Full wwPDB EM Validation Report ⓘ

Dec 18, 2022 – 02:07 pm GMT

PDB ID	:	7AOD
EMDB ID	:	EMD-11841
Title	:	Schizosaccharomyces pombe RNA polymerase I (dimer)
Authors	:	Heiss, F.; Daiss, J.; Becker, P.; Engel, C.
Deposited on	:	2020-10-14
Resolution	:	4.50 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:

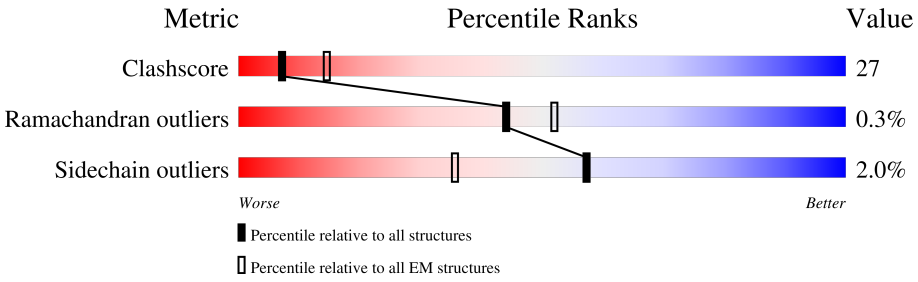
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 4.50 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	1689	25% 40% 41% • 18%
1	M	1689	25% 39% 42% • 18%
2	B	1174	22% 51% 47% ••
2	N	1174	22% 49% 49% ••
3	C	348	20% 43% 46% • 9%
3	O	348	22% 41% 49% • 9%
4	D	147	14% 13% 12% • 73%
4	P	147	15% 13% 13% • 73%

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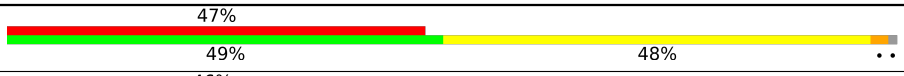
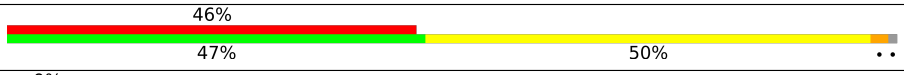
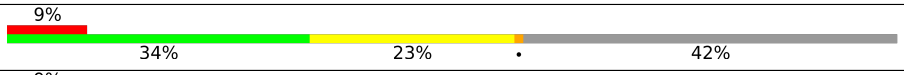
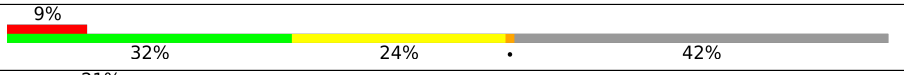
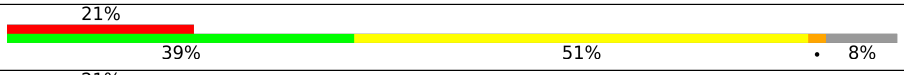
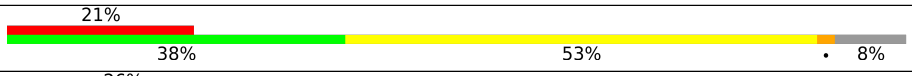
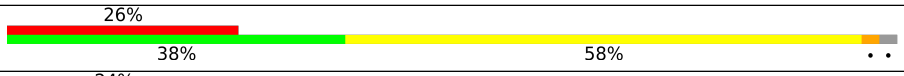
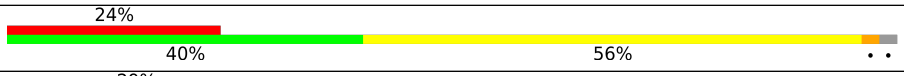
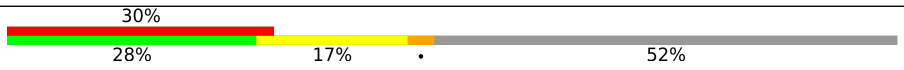
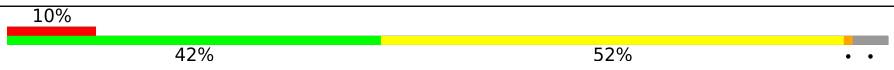
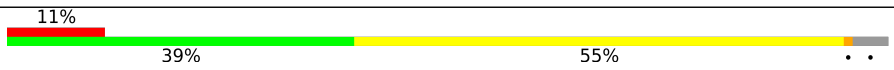
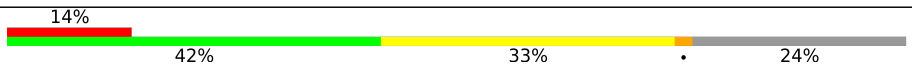
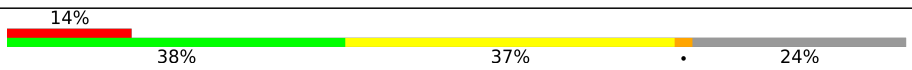
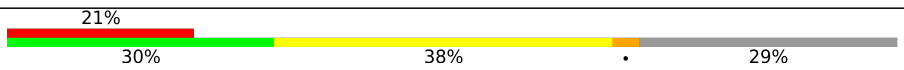
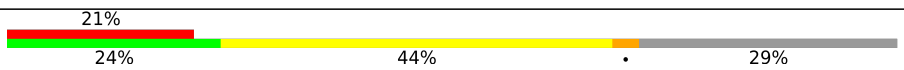
Mol	Chain	Length	Quality of chain
5	E	210	
5	Q	210	
6	F	142	
6	R	142	
7	G	173	
7	S	173	
8	H	125	
8	T	125	
9	I	119	
9	U	119	
10	J	71	
10	V	71	
11	K	125	
11	W	125	
12	L	63	
12	X	63	

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 59256 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 DNA-directed RNA polymerase I subunit rpa1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1384	Total	C	N	O	S	0	0
			10976	6965	1894	2059	58		
1	M	1384	Total	C	N	O	S	0	0
			10976	6965	1894	2059	58		

- Molecule 2 is a protein called Probable DNA-directed RNA polymerase I subunit RPA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1156	Total	C	N	O	S	0	0
			9127	5791	1592	1685	59		
2	N	1156	Total	C	N	O	S	0	0
			9127	5791	1592	1685	59		

- Molecule 3 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	317	Total	C	N	O	S	0	0
			2533	1621	430	475	7		
3	O	317	Total	C	N	O	S	0	0
			2533	1621	430	475	7		

- Molecule 4 is a protein called DNA-directed RNA polymerase I subunit rpa14.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	39	Total	C	N	O	S	0	0
			322	203	57	61	1		
4	P	39	Total	C	N	O	S	0	0
			322	203	57	61	1		

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	207	Total	C	N	O	S	0	0
			1663	1050	301	306	6		
5	Q	207	Total	C	N	O	S	0	0
			1663	1050	301	306	6		

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	82	Total	C	N	O	S	0	0
			650	413	111	123	3		
6	R	82	Total	C	N	O	S	0	0
			650	413	111	123	3		

- Molecule 7 is a protein called DNA-directed RNA polymerase I subunit rpa43.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	160	Total	C	N	O	S	0	0
			1267	817	210	236	4		
7	S	160	Total	C	N	O	S	0	0
			1267	817	210	236	4		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	123	Total	C	N	O	S	0	0
			990	628	166	193	3		
8	T	123	Total	C	N	O	S	0	0
			990	628	166	193	3		

- Molecule 9 is a protein called DNA-directed RNA polymerase I subunit RPA12.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	57	Total	C	N	O	S	0	0
			431	269	69	89	4		
9	U	57	Total	C	N	O	S	0	0
			431	269	69	89	4		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	68	Total	C	N	O	S	0	0
			550	350	93	100	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	V	68	Total 550	C 350	N 93	O 100	S 7	0	0

- Molecule 11 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	95	Total 745	C 472	N 123	O 146	S 4	0	0
11	W	95	Total 745	C 472	N 123	O 146	S 4	0	0

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	45	Total 368	C 225	N 74	O 61	S 8	0	0
12	X	45	Total 368	C 225	N 74	O 61	S 8	0	0

- Molecule 13 is ZINC ION (three-letter code: ZN) (formula: Zn).

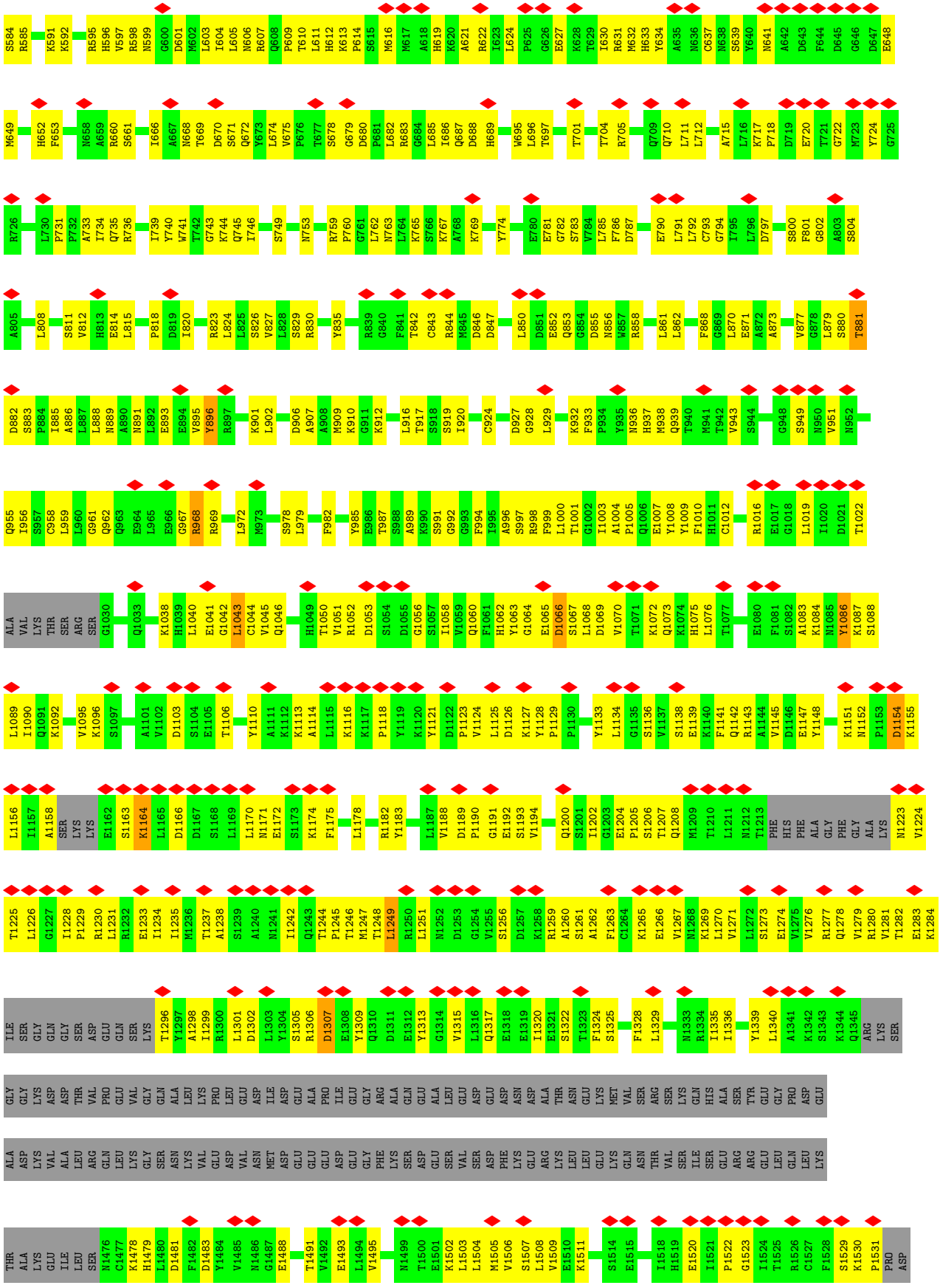
Mol	Chain	Residues	Atoms		AltConf
13	A	2	Total 2	Zn 2	0
13	B	1	Total 1	Zn 1	0
13	I	1	Total 1	Zn 1	0
13	J	1	Total 1	Zn 1	0
13	L	1	Total 1	Zn 1	0
13	M	2	Total 2	Zn 2	0
13	N	1	Total 1	Zn 1	0
13	U	1	Total 1	Zn 1	0
13	V	1	Total 1	Zn 1	0
13	X	1	Total 1	Zn 1	0

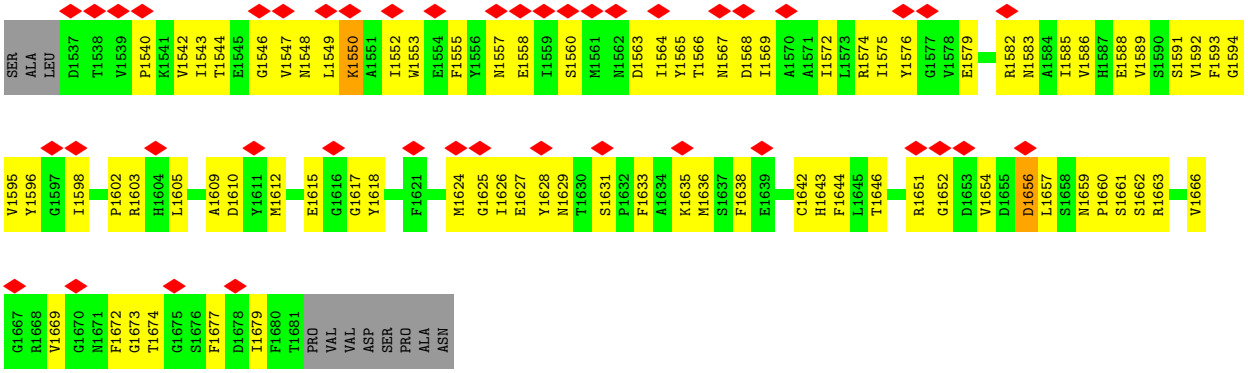
3 Residue-property plots (i)

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.

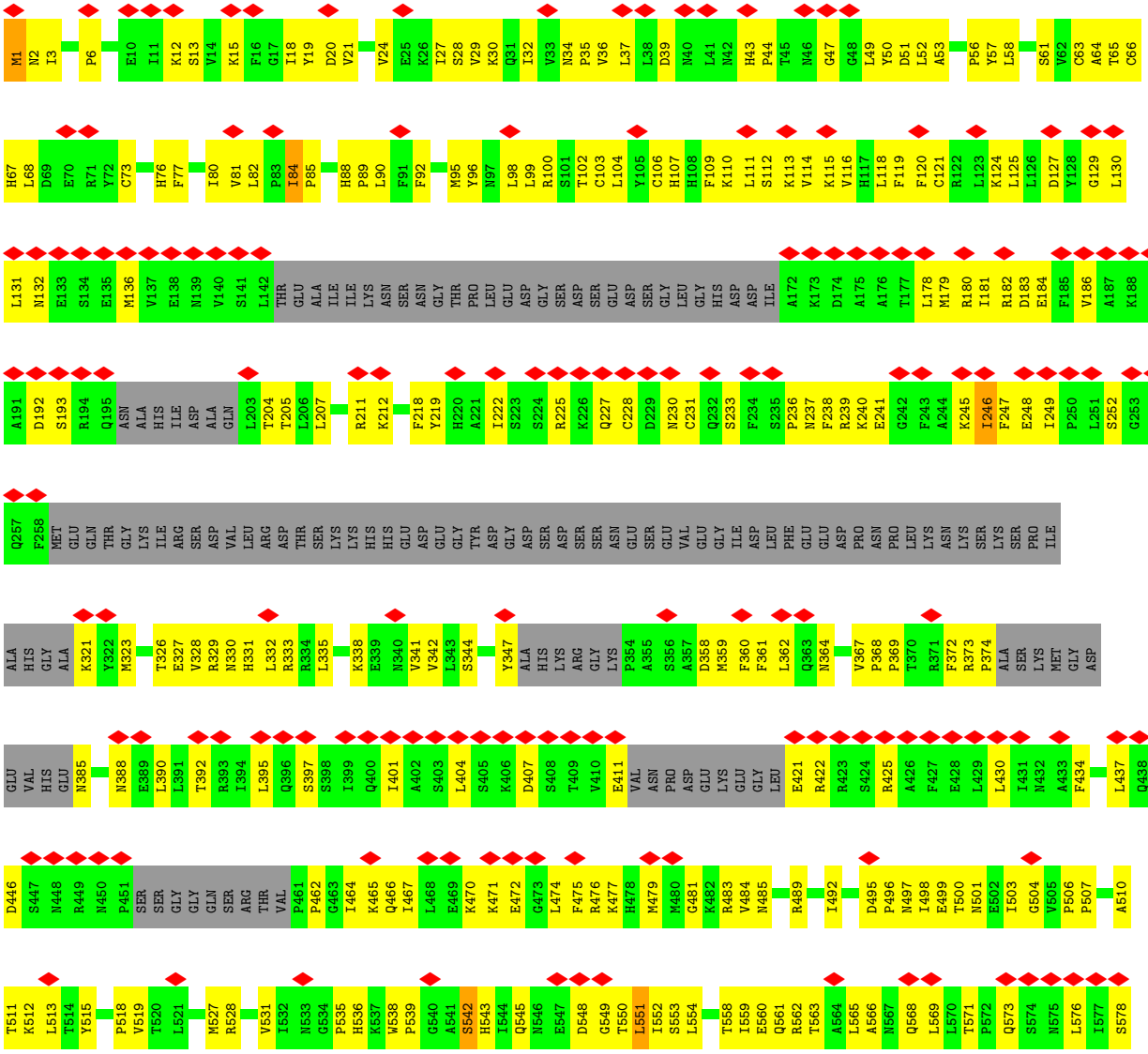
- Molecule 1: DNA-directed RNA polymerase I subunit rpa1

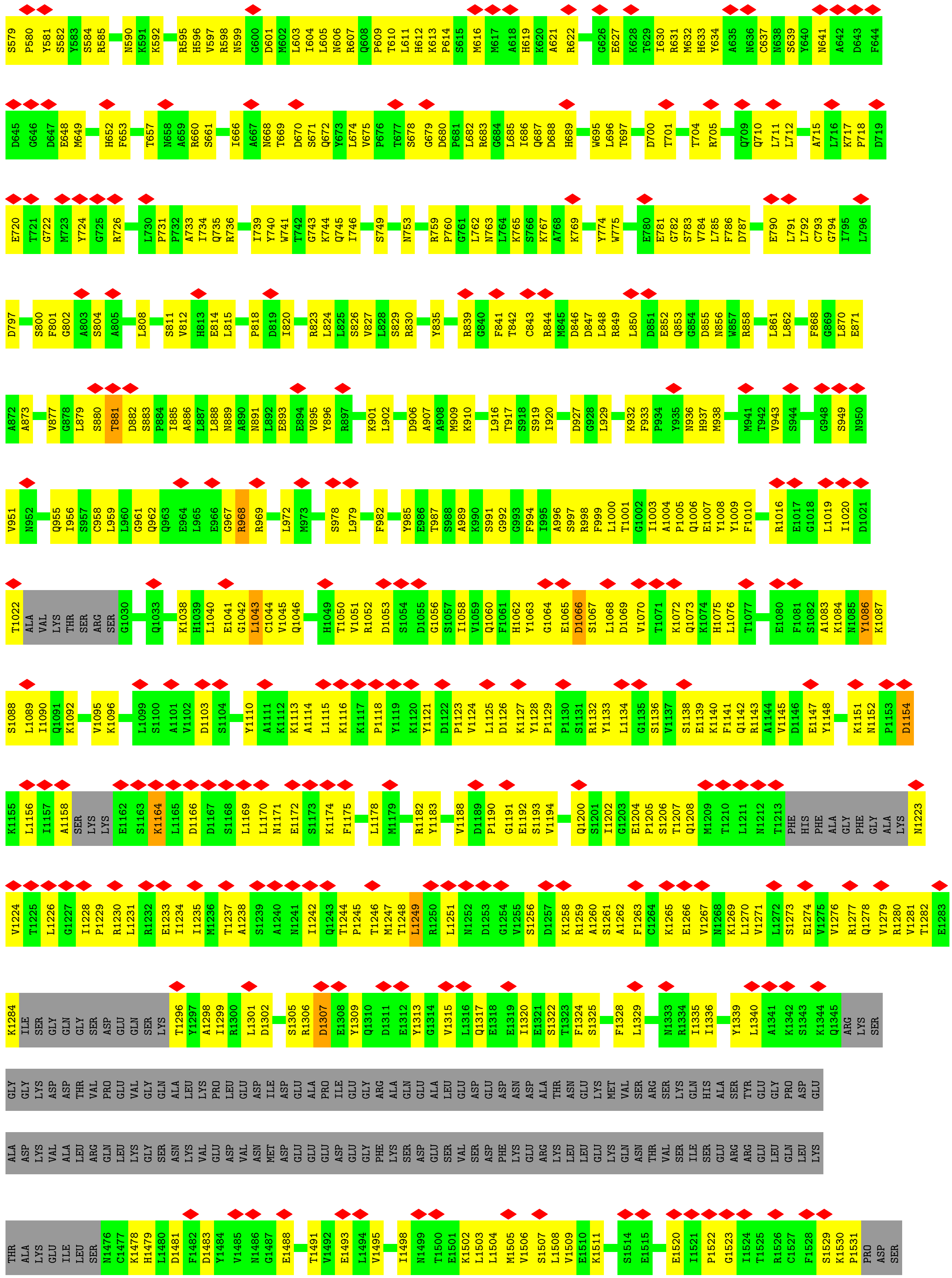
Chain A:

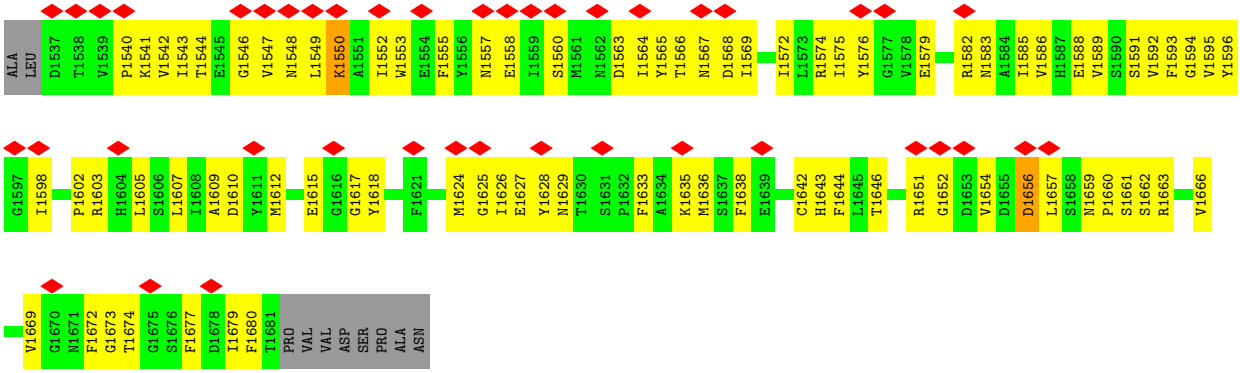

S584 R585 K591 K592 R595 H596 V597 R598 N599 G600 D601 M602 L603 I604 L605 N606 R607 Q608 P609 T610 L611 H612 K613 P614 S615 M616 M617 A618 H619 K620 A621 R622 I623 L624 P625 G626 E627 K628 T629 I630 R631 M632 H633 Y634 A635 N636 C637 N638 S639 Y640 N641 A642 D643 F644 D645 G646 D647 E648
M649 H652 F653 N658 A659 R660 S661 I666 A667 N668 T669 D670 S671 Q672 Y673 L674 V675 P676 T677 S678 G679 D680 P681 L682 R683 G684 L685 I686 Q687 D688 H689 W695 L696 T697 T701 T704 R705 Q709 Q710 L711 L712 A715 L716 K717 P718 D719 E720 T721 G722 M723 Y724 G725
R726 L730 P731 P732 A733 T734 Q735 R736 I739 Y740 W741 T742 G743 K744 Q745 I746 S749 N753 R759 P760 G761 L762 N763 L764 K765 S766 K767 A768 K769 Y774 E780 E781 G782 S783 V784 L785 F786 D787 E790 L791 L792 C793 G794 I795 L796 D797 S800 F801 G802 A803 S804
A805 L808 S811 V812 H813 E814 L815 P818 D819 I820 R823 L824 L825 S826 V827 L828 S829 R830 Y835 R839 G840 F841 T842 C843 R844 M845 D846 D847 L850 D851 E852 Q853 G854 D855 N856 W857 R858 L861 L862 F868 G869 L870 E871 A872 A873 V877 G878 L879 S880 T881
D882 S883 P884 I885 A886 L887 L888 N889 A890 N891 L892 E893 E894 V895 Y896 R897 K901 L902 D906 A907 A908 M909 K910 G911 K912 L916 T917 S918 S919 I920 C924 D927 G928 L929 K932 F933 P934 Y935 N936 H937 M938 Q939 T940 M941 T942 V943 S944 G948 S949 N950 V951 N952
Q955 I956 S957 C958 L959 L960 G961 Q962 Q963 E964 L965 E966 G967 R968 R969 L972 M973 S978 L979 F982 Y985 E986 T987 S988 A989 K990 S991 G992 G993 F994 T995 A996 S997 R998 F999 L1000 T1001 G1002 I1003 A1004 P1005 Q1006 E1007 Y1008 Y1009 F1010 H1011 C1012 R1016 E1017 G1018 L1019 I1020 D1021 T1022
ALA VAL LYS THR SER ARG SER G1030 Q1033 K1038 H1039 L1040 E1041 G1042 L1043 C1044 V1045 Q1046 H1049 T1050 V1051 R1052 D1053 S1054 D1065 G1056 S1057 I1058 V1059 Q1060 F1061 H1062 Y1063 G1064 E1065 D1066 S1067 L1068 D1069 V1070 T1071 K1072 Q1073 K1074 H1075 L1076 T1077 E1080 F1081 S1082 A1083 K1084 N1085 Y1086 K1087 S1088
L1089 I1090 Q1091 K1092 V1096 K1096 S1097 A1101 V1102 D1103 S1104 E1105 T1106 Y1110 A1111 K1112 K1113 A1114 L1115 K1116 K1117 P1118 Y1119 K1120 Y1121 D1122 P1123 V1124 L1125 D1126 K1127 Y1128 P1129 P1130 Y1133 L1134 G1135 S1136 V1137 S1138 E1139 K1140 F1141 Q1142 R1143 A1144 V1145 D1146 E1147 Y1148 K1151 N1152 P1153 D1154 K1155
L1156 I1157 A1158 SER LYS LYS E1162 S1163 K1164 L1165 D1166 D1167 S1168 L1169 L1170 N1171 E1172 S1173 K1174 F1175 L1178 R1182 Y1183 L1187 V1188 D1189 P1190 G1191 E1192 S1193 V1194 Q1200 S1201 I1202 G1203 E1204 P1205 S1206 T1207 Q1208 M1209 T1210 L1211 N1212 T1213 PHE HIS PHE ALA GLY PHE GLY ALA LYS N1223 V1224
T1225 L1226 G1227 I1228 P1229 R1230 L1231 R1232 E1233 I1234 I1235 M1236 T1237 A1238 S1239 A1240 N1241 I1242 Q1243 T1244 P1245 T1246 M1247 T1248 L1249 R1250 L1251 N1252 D1253 G1254 V1255 S1256 D1257 K1258 R1259 A1260 S1261 A1262 F1263 C1264 K1265 E1266 V1267 N1268 K1269 L1270 V1271 L1272 S1273 E1274 V1275 V1276 R1277 Q1278 V1279 R1280 V1281 T1282 E1283 K1284
ILE SER GLY GLN GLY SER ASP GLU GLN SER LYS T1296 Y1297 A1298 I1299 R1300 L1301 D1302 L1303 Y1304 S1305 R1306 D1307 E1308 Y1309 Q1310 D1311 E1312 Y1313 G1314 V1315 L1316 Q1317 E1318 E1319 I1320 E1321 S1322 T1323 F1324 S1325 F1328 L1329 N1333 R1334 I1335 I1336 Y1339 L1340 A1341 K1342 S1343 K1344 Q1345 ARG LYS SER
GLY GLY LYS ASP ASP THR VAL PRO GLU VAL GLY GLN ALA LEU LYS PRO LEU GLU ASP ILE ASP GLU ALA PRO ILE GLU GLY ARG ALA GLN GLU ALA LEU GLU ASP GLU ASP ASN ASP ALA THR ASN GLU LYS MET VAL SER ARG SER LYS GLN HIS ALA SER TYR GLU GLY GLY PRO ASP GLU
ALA ASP LYS VAL ALA LEU ARG GLN LEU LYS GLY SER ASN LYS VAL GLU ASP VAL ASN MET ASP GLU GLU ASP GLU GLY PHE LYS SER ASP GLU SER VAL SER ASP PHE LYS GLU ARG LYS LEU LEU GLU LYS GLN ASN THR VAL SER LYS GLN HIS ILE SER GLU ARG ARG GLU LEU GLN LEU LYS
THR ALA LYS GLU ILE LEU SER N1476 C1477 K1478 H1479 L1480 D1481 F1482 D1483 Y1484 V1485 N1486 G1487 E1488 T1491 V1492 E1493 L1494 V1495 N1499 T1500 E1501 K1502 L1503 L1504 M1505 V1506 S1507 L1508 V1509 E1510 K1511 S1514 E1515 I1518 H1519 E1520 I1521 P1522 G1523 I1524 T1525 R1526 C1527 F1528 S1529 K1530 P1531 PRO ASP



• Molecule 1: DNA-directed RNA polymerase I subunit rpa1

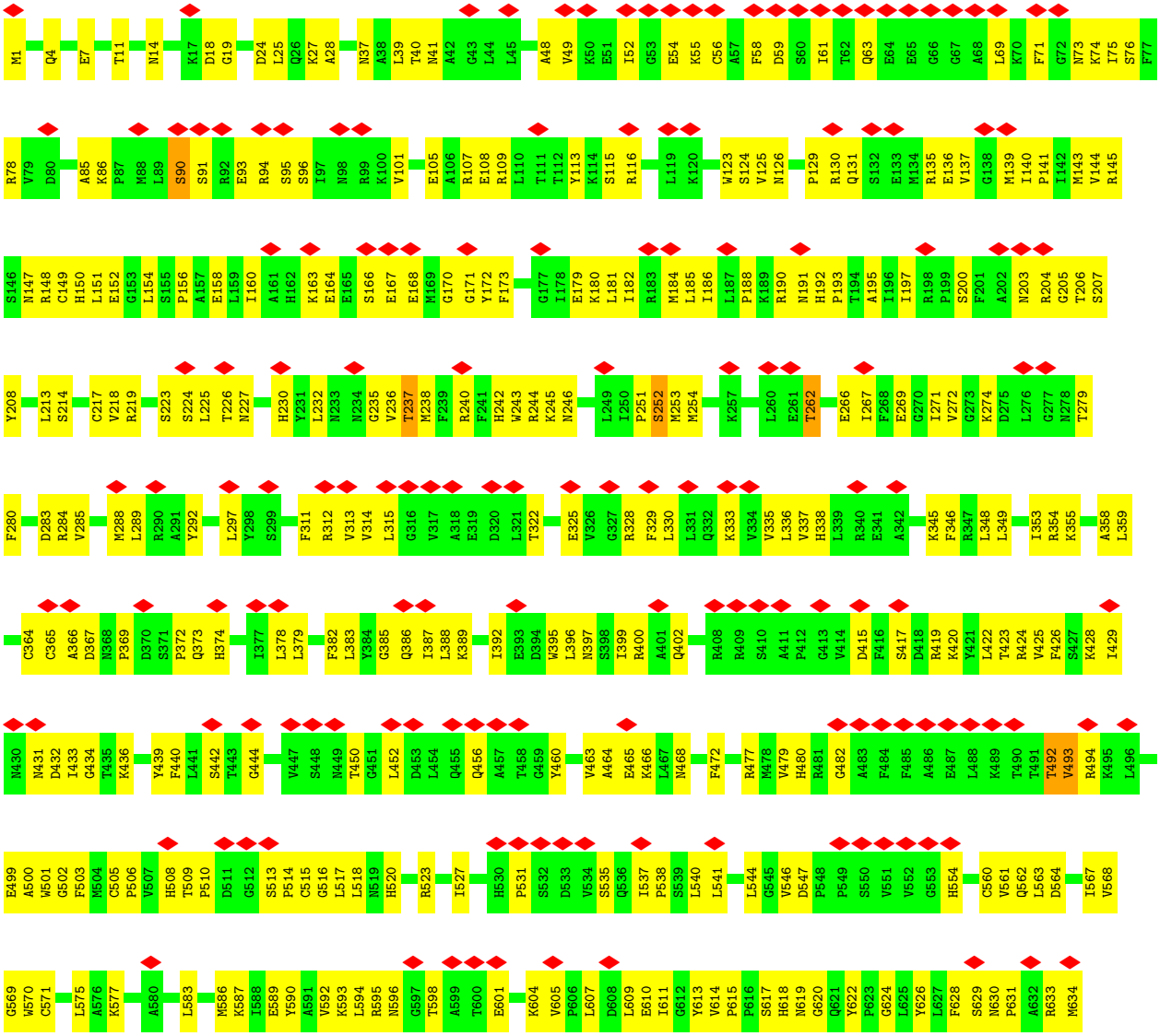


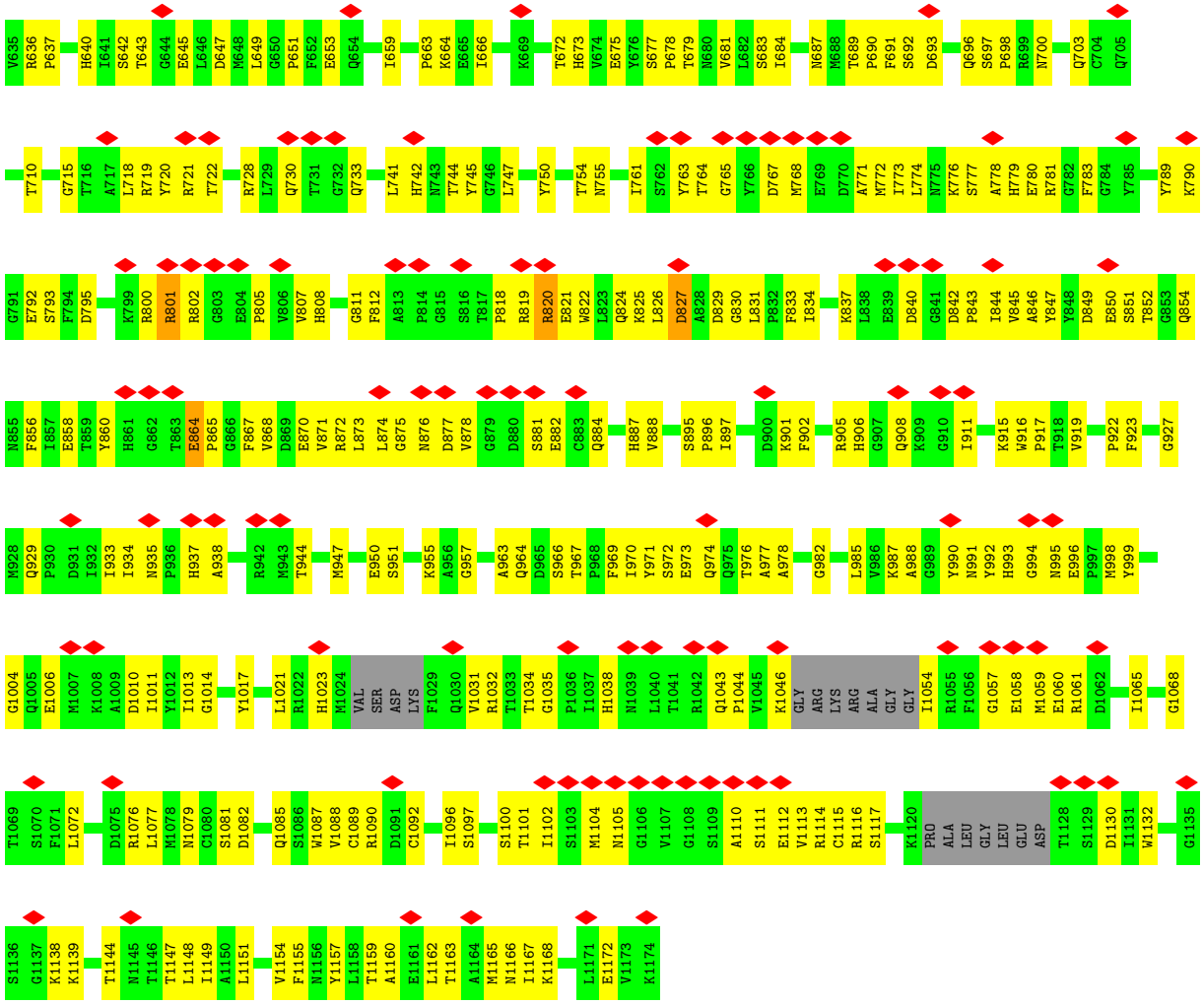

S579 P580 Y581 S582 Y583 S584 R585 N590 K591 K592 R595 H596 V597 R598 N599 G600 D601 M602 L603 I604 L605 N606 R607 Q608 P609 T610 L611 H612 K613 P614 S615 M616 M617 A618 H619 K620 A621 R622 G626 E627 K628 T629 I630 R631 M632 H633 Y634 A635 N636 C637 N638 S639 Y640 N641 A642 D643 F644
D645 G646 D647 E648 M649 H652 F653 T657 N658 A659 R660 S661 I666 A667 N668 T669 D670 S671 Q672 Y673 L674 V675 P676 T677 S678 G679 D680 P681 L682 R683 G684 L685 I686 Q687 D688 H689 W695 L696 T697 D700 T701 T704 R705 Q709 Q710 L711 L712 A715 L716 K717 P718 D719
E720 T721 G722 M723 Y724 G725 R726 L730 P731 P732 A733 I734 Q735 R736 I739 Y740 W741 T742 G743 K744 Q745 I746 S749 N753 R759 P760 G761 L762 N763 L764 K765 S766 K767 A768 K769 Y774 W775 E780 E781 G782 S783 V784 L785 F786 D787 E790 L791 L792 C793 G794 I795 L796
D797 S800 F801 G802 A803 S804 A805 L808 S811 V812 H813 E814 L815 P818 D819 I820 R823 L824 L825 S826 V827 L828 S829 R830 Y835 R839 G840 F841 T842 C843 R844 M845 D846 D847 L848 R849 L850 D851 E852 Q853 G854 D855 N856 W857 R858 L861 L862 F868 G869 L870 E871
A872 A873 V877 G878 L879 S880 T881 D882 S883 P884 I885 A886 L887 L888 N889 A890 N891 L892 E893 E894 V895 Y896 R897 K901 L902 D906 A907 A908 M909 K910 L916 T917 S918 S919 I920 D927 G928 L929 K932 F933 P934 Y935 N936 H937 M938 M941 T942 V943 S944 G948 S949 N950
V951 N952 Q955 I956 S957 C958 L959 L960 G961 Q962 Q963 E964 L965 E966 G967 R968 R969 L972 M973 S978 L979 F982 Y985 E986 T987 S988 A989 K990 S991 G992 G993 F994 I995 A996 S997 R998 F999 L1000 T1001 G1002 I1003 A1004 P1005 Q1006 E1007 Y1008 Y1009 F1010 R1016 E1017 G1018 L1019 I1020 D1021
T1022 ALA VAL LYS THR SER ARG SER G1030 Q1033 K1038 H1039 L1040 E1041 G1042 L1043 C1044 V1045 Q1046 H1049 T1050 V1051 R1052 D1053 S1054 D1055 G1056 S1057 I1058 V1059 Q1060 F1061 H1062 Y1063 G1064 E1065 D1066 S1067 L1068 D1069 V1070 T1071 K1072 Q1073 K1074 H1075 L1076 T1077 E1080 F1081 S1082 A1083 K1084 N1085 Y1086 K1087
S1088 L1089 I1090 Q1091 K1092 V1095 K1096 L1099 S1100 A1101 V1102 D1103 S1104 Y1110 A1111 K1112 K1113 A1114 L1115 K1116 K1117 P1118 Y1119 K1120 Y1121 D1122 P1123 V1124 L1125 D1126 K1127 Y1128 P1129 P1130 S1131 R1132 Y1133 L1134 G1135 S1136 V1137 S1138 E1139 K1140 F1141 Q1142 R1143 A1144 V1145 D1146 E1147 Y1148 K1151 N1152 P1153 D1154
K1155 L1156 I1157 A1158 SER LYS LYS E1162 S1163 K1164 L1165 D1166 D1167 S1168 L1169 L1170 N1171 E1172 S1173 K1174 F1175 L1178 M1179 R1182 Y1183 V1188 D1189 P1190 G1191 E1192 S1193 V1194 Q1200 S1201 I1202 G1203 E1204 P1205 S1206 T1207 Q1208 M1209 T1210 L1211 N1212 T1213 PHE HIS PHE ALA GLY PHE GLY ALA LYS N1223
V1224 T1225 L1226 G1227 I1228 P1229 R1230 L1231 R1232 E1233 I1234 I1235 M1236 T1237 A1238 S1239 A1240 N1241 I1242 Q1243 T1244 P1245 T1246 M1247 T1248 L1249 R1250 L1251 N1252 D1253 G1254 V1255 S1256 D1257 K1258 R1259 A1260 S1261 A1262 F1263 C1264 K1265 E1266 V1267 N1268 K1269 L1270 V1271 L1272 S1273 E1274 V1275 V1276 R1277 Q1278 V1279 R1280 V1281 T1282 E1283
K1284 ILE SER GLY GLN GLY SER ASP GLU GLN SER LYS T1296 Y1297 A1298 I1299 R1300 L1301 D1302 S1305 R1306 D1307 E1308 Y1309 Q1310 D1311 E1312 Y1313 G1314 V1315 L1316 Q1317 E1318 E1319 I1320 E1321 S1322 T1323 F1324 S1325 F1328 L1329 N1333 R1334 I1335 I1336 Y1339 L1340 A1341 K1342 S1343 K1344 Q1345 ARG LYS SER
GLY GLY LYS ASP ASP THR VAL PRO GLU VAL GLY GLN ALA LEU LYS PRO LEU GLU ASP ILE ASP GLU ALA PRO ILE GLU GLY ARG ALA GLN GLU ALA LEU GLU ASP GLU ASP ASN ASP ALA THR ASN GLU LYS MET VAL SER ARG SER LYS GLN HIS ALA SER TYR GLU GLY PRO ASP GLU
ALA ASP LYS VAL ALA LEU ARG GLN LEU LYS GLY SER ASN LYS VAL GLU ASP VAL ASN MET ASP GLU GLU GLU ASP GLU GLY PHE LYS SER ASP GLU SER VAL SER ASP PHE LYS GLU ARG LYS LEU LEU GLU LYS GLN ASN THR VAL SER ILE SER GLU ARG GLU LEU GLN LEU LYS
THR ALA LYS GLU ILE LEU SER N1476 C1477 K1478 H1479 L1480 D1481 F1482 D1483 Y1484 V1485 N1486 G1487 E1488 T1491 V1492 E1493 L1494 V1495 I1498 N1499 T1500 E1501 K1502 L1503 L1504 M1505 V1506 S1507 L1508 V1509 E1510 K1511 S1514 E1515 E1520 I1521 P1522 G1523 I1524 T1525 R1526 C1527 F1528 S1529 K1530 P1531 PRO ASP SER



• Molecule 2: Probable DNA-directed RNA polymerase I subunit RPA2

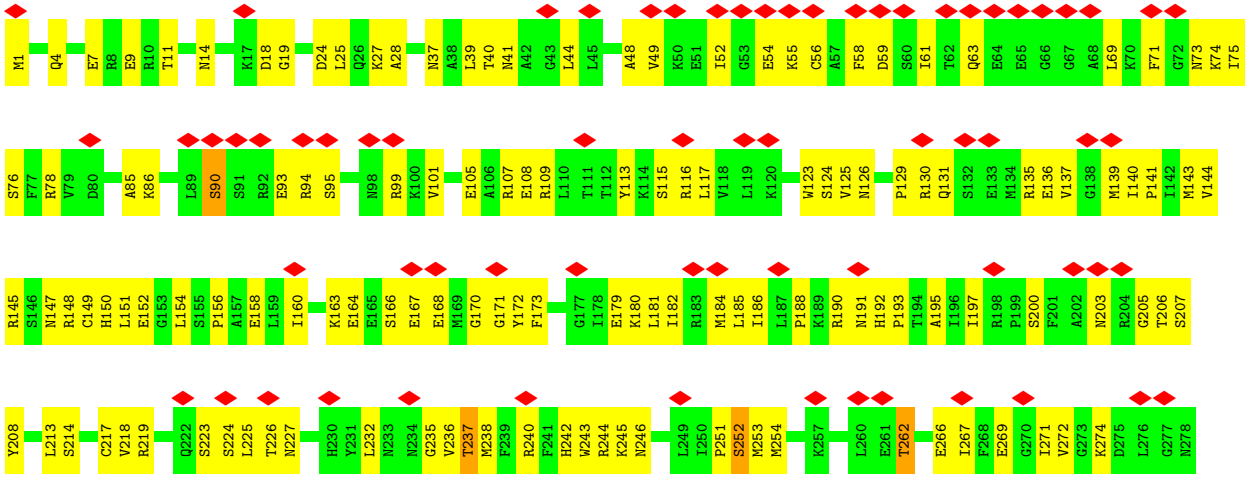
Chain B:

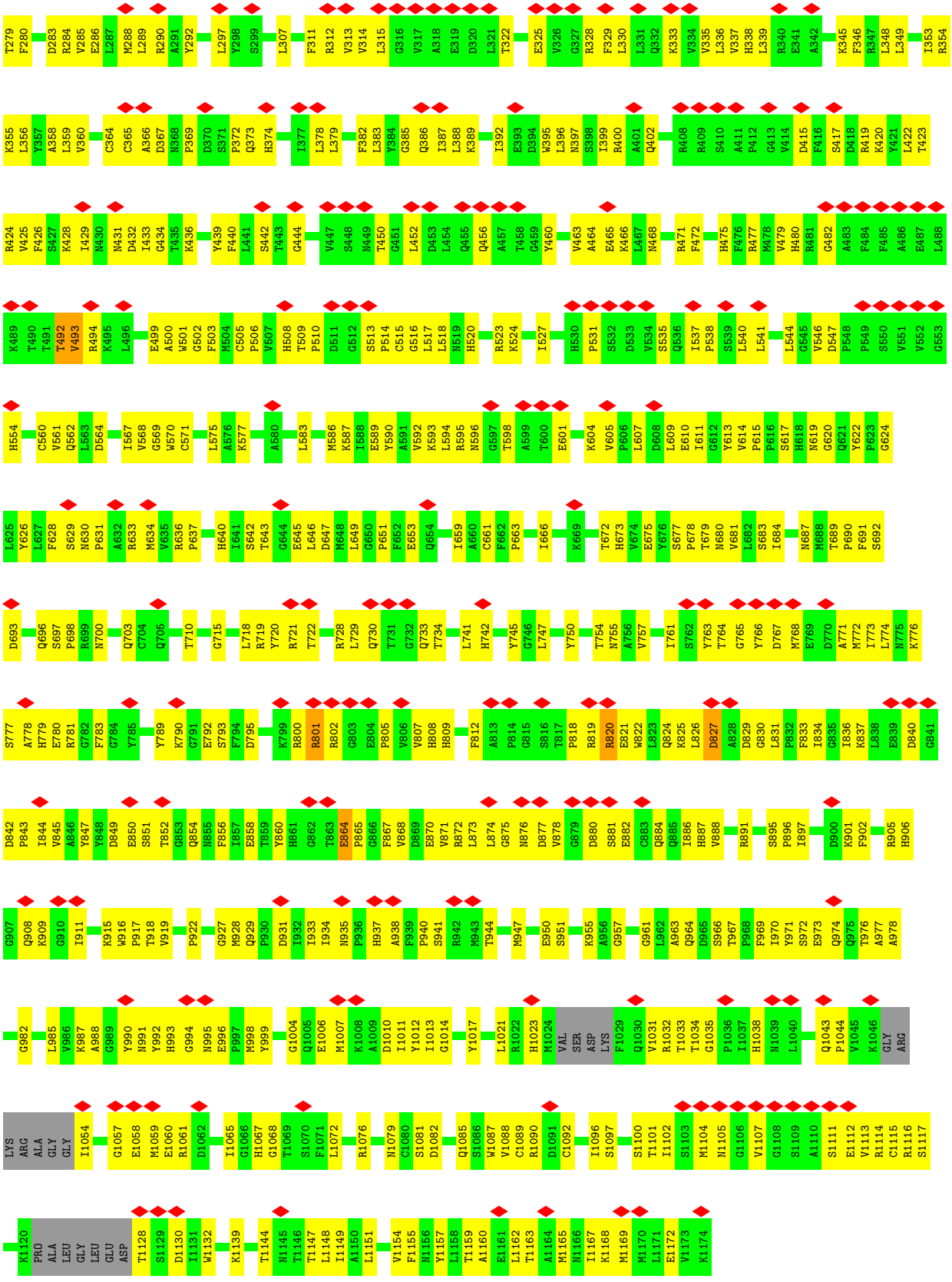




• Molecule 2: Probable DNA-directed RNA polymerase I subunit RPA2

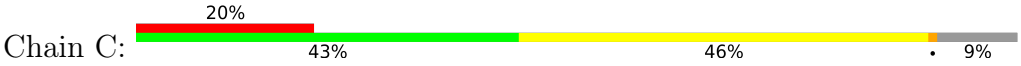
Chain N:

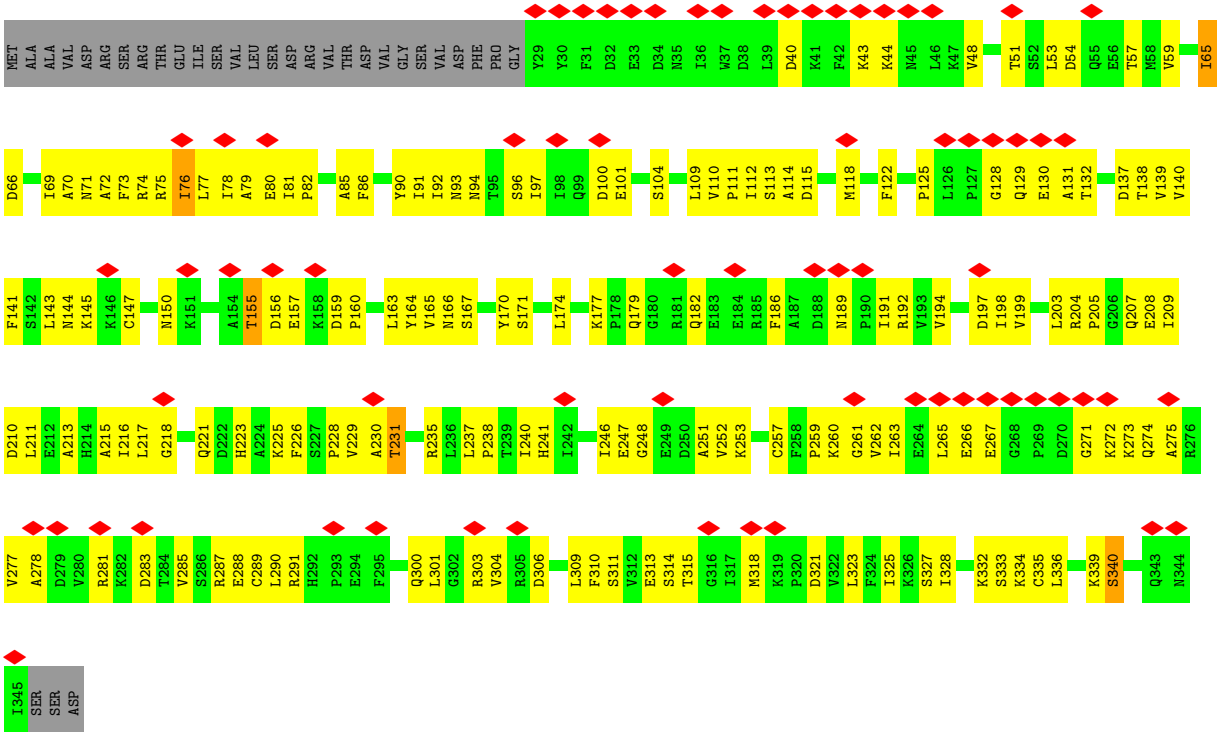




• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1

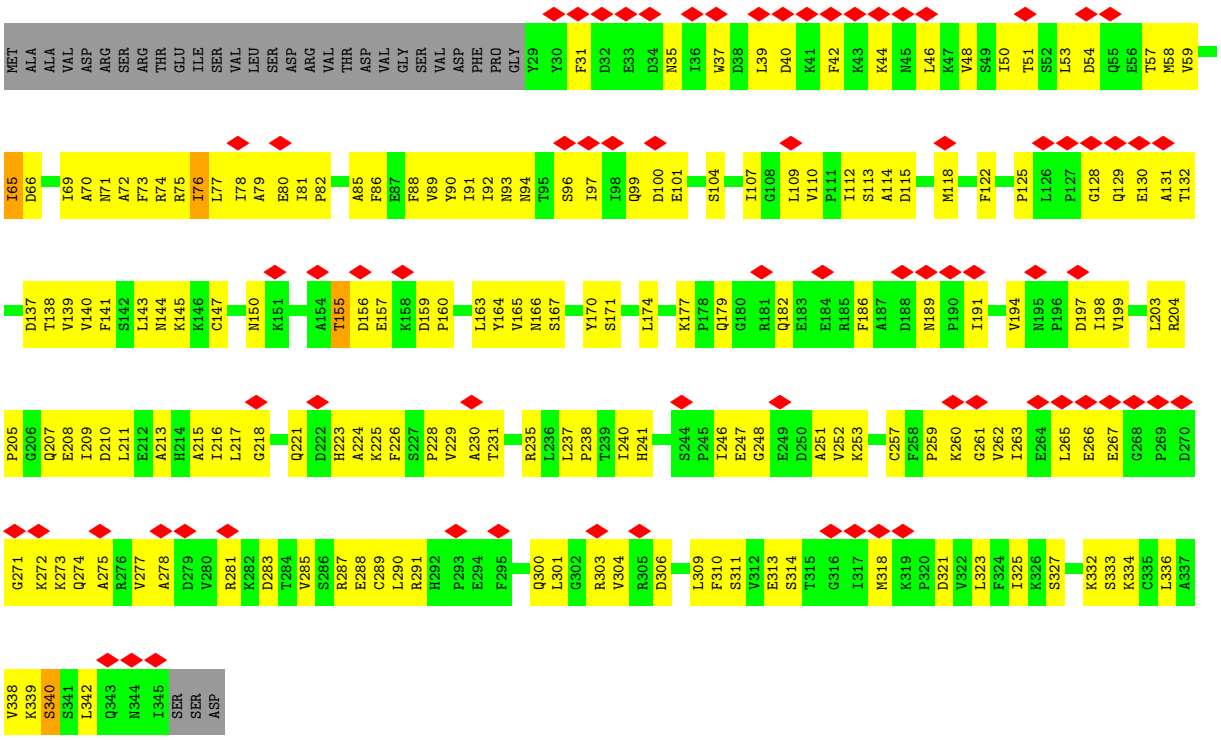
Chain C:





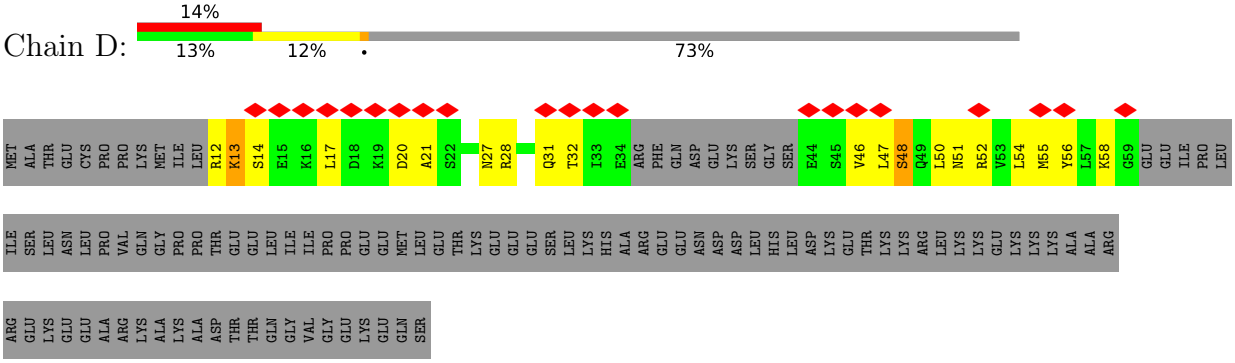
• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1

Chain O:



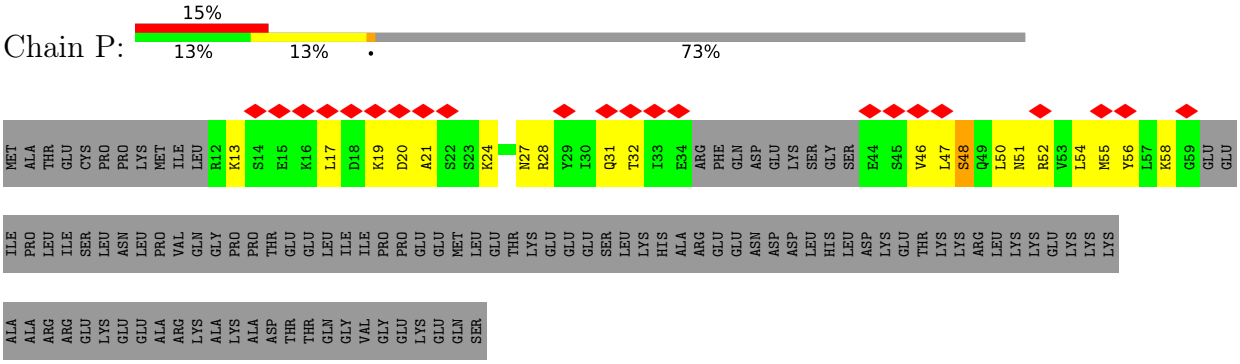
• Molecule 4: DNA-directed RNA polymerase I subunit rpa14

Chain D:



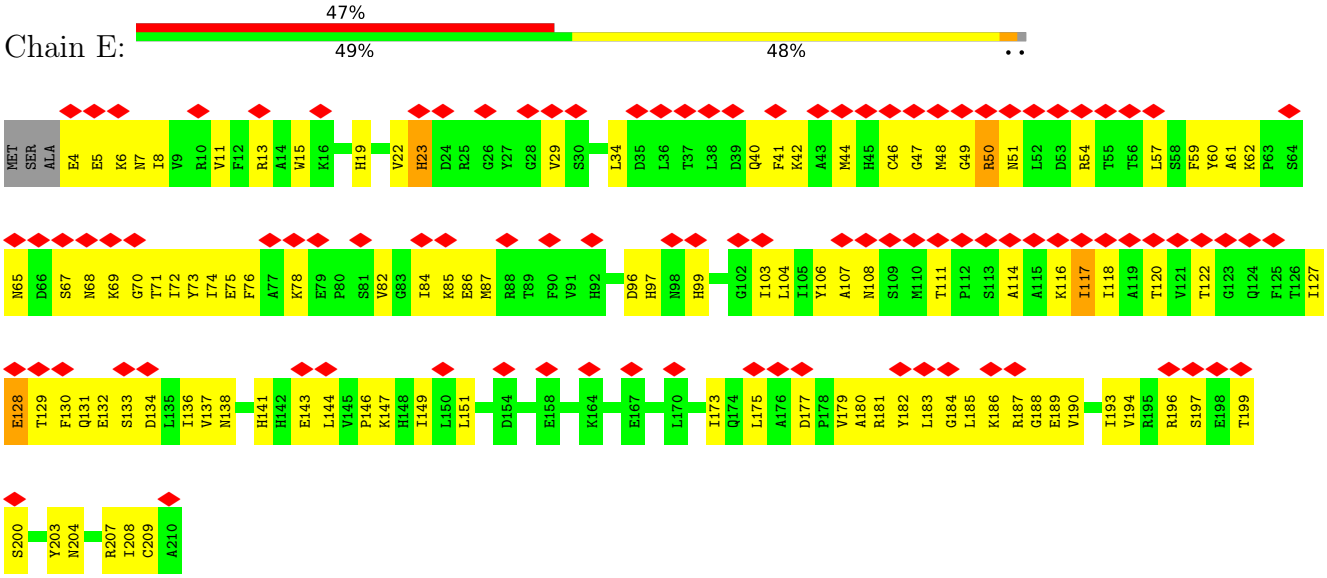
• Molecule 4: DNA-directed RNA polymerase I subunit rpa14

Chain P:



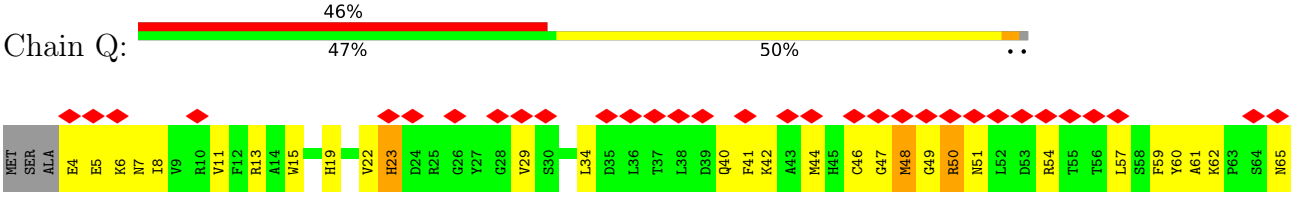
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

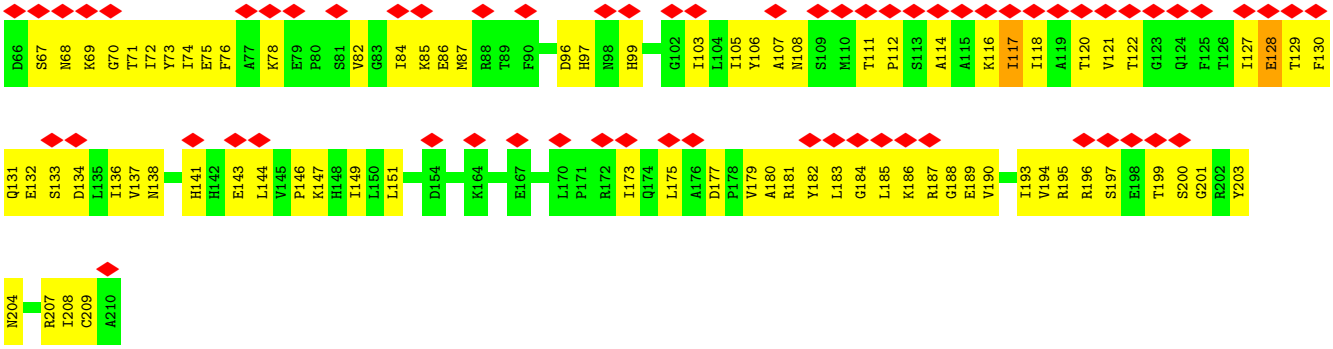
Chain E:



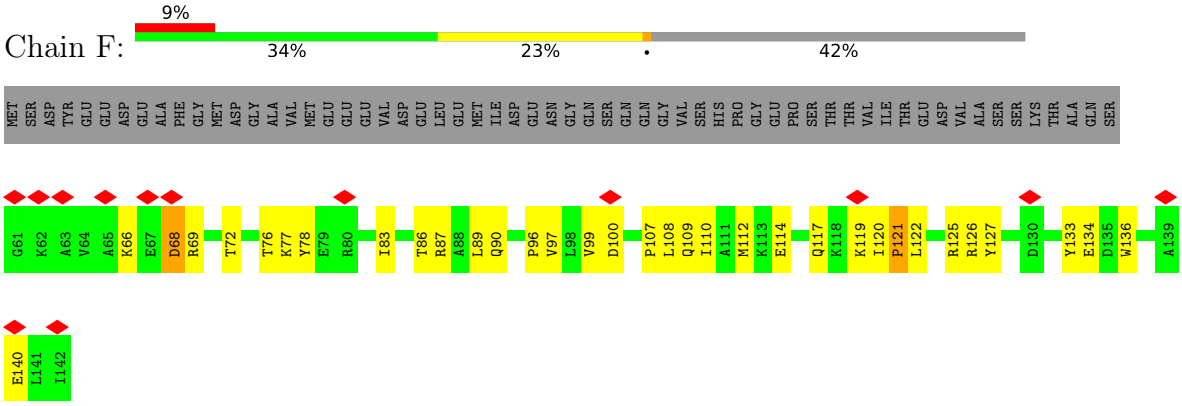
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain Q:

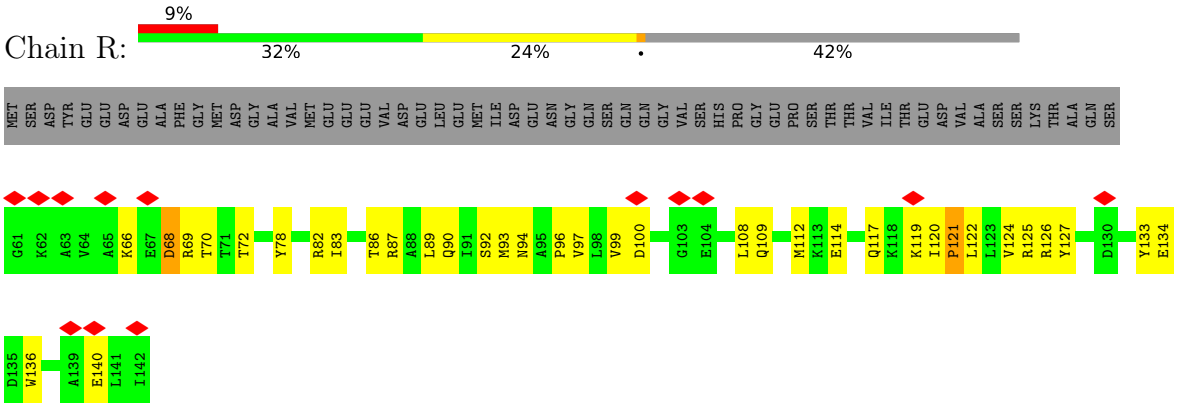




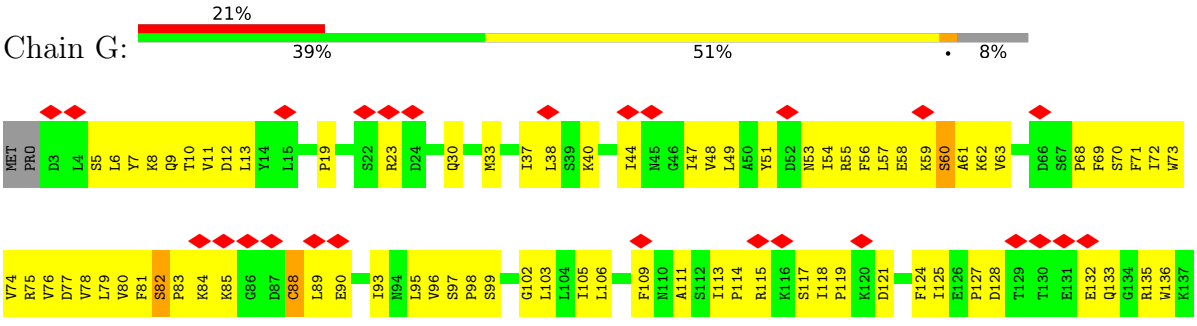
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

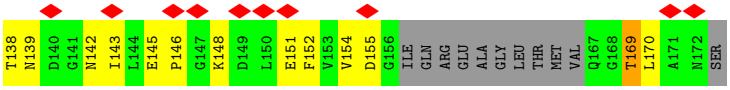


• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

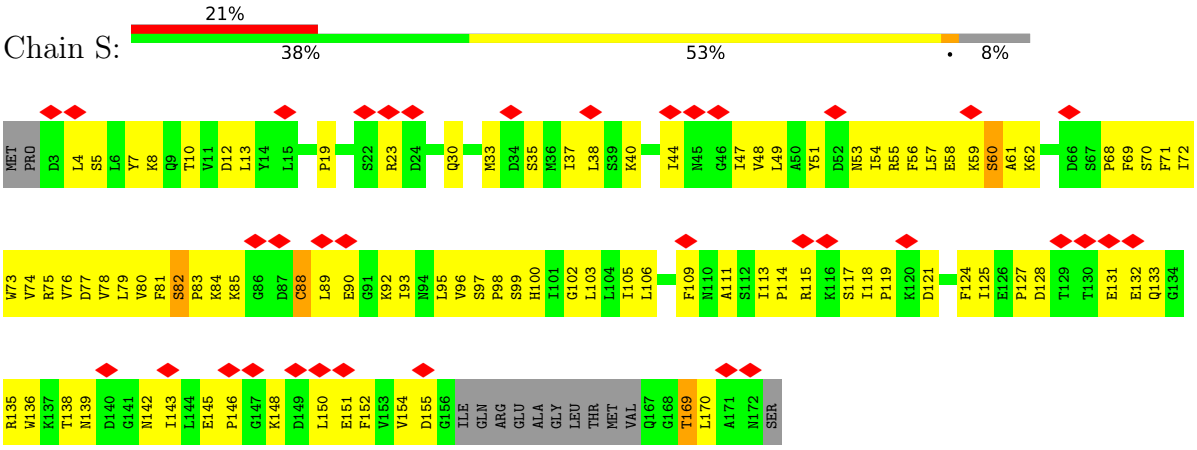


• Molecule 7: DNA-directed RNA polymerase I subunit rpa43

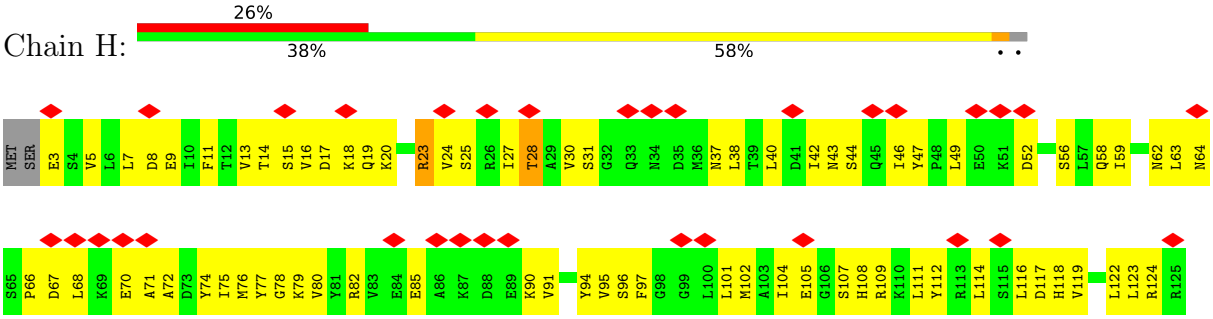




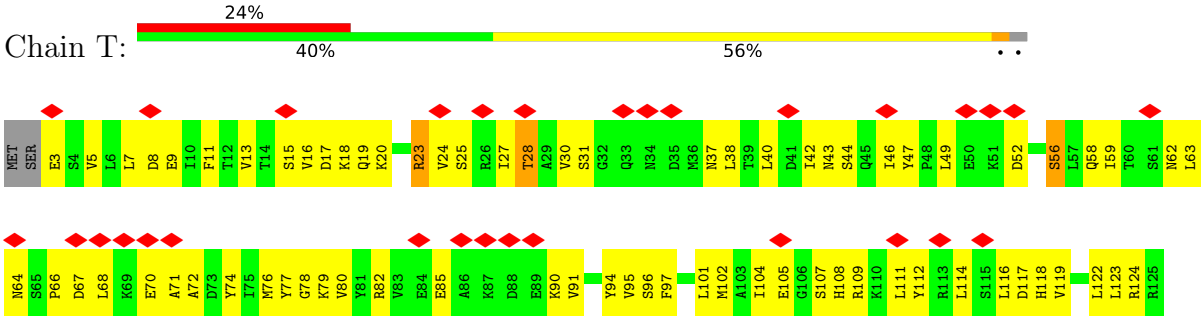
• Molecule 7: DNA-directed RNA polymerase I subunit rpa43



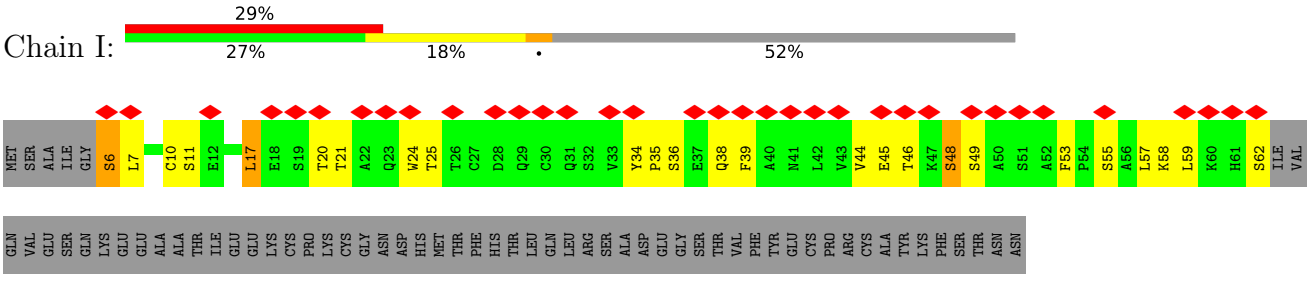
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

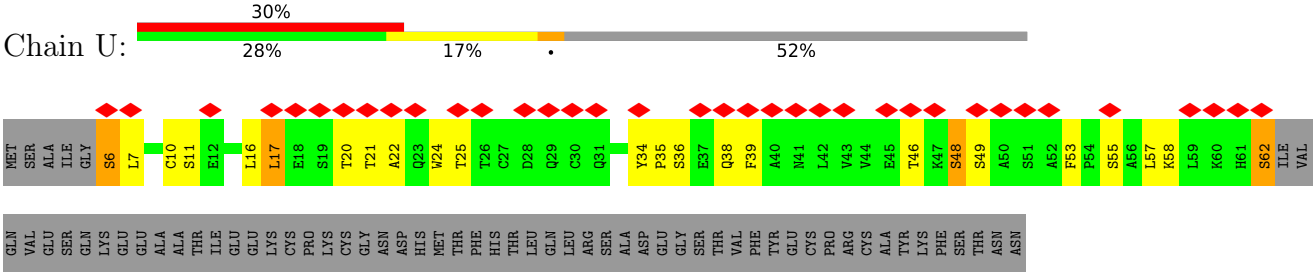


• Molecule 9: DNA-directed RNA polymerase I subunit RPA12



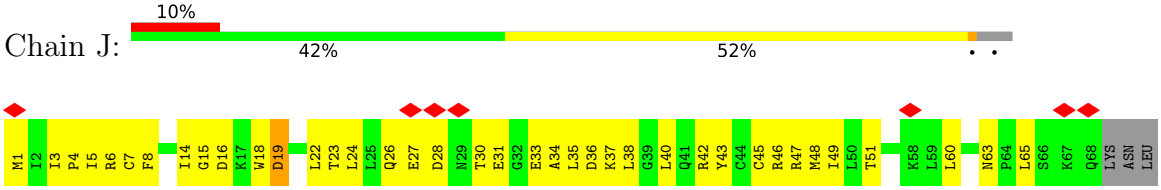
• Molecule 9: DNA-directed RNA polymerase I subunit RPA12

Chain U:



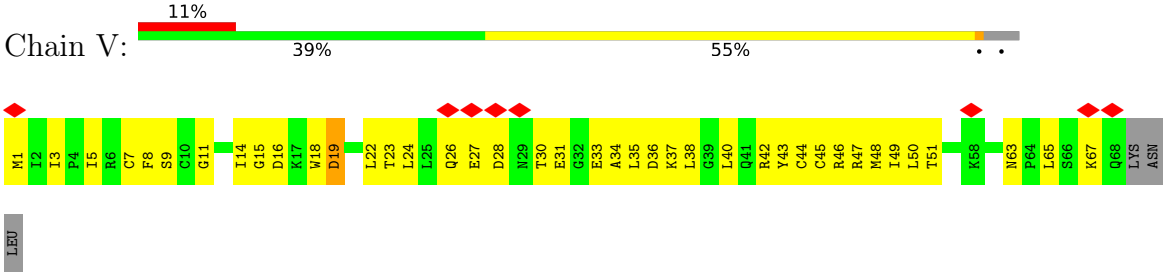
• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:



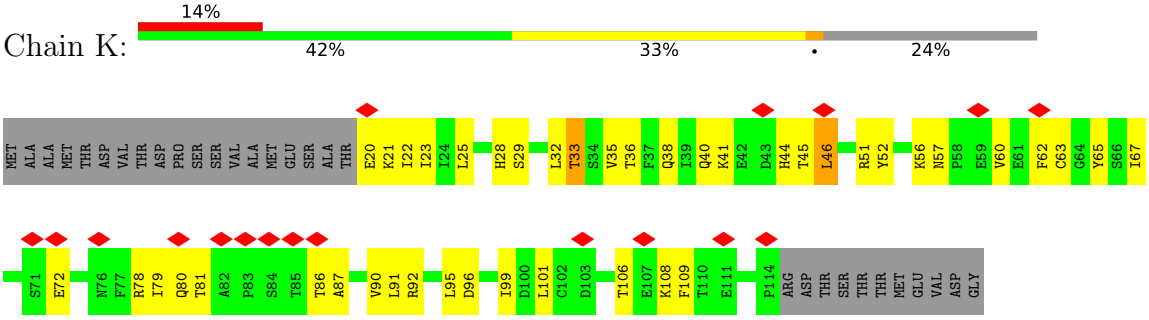
• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain V:



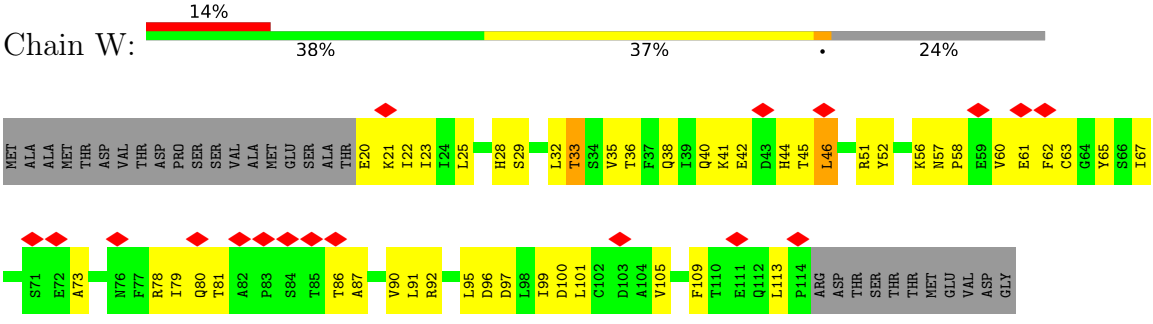
• Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2

Chain K:



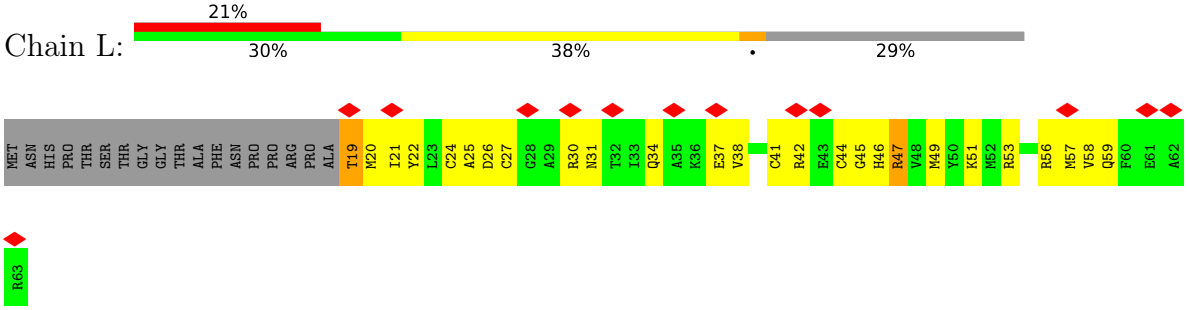
• Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2

Chain W:



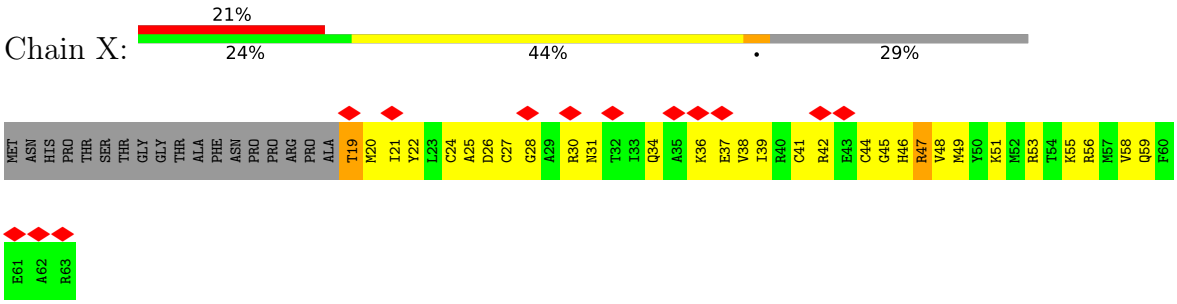
• Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L:



• Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain X:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	17102	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	86.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.099	Depositor
Minimum map value	-0.045	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.033	Depositor
Map size (Å)	382.86002, 382.86002, 382.86002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0635, 1.0635, 1.0635	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.37	0/11194	0.51	1/15122 (0.0%)
1	M	0.37	0/11194	0.51	1/15122 (0.0%)
2	B	0.40	0/9332	0.53	1/12615 (0.0%)
2	N	0.40	0/9332	0.53	1/12615 (0.0%)
3	C	0.37	0/2588	0.49	0/3505
3	O	0.37	0/2588	0.49	0/3505
4	D	0.31	0/323	0.50	0/427
4	P	0.31	0/323	0.50	0/427
5	E	0.35	0/1695	0.54	0/2287
5	Q	0.35	0/1695	0.54	0/2287
6	F	0.43	0/660	0.51	0/893
6	R	0.43	0/660	0.51	0/893
7	G	0.37	0/1295	0.52	0/1755
7	S	0.37	0/1295	0.52	0/1755
8	H	0.36	0/1004	0.58	0/1355
8	T	0.36	0/1004	0.59	0/1355
9	I	0.35	0/439	0.48	0/596
9	U	0.34	0/439	0.48	0/596
10	J	0.40	0/558	0.55	0/751
10	V	0.40	0/558	0.55	0/751
11	K	0.38	0/759	0.47	0/1030
11	W	0.38	0/759	0.47	0/1030
12	L	0.44	0/371	0.54	0/491
12	X	0.44	0/371	0.54	0/491
All	All	0.38	0/60436	0.52	4/81654 (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	4
1	M	0	4
2	B	0	1
2	N	0	1
5	E	0	4
5	Q	0	4
7	G	0	1
7	S	0	1
All	All	0	20

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1164	LYS	CD-CE-NZ	5.78	124.99	111.70
1	M	1164	LYS	CD-CE-NZ	5.78	124.99	111.70
2	N	934	ILE	C-N-CA	-5.51	107.93	121.70
2	B	934	ILE	C-N-CA	-5.49	107.97	121.70

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1656	ASP	Peptide
1	A	246	ILE	Peptide
1	A	84	ILE	Peptide
1	A	896	TYR	Peptide
2	B	90	SER	Peptide
5	E	128	GLU	Peptide
5	E	23	HIS	Peptide
5	E	50	ARG	Peptide
5	E	68	ASN	Peptide
7	G	60	SER	Peptide
1	M	1656	ASP	Peptide
1	M	246	ILE	Peptide
1	M	84	ILE	Peptide
1	M	896	TYR	Peptide
2	N	90	SER	Peptide
5	Q	128	GLU	Peptide
5	Q	23	HIS	Peptide
5	Q	50	ARG	Peptide
5	Q	68	ASN	Peptide

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Mol	Chain	Res	Type	Group
7	S	60	SER	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	10976	0	10980	628	0
1	M	10976	0	10980	641	0
2	B	9127	0	9092	497	0
2	N	9127	0	9092	546	0
3	C	2533	0	2540	152	0
3	O	2533	0	2540	171	0
4	D	322	0	338	21	0
4	P	322	0	338	18	0
5	E	1663	0	1684	78	0
5	Q	1663	0	1684	82	0
6	F	650	0	674	34	0
6	R	650	0	674	36	0
7	G	1267	0	1278	93	0
7	S	1267	0	1278	100	0
8	H	990	0	1001	65	0
8	T	990	0	1001	63	0
9	I	431	0	410	17	0
9	U	431	0	410	21	0
10	J	550	0	564	37	0
10	V	550	0	564	39	0
11	K	745	0	745	41	0
11	W	745	0	745	52	0
12	L	368	0	377	26	0
12	X	368	0	377	49	0
13	A	2	0	0	0	0
13	B	1	0	0	0	0
13	I	1	0	0	0	0
13	J	1	0	0	0	0
13	L	1	0	0	0	0
13	M	2	0	0	0	0
13	N	1	0	0	0	0
13	U	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	V	1	0	0	0	0
13	X	1	0	0	0	0
All	All	59256	0	59366	3163	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 27.

All (3163) 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)
2:N:696:GLN:HG2	2:N:698:PRO:HD2	1.45	0.98
2:B:696:GLN:HG2	2:B:698:PRO:HD2	1.45	0.96
1:A:735:GLN:HE22	8:H:77:TYR:HB2	1.30	0.95
1:A:1279:VAL:O	9:I:48:SER:OG	1.86	0.94
8:H:17:ASP:HA	8:H:18:LYS:HB2	1.51	0.92
1:M:774:TYR:O	8:T:20:LYS:NZ	2.02	0.92
2:B:1089:CYS:HB3	2:B:1092:CYS:SG	2.11	0.91
1:M:103:CYS:SG	1:M:106:CYS:HB3	2.11	0.90
1:A:103:CYS:SG	1:A:106:CYS:HB3	2.11	0.90
2:N:1089:CYS:HB3	2:N:1092:CYS:SG	2.11	0.90
8:T:17:ASP:HA	8:T:18:LYS:HB2	1.51	0.89
1:A:598:ARG:N	1:A:601:ASP:OD2	2.06	0.89
1:M:598:ARG:N	1:M:601:ASP:OD2	2.06	0.88
10:J:5:ILE:HG22	10:J:15:GLY:HA3	1.56	0.88
1:A:1306:ARG:HH21	1:A:1317:GLN:HG2	1.39	0.87
11:K:40:GLN:HG3	11:K:41:LYS:HG2	1.57	0.87
2:N:136:GLU:O	2:N:431:ASN:ND2	2.08	0.86
7:G:93:ILE:HD11	7:G:145:GLU:HA	1.57	0.86
1:M:1306:ARG:HH21	1:M:1317:GLN:HG2	1.40	0.86
2:N:967:THR:HB	2:N:970:ILE:HD11	1.58	0.86
2:B:136:GLU:O	2:B:431:ASN:ND2	2.08	0.85
10:V:5:ILE:HG22	10:V:15:GLY:HA3	1.56	0.85
1:A:1553:TRP:HB3	5:E:136:ILE:HD11	1.57	0.85
10:J:23:THR:OG1	10:J:27:GLU:OE1	1.95	0.85
2:B:967:THR:HB	2:B:970:ILE:HD11	1.58	0.85
1:A:1567:ASN:HB2	1:A:1569:ILE:HG23	1.57	0.85
7:S:93:ILE:HD11	7:S:145:GLU:HA	1.57	0.85
11:W:40:GLN:HG3	11:W:41:LYS:HG2	1.57	0.85
2:N:480:HIS:HD2	2:N:518:LEU:HB3	1.42	0.84
1:M:1567:ASN:HB2	1:M:1569:ILE:HG23	1.57	0.84
12:X:45:GLY:O	12:X:47:ARG:NH1	2.10	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:V:23:THR:OG1	10:V:27:GLU:OE1	1.95	0.83
3:O:93:ASN:HB2	12:X:55:LYS:HG2	1.60	0.83
1:A:1003:ILE:HD11	1:A:1008:TYR:HD2	1.42	0.83
1:M:1003:ILE:HD11	1:M:1008:TYR:HD2	1.42	0.83
2:B:480:HIS:HD2	2:B:518:LEU:HB3	1.42	0.83
2:B:1089:CYS:CB	2:B:1092:CYS:SG	2.67	0.83
2:N:1089:CYS:CB	2:N:1092:CYS:SG	2.67	0.83
12:L:45:GLY:O	12:L:47:ARG:NH1	2.10	0.82
2:B:630:ASN:O	2:B:633:ARG:NH1	2.13	0.82
2:N:630:ASN:O	2:N:633:ARG:NH1	2.13	0.82
12:L:27:CYS:HB3	12:L:44:CYS:SG	2.20	0.82
1:A:113:LYS:HG3	1:A:179:MET:HE1	1.62	0.82
12:X:27:CYS:HB3	12:X:44:CYS:SG	2.20	0.82
1:A:88:HIS:N	1:A:360:PHE:O	2.13	0.81
1:M:956:ILE:HA	1:M:999:PHE:HB2	1.62	0.81
1:M:1062:HIS:HB3	1:M:1066:ASP:HB3	1.62	0.81
2:B:927:GLY:O	2:B:929:GLN:NE2	2.13	0.81
1:A:956:ILE:HA	1:A:999:PHE:HB2	1.62	0.81
2:B:944:THR:HG22	2:B:947:MET:HB2	1.62	0.81
2:N:927:GLY:O	2:N:929:GLN:NE2	2.13	0.81
1:A:1062:HIS:HB3	1:A:1066:ASP:HB3	1.63	0.80
1:M:390:LEU:HD23	1:M:444:LEU:HA	1.62	0.80
1:M:113:LYS:HG3	1:M:179:MET:HE1	1.63	0.80
1:A:390:LEU:HD23	1:A:444:LEU:HA	1.62	0.80
2:N:730:GLN:O	10:V:1:MET:N	2.15	0.79
3:O:91:ILE:HD11	12:X:58:VAL:HB	1.63	0.79
1:M:88:HIS:N	1:M:360:PHE:O	2.13	0.79
2:N:944:THR:HG22	2:N:947:MET:HB2	1.62	0.79
2:N:999:TYR:HA	2:N:1006:GLU:HA	1.65	0.79
1:M:735:GLN:HE22	8:T:77:TYR:HB2	1.48	0.79
5:Q:7:ASN:HD21	5:Q:54:ARG:HH22	1.31	0.79
7:G:96:VAL:HG12	7:G:124:PHE:HE1	1.48	0.79
1:M:717:LYS:NZ	11:W:67:ILE:O	2.13	0.79
2:B:93:GLU:OE2	7:S:100:HIS:N	2.16	0.78
4:D:12:ARG:HA	7:G:11:VAL:HG23	1.66	0.78
1:A:1246:THR:H	1:A:1566:THR:HB	1.48	0.78
2:N:456:GLN:O	2:N:460:TYR:OH	2.01	0.78
1:A:565:LEU:HA	1:A:568:GLN:HE21	1.48	0.78
1:A:814:GLU:OE1	1:A:1072:LYS:NZ	2.16	0.78
2:B:999:TYR:HA	2:B:1006:GLU:HA	1.65	0.78
1:M:814:GLU:OE1	1:M:1072:LYS:NZ	2.16	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:814:GLU:O	1:A:1092:LYS:NZ	2.16	0.78
1:A:858:ARG:NH1	1:A:958:CYS:O	2.16	0.78
2:B:456:GLN:O	2:B:460:TYR:OH	2.01	0.78
1:M:1171:ASN:HB2	1:M:1174:LYS:HB2	1.66	0.78
1:M:1068:LEU:HD13	1:M:1188:VAL:HA	1.65	0.77
1:M:106:CYS:HA	1:M:231:CYS:HB2	1.66	0.77
1:M:565:LEU:HA	1:M:568:GLN:HE21	1.48	0.77
1:M:1060:GLN:NE2	1:M:1610:ASP:OD2	2.16	0.77
2:N:219:ARG:NH1	2:N:223:SER:O	2.17	0.77
2:B:219:ARG:NH1	2:B:223:SER:O	2.17	0.77
1:A:604:ILE:HB	1:A:652:HIS:HB2	1.67	0.77
7:S:96:VAL:HG12	7:S:124:PHE:HE1	1.48	0.77
12:X:19:THR:HB	12:X:34:GLN:HG2	1.66	0.77
1:A:1171:ASN:HB2	1:A:1174:LYS:HB2	1.66	0.77
1:A:1307:ASP:OD1	1:A:1307:ASP:N	2.14	0.77
1:M:1246:THR:H	1:M:1566:THR:HB	1.48	0.77
1:M:1307:ASP:N	1:M:1307:ASP:OD1	2.14	0.77
1:A:1068:LEU:HD13	1:A:1188:VAL:HA	1.65	0.77
5:E:7:ASN:HD21	5:E:54:ARG:HH22	1.31	0.77
1:M:814:GLU:O	1:M:1092:LYS:NZ	2.16	0.76
1:M:858:ARG:NH1	1:M:958:CYS:O	2.16	0.76
2:N:235:GLY:HA2	2:N:284:ARG:HH11	1.50	0.76
12:L:19:THR:HB	12:L:34:GLN:HG2	1.66	0.76
1:A:559:ILE:HG12	3:O:130:GLU:HB2	1.68	0.76
1:A:1060:GLN:NE2	1:A:1610:ASP:OD2	2.16	0.76
2:B:235:GLY:HA2	2:B:284:ARG:HH11	1.50	0.76
3:C:75:ARG:HH12	11:K:44:HIS:HB2	1.51	0.76
2:N:1090:ARG:NH2	2:N:1147:THR:OG1	2.18	0.76
3:O:94:ASN:ND2	3:O:100:ASP:OD1	2.19	0.76
7:S:49:LEU:HB2	7:S:79:LEU:HB3	1.68	0.76
2:B:123:TRP:HE1	2:B:422:LEU:HG	1.51	0.76
2:B:849:ASP:OD2	2:B:852:THR:N	2.19	0.76
1:M:1156:LEU:HD21	1:M:1172:GLU:HA	1.68	0.76
2:N:292:TYR:OH	2:N:297:LEU:O	2.03	0.76
1:A:895:VAL:HG13	1:A:901:LYS:HB3	1.69	0.75
1:M:604:ILE:HB	1:M:652:HIS:HB2	1.67	0.75
12:X:27:CYS:CB	12:X:44:CYS:SG	2.68	0.75
2:B:140:ILE:HG22	2:B:434:GLY:HA2	1.68	0.75
2:B:292:TYR:OH	2:B:297:LEU:O	2.03	0.75
3:O:155:THR:OG1	3:O:156:ASP:N	2.19	0.75
8:H:63:LEU:HG	8:H:68:LEU:HD12	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:1103:ASP:O	1:M:1134:LEU:N	2.18	0.75
8:T:63:LEU:HG	8:T:68:LEU:HD12	1.67	0.75
1:A:1114:ALA:HA	1:A:1121:TYR:HB3	1.68	0.75
2:N:880:ASP:HA	12:X:38:VAL:HG22	1.69	0.75
1:A:1156:LEU:HD21	1:A:1172:GLU:HA	1.68	0.75
2:N:123:TRP:HE1	2:N:422:LEU:HG	1.51	0.75
12:L:31:ASN:HD21	12:L:42:ARG:H	1.35	0.75
1:M:1114:ALA:HA	1:M:1121:TYR:HB3	1.68	0.75
1:M:1234:ILE:HG23	1:M:1235:ILE:HG12	1.67	0.75
2:N:849:ASP:OD2	2:N:852:THR:N	2.19	0.75
3:O:48:VAL:HG11	11:W:109:PHE:HD1	1.50	0.75
3:C:94:ASN:ND2	3:C:100:ASP:OD1	2.19	0.75
1:M:1479:HIS:HB2	1:M:1493:GLU:HB3	1.67	0.75
3:C:339:LYS:HZ1	11:K:92:ARG:HA	1.52	0.74
1:M:893:GLU:OE2	2:N:617:SER:OG	2.04	0.74
3:C:155:THR:OG1	3:C:156:ASP:N	2.19	0.74
7:G:49:LEU:HB2	7:G:79:LEU:HB3	1.68	0.74
2:N:54:GLU:OE1	2:N:78:ARG:NH2	2.20	0.74
1:A:476:ARG:HG3	2:B:1058:GLU:HG3	1.70	0.74
1:A:1234:ILE:HG23	1:A:1235:ILE:HG12	1.67	0.74
6:F:69:ARG:NH2	6:F:140:GLU:OE2	2.21	0.74
2:N:140:ILE:HG22	2:N:434:GLY:HA2	1.68	0.74
2:N:191:ASN:HD21	2:N:218:VAL:HG12	1.52	0.74
1:A:763:ASN:HA	1:A:787:ASP:HA	1.69	0.74
1:A:1479:HIS:HB2	1:A:1493:GLU:HB3	1.67	0.74
1:M:1281:VAL:O	9:U:46:THR:OG1	2.04	0.74
7:S:118:ILE:HG12	7:S:170:LEU:HD12	1.68	0.74
2:B:54:GLU:OE1	2:B:78:ARG:NH2	2.21	0.74
7:G:128:ASP:O	2:N:116:ARG:NH2	2.17	0.74
7:G:118:ILE:HG12	7:G:170:LEU:HD12	1.68	0.74
1:M:661:SER:HB3	6:R:108:LEU:HD11	1.69	0.74
1:M:763:ASN:HA	1:M:787:ASP:HA	1.69	0.74
3:O:75:ARG:HG2	11:W:45:THR:HB	1.70	0.74
2:B:1090:ARG:NH2	2:B:1147:THR:OG1	2.18	0.74
3:C:71:ASN:OD1	3:C:75:ARG:NH2	2.21	0.74
1:A:1065:GLU:HB3	5:E:200:SER:HB2	1.68	0.73
12:L:25:ALA:HB3	12:L:46:HIS:CE1	2.23	0.73
3:O:71:ASN:OD1	3:O:75:ARG:NH2	2.21	0.73
6:R:69:ARG:NH2	6:R:140:GLU:OE2	2.21	0.73
12:X:31:ASN:HD21	12:X:42:ARG:H	1.35	0.73
1:M:895:VAL:HG13	1:M:901:LYS:HB3	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1569:ILE:HA	1:A:1572:ILE:HG22	1.71	0.73
1:M:498:ILE:HG13	1:M:499:GLU:H	1.52	0.73
2:B:243:TRP:CD1	2:B:244:ARG:HG2	2.24	0.73
12:L:27:CYS:CB	12:L:44:CYS:SG	2.68	0.73
2:N:7:GLU:O	2:N:11:THR:OG1	2.04	0.73
12:X:25:ALA:HB3	12:X:46:HIS:CE1	2.23	0.73
2:N:54:GLU:HB3	2:N:78:ARG:HB3	1.71	0.73
1:A:705:ARG:HH12	11:K:60:VAL:HG13	1.53	0.73
1:M:1569:ILE:HA	1:M:1572:ILE:HG22	1.71	0.73
1:A:34:ASN:HB2	1:A:36:VAL:HG12	1.71	0.73
2:B:191:ASN:HD21	2:B:218:VAL:HG12	1.52	0.73
2:B:227:ASN:ND2	2:B:335:VAL:O	2.21	0.73
2:B:870:GLU:OE2	2:B:872:ARG:NH2	2.22	0.73
2:N:227:ASN:ND2	2:N:335:VAL:O	2.21	0.73
6:R:89:LEU:HG	7:S:68:PRO:HB3	1.71	0.73
1:A:498:ILE:HG13	1:A:499:GLU:H	1.52	0.72
12:X:21:ILE:HD11	12:X:30:ARG:HB3	1.71	0.72
1:A:106:CYS:HA	1:A:231:CYS:HB2	1.66	0.72
2:N:919:VAL:HB	3:O:78:ILE:HD13	1.71	0.72
2:B:494:ARG:NH2	2:B:513:SER:O	2.22	0.72
5:E:46:CYS:SG	5:E:47:GLY:N	2.61	0.72
7:G:59:LYS:HZ1	7:G:73:TRP:H	1.37	0.72
1:M:1205:PRO:HB2	1:M:1593:PHE:HE1	1.53	0.72
2:N:834:ILE:HD11	12:X:51:LYS:HD2	1.71	0.72
1:A:1230:ARG:NH1	1:A:1567:ASN:OD1	2.19	0.72
12:L:21:ILE:HD11	12:L:30:ARG:HB3	1.71	0.72
7:S:40:LYS:HG2	7:S:47:ILE:HG12	1.71	0.72
1:M:842:THR:HG21	2:N:1011:ILE:HA	1.71	0.72
1:A:106:CYS:SG	1:A:231:CYS:HB2	2.27	0.72
2:N:494:ARG:NH2	2:N:513:SER:O	2.22	0.72
3:C:130:GLU:HB2	1:M:559:ILE:HG12	1.70	0.72
5:Q:46:CYS:SG	5:Q:47:GLY:N	2.61	0.72
1:A:1103:ASP:O	1:A:1134:LEU:N	2.18	0.72
2:B:781:ARG:NH1	10:J:8:PHE:O	2.22	0.72
4:D:17:LEU:HD21	7:G:7:TYR:HA	1.72	0.72
5:E:65:ASN:OD1	5:E:67:SER:OG	2.08	0.72
1:A:1205:PRO:HB2	1:A:1593:PHE:HE1	1.53	0.71
2:N:243:TRP:CD1	2:N:244:ARG:HG2	2.24	0.71
2:N:870:GLU:OE2	2:N:872:ARG:NH2	2.22	0.71
1:A:710:GLN:NE2	11:K:65:TYR:O	2.23	0.71
2:B:54:GLU:HB3	2:B:78:ARG:HB3	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:20:ASP:OD1	4:D:21:ALA:N	2.24	0.71
7:G:40:LYS:HG2	7:G:47:ILE:HG12	1.71	0.71
2:N:237:THR:O	2:N:252:SER:OG	2.08	0.71
2:N:659:ILE:HG12	2:N:673:HIS:HB2	1.72	0.71
2:B:237:THR:O	2:B:252:SER:OG	2.08	0.71
1:A:786:PHE:HA	1:A:792:LEU:HG	1.71	0.71
2:B:659:ILE:HG12	2:B:673:HIS:HB2	1.72	0.71
1:M:476:ARG:HG3	2:N:1058:GLU:HG3	1.71	0.71
5:Q:65:ASN:OD1	5:Q:67:SER:OG	2.08	0.71
2:B:105:GLU:OE2	2:B:109:ARG:NH2	2.23	0.71
2:N:687:ASN:HD21	2:N:741:LEU:HD12	1.56	0.71
1:M:1504:LEU:HD21	2:N:284:ARG:CZ	2.20	0.71
2:N:440:PHE:O	2:N:444:GLY:N	2.24	0.71
1:M:34:ASN:HB2	1:M:36:VAL:HG12	1.71	0.71
2:B:546:VAL:HG12	2:B:571:CYS:HB3	1.72	0.71
2:B:1101:THR:O	2:B:1111:SER:OG	2.08	0.71
1:M:1657:LEU:HD12	1:M:1663:ARG:HA	1.72	0.71
1:M:604:ILE:HD11	2:N:1072:LEU:HD11	1.73	0.70
7:S:59:LYS:HZ1	7:S:73:TRP:H	1.39	0.70
1:A:121:CYS:HB3	1:A:186:VAL:HG21	1.73	0.70
2:B:7:GLU:O	2:B:11:THR:OG1	2.04	0.70
2:B:955:LYS:HE3	2:B:985:LEU:HD21	1.72	0.70
2:N:733:GLN:HE21	2:N:755:ASN:H	1.39	0.70
4:P:20:ASP:OD1	4:P:21:ALA:N	2.24	0.70
1:M:1089:LEU:HD23	1:M:1178:LEU:HD11	1.73	0.70
2:N:778:ALA:HB1	10:V:8:PHE:HB3	1.73	0.70
1:A:484:VAL:HG12	2:B:1081:SER:HB2	1.74	0.70
1:A:1657:LEU:HD12	1:A:1663:ARG:HA	1.72	0.70
1:M:248:GLU:HG2	1:M:249:ILE:H	1.57	0.70
2:B:1100:SER:HA	2:B:1113:VAL:HA	1.74	0.70
2:N:179:GLU:HB2	2:N:464:ALA:HB3	1.74	0.70
2:N:190:ARG:HD2	2:N:630:ASN:HD22	1.56	0.70
2:N:955:LYS:HE3	2:N:985:LEU:HD21	1.72	0.70
2:B:179:GLU:HB2	2:B:464:ALA:HB3	1.74	0.70
5:Q:61:ALA:O	5:Q:71:THR:OG1	2.10	0.70
8:T:40:LEU:HB3	8:T:102:MET:HG2	1.74	0.70
2:B:687:ASN:HD21	2:B:741:LEU:HD12	1.56	0.70
1:M:1602:PRO:HA	1:M:1605:LEU:HD13	1.73	0.70
2:N:1100:SER:HA	2:N:1113:VAL:HA	1.74	0.70
1:A:1602:PRO:HA	1:A:1605:LEU:HD13	1.73	0.70
2:B:733:GLN:HE21	2:B:755:ASN:H	1.39	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:121:CYS:HB3	1:M:186:VAL:HG21	1.73	0.70
1:M:786:PHE:HA	1:M:792:LEU:HG	1.72	0.70
2:N:546:VAL:HG12	2:N:571:CYS:HB3	1.72	0.70
1:A:604:ILE:HD11	2:B:1072:LEU:HD11	1.72	0.70
1:A:718:PRO:O	1:A:722:GLY:N	2.22	0.70
1:A:1151:LYS:HG3	1:A:1152:ASN:H	1.57	0.70
3:C:339:LYS:NZ	11:K:92:ARG:HA	2.07	0.70
1:A:248:GLU:HG2	1:A:249:ILE:H	1.57	0.69
2:B:501:TRP:NE1	2:B:675:GLU:OE2	2.25	0.69
1:M:1116:LYS:HG2	1:M:1118:PRO:HD2	1.74	0.69
1:A:1001:THR:HG21	2:B:973:GLU:HA	1.72	0.69
2:B:190:ARG:HD2	2:B:630:ASN:HD22	1.55	0.69
1:M:484:VAL:HG12	2:N:1081:SER:HB2	1.74	0.69
1:M:705:ARG:HH12	11:W:60:VAL:HG13	1.56	0.69
2:N:1101:THR:O	2:N:1111:SER:OG	2.08	0.69
1:A:503:ILE:HD12	1:A:605:LEU:HD11	1.74	0.69
1:A:1089:LEU:HD23	1:A:1178:LEU:HD11	1.73	0.69
1:M:503:ILE:HD12	1:M:605:LEU:HD11	1.75	0.69
1:A:1116:LYS:HG2	1:A:1118:PRO:HD2	1.74	0.69
8:H:40:LEU:HB3	8:H:102:MET:HG2	1.74	0.69
1:A:909:MET:SD	1:A:969:ARG:NH1	2.66	0.69
1:A:1103:ASP:HB3	1:A:1133:TYR:HD2	1.58	0.69
11:K:32:LEU:O	11:K:86:THR:OG1	2.10	0.69
1:M:28:SER:O	2:N:1116:ARG:NH2	2.25	0.69
1:A:1251:LEU:HB2	1:A:1540:PRO:HB2	1.75	0.69
8:H:90:LYS:HE3	8:H:105:GLU:HG2	1.75	0.69
1:M:909:MET:SD	1:M:969:ARG:NH1	2.66	0.69
1:M:678:SER:HA	1:M:1070:VAL:HG11	1.74	0.69
2:N:105:GLU:OE2	2:N:109:ARG:NH2	2.23	0.69
2:N:232:LEU:HD12	2:N:235:GLY:H	1.58	0.69
2:N:501:TRP:NE1	2:N:675:GLU:OE2	2.25	0.69
3:O:262:VAL:HG13	3:O:263:ILE:HG12	1.75	0.69
1:A:88:HIS:HD2	1:A:362:LEU:HD21	1.57	0.69
7:S:135:ARG:NE	7:S:145:GLU:HB2	2.08	0.69
8:T:90:LYS:HE3	8:T:105:GLU:HG2	1.75	0.69
1:A:678:SER:HA	1:A:1070:VAL:HG11	1.74	0.68
1:A:793:CYS:SG	1:A:794:GLY:N	2.66	0.68
3:C:262:VAL:HG13	3:C:263:ILE:HG12	1.75	0.68
1:M:1661:SER:OG	2:N:1061:ARG:NH1	2.26	0.68
1:A:1242:ILE:HG21	1:A:1567:ASN:HD21	1.58	0.68
5:E:61:ALA:O	5:E:71:THR:OG1	2.10	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:135:ARG:NE	7:G:145:GLU:HB2	2.08	0.68
1:M:106:CYS:SG	1:M:231:CYS:HB2	2.27	0.68
1:M:710:GLN:NE2	11:W:65:TYR:O	2.26	0.68
1:M:1242:ILE:HG21	1:M:1567:ASN:HD21	1.58	0.68
2:N:59:ASP:OD2	2:N:73:ASN:ND2	2.24	0.68
1:A:180:ARG:NH1	1:A:183:ASP:OD2	2.27	0.68
1:A:604:ILE:N	1:A:652:HIS:O	2.26	0.68
2:B:108:GLU:HA	2:B:722:THR:HG21	1.74	0.68
2:B:232:LEU:HD12	2:B:235:GLY:H	1.58	0.68
2:B:440:PHE:O	2:B:444:GLY:N	2.24	0.68
1:M:604:ILE:N	1:M:652:HIS:O	2.26	0.68
1:M:793:CYS:SG	1:M:794:GLY:N	2.67	0.68
1:M:1151:LYS:HG3	1:M:1152:ASN:H	1.57	0.68
11:W:32:LEU:O	11:W:86:THR:OG1	2.10	0.68
1:A:330:ASN:HA	1:A:333:ARG:HD3	1.76	0.68
1:A:1192:GLU:HG2	1:A:1194:VAL:HG22	1.75	0.68
1:M:99:LEU:O	1:M:102:THR:OG1	2.08	0.68
1:M:330:ASN:HA	1:M:333:ARG:HD3	1.76	0.68
7:S:118:ILE:HA	7:S:170:LEU:HB2	1.75	0.68
7:S:99:SER:HA	7:S:115:ARG:NH1	2.09	0.68
1:M:88:HIS:HD2	1:M:362:LEU:HD21	1.57	0.68
1:A:653:PHE:O	2:B:1076:ARG:NH2	2.27	0.68
2:B:1113:VAL:O	2:B:1114:ARG:NH1	2.27	0.68
7:G:124:PHE:HB2	7:G:136:TRP:CE3	2.29	0.68
2:B:61:ILE:O	2:B:69:LEU:HB2	1.95	0.67
2:B:790:LYS:NZ	2:B:792:GLU:OE2	2.27	0.67
3:C:90:TYR:HE1	1:M:560:GLU:HG2	1.60	0.67
1:M:1103:ASP:HB3	1:M:1133:TYR:HD2	1.58	0.67
7:S:124:PHE:HB2	7:S:136:TRP:CE3	2.29	0.67
2:B:59:ASP:OD2	2:B:73:ASN:ND2	2.24	0.67
1:M:1324:PHE:O	1:M:1328:PHE:HB3	1.95	0.67
2:N:61:ILE:O	2:N:69:LEU:HB2	1.95	0.67
2:N:955:LYS:NZ	2:N:994:GLY:O	2.28	0.67
1:A:781:GLU:O	1:A:783:SER:N	2.28	0.67
3:C:223:HIS:CG	3:C:225:LYS:HE3	2.30	0.67
1:M:718:PRO:O	1:M:722:GLY:N	2.22	0.67
1:M:1279:VAL:O	9:U:48:SER:OG	2.11	0.67
2:N:108:GLU:HA	2:N:722:THR:HG21	1.74	0.67
3:O:223:HIS:CG	3:O:225:LYS:HE3	2.30	0.67
3:C:171:SER:N	3:C:198:ILE:O	2.28	0.67
1:M:180:ARG:NH1	1:M:183:ASP:OD2	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:1090:ARG:HH21	2:N:1147:THR:HG1	1.43	0.67
3:O:94:ASN:O	12:X:53:ARG:NH1	2.25	0.67
3:C:237:LEU:HD12	3:C:238:PRO:HD2	1.76	0.67
7:G:118:ILE:HA	7:G:170:LEU:HB2	1.76	0.67
1:A:1504:LEU:HD21	2:B:284:ARG:CZ	2.24	0.67
1:M:1251:LEU:HB2	1:M:1540:PRO:HB2	1.75	0.67
8:H:74:TYR:N	8:H:123:LEU:O	2.28	0.67
11:K:25:LEU:HD11	11:K:38:GLN:HB2	1.76	0.67
1:M:1192:GLU:HG2	1:M:1194:VAL:HG22	1.75	0.67
1:M:998:ARG:HE	1:M:1000:LEU:HD23	1.60	0.67
2:N:144:VAL:HB	2:N:170:GLY:HA2	1.77	0.67
1:A:1522:PRO:HD2	1:A:1550:LYS:HZ1	1.60	0.66
6:F:96:PRO:HB2	7:G:23:ARG:HH11	1.59	0.66
8:H:42:ILE:HD13	8:H:49:LEU:HD12	1.77	0.66
3:O:237:LEU:HD12	3:O:238:PRO:HD2	1.76	0.66
2:B:144:VAL:HB	2:B:170:GLY:HA2	1.77	0.66
7:G:99:SER:HA	7:G:115:ARG:NH1	2.09	0.66
1:M:1230:ARG:NH1	1:M:1567:ASN:OD1	2.19	0.66
11:W:25:LEU:HD11	11:W:38:GLN:HB2	1.76	0.66
1:A:998:ARG:HE	1:A:1000:LEU:HD23	1.60	0.66
2:B:955:LYS:NZ	2:B:994:GLY:O	2.28	0.66
2:N:185:LEU:HB2	2:N:378:LEU:HD21	1.78	0.66
2:N:1113:VAL:O	2:N:1114:ARG:NH1	2.27	0.66
3:O:204:ARG:N	3:O:207:GLN:HE21	1.93	0.66
1:A:212:LYS:HD3	1:A:1628:TYR:HE1	1.61	0.66
8:T:42:ILE:HD13	8:T:49:LEU:HD12	1.77	0.66
1:A:247:PHE:O	1:A:321:LYS:N	2.29	0.66
1:M:1660:PRO:HA	1:M:1663:ARG:HB2	1.76	0.66
2:N:480:HIS:CD2	2:N:518:LEU:HB3	2.28	0.66
3:O:92:ILE:HG12	3:O:211:LEU:HA	1.78	0.66
1:M:212:LYS:HD3	1:M:1628:TYR:HE1	1.61	0.66
1:M:1038:LYS:HG2	1:M:1638:PHE:CD2	2.30	0.66
2:N:99:ARG:HH22	12:X:46:HIS:HA	1.61	0.66
2:N:672:THR:HG23	2:N:673:HIS:HD1	1.61	0.66
2:B:781:ARG:HD3	10:J:8:PHE:HA	1.76	0.66
3:C:339:LYS:HZ2	11:K:92:ARG:HG3	1.61	0.66
10:J:40:LEU:O	10:J:46:ARG:NH1	2.26	0.66
1:M:131:LEU:HD21	1:M:207:LEU:HG	1.78	0.66
3:C:92:ILE:HG12	3:C:211:LEU:HA	1.78	0.66
5:E:49:GLY:HA2	5:E:50:ARG:HB2	1.78	0.66
1:M:781:GLU:O	1:M:783:SER:N	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:786:PHE:HB2	1:A:790:GLU:O	1.96	0.65
1:M:247:PHE:O	1:M:321:LYS:N	2.29	0.65
2:N:561:VAL:HG13	2:N:568:VAL:HG23	1.78	0.65
2:N:208:TYR:HA	2:N:232:LEU:HA	1.78	0.65
5:Q:49:GLY:HA2	5:Q:50:ARG:HB2	1.78	0.65
8:T:74:TYR:N	8:T:123:LEU:O	2.28	0.65
10:V:19:ASP:O	10:V:23:THR:HG22	1.96	0.65
1:A:1324:PHE:O	1:A:1328:PHE:HB3	1.95	0.65
1:A:1660:PRO:HA	1:A:1663:ARG:HB2	1.76	0.65
3:C:204:ARG:N	3:C:207:GLN:HE21	1.93	0.65
3:C:315:THR:HG21	10:J:6:ARG:NH2	2.10	0.65
8:H:79:LYS:HA	8:H:118:HIS:HA	1.78	0.65
10:J:19:ASP:O	10:J:23:THR:HG22	1.96	0.65
1:M:102:THR:HG22	1:M:335:LEU:HD22	1.79	0.65
10:V:27:GLU:O	10:V:27:GLU:HG2	1.96	0.65
2:B:185:LEU:HB2	2:B:378:LEU:HD21	1.78	0.65
2:B:719:ARG:O	2:B:872:ARG:NH2	2.30	0.65
2:N:790:LYS:NZ	2:N:792:GLU:OE2	2.27	0.65
1:A:77:PHE:CE1	1:A:369:PRO:HD3	2.32	0.65
1:A:131:LEU:HD21	1:A:207:LEU:HG	1.78	0.65
1:A:1051:VAL:HG21	1:A:1063:TYR:HB2	1.79	0.65
2:B:761:ILE:HD13	2:B:1011:ILE:HD12	1.78	0.65
1:M:77:PHE:CE1	1:M:369:PRO:HD3	2.32	0.65
3:O:240:ILE:HB	3:O:277:VAL:HG11	1.79	0.65
1:A:1228:ILE:HG13	1:A:1229:PRO:HD3	1.77	0.65
1:M:1228:ILE:HG13	1:M:1229:PRO:HD3	1.77	0.65
2:N:719:ARG:O	2:N:872:ARG:NH2	2.30	0.65
2:B:164:GLU:N	2:B:164:GLU:OE1	2.30	0.65
2:B:208:TYR:HA	2:B:232:LEU:HA	1.78	0.65
2:N:595:ARG:NH1	2:N:645:GLU:OE2	2.29	0.65
1:A:607:ARG:HH12	1:A:609:PRO:HD2	1.62	0.65
1:A:612:HIS:CD2	1:A:614:PRO:HD2	2.32	0.65
3:C:240:ILE:HB	3:C:277:VAL:HG11	1.79	0.65
1:M:1553:TRP:HB3	5:Q:136:ILE:HD11	1.78	0.65
3:O:101:GLU:OE1	3:O:101:GLU:N	2.28	0.65
1:A:1038:LYS:HG2	1:A:1638:PHE:CD2	2.31	0.65
1:A:1661:SER:OG	2:B:1061:ARG:NH1	2.29	0.65
1:A:1673:GLY:HA2	6:F:78:TYR:CD1	2.32	0.64
2:N:164:GLU:OE1	2:N:164:GLU:N	2.30	0.64
6:R:68:ASP:OD2	6:R:68:ASP:N	2.28	0.64
1:A:39:ASP:OD1	1:A:43:HIS:N	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1242:ILE:HD13	1:A:1568:ASP:H	1.63	0.64
2:B:864:GLU:HG2	2:B:865:PRO:HD2	1.79	0.64
1:M:687:GLN:HB2	2:N:937:HIS:CD2	2.32	0.64
2:N:63:GLN:HB3	2:N:69:LEU:HB3	1.80	0.64
4:P:47:LEU:O	4:P:51:ASN:ND2	2.31	0.64
1:A:687:GLN:HB2	2:B:937:HIS:CD2	2.33	0.64
3:C:101:GLU:OE1	3:C:101:GLU:N	2.28	0.64
1:M:786:PHE:HB2	1:M:790:GLU:O	1.96	0.64
2:N:761:ILE:HD13	2:N:1011:ILE:HD12	1.78	0.64
2:N:906:HIS:NE2	2:N:950:GLU:OE1	2.30	0.64
12:X:19:THR:OG1	12:X:20:MET:N	2.26	0.64
2:B:906:HIS:NE2	2:B:950:GLU:OE1	2.30	0.64
10:J:27:GLU:O	10:J:27:GLU:HG2	1.97	0.64
1:A:102:THR:HG22	1:A:335:LEU:HD22	1.79	0.64
1:A:797:ASP:N	1:A:800:SER:OG	2.30	0.64
4:D:13:LYS:HE3	7:G:10:THR:OG1	1.98	0.64
7:G:30:GLN:HA	7:G:33:MET:HB2	1.79	0.64
1:A:515:TYR:OH	1:A:595:ARG:NH1	2.31	0.64
1:A:1138:SER:HB3	1:A:1141:PHE:HB2	1.80	0.64
2:B:728:ARG:NH2	2:B:789:TYR:OH	2.31	0.64
7:G:115:ARG:HA	7:G:118:ILE:HD12	1.80	0.64
1:A:404:LEU:HG	1:A:430:LEU:HD23	1.80	0.64
2:B:561:VAL:HG13	2:B:568:VAL:HG23	1.78	0.64
2:B:905:ARG:NH2	2:B:950:GLU:OE2	2.26	0.64
2:N:205:GLY:O	2:N:208:TYR:N	2.28	0.64
7:S:30:GLN:HA	7:S:33:MET:HB2	1.79	0.64
1:A:820:ILE:HD13	1:A:823:ARG:HD3	1.80	0.64
1:A:989:ALA:HB1	1:A:994:PHE:HB3	1.80	0.64
2:B:205:GLY:O	2:B:208:TYR:N	2.28	0.64
1:M:612:HIS:CD2	1:M:614:PRO:HD2	2.32	0.64
1:M:989:ALA:HB1	1:M:994:PHE:HB3	1.80	0.64
2:N:728:ARG:NH2	2:N:789:TYR:OH	2.31	0.64
2:B:595:ARG:NH1	2:B:645:GLU:OE2	2.30	0.64
2:B:1160:ALA:O	2:B:1163:THR:OG1	2.15	0.64
1:M:607:ARG:HH12	1:M:609:PRO:HD2	1.62	0.64
1:M:1051:VAL:HG21	1:M:1063:TYR:HB2	1.79	0.64
2:N:864:GLU:HG2	2:N:865:PRO:HD2	1.79	0.64
2:B:480:HIS:CD2	2:B:518:LEU:HB3	2.28	0.64
1:A:53:ALA:O	1:A:65:THR:OG1	2.13	0.63
2:B:40:THR:OG1	2:B:148:ARG:NH1	2.31	0.63
1:M:812:VAL:HG11	1:M:824:LEU:HD13	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:149:CYS:SG	2:N:150:HIS:N	2.71	0.63
2:N:691:PHE:N	2:N:966:SER:OG	2.31	0.63
1:A:661:SER:HB3	6:F:108:LEU:HD11	1.80	0.63
3:C:125:PRO:HB3	3:C:132:THR:HG21	1.80	0.63
6:F:89:LEU:HG	7:G:68:PRO:HB3	1.79	0.63
6:F:125:ARG:HB3	6:F:127:TYR:HE2	1.63	0.63
2:N:905:ARG:NH2	2:N:950:GLU:OE2	2.26	0.63
6:R:125:ARG:HB3	6:R:127:TYR:HE2	1.63	0.63
1:A:99:LEU:O	1:A:102:THR:OG1	2.08	0.63
2:B:63:GLN:HB3	2:B:69:LEU:HB3	1.79	0.63
2:B:149:CYS:SG	2:B:150:HIS:N	2.71	0.63
4:D:47:LEU:O	4:D:51:ASN:ND2	2.31	0.63
1:M:56:PRO:HG3	1:M:63:CYS:HB2	1.80	0.63
8:T:79:LYS:HA	8:T:118:HIS:HA	1.78	0.63
1:A:842:THR:HG21	2:B:1011:ILE:HA	1.81	0.63
1:M:515:TYR:OH	1:M:595:ARG:NH1	2.31	0.63
1:M:1001:THR:HG21	2:N:973:GLU:HA	1.80	0.63
2:N:40:THR:OG1	2:N:148:ARG:NH1	2.31	0.63
3:O:125:PRO:HB3	3:O:132:THR:HG21	1.80	0.63
1:A:1038:LYS:HZ1	1:A:1626:ILE:HA	1.62	0.63
3:C:65:ILE:HD11	3:C:69:ILE:HB	1.81	0.63
1:M:1281:VAL:HG21	1:M:1505:MET:HG2	1.80	0.63
2:N:1097:SER:OG	2:N:1115:CYS:SG	2.56	0.63
5:E:177:ASP:OD1	5:E:179:VAL:N	2.31	0.63
6:F:87:ARG:NH1	6:F:90:GLN:OE1	2.32	0.63
12:L:19:THR:OG1	12:L:20:MET:N	2.26	0.63
3:O:334:LYS:HE2	11:W:46:LEU:HD12	1.81	0.63
5:Q:177:ASP:OD1	5:Q:179:VAL:N	2.31	0.63
1:A:895:VAL:HA	1:A:901:LYS:HD3	1.81	0.63
1:M:820:ILE:HD13	1:M:823:ARG:HD3	1.80	0.63
1:M:1132:ARG:NH2	6:R:70:THR:HG23	2.13	0.63
1:A:812:VAL:HG11	1:A:824:LEU:HD13	1.79	0.63
1:M:1242:ILE:HD13	1:M:1568:ASP:H	1.63	0.63
9:U:6:SER:O	9:U:6:SER:OG	2.15	0.63
1:A:893:GLU:OE2	2:B:617:SER:OG	2.17	0.62
2:B:718:LEU:HA	2:B:721:ARG:HG3	1.80	0.62
1:M:765:LYS:HB2	1:M:785:LEU:HD13	1.81	0.62
1:A:446:ASP:OD1	1:A:465:LYS:NZ	2.32	0.62
1:A:471:LYS:HZ2	1:A:476:ARG:HH21	1.45	0.62
1:M:1138:SER:HB3	1:M:1141:PHE:HB2	1.80	0.62
2:N:718:LEU:HA	2:N:721:ARG:HG3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1588:GLU:O	1:A:1591:SER:OG	2.16	0.62
5:E:182:TYR:HD2	5:E:183:LEU:HD22	1.64	0.62
1:M:29:VAL:HG12	1:M:30:LYS:HG2	1.81	0.62
2:N:55:LYS:NZ	2:N:397:ASN:OD1	2.31	0.62
1:A:1572:ILE:O	1:A:1576:TYR:HB2	1.99	0.62
2:B:733:GLN:NE2	2:B:754:THR:OG1	2.31	0.62
5:E:42:LYS:O	5:E:46:CYS:HB2	2.00	0.62
1:M:404:LEU:HG	1:M:430:LEU:HD23	1.80	0.62
3:O:171:SER:N	3:O:198:ILE:O	2.28	0.62
1:A:56:PRO:HG3	1:A:63:CYS:HB2	1.80	0.62
1:M:39:ASP:OD1	1:M:43:HIS:N	2.29	0.62
2:N:1112:GLU:HG2	2:N:1114:ARG:HH12	1.64	0.62
5:Q:74:ILE:HG22	5:Q:103:ILE:HD12	1.81	0.62
5:E:59:PHE:HB2	5:E:74:ILE:HD11	1.82	0.62
1:M:82:LEU:HB2	1:M:84:ILE:HD13	1.82	0.62
1:M:471:LYS:HZ2	1:M:476:ARG:HH21	1.45	0.62
1:M:1563:ASP:N	1:M:1563:ASP:OD1	2.32	0.62
1:M:1635:LYS:HB3	1:M:1644:PHE:CD2	2.35	0.62
5:Q:42:LYS:O	5:Q:46:CYS:HB2	2.00	0.62
5:E:74:ILE:HG22	5:E:103:ILE:HD12	1.81	0.62
2:N:818:PRO:HB3	2:N:820:ARG:NH1	2.15	0.62
6:R:125:ARG:HB3	6:R:127:TYR:CE2	2.35	0.62
1:A:1281:VAL:HG21	1:A:1505:MET:HG2	1.80	0.62
2:B:336:LEU:HB2	2:B:345:LYS:HD3	1.82	0.62
1:M:797:ASP:N	1:M:800:SER:OG	2.30	0.62
8:H:24:VAL:HG22	8:H:43:ASN:HA	1.82	0.62
2:N:99:ARG:HH22	12:X:47:ARG:NH1	1.97	0.62
3:O:50:ILE:HD12	11:W:113:LEU:HB3	1.82	0.62
1:A:15:LYS:HB2	1:A:1654:VAL:HG22	1.81	0.62
1:A:634:TYR:CZ	2:B:768:MET:HB2	2.35	0.62
1:A:886:ALA:HA	1:A:889:ASN:HD22	1.63	0.62
2:B:54:GLU:HB3	2:B:78:ARG:HD3	1.82	0.62
2:B:1112:GLU:HG2	2:B:1114:ARG:HH12	1.64	0.62
6:F:125:ARG:HB3	6:F:127:TYR:CE2	2.35	0.62
1:M:27:ILE:O	2:N:1116:ARG:NE	2.32	0.62
1:M:717:LYS:HD3	1:M:720:GLU:HG3	1.82	0.62
1:M:895:VAL:HA	1:M:901:LYS:HD3	1.81	0.62
1:M:1065:GLU:HB3	5:Q:200:SER:HB2	1.80	0.62
2:N:244:ARG:O	2:N:246:ASN:ND2	2.33	0.62
2:N:336:LEU:HB2	2:N:345:LYS:HD3	1.82	0.62
7:G:12:ASP:OD2	7:G:75:ARG:NE	2.25	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:1070:VAL:HA	1:M:1073:GLN:HE21	1.65	0.61
3:O:65:ILE:HD11	3:O:69:ILE:HB	1.81	0.61
10:J:35:LEU:HA	10:J:38:LEU:HD13	1.82	0.61
1:M:886:ALA:HA	1:M:889:ASN:HD22	1.64	0.61
2:B:691:PHE:N	2:B:966:SER:OG	2.32	0.61
2:B:829:ASP:OD2	12:L:22:TYR:OH	2.18	0.61
2:N:780:GLU:OE1	3:O:224:ALA:N	2.26	0.61
7:S:115:ARG:HA	7:S:118:ILE:HD12	1.80	0.61
1:A:774:TYR:O	8:H:20:LYS:NZ	2.26	0.61
2:B:818:PRO:HB3	2:B:820:ARG:NH1	2.15	0.61
1:M:962:GLN:NE2	1:M:992:GLY:O	2.17	0.61
1:M:1572:ILE:O	1:M:1576:TYR:HB2	1.99	0.61
2:N:733:GLN:NE2	2:N:754:THR:OG1	2.31	0.61
5:Q:182:TYR:HD2	5:Q:183:LEU:HD22	1.64	0.61
1:A:29:VAL:HG12	1:A:30:LYS:HG2	1.82	0.61
2:N:715:GLY:HA2	2:N:750:TYR:HE1	1.66	0.61
2:N:891:ARG:NH1	3:O:101:GLU:OE1	2.34	0.61
3:O:223:HIS:HD2	3:O:225:LYS:H	1.49	0.61
12:X:26:ASP:OD1	12:X:27:CYS:N	2.32	0.61
1:A:717:LYS:HD3	1:A:720:GLU:HG3	1.82	0.61
1:A:1602:PRO:HB2	5:E:199:THR:HG21	1.82	0.61
3:O:88:PHE:HB3	12:X:59:GLN:NE2	2.15	0.61
10:V:40:LEU:O	10:V:46:ARG:NH1	2.26	0.61
1:A:67:HIS:ND1	2:B:1102:ILE:HD11	2.16	0.61
1:A:916:LEU:O	1:A:919:SER:OG	2.12	0.61
1:M:15:LYS:HB2	1:M:1654:VAL:HG22	1.81	0.61
5:Q:59:PHE:HB2	5:Q:74:ILE:HD11	1.82	0.61
1:M:1251:LEU:HD13	1:M:1558:GLU:HB3	1.83	0.61
2:N:1160:ALA:O	2:N:1163:THR:OG1	2.15	0.61
1:A:82:LEU:HB2	1:A:84:ILE:HD13	1.82	0.61
1:A:668:ASN:N	1:A:668:ASN:OD1	2.34	0.61
1:A:1635:LYS:HB3	1:A:1644:PHE:CD2	2.35	0.61
11:K:36:THR:HG22	11:K:78:ARG:HD3	1.83	0.61
1:M:1038:LYS:HZ3	1:M:1629:ASN:HD22	1.48	0.61
1:M:1246:THR:OG1	1:M:1566:THR:OG1	2.11	0.61
2:B:571:CYS:HB2	2:B:575:LEU:HD23	1.82	0.61
1:M:446:ASP:OD1	1:M:465:LYS:NZ	2.32	0.61
3:O:91:ILE:HG12	12:X:58:VAL:O	2.00	0.61
8:T:24:VAL:HG22	8:T:43:ASN:HA	1.81	0.61
11:W:36:THR:HG22	11:W:78:ARG:HD3	1.83	0.61
1:A:1226:LEU:HD21	1:A:1595:VAL:HG21	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:81:VAL:HA	1:M:364:ASN:HB3	1.83	0.60
2:B:715:GLY:HA2	2:B:750:TYR:HE1	1.66	0.60
2:B:995:ASN:HB3	2:B:1010:ASP:HB3	1.83	0.60
1:M:968:ARG:HG3	1:M:969:ARG:H	1.65	0.60
5:Q:84:ILE:HG23	5:Q:85:LYS:HE3	1.83	0.60
10:V:35:LEU:HA	10:V:38:LEU:HD13	1.82	0.60
1:A:52:LEU:O	1:A:64:ALA:N	2.30	0.60
1:A:411:GLU:HB3	1:A:422:ARG:NH2	2.16	0.60
1:A:765:LYS:HB2	1:A:785:LEU:HD13	1.81	0.60
1:A:968:ARG:HG3	1:A:969:ARG:H	1.65	0.60
1:A:1044:CYS:SG	1:A:1046:GLN:NE2	2.74	0.60
2:B:156:PRO:HB3	2:B:166:SER:OG	2.02	0.60
2:B:279:THR:HG23	9:I:46:THR:HG22	1.83	0.60
1:M:13:SER:OG	2:N:1172:GLU:OE2	2.14	0.60
1:M:411:GLU:HB3	1:M:422:ARG:NH2	2.16	0.60
2:N:571:CYS:HB2	2:N:575:LEU:HD23	1.82	0.60
1:A:19:TYR:CD2	2:B:1168:LYS:HD2	2.36	0.60
1:A:612:HIS:CE1	1:A:1204:GLU:HG3	2.36	0.60
1:A:612:HIS:ND1	1:A:1204:GLU:HG3	2.17	0.60
2:B:116:ARG:HD3	7:S:131:GLU:OE1	2.00	0.60
1:M:612:HIS:ND1	1:M:1204:GLU:HG3	2.17	0.60
2:N:54:GLU:HB3	2:N:78:ARG:HD3	1.82	0.60
2:N:99:ARG:NH2	12:X:47:ARG:HH12	1.99	0.60
1:A:77:PHE:CE1	1:A:368:PRO:HA	2.37	0.60
1:A:560:GLU:HG2	3:O:90:TYR:HE1	1.64	0.60
1:A:1305:SER:O	1:A:1309:TYR:N	2.35	0.60
7:G:56:PHE:HB3	7:G:74:VAL:HG22	1.84	0.60
1:M:3:ILE:HG21	6:R:89:LEU:HD11	1.82	0.60
1:M:760:PRO:HD2	1:M:1088:SER:HA	1.84	0.60
1:M:1238:ALA:HB1	1:M:1618:TYR:CE2	2.36	0.60
1:M:1588:GLU:O	1:M:1591:SER:OG	2.16	0.60
2:N:593:LYS:HB3	2:N:598:THR:HG21	1.83	0.60
1:A:462:PRO:HA	1:A:466:GLN:OE1	2.02	0.60
1:A:1044:CYS:O	1:A:1046:GLN:NE2	2.34	0.60
2:B:587:LYS:HD2	2:B:607:LEU:HA	1.84	0.60
1:M:1045:VAL:O	1:M:1191:GLY:N	2.34	0.60
2:N:587:LYS:HD2	2:N:607:LEU:HA	1.84	0.60
2:N:822:TRP:HB3	2:N:826:LEU:HD12	1.84	0.60
1:A:613:LYS:NZ	1:A:672:GLN:OE1	2.35	0.60
1:M:660:ARG:NH1	6:R:108:LEU:HD13	2.17	0.60
1:M:1044:CYS:SG	1:M:1046:GLN:NE2	2.74	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:1271:VAL:HG12	1:M:1273:SER:H	1.66	0.60
1:A:512:LYS:HD3	2:B:1031:VAL:HG11	1.82	0.60
1:A:1563:ASP:OD1	1:A:1563:ASP:N	2.32	0.60
2:B:205:GLY:HA3	2:B:208:TYR:CD2	2.36	0.60
2:B:217:CYS:HB2	2:B:338:HIS:ND1	2.17	0.60
1:M:499:GLU:O	1:M:633:HIS:HB2	2.02	0.60
1:A:1070:VAL:HA	1:A:1073:GLN:HE21	1.65	0.60
1:A:1238:ALA:HB1	1:A:1618:TYR:CE2	2.36	0.60
1:A:1251:LEU:HD13	1:A:1558:GLU:HB3	1.83	0.60
1:A:1582:ARG:NH1	5:E:197:SER:OG	2.34	0.60
2:B:244:ARG:O	2:B:246:ASN:ND2	2.33	0.60
2:B:1032:ARG:HE	2:B:1044:PRO:HB3	1.67	0.60
2:N:1032:ARG:HE	2:N:1044:PRO:HB3	1.67	0.60
1:A:1309:TYR:O	1:A:1313:TYR:HB2	2.02	0.60
2:B:593:LYS:HB3	2:B:598:THR:HG21	1.83	0.60
1:M:613:LYS:NZ	1:M:672:GLN:OE1	2.35	0.60
1:M:1226:LEU:HD21	1:M:1595:VAL:HG21	1.83	0.60
2:N:205:GLY:HA3	2:N:208:TYR:CD2	2.36	0.60
2:B:1097:SER:HB2	2:B:1117:SER:H	1.67	0.59
6:F:96:PRO:CB	7:G:23:ARG:HH11	2.15	0.59
1:M:612:HIS:CE1	1:M:1204:GLU:HG3	2.36	0.59
1:M:1044:CYS:O	1:M:1046:GLN:NE2	2.34	0.59
2:N:156:PRO:HB3	2:N:166:SER:OG	2.02	0.59
2:N:777:SER:OG	2:N:781:ARG:NH1	2.35	0.59
3:O:128:GLY:N	3:O:129:GLN:OE1	2.34	0.59
1:A:543:HIS:HB2	1:A:552:ILE:O	2.02	0.59
2:B:1097:SER:OG	2:B:1115:CYS:SG	2.56	0.59
3:C:90:TYR:HA	12:L:59:GLN:OE1	2.02	0.59
7:G:70:SER:OG	7:G:71:PHE:N	2.35	0.59
9:I:6:SER:O	9:I:6:SER:OG	2.16	0.59
3:O:229:VAL:HA	3:O:314:SER:HA	1.83	0.59
1:A:1045:VAL:O	1:A:1191:GLY:N	2.34	0.59
2:B:14:ASN:OD1	2:B:14:ASN:N	2.35	0.59
2:B:232:LEU:HG	2:B:236:VAL:O	2.02	0.59
3:C:223:HIS:HD2	3:C:225:LYS:H	1.49	0.59
4:D:28:ARG:O	4:D:32:THR:HG23	2.02	0.59
5:E:84:ILE:HG23	5:E:85:LYS:HE3	1.83	0.59
7:G:105:ILE:HG23	7:G:109:PHE:HB2	1.84	0.59
1:M:850:LEU:HA	1:M:929:LEU:HA	1.83	0.59
1:A:736:ARG:HD3	8:H:75:ILE:HD12	1.85	0.59
3:C:128:GLY:N	3:C:129:GLN:OE1	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:77:PHE:CE1	1:M:368:PRO:HA	2.37	0.59
1:A:850:LEU:HA	1:A:929:LEU:HA	1.83	0.59
1:A:1271:VAL:HG12	1:A:1273:SER:H	1.66	0.59
6:F:68:ASP:OD2	6:F:68:ASP:N	2.28	0.59
2:N:733:GLN:NE2	2:N:755:ASN:H	2.01	0.59
1:A:734:ILE:HD11	1:A:740:TYR:HB2	1.83	0.59
1:M:462:PRO:HA	1:M:466:GLN:OE1	2.02	0.59
1:M:885:ILE:HG22	1:M:889:ASN:HD21	1.67	0.59
1:M:1522:PRO:HD2	1:M:1550:LYS:HZ1	1.66	0.59
2:N:217:CYS:HB2	2:N:338:HIS:ND1	2.17	0.59
4:P:27:ASN:OD1	4:P:31:GLN:NE2	2.36	0.59
7:S:105:ILE:HG23	7:S:109:PHE:HB2	1.84	0.59
1:M:734:ILE:HD11	1:M:740:TYR:HB2	1.83	0.59
1:M:1305:SER:O	1:M:1309:TYR:N	2.35	0.59
1:A:81:VAL:HA	1:A:364:ASN:HB3	1.83	0.59
1:A:240:LYS:HA	1:A:246:ILE:HG22	1.85	0.59
1:A:499:GLU:O	1:A:633:HIS:HB2	2.02	0.59
1:A:1038:LYS:HE3	1:A:1626:ILE:HG23	1.85	0.59
2:B:733:GLN:NE2	2:B:755:ASN:H	2.01	0.59
3:C:334:LYS:HE2	11:K:46:LEU:HD12	1.82	0.59
2:N:232:LEU:HG	2:N:236:VAL:O	2.02	0.59
2:N:1097:SER:HB2	2:N:1117:SER:H	1.67	0.59
4:P:17:LEU:O	7:S:4:LEU:HD21	2.03	0.59
6:R:93:MET:HG3	7:S:68:PRO:HG3	1.83	0.59
8:T:38:LEU:HD21	8:T:40:LEU:HD22	1.85	0.59
1:A:760:PRO:HD2	1:A:1088:SER:HA	1.84	0.59
2:B:822:TRP:HB3	2:B:826:LEU:HD12	1.84	0.59
3:C:75:ARG:HG2	11:K:45:THR:HB	1.84	0.59
6:F:97:VAL:HG22	6:F:99:VAL:H	1.67	0.59
7:G:44:ILE:HG21	7:G:80:VAL:HG11	1.85	0.59
2:N:728:ARG:HH22	3:O:99:GLN:HE22	1.50	0.59
7:S:70:SER:OG	7:S:71:PHE:N	2.36	0.59
2:B:208:TYR:CD1	2:B:232:LEU:HB3	2.38	0.59
2:B:218:VAL:HA	2:B:224:SER:HA	1.85	0.59
2:B:777:SER:OG	2:B:781:ARG:NH1	2.36	0.59
3:C:336:LEU:O	3:C:340:SER:OG	2.21	0.59
4:D:27:ASN:OD1	4:D:31:GLN:NE2	2.36	0.59
6:F:114:GLU:OE1	6:F:119:LYS:HB2	2.03	0.59
1:M:543:HIS:HB2	1:M:552:ILE:O	2.02	0.59
1:M:717:LYS:HZ1	11:W:67:ILE:C	2.04	0.59
1:M:1038:LYS:HE3	1:M:1626:ILE:HG23	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:59:VAL:HG12	3:O:311:SER:HA	1.85	0.59
1:A:12:LYS:HB3	2:B:1172:GLU:OE2	2.02	0.58
1:M:1309:TYR:O	1:M:1313:TYR:HB2	2.02	0.58
2:N:918:THR:HG23	3:O:78:ILE:HD11	1.85	0.58
2:N:995:ASN:HB3	2:N:1010:ASP:HB3	1.83	0.58
6:R:97:VAL:HG22	6:R:99:VAL:H	1.67	0.58
1:A:1569:ILE:HG21	1:A:1585:ILE:HG22	1.85	0.58
2:B:636:ARG:HH22	2:B:675:GLU:CD	2.07	0.58
8:H:43:ASN:OD1	8:H:46:ILE:N	2.23	0.58
1:M:240:LYS:HA	1:M:246:ILE:HG22	1.85	0.58
2:N:636:ARG:HH22	2:N:675:GLU:CD	2.07	0.58
5:Q:188:GLY:N	5:Q:209:CYS:O	2.36	0.58
3:C:59:VAL:HG12	3:C:311:SER:HA	1.85	0.58
9:I:55:SER:HB3	9:I:58:LYS:HB2	1.84	0.58
1:M:178:LEU:HA	1:M:181:ILE:HD12	1.86	0.58
1:M:734:ILE:HG22	8:T:76:MET:HG2	1.84	0.58
3:O:339:LYS:NZ	11:W:92:ARG:HA	2.18	0.58
2:B:200:SER:HA	2:B:203:ASN:HD21	1.68	0.58
2:B:235:GLY:HA2	2:B:284:ARG:NH1	2.17	0.58
3:C:229:VAL:HA	3:C:314:SER:HA	1.83	0.58
2:N:37:ASN:HB3	2:N:41:ASN:HD21	1.68	0.58
2:N:793:SER:OG	2:N:887:HIS:ND1	2.33	0.58
3:O:35:ASN:O	11:W:56:LYS:HD2	2.03	0.58
3:O:336:LEU:O	3:O:340:SER:OG	2.21	0.58
7:S:44:ILE:HG21	7:S:80:VAL:HG11	1.85	0.58
7:S:56:PHE:HB3	7:S:74:VAL:HG22	1.84	0.58
1:A:870:LEU:HD12	1:A:987:THR:HG21	1.85	0.58
1:M:917:THR:HG23	1:M:959:LEU:HD11	1.85	0.58
1:M:1569:ILE:HG21	1:M:1585:ILE:HG22	1.85	0.58
3:O:338:VAL:HG13	11:W:22:ILE:HG21	1.84	0.58
4:P:28:ARG:O	4:P:32:THR:HG23	2.03	0.58
6:R:87:ARG:NH1	6:R:90:GLN:OE1	2.32	0.58
9:U:55:SER:HB3	9:U:58:LYS:HB2	1.84	0.58
2:B:55:LYS:NZ	2:B:397:ASN:OD1	2.31	0.58
12:L:26:ASP:OD1	12:L:27:CYS:N	2.32	0.58
2:N:208:TYR:CD1	2:N:232:LEU:HB3	2.38	0.58
7:S:117:SER:HB2	7:S:169:THR:HA	1.86	0.58
1:A:885:ILE:HG22	1:A:889:ASN:HD21	1.67	0.58
2:B:824:GLN:O	12:L:56:ARG:NH2	2.37	0.58
8:H:38:LEU:HD21	8:H:40:LEU:HD22	1.85	0.58
1:M:1064:GLY:O	1:M:1603:ARG:HG2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:W:79:ILE:HD11	11:W:91:LEU:HD13	1.86	0.58
1:A:558:THR:N	1:A:561:GLN:OE1	2.22	0.58
2:B:37:ASN:HB3	2:B:41:ASN:HD21	1.68	0.58
3:C:91:ILE:HA	3:C:211:LEU:HB3	1.86	0.58
7:G:121:ASP:N	7:G:121:ASP:OD1	2.36	0.58
1:M:870:LEU:HD12	1:M:987:THR:HG21	1.85	0.58
1:M:1003:ILE:HD11	1:M:1008:TYR:CD2	2.32	0.58
1:M:1270:LEU:HD22	1:M:1313:TYR:CD1	2.39	0.58
2:N:200:SER:HA	2:N:203:ASN:HD21	1.68	0.58
6:R:96:PRO:HG3	7:S:23:ARG:HG2	1.84	0.58
1:A:178:LEU:HA	1:A:181:ILE:HD12	1.86	0.58
1:M:1038:LYS:HZ1	1:M:1626:ILE:HA	1.68	0.58
2:N:880:ASP:HA	12:X:38:VAL:CG2	2.34	0.58
1:A:77:PHE:CD1	1:A:368:PRO:HA	2.39	0.57
1:A:917:THR:HG23	1:A:959:LEU:HD11	1.85	0.57
1:A:1673:GLY:HA2	6:F:78:TYR:CE1	2.39	0.57
11:K:57:ASN:O	11:K:60:VAL:HG12	2.05	0.57
1:M:558:THR:N	1:M:561:GLN:OE1	2.22	0.57
2:N:283:ASP:OD1	2:N:284:ARG:N	2.37	0.57
8:T:96:SER:HA	8:T:101:LEU:HD23	1.86	0.57
1:A:1:MET:HB2	2:B:1079:ASN:HB3	1.85	0.57
1:A:774:TYR:HB3	1:A:933:PHE:CD2	2.39	0.57
1:A:1270:LEU:HD22	1:A:1313:TYR:CD1	2.39	0.57
8:H:80:VAL:HB	8:H:95:VAL:HG22	1.87	0.57
1:M:19:TYR:CD2	2:N:1168:LYS:HD2	2.38	0.57
1:M:388:ASN:O	1:M:392:THR:HG23	2.04	0.57
1:M:668:ASN:OD1	1:M:668:ASN:N	2.34	0.57
2:N:218:VAL:HA	2:N:224:SER:HA	1.85	0.57
4:P:56:TYR:CE1	7:S:106:LEU:HD23	2.39	0.57
1:A:1550:LYS:HA	1:A:1553:TRP:HD1	1.69	0.57
1:M:979:LEU:HD22	1:M:1010:PHE:CZ	2.39	0.57
2:N:123:TRP:HE3	2:N:131:GLN:O	1.88	0.57
5:Q:173:ILE:N	5:Q:208:ILE:O	2.37	0.57
1:A:388:ASN:O	1:A:392:THR:HG23	2.04	0.57
1:M:53:ALA:O	1:M:65:THR:OG1	2.13	0.57
1:M:1498:ILE:HD11	9:U:22:ALA:HB2	1.87	0.57
3:O:137:ASP:HB3	3:O:138:THR:HG23	1.86	0.57
1:A:1064:GLY:O	1:A:1603:ARG:HG2	2.04	0.57
2:B:58:PHE:HB3	2:B:74:LYS:HA	1.86	0.57
2:B:123:TRP:HE3	2:B:131:GLN:O	1.88	0.57
2:B:225:LEU:HD12	2:B:226:THR:H	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:373:GLN:HA	2:B:651:PRO:O	2.05	0.57
2:B:518:LEU:HD23	2:B:518:LEU:H	1.69	0.57
7:G:145:GLU:HB3	7:G:146:PRO:HD3	1.86	0.57
1:M:130:LEU:HD21	1:M:193:SER:HB3	1.87	0.57
8:T:80:VAL:HB	8:T:95:VAL:HG22	1.87	0.57
1:A:211:ARG:NH2	1:A:1651:ARG:HD2	2.20	0.57
1:A:705:ARG:NH1	11:K:60:VAL:O	2.37	0.57
2:B:208:TYR:HD1	2:B:232:LEU:HB3	1.70	0.57
1:M:77:PHE:CD1	1:M:368:PRO:HA	2.39	0.57
2:N:58:PHE:HB3	2:N:74:LYS:HA	1.86	0.57
2:B:184:MET:HB2	2:B:479:VAL:HG22	1.87	0.57
2:B:1034:THR:HG22	2:B:1035:GLY:H	1.69	0.57
3:C:137:ASP:HB3	3:C:138:THR:HG23	1.86	0.57
5:E:188:GLY:N	5:E:209:CYS:O	2.36	0.57
7:G:19:PRO:HD3	7:G:69:PHE:HB3	1.86	0.57
7:G:117:SER:HB2	7:G:169:THR:HA	1.86	0.57
1:M:1550:LYS:HA	1:M:1553:TRP:HD1	1.69	0.57
2:N:18:ASP:OD2	2:N:19:GLY:N	2.38	0.57
2:N:824:GLN:O	12:X:56:ARG:NH2	2.38	0.57
5:E:54:ARG:HB3	5:E:78:LYS:HD3	1.86	0.57
2:B:831:LEU:HD13	2:B:845:VAL:HG12	1.87	0.57
5:E:15:TRP:O	5:E:19:HIS:N	2.38	0.57
2:N:531:PRO:HB3	2:N:631:PRO:HD3	1.87	0.57
6:R:114:GLU:OE1	6:R:119:LYS:HB2	2.03	0.57
1:A:736:ARG:NH2	8:H:68:LEU:O	2.38	0.57
1:A:979:LEU:HD22	1:A:1010:PHE:CZ	2.39	0.57
1:A:1233:GLU:HA	1:A:1237:THR:HG22	1.87	0.57
3:C:77:LEU:HG	3:C:229:VAL:HG11	1.87	0.57
8:H:96:SER:HA	8:H:101:LEU:HD23	1.86	0.57
11:K:79:ILE:HD11	11:K:91:LEU:HD13	1.86	0.57
2:N:14:ASN:OD1	2:N:14:ASN:N	2.35	0.57
11:W:57:ASN:O	11:W:60:VAL:HG12	2.04	0.57
1:A:696:LEU:HB2	1:A:835:TYR:CE2	2.40	0.56
1:A:962:GLN:NE2	1:A:992:GLY:O	2.17	0.56
2:B:271:ILE:HG23	2:B:272:VAL:HG13	1.87	0.56
2:B:687:ASN:ND2	2:B:741:LEU:HD12	2.20	0.56
3:C:96:SER:OG	3:C:97:ILE:N	2.38	0.56
5:E:173:ILE:N	5:E:208:ILE:O	2.37	0.56
7:G:37:ILE:HG13	7:G:38:LEU:HD23	1.87	0.56
1:M:774:TYR:HB3	1:M:933:PHE:CD2	2.39	0.56
7:S:37:ILE:HG13	7:S:38:LEU:HD23	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:T:7:LEU:HB2	8:T:59:ILE:HG12	1.87	0.56
1:A:130:LEU:HD21	1:A:193:SER:HB3	1.87	0.56
2:B:283:ASP:OD1	2:B:284:ARG:N	2.37	0.56
2:B:502:GLY:HA2	2:B:681:VAL:HA	1.87	0.56
7:G:97:SER:HB2	2:N:93:GLU:CD	2.26	0.56
8:H:7:LEU:HB2	8:H:59:ILE:HG12	1.87	0.56
1:M:685:LEU:HB3	1:M:689:HIS:HB2	1.87	0.56
2:N:225:LEU:HD12	2:N:226:THR:H	1.69	0.56
2:N:587:LYS:HA	2:N:605:VAL:HG23	1.87	0.56
3:O:91:ILE:HA	3:O:211:LEU:HB3	1.86	0.56
1:A:528:ARG:HG3	1:A:566:ALA:HB1	1.87	0.56
1:A:542:SER:OG	1:A:543:HIS:N	2.38	0.56
2:B:18:ASP:OD2	2:B:19:GLY:N	2.38	0.56
2:B:336:LEU:HB3	2:B:338:HIS:CE1	2.40	0.56
2:B:399:ILE:HG22	2:B:429:ILE:HG21	1.88	0.56
4:D:48:SER:HA	4:D:51:ASN:HD22	1.71	0.56
1:M:77:PHE:CD2	2:N:1096:ILE:HG12	2.41	0.56
1:M:852:GLU:O	1:M:856:ASN:ND2	2.38	0.56
2:N:184:MET:HB2	2:N:479:VAL:HG22	1.87	0.56
2:N:235:GLY:HA2	2:N:284:ARG:NH1	2.17	0.56
2:N:439:TYR:O	2:N:442:SER:OG	2.21	0.56
2:N:523:ARG:NE	2:N:741:LEU:HD13	2.20	0.56
2:N:852:THR:OG1	2:N:854:GLN:HG2	2.06	0.56
5:Q:15:TRP:O	5:Q:19:HIS:N	2.38	0.56
7:S:19:PRO:HD3	7:S:69:PHE:HB3	1.86	0.56
8:T:43:ASN:OD1	8:T:46:ILE:N	2.23	0.56
1:A:492:ILE:HG13	1:A:630:ILE:HD11	1.88	0.56
2:B:135:ARG:NH2	2:B:426:PHE:HB3	2.20	0.56
1:M:542:SER:O	1:M:554:LEU:HB2	2.06	0.56
1:M:606:ASN:OD1	1:M:607:ARG:N	2.39	0.56
2:N:336:LEU:HB3	2:N:338:HIS:CE1	2.40	0.56
3:O:75:ARG:HH12	11:W:44:HIS:HB2	1.70	0.56
3:O:143:LEU:HD23	3:O:174:LEU:HG	1.88	0.56
5:Q:54:ARG:HB3	5:Q:78:LYS:HD3	1.86	0.56
1:A:498:ILE:HG13	1:A:499:GLU:N	2.21	0.56
2:B:523:ARG:NE	2:B:741:LEU:HD13	2.20	0.56
2:B:793:SER:OG	2:B:887:HIS:ND1	2.32	0.56
2:N:518:LEU:HD23	2:N:518:LEU:H	1.69	0.56
3:O:79:ALA:HB1	3:O:221:GLN:N	2.21	0.56
7:S:145:GLU:HB3	7:S:146:PRO:HD3	1.86	0.56
2:B:844:ILE:HG22	2:B:845:VAL:HG13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:230:ALA:N	3:C:313:GLU:O	2.39	0.56
3:C:315:THR:HG21	10:J:6:ARG:HH22	1.69	0.56
1:M:498:ILE:HG13	1:M:499:GLU:N	2.21	0.56
2:N:399:ILE:HG22	2:N:429:ILE:HG21	1.88	0.56
2:N:1034:THR:HG22	2:N:1035:GLY:H	1.69	0.56
3:O:96:SER:OG	3:O:97:ILE:N	2.38	0.56
1:A:852:GLU:O	1:A:856:ASN:ND2	2.38	0.56
2:B:531:PRO:HB3	2:B:631:PRO:HD3	1.87	0.56
3:C:79:ALA:HB1	3:C:221:GLN:N	2.21	0.56
7:G:61:ALA:HB2	7:G:72:ILE:HB	1.87	0.56
1:M:1335:ILE:HD11	1:M:1511:LYS:HE3	1.87	0.56
2:N:135:ARG:NH2	2:N:426:PHE:HB3	2.20	0.56
2:N:315:LEU:HD21	2:N:330:LEU:HD21	1.87	0.56
2:N:844:ILE:HG22	2:N:845:VAL:HG13	1.87	0.56
3:O:241:HIS:CE1	3:O:300:GLN:HB3	2.41	0.56
1:A:542:SER:O	1:A:554:LEU:HB2	2.06	0.56
2:B:315:LEU:HD21	2:B:330:LEU:HD21	1.87	0.56
3:C:204:ARG:HB2	10:J:63:ASN:HD21	1.71	0.56
5:E:146:PRO:HB3	5:E:194:VAL:O	2.06	0.56
1:M:211:ARG:NH2	1:M:1651:ARG:HD2	2.20	0.56
1:M:726:ARG:HA	11:W:78:ARG:HH21	1.71	0.56
2:N:364:CYS:SG	2:N:622:TYR:N	2.79	0.56
2:N:373:GLN:HA	2:N:651:PRO:O	2.05	0.56
1:A:481:GLY:HA2	2:B:1057:GLY:HA3	1.88	0.56
1:A:955:GLN:HA	1:A:959:LEU:O	2.06	0.56
1:M:955:GLN:HA	1:M:959:LEU:O	2.06	0.56
2:N:540:LEU:O	2:N:544:LEU:HB2	2.06	0.56
3:O:35:ASN:O	11:W:56:LYS:HA	2.06	0.56
2:B:109:ARG:HD2	2:B:875:GLY:O	2.06	0.56
2:B:540:LEU:O	2:B:544:LEU:HB2	2.06	0.56
2:B:1087:TRP:HA	2:B:1147:THR:O	2.06	0.56
1:M:111:LEU:HD11	1:M:222:ILE:HG22	1.88	0.56
1:M:219:TYR:HA	1:M:222:ILE:HG12	1.87	0.56
1:M:1001:THR:HG23	2:N:976:THR:HG23	1.89	0.56
2:N:365:CYS:N	2:N:620:GLY:O	2.27	0.56
2:N:831:LEU:HD13	2:N:845:VAL:HG12	1.87	0.56
3:O:77:LEU:HG	3:O:229:VAL:HG11	1.87	0.56
1:A:219:TYR:HA	1:A:222:ILE:HG12	1.88	0.55
2:B:285:VAL:O	2:B:289:LEU:HG	2.06	0.55
2:B:364:CYS:SG	2:B:622:TYR:N	2.79	0.55
2:B:439:TYR:O	2:B:442:SER:OG	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:116:VAL:HG12	1:M:342:VAL:HG21	1.88	0.55
2:N:891:ARG:HD3	3:O:99:GLN:HG2	1.88	0.55
8:T:95:VAL:HG11	8:T:119:VAL:HG21	1.87	0.55
1:A:116:VAL:HG12	1:A:342:VAL:HG21	1.88	0.55
1:A:606:ASN:OD1	1:A:607:ARG:N	2.39	0.55
1:A:712:LEU:HD11	1:A:753:ASN:ND2	2.22	0.55
1:A:1038:LYS:HZ3	1:A:1629:ASN:HD22	1.54	0.55
2:B:587:LYS:HA	2:B:605:VAL:HG23	1.87	0.55
3:C:143:LEU:HD23	3:C:174:LEU:HG	1.88	0.55
3:C:145:LYS:HD3	3:C:166:ASN:HB3	1.88	0.55
3:C:167:SER:OG	3:C:203:LEU:O	2.17	0.55
4:D:17:LEU:CD2	7:G:7:TYR:HA	2.35	0.55
6:F:96:PRO:HG3	7:G:23:ARG:HG2	1.88	0.55
8:H:95:VAL:HG11	8:H:119:VAL:HG21	1.87	0.55
1:M:492:ILE:HG13	1:M:630:ILE:HD11	1.88	0.55
1:M:507:PRO:O	1:M:511:THR:HG23	2.07	0.55
5:Q:49:GLY:HA3	5:Q:51:ASN:H	1.70	0.55
7:S:121:ASP:OD1	7:S:121:ASP:N	2.37	0.55
1:A:685:LEU:HB3	1:A:689:HIS:HB2	1.87	0.55
1:A:759:ARG:NH2	1:A:1092:LYS:HB2	2.22	0.55
5:E:49:GLY:HA3	5:E:51:ASN:H	1.71	0.55
1:M:528:ARG:HG3	1:M:566:ALA:HB1	1.87	0.55
1:M:696:LEU:HB2	1:M:835:TYR:CE2	2.40	0.55
1:M:1233:GLU:HA	1:M:1237:THR:HG22	1.87	0.55
2:N:1087:TRP:HA	2:N:1147:THR:O	2.06	0.55
3:O:230:ALA:N	3:O:313:GLU:O	2.39	0.55
1:A:88:HIS:CD2	1:A:362:LEU:HD21	2.41	0.55
1:A:507:PRO:O	1:A:511:THR:HG23	2.07	0.55
1:A:1263:PHE:HE1	1:A:1555:PHE:CG	2.24	0.55
1:A:1335:ILE:HD11	1:A:1511:LYS:HE3	1.87	0.55
2:B:123:TRP:NE1	2:B:422:LEU:HG	2.22	0.55
2:B:365:CYS:N	2:B:620:GLY:O	2.27	0.55
5:E:13:ARG:HE	5:E:137:VAL:HG12	1.71	0.55
1:M:470:LYS:C	1:M:472:GLU:H	2.09	0.55
1:M:916:LEU:O	1:M:919:SER:OG	2.12	0.55
1:M:1680:PHE:O	6:R:122:LEU:HA	2.06	0.55
2:N:109:ARG:HD2	2:N:875:GLY:O	2.06	0.55
2:N:271:ILE:HG23	2:N:272:VAL:HG13	1.87	0.55
2:B:386:GLN:HE21	2:B:452:LEU:HD22	1.72	0.55
3:C:262:VAL:HG21	3:C:283:ASP:HB2	1.89	0.55
3:C:335:CYS:HB3	11:K:99:ILE:HG12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:52:LEU:O	1:M:64:ALA:N	2.30	0.55
1:M:1020:ILE:HG22	2:N:515:CYS:SG	2.47	0.55
2:B:145:ARG:HB3	2:B:170:GLY:HA3	1.89	0.55
2:B:852:THR:OG1	2:B:854:GLN:HG2	2.06	0.55
3:C:241:HIS:CE1	3:C:300:GLN:HB3	2.41	0.55
1:M:542:SER:OG	1:M:543:HIS:N	2.38	0.55
1:M:1263:PHE:HE1	1:M:1555:PHE:CG	2.24	0.55
1:M:1522:PRO:HD2	1:M:1550:LYS:NZ	2.22	0.55
2:N:502:GLY:HA2	2:N:681:VAL:HA	1.87	0.55
7:S:12:ASP:OD2	7:S:75:ARG:NE	2.25	0.55
2:N:208:TYR:HD1	2:N:232:LEU:HB3	1.70	0.55
2:N:285:VAL:O	2:N:289:LEU:HG	2.06	0.55
1:A:862:LEU:HD13	1:A:996:ALA:HB1	1.89	0.55
1:A:1139:GLU:O	1:A:1143:ARG:HG2	2.07	0.55
2:B:614:VAL:HB	2:B:624:GLY:H	1.72	0.55
1:M:712:LEU:HD11	1:M:753:ASN:ND2	2.22	0.55
1:M:1602:PRO:HB2	5:Q:199:THR:HG21	1.89	0.55
5:Q:13:ARG:HE	5:Q:137:VAL:HG12	1.71	0.55
2:B:874:LEU:HD11	2:B:887:HIS:HB2	1.89	0.55
1:M:32:ILE:HA	1:M:47:GLY:O	2.07	0.55
1:M:653:PHE:O	2:N:1076:ARG:NH2	2.40	0.55
1:M:862:LEU:HD13	1:M:996:ALA:HB1	1.89	0.55
2:N:503:PHE:CE1	2:N:636:ARG:HB3	2.42	0.55
1:M:949:SER:OG	1:M:951:VAL:HG22	2.07	0.54
1:M:1249:LEU:HD12	1:M:1542:VAL:CG1	2.38	0.54
3:O:144:ASN:HA	3:O:209:ILE:O	2.07	0.54
5:Q:146:PRO:HB3	5:Q:194:VAL:O	2.06	0.54
1:A:32:ILE:HA	1:A:47:GLY:O	2.07	0.54
5:E:73:TYR:CE2	5:E:75:GLU:HB3	2.42	0.54
11:K:81:THR:HG21	11:K:90:VAL:HG21	1.89	0.54
1:M:1062:HIS:CB	1:M:1066:ASP:HB3	2.36	0.54
3:O:88:PHE:HB3	12:X:59:GLN:HE21	1.71	0.54
3:O:262:VAL:HG21	3:O:283:ASP:HB2	1.89	0.54
3:O:288:GLU:OE2	3:O:291:ARG:NH2	2.40	0.54
1:A:470:LYS:C	1:A:472:GLU:H	2.09	0.54
1:A:1003:ILE:HD11	1:A:1008:TYR:CD2	2.32	0.54
1:A:1246:THR:OG1	1:A:1566:THR:OG1	2.11	0.54
1:A:1249:LEU:HD12	1:A:1542:VAL:CG1	2.38	0.54
1:A:1522:PRO:HD2	1:A:1550:LYS:NZ	2.22	0.54
2:B:237:THR:HG21	2:B:353:ILE:HD13	1.90	0.54
2:B:957:GLY:N	2:B:964:GLN:HE21	2.05	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1085:GLN:HB3	2:B:1148:LEU:HD21	1.90	0.54
2:N:145:ARG:HB3	2:N:170:GLY:HA3	1.89	0.54
1:A:111:LEU:HD11	1:A:222:ILE:HG22	1.88	0.54
4:D:13:LYS:HE3	7:G:10:THR:HG1	1.72	0.54
1:M:35:PRO:HG3	1:M:395:LEU:HG	1.89	0.54
1:M:1248:THR:HB	1:M:1564:ILE:HB	1.89	0.54
1:M:1279:VAL:HG13	1:M:1301:LEU:HA	1.88	0.54
2:N:386:GLN:HE21	2:N:452:LEU:HD22	1.72	0.54
5:Q:73:TYR:CE2	5:Q:75:GLU:HB3	2.42	0.54
7:S:61:ALA:HB2	7:S:72:ILE:HB	1.87	0.54
11:W:81:THR:HG21	11:W:90:VAL:HG21	1.89	0.54
1:A:910:LYS:NZ	1:A:967:GLY:O	2.41	0.54
1:A:1279:VAL:HG13	1:A:1301:LEU:HA	1.88	0.54
2:B:882:GLU:HB2	2:B:884:GLN:HE21	1.71	0.54
2:B:985:LEU:HG	2:B:990:TYR:HB2	1.89	0.54
10:J:24:LEU:O	10:J:28:ASP:HB2	2.08	0.54
1:M:67:HIS:ND1	2:N:1102:ILE:HD11	2.22	0.54
1:M:1009:TYR:OH	2:N:500:ALA:HB3	2.08	0.54
1:M:1139:GLU:O	1:M:1143:ARG:HG2	2.07	0.54
2:N:614:VAL:HB	2:N:624:GLY:H	1.72	0.54
2:N:677:SER:OG	2:N:679:THR:HB	2.07	0.54
2:N:875:GLY:HA2	12:X:39:ILE:HG21	1.89	0.54
3:O:145:LYS:HD3	3:O:166:ASN:HB3	1.88	0.54
4:P:48:SER:HA	4:P:51:ASN:HD22	1.71	0.54
1:A:949:SER:OG	1:A:951:VAL:HG22	2.07	0.54
2:B:116:ARG:HA	2:B:139:MET:HG2	1.90	0.54
3:C:144:ASN:HA	3:C:209:ILE:O	2.07	0.54
6:F:96:PRO:HB2	7:G:23:ARG:NH1	2.23	0.54
1:M:1478:LYS:HG3	1:M:1495:VAL:HG23	1.90	0.54
2:N:99:ARG:HH22	12:X:47:ARG:HH12	1.52	0.54
2:N:147:ASN:HA	2:N:152:GLU:OE1	2.08	0.54
2:N:882:GLU:HB2	2:N:884:GLN:HE21	1.71	0.54
2:N:957:GLY:N	2:N:964:GLN:HE21	2.05	0.54
1:A:35:PRO:HG3	1:A:395:LEU:HG	1.89	0.54
2:B:677:SER:OG	2:B:679:THR:HB	2.07	0.54
5:E:71:THR:HG23	5:E:99:HIS:HD2	1.73	0.54
7:G:7:TYR:HD2	7:G:82:SER:HB3	1.73	0.54
1:M:88:HIS:CD2	1:M:362:LEU:HD21	2.41	0.54
1:M:759:ARG:NH2	1:M:1092:LYS:HB2	2.22	0.54
1:M:846:ASP:HB3	2:N:993:HIS:CG	2.42	0.54
3:O:204:ARG:H	3:O:207:GLN:HE21	1.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:ARG:O	1:A:332:LEU:HG	2.08	0.54
1:A:372:PHE:CE1	2:B:1157:TYR:HA	2.43	0.54
1:A:1277:ARG:HG2	1:A:1278:GLN:H	1.73	0.54
7:G:57:LEU:O	7:G:59:LYS:HG3	2.08	0.54
7:G:128:ASP:C	2:N:116:ARG:HH22	2.10	0.54
1:M:13:SER:HA	1:M:1656:ASP:O	2.08	0.54
1:M:329:ARG:O	1:M:332:LEU:HG	2.08	0.54
1:M:704:THR:HG22	1:M:705:ARG:H	1.72	0.54
1:M:1277:ARG:HG2	1:M:1278:GLN:H	1.73	0.54
1:M:1582:ARG:NH1	5:Q:197:SER:OG	2.39	0.54
2:N:116:ARG:HA	2:N:139:MET:HG2	1.90	0.54
2:B:935:ASN:OD1	2:B:937:HIS:ND1	2.41	0.54
1:M:464:ILE:O	1:M:467:ILE:HG12	2.07	0.54
2:N:985:LEU:HG	2:N:990:TYR:HB2	1.89	0.54
1:A:247:PHE:N	1:A:321:LYS:O	2.41	0.54
2:B:503:PHE:CE1	2:B:636:ARG:HB3	2.42	0.54
2:B:901:LYS:HB2	2:B:1021:LEU:HD22	1.89	0.54
2:B:976:THR:HG22	2:B:978:ALA:H	1.72	0.54
9:I:24:TRP:NE1	9:I:34:TYR:O	2.41	0.54
2:N:237:THR:HG21	2:N:353:ILE:HD13	1.90	0.54
2:N:976:THR:HG22	2:N:978:ALA:H	1.72	0.54
7:S:114:PRO:HD2	7:S:117:SER:OG	2.08	0.54
1:A:98:LEU:HD23	1:A:360:PHE:HE2	1.74	0.53
1:A:1151:LYS:HG3	1:A:1152:ASN:N	2.22	0.53
2:B:693:ASP:OD1	2:B:693:ASP:N	2.32	0.53
1:M:80:ILE:HD11	1:M:395:LEU:HD13	1.90	0.53
2:N:687:ASN:ND2	2:N:741:LEU:HD12	2.20	0.53
2:N:919:VAL:HG21	3:O:75:ARG:HD3	1.89	0.53
5:Q:180:ALA:HA	5:Q:185:LEU:HD12	1.90	0.53
1:A:464:ILE:O	1:A:467:ILE:HG12	2.07	0.53
2:B:107:ARG:NH1	2:B:721:ARG:HH22	2.06	0.53
2:B:243:TRP:HD1	2:B:244:ARG:HG2	1.72	0.53
7:G:5:SER:HG	7:G:81:PHE:HE1	1.56	0.53
7:G:114:PRO:HD2	7:G:117:SER:OG	2.08	0.53
9:I:20:THR:OG1	9:I:36:SER:HB3	2.08	0.53
9:I:24:TRP:HA	9:I:36:SER:OG	2.08	0.53
1:M:247:PHE:N	1:M:321:LYS:O	2.41	0.53
1:M:997:SER:OG	1:M:1003:ILE:HG22	2.08	0.53
2:N:154:LEU:HD22	2:N:158:GLU:HG3	1.89	0.53
2:N:971:TYR:CG	2:N:977:ALA:HB2	2.44	0.53
9:U:20:THR:OG1	9:U:36:SER:HB3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:X:24:CYS:HA	12:X:49:MET:HG2	1.89	0.53
2:B:842:ASP:OD1	2:B:843:PRO:HD2	2.08	0.53
2:N:372:PRO:HB2	2:N:499:GLU:OE1	2.08	0.53
2:N:874:LEU:HD11	2:N:887:HIS:HB2	1.89	0.53
1:A:471:LYS:NZ	1:A:476:ARG:HH21	2.07	0.53
1:A:704:THR:HG22	1:A:705:ARG:H	1.72	0.53
2:B:820:ARG:HG2	2:B:821:GLU:HG3	1.91	0.53
3:C:204:ARG:HG3	10:J:60:LEU:HD22	1.91	0.53
5:E:106:TYR:O	5:E:131:GLN:HB2	2.09	0.53
6:F:72:THR:O	6:F:126:ARG:NH1	2.30	0.53
11:K:52:TYR:O	11:K:56:LYS:HG2	2.09	0.53
1:M:559:ILE:O	1:M:563:THR:OG1	2.22	0.53
1:M:893:GLU:HB2	1:M:985:TYR:CZ	2.44	0.53
2:N:820:ARG:HG2	2:N:821:GLU:HG3	1.91	0.53
2:B:147:ASN:HA	2:B:152:GLU:OE1	2.08	0.53
2:B:253:MET:HB2	2:B:288:MET:SD	2.48	0.53
1:M:844:ARG:HD2	2:N:995:ASN:HD21	1.74	0.53
2:N:253:MET:HB2	2:N:288:MET:SD	2.48	0.53
3:O:114:ALA:HB2	3:O:191:ILE:HG23	1.90	0.53
10:V:47:ARG:NH1	10:V:48:MET:SD	2.82	0.53
1:A:113:LYS:HB3	1:A:230:ASN:HD21	1.74	0.53
1:A:902:LEU:HD22	1:A:968:ARG:HH21	1.74	0.53
1:A:1248:THR:HB	1:A:1564:ILE:HB	1.90	0.53
3:C:86:PHE:CD2	3:C:215:ALA:HB2	2.44	0.53
4:D:54:LEU:O	4:D:58:LYS:HG2	2.08	0.53
12:L:24:CYS:HA	12:L:49:MET:HG2	1.89	0.53
1:M:582:SER:OG	7:S:35:SER:O	2.26	0.53
1:M:1309:TYR:OH	1:M:1315:VAL:HG23	2.09	0.53
2:N:935:ASN:OD1	2:N:937:HIS:ND1	2.41	0.53
4:P:47:LEU:HA	4:P:50:LEU:HD12	1.90	0.53
8:T:24:VAL:HG13	8:T:42:ILE:C	2.29	0.53
11:W:52:TYR:O	11:W:56:LYS:HG2	2.09	0.53
1:A:660:ARG:NH1	6:F:108:LEU:HD13	2.23	0.53
1:A:997:SER:OG	1:A:1003:ILE:HG22	2.08	0.53
1:A:1306:ARG:HA	1:A:1309:TYR:HB3	1.91	0.53
2:B:985:LEU:HD12	2:B:988:ALA:HB3	1.90	0.53
4:D:47:LEU:HA	4:D:50:LEU:HD12	1.90	0.53
11:K:60:VAL:HA	11:K:81:THR:HG22	1.91	0.53
1:M:844:ARG:HD2	2:N:995:ASN:ND2	2.23	0.53
2:N:312:ARG:NH1	2:N:322:THR:O	2.40	0.53
2:N:505:CYS:SG	2:N:683:SER:N	2.77	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:891:ARG:CD	3:O:99:GLN:HG2	2.38	0.53
6:R:72:THR:O	6:R:126:ARG:NH1	2.30	0.53
9:U:24:TRP:HA	9:U:36:SER:OG	2.08	0.53
9:U:24:TRP:NE1	9:U:34:TYR:O	2.41	0.53
10:V:67:LYS:HG3	12:X:28:GLY:O	2.09	0.53
1:A:13:SER:HA	1:A:1656:ASP:O	2.08	0.53
1:A:80:ILE:HD11	1:A:395:LEU:HD13	1.90	0.53
1:A:1309:TYR:OH	1:A:1315:VAL:HG23	2.09	0.53
2:B:154:LEU:HD22	2:B:158:GLU:HG3	1.90	0.53
2:B:763:TYR:CE2	2:B:922:PRO:HD3	2.44	0.53
8:H:108:HIS:ND1	8:H:108:HIS:O	2.42	0.53
11:K:51:ARG:HG3	11:K:63:CYS:SG	2.49	0.53
1:M:910:LYS:NZ	1:M:967:GLY:O	2.41	0.53
3:O:76:ILE:HA	3:O:80:GLU:HB2	1.91	0.53
3:O:167:SER:O	3:O:203:LEU:N	2.23	0.53
1:A:852:GLU:HA	1:A:855:ASP:HB3	1.89	0.53
2:B:971:TYR:CG	2:B:977:ALA:HB2	2.44	0.53
8:H:24:VAL:HG13	8:H:42:ILE:C	2.29	0.53
10:J:47:ARG:NH1	10:J:48:MET:SD	2.82	0.53
1:M:326:THR:HG23	1:M:329:ARG:NH1	2.24	0.53
1:M:518:PRO:HB2	6:R:92:SER:O	2.08	0.53
1:M:1306:ARG:HA	1:M:1309:TYR:HB3	1.91	0.53
1:M:1663:ARG:HD2	1:M:1669:VAL:O	2.09	0.53
2:N:279:THR:HG23	9:U:46:THR:HG22	1.91	0.53
3:O:86:PHE:CD2	3:O:215:ALA:HB2	2.44	0.53
3:O:204:ARG:HB2	10:V:63:ASN:HD21	1.74	0.53
1:A:743:GLY:HA2	1:A:746:ILE:HD12	1.90	0.53
1:A:1062:HIS:CB	1:A:1066:ASP:HB3	2.36	0.53
1:A:1478:LYS:HG3	1:A:1495:VAL:HG23	1.90	0.53
2:B:372:PRO:HB2	2:B:499:GLU:OE1	2.08	0.53
2:B:919:VAL:HB	3:C:78:ILE:HD13	1.91	0.53
3:C:167:SER:O	3:C:203:LEU:N	2.23	0.53
3:C:247:GLU:HA	3:C:273:LYS:O	2.09	0.53
3:C:288:GLU:OE2	3:C:291:ARG:NH2	2.40	0.53
8:H:66:PRO:O	8:H:70:GLU:HG2	2.09	0.53
10:J:31:GLU:OE1	10:J:31:GLU:N	2.33	0.53
1:M:113:LYS:HB3	1:M:230:ASN:HD21	1.74	0.53
1:M:731:PRO:O	1:M:745:GLN:NE2	2.42	0.53
1:M:1005:PRO:HG3	2:N:969:PHE:CG	2.44	0.53
1:M:1075:HIS:HB2	1:M:1182:ARG:NH2	2.24	0.53
2:N:901:LYS:HB2	2:N:1021:LEU:HD22	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:1128:THR:N	7:S:84:LYS:HZ1	2.07	0.53
2:N:1163:THR:HG22	2:N:1168:LYS:HG2	1.89	0.53
5:Q:106:TYR:O	5:Q:131:GLN:HB2	2.09	0.53
2:B:514:PRO:HA	2:B:517:LEU:HD12	1.91	0.52
1:M:852:GLU:HA	1:M:855:ASP:HB3	1.89	0.52
1:M:1151:LYS:HG3	1:M:1152:ASN:N	2.22	0.52
2:N:107:ARG:NH1	2:N:721:ARG:HH22	2.06	0.52
2:N:1085:GLN:HB3	2:N:1148:LEU:HD21	1.90	0.52
7:S:57:LEU:O	7:S:59:LYS:HG3	2.08	0.52
1:A:504:GLY:HA2	1:A:622:ARG:O	2.09	0.52
1:A:637:CYS:O	1:A:641:ASN:N	2.42	0.52
1:A:1663:ARG:HD2	1:A:1669:VAL:O	2.09	0.52
3:C:77:LEU:HD11	3:C:323:LEU:HB3	1.91	0.52
2:N:509:THR:CG2	2:N:516:GLY:H	2.23	0.52
2:N:733:GLN:HB2	10:V:51:THR:O	2.10	0.52
2:N:809:HIS:NE2	12:X:36:LYS:HE3	2.23	0.52
10:V:24:LEU:O	10:V:28:ASP:HB2	2.08	0.52
1:A:28:SER:O	2:B:1116:ARG:NH2	2.42	0.52
3:C:76:ILE:HA	3:C:80:GLU:HB2	1.91	0.52
5:E:177:ASP:OD1	5:E:179:VAL:HG22	2.09	0.52
6:F:69:ARG:HD2	6:F:136:TRP:NE1	2.25	0.52
8:H:70:GLU:HG3	8:H:71:ALA:N	2.24	0.52
1:M:401:ILE:HG13	1:M:437:LEU:HD13	1.91	0.52
1:M:639:SER:HA	1:M:682:LEU:HD11	1.91	0.52
2:N:217:CYS:SG	2:N:337:VAL:HG22	2.49	0.52
2:N:286:GLU:HB2	9:U:7:LEU:HD11	1.91	0.52
2:N:842:ASP:OD1	2:N:843:PRO:HD2	2.08	0.52
4:P:54:LEU:O	4:P:58:LYS:HG2	2.08	0.52
5:Q:71:THR:HG23	5:Q:99:HIS:HD2	1.73	0.52
5:Q:96:ASP:OD2	5:Q:97:HIS:ND1	2.43	0.52
5:Q:147:LYS:HE3	5:Q:149:ILE:HD11	1.91	0.52
6:R:100:ASP:N	6:R:100:ASP:OD1	2.42	0.52
8:T:108:HIS:O	8:T:108:HIS:ND1	2.42	0.52
11:W:21:LYS:HG3	11:W:22:ILE:HG23	1.91	0.52
1:A:66:CYS:HB3	1:A:76:HIS:CE1	2.43	0.52
1:A:722:GLY:O	1:A:724:TYR:HD1	1.92	0.52
2:B:523:ARG:HE	2:B:745:TYR:HE2	1.58	0.52
11:K:21:LYS:HG3	11:K:22:ILE:HG23	1.92	0.52
1:M:611:LEU:HD23	1:M:1204:GLU:HA	1.91	0.52
1:M:1522:PRO:O	1:M:1548:ASN:ND2	2.42	0.52
2:N:728:ARG:HH22	3:O:99:GLN:NE2	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:985:LEU:HD12	2:N:988:ALA:HB3	1.90	0.52
2:B:91:SER:O	7:S:132:GLU:HG3	2.09	0.52
2:B:93:GLU:OE2	7:S:99:SER:OG	2.15	0.52
2:B:1060:GLU:OE1	2:B:1060:GLU:N	2.36	0.52
2:B:1163:THR:HG22	2:B:1168:LYS:HG2	1.90	0.52
3:C:246:ILE:HD12	3:C:251:ALA:HA	1.91	0.52
5:E:96:ASP:OD2	5:E:97:HIS:ND1	2.43	0.52
7:S:58:GLU:OE2	7:S:60:SER:N	2.43	0.52
11:W:60:VAL:HA	11:W:81:THR:HG22	1.91	0.52
1:A:109:PHE:CZ	1:A:335:LEU:HD21	2.45	0.52
1:A:326:THR:HG23	1:A:329:ARG:NH1	2.24	0.52
2:B:217:CYS:SG	2:B:337:VAL:HG22	2.49	0.52
3:C:114:ALA:HB2	3:C:191:ILE:HG23	1.91	0.52
5:E:180:ALA:HA	5:E:185:LEU:HD12	1.90	0.52
1:M:218:PHE:O	1:M:222:ILE:HG23	2.10	0.52
1:M:481:GLY:HA2	2:N:1057:GLY:HA3	1.91	0.52
1:M:722:GLY:O	1:M:724:TYR:HD1	1.92	0.52
1:M:1279:VAL:HG23	9:U:53:PHE:CE2	2.45	0.52
2:N:523:ARG:HE	2:N:745:TYR:HE2	1.58	0.52
2:N:755:ASN:OD1	2:N:1017:TYR:HD1	1.93	0.52
1:A:106:CYS:SG	1:A:231:CYS:N	2.83	0.52
2:B:509:THR:CG2	2:B:516:GLY:H	2.23	0.52
2:B:715:GLY:HA2	2:B:750:TYR:CE1	2.45	0.52
1:M:109:PHE:CZ	1:M:335:LEU:HD21	2.45	0.52
1:M:634:TYR:O	1:M:637:CYS:N	2.38	0.52
2:N:836:ILE:HD13	12:X:56:ARG:HE	1.75	0.52
2:N:1032:ARG:HH12	2:N:1035:GLY:HA3	1.75	0.52
6:R:69:ARG:HD2	6:R:136:TRP:NE1	2.25	0.52
7:S:98:PRO:HD3	7:S:124:PHE:CE2	2.45	0.52
8:T:13:VAL:HB	8:T:52:ASP:N	2.25	0.52
1:A:401:ILE:HG13	1:A:437:LEU:HD13	1.91	0.52
1:A:639:SER:HA	1:A:682:LEU:HD11	1.91	0.52
2:B:613:TYR:CE2	2:B:615:PRO:HG3	2.45	0.52
2:B:742:HIS:NE2	2:B:747:LEU:HB3	2.25	0.52
3:C:122:PHE:HA	3:C:137:ASP:OD1	2.10	0.52
8:H:14:THR:OG1	8:H:28:THR:O	2.24	0.52
1:M:12:LYS:HB3	2:N:1172:GLU:OE2	2.10	0.52
1:M:98:LEU:HD23	1:M:360:PHE:HE2	1.73	0.52
1:M:545:GLN:HE21	1:M:549:GLY:HA2	1.75	0.52
1:M:1038:LYS:HG2	1:M:1638:PHE:HD2	1.74	0.52
2:N:245:LYS:HG2	2:N:450:THR:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:PHE:HE2	1:A:1636:MET:HB3	1.75	0.52
1:M:902:LEU:HD22	1:M:968:ARG:HH21	1.74	0.52
2:N:514:PRO:HA	2:N:517:LEU:HD12	1.91	0.52
3:O:89:VAL:N	12:X:59:GLN:HE22	2.07	0.52
3:O:109:LEU:HD23	3:O:225:LYS:HB3	1.92	0.52
3:O:247:GLU:HA	3:O:273:LYS:O	2.10	0.52
5:Q:60:TYR:HB2	5:Q:72:ILE:O	2.10	0.52
8:T:66:PRO:O	8:T:70:GLU:HG2	2.09	0.52
11:W:51:ARG:HG3	11:W:63:CYS:SG	2.49	0.52
1:A:576:LEU:HD23	1:A:579:SER:HA	1.92	0.52
1:A:731:PRO:O	1:A:745:GLN:NE2	2.42	0.52
1:A:1075:HIS:HB2	1:A:1182:ARG:NH2	2.24	0.52
3:C:285:VAL:O	3:C:287:ARG:HG3	2.10	0.52
5:E:60:TYR:HB2	5:E:72:ILE:O	2.10	0.52
7:G:98:PRO:HD3	7:G:124:PHE:CE2	2.45	0.52
1:M:743:GLY:HA2	1:M:746:ILE:HD12	1.91	0.52
3:O:246:ILE:HD12	3:O:251:ALA:HA	1.91	0.52
7:S:7:TYR:HD2	7:S:82:SER:HB3	1.73	0.52
7:S:10:THR:HG22	7:S:77:ASP:HB3	1.92	0.52
1:A:560:GLU:HG2	3:O:90:TYR:CE1	2.44	0.51
1:A:893:GLU:HB2	1:A:985:TYR:CZ	2.44	0.51
7:G:99:SER:HA	7:G:115:ARG:HH11	1.75	0.51
8:H:13:VAL:HB	8:H:52:ASP:N	2.25	0.51
9:I:10:CYS:SG	9:I:11:SER:N	2.83	0.51
12:L:22:TYR:HD2	12:L:51:LYS:HA	1.75	0.51
1:M:88:HIS:CE1	1:M:90:LEU:HB2	2.45	0.51
3:O:48:VAL:HG11	11:W:109:PHE:CD1	2.40	0.51
3:O:140:VAL:HA	3:O:213:ALA:O	2.11	0.51
9:U:10:CYS:SG	9:U:11:SER:N	2.83	0.51
9:U:25:THR:HG21	9:U:39:PHE:HZ	1.75	0.51
1:A:1642:CYS:SG	1:A:1643:HIS:N	2.83	0.51
2:B:689:THR:HB	2:B:692:SER:HB3	1.93	0.51
1:M:6:PRO:HA	7:S:69:PHE:HE2	1.74	0.51
1:M:634:TYR:CZ	2:N:768:MET:HB2	2.45	0.51
1:M:637:CYS:O	1:M:641:ASN:N	2.42	0.51
4:P:56:TYR:CD1	7:S:106:LEU:HA	2.46	0.51
5:Q:177:ASP:OD1	5:Q:179:VAL:HG22	2.09	0.51
1:A:110:LYS:HB2	1:A:225:ARG:HB2	1.91	0.51
1:A:611:LEU:HD23	1:A:1204:GLU:HA	1.91	0.51
1:A:797:ASP:H	1:A:800:SER:HG	1.56	0.51
3:C:204:ARG:H	3:C:207:GLN:HE21	1.55	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:58:GLU:OE2	7:G:60:SER:N	2.43	0.51
9:I:25:THR:HG21	9:I:39:PHE:HZ	1.75	0.51
1:M:110:LYS:HB2	1:M:225:ARG:HB2	1.91	0.51
2:N:39:LEU:HD11	2:N:385:GLY:HA3	1.92	0.51
2:N:613:TYR:CE2	2:N:615:PRO:HG3	2.45	0.51
2:N:763:TYR:CE2	2:N:922:PRO:HD3	2.44	0.51
2:N:928:MET:HB3	10:V:42:ARG:HD3	1.91	0.51
1:A:88:HIS:CE1	1:A:90:LEU:HB2	2.46	0.51
1:A:513:LEU:HD22	1:A:597:VAL:HG11	1.92	0.51
1:A:634:TYR:O	1:A:637:CYS:N	2.38	0.51
1:A:733:ALA:O	8:H:77:TYR:N	2.43	0.51
3:C:111:PRO:HB3	10:J:6:ARG:HH21	1.75	0.51
3:C:140:VAL:HA	3:C:213:ALA:O	2.11	0.51
5:E:147:LYS:HE3	5:E:149:ILE:HD11	1.91	0.51
1:M:715:ALA:O	1:M:827:VAL:HG23	2.11	0.51
2:N:9:GLU:HG3	10:V:22:LEU:HD21	1.91	0.51
2:N:232:LEU:HD23	2:N:238:MET:HG2	1.92	0.51
2:N:354:ARG:HH12	2:N:358:ALA:HB2	1.76	0.51
2:N:689:THR:HB	2:N:692:SER:HB3	1.93	0.51
3:O:77:LEU:HD11	3:O:323:LEU:HB3	1.91	0.51
1:A:545:GLN:HE21	1:A:549:GLY:HA2	1.75	0.51
1:A:1126:ASP:OD2	5:E:204:ASN:HB2	2.10	0.51
2:B:312:ARG:NH1	2:B:322:THR:O	2.40	0.51
2:B:877:ASP:OD1	2:B:881:SER:OG	2.18	0.51
5:E:128:GLU:HA	5:E:129:THR:OG1	2.10	0.51
5:E:128:GLU:OE2	5:E:184:GLY:HA2	2.11	0.51
1:M:504:GLY:HA2	1:M:622:ARG:O	2.09	0.51
1:M:680:ASP:N	1:M:680:ASP:OD2	2.44	0.51
1:M:998:ARG:NE	1:M:1000:LEU:HD23	2.26	0.51
1:M:1674:THR:HB	6:R:82:ARG:HB2	1.91	0.51
2:N:999:TYR:HB3	2:N:1004:GLY:O	2.11	0.51
5:Q:128:GLU:OE2	5:Q:184:GLY:HA2	2.11	0.51
8:T:70:GLU:HG3	8:T:71:ALA:N	2.24	0.51
1:A:605:LEU:HD12	1:A:619:HIS:ND1	2.26	0.51
1:A:612:HIS:HA	1:A:1200:GLN:CD	2.31	0.51
2:B:39:LEU:HD11	2:B:385:GLY:HA3	1.92	0.51
2:B:191:ASN:ND2	2:B:218:VAL:HG12	2.24	0.51
2:B:562:GLN:HB2	2:B:626:TYR:HD1	1.76	0.51
2:B:882:GLU:OE1	2:B:882:GLU:N	2.43	0.51
3:C:140:VAL:HG23	3:C:177:LYS:HB2	1.93	0.51
8:H:47:TYR:CD1	8:H:74:TYR:HB2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:106:CYS:SG	1:M:231:CYS:N	2.83	0.51
1:M:374:PRO:O	1:M:385:ASN:ND2	2.44	0.51
1:M:1245:PRO:O	1:M:1546:GLY:N	2.42	0.51
2:N:40:THR:HG23	2:N:41:ASN:H	1.75	0.51
2:N:123:TRP:NE1	2:N:422:LEU:HG	2.22	0.51
8:T:82:ARG:HB3	8:T:94:TYR:HB2	1.93	0.51
2:B:4:GLN:HB3	2:B:7:GLU:HB2	1.93	0.51
3:C:51:THR:OG1	3:C:59:VAL:O	2.23	0.51
3:C:109:LEU:HD23	3:C:225:LYS:HB3	1.92	0.51
6:F:100:ASP:OD1	6:F:100:ASP:N	2.42	0.51
7:G:10:THR:HG22	7:G:77:ASP:HB3	1.92	0.51
11:K:20:GLU:HB3	11:K:23:ILE:HD11	1.93	0.51
1:M:841:PHE:O	2:N:761:ILE:HD12	2.11	0.51
1:M:1642:CYS:SG	1:M:1643:HIS:N	2.83	0.51
2:N:271:ILE:HD13	2:N:353:ILE:HG23	1.92	0.51
2:N:290:ARG:HD3	9:U:16:LEU:HD22	1.93	0.51
3:O:122:PHE:HA	3:O:137:ASP:OD1	2.10	0.51
3:O:285:VAL:O	3:O:287:ARG:HG3	2.10	0.51
1:A:328:VAL:HA	1:A:331:HIS:ND1	2.26	0.51
2:B:271:ILE:HD13	2:B:353:ILE:HG23	1.92	0.51
2:B:354:ARG:HH12	2:B:358:ALA:HB2	1.76	0.51
2:B:653:GLU:N	2:B:653:GLU:OE1	2.44	0.51
2:B:755:ASN:OD1	2:B:1017:TYR:HD1	1.93	0.51
2:B:1032:ARG:HH12	2:B:1035:GLY:HA3	1.75	0.51
2:B:1043:GLN:HE21	2:B:1154:VAL:HG21	1.76	0.51
3:C:246:ILE:HD11	3:C:275:ALA:HB3	1.93	0.51
1:M:471:LYS:NZ	1:M:476:ARG:HH21	2.07	0.51
2:N:562:GLN:HB2	2:N:626:TYR:HD1	1.76	0.51
2:B:40:THR:HG23	2:B:41:ASN:H	1.75	0.51
2:B:767:ASP:HA	2:B:771:ALA:HB3	1.93	0.51
2:N:742:HIS:NE2	2:N:747:LEU:HB3	2.25	0.51
1:A:510:ALA:HA	1:A:597:VAL:HG22	1.93	0.51
1:A:1522:PRO:O	1:A:1548:ASN:ND2	2.42	0.51
1:A:1642:CYS:O	1:A:1646:THR:HG23	2.10	0.51
2:B:24:ASP:HA	2:B:27:LYS:HE2	1.92	0.51
2:B:245:LYS:HG2	2:B:450:THR:HA	1.91	0.51
3:C:223:HIS:CD2	3:C:225:LYS:HG2	2.46	0.51
1:M:605:LEU:HD12	1:M:619:HIS:ND1	2.26	0.51
1:M:613:LYS:HG2	1:M:614:PRO:HD3	1.93	0.51
2:N:163:LYS:HB3	2:N:720:TYR:CD1	2.46	0.51
2:N:191:ASN:ND2	2:N:218:VAL:HG12	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:818:PRO:O	2:N:822:TRP:HB2	2.11	0.51
3:O:140:VAL:HG23	3:O:177:LYS:HB2	1.93	0.51
5:Q:143:GLU:HB2	5:Q:144:LEU:HD12	1.92	0.51
12:X:22:TYR:HD2	12:X:51:LYS:HA	1.75	0.51
1:A:19:TYR:O	2:B:1166:ASN:ND2	2.42	0.50
1:A:182:ARG:O	1:A:186:VAL:HG23	2.11	0.50
1:A:218:PHE:O	1:A:222:ILE:HG23	2.10	0.50
1:A:715:ALA:O	1:A:827:VAL:HG23	2.11	0.50
1:A:1073:GLN:HA	1:A:1076:LEU:HG	1.92	0.50
2:B:999:TYR:HB3	2:B:1004:GLY:O	2.11	0.50
7:G:10:THR:HA	7:G:77:ASP:HA	1.92	0.50
1:M:107:HIS:O	1:M:338:LYS:HD2	2.11	0.50
2:N:547:ASP:OD1	2:N:547:ASP:N	2.43	0.50
3:O:37:TRP:NE1	11:W:97:ASP:HB3	2.26	0.50
5:Q:128:GLU:HA	5:Q:129:THR:OG1	2.10	0.50
2:B:502:GLY:N	2:B:681:VAL:HG23	2.26	0.50
3:C:266:GLU:HB2	3:C:274:GLN:HB2	1.93	0.50
5:E:8:ILE:HG13	5:E:41:PHE:HE2	1.76	0.50
1:M:576:LEU:HD23	1:M:579:SER:HA	1.92	0.50
2:N:1043:GLN:HE21	2:N:1154:VAL:HG21	1.76	0.50
5:Q:8:ILE:HG13	5:Q:41:PHE:HE2	1.76	0.50
7:S:51:TYR:HA	7:S:77:ASP:O	2.11	0.50
1:A:129:GLY:HA2	1:A:207:LEU:HD21	1.94	0.50
1:A:239:ARG:HD2	1:A:240:LYS:O	2.11	0.50
1:A:559:ILE:O	1:A:563:THR:OG1	2.22	0.50
1:A:613:LYS:HG2	1:A:614:PRO:HD3	1.93	0.50
1:A:998:ARG:NE	1:A:1000:LEU:HD23	2.26	0.50
3:C:259:PRO:O	3:C:262:VAL:HG12	2.12	0.50
1:M:66:CYS:HB3	1:M:76:HIS:CE1	2.43	0.50
1:M:475:PHE:HA	1:M:479:MET:HB3	1.93	0.50
1:M:1238:ALA:HB1	1:M:1618:TYR:HE2	1.76	0.50
1:M:1642:CYS:O	1:M:1646:THR:HG23	2.10	0.50
2:N:208:TYR:OH	2:N:238:MET:HG3	2.11	0.50
8:T:47:TYR:CD1	8:T:74:TYR:HB2	2.46	0.50
1:A:212:LYS:HD3	1:A:1628:TYR:CE1	2.44	0.50
1:A:372:PHE:HE1	2:B:1157:TYR:HA	1.74	0.50
1:A:687:GLN:HG2	1:A:688:ASP:H	1.75	0.50
1:A:1154:ASP:N	1:A:1154:ASP:OD1	2.45	0.50
1:A:1574:ARG:HG2	1:A:1575:ILE:HG23	1.93	0.50
1:A:1579:GLU:HB3	5:E:146:PRO:HD2	1.92	0.50
2:B:232:LEU:HD23	2:B:238:MET:HG2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:818:PRO:O	2:B:822:TRP:HB2	2.11	0.50
7:G:51:TYR:HA	7:G:77:ASP:O	2.11	0.50
7:G:98:PRO:HB3	7:G:124:PHE:CB	2.42	0.50
1:M:67:HIS:CG	2:N:1102:ILE:HD11	2.46	0.50
1:M:1038:LYS:NZ	1:M:1626:ILE:HA	2.27	0.50
1:M:1615:GLU:HG3	1:M:1617:GLY:H	1.76	0.50
2:N:4:GLN:HB3	2:N:7:GLU:HB2	1.93	0.50
2:N:205:GLY:O	2:N:207:SER:N	2.44	0.50
2:N:502:GLY:N	2:N:681:VAL:HG23	2.26	0.50
5:Q:130:PHE:HE1	5:Q:181:ARG:HG3	1.77	0.50
1:A:106:CYS:HA	1:A:231:CYS:CB	2.39	0.50
1:A:374:PRO:O	1:A:385:ASN:ND2	2.44	0.50
1:A:581:TYR:CE2	2:B:1110:ALA:HB2	2.47	0.50
1:A:1481:ASP:HB2	1:A:1491:THR:HB	1.93	0.50
2:B:205:GLY:O	2:B:207:SER:N	2.44	0.50
5:E:143:GLU:HB2	5:E:144:LEU:HD12	1.92	0.50
1:M:182:ARG:O	1:M:186:VAL:HG23	2.11	0.50
1:M:612:HIS:HA	1:M:1200:GLN:CD	2.31	0.50
1:M:687:GLN:HG2	1:M:688:ASP:H	1.75	0.50
2:N:505:CYS:HB2	2:N:683:SER:HB2	1.93	0.50
2:N:715:GLY:HA2	2:N:750:TYR:CE1	2.45	0.50
3:O:223:HIS:CD2	3:O:225:LYS:HG2	2.46	0.50
10:V:43:TYR:HA	10:V:46:ARG:HB3	1.94	0.50
1:A:368:PRO:HD2	1:A:373:ARG:HD3	1.93	0.50
1:A:1282:THR:OG1	1:A:1298:ALA:O	2.28	0.50
2:B:91:SER:OG	7:S:132:GLU:HG2	2.11	0.50
2:B:180:LYS:NZ	2:B:463:VAL:HB	2.26	0.50
2:B:492:THR:OG1	2:B:493:VAL:N	2.33	0.50
2:B:991:ASN:OD1	2:B:992:TYR:N	2.44	0.50
2:N:502:GLY:H	2:N:681:VAL:HG23	1.76	0.50
5:Q:131:GLN:HE21	5:Q:134:ASP:HB2	1.76	0.50
6:R:134:GLU:OE1	6:R:134:GLU:N	2.45	0.50
1:A:744:LYS:HA	1:A:791:LEU:HD23	1.94	0.50
3:C:122:PHE:HE2	3:C:125:PRO:HD3	1.77	0.50
5:E:131:GLN:HE21	5:E:134:ASP:HB2	1.76	0.50
7:G:135:ARG:NH2	7:G:145:GLU:OE1	2.45	0.50
10:J:3:ILE:HD11	10:J:49:ILE:HG22	1.92	0.50
1:M:475:PHE:HE2	1:M:1636:MET:HB3	1.75	0.50
1:M:1073:GLN:HA	1:M:1076:LEU:HG	1.92	0.50
1:M:1574:ARG:HG2	1:M:1575:ILE:HG23	1.93	0.50
2:N:99:ARG:NH2	12:X:47:ARG:NH1	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:259:PRO:O	3:O:262:VAL:HG12	2.12	0.50
7:S:10:THR:HA	7:S:77:ASP:HA	1.92	0.50
7:S:98:PRO:HB3	7:S:124:PHE:CB	2.42	0.50
1:A:483:ARG:HA	2:B:1054:ILE:O	2.10	0.50
1:A:607:ARG:HB2	1:A:649:MET:HE3	1.93	0.50
1:A:746:ILE:O	1:A:749:SER:OG	2.22	0.50
1:A:1086:TYR:HD1	1:A:1178:LEU:HD22	1.77	0.50
1:A:1238:ALA:HB1	1:A:1618:TYR:HE2	1.76	0.50
1:A:1550:LYS:HA	1:A:1553:TRP:CD1	2.46	0.50
2:B:547:ASP:N	2:B:547:ASP:OD1	2.43	0.50
7:G:145:GLU:OE2	7:G:148:LYS:NZ	2.45	0.50
1:M:106:CYS:HA	1:M:231:CYS:CB	2.39	0.50
1:M:510:ALA:HA	1:M:597:VAL:HG22	1.94	0.50
1:M:513:LEU:HD22	1:M:597:VAL:HG11	1.93	0.50
1:M:1052:ARG:NH1	1:M:1056:GLY:O	2.45	0.50
2:N:24:ASP:HA	2:N:27:LYS:HE2	1.92	0.50
2:N:577:LYS:HB2	2:N:613:TYR:CZ	2.47	0.50
2:N:767:ASP:HA	2:N:771:ALA:HB3	1.93	0.50
2:N:801:ARG:HG2	2:N:802:ARG:N	2.27	0.50
2:N:991:ASN:OD1	2:N:992:TYR:N	2.44	0.50
1:A:680:ASP:OD2	1:A:680:ASP:N	2.44	0.50
1:A:759:ARG:NH2	1:A:815:LEU:O	2.45	0.50
1:A:1549:LEU:HA	1:A:1552:ILE:HG12	1.94	0.50
2:B:208:TYR:OH	2:B:238:MET:HG3	2.11	0.50
2:B:505:CYS:SG	2:B:683:SER:N	2.77	0.50
7:G:113:ILE:HG21	7:G:170:LEU:HG	1.94	0.50
10:J:3:ILE:HD13	10:J:18:TRP:HB2	1.94	0.50
1:M:328:VAL:HA	1:M:331:HIS:ND1	2.26	0.50
1:M:1244:THR:O	1:M:1566:THR:HG21	2.12	0.50
10:V:3:ILE:HD11	10:V:49:ILE:HG22	1.92	0.50
1:A:1045:VAL:HB	1:A:1191:GLY:H	1.76	0.49
1:A:1052:ARG:HG2	1:A:1058:ILE:HA	1.94	0.49
2:B:502:GLY:H	2:B:681:VAL:HG23	1.76	0.49
5:E:136:ILE:HG13	5:E:137:VAL:HG13	1.94	0.49
10:J:43:TYR:HA	10:J:46:ARG:HB3	1.94	0.49
1:M:739:ILE:HD12	1:M:741:TRP:CH2	2.47	0.49
1:M:763:ASN:ND2	1:M:1084:LYS:HG3	2.27	0.49
1:M:1277:ARG:HB3	1:M:1302:ASP:HB3	1.94	0.49
1:M:1679:ILE:HD12	6:R:83:ILE:HG12	1.93	0.49
2:N:180:LYS:NZ	2:N:463:VAL:HB	2.26	0.49
2:N:583:LEU:HD23	2:N:611:ILE:HG12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:653:GLU:OE1	2:N:653:GLU:N	2.44	0.49
2:N:683:SER:OG	2:N:684:ILE:N	2.45	0.49
8:T:9:GLU:HB2	8:T:11:PHE:CE2	2.47	0.49
1:A:545:GLN:OE1	1:A:592:LYS:HD2	2.12	0.49
1:A:701:THR:CG2	1:A:743:GLY:H	2.25	0.49
1:A:763:ASN:ND2	1:A:1084:LYS:HG3	2.27	0.49
1:A:1244:THR:O	1:A:1566:THR:HG21	2.12	0.49
1:A:1615:GLU:HG3	1:A:1617:GLY:H	1.76	0.49
2:B:395:TRP:HE3	2:B:396:LEU:HD12	1.76	0.49
2:B:577:LYS:HB2	2:B:613:TYR:CZ	2.47	0.49
1:M:96:TYR:OH	1:M:100:ARG:NH2	2.33	0.49
1:M:701:THR:CG2	1:M:743:GLY:H	2.25	0.49
1:M:759:ARG:NH2	1:M:815:LEU:O	2.45	0.49
1:M:1596:TYR:HB2	1:M:1598:ILE:HG22	1.95	0.49
1:M:1672:PHE:CD1	2:N:1068:GLY:HA2	2.47	0.49
2:N:85:ALA:O	2:N:115:SER:OG	2.20	0.49
3:O:208:GLU:OE1	3:O:210:ASP:HB2	2.12	0.49
1:A:1596:TYR:HB2	1:A:1598:ILE:HG22	1.94	0.49
2:B:589:GLU:O	2:B:592:VAL:HG12	2.13	0.49
5:E:118:ILE:O	5:E:122:THR:HG23	2.12	0.49
1:M:483:ARG:HA	2:N:1054:ILE:O	2.12	0.49
1:M:1065:GLU:O	1:M:1067:SER:N	2.46	0.49
2:N:48:ALA:O	2:N:52:ILE:HG13	2.12	0.49
2:N:125:VAL:HG23	2:N:129:PRO:HG3	1.94	0.49
2:N:849:ASP:HB3	2:N:852:THR:OG1	2.12	0.49
6:R:125:ARG:HA	6:R:134:GLU:O	2.12	0.49
11:W:20:GLU:HB3	11:W:23:ILE:HD11	1.93	0.49
1:A:666:ILE:O	1:A:671:SER:OG	2.30	0.49
2:B:48:ALA:O	2:B:52:ILE:HG13	2.12	0.49
2:B:93:GLU:OE1	7:S:97:SER:HB2	2.12	0.49
2:B:163:LYS:HB3	2:B:720:TYR:CD1	2.46	0.49
2:B:468:ASN:ND2	2:B:710:THR:HB	2.27	0.49
2:B:822:TRP:N	2:B:822:TRP:CD1	2.80	0.49
4:D:56:TYR:CE1	7:G:106:LEU:HD23	2.47	0.49
8:H:82:ARG:HB3	8:H:94:TYR:HB2	1.93	0.49
1:M:239:ARG:HD2	1:M:240:LYS:O	2.12	0.49
1:M:666:ILE:O	1:M:671:SER:OG	2.30	0.49
1:M:1223:ASN:OD1	1:M:1224:VAL:N	2.46	0.49
3:O:238:PRO:HA	3:O:303:ARG:HA	1.95	0.49
5:Q:118:ILE:O	5:Q:122:THR:HG23	2.12	0.49
10:V:63:ASN:HB3	10:V:65:LEU:HD23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1148:TYR:HA	1:A:1151:LYS:HG2	1.93	0.49
1:A:1579:GLU:CB	5:E:146:PRO:HD2	2.42	0.49
2:B:280:PHE:O	2:B:284:ARG:HG2	2.12	0.49
2:B:335:VAL:HG23	2:B:336:LEU:N	2.28	0.49
2:B:433:ILE:O	2:B:436:LYS:N	2.44	0.49
2:B:966:SER:OG	2:B:966:SER:O	2.30	0.49
6:F:125:ARG:HA	6:F:134:GLU:O	2.12	0.49
6:F:134:GLU:N	6:F:134:GLU:OE1	2.45	0.49
9:I:10:CYS:HB2	9:I:17:LEU:HD21	1.95	0.49
1:M:775:TRP:O	8:T:20:LYS:HD2	2.12	0.49
2:N:191:ASN:HD22	2:N:217:CYS:HA	1.78	0.49
2:N:335:VAL:HG23	2:N:336:LEU:N	2.28	0.49
2:N:468:ASN:ND2	2:N:710:THR:HB	2.27	0.49
2:N:966:SER:OG	2:N:966:SER:O	2.30	0.49
3:O:122:PHE:HE2	3:O:125:PRO:HD3	1.77	0.49
3:O:141:PHE:HB3	3:O:174:LEU:HD22	1.95	0.49
3:O:246:ILE:HD11	3:O:275:ALA:HB3	1.93	0.49
3:O:266:GLU:HB2	3:O:274:GLN:HB2	1.93	0.49
3:O:339:LYS:HZ1	11:W:92:ARG:HA	1.77	0.49
5:Q:138:ASN:HD22	5:Q:141:HIS:CE1	2.30	0.49
6:R:96:PRO:HB2	7:S:23:ARG:HH11	1.78	0.49
10:V:16:ASP:OD1	10:V:16:ASP:N	2.46	0.49
1:A:1245:PRO:O	1:A:1546:GLY:N	2.42	0.49
1:A:1277:ARG:HB3	1:A:1302:ASP:HB3	1.94	0.49
2:B:505:CYS:HB2	2:B:683:SER:HB2	1.93	0.49
6:F:90:GLN:HE22	6:F:122:LEU:HD11	1.78	0.49
1:M:744:LYS:HA	1:M:791:LEU:HD23	1.94	0.49
1:M:1045:VAL:HB	1:M:1191:GLY:H	1.76	0.49
1:M:1129:PRO:HD2	1:M:1133:TYR:CE1	2.48	0.49
1:M:1481:ASP:HB2	1:M:1491:THR:HB	1.93	0.49
3:O:125:PRO:HB2	3:O:129:GLN:HB2	1.95	0.49
5:Q:136:ILE:HG13	5:Q:137:VAL:HG13	1.94	0.49
6:R:90:GLN:HE22	6:R:122:LEU:HD11	1.78	0.49
1:A:1052:ARG:NH1	1:A:1056:GLY:O	2.45	0.49
2:B:86:LYS:HB3	2:B:150:HIS:CE1	2.48	0.49
2:B:349:LEU:O	2:B:353:ILE:HG22	2.12	0.49
2:B:672:THR:HG23	2:B:673:HIS:ND1	2.27	0.49
4:D:17:LEU:HD21	7:G:6:LEU:O	2.12	0.49
5:E:130:PHE:HE1	5:E:181:ARG:HG3	1.77	0.49
1:M:368:PRO:HD2	1:M:373:ARG:HD3	1.93	0.49
1:M:746:ILE:O	1:M:749:SER:OG	2.22	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:1052:ARG:HG2	1:M:1058:ILE:HA	1.94	0.49
1:A:67:HIS:CG	2:B:1102:ILE:HD11	2.47	0.49
1:A:739:ILE:HD12	1:A:741:TRP:CH2	2.47	0.49
1:A:1038:LYS:NZ	1:A:1626:ILE:HA	2.27	0.49
1:A:1672:PHE:CD1	2:B:1068:GLY:HA2	2.47	0.49
2:B:93:GLU:CD	7:S:97:SER:HB2	2.33	0.49
2:B:849:ASP:HB3	2:B:852:THR:OG1	2.12	0.49
3:C:318:MET:HB2	3:C:323:LEU:HD22	1.94	0.49
10:J:63:ASN:HB3	10:J:65:LEU:HD23	1.94	0.49
2:N:86:LYS:HB3	2:N:150:HIS:CE1	2.48	0.49
2:N:108:GLU:HG2	12:X:48:VAL:HG11	1.94	0.49
2:N:163:LYS:HD2	2:N:720:TYR:CD2	2.48	0.49
2:N:395:TRP:HE3	2:N:396:LEU:HD12	1.77	0.49
2:N:589:GLU:O	2:N:592:VAL:HG12	2.13	0.49
2:N:672:THR:HG23	2:N:673:HIS:ND1	2.27	0.49
7:S:113:ILE:HG21	7:S:170:LEU:HG	1.94	0.49
7:S:135:ARG:NH2	7:S:145:GLU:OE1	2.45	0.49
8:T:78:GLY:HA3	8:T:97:PHE:HD1	1.78	0.49
1:M:227:GLN:OE1	1:M:227:GLN:N	2.46	0.49
1:M:1148:TYR:HA	1:M:1151:LYS:HG2	1.94	0.49
1:A:96:TYR:OH	1:A:100:ARG:NH2	2.33	0.49
1:A:853:GLN:HA	1:A:856:ASN:HD21	1.77	0.49
2:B:85:ALA:O	2:B:115:SER:OG	2.20	0.49
2:B:503:PHE:HE1	2:B:636:ARG:HB3	1.78	0.49
8:H:78:GLY:HA3	8:H:97:PHE:HD1	1.78	0.49
1:M:129:GLY:HA2	1:M:207:LEU:HD21	1.94	0.49
1:M:1306:ARG:NH2	1:M:1317:GLN:HG2	2.20	0.49
2:N:415:ASP:OD2	2:N:417:SER:OG	2.23	0.49
2:N:466:LYS:HE2	2:N:472:PHE:CE1	2.48	0.49
2:N:742:HIS:CE1	2:N:747:LEU:HB3	2.48	0.49
3:O:51:THR:OG1	3:O:59:VAL:O	2.23	0.49
9:U:35:PRO:HB2	9:U:38:GLN:HG3	1.95	0.49
1:A:475:PHE:HA	1:A:479:MET:HB3	1.93	0.48
1:A:1065:GLU:O	1:A:1067:SER:N	2.46	0.48
2:B:156:PRO:O	2:B:160:ILE:HG12	2.13	0.48
2:B:163:LYS:HD2	2:B:720:TYR:CD2	2.48	0.48
2:B:583:LEU:HD23	2:B:611:ILE:HG12	1.94	0.48
2:B:772:MET:SD	2:B:902:PHE:HB2	2.53	0.48
1:M:212:LYS:HD3	1:M:1628:TYR:CE1	2.44	0.48
1:M:1086:TYR:HD1	1:M:1178:LEU:HD22	1.77	0.48
1:M:1585:ILE:HD11	1:M:1609:ALA:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:156:PRO:O	2:N:160:ILE:HG12	2.13	0.48
2:N:280:PHE:O	2:N:284:ARG:HG2	2.12	0.48
2:N:776:LYS:O	2:N:780:GLU:HG3	2.13	0.48
2:N:882:GLU:OE1	2:N:882:GLU:N	2.43	0.48
3:O:51:THR:OG1	3:O:59:VAL:HG23	2.13	0.48
1:A:227:GLN:OE1	1:A:227:GLN:N	2.46	0.48
1:A:228:CYS:HB2	1:A:233:SER:H	1.78	0.48
1:A:844:ARG:HD2	2:B:995:ASN:HD21	1.77	0.48
2:B:125:VAL:HG23	2:B:129:PRO:HG3	1.94	0.48
2:B:830:GLY:O	2:B:845:VAL:HA	2.13	0.48
3:C:125:PRO:HB2	3:C:129:GLN:HB2	1.95	0.48
4:D:52:ARG:HA	4:D:55:MET:HE2	1.95	0.48
5:E:131:GLN:NE2	5:E:132:GLU:O	2.46	0.48
8:H:9:GLU:HB2	8:H:11:PHE:CE2	2.47	0.48
1:M:228:CYS:CB	1:M:231:CYS:HB3	2.44	0.48
1:M:1154:ASP:OD1	1:M:1154:ASP:N	2.45	0.48
1:M:1256:SER:O	1:M:1260:ALA:N	2.38	0.48
2:N:509:THR:HG21	2:N:516:GLY:H	1.78	0.48
2:N:592:VAL:O	2:N:596:ASN:ND2	2.46	0.48
2:N:880:ASP:H	12:X:38:VAL:HG13	1.78	0.48
2:N:928:MET:HG3	10:V:44:CYS:HB3	1.95	0.48
3:O:145:LYS:O	3:O:208:GLU:HG2	2.13	0.48
7:S:145:GLU:OE2	7:S:148:LYS:NZ	2.45	0.48
9:U:10:CYS:HB2	9:U:17:LEU:HD21	1.95	0.48
10:V:3:ILE:HD13	10:V:18:TRP:HB2	1.94	0.48
12:X:31:ASN:ND2	12:X:42:ARG:H	2.08	0.48
1:A:112:SER:OG	1:A:114:VAL:HG12	2.13	0.48
1:A:1129:PRO:HD2	1:A:1133:TYR:CE1	2.48	0.48
1:A:1520:GLU:OE1	1:A:1523:GLY:N	2.40	0.48
2:B:466:LYS:HE2	2:B:472:PHE:CE1	2.48	0.48
2:B:592:VAL:O	2:B:596:ASN:ND2	2.46	0.48
2:B:801:ARG:HG2	2:B:802:ARG:N	2.27	0.48
3:C:85:ALA:HB3	3:C:226:PHE:CE1	2.49	0.48
3:C:141:PHE:HB3	3:C:174:LEU:HD22	1.95	0.48
5:E:138:ASN:HD22	5:E:141:HIS:CE1	2.30	0.48
1:M:125:LEU:HD11	1:M:130:LEU:HD22	1.95	0.48
1:M:1549:LEU:HA	1:M:1552:ILE:HG12	1.94	0.48
2:N:825:LYS:HG3	2:N:842:ASP:OD1	2.13	0.48
2:N:830:GLY:O	2:N:845:VAL:HA	2.14	0.48
3:O:318:MET:HB2	3:O:323:LEU:HD22	1.94	0.48
1:A:1242:ILE:HG21	1:A:1567:ASN:ND2	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1585:ILE:HD11	1:A:1609:ALA:HA	1.95	0.48
1:A:1624:MET:HG2	1:A:1625:GLY:N	2.28	0.48
3:C:208:GLU:OE1	3:C:210:ASP:HB2	2.12	0.48
3:C:238:PRO:HA	3:C:303:ARG:HA	1.95	0.48
1:M:112:SER:OG	1:M:114:VAL:HG12	2.13	0.48
1:M:501:ASN:HA	1:M:669:THR:HG21	1.96	0.48
1:M:545:GLN:OE1	1:M:592:LYS:HD2	2.12	0.48
1:M:1095:VAL:HG23	1:M:1096:LYS:HD2	1.95	0.48
1:M:1129:PRO:HD2	1:M:1133:TYR:HE1	1.79	0.48
1:M:1284:LYS:HB3	1:M:1296:THR:HB	1.95	0.48
2:N:479:VAL:HG12	2:N:480:HIS:N	2.29	0.48
5:Q:107:ALA:HA	5:Q:108:ASN:HA	1.60	0.48
5:Q:131:GLN:NE2	5:Q:132:GLU:O	2.47	0.48
7:S:99:SER:HA	7:S:115:ARG:HH11	1.75	0.48
8:T:80:VAL:HA	8:T:95:VAL:HA	1.95	0.48
1:A:1284:LYS:HB3	1:A:1296:THR:HB	1.95	0.48
2:B:415:ASP:OD2	2:B:417:SER:OG	2.22	0.48
2:B:649:LEU:HD12	2:B:653:GLU:HB2	1.95	0.48
3:C:150:ASN:HB2	3:C:165:VAL:HG13	1.95	0.48
1:M:853:GLN:HA	1:M:856:ASN:HD21	1.78	0.48
1:M:1550:LYS:HA	1:M:1553:TRP:CD1	2.46	0.48
2:N:243:TRP:HD1	2:N:244:ARG:HG2	1.72	0.48
2:N:649:LEU:HD12	2:N:653:GLU:HB2	1.96	0.48
2:N:772:MET:SD	2:N:902:PHE:HB2	2.53	0.48
1:A:107:HIS:O	1:A:338:LYS:HD2	2.11	0.48
1:A:241:GLU:N	1:A:245:LYS:O	2.47	0.48
1:A:1129:PRO:HD2	1:A:1133:TYR:HE1	1.78	0.48
2:B:402:GLN:NE2	2:B:428:LYS:HD3	2.29	0.48
2:B:479:VAL:HG12	2:B:480:HIS:N	2.29	0.48
2:B:742:HIS:CE1	2:B:747:LEU:HB3	2.48	0.48
2:B:801:ARG:HG2	2:B:802:ARG:H	1.79	0.48
2:B:1082:ASP:N	2:B:1082:ASP:OD1	2.47	0.48
1:M:1126:ASP:OD2	5:Q:204:ASN:HB2	2.14	0.48
1:M:1151:LYS:NZ	1:M:1152:ASN:HB3	2.28	0.48
1:M:1624:MET:HG2	1:M:1625:GLY:N	2.28	0.48
2:N:107:ARG:HH11	2:N:721:ARG:HH22	1.61	0.48
2:N:349:LEU:O	2:N:353:ILE:HG22	2.12	0.48
3:O:167:SER:OG	3:O:203:LEU:O	2.17	0.48
1:A:1339:TYR:CE2	1:A:1508:LEU:HD21	2.49	0.48
2:B:191:ASN:HD22	2:B:217:CYS:HA	1.78	0.48
2:B:266:GLU:HA	2:B:269:GLU:OE1	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:325:GLU:CD	2:B:328:ARG:HE	2.17	0.48
11:K:62:PHE:HB3	11:K:80:GLN:HB2	1.96	0.48
2:N:433:ILE:HA	2:N:436:LYS:HZ2	1.78	0.48
2:N:999:TYR:CD2	2:N:1006:GLU:HB3	2.49	0.48
2:N:1159:THR:O	2:N:1163:THR:HG23	2.14	0.48
1:A:711:LEU:HD23	1:A:746:ILE:HD13	1.95	0.48
1:A:1151:LYS:HZ3	1:A:1152:ASN:HB3	1.79	0.48
1:A:1151:LYS:NZ	1:A:1152:ASN:HB3	2.28	0.48
2:B:123:TRP:HE1	2:B:422:LEU:CG	2.24	0.48
2:B:537:ILE:HB	2:B:538:PRO:HD3	1.95	0.48
2:B:604:LYS:HG3	2:B:605:VAL:HG13	1.96	0.48
3:C:145:LYS:O	3:C:208:GLU:HG2	2.14	0.48
1:M:98:LEU:O	1:M:102:THR:HG23	2.14	0.48
1:M:241:GLU:N	1:M:245:LYS:O	2.47	0.48
1:M:1040:LEU:HA	1:M:1043:LEU:HD23	1.95	0.48
1:M:1339:TYR:CE2	1:M:1508:LEU:HD21	2.49	0.48
2:N:336:LEU:HD22	2:N:338:HIS:HE1	1.79	0.48
2:N:822:TRP:N	2:N:822:TRP:CD1	2.80	0.48
5:Q:111:THR:HG23	5:Q:114:ALA:HB3	1.96	0.48
10:V:23:THR:HA	10:V:26:GLN:HB3	1.96	0.48
1:A:1123:PRO:HG2	5:E:203:TYR:HA	1.94	0.48
2:B:1100:SER:HA	2:B:1113:VAL:HG12	1.96	0.48
5:E:111:THR:HG23	5:E:114:ALA:HB3	1.96	0.48
8:H:80:VAL:HG12	8:H:117:ASP:O	2.13	0.48
9:I:35:PRO:HB2	9:I:38:GLN:HG3	1.95	0.48
1:M:850:LEU:HD13	1:M:929:LEU:HB3	1.95	0.48
2:N:55:LYS:O	2:N:76:SER:HA	2.14	0.48
2:N:266:GLU:HA	2:N:269:GLU:OE1	2.14	0.48
2:N:1060:GLU:OE1	2:N:1060:GLU:N	2.36	0.48
2:N:1082:ASP:OD1	2:N:1082:ASP:N	2.47	0.48
3:O:39:LEU:HD22	11:W:100:ASP:HB3	1.96	0.48
1:A:98:LEU:O	1:A:102:THR:HG23	2.14	0.48
2:B:637:PRO:HA	2:B:647:ASP:O	2.14	0.48
2:B:998:MET:SD	2:B:1013:ILE:HD11	2.54	0.48
2:B:1159:THR:O	2:B:1163:THR:HG23	2.14	0.48
1:M:228:CYS:HB2	1:M:233:SER:H	1.78	0.48
1:M:1242:ILE:HG21	1:M:1567:ASN:ND2	2.27	0.48
2:N:919:VAL:CG2	3:O:78:ILE:HG21	2.44	0.48
2:N:1100:SER:HA	2:N:1113:VAL:HG12	1.96	0.48
3:O:37:TRP:CD1	11:W:97:ASP:HB3	2.49	0.48
3:O:85:ALA:HA	3:O:112:ILE:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:LEU:HD11	1:A:130:LEU:HD22	1.95	0.47
1:A:1069:ASP:OD1	1:A:1070:VAL:HG22	2.14	0.47
1:A:1205:PRO:HA	1:A:1208:GLN:HB2	1.96	0.47
1:A:1299:ILE:O	1:A:1491:THR:HA	2.14	0.47
8:H:37:ASN:O	8:H:104:ILE:HD12	2.14	0.47
10:J:16:ASP:N	10:J:16:ASP:OD1	2.46	0.47
1:M:1046:GLN:OE1	1:M:1052:ARG:N	2.45	0.47
1:M:1309:TYR:CZ	1:M:1320:ILE:HD11	2.49	0.47
2:N:325:GLU:CD	2:N:328:ARG:HE	2.17	0.47
2:N:492:THR:OG1	2:N:493:VAL:N	2.33	0.47
3:O:150:ASN:HB2	3:O:165:VAL:HG13	1.95	0.47
4:P:52:ARG:HA	4:P:55:MET:HE3	1.95	0.47
1:A:1588:GLU:O	1:A:1592:VAL:HG23	2.15	0.47
2:B:776:LYS:O	2:B:780:GLU:HG3	2.13	0.47
8:H:74:TYR:HB3	8:H:123:LEU:HB3	1.96	0.47
8:H:80:VAL:HA	8:H:95:VAL:HA	1.95	0.47
1:M:63:CYS:HB3	1:M:66:CYS:SG	2.54	0.47
1:M:767:LYS:HD3	1:M:783:SER:HB3	1.95	0.47
1:M:1206:SER:OG	1:M:1207:THR:N	2.47	0.47
1:M:1235:ILE:HG23	1:M:1612:MET:HE1	1.96	0.47
1:A:1095:VAL:HG23	1:A:1096:LYS:HD2	1.95	0.47
1:A:1309:TYR:CZ	1:A:1320:ILE:HD11	2.49	0.47
2:B:75:ILE:HA	2:B:124:SER:O	2.15	0.47
2:B:683:SER:OG	2:B:684:ILE:N	2.45	0.47
2:B:825:LYS:HG3	2:B:842:ASP:OD1	2.14	0.47
1:M:711:LEU:HD23	1:M:746:ILE:HD13	1.95	0.47
3:O:130:GLU:OE2	3:O:130:GLU:N	2.31	0.47
3:O:130:GLU:HG2	3:O:131:ALA:H	1.78	0.47
7:S:5:SER:HG	7:S:81:PHE:HE1	1.61	0.47
8:T:30:VAL:HB	8:T:37:ASN:HD22	1.80	0.47
1:A:118:LEU:HB2	1:A:182:ARG:NH1	2.29	0.47
1:A:407:ASP:O	1:A:411:GLU:N	2.48	0.47
1:A:1066:ASP:OD1	1:A:1183:TYR:OH	2.29	0.47
1:A:1235:ILE:HG23	1:A:1612:MET:HE1	1.95	0.47
1:A:1247:MET:SD	1:A:1547:VAL:HA	2.54	0.47
3:C:115:ASP:OD2	3:C:118:MET:N	2.48	0.47
3:C:130:GLU:HG2	3:C:131:ALA:H	1.78	0.47
1:M:1041:GLU:OE2	2:N:1061:ARG:NH1	2.48	0.47
1:M:1069:ASP:OD1	1:M:1070:VAL:HG22	2.14	0.47
1:M:1588:GLU:O	1:M:1592:VAL:HG23	2.15	0.47
2:N:996:GLU:N	2:N:1011:ILE:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:95:SER:O	2:B:95:SER:OG	2.32	0.47
2:B:137:VAL:HA	2:B:431:ASN:O	2.15	0.47
2:B:336:LEU:HD22	2:B:338:HIS:HE1	1.79	0.47
2:B:420:LYS:O	2:B:423:THR:OG1	2.24	0.47
2:B:561:VAL:HG12	2:B:569:GLY:O	2.14	0.47
2:B:1130:ASP:OD1	2:B:1130:ASP:N	2.47	0.47
3:C:82:PRO:HB2	3:C:217:LEU:HD22	1.96	0.47
3:C:91:ILE:HD11	12:L:58:VAL:HB	1.97	0.47
3:C:155:THR:HG1	3:C:156:ASP:H	1.61	0.47
7:G:138:THR:HG22	7:G:142:ASN:O	2.14	0.47
1:M:1299:ILE:O	1:M:1491:THR:HA	2.14	0.47
2:N:503:PHE:HE1	2:N:636:ARG:HB3	1.78	0.47
2:N:998:MET:SD	2:N:1013:ILE:HD11	2.54	0.47
2:N:1162:LEU:HG	2:N:1167:ILE:O	2.14	0.47
7:S:138:THR:HG22	7:S:142:ASN:O	2.14	0.47
1:A:219:TYR:OH	1:A:347:TYR:OH	2.28	0.47
1:A:686:ILE:HB	1:A:687:GLN:OE1	2.15	0.47
1:A:1038:LYS:HG2	1:A:1638:PHE:HD2	1.74	0.47
1:A:1042:GLY:HA3	1:A:1053:ASP:OD2	2.14	0.47
2:B:55:LYS:O	2:B:76:SER:HA	2.14	0.47
1:M:496:PRO:HD2	2:N:766:TYR:CZ	2.49	0.47
3:O:85:ALA:HB3	3:O:226:PHE:CE1	2.49	0.47
8:T:17:ASP:OD1	8:T:17:ASP:N	2.47	0.47
1:A:228:CYS:CB	1:A:231:CYS:HB3	2.43	0.47
1:A:850:LEU:HD13	1:A:929:LEU:HB3	1.95	0.47
1:A:972:LEU:HA	1:A:972:LEU:HD23	1.61	0.47
1:A:1125:LEU:HD23	1:A:1136:SER:OG	2.15	0.47
1:A:1189:ASP:OD2	6:F:76:THR:HB	2.15	0.47
1:A:1206:SER:OG	1:A:1207:THR:N	2.47	0.47
1:A:1223:ASN:OD1	1:A:1224:VAL:N	2.46	0.47
2:B:37:ASN:OD1	2:B:147:ASN:HB2	2.15	0.47
2:B:55:LYS:HB3	2:B:400:ARG:HD2	1.97	0.47
2:B:219:ARG:HH11	2:B:223:SER:HB2	1.80	0.47
2:B:355:LYS:HG3	2:B:622:TYR:CD2	2.49	0.47
2:B:383:LEU:O	2:B:387:ILE:HG12	2.15	0.47
2:B:386:GLN:NE2	2:B:452:LEU:HD22	2.30	0.47
2:B:999:TYR:CD2	2:B:1006:GLU:HB3	2.49	0.47
3:C:51:THR:OG1	3:C:59:VAL:HG23	2.13	0.47
3:C:85:ALA:HA	3:C:112:ILE:HD12	1.96	0.47
5:E:151:LEU:HB2	5:E:190:VAL:HG13	1.97	0.47
7:G:54:ILE:HA	7:G:76:VAL:HG12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:72:ALA:HB2	8:H:122:LEU:HB3	1.97	0.47
1:M:84:ILE:HD11	1:M:401:ILE:HG21	1.96	0.47
1:M:114:VAL:HG22	1:M:182:ARG:NH1	2.29	0.47
1:M:407:ASP:O	1:M:411:GLU:N	2.48	0.47
1:M:880:SER:OG	1:M:881:THR:N	2.48	0.47
1:M:1062:HIS:NE2	1:M:1125:LEU:O	2.47	0.47
1:M:1125:LEU:HD23	1:M:1136:SER:OG	2.15	0.47
1:M:1579:GLU:OE2	5:Q:193:ILE:HD12	2.15	0.47
2:N:355:LYS:HG3	2:N:622:TYR:CD2	2.49	0.47
2:N:402:GLN:NE2	2:N:428:LYS:HD3	2.29	0.47
2:N:433:ILE:O	2:N:436:LYS:N	2.44	0.47
2:N:561:VAL:HG12	2:N:569:GLY:O	2.14	0.47
2:N:637:PRO:HA	2:N:647:ASP:O	2.14	0.47
2:N:693:ASP:OD2	2:N:969:PHE:N	2.36	0.47
2:N:1130:ASP:OD1	2:N:1130:ASP:N	2.47	0.47
2:N:1147:THR:HG22	2:N:1148:LEU:H	1.80	0.47
3:O:82:PRO:HB2	3:O:217:LEU:HD22	1.96	0.47
3:O:93:ASN:O	3:O:210:ASP:N	2.48	0.47
5:Q:116:LYS:HG3	5:Q:117:ILE:N	2.29	0.47
7:S:54:ILE:HA	7:S:76:VAL:HG12	1.96	0.47
8:T:25:SER:HB3	8:T:44:SER:OG	2.15	0.47
8:T:80:VAL:HG12	8:T:117:ASP:O	2.13	0.47
10:V:7:CYS:HB3	10:V:14:ILE:HD13	1.97	0.47
11:W:62:PHE:HB3	11:W:80:GLN:HB2	1.96	0.47
1:A:66:CYS:SG	1:A:73:CYS:CB	3.01	0.47
1:A:501:ASN:HA	1:A:669:THR:HG21	1.96	0.47
1:A:519:VAL:HG21	1:A:569:LEU:HD21	1.96	0.47
1:A:767:LYS:HD3	1:A:783:SER:HB3	1.95	0.47
2:B:1162:LEU:HG	2:B:1167:ILE:O	2.14	0.47
3:C:101:GLU:O	3:C:104:SER:OG	2.31	0.47
8:H:25:SER:HB3	8:H:44:SER:OG	2.15	0.47
1:M:3:ILE:HG22	7:S:68:PRO:HD3	1.96	0.47
1:M:610:THR:HG21	2:N:1060:GLU:HG3	1.96	0.47
1:M:1231:LEU:HA	1:M:1234:ILE:HG22	1.97	0.47
1:M:1589:VAL:HG13	1:M:1605:LEU:HD23	1.96	0.47
1:M:1674:THR:HA	1:M:1677:PHE:CZ	2.50	0.47
2:N:37:ASN:OD1	2:N:147:ASN:HB2	2.15	0.47
2:N:801:ARG:HG2	2:N:802:ARG:H	1.79	0.47
2:N:1088:VAL:HG12	2:N:1149:ILE:HD11	1.97	0.47
3:O:266:GLU:N	3:O:274:GLN:O	2.41	0.47
1:A:63:CYS:HB3	1:A:66:CYS:SG	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:ASN:OD1	1:A:238:PHE:N	2.46	0.47
1:A:472:GLU:HA	1:A:477:LYS:NZ	2.29	0.47
1:A:808:LEU:O	1:A:812:VAL:HG23	2.15	0.47
1:A:844:ARG:HD2	2:B:995:ASN:ND2	2.30	0.47
1:A:901:LYS:HG2	9:I:59:LEU:HD11	1.95	0.47
2:B:509:THR:HG21	2:B:516:GLY:H	1.78	0.47
2:B:772:MET:HG2	2:B:911:ILE:N	2.30	0.47
2:B:919:VAL:HG21	3:C:75:ARG:HD3	1.97	0.47
2:B:996:GLU:N	2:B:1011:ILE:O	2.47	0.47
5:E:116:LYS:HG3	5:E:117:ILE:N	2.29	0.47
5:E:117:ILE:HD12	5:E:117:ILE:HA	1.82	0.47
10:J:7:CYS:HB3	10:J:14:ILE:HD13	1.97	0.47
1:M:219:TYR:OH	1:M:347:TYR:OH	2.28	0.47
1:M:472:GLU:HA	1:M:477:LYS:NZ	2.29	0.47
1:M:512:LYS:HD3	2:N:1031:VAL:HG11	1.96	0.47
3:O:76:ILE:HG22	3:O:80:GLU:HB2	1.96	0.47
8:T:37:ASN:O	8:T:104:ILE:HD12	2.14	0.47
8:T:74:TYR:HB3	8:T:123:LEU:HB3	1.96	0.47
1:A:114:VAL:HG22	1:A:182:ARG:NH1	2.29	0.47
1:A:1040:LEU:HA	1:A:1043:LEU:HD23	1.96	0.47
2:B:107:ARG:HH11	2:B:721:ARG:HH22	1.62	0.47
3:C:129:GLN:OE1	3:C:129:GLN:N	2.48	0.47
7:G:84:LYS:HA	7:G:84:LYS:HD2	1.71	0.47
7:G:95:LEU:HG	7:G:102:GLY:HA3	1.97	0.47
1:M:364:ASN:N	1:M:364:ASN:OD1	2.48	0.47
1:M:675:VAL:HG12	1:M:682:LEU:HD22	1.97	0.47
1:M:1205:PRO:HA	1:M:1208:GLN:HB2	1.96	0.47
2:N:1:MET:O	2:N:963:ALA:HB3	2.15	0.47
2:N:86:LYS:HD3	2:N:148:ARG:HD2	1.97	0.47
2:N:185:LEU:HB2	2:N:378:LEU:CD2	2.44	0.47
3:O:342:LEU:N	11:W:22:ILE:HD11	2.30	0.47
7:S:95:LEU:HG	7:S:102:GLY:HA3	1.97	0.47
1:A:84:ILE:HD11	1:A:401:ILE:HG21	1.96	0.46
1:A:1110:TYR:CZ	1:A:1127:LYS:HE2	2.50	0.46
1:A:1269:LYS:HD2	1:A:1520:GLU:HG3	1.97	0.46
1:A:1282:THR:HG22	9:I:45:GLU:OE1	2.15	0.46
2:B:41:ASN:HD22	2:B:147:ASN:ND2	2.13	0.46
8:H:8:ASP:HA	8:H:58:GLN:HG2	1.97	0.46
1:M:1042:GLY:HA3	1:M:1053:ASP:OD2	2.14	0.46
1:M:1087:LYS:HA	1:M:1090:ILE:HG22	1.97	0.46
2:N:197:ILE:HD13	2:N:366:ALA:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:604:LYS:HG3	2:N:605:VAL:HG13	1.96	0.46
8:T:72:ALA:HB2	8:T:122:LEU:HB3	1.97	0.46
10:V:31:GLU:OE1	10:V:31:GLU:N	2.33	0.46
1:A:1633:PHE:HB2	1:A:1662:SER:HB2	1.98	0.46
2:B:197:ILE:HD13	2:B:366:ALA:HB2	1.97	0.46
2:B:610:GLU:HG2	2:B:633:ARG:NH2	2.30	0.46
2:B:807:VAL:HG23	2:B:850:GLU:HB2	1.96	0.46
3:C:74:ARG:O	3:C:78:ILE:HG22	2.15	0.46
3:C:266:GLU:N	3:C:274:GLN:O	2.41	0.46
11:K:25:LEU:HB2	11:K:36:THR:OG1	2.16	0.46
1:M:121:CYS:HB3	1:M:186:VAL:CG2	2.44	0.46
1:M:519:VAL:HG21	1:M:569:LEU:HD21	1.96	0.46
1:M:1110:TYR:CZ	1:M:1127:LYS:HE2	2.50	0.46
2:N:137:VAL:HA	2:N:431:ASN:O	2.15	0.46
2:N:690:PRO:HG3	2:N:905:ARG:NH2	2.31	0.46
2:N:693:ASP:OD1	2:N:693:ASP:N	2.32	0.46
3:O:115:ASP:OD2	3:O:118:MET:N	2.48	0.46
3:O:129:GLN:OE1	3:O:129:GLN:N	2.48	0.46
3:O:218:GLY:HA3	3:O:226:PHE:CE2	2.51	0.46
1:A:241:GLU:HB2	1:A:245:LYS:HB2	1.98	0.46
1:A:1087:LYS:HA	1:A:1090:ILE:HG22	1.97	0.46
1:A:1231:LEU:HA	1:A:1234:ILE:HG22	1.97	0.46
2:B:1:MET:O	2:B:963:ALA:HB3	2.15	0.46
2:B:86:LYS:HD3	2:B:148:ARG:HD2	1.97	0.46
2:B:311:PHE:O	2:B:315:LEU:HD23	2.16	0.46
2:B:774:LEU:O	2:B:915:LYS:HA	2.16	0.46
2:B:1087:TRP:CD1	2:B:1113:VAL:HG21	2.51	0.46
3:C:218:GLY:HA3	3:C:226:PHE:CE2	2.50	0.46
8:H:30:VAL:HB	8:H:37:ASN:HD22	1.80	0.46
1:M:118:LEU:HB2	1:M:182:ARG:NH1	2.29	0.46
1:M:1068:LEU:HA	1:M:1188:VAL:HG22	1.98	0.46
1:M:1541:LYS:HE3	1:M:1541:LYS:HB2	1.70	0.46
2:N:95:SER:O	2:N:95:SER:OG	2.32	0.46
2:N:383:LEU:O	2:N:387:ILE:HG12	2.15	0.46
2:N:537:ILE:HB	2:N:538:PRO:HD3	1.95	0.46
2:N:774:LEU:O	2:N:915:LYS:HA	2.16	0.46
2:N:807:VAL:HG23	2:N:850:GLU:HB2	1.96	0.46
2:N:972:SER:OG	2:N:974:GLN:HG2	2.16	0.46
7:S:70:SER:HG	7:S:71:PHE:H	1.62	0.46
1:A:57:TYR:N	1:A:61:SER:OG	2.49	0.46
1:A:734:ILE:HG22	8:H:76:MET:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:78:ARG:HH11	2:B:130:ARG:HE	1.64	0.46
2:B:185:LEU:HB2	2:B:378:LEU:CD2	2.44	0.46
2:B:972:SER:OG	2:B:974:GLN:HG2	2.16	0.46
5:E:22:VAL:HG11	5:E:29:VAL:HB	1.96	0.46
10:J:23:THR:HA	10:J:26:GLN:HB3	1.96	0.46
1:M:115:LYS:HE3	1:M:115:LYS:HB2	1.60	0.46
2:N:41:ASN:HD22	2:N:147:ASN:ND2	2.13	0.46
5:Q:22:VAL:HG11	5:Q:29:VAL:HB	1.96	0.46
5:Q:106:TYR:CZ	5:Q:131:GLN:HB3	2.50	0.46
1:A:1062:HIS:NE2	1:A:1125:LEU:O	2.47	0.46
2:B:116:ARG:NH2	7:S:128:ASP:O	2.46	0.46
2:B:827:ASP:HA	2:B:833:PHE:CE1	2.51	0.46
2:B:1147:THR:HG22	2:B:1148:LEU:H	1.80	0.46
4:D:27:ASN:O	4:D:31:GLN:NE2	2.41	0.46
1:M:241:GLU:HB2	1:M:245:LYS:HB2	1.98	0.46
1:M:252:SER:O	1:M:256:LEU:N	2.48	0.46
1:M:843:CYS:SG	1:M:938:MET:HB2	2.56	0.46
1:M:1140:LYS:HB3	5:Q:201:GLY:H	1.80	0.46
2:N:75:ILE:HA	2:N:124:SER:O	2.15	0.46
2:N:728:ARG:NH2	3:O:99:GLN:HE22	2.14	0.46
2:N:1169:MET:SD	2:N:1169:MET:N	2.81	0.46
5:Q:62:LYS:HA	5:Q:71:THR:HG1	1.80	0.46
5:Q:151:LEU:HB2	5:Q:190:VAL:HG13	1.97	0.46
11:W:25:LEU:HB2	11:W:36:THR:OG1	2.16	0.46
1:A:77:PHE:HE1	1:A:369:PRO:HD3	1.79	0.46
1:A:181:ILE:O	1:A:184:GLU:HG2	2.16	0.46
1:A:1068:LEU:HA	1:A:1188:VAL:HG22	1.98	0.46
1:A:1193:SER:O	1:A:1193:SER:OG	2.34	0.46
1:A:1674:THR:HA	1:A:1677:PHE:CZ	2.50	0.46
2:B:873:LEU:HD23	2:B:873:LEU:HA	1.76	0.46
5:E:96:ASP:OD2	5:E:97:HIS:N	2.49	0.46
5:E:106:TYR:CZ	5:E:131:GLN:HB3	2.50	0.46
8:H:108:HIS:O	8:H:112:TYR:HB2	2.15	0.46
1:M:106:CYS:SG	1:M:230:ASN:HB2	2.56	0.46
1:M:485:ASN:HB3	2:N:1033:THR:O	2.15	0.46
1:M:686:ILE:HB	1:M:687:GLN:OE1	2.15	0.46
2:N:219:ARG:HH11	2:N:223:SER:HB2	1.80	0.46
2:N:311:PHE:O	2:N:315:LEU:HD23	2.15	0.46
2:N:386:GLN:NE2	2:N:452:LEU:HD22	2.30	0.46
2:N:772:MET:HG2	2:N:911:ILE:N	2.30	0.46
1:A:1679:ILE:O	7:G:63:VAL:HG12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:48:ALA:HB1	2:B:389:LYS:HG3	1.98	0.46
2:B:144:VAL:HG21	2:B:172:TYR:CE2	2.51	0.46
3:C:76:ILE:HG22	3:C:80:GLU:HB2	1.96	0.46
1:M:57:TYR:N	1:M:61:SER:OG	2.49	0.46
1:M:475:PHE:HA	1:M:479:MET:CB	2.46	0.46
1:M:613:LYS:HB2	2:N:1067:HIS:CE1	2.50	0.46
2:N:99:ARG:CZ	12:X:47:ARG:HH12	2.29	0.46
2:N:135:ARG:HA	2:N:135:ARG:HD2	1.73	0.46
2:N:144:VAL:HG21	2:N:172:TYR:CE2	2.51	0.46
2:N:987:LYS:HD3	2:N:987:LYS:HA	1.68	0.46
1:A:106:CYS:SG	1:A:231:CYS:CB	3.03	0.46
1:A:843:CYS:SG	1:A:938:MET:HB2	2.56	0.46
2:B:690:PRO:HG3	2:B:905:ARG:NH2	2.31	0.46
8:H:16:VAL:HG13	8:H:27:ILE:HG22	1.98	0.46
8:H:23:ARG:HB3	8:H:24:VAL:H	1.62	0.46
12:L:57:MET:HG2	1:M:561:GLN:HA	1.97	0.46
1:M:808:LEU:O	1:M:812:VAL:HG23	2.15	0.46
1:M:861:LEU:HD13	1:M:920:ILE:HG22	1.98	0.46
1:M:1247:MET:SD	1:M:1547:VAL:HA	2.55	0.46
2:N:778:ALA:O	2:N:783:PHE:HB2	2.16	0.46
2:N:827:ASP:HA	2:N:833:PHE:CE1	2.51	0.46
2:N:882:GLU:O	2:N:884:GLN:HG2	2.16	0.46
2:N:1087:TRP:CD1	2:N:1113:VAL:HG21	2.51	0.46
3:O:334:LYS:HD2	11:W:42:GLU:OE2	2.15	0.46
5:Q:96:ASP:OD2	5:Q:97:HIS:N	2.49	0.46
7:S:81:PHE:O	7:S:83:PRO:HD3	2.16	0.46
8:T:8:ASP:HA	8:T:58:GLN:HG2	1.97	0.46
1:A:106:CYS:SG	1:A:230:ASN:HB2	2.56	0.46
1:A:475:PHE:HA	1:A:479:MET:CB	2.46	0.46
1:A:675:VAL:HG12	1:A:682:LEU:HD22	1.98	0.46
1:A:1306:ARG:NH2	1:A:1317:GLN:HG2	2.20	0.46
2:B:195:ALA:HB1	2:B:359:LEU:HD22	1.97	0.46
2:B:916:TRP:CD1	2:B:917:PRO:HD2	2.51	0.46
7:G:81:PHE:O	7:G:83:PRO:HD3	2.16	0.46
8:H:17:ASP:N	8:H:17:ASP:OD1	2.46	0.46
1:M:27:ILE:HG21	2:N:1096:ILE:HG23	1.96	0.46
1:M:736:ARG:NH2	8:T:68:LEU:O	2.49	0.46
1:M:767:LYS:HA	1:M:783:SER:HB2	1.98	0.46
1:M:868:PHE:O	1:M:871:GLU:HB2	2.16	0.46
2:N:822:TRP:O	2:N:826:LEU:N	2.45	0.46
2:N:844:ILE:N	2:N:858:GLU:O	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:916:TRP:CD1	2:N:917:PRO:HD2	2.51	0.46
2:N:1112:GLU:CD	2:N:1114:ARG:HH22	2.19	0.46
1:A:2:ASN:ND2	1:A:545:GLN:HE22	2.13	0.46
1:A:513:LEU:HD21	1:A:653:PHE:CG	2.51	0.46
1:A:767:LYS:HA	1:A:783:SER:HB2	1.97	0.46
1:A:868:PHE:O	1:A:871:GLU:HB2	2.16	0.46
1:A:1262:ALA:O	1:A:1266:GLU:HG2	2.16	0.46
1:A:1589:VAL:HG13	1:A:1605:LEU:HD23	1.96	0.46
2:B:186:ILE:HG13	2:B:479:VAL:HG11	1.98	0.46
2:B:876:ASN:ND2	2:B:884:GLN:HB2	2.31	0.46
2:B:882:GLU:O	2:B:884:GLN:HG2	2.16	0.46
2:B:1112:GLU:CD	2:B:1114:ARG:HH22	2.19	0.46
3:C:253:LYS:HB2	3:C:253:LYS:HE2	1.81	0.46
6:F:121:PRO:O	6:F:122:LEU:HB2	2.16	0.46
7:G:93:ILE:HD12	7:G:96:VAL:HG21	1.98	0.46
1:M:2:ASN:ND2	1:M:545:GLN:HE22	2.13	0.46
1:M:657:THR:HG22	6:R:89:LEU:HD13	1.98	0.46
1:M:1193:SER:O	1:M:1193:SER:OG	2.34	0.46
1:M:1262:ALA:O	1:M:1266:GLU:HG2	2.16	0.46
2:N:27:LYS:HE2	2:N:27:LYS:HB3	1.60	0.46
2:N:663:PRO:HA	2:N:666:ILE:HD11	1.98	0.46
2:N:851:SER:OG	2:N:852:THR:N	2.49	0.46
2:N:1151:LEU:HD13	2:N:1155:PHE:HD2	1.81	0.46
3:O:253:LYS:HE2	3:O:253:LYS:HB2	1.80	0.46
8:T:108:HIS:O	8:T:112:TYR:HB2	2.16	0.46
8:T:109:ARG:C	8:T:111:LEU:H	2.20	0.46
1:A:538:TRP:CE2	1:A:539:PRO:HB3	2.51	0.45
1:A:880:SER:OG	1:A:881:THR:N	2.48	0.45
1:A:968:ARG:NH1	1:A:969:ARG:O	2.49	0.45
7:G:85:LYS:HA	7:G:154:VAL:HB	1.98	0.45
7:G:99:SER:OG	2:N:93:GLU:OE2	2.31	0.45
10:J:3:ILE:HA	10:J:4:PRO:HD3	1.86	0.45
1:M:1019:LEU:O	1:M:1022:THR:OG1	2.26	0.45
2:N:55:LYS:HB3	2:N:400:ARG:HD2	1.97	0.45
3:O:144:ASN:HB3	3:O:210:ASP:OD1	2.16	0.45
10:V:51:THR:O	10:V:51:THR:OG1	2.32	0.45
1:A:44:PRO:HB3	1:A:50:TYR:O	2.16	0.45
1:A:115:LYS:HB2	1:A:115:LYS:HE3	1.61	0.45
1:A:1142:GLN:HA	1:A:1145:VAL:HG12	1.99	0.45
1:A:1155:LYS:HD2	1:A:1155:LYS:HA	1.77	0.45
5:E:69:LYS:HA	5:E:70:GLY:HA2	1.58	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:1:MET:HB2	2:N:1079:ASN:HB3	1.97	0.45
1:M:237:ASN:OD1	1:M:238:PHE:N	2.46	0.45
1:M:472:GLU:HA	1:M:477:LYS:HZ1	1.80	0.45
2:N:78:ARG:HH11	2:N:130:ARG:HE	1.64	0.45
2:N:876:ASN:ND2	2:N:884:GLN:HB2	2.31	0.45
1:A:472:GLU:HA	1:A:477:LYS:HZ1	1.81	0.45
1:A:1113:LYS:HB3	1:A:1121:TYR:CE1	2.51	0.45
1:M:576:LEU:HB3	1:M:579:SER:HA	1.99	0.45
1:M:1633:PHE:HB2	1:M:1662:SER:HB2	1.98	0.45
2:N:590:TYR:CD1	2:N:594:LEU:HD23	2.51	0.45
2:N:829:ASP:OD2	12:X:20:MET:HG3	2.17	0.45
2:N:931:ASP:OD1	10:V:9:SER:HA	2.16	0.45
3:O:74:ARG:O	3:O:78:ILE:HG22	2.15	0.45
5:Q:118:ILE:HG22	5:Q:127:ILE:HD13	1.98	0.45
7:S:98:PRO:HD2	7:S:132:GLU:OE1	2.16	0.45
8:T:19:GLN:OE1	8:T:19:GLN:N	2.50	0.45
1:A:687:GLN:HG2	1:A:688:ASP:N	2.31	0.45
1:A:762:LEU:HD11	1:A:811:SER:OG	2.17	0.45
1:A:802:GLY:O	1:A:804:SER:N	2.49	0.45
1:A:846:ASP:HB3	2:B:993:HIS:CG	2.52	0.45
1:A:861:LEU:HD13	1:A:920:ILE:HG22	1.98	0.45
1:A:1046:GLN:OE1	1:A:1052:ARG:N	2.45	0.45
1:A:1505:MET:O	1:A:1509:VAL:HG22	2.17	0.45
2:B:185:LEU:H	2:B:378:LEU:HG	1.82	0.45
2:B:348:LEU:HA	2:B:567:ILE:HD11	1.98	0.45
2:B:851:SER:OG	2:B:852:THR:N	2.49	0.45
3:C:115:ASP:OD2	3:C:118:MET:HG2	2.16	0.45
1:M:979:LEU:HB3	1:M:982:PHE:HD2	1.81	0.45
1:M:1158:ALA:HB3	1:M:1166:ASP:OD2	2.16	0.45
1:M:1231:LEU:HA	1:M:1231:LEU:HD12	1.71	0.45
2:N:143:MET:HB2	2:N:173:PHE:CE1	2.52	0.45
2:N:195:ALA:HB1	2:N:359:LEU:HD22	1.97	0.45
5:Q:7:ASN:ND2	5:Q:54:ARG:HH22	2.08	0.45
6:R:121:PRO:O	6:R:122:LEU:HB2	2.16	0.45
7:S:125:ILE:O	7:S:125:ILE:HG13	2.16	0.45
1:A:401:ILE:HD12	1:A:434:PHE:HD1	1.82	0.45
1:A:1158:ALA:HB3	1:A:1166:ASP:OD2	2.16	0.45
2:B:166:SER:HB3	2:B:167:GLU:OE1	2.17	0.45
2:B:1090:ARG:HE	2:B:1090:ARG:HB2	1.53	0.45
2:B:1151:LEU:HD13	2:B:1155:PHE:HD2	1.81	0.45
1:M:1269:LYS:HD2	1:M:1520:GLU:HG3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:985:LEU:CG	2:N:990:TYR:HB2	2.47	0.45
3:O:155:THR:HG1	3:O:156:ASP:H	1.60	0.45
3:O:290:LEU:HD21	3:O:301:LEU:HD13	1.98	0.45
8:T:16:VAL:HG22	8:T:27:ILE:HG22	1.99	0.45
12:X:41:CYS:N	12:X:46:HIS:O	2.39	0.45
1:A:888:LEU:HA	1:A:891:ASN:HD22	1.82	0.45
1:A:906:ASP:OD1	1:A:907:ALA:N	2.49	0.45
2:B:822:TRP:O	2:B:826:LEU:N	2.45	0.45
5:E:103:ILE:HA	5:E:128:GLU:O	2.16	0.45
7:G:48:VAL:HG13	7:G:78:VAL:HG23	1.98	0.45
7:G:125:ILE:O	7:G:125:ILE:HG13	2.16	0.45
8:H:19:GLN:N	8:H:19:GLN:OE1	2.50	0.45
1:M:181:ILE:O	1:M:184:GLU:HG2	2.16	0.45
1:M:774:TYR:CZ	1:M:943:VAL:HG21	2.52	0.45
1:M:880:SER:OG	1:M:882:ASP:OD1	2.20	0.45
1:M:968:ARG:NH1	1:M:969:ARG:O	2.49	0.45
1:M:1113:LYS:HB3	1:M:1121:TYR:CE1	2.51	0.45
1:M:1140:LYS:CB	5:Q:201:GLY:H	2.30	0.45
1:M:1591:SER:O	1:M:1594:GLY:N	2.49	0.45
2:N:610:GLU:HG2	2:N:633:ARG:NH2	2.30	0.45
2:N:876:ASN:CG	2:N:884:GLN:HB2	2.37	0.45
2:N:982:GLY:HA3	2:N:992:TYR:CE1	2.52	0.45
3:O:69:ILE:HG22	3:O:73:PHE:CE2	2.52	0.45
5:Q:132:GLU:C	5:Q:134:ASP:H	2.20	0.45
7:S:85:LYS:HA	7:S:154:VAL:HB	1.98	0.45
1:A:499:GLU:HG3	1:A:501:ASN:H	1.81	0.45
1:A:1283:GLU:HB2	9:I:44:VAL:O	2.17	0.45
1:A:1591:SER:O	1:A:1594:GLY:N	2.49	0.45
2:B:27:LYS:HE2	2:B:27:LYS:HB3	1.60	0.45
2:B:982:GLY:HA3	2:B:992:TYR:CE1	2.52	0.45
6:F:96:PRO:HG3	7:G:23:ARG:HD3	1.97	0.45
8:H:109:ARG:C	8:H:111:LEU:H	2.20	0.45
1:M:513:LEU:HD21	1:M:653:PHE:CG	2.51	0.45
1:M:606:ASN:HD22	1:M:616:MET:HG3	1.81	0.45
1:M:687:GLN:HG2	1:M:688:ASP:N	2.31	0.45
1:M:906:ASP:OD1	1:M:907:ALA:N	2.49	0.45
2:N:113:TYR:O	2:N:141:PRO:HA	2.17	0.45
2:N:213:LEU:HD23	2:N:214:SER:N	2.32	0.45
5:Q:8:ILE:HD11	5:Q:42:LYS:HG2	1.99	0.45
2:B:137:VAL:HG22	2:B:433:ILE:HG12	1.99	0.45
2:B:274:LYS:HD2	2:B:554:HIS:NE2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:663:PRO:HA	2:B:666:ILE:HD11	1.98	0.45
2:B:876:ASN:CG	2:B:884:GLN:HB2	2.37	0.45
10:J:51:THR:O	10:J:51:THR:OG1	2.32	0.45
1:M:44:PRO:HB3	1:M:50:TYR:O	2.17	0.45
1:M:538:TRP:CE2	1:M:539:PRO:HB3	2.51	0.45
1:M:762:LEU:HD11	1:M:811:SER:OG	2.17	0.45
1:M:927:ASP:HA	1:M:932:LYS:NZ	2.32	0.45
1:M:1004:ALA:N	1:M:1007:GLU:OE1	2.27	0.45
1:M:1066:ASP:OD1	1:M:1183:TYR:OH	2.29	0.45
1:M:1282:THR:OG1	1:M:1298:ALA:O	2.28	0.45
2:N:137:VAL:HG22	2:N:433:ILE:HG12	1.99	0.45
3:O:94:ASN:O	12:X:53:ARG:HD3	2.17	0.45
9:U:24:TRP:CZ2	9:U:35:PRO:HA	2.52	0.45
1:A:1231:LEU:HA	1:A:1231:LEU:HD12	1.71	0.45
1:A:1483:ASP:HB3	1:A:1488:GLU:H	1.82	0.45
2:B:1088:VAL:HG12	2:B:1149:ILE:HD11	1.97	0.45
3:C:304:VAL:HG12	3:C:306:ASP:H	1.81	0.45
8:H:85:GLU:HG2	8:H:91:VAL:HG12	1.99	0.45
1:M:132:ASN:O	1:M:136:MET:HG2	2.17	0.45
1:M:237:ASN:O	1:M:248:GLU:HB3	2.17	0.45
2:N:48:ALA:HB1	2:N:389:LYS:HG3	1.98	0.45
3:O:147:CYS:O	3:O:205:PRO:HA	2.17	0.45
8:T:85:GLU:HG2	8:T:91:VAL:HG12	1.99	0.45
1:A:120:PHE:HB2	1:A:342:VAL:HG22	1.99	0.45
1:A:576:LEU:HG	1:A:578:SER:H	1.81	0.45
1:A:1325:SER:O	1:A:1329:LEU:HB2	2.17	0.45
1:A:1506:VAL:HG13	1:A:1507:SER:H	1.82	0.45
3:C:93:ASN:O	3:C:210:ASP:N	2.48	0.45
3:C:113:SER:OG	3:C:192:ARG:O	2.33	0.45
3:C:144:ASN:HB3	3:C:210:ASP:OD1	2.16	0.45
3:C:147:CYS:O	3:C:205:PRO:HA	2.17	0.45
5:E:7:ASN:ND2	5:E:54:ARG:HH22	2.08	0.45
5:E:118:ILE:HG22	5:E:127:ILE:HD13	1.99	0.45
7:G:88:CYS:O	7:G:89:LEU:HD22	2.17	0.45
7:G:96:VAL:HG12	7:G:124:PHE:CE1	2.39	0.45
9:I:24:TRP:CZ2	9:I:35:PRO:HA	2.52	0.45
12:L:31:ASN:ND2	12:L:42:ARG:H	2.08	0.45
1:M:503:ILE:HG13	1:M:631:ARG:O	2.17	0.45
1:M:978:SER:HB2	1:M:991:SER:OG	2.17	0.45
1:M:1280:ARG:O	1:M:1299:ILE:HD12	2.17	0.45
1:M:1505:MET:O	1:M:1509:VAL:HG22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:57:THR:HA	3:O:313:GLU:OE1	2.17	0.45
7:S:88:CYS:O	7:S:89:LEU:HD22	2.17	0.45
1:A:774:TYR:CZ	1:A:943:VAL:HG21	2.52	0.44
1:A:978:SER:HB2	1:A:991:SER:OG	2.17	0.44
1:A:1280:ARG:O	1:A:1299:ILE:HD12	2.17	0.44
1:A:1504:LEU:O	1:A:1508:LEU:HG	2.18	0.44
4:D:17:LEU:HD13	7:G:8:LYS:N	2.32	0.44
6:F:117:GLN:HB2	6:F:119:LYS:HG3	1.98	0.44
6:F:126:ARG:O	6:F:133:TYR:HA	2.17	0.44
1:M:499:GLU:HG3	1:M:501:ASN:H	1.81	0.44
1:M:726:ARG:NH2	11:W:61:GLU:OE1	2.50	0.44
1:M:1483:ASP:HB3	1:M:1488:GLU:H	1.82	0.44
1:M:1530:LYS:HD2	1:M:1531:PRO:HD2	1.98	0.44
1:M:1585:ILE:HG13	1:M:1586:VAL:N	2.32	0.44
2:N:186:ILE:HG13	2:N:479:VAL:HG11	1.98	0.44
2:N:388:LEU:O	2:N:392:ILE:HG12	2.17	0.44
2:N:610:GLU:HB2	2:N:653:GLU:OE2	2.17	0.44
3:O:304:VAL:HG12	3:O:306:ASP:H	1.81	0.44
7:S:48:VAL:HG13	7:S:78:VAL:HG23	1.98	0.44
1:A:29:VAL:HG11	1:A:65:THR:OG1	2.18	0.44
1:A:68:LEU:HD23	1:A:68:LEU:HA	1.78	0.44
1:A:606:ASN:HD22	1:A:616:MET:HG3	1.81	0.44
1:A:1138:SER:HB3	1:A:1141:PHE:CB	2.47	0.44
1:A:1147:GLU:O	1:A:1151:LYS:HG2	2.17	0.44
1:A:1560:SER:O	1:A:1560:SER:OG	2.31	0.44
2:B:125:VAL:O	2:B:126:ASN:ND2	2.50	0.44
2:B:346:PHE:HA	2:B:349:LEU:HD12	2.00	0.44
2:B:733:GLN:HB2	10:J:51:THR:O	2.18	0.44
3:C:48:VAL:HG11	11:K:109:PHE:HD1	1.82	0.44
7:G:98:PRO:HD2	7:G:132:GLU:OE1	2.16	0.44
1:M:848:LEU:HA	1:M:848:LEU:HD23	1.71	0.44
1:M:1006:GLN:NE2	2:N:661:CYS:SG	2.64	0.44
1:M:1506:VAL:HG13	1:M:1507:SER:H	1.82	0.44
2:N:185:LEU:H	2:N:378:LEU:HG	1.82	0.44
7:S:85:LYS:HB3	7:S:155:ASP:C	2.38	0.44
8:T:16:VAL:HG13	8:T:27:ILE:HG22	1.98	0.44
1:A:18:ILE:HD13	1:A:359:MET:HA	1.99	0.44
1:A:503:ILE:HG13	1:A:631:ARG:O	2.17	0.44
1:A:927:ASP:HA	1:A:932:LYS:NZ	2.32	0.44
1:A:979:LEU:HB3	1:A:982:PHE:HD2	1.81	0.44
1:A:1267:VAL:HG12	1:A:1555:PHE:CZ	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:57:THR:HA	3:C:313:GLU:OE1	2.17	0.44
3:C:65:ILE:HG13	3:C:66:ASP:N	2.32	0.44
5:E:132:GLU:C	5:E:134:ASP:H	2.20	0.44
1:M:802:GLY:O	1:M:804:SER:N	2.48	0.44
1:M:888:LEU:HA	1:M:891:ASN:HD22	1.82	0.44
2:N:125:VAL:O	2:N:126:ASN:ND2	2.50	0.44
3:O:65:ILE:HG13	3:O:66:ASP:N	2.32	0.44
3:O:101:GLU:O	3:O:104:SER:OG	2.31	0.44
3:O:235:ARG:HH11	3:O:309:LEU:HD23	1.82	0.44
5:Q:194:VAL:HG13	5:Q:204:ASN:OD1	2.17	0.44
6:R:120:ILE:HA	6:R:121:PRO:HD3	1.90	0.44
1:A:334:ARG:HD3	1:A:334:ARG:HA	1.87	0.44
1:A:364:ASN:OD1	1:A:364:ASN:N	2.48	0.44
1:A:701:THR:HG23	1:A:743:GLY:H	1.83	0.44
1:A:739:ILE:HD12	1:A:741:TRP:HH2	1.83	0.44
2:B:49:VAL:O	2:B:52:ILE:HB	2.17	0.44
2:B:778:ALA:O	2:B:783:PHE:HB2	2.16	0.44
2:B:849:ASP:HB3	2:B:852:THR:HG1	1.81	0.44
2:B:951:SER:OG	2:B:1014:GLY:HA3	2.17	0.44
7:G:121:ASP:HB2	7:G:139:ASN:HB3	2.00	0.44
8:H:16:VAL:HG22	8:H:27:ILE:HG22	1.99	0.44
1:M:29:VAL:HG11	1:M:65:THR:OG1	2.18	0.44
1:M:605:LEU:HA	1:M:605:LEU:HD23	1.74	0.44
1:M:842:THR:O	1:M:937:HIS:ND1	2.50	0.44
2:N:71:PHE:HE2	2:N:74:LYS:HB2	1.83	0.44
2:N:274:LYS:HD2	2:N:554:HIS:NE2	2.32	0.44
2:N:812:PHE:CE1	2:N:822:TRP:HE3	2.35	0.44
3:O:338:VAL:HG13	11:W:22:ILE:HD13	2.00	0.44
5:Q:103:ILE:HA	5:Q:128:GLU:O	2.17	0.44
7:S:84:LYS:HA	7:S:84:LYS:HD2	1.71	0.44
8:T:70:GLU:HG3	8:T:71:ALA:H	1.82	0.44
1:A:58:LEU:HD23	1:A:58:LEU:HA	1.79	0.44
1:A:178:LEU:HD21	1:A:182:ARG:NH2	2.33	0.44
1:A:341:VAL:O	1:A:344:SER:OG	2.30	0.44
1:A:500:THR:HG22	1:A:826:SER:OG	2.18	0.44
1:A:548:ASP:OD2	1:A:550:THR:HG23	2.18	0.44
1:A:576:LEU:HB3	1:A:579:SER:HA	1.99	0.44
1:A:1256:SER:O	1:A:1260:ALA:N	2.38	0.44
2:B:329:PHE:O	2:B:333:LYS:HG2	2.17	0.44
2:B:480:HIS:CE1	2:B:482:GLY:H	2.36	0.44
2:B:610:GLU:HB2	2:B:653:GLU:OE2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:72:ALA:O	3:C:76:ILE:HG12	2.17	0.44
1:M:120:PHE:HB2	1:M:342:VAL:HG22	1.99	0.44
1:M:769:LYS:N	1:M:797:ASP:OD2	2.48	0.44
1:M:1123:PRO:HG2	5:Q:203:TYR:HA	2.00	0.44
1:M:1498:ILE:CD1	9:U:22:ALA:HB2	2.47	0.44
1:M:1520:GLU:OE1	1:M:1523:GLY:N	2.40	0.44
2:N:99:ARG:NH1	12:X:47:ARG:HH12	2.15	0.44
3:O:115:ASP:OD2	3:O:118:MET:HG2	2.16	0.44
6:R:126:ARG:O	6:R:133:TYR:HA	2.17	0.44
7:S:121:ASP:HB2	7:S:139:ASN:HB3	1.99	0.44
11:W:96:ASP:HA	11:W:99:ILE:HD12	2.00	0.44
1:A:111:LEU:CD1	1:A:222:ILE:HG22	2.48	0.44
1:A:842:THR:O	1:A:937:HIS:ND1	2.51	0.44
1:A:1530:LYS:HD2	1:A:1531:PRO:HD2	1.98	0.44
2:B:1032:ARG:NE	2:B:1044:PRO:HB3	2.32	0.44
2:B:1090:ARG:HH21	2:B:1147:THR:HG1	1.52	0.44
7:G:61:ALA:CB	7:G:72:ILE:HB	2.47	0.44
1:M:1147:GLU:O	1:M:1151:LYS:HG2	2.17	0.44
3:O:42:PHE:CZ	11:W:101:LEU:HG	2.53	0.44
11:W:29:SER:OG	11:W:33:THR:N	2.51	0.44
1:A:1:MET:CB	2:B:1079:ASN:HB3	2.47	0.44
1:A:24:VAL:O	1:A:28:SER:OG	2.25	0.44
1:A:237:ASN:O	1:A:248:GLU:HB3	2.17	0.44
1:A:247:PHE:CE2	1:A:323:MET:HB2	2.53	0.44
1:A:252:SER:O	1:A:256:LEU:N	2.48	0.44
1:A:829:SER:OG	1:A:830:ARG:N	2.51	0.44
1:A:1050:THR:OG1	1:A:1050:THR:O	2.36	0.44
1:A:1070:VAL:HA	1:A:1073:GLN:HG3	2.00	0.44
2:B:54:GLU:CB	2:B:78:ARG:HB3	2.44	0.44
2:B:143:MET:HB2	2:B:173:PHE:CE1	2.52	0.44
2:B:505:CYS:SG	2:B:506:PRO:HD2	2.58	0.44
3:C:69:ILE:HG21	11:K:101:LEU:HD21	1.98	0.44
3:C:204:ARG:NE	10:J:60:LEU:HB3	2.32	0.44
5:E:175:LEU:HD21	5:E:187:ARG:HG2	2.00	0.44
5:E:194:VAL:HG13	5:E:204:ASN:OD1	2.16	0.44
11:K:96:ASP:HA	11:K:99:ILE:HD12	2.00	0.44
1:M:401:ILE:HD12	1:M:434:PHE:HD1	1.82	0.44
1:M:476:ARG:NH1	1:M:1638:PHE:HA	2.33	0.44
1:M:879:LEU:HD23	1:M:883:SER:HB3	1.99	0.44
1:M:1052:ARG:HG2	1:M:1058:ILE:HD13	1.99	0.44
2:N:49:VAL:O	2:N:52:ILE:HB	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:236:VAL:HG12	2:N:237:THR:N	2.32	0.44
2:N:329:PHE:O	2:N:333:LYS:HG2	2.17	0.44
2:N:346:PHE:HA	2:N:349:LEU:HD12	2.00	0.44
2:N:348:LEU:HA	2:N:567:ILE:HD11	1.99	0.44
1:A:1041:GLU:OE2	2:B:1061:ARG:NH1	2.50	0.44
1:A:1279:VAL:HG23	9:I:53:PHE:CE2	2.53	0.44
2:B:388:LEU:O	2:B:392:ILE:HG12	2.17	0.44
2:B:812:PHE:CE1	2:B:822:TRP:HE3	2.35	0.44
2:B:985:LEU:CG	2:B:990:TYR:HB2	2.47	0.44
1:M:114:VAL:HG21	1:M:178:LEU:HD23	2.00	0.44
1:M:800:SER:O	1:M:808:LEU:N	2.48	0.44
1:M:1142:GLN:HA	1:M:1145:VAL:HG12	1.99	0.44
1:M:1267:VAL:HG12	1:M:1555:PHE:CZ	2.51	0.44
2:N:166:SER:HB3	2:N:167:GLU:OE1	2.17	0.44
2:N:420:LYS:O	2:N:423:THR:OG1	2.24	0.44
2:N:836:ILE:HD13	12:X:56:ARG:NE	2.32	0.44
2:N:844:ILE:HD11	2:N:860:TYR:HA	2.00	0.44
2:N:895:SER:O	2:N:897:ILE:HG23	2.18	0.44
6:R:117:GLN:HB2	6:R:119:LYS:HG3	1.98	0.44
1:A:121:CYS:HB3	1:A:186:VAL:CG2	2.44	0.44
1:A:132:ASN:O	1:A:136:MET:HG2	2.17	0.44
1:A:736:ARG:HD3	8:H:75:ILE:CD1	2.48	0.44
2:B:113:TYR:O	2:B:141:PRO:HA	2.17	0.44
2:B:213:LEU:HD23	2:B:214:SER:N	2.32	0.44
2:B:235:GLY:CA	2:B:284:ARG:HH11	2.26	0.44
2:B:433:ILE:HA	2:B:436:LYS:HZ2	1.83	0.44
2:B:590:TYR:CD1	2:B:594:LEU:HD23	2.51	0.44
7:G:37:ILE:HA	7:G:48:VAL:HB	1.99	0.44
7:G:85:LYS:HB3	7:G:155:ASP:C	2.38	0.44
7:G:97:SER:HB2	2:N:93:GLU:OE1	2.17	0.44
10:J:40:LEU:HD13	10:J:46:ARG:HA	2.00	0.44
1:M:247:PHE:CE2	1:M:323:MET:HB2	2.53	0.44
1:M:1247:MET:HE2	1:M:1544:THR:OG1	2.18	0.44
2:N:240:ARG:NE	2:N:242:HIS:HE1	2.15	0.44
2:N:339:LEU:HD23	2:N:339:LEU:HA	1.83	0.44
5:Q:4:GLU:OE2	5:Q:5:GLU:HB2	2.18	0.44
7:S:93:ILE:HD12	7:S:96:VAL:HG21	1.98	0.44
8:T:80:VAL:HG13	8:T:116:LEU:HA	2.00	0.44
1:A:769:LYS:N	1:A:797:ASP:OD2	2.48	0.43
1:A:1249:LEU:HD12	1:A:1542:VAL:HG13	2.00	0.43
1:A:1631:SER:O	1:A:1631:SER:OG	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1659:ASN:OD1	1:A:1659:ASN:N	2.49	0.43
1:A:1672:PHE:CZ	2:B:1065:ILE:HG22	2.53	0.43
2:B:28:ALA:O	2:B:477:ARG:HD3	2.18	0.43
2:B:772:MET:HG2	2:B:911:ILE:H	1.83	0.43
2:B:837:LYS:HA	2:B:867:PHE:HD1	1.83	0.43
2:B:1061:ARG:O	2:B:1065:ILE:HG12	2.18	0.43
2:B:1077:LEU:HA	2:B:1077:LEU:HD23	1.78	0.43
3:C:69:ILE:HG22	3:C:73:PHE:CE2	2.52	0.43
3:C:290:LEU:HD21	3:C:301:LEU:HD13	1.98	0.43
3:C:321:ASP:O	3:C:325:ILE:HG13	2.18	0.43
5:E:4:GLU:OE2	5:E:5:GLU:HB2	2.18	0.43
5:E:107:ALA:HA	5:E:108:ASN:HA	1.60	0.43
8:H:70:GLU:HG3	8:H:71:ALA:H	1.82	0.43
1:M:111:LEU:CD1	1:M:222:ILE:HG22	2.48	0.43
1:M:500:THR:HG22	1:M:826:SER:OG	2.18	0.43
1:M:1276:VAL:HG22	1:M:1277:ARG:O	2.18	0.43
2:N:99:ARG:NH2	12:X:46:HIS:HA	2.30	0.43
2:N:145:ARG:HH21	2:N:168:GLU:HB3	1.83	0.43
2:N:819:ARG:NH1	2:N:820:ARG:HA	2.33	0.43
2:N:837:LYS:HA	2:N:867:PHE:HD1	1.83	0.43
7:S:92:LYS:HA	7:S:92:LYS:HD3	1.80	0.43
1:A:104:LEU:HD12	1:A:236:PRO:HG2	2.00	0.43
1:A:682:LEU:HD23	1:A:683:ARG:H	1.82	0.43
1:A:1585:ILE:HG13	1:A:1586:VAL:N	2.32	0.43
2:B:94:ARG:HG3	2:B:878:VAL:HG22	2.00	0.43
2:B:537:ILE:O	2:B:541:LEU:HG	2.18	0.43
2:B:844:ILE:HD11	2:B:860:TYR:HA	2.00	0.43
2:B:895:SER:O	2:B:897:ILE:HG23	2.18	0.43
2:B:1021:LEU:HD23	2:B:1023:HIS:CE1	2.54	0.43
3:C:235:ARG:HH11	3:C:309:LEU:HD23	1.82	0.43
3:C:260:LYS:HD3	3:C:260:LYS:HA	1.69	0.43
7:G:125:ILE:HG12	7:G:135:ARG:HB2	2.00	0.43
12:L:34:GLN:HB2	2:N:1107:VAL:HG11	2.00	0.43
1:M:92:PHE:O	1:M:95:MET:HE3	2.19	0.43
1:M:576:LEU:HG	1:M:578:SER:H	1.81	0.43
1:M:1070:VAL:HA	1:M:1073:GLN:NE2	2.32	0.43
1:M:1140:LYS:H	5:Q:201:GLY:CA	2.31	0.43
2:N:757:VAL:HG21	10:V:9:SER:HB3	2.00	0.43
2:N:877:ASP:OD1	2:N:881:SER:OG	2.19	0.43
3:O:339:LYS:HZ2	11:W:92:ARG:HG3	1.83	0.43
4:P:19:LYS:HE2	4:P:19:LYS:HB2	1.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Q:175:LEU:HD21	5:Q:187:ARG:HG2	2.00	0.43
7:S:61:ALA:CB	7:S:72:ILE:HB	2.47	0.43
8:T:71:ALA:HB1	8:T:124:ARG:HH21	1.83	0.43
8:T:72:ALA:CB	8:T:122:LEU:HB3	2.48	0.43
1:A:34:ASN:OD1	1:A:34:ASN:N	2.45	0.43
1:A:327:GLU:HG3	1:A:328:VAL:H	1.83	0.43
1:A:495:ASP:N	1:A:632:MET:O	2.51	0.43
1:A:1004:ALA:N	1:A:1007:GLU:OE1	2.27	0.43
2:B:71:PHE:HE2	2:B:74:LYS:HB2	1.82	0.43
2:B:236:VAL:HG12	2:B:237:THR:N	2.32	0.43
2:B:540:LEU:HD21	2:B:586:MET:SD	2.59	0.43
3:C:90:TYR:CE1	1:M:560:GLU:HG2	2.47	0.43
5:E:8:ILE:HD11	5:E:42:LYS:HG2	1.99	0.43
6:F:109:GLN:O	6:F:112:MET:HB2	2.19	0.43
8:H:80:VAL:HG13	8:H:116:LEU:HA	2.00	0.43
1:M:401:ILE:HD12	1:M:434:PHE:CD1	2.53	0.43
1:M:700:ASP:O	8:T:23:ARG:NH1	2.52	0.43
1:M:839:ARG:O	2:N:1007:MET:HB3	2.19	0.43
1:M:1325:SER:O	1:M:1329:LEU:HB2	2.17	0.43
1:M:1582:ARG:NH2	5:Q:195:ARG:HD3	2.33	0.43
2:N:90:SER:HB3	2:N:878:VAL:HG23	2.00	0.43
2:N:251:PRO:HG2	2:N:254:MET:HB2	2.01	0.43
2:N:379:LEU:HD12	2:N:382:PHE:CE2	2.53	0.43
2:N:592:VAL:HB	2:N:645:GLU:HG2	2.00	0.43
2:N:728:ARG:NH2	3:O:99:GLN:NE2	2.66	0.43
2:N:951:SER:OG	2:N:1014:GLY:HA3	2.17	0.43
2:N:1061:ARG:O	2:N:1065:ILE:HG12	2.18	0.43
7:S:37:ILE:HA	7:S:48:VAL:HB	1.99	0.43
1:A:21:VAL:HG23	1:A:364:ASN:OD1	2.19	0.43
1:A:879:LEU:HD23	1:A:883:SER:HB3	1.99	0.43
1:A:951:VAL:O	1:A:955:GLN:HG3	2.18	0.43
1:A:1009:TYR:OH	2:B:500:ALA:HB3	2.18	0.43
1:A:1276:VAL:HG22	1:A:1277:ARG:O	2.18	0.43
2:B:240:ARG:NE	2:B:242:HIS:HE1	2.16	0.43
2:B:733:GLN:OE1	10:J:51:THR:HG23	2.19	0.43
2:B:987:LYS:HD3	2:B:987:LYS:HA	1.68	0.43
3:C:170:TYR:HA	3:C:199:VAL:HA	1.99	0.43
3:C:231:THR:HG21	10:J:42:ARG:CZ	2.48	0.43
8:H:71:ALA:HB1	8:H:124:ARG:HH21	1.83	0.43
1:M:66:CYS:SG	1:M:73:CYS:CB	3.01	0.43
1:M:90:LEU:HD23	1:M:90:LEU:HA	1.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:327:GLU:HG3	1:M:328:VAL:H	1.83	0.43
1:M:483:ARG:HG3	2:N:1054:ILE:C	2.39	0.43
1:M:951:VAL:O	1:M:955:GLN:HG3	2.18	0.43
1:M:1050:THR:O	1:M:1050:THR:OG1	2.36	0.43
1:M:1151:LYS:HZ3	1:M:1152:ASN:HB3	1.83	0.43
1:M:1530:LYS:HB3	1:M:1543:ILE:HD13	2.01	0.43
2:N:181:LEU:HD12	2:N:182:ILE:H	1.84	0.43
2:N:754:THR:OG1	2:N:755:ASN:N	2.50	0.43
2:N:772:MET:HG2	2:N:911:ILE:H	1.83	0.43
2:N:875:GLY:HA2	12:X:39:ILE:CG2	2.48	0.43
2:N:1021:LEU:HD23	2:N:1023:HIS:CE1	2.54	0.43
3:O:46:LEU:HD11	11:W:105:VAL:HG22	2.01	0.43
1:A:19:TYR:CE2	2:B:1168:LYS:HD2	2.53	0.43
1:A:82:LEU:HB2	1:A:84:ILE:CD1	2.48	0.43
1:A:358:ASP:HA	1:A:361:PHE:CE1	2.53	0.43
1:A:476:ARG:NH1	1:A:1638:PHE:HA	2.33	0.43
1:A:483:ARG:HG3	2:B:1054:ILE:C	2.38	0.43
1:A:1041:GLU:HG2	1:A:1659:ASN:HB2	2.01	0.43
1:A:1052:ARG:HG2	1:A:1058:ILE:HD13	2.00	0.43
2:B:700:ASN:O	2:B:703:GLN:HB3	2.18	0.43
2:B:754:THR:OG1	2:B:755:ASN:N	2.50	0.43
3:C:257:CYS:SG	3:C:288:GLU:HG3	2.59	0.43
3:C:328:ILE:HG21	11:K:106:THR:HG22	1.99	0.43
5:E:57:LEU:HB2	5:E:76:PHE:HB2	2.00	0.43
7:G:70:SER:HG	7:G:71:PHE:H	1.64	0.43
1:M:358:ASP:HA	1:M:361:PHE:CE1	2.53	0.43
1:M:578:SER:HB2	1:M:584:SER:HB2	2.00	0.43
1:M:829:SER:OG	1:M:830:ARG:N	2.51	0.43
2:N:480:HIS:CE1	2:N:482:GLY:H	2.36	0.43
3:O:78:ILE:HG23	3:O:79:ALA:H	1.84	0.43
1:A:401:ILE:HD12	1:A:434:PHE:CD1	2.53	0.43
1:A:880:SER:OG	1:A:882:ASP:OD1	2.20	0.43
1:A:1110:TYR:OH	1:A:1127:LYS:HE2	2.18	0.43
1:A:1189:ASP:OD1	6:F:77:LYS:HB3	2.17	0.43
1:A:1246:THR:H	1:A:1566:THR:CB	2.24	0.43
1:A:1320:ILE:O	1:A:1324:PHE:HB3	2.18	0.43
2:B:181:LEU:HD12	2:B:182:ILE:N	2.34	0.43
3:C:70:ALA:HB1	3:C:310:PHE:HZ	1.83	0.43
3:C:267:GLU:O	3:C:267:GLU:HG2	2.19	0.43
8:H:72:ALA:CB	8:H:122:LEU:HB3	2.48	0.43
10:J:24:LEU:HD13	10:J:34:ALA:HB1	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:74:LYS:H	2:N:126:ASN:ND2	2.16	0.43
2:N:778:ALA:CB	10:V:8:PHE:HB3	2.45	0.43
3:O:170:TYR:HA	3:O:199:VAL:HA	1.99	0.43
5:Q:57:LEU:HB2	5:Q:76:PHE:HB2	2.00	0.43
8:T:11:PHE:HA	8:T:31:SER:HB2	2.00	0.43
1:A:92:PHE:O	1:A:95:MET:HE3	2.19	0.43
1:A:119:PHE:CD2	1:A:218:PHE:HB2	2.54	0.43
2:B:74:LYS:H	2:B:126:ASN:ND2	2.17	0.43
2:B:90:SER:HB3	2:B:878:VAL:HG23	2.00	0.43
2:B:227:ASN:N	2:B:227:ASN:OD1	2.52	0.43
2:B:819:ARG:NH1	2:B:820:ARG:HA	2.33	0.43
3:C:78:ILE:HG23	3:C:79:ALA:H	1.84	0.43
3:C:265:LEU:HD23	3:C:265:LEU:HA	1.75	0.43
1:M:595:ARG:NH2	1:M:596:HIS:O	2.52	0.43
1:M:670:ASP:OD1	1:M:818:PRO:HB2	2.19	0.43
1:M:1110:TYR:OH	1:M:1127:LYS:HE2	2.18	0.43
1:M:1249:LEU:HD12	1:M:1542:VAL:HG13	2.00	0.43
7:S:62:LYS:C	7:S:70:SER:HG	2.18	0.43
1:A:27:ILE:HG21	2:B:1096:ILE:HG23	1.99	0.43
1:A:1066:ASP:OD1	1:A:1067:SER:N	2.52	0.43
1:A:1103:ASP:OD2	1:A:1106:THR:OG1	2.25	0.43
2:B:402:GLN:HG3	2:B:425:VAL:HG23	2.01	0.43
2:B:684:ILE:H	2:B:684:ILE:HG13	1.69	0.43
3:C:43:LYS:HE2	11:K:108:LYS:HE2	1.99	0.43
1:M:18:ILE:HD13	1:M:359:MET:HA	1.99	0.43
1:M:30:LYS:HE2	1:M:51:ASP:OD1	2.19	0.43
1:M:682:LEU:HD23	1:M:683:ARG:H	1.82	0.43
1:M:701:THR:HG23	1:M:743:GLY:H	1.83	0.43
1:M:1001:THR:HA	2:N:976:THR:HG23	2.01	0.43
1:M:1504:LEU:O	1:M:1508:LEU:HG	2.18	0.43
2:N:94:ARG:HG3	2:N:878:VAL:HG22	2.00	0.43
2:N:235:GLY:CA	2:N:284:ARG:HH11	2.26	0.43
2:N:589:GLU:O	2:N:593:LYS:HG3	2.19	0.43
2:N:795:ASP:HA	2:N:884:GLN:O	2.19	0.43
10:V:22:LEU:HA	10:V:22:LEU:HD12	1.76	0.43
1:A:891:ASN:O	1:A:895:VAL:HG23	2.19	0.43
1:A:1045:VAL:HG12	1:A:1190:PRO:HA	2.01	0.43
1:A:1070:VAL:HA	1:A:1073:GLN:NE2	2.32	0.43
1:A:1083:ALA:HB2	1:A:1175:PHE:CE1	2.54	0.43
1:A:1624:MET:SD	1:A:1624:MET:N	2.91	0.43
2:B:145:ARG:HH21	2:B:168:GLU:HB3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:197:ILE:HD13	2:B:366:ALA:CB	2.49	0.43
2:B:251:PRO:HG2	2:B:254:MET:HB2	2.01	0.43
2:B:379:LEU:HD12	2:B:382:PHE:CE2	2.53	0.43
3:C:318:MET:HB2	3:C:323:LEU:CD2	2.49	0.43
5:E:40:GLN:O	5:E:44:MET:HG2	2.19	0.43
5:E:82:VAL:HB	5:E:86:GLU:HB2	2.01	0.43
9:I:7:LEU:HD23	9:I:7:LEU:HA	1.81	0.43
1:M:178:LEU:HD21	1:M:182:ARG:NH2	2.33	0.43
1:M:1041:GLU:CD	2:N:1061:ARG:HH12	2.22	0.43
1:M:1229:PRO:O	1:M:1233:GLU:HG2	2.19	0.43
2:N:181:LEU:HD12	2:N:182:ILE:N	2.34	0.43
2:N:643:THR:HG23	2:N:645:GLU:H	1.84	0.43
3:O:40:ASP:O	3:O:44:LYS:HG2	2.19	0.43
3:O:72:ALA:O	3:O:76:ILE:HG12	2.17	0.43
3:O:257:CYS:SG	3:O:288:GLU:HG3	2.59	0.43
1:A:873:ALA:O	1:A:877:VAL:HG23	2.18	0.43
2:B:868:VAL:HG13	2:B:888:VAL:HG23	2.01	0.43
2:B:1138:LYS:H	2:B:1138:LYS:HG3	1.69	0.43
3:C:138:THR:HG22	3:C:216:ILE:HG22	2.01	0.43
5:E:186:LYS:O	5:E:189:GLU:HG2	2.19	0.43
11:K:86:THR:OG1	11:K:87:ALA:N	2.52	0.43
1:M:475:PHE:HA	1:M:475:PHE:HD1	1.72	0.43
1:M:1083:ALA:HB2	1:M:1175:PHE:CE1	2.54	0.43
2:N:505:CYS:SG	2:N:506:PRO:HD2	2.58	0.43
2:N:868:VAL:HG13	2:N:888:VAL:HG23	2.01	0.43
3:O:321:ASP:O	3:O:325:ILE:HG13	2.18	0.43
3:O:332:LYS:HB2	3:O:332:LYS:HE3	1.74	0.43
1:A:27:ILE:O	2:B:1116:ARG:NE	2.51	0.42
1:A:595:ARG:NH2	1:A:596:HIS:O	2.52	0.42
1:A:670:ASP:OD1	1:A:818:PRO:HB2	2.19	0.42
2:B:854:GLN:HG3	2:B:856:PHE:CE2	2.54	0.42
3:C:77:LEU:HD13	3:C:327:SER:OG	2.19	0.42
3:C:335:CYS:HB3	11:K:99:ILE:CG1	2.49	0.42
7:G:62:LYS:C	7:G:70:SER:HG	2.17	0.42
8:H:11:PHE:HA	8:H:31:SER:CB	2.49	0.42
12:L:37:GLU:HG2	12:L:38:VAL:O	2.19	0.42
1:M:104:LEU:HD12	1:M:236:PRO:HG2	2.00	0.42
1:M:548:ASP:OD2	1:M:550:THR:HG23	2.18	0.42
1:M:603:LEU:HD22	1:M:621:ALA:HB2	2.00	0.42
1:M:873:ALA:O	1:M:877:VAL:HG23	2.18	0.42
1:M:1115:LEU:HD23	1:M:1115:LEU:HA	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:1246:THR:H	1:M:1566:THR:CB	2.24	0.42
1:M:1320:ILE:O	1:M:1324:PHE:HB3	2.18	0.42
2:N:28:ALA:O	2:N:477:ARG:HD3	2.18	0.42
2:N:143:MET:CE	2:N:171:GLY:HA2	2.49	0.42
2:N:402:GLN:HG3	2:N:425:VAL:HG23	2.01	0.42
2:N:540:LEU:HD21	2:N:586:MET:SD	2.59	0.42
2:N:781:ARG:NH1	10:V:8:PHE:O	2.51	0.42
3:O:70:ALA:HB1	3:O:310:PHE:HZ	1.83	0.42
3:O:90:TYR:HA	12:X:59:GLN:OE1	2.19	0.42
7:S:98:PRO:O	7:S:115:ARG:NH1	2.53	0.42
1:A:578:SER:HB2	1:A:584:SER:HB2	2.00	0.42
2:B:508:HIS:CE1	2:B:520:HIS:CG	3.08	0.42
2:B:589:GLU:O	2:B:593:LYS:HG3	2.19	0.42
3:C:291:ARG:HE	3:C:291:ARG:HB3	1.65	0.42
3:C:332:LYS:HE3	3:C:332:LYS:HB2	1.74	0.42
5:E:4:GLU:N	5:E:6:LYS:HE2	2.34	0.42
10:J:47:ARG:H	10:J:47:ARG:HG3	1.70	0.42
12:L:20:MET:HB3	12:L:22:TYR:CZ	2.55	0.42
1:M:372:PHE:CE1	2:N:1157:TYR:HA	2.55	0.42
1:M:1070:VAL:HA	1:M:1073:GLN:HG3	2.00	0.42
1:M:1156:LEU:HA	1:M:1170:LEU:HD13	2.01	0.42
1:M:1560:SER:O	1:M:1560:SER:OG	2.31	0.42
1:M:1673:GLY:HA2	6:R:78:TYR:CD1	2.54	0.42
2:N:642:SER:OG	2:N:643:THR:N	2.53	0.42
2:N:700:ASN:O	2:N:703:GLN:HB3	2.19	0.42
2:N:1114:ARG:HG3	2:N:1132:TRP:NE1	2.34	0.42
3:O:89:VAL:H	12:X:59:GLN:NE2	2.17	0.42
3:O:267:GLU:HG2	3:O:267:GLU:O	2.19	0.42
5:Q:85:LYS:HA	5:Q:85:LYS:HD3	1.92	0.42
5:Q:147:LYS:HB3	5:Q:194:VAL:HB	2.01	0.42
6:R:109:GLN:O	6:R:112:MET:HB2	2.19	0.42
10:V:24:LEU:HD13	10:V:34:ALA:HB1	2.00	0.42
1:A:212:LYS:HE3	1:A:1627:GLU:OE2	2.19	0.42
2:B:192:HIS:HD2	2:B:193:PRO:HD2	1.84	0.42
2:B:642:SER:OG	2:B:643:THR:N	2.52	0.42
2:B:643:THR:HG23	2:B:645:GLU:H	1.84	0.42
2:B:840:ASP:HA	2:B:860:TYR:HD2	1.84	0.42
3:C:86:PHE:CD1	3:C:112:ILE:HD11	2.54	0.42
3:C:113:SER:O	3:C:191:ILE:HG23	2.19	0.42
6:F:120:ILE:HA	6:F:121:PRO:HD3	1.90	0.42
7:G:13:LEU:O	7:G:73:TRP:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:98:PRO:O	7:G:115:ARG:NH1	2.53	0.42
1:M:119:PHE:CD2	1:M:218:PHE:HB2	2.54	0.42
1:M:212:LYS:HE3	1:M:1627:GLU:OE2	2.19	0.42
1:M:1605:LEU:H	1:M:1605:LEU:HD12	1.85	0.42
2:N:195:ALA:HB3	2:N:367:ASP:H	1.85	0.42
2:N:227:ASN:OD1	2:N:227:ASN:N	2.52	0.42
2:N:537:ILE:O	2:N:541:LEU:HG	2.18	0.42
3:O:113:SER:HB3	3:O:194:VAL:HB	2.01	0.42
3:O:265:LEU:HD23	3:O:265:LEU:HA	1.75	0.42
3:O:318:MET:HB2	3:O:323:LEU:CD2	2.49	0.42
8:T:56:SER:HG	8:T:124:ARG:HB3	1.82	0.42
1:A:30:LYS:HE2	1:A:51:ASP:OD1	2.19	0.42
1:A:114:VAL:HG21	1:A:178:LEU:HD23	2.00	0.42
1:A:421:GLU:O	1:A:425:ARG:HG2	2.20	0.42
2:B:101:VAL:HG23	2:B:101:VAL:O	2.20	0.42
2:B:463:VAL:O	2:B:465:GLU:N	2.53	0.42
2:B:592:VAL:HB	2:B:645:GLU:HG2	2.00	0.42
2:B:1114:ARG:HG3	2:B:1132:TRP:NE1	2.34	0.42
7:G:78:VAL:HG22	7:G:79:LEU:H	1.84	0.42
8:H:71:ALA:HB1	8:H:124:ARG:HE	1.84	0.42
1:M:21:VAL:HG23	1:M:364:ASN:OD1	2.19	0.42
1:M:367:VAL:HA	1:M:368:PRO:HD3	1.86	0.42
1:M:543:HIS:HE1	1:M:551:LEU:HD11	1.84	0.42
1:M:1066:ASP:OD1	1:M:1067:SER:N	2.52	0.42
1:M:1607:LEU:HD12	1:M:1607:LEU:HA	1.80	0.42
2:N:590:TYR:HA	2:N:593:LYS:HD2	2.01	0.42
2:N:1034:THR:HG22	2:N:1035:GLY:N	2.34	0.42
4:P:46:VAL:HG23	4:P:47:LEU:H	1.84	0.42
5:Q:4:GLU:N	5:Q:6:LYS:HE2	2.34	0.42
7:S:78:VAL:HG22	7:S:79:LEU:H	1.84	0.42
7:S:88:CYS:HA	7:S:152:PHE:O	2.19	0.42
7:S:124:PHE:HB2	7:S:136:TRP:HE3	1.83	0.42
7:S:125:ILE:HG12	7:S:135:ARG:HB2	2.00	0.42
1:A:543:HIS:HE1	1:A:551:LEU:HD11	1.84	0.42
1:A:578:SER:HB3	1:A:581:TYR:O	2.19	0.42
1:A:603:LEU:HD22	1:A:621:ALA:HB2	2.00	0.42
1:A:1229:PRO:O	1:A:1233:GLU:HG2	2.19	0.42
1:A:1605:LEU:H	1:A:1605:LEU:HD12	1.85	0.42
2:B:365:CYS:HB2	2:B:619:ASN:O	2.19	0.42
2:B:609:LEU:HD12	2:B:629:SER:HB3	2.02	0.42
2:B:811:GLY:N	2:B:846:ALA:O	2.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:218:GLY:HA3	3:C:226:PHE:CZ	2.54	0.42
4:D:46:VAL:HG23	4:D:47:LEU:H	1.84	0.42
8:H:24:VAL:HG13	8:H:42:ILE:O	2.20	0.42
11:K:52:TYR:CE1	11:K:56:LYS:HE3	2.55	0.42
12:L:41:CYS:N	12:L:46:HIS:O	2.39	0.42
1:M:15:LYS:NZ	1:M:1652:GLY:O	2.52	0.42
1:M:58:LEU:HD23	1:M:58:LEU:HA	1.79	0.42
1:M:599:ASN:HD22	1:M:622:ARG:HA	1.84	0.42
1:M:847:ASP:OD2	1:M:936:ASN:ND2	2.53	0.42
2:N:78:ARG:NH1	2:N:130:ARG:HE	2.17	0.42
2:N:101:VAL:HG23	2:N:101:VAL:O	2.20	0.42
2:N:143:MET:HE3	2:N:171:GLY:HA2	2.02	0.42
2:N:197:ILE:HD13	2:N:366:ALA:CB	2.49	0.42
2:N:595:ARG:NH2	2:N:645:GLU:OE2	2.53	0.42
3:O:86:PHE:CD1	3:O:112:ILE:HD11	2.54	0.42
3:O:218:GLY:HA3	3:O:226:PHE:CZ	2.54	0.42
7:S:77:ASP:OD1	7:S:77:ASP:N	2.51	0.42
8:T:11:PHE:HA	8:T:31:SER:CB	2.49	0.42
8:T:71:ALA:HB1	8:T:124:ARG:HE	1.84	0.42
1:A:136:MET:HE1	5:E:187:ARG:HD2	2.02	0.42
1:A:695:TRP:CZ2	1:A:937:HIS:HD2	2.37	0.42
1:A:959:LEU:HA	1:A:997:SER:O	2.19	0.42
1:A:1502:LYS:C	1:A:1503:LEU:HD12	2.39	0.42
2:B:96:SER:O	7:S:95:LEU:HD22	2.19	0.42
2:B:116:ARG:NE	7:S:131:GLU:HB2	2.35	0.42
2:B:181:LEU:HD12	2:B:182:ILE:H	1.84	0.42
2:B:821:GLU:HB2	2:B:822:TRP:HD1	1.85	0.42
2:B:834:ILE:HD11	2:B:871:VAL:HG22	2.02	0.42
7:G:59:LYS:NZ	7:G:73:TRP:HB2	2.34	0.42
8:H:11:PHE:HA	8:H:31:SER:HB2	2.00	0.42
1:M:578:SER:HB3	1:M:581:TYR:O	2.19	0.42
1:M:695:TRP:CZ2	1:M:937:HIS:HD2	2.37	0.42
1:M:739:ILE:HD12	1:M:741:TRP:HH2	1.83	0.42
1:M:1259:ARG:NH2	1:M:1557:ASN:HD21	2.17	0.42
2:N:192:HIS:HD2	2:N:193:PRO:HD2	1.84	0.42
2:N:609:LEU:HD12	2:N:629:SER:HB3	2.02	0.42
3:O:261:GLY:O	3:O:278:ALA:HB3	2.20	0.42
4:P:56:TYR:CE1	7:S:106:LEU:HA	2.55	0.42
1:A:37:LEU:HD11	1:A:50:TYR:CD2	2.55	0.42
1:A:88:HIS:CD2	1:A:362:LEU:HD11	2.55	0.42
1:A:610:THR:O	2:B:1059:MET:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:924:CYS:O	1:A:928:GLY:N	2.40	0.42
1:A:1001:THR:HG23	2:B:976:THR:HG23	2.01	0.42
1:A:1530:LYS:HB3	1:A:1543:ILE:HD13	2.01	0.42
1:A:1657:LEU:HD11	1:A:1663:ARG:HD3	2.01	0.42
2:B:348:LEU:HD13	2:B:567:ILE:HG13	2.02	0.42
2:B:872:ARG:HB2	2:B:887:HIS:HB3	2.02	0.42
3:C:125:PRO:HB2	3:C:129:GLN:CB	2.50	0.42
1:M:421:GLU:O	1:M:425:ARG:HG2	2.20	0.42
1:M:610:THR:O	2:N:1059:MET:HG2	2.19	0.42
1:M:891:ASN:O	1:M:895:VAL:HG23	2.19	0.42
1:M:901:LYS:HE2	9:U:62:SER:HB2	2.01	0.42
2:N:419:ARG:O	2:N:423:THR:HG23	2.20	0.42
2:N:873:LEU:HD23	2:N:873:LEU:HA	1.76	0.42
3:O:186:PHE:HB3	3:O:189:ASN:O	2.20	0.42
5:Q:40:GLN:O	5:Q:44:MET:HG2	2.19	0.42
9:U:7:LEU:HA	9:U:7:LEU:HD23	1.81	0.42
10:V:40:LEU:HD13	10:V:46:ARG:HA	2.00	0.42
1:A:599:ASN:HD22	1:A:622:ARG:HA	1.84	0.42
1:A:1256:SER:H	1:A:1259:ARG:HB3	1.84	0.42
1:A:1582:ARG:O	1:A:1586:VAL:HG23	2.20	0.42
3:C:40:ASP:O	3:C:44:LYS:HG2	2.19	0.42
3:C:81:ILE:HD11	3:C:228:PRO:HG3	2.02	0.42
3:C:113:SER:HB3	3:C:194:VAL:HB	2.02	0.42
7:G:88:CYS:HA	7:G:152:PHE:O	2.19	0.42
8:H:59:ILE:HG13	8:H:59:ILE:O	2.20	0.42
1:M:2:ASN:HD21	1:M:545:GLN:HE22	1.67	0.42
1:M:543:HIS:HA	1:M:554:LEU:HD12	2.02	0.42
2:N:365:CYS:HB2	2:N:619:ASN:O	2.19	0.42
2:N:834:ILE:HD11	2:N:871:VAL:HG22	2.02	0.42
3:O:53:LEU:HD23	3:O:54:ASP:N	2.35	0.42
11:W:44:HIS:CD2	11:W:44:HIS:H	2.38	0.42
1:A:774:TYR:HD1	1:A:933:PHE:CD1	2.38	0.42
1:A:847:ASP:OD2	1:A:936:ASN:ND2	2.53	0.42
1:A:1156:LEU:HA	1:A:1170:LEU:HD13	2.01	0.42
2:B:151:LEU:HA	2:B:154:LEU:HD12	2.02	0.42
2:B:595:ARG:NH2	2:B:645:GLU:OE2	2.53	0.42
2:B:1162:LEU:HD12	2:B:1162:LEU:HA	1.83	0.42
3:C:147:CYS:HB3	3:C:204:ARG:O	2.18	0.42
3:C:157:GLU:O	3:C:159:ASP:N	2.50	0.42
3:C:160:PRO:HG3	3:C:204:ARG:NH1	2.35	0.42
5:E:147:LYS:HB3	5:E:194:VAL:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:67:ASP:OD1	8:H:71:ALA:HB3	2.20	0.42
8:H:114:LEU:HD13	8:H:114:LEU:HA	1.86	0.42
12:L:41:CYS:HB3	12:L:45:GLY:H	1.85	0.42
1:M:397:SER:O	1:M:401:ILE:HG12	2.20	0.42
1:M:733:ALA:O	8:T:77:TYR:N	2.53	0.42
1:M:1038:LYS:NZ	1:M:1629:ASN:HD22	2.17	0.42
1:M:1045:VAL:HG12	1:M:1190:PRO:HA	2.01	0.42
1:M:1624:MET:SD	1:M:1624:MET:N	2.91	0.42
1:M:1679:ILE:HA	6:R:124:VAL:HA	2.01	0.42
2:N:279:THR:HG21	9:U:46:THR:HA	2.01	0.42
2:N:840:ASP:HA	2:N:860:TYR:HD2	1.84	0.42
2:N:854:GLN:HG3	2:N:856:PHE:CE2	2.54	0.42
3:O:78:ILE:HG23	3:O:79:ALA:N	2.35	0.42
3:O:138:THR:HG22	3:O:216:ILE:HG22	2.01	0.42
8:T:24:VAL:HG13	8:T:42:ILE:O	2.20	0.42
1:A:511:THR:HA	1:A:596:HIS:CE1	2.55	0.42
1:A:543:HIS:CE1	1:A:551:LEU:HD11	2.55	0.42
1:A:893:GLU:HG2	2:B:618:HIS:CE1	2.55	0.42
2:B:419:ARG:O	2:B:423:THR:HG23	2.20	0.42
2:B:781:ARG:HB3	10:J:8:PHE:HD1	1.85	0.42
2:B:795:ASP:HA	2:B:884:GLN:O	2.19	0.42
3:C:78:ILE:HG23	3:C:79:ALA:N	2.35	0.42
3:C:179:GLN:HB2	3:C:182:GLN:NE2	2.35	0.42
3:C:203:LEU:HD22	3:C:207:GLN:HG3	2.02	0.42
3:C:334:LYS:HB3	11:K:46:LEU:HD12	2.01	0.42
5:E:71:THR:HG1	5:E:72:ILE:H	1.68	0.42
11:K:44:HIS:CD2	11:K:44:HIS:H	2.38	0.42
1:M:37:LEU:HD11	1:M:50:TYR:CD2	2.55	0.42
1:M:68:LEU:HA	1:M:68:LEU:HD23	1.78	0.42
1:M:77:PHE:CE2	2:N:1096:ILE:HG12	2.55	0.42
1:M:82:LEU:HB2	1:M:84:ILE:CD1	2.48	0.42
1:M:495:ASP:N	1:M:632:MET:O	2.52	0.42
1:M:531:VAL:HG21	1:M:569:LEU:CD1	2.50	0.42
1:M:674:LEU:HD22	1:M:679:GLY:O	2.20	0.42
1:M:759:ARG:CZ	1:M:1092:LYS:HB2	2.50	0.42
1:M:885:ILE:HG22	1:M:889:ASN:ND2	2.35	0.42
1:M:962:GLN:OE1	1:M:994:PHE:HB2	2.20	0.42
2:N:39:LEU:HA	2:N:39:LEU:HD12	1.75	0.42
2:N:180:LYS:HD3	2:N:180:LYS:HA	1.68	0.42
2:N:564:ASP:HA	2:N:628:PHE:CD1	2.55	0.42
2:N:1032:ARG:NH1	2:N:1035:GLY:HA3	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:179:GLN:HB2	3:O:182:GLN:NE2	2.35	0.42
8:T:59:ILE:O	8:T:59:ILE:HG13	2.20	0.42
1:A:390:LEU:HB3	1:A:444:LEU:HD13	2.02	0.41
1:A:489:ARG:NH2	1:A:648:GLU:OE2	2.53	0.41
1:A:495:ASP:OD1	1:A:497:ASN:N	2.53	0.41
2:B:91:SER:OG	7:S:131:GLU:HB3	2.20	0.41
2:B:367:ASP:O	2:B:369:PRO:HD3	2.20	0.41
2:B:402:GLN:HE21	2:B:428:LYS:HD3	1.84	0.41
3:C:237:LEU:HD11	3:C:281:ARG:HG2	2.02	0.41
4:D:17:LEU:HD23	4:D:17:LEU:N	2.35	0.41
5:E:54:ARG:CB	5:E:78:LYS:HD3	2.50	0.41
1:M:88:HIS:CD2	1:M:362:LEU:HD11	2.54	0.41
1:M:489:ARG:NH2	1:M:648:GLU:OE2	2.53	0.41
1:M:959:LEU:HA	1:M:997:SER:O	2.19	0.41
1:M:1041:GLU:HG2	1:M:1659:ASN:HB2	2.01	0.41
1:M:1138:SER:HB3	1:M:1141:PHE:CB	2.47	0.41
1:M:1662:SER:O	1:M:1666:VAL:HG22	2.20	0.41
2:N:508:HIS:CE1	2:N:520:HIS:CG	3.08	0.41
2:N:510:PRO:O	2:N:515:CYS:HA	2.20	0.41
2:N:678:PRO:O	2:N:681:VAL:HG12	2.20	0.41
2:N:821:GLU:HB2	2:N:822:TRP:HD1	1.85	0.41
2:N:1165:MET:O	2:N:1167:ILE:HD12	2.20	0.41
3:O:147:CYS:HB3	3:O:204:ARG:O	2.19	0.41
5:Q:186:LYS:O	5:Q:189:GLU:HG2	2.19	0.41
7:S:13:LEU:O	7:S:73:TRP:HA	2.20	0.41
7:S:59:LYS:NZ	7:S:73:TRP:HB2	2.35	0.41
11:W:52:TYR:CE1	11:W:56:LYS:HE3	2.55	0.41
1:A:96:TYR:CD1	1:A:240:LYS:HB3	2.55	0.41
1:A:571:THR:HG23	1:A:573:GLN:HG2	2.03	0.41
1:A:613:LYS:CG	1:A:614:PRO:HD3	2.50	0.41
1:A:674:LEU:HD22	1:A:679:GLY:O	2.20	0.41
1:A:697:THR:O	1:A:744:LYS:HE2	2.21	0.41
1:A:763:ASN:OD1	1:A:763:ASN:N	2.54	0.41
1:A:1247:MET:HE2	1:A:1544:THR:OG1	2.19	0.41
2:B:143:MET:CE	2:B:171:GLY:HA2	2.50	0.41
2:B:190:ARG:HB2	2:B:630:ASN:ND2	2.35	0.41
2:B:237:THR:OG1	2:B:252:SER:OG	2.13	0.41
7:G:44:ILE:HD12	7:G:44:ILE:HA	1.93	0.41
1:M:495:ASP:OD1	1:M:497:ASN:N	2.53	0.41
1:M:607:ARG:HB2	1:M:649:MET:HE3	2.02	0.41
1:M:1549:LEU:HD11	1:M:1565:TYR:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:1582:ARG:O	1:M:1586:VAL:HG23	2.20	0.41
2:N:24:ASP:OD2	2:N:25:LEU:N	2.53	0.41
2:N:348:LEU:HD13	2:N:567:ILE:HG13	2.02	0.41
2:N:463:VAL:O	2:N:465:GLU:N	2.53	0.41
2:N:1032:ARG:NE	2:N:1044:PRO:HB3	2.32	0.41
7:S:98:PRO:HD3	7:S:124:PHE:CD2	2.55	0.41
11:W:28:HIS:HB3	11:W:35:VAL:HG23	2.02	0.41
12:X:20:MET:HB3	12:X:22:TYR:CZ	2.55	0.41
12:X:41:CYS:HB3	12:X:45:GLY:H	1.85	0.41
1:A:2:ASN:HD21	1:A:545:GLN:HE22	1.66	0.41
1:A:531:VAL:HG21	1:A:569:LEU:CD1	2.50	0.41
1:A:558:THR:HG22	1:A:561:GLN:CD	2.40	0.41
1:A:717:LYS:NZ	11:K:67:ILE:O	2.46	0.41
1:A:1124:VAL:HG22	1:A:1128:TYR:HB2	2.02	0.41
1:A:1572:ILE:HG13	1:A:1576:TYR:HD2	1.85	0.41
2:B:74:LYS:HB3	2:B:126:ASN:HB3	2.03	0.41
2:B:192:HIS:HB2	2:B:628:PHE:CZ	2.55	0.41
2:B:510:PRO:O	2:B:515:CYS:HA	2.20	0.41
2:B:590:TYR:OH	2:B:601:GLU:N	2.53	0.41
2:B:1165:MET:O	2:B:1167:ILE:HD12	2.20	0.41
7:G:85:LYS:HD3	7:G:155:ASP:O	2.21	0.41
7:G:98:PRO:HD3	7:G:124:PHE:CD2	2.56	0.41
7:G:119:PRO:HB2	7:G:121:ASP:OD1	2.19	0.41
11:K:29:SER:OG	11:K:33:THR:N	2.50	0.41
1:M:511:THR:HA	1:M:596:HIS:CE1	2.55	0.41
1:M:685:LEU:HD13	1:M:689:HIS:HB3	2.03	0.41
1:M:1251:LEU:HD13	1:M:1251:LEU:HA	1.87	0.41
1:M:1336:ILE:O	1:M:1340:LEU:HD23	2.20	0.41
2:N:123:TRP:HE1	2:N:422:LEU:CG	2.24	0.41
2:N:190:ARG:HB2	2:N:630:ASN:ND2	2.35	0.41
2:N:197:ILE:HD11	2:N:359:LEU:HD21	2.01	0.41
2:N:354:ARG:NH1	2:N:358:ALA:HB2	2.34	0.41
3:O:50:ILE:CD1	11:W:113:LEU:HB3	2.48	0.41
5:Q:23:HIS:HE1	5:Q:34:LEU:HD11	1.85	0.41
8:T:15:SER:HB3	8:T:28:THR:CG2	2.50	0.41
1:A:1005:PRO:HG3	2:B:969:PHE:CG	2.56	0.41
1:A:1259:ARG:NH2	1:A:1557:ASN:HD21	2.17	0.41
1:A:1549:LEU:HD11	1:A:1565:TYR:CE2	2.55	0.41
2:B:56:CYS:SG	2:B:76:SER:HB2	2.60	0.41
2:B:78:ARG:NH1	2:B:130:ARG:HE	2.17	0.41
2:B:188:PRO:HA	2:B:374:HIS:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:271:ILE:HG13	2:B:272:VAL:HG13	2.03	0.41
2:B:609:LEU:HG	2:B:628:PHE:O	2.20	0.41
2:B:1032:ARG:NH1	2:B:1035:GLY:HA3	2.35	0.41
1:M:527:MET:O	1:M:531:VAL:HG23	2.21	0.41
1:M:613:LYS:CG	1:M:614:PRO:HD3	2.50	0.41
1:M:1502:LYS:C	1:M:1503:LEU:HD12	2.39	0.41
2:N:56:CYS:SG	2:N:76:SER:HB2	2.60	0.41
2:N:117:LEU:HD22	2:N:140:ILE:HG21	2.03	0.41
2:N:262:THR:HG22	2:N:266:GLU:HB2	2.01	0.41
2:N:590:TYR:OH	2:N:601:GLU:N	2.53	0.41
2:N:734:THR:OG1	10:V:51:THR:OG1	2.19	0.41
2:N:908:GLN:NE2	2:N:938:ALA:HB1	2.36	0.41
2:N:940:PRO:O	2:N:941:SER:OG	2.33	0.41
2:N:985:LEU:HD12	2:N:985:LEU:HA	1.83	0.41
3:O:160:PRO:HG3	3:O:204:ARG:NH1	2.35	0.41
7:S:8:LYS:HE2	7:S:8:LYS:HB2	1.76	0.41
7:S:53:ASN:HB3	7:S:55:ARG:NH1	2.35	0.41
8:T:3:GLU:HG3	8:T:5:VAL:HG23	2.02	0.41
11:W:86:THR:OG1	11:W:87:ALA:N	2.52	0.41
12:X:37:GLU:HG2	12:X:38:VAL:O	2.19	0.41
1:A:759:ARG:CZ	1:A:1092:LYS:HB2	2.50	0.41
2:B:167:GLU:OE1	2:B:167:GLU:N	2.53	0.41
2:B:630:ASN:OD1	2:B:633:ARG:HD3	2.21	0.41
3:C:163:LEU:HG	3:C:164:TYR:CE1	2.56	0.41
5:E:62:LYS:HA	5:E:71:THR:HG1	1.84	0.41
8:H:15:SER:HB3	8:H:28:THR:CG2	2.50	0.41
10:J:33:GLU:O	10:J:36:ASP:HB2	2.20	0.41
1:M:106:CYS:SG	1:M:231:CYS:CB	3.03	0.41
1:M:607:ARG:HB2	1:M:649:MET:CE	2.51	0.41
1:M:849:ARG:HH12	2:N:993:HIS:CE1	2.38	0.41
1:M:972:LEU:HD23	1:M:972:LEU:HA	1.61	0.41
1:M:1659:ASN:OD1	1:M:1659:ASN:N	2.49	0.41
2:N:1104:MET:HG3	2:N:1105:ASN:N	2.35	0.41
3:O:77:LEU:HD13	3:O:327:SER:OG	2.19	0.41
3:O:81:ILE:HD11	3:O:228:PRO:HG3	2.02	0.41
3:O:260:LYS:HA	3:O:260:LYS:HD3	1.69	0.41
5:Q:82:VAL:HB	5:Q:86:GLU:HB2	2.01	0.41
7:S:127:PRO:HG2	7:S:133:GLN:O	2.21	0.41
8:T:107:SER:OG	8:T:109:ARG:NH1	2.53	0.41
1:A:77:PHE:CD2	2:B:1096:ILE:HG12	2.55	0.41
1:A:246:ILE:O	1:A:247:PHE:CG	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:ARG:HH11	1:A:361:PHE:HZ	1.68	0.41
1:A:397:SER:O	1:A:401:ILE:HG12	2.20	0.41
1:A:685:LEU:HD12	1:A:801:PHE:CD2	2.56	0.41
1:A:688:ASP:HA	2:B:937:HIS:CE1	2.55	0.41
1:A:1261:SER:HB2	1:A:1265:LYS:HE3	2.03	0.41
1:A:1583:ASN:OD1	1:A:1583:ASN:N	2.54	0.41
2:B:424:ARG:O	2:B:428:LYS:HG3	2.20	0.41
2:B:664:LYS:HE3	2:B:664:LYS:HB2	1.87	0.41
2:B:697:SER:OG	2:B:698:PRO:HD3	2.21	0.41
3:C:53:LEU:HD23	3:C:54:ASP:N	2.35	0.41
3:C:109:LEU:CD2	3:C:225:LYS:HB3	2.51	0.41
3:C:186:PHE:HB3	3:C:189:ASN:O	2.20	0.41
3:C:248:GLY:O	3:C:252:VAL:HG23	2.21	0.41
5:E:193:ILE:O	5:E:204:ASN:HA	2.21	0.41
8:H:107:SER:OG	8:H:109:ARG:NH1	2.53	0.41
11:K:28:HIS:HB3	11:K:35:VAL:HG23	2.02	0.41
1:M:246:ILE:O	1:M:247:PHE:CG	2.74	0.41
1:M:1657:LEU:HD11	1:M:1663:ARG:HD3	2.01	0.41
2:N:179:GLU:CB	2:N:464:ALA:HB3	2.48	0.41
2:N:271:ILE:HG13	2:N:272:VAL:HG13	2.03	0.41
2:N:527:ILE:HD13	2:N:634:MET:HA	2.02	0.41
2:N:535:SER:O	2:N:538:PRO:HD2	2.21	0.41
2:N:961:GLY:HA2	10:V:50:LEU:HD11	2.02	0.41
3:O:109:LEU:CD2	3:O:225:LYS:HB3	2.51	0.41
3:O:125:PRO:HB2	3:O:129:GLN:CB	2.50	0.41
3:O:144:ASN:OD1	3:O:144:ASN:N	2.54	0.41
5:Q:54:ARG:CB	5:Q:78:LYS:HD3	2.50	0.41
7:S:90:GLU:HB3	7:S:151:GLU:CD	2.41	0.41
1:A:346:LEU:HD12	1:A:346:LEU:HA	1.73	0.41
1:A:1226:LEU:HD11	1:A:1595:VAL:HG11	2.02	0.41
2:B:197:ILE:HD11	2:B:359:LEU:HD21	2.01	0.41
2:B:262:THR:HG22	2:B:266:GLU:HB2	2.01	0.41
2:B:590:TYR:HA	2:B:593:LYS:HD2	2.01	0.41
3:C:94:ASN:O	12:L:53:ARG:NH1	2.54	0.41
7:G:135:ARG:NE	7:G:135:ARG:HA	2.36	0.41
1:M:77:PHE:HE1	1:M:369:PRO:HD3	1.79	0.41
1:M:475:PHE:CE2	1:M:1636:MET:HB3	2.55	0.41
1:M:492:ILE:HD11	1:M:649:MET:HB2	2.02	0.41
1:M:506:PRO:HB3	1:M:627:GLU:O	2.21	0.41
1:M:774:TYR:HD1	1:M:933:PHE:CD1	2.38	0.41
1:M:1256:SER:H	1:M:1259:ARG:HB3	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:1261:SER:HB2	1:M:1265:LYS:HE3	2.03	0.41
1:M:1274:GLU:HB3	1:M:1313:TYR:OH	2.21	0.41
2:N:151:LEU:HA	2:N:154:LEU:HD12	2.01	0.41
2:N:192:HIS:HB2	2:N:628:PHE:CZ	2.56	0.41
2:N:313:VAL:HG13	2:N:314:VAL:H	1.85	0.41
2:N:367:ASP:O	2:N:369:PRO:HD3	2.20	0.41
2:N:402:GLN:HE21	2:N:428:LYS:HD3	1.84	0.41
2:N:420:LYS:HB3	2:N:420:LYS:HE2	1.70	0.41
2:N:684:ILE:H	2:N:684:ILE:HG13	1.69	0.41
2:N:779:HIS:CD2	2:N:896:PRO:HB2	2.56	0.41
3:O:248:GLY:O	3:O:252:VAL:HG23	2.21	0.41
3:O:289:CYS:SG	3:O:290:LEU:N	2.94	0.41
7:S:59:LYS:HZ1	7:S:73:TRP:HB2	1.86	0.41
1:A:15:LYS:NZ	1:A:1652:GLY:O	2.52	0.41
1:A:595:ARG:HG3	1:A:596:HIS:O	2.21	0.41
1:A:607:ARG:HB2	1:A:649:MET:CE	2.51	0.41
1:A:1662:SER:O	1:A:1666:VAL:HG22	2.20	0.41
2:B:195:ALA:HB3	2:B:367:ASP:H	1.85	0.41
2:B:354:ARG:NH1	2:B:358:ALA:HB2	2.34	0.41
2:B:808:HIS:HB3	2:B:847:TYR:CD2	2.56	0.41
3:C:289:CYS:SG	3:C:290:LEU:N	2.94	0.41
7:G:90:GLU:HB3	7:G:151:GLU:CD	2.41	0.41
10:J:30:THR:HG21	10:J:37:LYS:NZ	2.36	0.41
11:K:32:LEU:HD12	11:K:32:LEU:HA	1.94	0.41
1:M:96:TYR:CD1	1:M:240:LYS:HB3	2.55	0.41
1:M:338:LYS:HE2	1:M:338:LYS:HB2	1.82	0.41
2:N:109:ARG:HA	2:N:874:LEU:HD23	2.03	0.41
2:N:307:LEU:HD12	2:N:307:LEU:HA	1.95	0.41
2:N:808:HIS:HB3	2:N:847:TYR:CD2	2.56	0.41
3:O:31:PHE:CD2	11:W:58:PRO:HB3	2.56	0.41
3:O:50:ILE:HG23	3:O:58:MET:HE2	2.03	0.41
3:O:113:SER:O	3:O:191:ILE:HG23	2.20	0.41
10:V:30:THR:HG21	10:V:37:LYS:NZ	2.36	0.41
10:V:33:GLU:O	10:V:36:ASP:HB2	2.20	0.41
11:W:41:LYS:N	11:W:73:ALA:O	2.54	0.41
1:A:136:MET:CE	5:E:187:ARG:HD2	2.50	0.41
1:A:513:LEU:HD22	1:A:597:VAL:CG1	2.51	0.41
1:A:824:LEU:HA	1:A:827:VAL:HG12	2.02	0.41
1:A:919:SER:OG	1:A:920:ILE:N	2.54	0.41
1:A:962:GLN:OE1	1:A:994:PHE:HB2	2.20	0.41
1:A:998:ARG:NH2	1:A:1001:THR:OG1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1086:TYR:CD1	1:A:1178:LEU:HD13	2.56	0.41
1:A:1202:ILE:C	1:A:1205:PRO:HD2	2.42	0.41
1:A:1274:GLU:HB3	1:A:1313:TYR:OH	2.21	0.41
1:A:1336:ILE:O	1:A:1340:LEU:HD23	2.20	0.41
2:B:24:ASP:OD2	2:B:25:LEU:N	2.53	0.41
2:B:116:ARG:HD3	7:S:131:GLU:CD	2.40	0.41
2:B:271:ILE:O	2:B:354:ARG:HD3	2.21	0.41
2:B:313:VAL:HG13	2:B:314:VAL:H	1.85	0.41
2:B:432:ASP:O	2:B:436:LYS:NZ	2.53	0.41
2:B:527:ILE:HD13	2:B:634:MET:HA	2.02	0.41
2:B:564:ASP:HA	2:B:628:PHE:CD1	2.55	0.41
2:B:678:PRO:O	2:B:681:VAL:HG12	2.20	0.41
2:B:765:GLY:O	2:B:768:MET:HE1	2.21	0.41
2:B:844:ILE:N	2:B:858:GLU:O	2.44	0.41
2:B:1034:THR:HG22	2:B:1035:GLY:N	2.34	0.41
3:C:261:GLY:O	3:C:278:ALA:HB3	2.20	0.41
4:D:14:SER:HA	7:G:9:GLN:HB3	2.03	0.41
5:E:75:GLU:HG3	5:E:104:LEU:HD23	2.03	0.41
7:G:53:ASN:HB3	7:G:55:ARG:NH1	2.35	0.41
8:H:107:SER:C	8:H:109:ARG:H	2.24	0.41
10:J:22:LEU:HD12	10:J:22:LEU:HA	1.76	0.41
11:K:95:LEU:O	11:K:99:ILE:HG13	2.20	0.41
1:M:474:LEU:HA	1:M:474:LEU:HD13	1.84	0.41
1:M:543:HIS:CE1	1:M:551:LEU:HD11	2.55	0.41
1:M:558:THR:HG22	1:M:561:GLN:CD	2.41	0.41
1:M:571:THR:HG23	1:M:573:GLN:HG2	2.02	0.41
1:M:998:ARG:NH2	1:M:1001:THR:OG1	2.54	0.41
1:M:1124:VAL:HG22	1:M:1128:TYR:HB2	2.03	0.41
1:M:1169:LEU:O	1:M:1170:LEU:HG	2.21	0.41
1:M:1202:ILE:C	1:M:1205:PRO:HD2	2.42	0.41
1:M:1258:LYS:HE3	1:M:1258:LYS:HB3	1.88	0.41
1:M:1624:MET:HG2	1:M:1625:GLY:H	1.85	0.41
2:N:44:LEU:HD12	2:N:44:LEU:HA	1.89	0.41
2:N:188:PRO:HA	2:N:374:HIS:O	2.20	0.41
2:N:290:ARG:HA	2:N:290:ARG:HD2	1.85	0.41
2:N:424:ARG:O	2:N:428:LYS:HG3	2.20	0.41
2:N:630:ASN:OD1	2:N:633:ARG:HD3	2.21	0.41
2:N:637:PRO:HB2	2:N:646:LEU:HD11	2.03	0.41
2:N:741:LEU:HD23	2:N:741:LEU:HA	1.81	0.41
2:N:765:GLY:O	2:N:768:MET:HE1	2.21	0.41
2:N:781:ARG:HD3	10:V:7:CYS:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:845:VAL:HG11	2:N:886:ILE:HD12	2.02	0.41
3:O:109:LEU:HD23	3:O:109:LEU:HA	1.71	0.41
3:O:203:LEU:HA	3:O:207:GLN:NE2	2.36	0.41
3:O:230:ALA:O	10:V:11:GLY:HA3	2.21	0.41
4:P:17:LEU:N	4:P:17:LEU:HD23	2.35	0.41
4:P:27:ASN:O	4:P:31:GLN:NE2	2.41	0.41
5:Q:69:LYS:HA	5:Q:70:GLY:HA2	1.58	0.41
5:Q:111:THR:HA	5:Q:112:PRO:HD3	1.97	0.41
5:Q:128:GLU:HG3	5:Q:129:THR:OG1	2.21	0.41
5:Q:193:ILE:O	5:Q:204:ASN:HA	2.21	0.41
7:S:56:PHE:HA	7:S:74:VAL:HA	2.03	0.41
10:V:40:LEU:HA	10:V:40:LEU:HD23	1.85	0.41
11:W:40:GLN:HG3	11:W:41:LYS:CG	2.41	0.41
11:W:95:LEU:O	11:W:99:ILE:HG13	2.20	0.41
12:X:25:ALA:HB3	12:X:46:HIS:ND1	2.36	0.41
1:A:3:ILE:HG21	6:F:89:LEU:HD11	2.03	0.41
1:A:204:THR:HG22	1:A:205:THR:H	1.86	0.41
1:A:527:MET:O	1:A:531:VAL:HG23	2.21	0.41
1:A:603:LEU:HD23	1:A:603:LEU:H	1.86	0.41
1:A:671:SER:O	1:A:672:GLN:NE2	2.54	0.41
1:A:762:LEU:HD22	1:A:786:PHE:CZ	2.56	0.41
2:B:56:CYS:HA	2:B:75:ILE:O	2.21	0.41
2:B:422:LEU:HA	2:B:425:VAL:HG12	2.03	0.41
2:B:535:SER:O	2:B:538:PRO:HD2	2.21	0.41
2:B:640:HIS:HA	2:B:673:HIS:CD2	2.56	0.41
3:C:91:ILE:HG12	12:L:58:VAL:O	2.21	0.41
6:F:66:LYS:HG3	6:F:69:ARG:NH2	2.36	0.41
8:H:30:VAL:HG12	8:H:38:LEU:H	1.86	0.41
8:H:62:ASN:HB2	8:H:64:ASN:OD1	2.21	0.41
1:M:37:LEU:CD1	1:M:49:LEU:HB3	2.51	0.41
1:M:820:ILE:HD13	1:M:820:ILE:HA	1.86	0.41
1:M:919:SER:OG	1:M:920:ILE:N	2.54	0.41
1:M:1226:LEU:HD11	1:M:1595:VAL:HG11	2.02	0.41
1:M:1572:ILE:HG13	1:M:1576:TYR:HD2	1.85	0.41
2:N:74:LYS:HB3	2:N:126:ASN:HB3	2.03	0.41
2:N:167:GLU:OE1	2:N:167:GLU:N	2.53	0.41
2:N:640:HIS:HA	2:N:673:HIS:CD2	2.56	0.41
3:O:42:PHE:CE2	11:W:101:LEU:HG	2.56	0.41
4:P:27:ASN:O	4:P:31:GLN:HG2	2.21	0.41
5:Q:87:MET:HG2	5:Q:118:ILE:HG12	2.02	0.41
5:Q:105:ILE:HG23	5:Q:132:GLU:N	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:66:LYS:HG3	6:R:69:ARG:NH2	2.36	0.41
1:A:37:LEU:CD1	1:A:49:LEU:HB3	2.51	0.40
1:A:204:THR:HG22	1:A:205:THR:N	2.36	0.40
1:A:471:LYS:HA	1:A:471:LYS:HD2	1.95	0.40
1:A:511:THR:HA	1:A:596:HIS:NE2	2.36	0.40
1:A:543:HIS:HA	1:A:554:LEU:HD12	2.02	0.40
1:A:1125:LEU:HD11	1:A:1138:SER:HA	2.03	0.40
1:A:1624:MET:HG2	1:A:1625:GLY:H	1.85	0.40
2:B:562:GLN:OE1	2:B:567:ILE:HG12	2.21	0.40
3:C:144:ASN:N	3:C:144:ASN:OD1	2.54	0.40
12:L:57:MET:HE3	12:L:59:GLN:HB2	2.03	0.40
1:M:559:ILE:HG13	1:M:560:GLU:N	2.36	0.40
1:M:603:LEU:H	1:M:603:LEU:HD23	1.86	0.40
1:M:979:LEU:HB3	1:M:982:PHE:CD2	2.56	0.40
1:M:1582:ARG:CZ	5:Q:195:ARG:HD3	2.51	0.40
2:N:471:ARG:HG3	2:N:475:HIS:NE2	2.37	0.40
3:O:163:LEU:HG	3:O:164:TYR:CE1	2.56	0.40
3:O:237:LEU:HD11	3:O:281:ARG:HG2	2.02	0.40
3:O:271:GLY:O	3:O:272:LYS:HD2	2.21	0.40
5:Q:173:ILE:HG13	5:Q:207:ARG:HB3	2.03	0.40
7:S:85:LYS:HD3	7:S:155:ASP:O	2.21	0.40
8:T:67:ASP:OD1	8:T:71:ALA:HB3	2.20	0.40
1:A:96:TYR:CE1	1:A:240:LYS:HB3	2.56	0.40
1:A:569:LEU:O	1:A:591:LYS:HD2	2.22	0.40
1:A:606:ASN:HB2	1:A:616:MET:HG3	2.03	0.40
1:A:896:TYR:OH	1:A:985:TYR:CD1	2.71	0.40
1:A:979:LEU:HB3	1:A:982:PHE:CD2	2.56	0.40
1:A:1063:TYR:O	1:A:1066:ASP:HA	2.21	0.40
2:B:191:ASN:ND2	2:B:217:CYS:HA	2.36	0.40
2:B:208:TYR:CZ	2:B:238:MET:HG3	2.56	0.40
2:B:560:CYS:HB2	2:B:570:TRP:CZ3	2.56	0.40
2:B:741:LEU:HA	2:B:744:THR:HB	2.04	0.40
2:B:800:ARG:HD3	2:B:805:PRO:C	2.42	0.40
2:B:908:GLN:NE2	2:B:938:ALA:HB1	2.36	0.40
2:B:1104:MET:HG3	2:B:1105:ASN:N	2.35	0.40
3:C:76:ILE:HG12	3:C:76:ILE:H	1.42	0.40
5:E:87:MET:HG2	5:E:118:ILE:HG12	2.02	0.40
6:F:107:PRO:HA	6:F:110:ILE:HD12	2.03	0.40
12:L:22:TYR:HE2	12:L:51:LYS:HG3	1.86	0.40
1:M:49:LEU:HD21	1:M:388:ASN:HB3	2.02	0.40
1:M:685:LEU:HD12	1:M:801:PHE:CD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:688:ASP:HA	2:N:937:HIS:CE1	2.56	0.40
1:M:762:LEU:HD22	1:M:786:PHE:CZ	2.56	0.40
1:M:824:LEU:HA	1:M:827:VAL:HG12	2.02	0.40
1:M:1063:TYR:O	1:M:1066:ASP:HA	2.21	0.40
2:N:356:LEU:O	2:N:360:VAL:HG23	2.22	0.40
2:N:524:LYS:HB3	2:N:680:ASN:OD1	2.22	0.40
2:N:872:ARG:HB2	2:N:887:HIS:HB3	2.02	0.40
2:N:909:LYS:HB3	2:N:909:LYS:HE2	1.91	0.40
4:P:20:ASP:O	4:P:24:LYS:HD3	2.21	0.40
7:S:119:PRO:HB2	7:S:121:ASP:OD1	2.20	0.40
1:A:49:LEU:HD21	1:A:388:ASN:HB3	2.02	0.40
1:A:506:PRO:HB3	1:A:627:GLU:O	2.21	0.40
1:A:826:SER:O	1:A:829:SER:OG	2.21	0.40
1:A:961:GLY:HA2	1:A:994:PHE:CE1	2.56	0.40
1:A:1163:SER:HA	1:A:1166:ASP:CG	2.42	0.40
2:B:145:ARG:NH2	2:B:168:GLU:HB3	2.37	0.40
2:B:563:LEU:HD12	2:B:563:LEU:HA	1.93	0.40
2:B:779:HIS:CD2	2:B:896:PRO:HB2	2.56	0.40
7:G:97:SER:OG	7:G:132:GLU:HB3	2.21	0.40
7:G:127:PRO:HG2	7:G:133:GLN:O	2.21	0.40
7:G:170:LEU:HD23	7:G:170:LEU:HA	1.87	0.40
11:K:72:GLU:H	11:K:72:GLU:HG2	1.47	0.40
1:M:20:ASP:O	1:M:24:VAL:HG23	2.21	0.40
1:M:341:VAL:O	1:M:344:SER:OG	2.30	0.40
1:M:390:LEU:HB3	1:M:444:LEU:HD13	2.02	0.40
1:M:535:PRO:O	1:M:536:HIS:HD2	2.05	0.40
1:M:590:ASN:HD21	6:R:94:ASN:ND2	2.19	0.40
1:M:961:GLY:HA2	1:M:994:PHE:CE1	2.56	0.40
1:M:1583:ASN:OD1	1:M:1583:ASN:N	2.54	0.40
2:N:271:ILE:O	2:N:354:ARG:HD3	2.21	0.40
2:N:432:ASP:O	2:N:436:LYS:NZ	2.53	0.40
2:N:560:CYS:HB2	2:N:570:TRP:CZ3	2.56	0.40
2:N:609:LEU:HG	2:N:628:PHE:O	2.20	0.40
2:N:729:LEU:HD23	2:N:730:GLN:N	2.37	0.40
5:Q:48:MET:H	5:Q:48:MET:HG2	1.47	0.40
5:Q:118:ILE:HA	5:Q:121:VAL:HG22	2.03	0.40
7:S:82:SER:O	7:S:82:SER:OG	2.30	0.40
7:S:103:LEU:HB2	7:S:111:ALA:HB3	2.03	0.40
8:T:56:SER:OG	8:T:124:ARG:HB3	2.22	0.40
8:T:114:LEU:HA	8:T:114:LEU:HD13	1.86	0.40
1:A:492:ILE:HD11	1:A:649:MET:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:559:ILE:HG13	1:A:560:GLU:N	2.36	0.40
1:A:912:LYS:HB2	1:A:912:LYS:HE2	1.87	0.40
1:A:939:GLN:O	1:A:943:VAL:HG12	2.21	0.40
2:B:204:ARG:HH22	2:B:230:HIS:CD2	2.40	0.40
2:B:730:GLN:O	10:J:1:MET:N	2.54	0.40
3:C:335:CYS:CB	11:K:99:ILE:HG12	2.52	0.40
5:E:128:GLU:HG3	5:E:129:THR:OG1	2.21	0.40
5:E:173:ILE:HG13	5:E:207:ARG:HB3	2.03	0.40
8:H:3:GLU:HG3	8:H:5:VAL:HG23	2.02	0.40
1:M:204:THR:HG22	1:M:205:THR:H	1.86	0.40
1:M:513:LEU:HD22	1:M:597:VAL:CG1	2.51	0.40
1:M:784:VAL:HA	1:M:794:GLY:HA3	2.04	0.40
1:M:1068:LEU:HG	1:M:1069:ASP:N	2.37	0.40
1:M:1125:LEU:HD11	1:M:1138:SER:HA	2.03	0.40
2:N:56:CYS:HA	2:N:75:ILE:O	2.21	0.40
2:N:208:TYR:CZ	2:N:238:MET:HG3	2.56	0.40
2:N:800:ARG:HD3	2:N:805:PRO:C	2.42	0.40
2:N:1038:HIS:N	2:N:1043:GLN:O	2.55	0.40
3:O:107:ILE:C	3:O:109:LEU:N	2.75	0.40
6:R:121:PRO:HB2	6:R:122:LEU:HD12	2.03	0.40
7:S:103:LEU:HD21	7:S:150:LEU:HB3	2.04	0.40
8:T:62:ASN:HB2	8:T:64:ASN:OD1	2.21	0.40
12:X:22:TYR:HE2	12:X:51:LYS:HG3	1.86	0.40
1:A:20:ASP:O	1:A:24:VAL:HG23	2.21	0.40
1:A:347:TYR:HA	1:A:1651:ARG:HA	2.03	0.40
1:A:471:LYS:NZ	1:A:476:ARG:HD2	2.36	0.40
1:A:483:ARG:HD2	2:B:1046:LYS:NZ	2.37	0.40
1:A:622:ARG:NH1	1:A:624:LEU:HD11	2.37	0.40
1:A:1012:CYS:SG	2:B:506:PRO:HB2	2.61	0.40
1:A:1019:LEU:O	1:A:1022:THR:OG1	2.26	0.40
1:A:1038:LYS:NZ	1:A:1629:ASN:HD22	2.17	0.40
1:A:1225:THR:H	1:A:1244:THR:HG21	1.87	0.40
1:A:1679:ILE:HD12	6:F:83:ILE:HG12	2.02	0.40
2:B:923:PHE:HB3	2:B:929:GLN:OE1	2.22	0.40
2:B:985:LEU:HD23	2:B:991:ASN:O	2.21	0.40
2:B:1038:HIS:N	2:B:1043:GLN:O	2.55	0.40
3:C:94:ASN:OD1	3:C:209:ILE:HG12	2.21	0.40
3:C:174:LEU:HD23	3:C:174:LEU:HA	1.80	0.40
3:C:271:GLY:O	3:C:272:LYS:HD2	2.21	0.40
4:D:27:ASN:O	4:D:31:GLN:HG2	2.22	0.40
5:E:23:HIS:HE1	5:E:34:LEU:HD11	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:103:LEU:HB2	7:G:111:ALA:HB3	2.04	0.40
8:H:30:VAL:HB	8:H:37:ASN:HA	2.04	0.40
1:M:88:HIS:HA	1:M:89:PRO:HD3	1.92	0.40
1:M:124:LYS:O	1:M:127:ASP:HB3	2.22	0.40
1:M:559:ILE:HA	1:M:562:ARG:HG3	2.03	0.40
1:M:595:ARG:HG3	1:M:596:HIS:O	2.21	0.40
1:M:697:THR:O	1:M:744:LYS:HE2	2.21	0.40
1:M:849:ARG:HH12	2:N:993:HIS:HE1	1.67	0.40
2:N:425:VAL:O	2:N:428:LYS:HB2	2.21	0.40
2:N:562:GLN:OE1	2:N:567:ILE:HG12	2.21	0.40
2:N:697:SER:OG	2:N:698:PRO:HD3	2.21	0.40
2:N:951:SER:HB3	2:N:1012:TYR:OH	2.22	0.40
2:N:985:LEU:HD23	2:N:991:ASN:O	2.21	0.40
3:O:157:GLU:O	3:O:159:ASP:N	2.50	0.40
7:S:96:VAL:HG12	7:S:124:PHE:CE1	2.39	0.40
8:T:47:TYR:CE1	8:T:74:TYR:HB2	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	1356/1689 (80%)	1213 (90%)	136 (10%)	7 (0%)	29	68
1	M	1356/1689 (80%)	1214 (90%)	135 (10%)	7 (0%)	29	68
2	B	1148/1174 (98%)	1015 (88%)	129 (11%)	4 (0%)	41	76
2	N	1148/1174 (98%)	1015 (88%)	129 (11%)	4 (0%)	41	76
3	C	315/348 (90%)	290 (92%)	25 (8%)	0	100	100
3	O	315/348 (90%)	290 (92%)	25 (8%)	0	100	100
4	D	35/147 (24%)	34 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	P	35/147 (24%)	34 (97%)	1 (3%)	0	100	100
5	E	205/210 (98%)	180 (88%)	25 (12%)	0	100	100
5	Q	205/210 (98%)	179 (87%)	26 (13%)	0	100	100
6	F	80/142 (56%)	75 (94%)	4 (5%)	1 (1%)	12	48
6	R	80/142 (56%)	75 (94%)	4 (5%)	1 (1%)	12	48
7	G	156/173 (90%)	139 (89%)	17 (11%)	0	100	100
7	S	156/173 (90%)	139 (89%)	17 (11%)	0	100	100
8	H	121/125 (97%)	95 (78%)	26 (22%)	0	100	100
8	T	121/125 (97%)	95 (78%)	26 (22%)	0	100	100
9	I	55/119 (46%)	50 (91%)	5 (9%)	0	100	100
9	U	55/119 (46%)	50 (91%)	5 (9%)	0	100	100
10	J	66/71 (93%)	46 (70%)	20 (30%)	0	100	100
10	V	66/71 (93%)	46 (70%)	20 (30%)	0	100	100
11	K	93/125 (74%)	90 (97%)	3 (3%)	0	100	100
11	W	93/125 (74%)	90 (97%)	3 (3%)	0	100	100
12	L	43/63 (68%)	40 (93%)	3 (7%)	0	100	100
12	X	43/63 (68%)	40 (93%)	3 (7%)	0	100	100
All	All	7346/8772 (84%)	6534 (89%)	788 (11%)	24 (0%)	44	76

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1066	ASP
1	M	1066	ASP
1	A	1154	ASP
1	M	1154	ASP
2	B	206	THR
2	N	206	THR
1	A	1043	LEU
2	B	492	THR
2	B	827	ASP
1	M	1043	LEU
2	N	492	THR
2	N	827	ASP
1	A	968	ARG
2	B	493	VAL

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Mol	Chain	Res	Type
1	M	968	ARG
2	N	493	VAL
1	A	85	PRO
1	A	782	GLY
1	M	85	PRO
1	M	782	GLY
1	A	580	PRO
1	M	580	PRO
6	F	121	PRO
6	R	121	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	1225/1484 (82%)	1210 (99%)	15 (1%)	71	84
1	M	1225/1484 (82%)	1210 (99%)	15 (1%)	71	84
2	B	1001/1013 (99%)	989 (99%)	12 (1%)	71	84
2	N	1001/1013 (99%)	989 (99%)	12 (1%)	71	84
3	C	281/308 (91%)	272 (97%)	9 (3%)	39	62
3	O	281/308 (91%)	272 (97%)	9 (3%)	39	62
4	D	37/134 (28%)	35 (95%)	2 (5%)	22	49
4	P	37/134 (28%)	35 (95%)	2 (5%)	22	49
5	E	182/184 (99%)	176 (97%)	6 (3%)	38	61
5	Q	182/184 (99%)	176 (97%)	6 (3%)	38	61
6	F	70/121 (58%)	68 (97%)	2 (3%)	42	64
6	R	70/121 (58%)	68 (97%)	2 (3%)	42	64
7	G	143/154 (93%)	139 (97%)	4 (3%)	43	65
7	S	143/154 (93%)	139 (97%)	4 (3%)	43	65
8	H	112/114 (98%)	109 (97%)	3 (3%)	44	66
8	T	112/114 (98%)	109 (97%)	3 (3%)	44	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
9	I	51/105 (49%)	44 (86%)	7 (14%)	3 19
9	U	51/105 (49%)	44 (86%)	7 (14%)	3 19
10	J	63/66 (96%)	61 (97%)	2 (3%)	39 62
10	V	63/66 (96%)	61 (97%)	2 (3%)	39 62
11	K	86/111 (78%)	84 (98%)	2 (2%)	50 70
11	W	86/111 (78%)	84 (98%)	2 (2%)	50 70
12	L	39/53 (74%)	37 (95%)	2 (5%)	24 50
12	X	39/53 (74%)	37 (95%)	2 (5%)	24 50
All	All	6580/7694 (86%)	6448 (98%)	132 (2%)	57 73

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	192	ASP
1	A	542	SER
1	A	551	LEU
1	A	553	SER
1	A	585	ARG
1	A	881	THR
1	A	1016	ARG
1	A	1086	TYR
1	A	1164	LYS
1	A	1249	LEU
1	A	1307	ASP
1	A	1322	SER
1	A	1529	SER
1	A	1550	LYS
2	B	237	THR
2	B	252	SER
2	B	262	THR
2	B	267	ILE
2	B	764	THR
2	B	773	ILE
2	B	801	ARG
2	B	820	ARG
2	B	864	GLU
2	B	933	ILE
2	B	1139	LYS

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Mol	Chain	Res	Type
2	B	1144	THR
3	C	65	ILE
3	C	76	ILE
3	C	110	VAL
3	C	139	VAL
3	C	155	THR
3	C	197	ASP
3	C	231	THR
3	C	333	SER
3	C	340	SER
4	D	13	LYS
4	D	48	SER
5	E	11	VAL
5	E	48	MET
5	E	117	ILE
5	E	120	THR
5	E	133	SER
5	E	196	ARG
6	F	68	ASP
6	F	86	THR
7	G	82	SER
7	G	88	CYS
7	G	143	ILE
7	G	169	THR
8	H	23	ARG
8	H	28	THR
8	H	56	SER
9	I	6	SER
9	I	17	LEU
9	I	21	THR
9	I	48	SER
9	I	49	SER
9	I	57	LEU
9	I	62	SER
10	J	19	ASP
10	J	45	CYS
11	K	33	THR
11	K	46	LEU
12	L	19	THR
12	L	47	ARG
1	M	1	MET
1	M	192	ASP

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Mol	Chain	Res	Type
1	M	542	SER
1	M	551	LEU
1	M	553	SER
1	M	585	ARG
1	M	881	THR
1	M	1016	ARG
1	M	1086	TYR
1	M	1164	LYS
1	M	1249	LEU
1	M	1307	ASP
1	M	1322	SER
1	M	1529	SER
1	M	1550	LYS
2	N	237	THR
2	N	252	SER
2	N	262	THR
2	N	267	ILE
2	N	764	THR
2	N	773	ILE
2	N	801	ARG
2	N	820	ARG
2	N	864	GLU
2	N	933	ILE
2	N	1139	LYS
2	N	1144	THR
3	O	65	ILE
3	O	76	ILE
3	O	110	VAL
3	O	139	VAL
3	O	155	THR
3	O	197	ASP
3	O	231	THR
3	O	333	SER
3	O	340	SER
4	P	13	LYS
4	P	48	SER
5	Q	11	VAL
5	Q	48	MET
5	Q	117	ILE
5	Q	120	THR
5	Q	133	SER
5	Q	196	ARG

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Mol	Chain	Res	Type
6	R	68	ASP
6	R	86	THR
7	S	82	SER
7	S	88	CYS
7	S	143	ILE
7	S	169	THR
8	T	23	ARG
8	T	28	THR
8	T	56	SER
9	U	6	SER
9	U	17	LEU
9	U	21	THR
9	U	48	SER
9	U	49	SER
9	U	57	LEU
9	U	62	SER
10	V	19	ASP
10	V	45	CYS
11	W	33	THR
11	W	46	LEU
12	X	19	THR
12	X	47	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (123) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	232	GLN
1	A	257	GLN
1	A	501	ASN
1	A	533	ASN
1	A	536	HIS
1	A	543	HIS
1	A	545	GLN
1	A	546	ASN
1	A	568	GLN
1	A	599	ASN
1	A	753	ASN
1	A	856	ASN
1	A	860	GLN
1	A	889	ASN
1	A	891	ASN

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Mol	Chain	Res	Type
1	A	937	HIS
1	A	1073	GLN
1	A	1075	HIS
1	A	1152	ASN
1	A	1479	HIS
1	A	1519	HIS
1	A	1557	ASN
1	A	1604	HIS
1	A	1629	ASN
2	B	126	ASN
2	B	147	ASN
2	B	191	ASN
2	B	192	HIS
2	B	230	HIS
2	B	300	GLN
2	B	374	HIS
2	B	386	GLN
2	B	402	GLN
2	B	404	ASN
2	B	640	HIS
2	B	687	ASN
2	B	733	GLN
2	B	752	ASN
2	B	779	HIS
2	B	908	GLN
2	B	964	GLN
2	B	1023	HIS
2	B	1038	HIS
2	B	1043	GLN
3	C	133	HIS
3	C	182	GLN
3	C	207	GLN
3	C	214	HIS
3	C	223	HIS
4	D	51	ASN
5	E	7	ASN
5	E	99	HIS
5	E	131	GLN
7	G	21	HIS
7	G	100	HIS
7	G	167	GLN
8	H	37	ASN

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Mol	Chain	Res	Type
8	H	118	HIS
10	J	63	ASN
12	L	31	ASN
1	M	60	ASN
1	M	232	GLN
1	M	257	GLN
1	M	501	ASN
1	M	533	ASN
1	M	536	HIS
1	M	543	HIS
1	M	545	GLN
1	M	546	ASN
1	M	568	GLN
1	M	590	ASN
1	M	599	ASN
1	M	753	ASN
1	M	856	ASN
1	M	860	GLN
1	M	889	ASN
1	M	891	ASN
1	M	937	HIS
1	M	1073	GLN
1	M	1075	HIS
1	M	1152	ASN
1	M	1479	HIS
1	M	1519	HIS
1	M	1557	ASN
1	M	1604	HIS
1	M	1629	ASN
2	N	126	ASN
2	N	147	ASN
2	N	191	ASN
2	N	192	HIS
2	N	230	HIS
2	N	300	GLN
2	N	374	HIS
2	N	386	GLN
2	N	402	GLN
2	N	404	ASN
2	N	640	HIS
2	N	687	ASN
2	N	733	GLN

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Mol	Chain	Res	Type
2	N	752	ASN
2	N	779	HIS
2	N	908	GLN
2	N	964	GLN
2	N	1023	HIS
2	N	1038	HIS
2	N	1043	GLN
3	O	45	ASN
3	O	99	GLN
3	O	182	GLN
3	O	207	GLN
3	O	214	HIS
3	O	223	HIS
4	P	51	ASN
5	Q	7	ASN
5	Q	99	HIS
5	Q	131	GLN
7	S	21	HIS
7	S	100	HIS
7	S	167	GLN
8	T	37	ASN
8	T	118	HIS
12	X	31	ASN

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

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

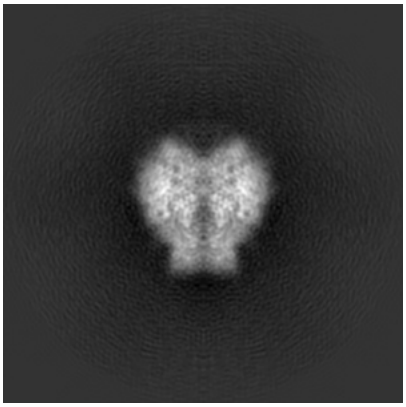
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11841. These allow visual inspection of the internal detail of the map and identification of artifacts.

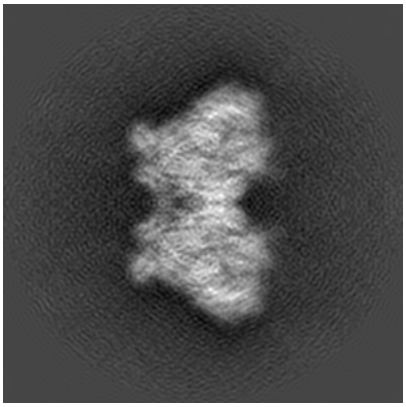
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

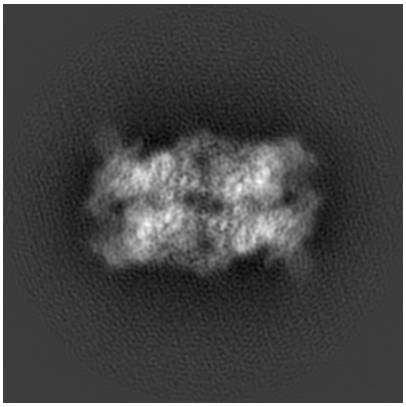
6.1.1 Primary map



X



Y

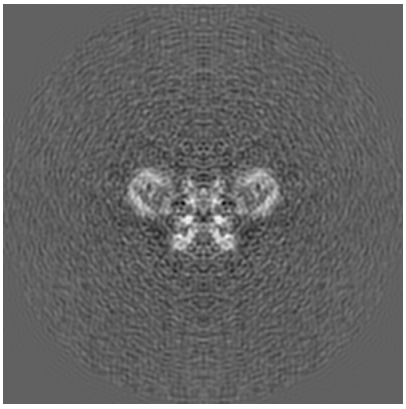


Z

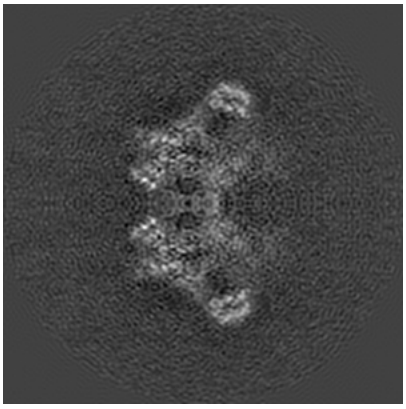
The images above show the map projected in three orthogonal directions.

6.2 Central slices

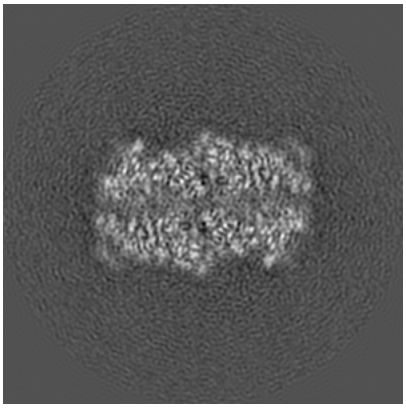
6.2.1 Primary map



X Index: 180



Y Index: 180

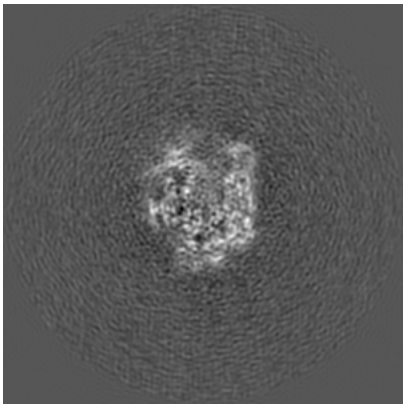


Z Index: 180

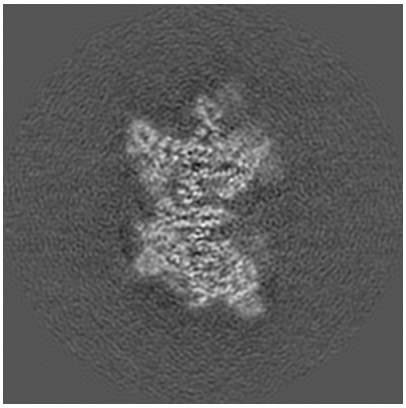
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

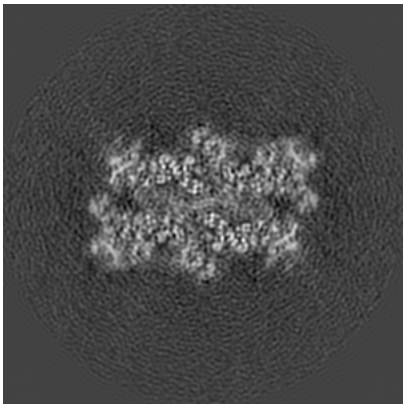
6.3.1 Primary map



X Index: 145



Y Index: 200

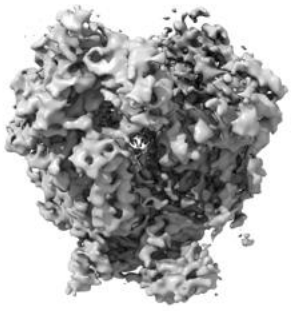


Z Index: 189

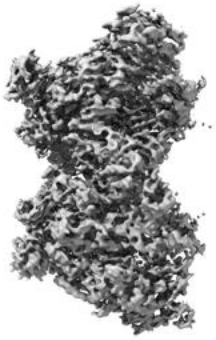
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

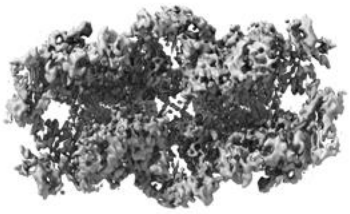
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.033. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

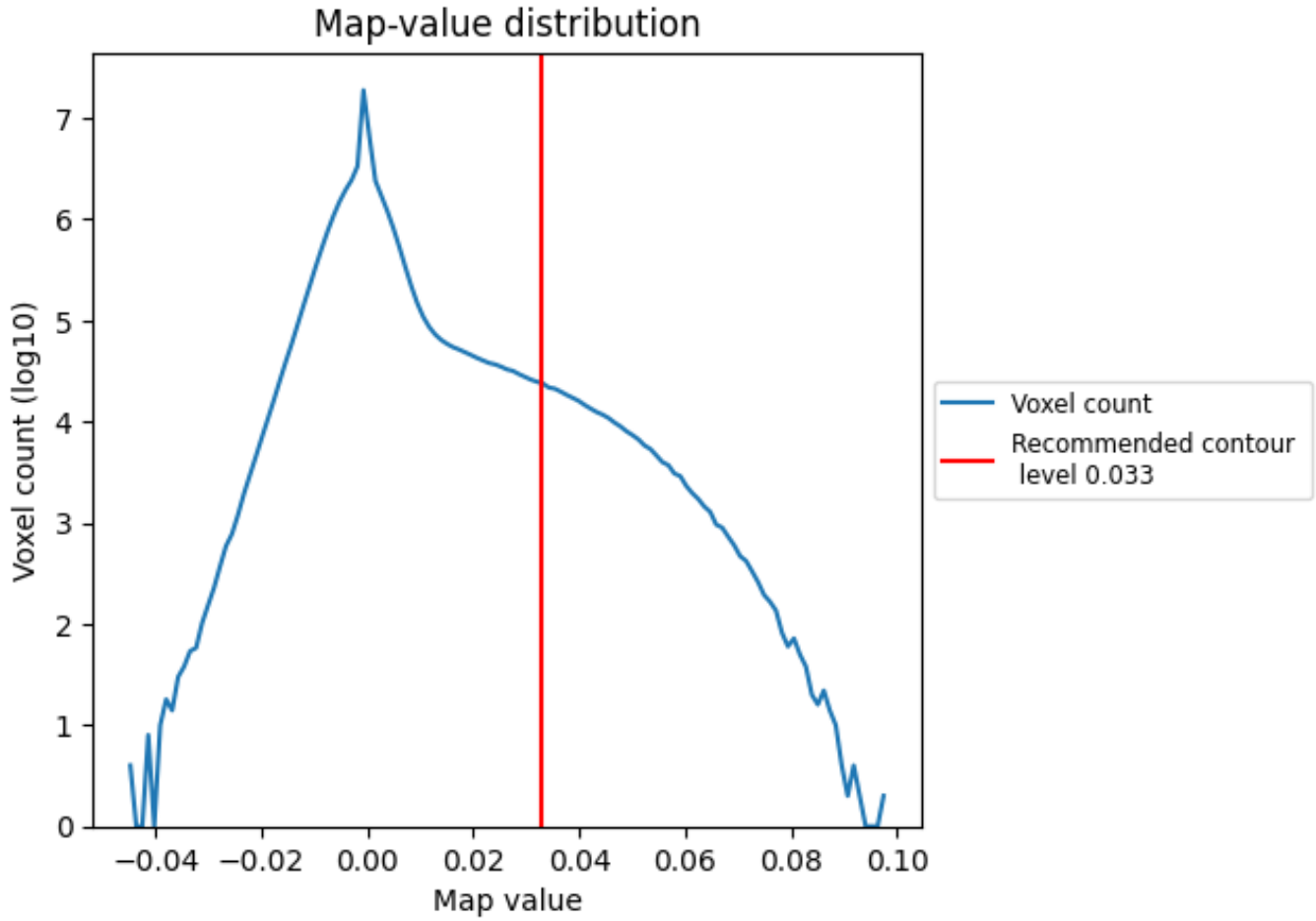
6.5 Mask visualisation (i)

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

7 Map analysis

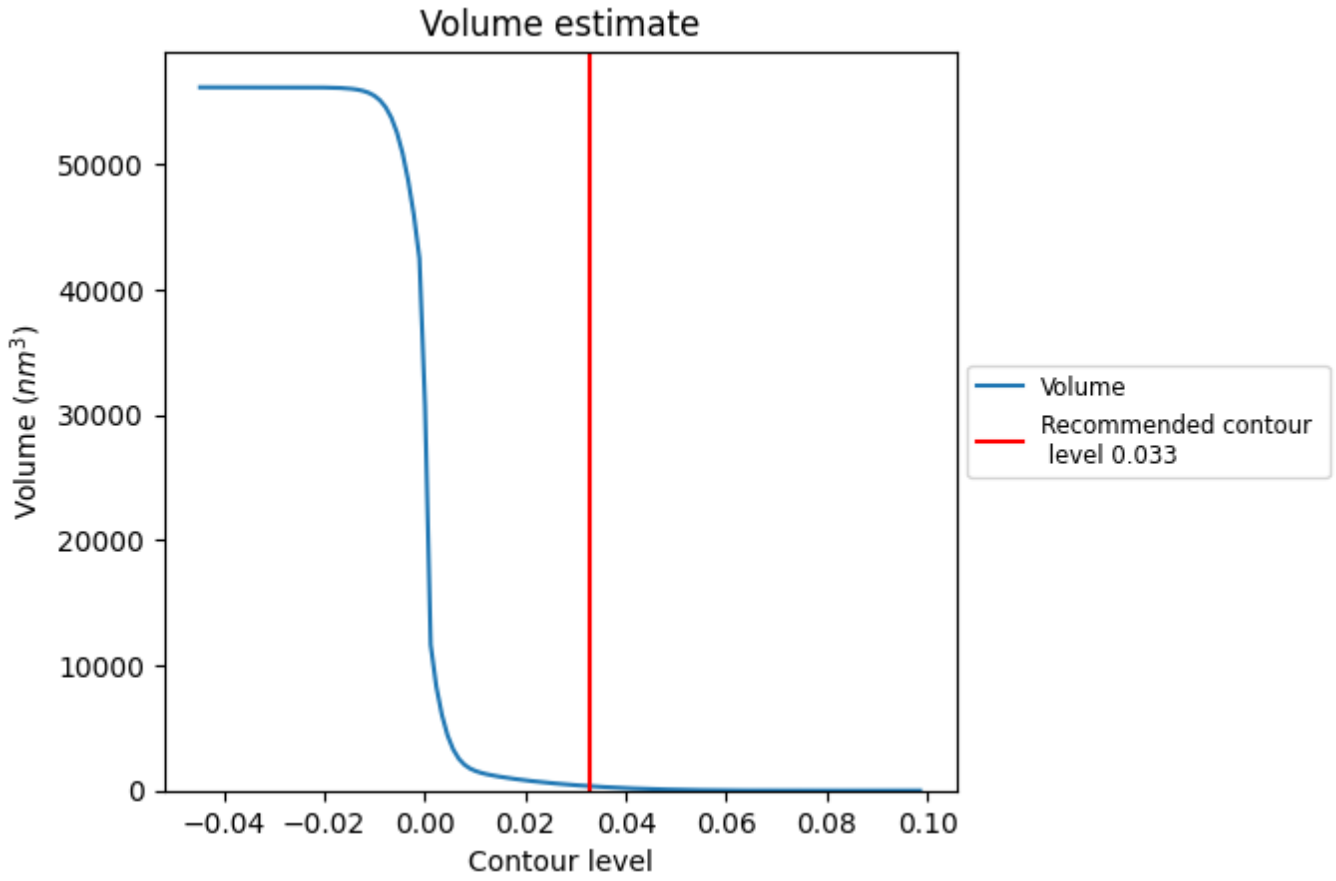
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

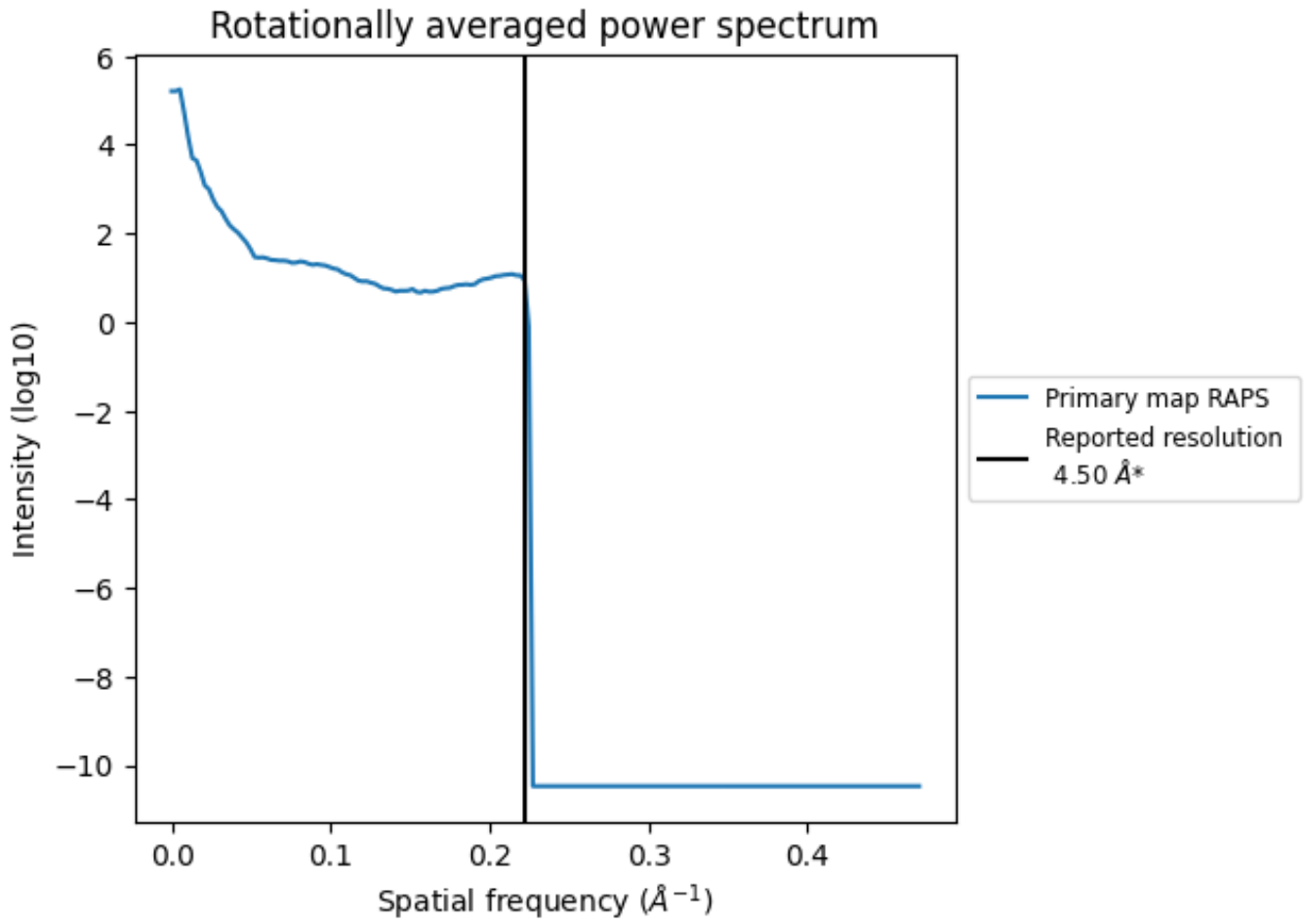
7.2 Volume estimate



The volume at the recommended contour level is 347 nm^3; this corresponds to an approximate mass of 314 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 0.222 Å^{-1}

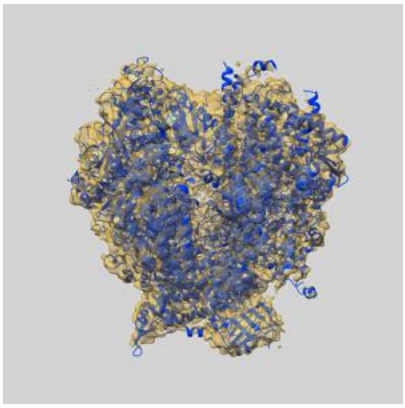
8 Fourier-Shell correlation

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

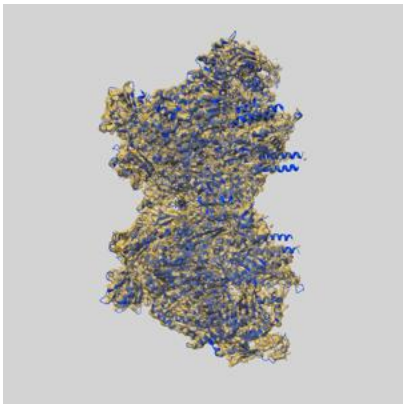
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-11841 and PDB model 7AOD. Per-residue inclusion information can be found in section 3 on page 7.

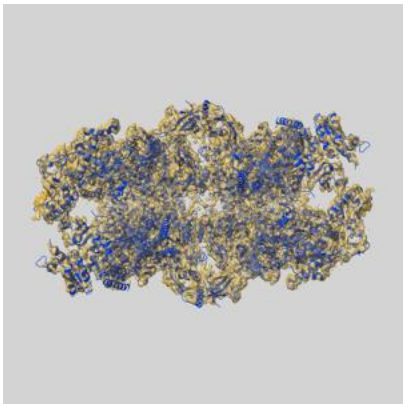
9.1 Map-model overlay



X



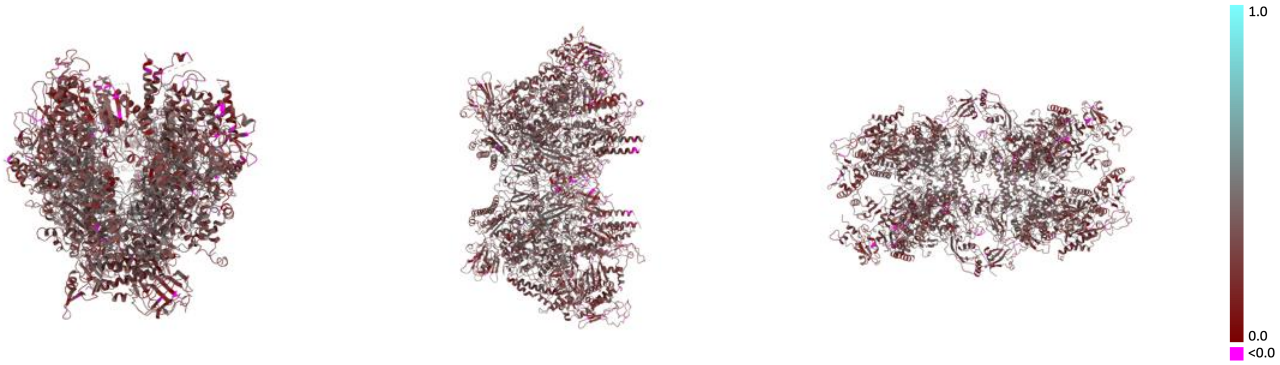
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.033 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.

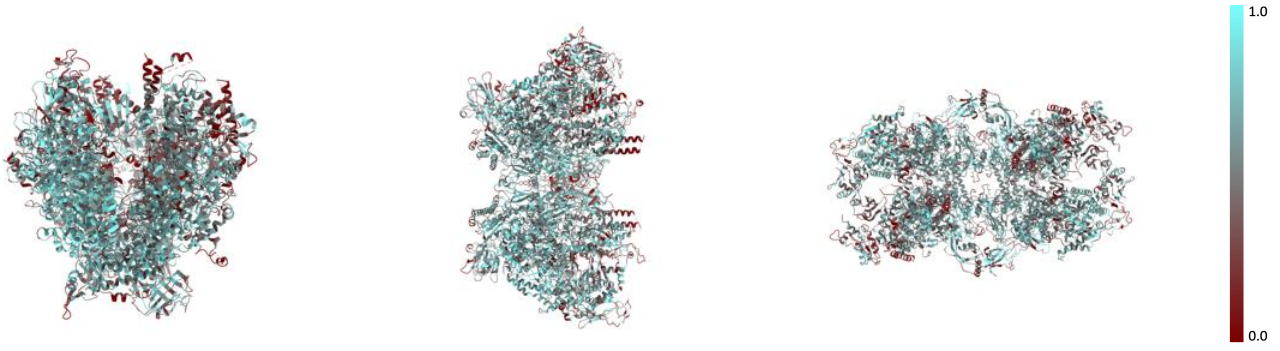
9.2 Q-score mapped to coordinate model (i)



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.

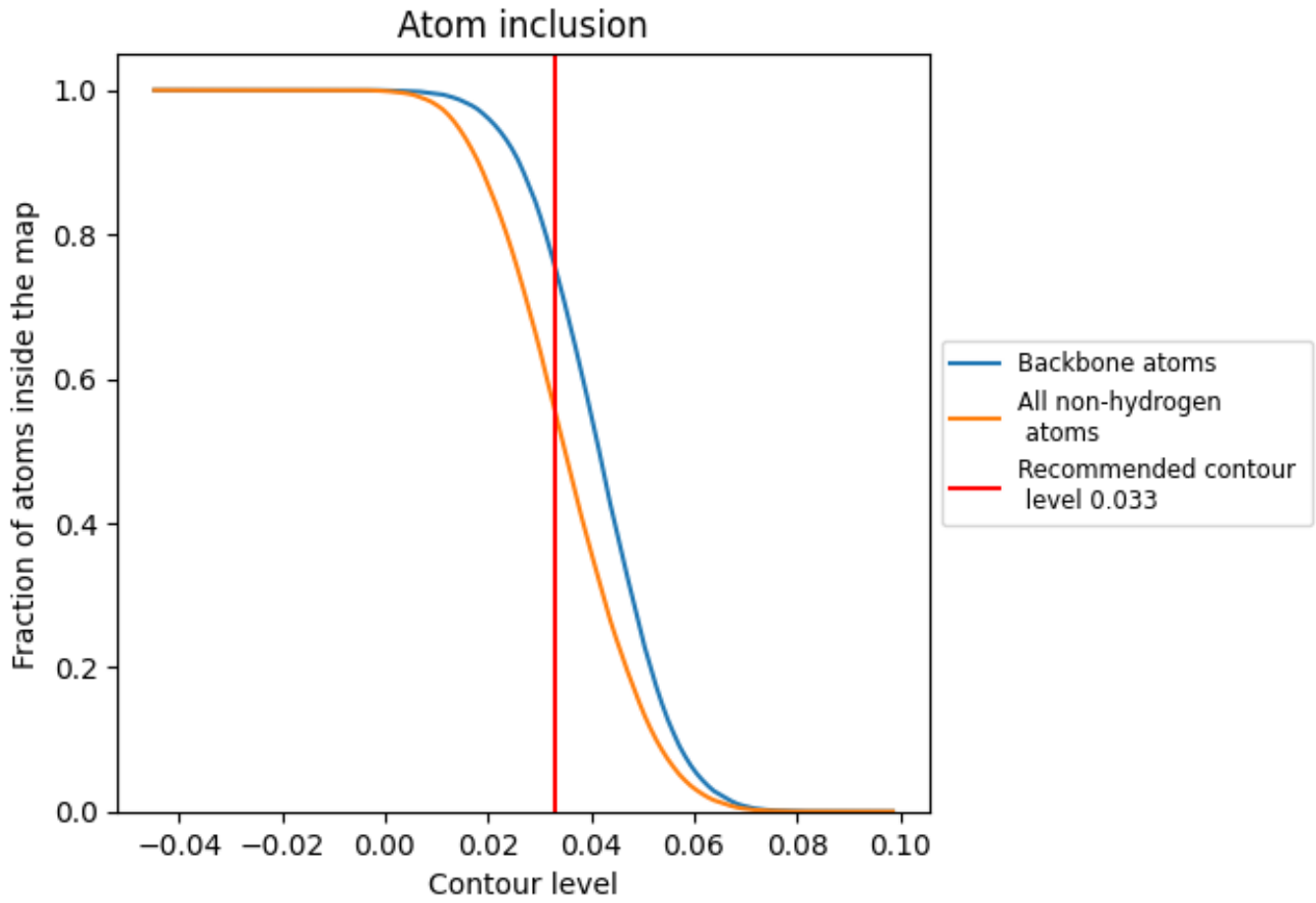
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.033).

9.4 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 56% 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 (0.033) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5553	0.3090
A	0.5317	0.3070
B	0.5945	0.3230
C	0.5726	0.3120
D	0.3949	0.2420
E	0.4360	0.2740
F	0.6224	0.3460
G	0.5962	0.2870
H	0.5444	0.2730
I	0.3302	0.2280
J	0.7013	0.3360
K	0.6011	0.2960
L	0.5439	0.3340
M	0.5304	0.3070
N	0.5951	0.3220
O	0.5754	0.3190
P	0.3822	0.2390
Q	0.4458	0.2780
R	0.6161	0.3530
S	0.5986	0.2910
T	0.5517	0.2720
U	0.3326	0.2410
V	0.7069	0.3460
W	0.5997	0.2950
X	0.5496	0.3400