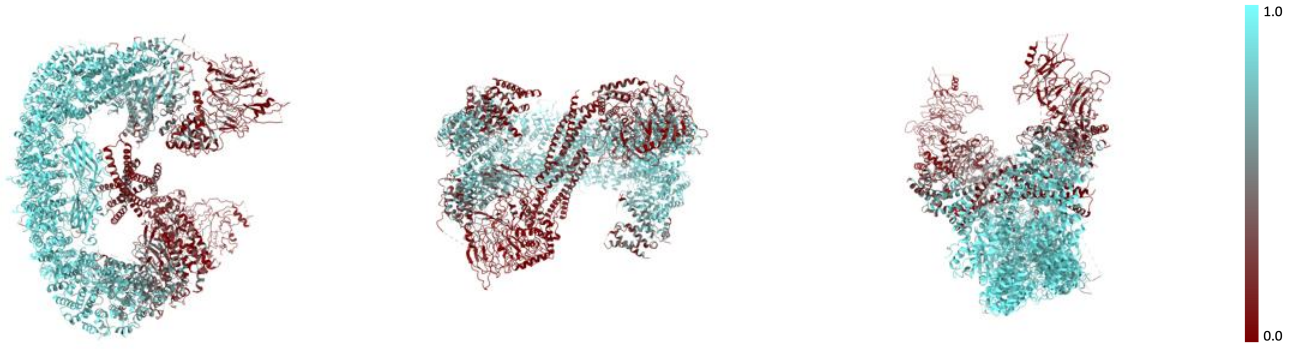
9.2 Q-score mapped to coordinate model (i)



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.

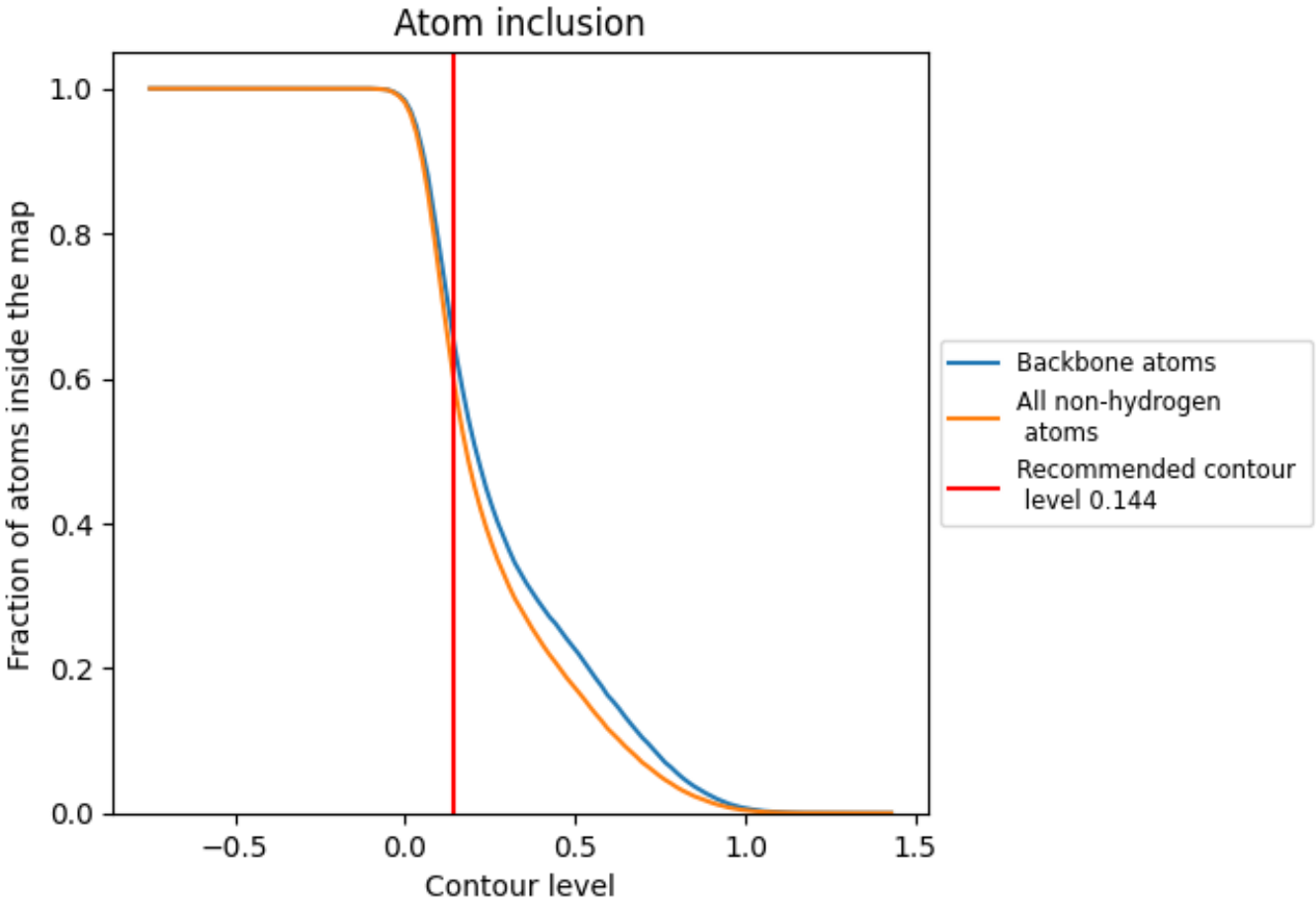
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.144).

9.4 Atom inclusion (i)



At the recommended contour level, 65% of all backbone atoms, 59% 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 (0.144) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5934	0.3340
A	0.5922	0.3380
B	0.6391	0.3550
C	0.1931	0.0830
D	0.1491	0.0780