Full wwPDB EM Validation Report (i)

Sep 28, 2024 – 09:37 pm BST

PDB ID	:	5LCW
EMDB ID	:	EMD-4037
Title	:	Cryo-EM structure of the Anaphase-promoting complex/Cyclosome, in complex with the Mitotic checkpoint complex (APC/C-MCC) at 4.2 angstrom resolution
Authors	:	Alfieri, C.; Chang, L.; Zhang, Z.; Yang, J.; Maslen, S.; Skehel, M.; Barford, D.
Deposited on	:	2016-06-22
Resolution	:	4.20 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 (i) 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 (i)) were used in the production of this report:

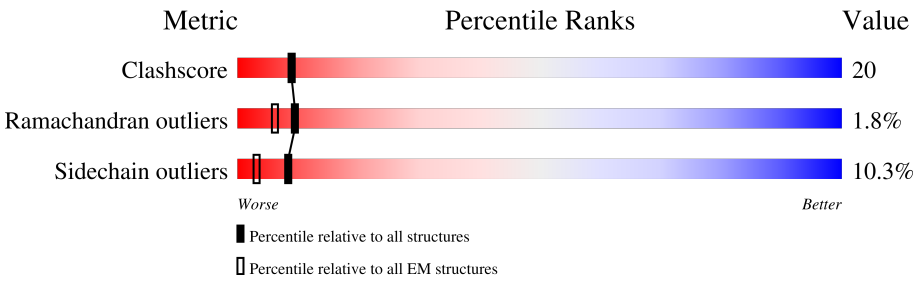
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.20 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1944	11% 45% 25% • 26%
2	B	84	79% 40% 42% 8% • 6%
3	C	597	11% 55% 30% • 12%
3	P	597	8% 54% 24% • 18%
4	D	121	7% 6% 8% • 85%
5	E	110	• 34% 15% • 49%
6	F	824	• 40% 17% • 41%
6	H	824	40% 17% • 41%

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Mol	Chain	Length	Quality of chain
7	G	85	16% 12% • 71%
7	W	85	• 18% 9% • 71%
8	I	808	19% 55% 33% • 9%
9	J	620	• 50% 26% 5% 19%
9	K	620	• 48% 28% • 20%
10	L	185	9% 61% 34% • •
11	M	74	15% 47% 28% • 20%
12	N	822	23% 48% 28% 7% • 14%
13	O	755	17% 57% 28% 6% 9%
14	Q	374	22% 74% 19% • 5%
15	R	499	15% 56% 19% • 23%
16	S	342	21% 47% 29% 5% 19%
17	X	599	13% 53% 26% • 19%
17	Y	599	7% 52% 27% • 17%
18	Z	205	26% 69% 21% • 5%

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 72075 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 Anaphase-promoting complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1441	10949	7039	1853	1983	74	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	356	PHE	PRO	conflict	UNP Q9H1A4

- Molecule 2 is a protein called Anaphase-promoting complex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	79	643	411	116	100	16	0	0

- Molecule 3 is a protein called Cell division cycle protein 23 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	524	4306	2774	727	781	24	0	0
3	P	491	4043	2611	679	729	24	0	0

- Molecule 4 is a protein called Anaphase-promoting complex subunit 15.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	D	18	153	104	23	26	0	0

- Molecule 5 is a protein called Anaphase-promoting complex subunit 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	56	450	290	74	85	1	0	0

- Molecule 6 is a protein called Cell division cycle protein 27 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	483	3849	2470	649	704	26	0	0
6	H	483	3853	2473	650	704	26	0	0

- Molecule 7 is a protein called Anaphase-promoting complex subunit CDC26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	25	213	133	40	39	1	0	0
7	W	25	213	133	40	39	1	0	0

- Molecule 8 is a protein called Anaphase-promoting complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	I	733	5716	3665	951	1067	33	0	0

- Molecule 9 is a protein called Cell division cycle protein 16 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	J	504	4047	2601	684	737	25	0	0
9	K	493	3988	2563	672	729	24	0	0

- Molecule 10 is a protein called Anaphase-promoting complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	L	182	1435	898	263	268	6	0	0

- Molecule 11 is a protein called Anaphase-promoting complex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	M	59	493	310	79	102	2	0	0

- Molecule 12 is a protein called Anaphase-promoting complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	N	703	5403	3436	971	971	25	0	0

- Molecule 13 is a protein called Anaphase-promoting complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	O	685	5402	3446	940	988	28	0	0

- Molecule 14 is a protein called Cell division cycle protein 20 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	Q	354	2671	1676	488	496	11	0	0

- Molecule 15 is a protein called Cell division cycle protein 20 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	R	383	2953	1855	538	548	12	0	0

- Molecule 16 is a protein called Mitotic checkpoint serine/threonine-protein kinase BUB1 beta,Mitotic checkpoint serine/threonine-protein kinase BUB1 beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	S	277	2077	1292	380	400	5	0	0

- Molecule 17 is a protein called Anaphase-promoting complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	X	484	3773	2393	652	704	24	0	0
17	Y	496	3868	2449	669	724	26	0	0

- Molecule 18 is a protein called Mitotic spindle assembly checkpoint protein MAD2A.

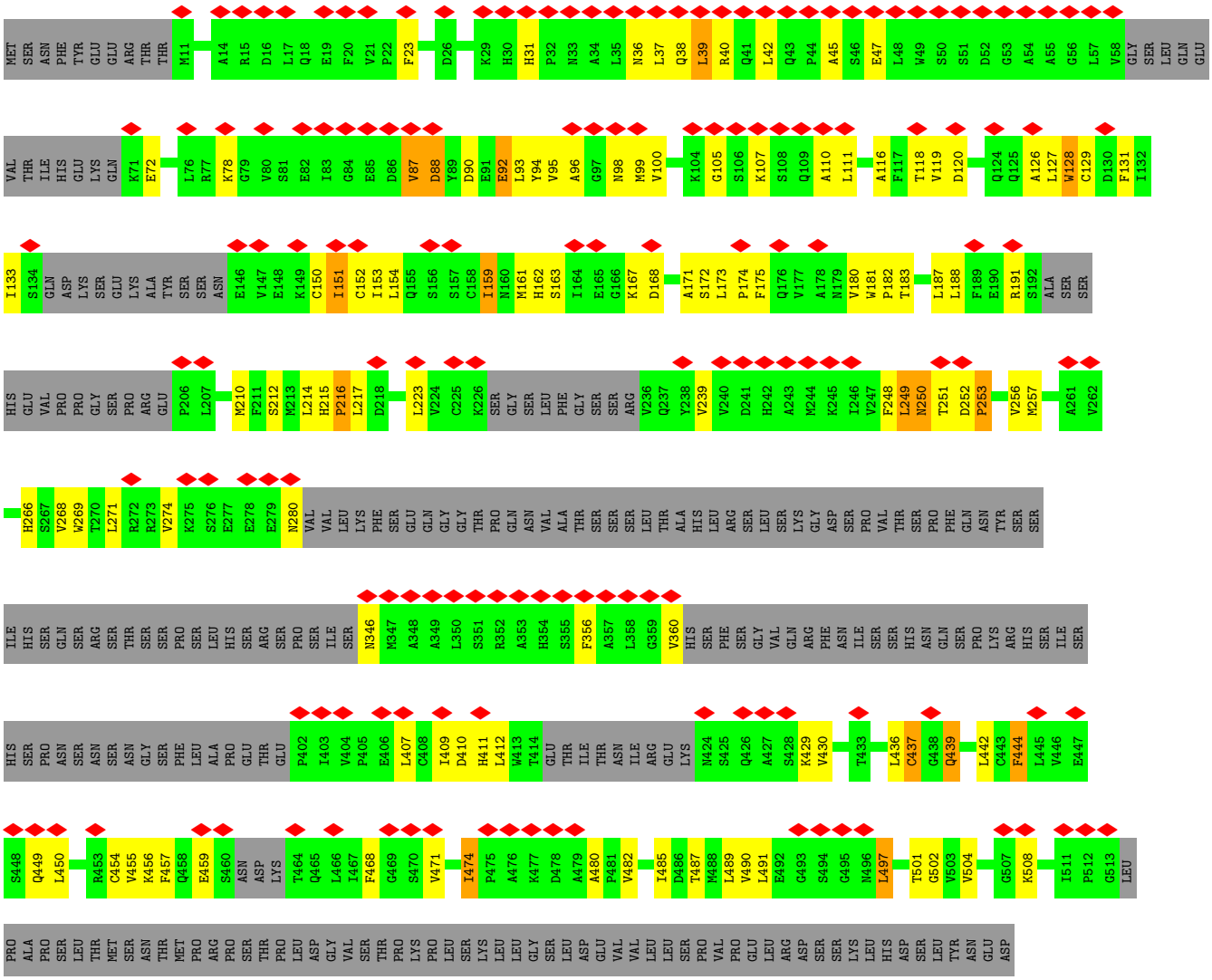
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	Z	195	1577	1012	256	305	4	0	0

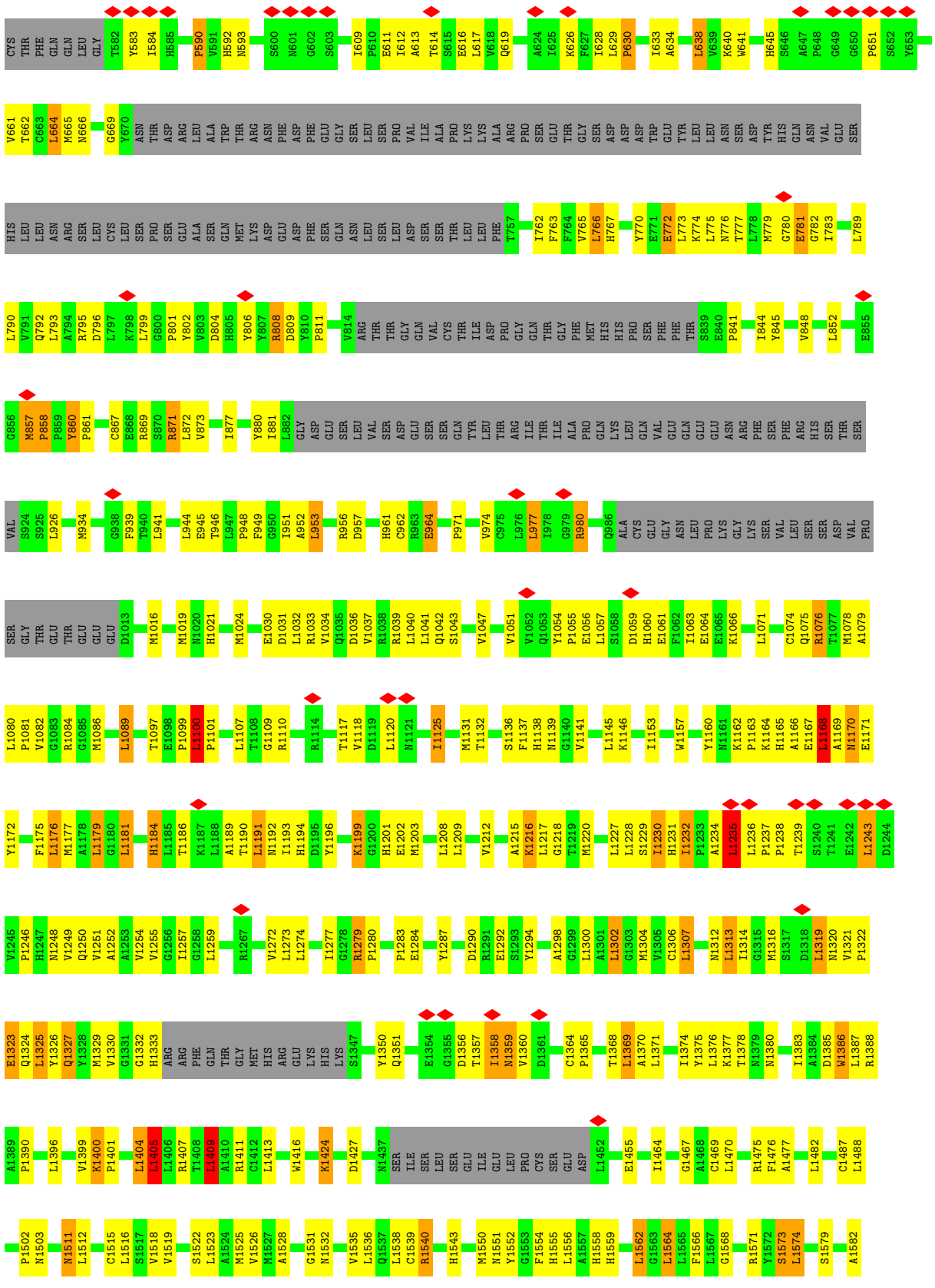
3 Residue-property plots (i)

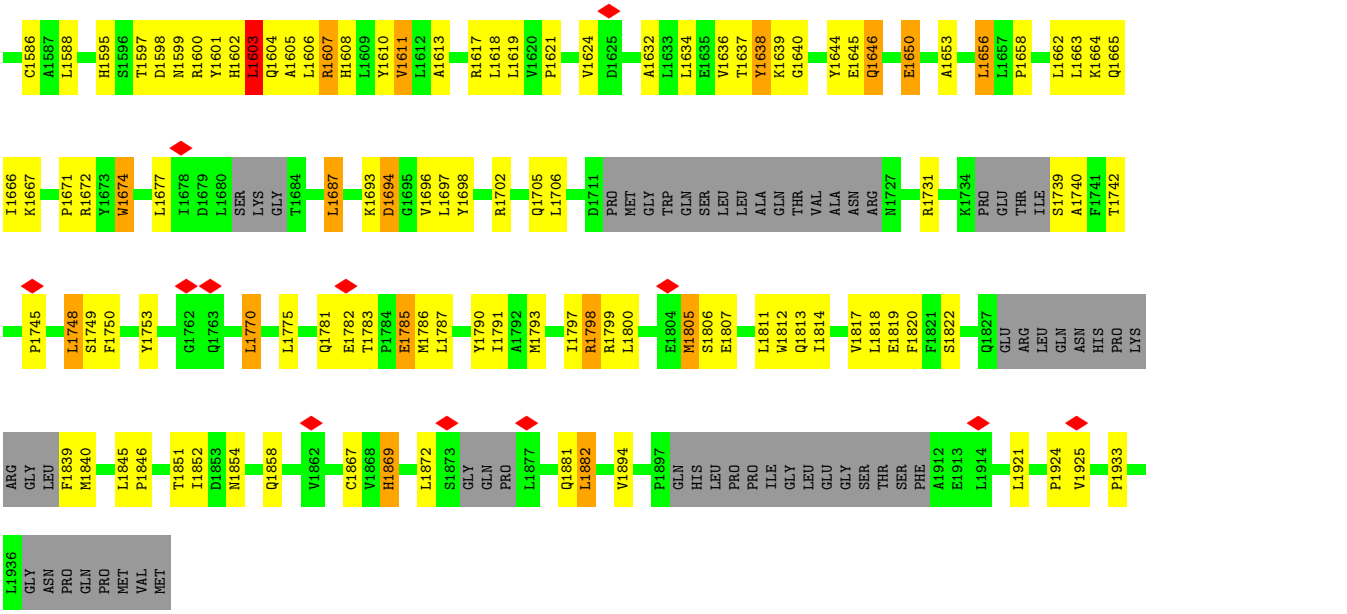
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Anaphase-promoting complex subunit 1

Chain A:

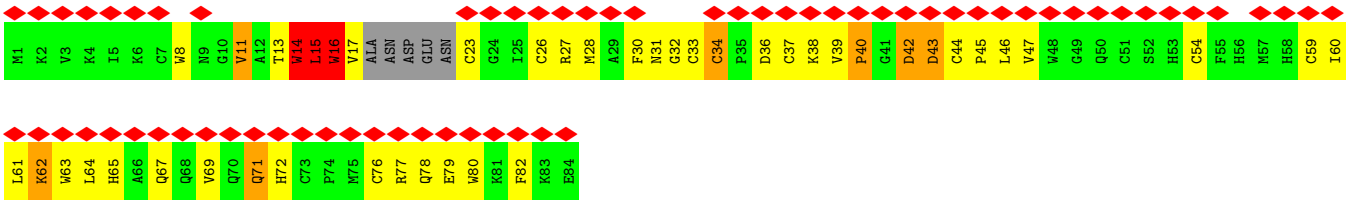



CYS THR PHE GLN GLN LEU GLY T582 Y583 I584 H585 P590 V591 H592 N593 S600 N601 G602 S603 I609 P610 E611 I612 A613 T614 S615 E616 L617 V618 Q619 A624 I625 K626 F627 I628 L629 P630 I633 A634 L638 V639 K640 W641 H645 S646 A647 P648 G649 G650 P651 S652 Y653
V661 T662 C663 L664 M665 N666 G669 Y670 ASN THR ASP ARG LEU ALA TRP THR ARG ASN PHE ASP PHE GLU GLY SER LEU SER PRO VAL ILE ALA PRO LYS LYS ALA ARG PRO SER GLU THR GLY SER ASP ASP TRP GLU TYR LEU LEU ASN SER ASP TYR HIS GLN ASN VAL GLU SER
HIS LEU LEU ASN ARG SER LEU CYS LEU SER PRO SER GLU ALA SER GLN MET LYS ASP GLU ASP PHE SER GLN ASN LEU LEU SER LEU ASP SER SER THR LEU LEU PHE T757 I762 F763 F764 V765 L766 H767 Y770 E771 E772 L773 K774 L775 N776 T777 L778 M779 G780 E781 G782 I783 L789
L790 V791 Q792 L793 A794 R795 D796 L797 K798 L799 G800 P801 Y802 V803 D804 H805 Y806 Y807 R808 D809 Y810 P811 V814 ARG THR THR GLY GLN VAL CYS THR ILE ASP PRO GLY GLN THR GLY PHE MET HIS HIS PRO SER PHE PHE THR S839 E840 P841 I844 Y845 V848 L852 E855
G856 M857 P858 P859 Y860 P861 C867 E868 R869 S870 R871 L872 V873 I877 Y880 I881 L882 GLY ASP GLU SER LEU VAL SER ASP GLU SER SER GLN TYR LEU THR ARG ILE THR ILE ALA PRO GLN LYS LEU GLN VAL GLU GLN GLU GLU ASN ARG PHE SER PHE ARG HIS SER THR SER
VAL S924 S925 L926 M934 G938 F939 T940 L941 L944 E945 T946 L947 P948 F949 G950 I951 A952 L953 R956 D957 H961 C962 R963 E964 P971 V974 C975 L976 L977 I978 G979 R980 Q986 ALA CYS GLU GLY ASN LEU PRO LYS GLY LYS SER VAL LEU SER SER ASP VAL PRO
SER GLY THR GLU THR GLU GLU GLU D1013 M1016 M1019 N1020 H1021 M1024 E1030 D1031 L1032 R1033 V1034 Q1035 D1036 V1037 R1038 R1039 L1040 L1041 Q1042 S1043 V1047 V1051 V1052 Q1053 Y1054 P1055 E1056 L1057 S1058 D1059 H1060 E1061 F1062 I1063 E1064 E1065 K1066 L1071 C1074 Q1075 R1076 T1077 M1078 A1079
L1080 P1081 V1082 G1083 R1084 G1085 M1086 L1089 T1097 E1098 P1099 L1100 P1101 L1107 T1108 G1109 R1110 R1114 T1117 V1118 D1119 L1120 N1121 I1125 M1131 T1132 S1136 F1137 H1138 N1139 G1140 V1141 L1145 K1146 I1153 W1157 Y1160 N1161 K1162 P1163 K1164 H1165 A1166 E1167 L1168 A1169 N1170 E1171
Y1172 F1175 L1176 M1177 A1178 L1179 G1180 L1181 H1184 L1185 T1186 K1187 L1188 A1189 T1190 L1191 N1192 I1193 H1194 D1195 Y1196 K1199 G1200 H1201 E1202 M1203 L1208 L1209 V1212 A1215 K1216 L1217 G1218 T1219 M1220 L1227 L1228 S1229 I1230 H1231 I1232 P1233 A1234 L1235 L1236 P1237 P1238 T1239 S1240 T1241 E1242 L1243 D1244
V1245 P1246 H1247 N1248 V1249 Q1250 V1251 A1252 A1253 V1254 V1255 G1256 I1257 G1258 L1259 R1267 V1272 L1273 L1274 I1277 G1278 R1279 P1280 P1283 E1284 Y1287 D1290 R1291 E1292 S1293 Y1294 A1298 G1299 L1300 A1301 L1302 G1303 M1304 V1305 C1306 L1307 N1312 L1313 I1314 G1315 M1316 S1317 D1318 L1319 N1320 V1321 P1322
E1323 Q1324 L1325 Y1326 Q1327 Y1328 M1329 V1330 G1331 G1332 H1333 ARG ARG PHE GLN THR GLY MET HIS ARG GLU LYS HIS LYS S1347 Y1350 Q1351 E1354 G1355 D1356 T1357 I1358 N1359 V1360 D1361 C1364 P1365 T1368 L1369 A1370 L1371 I1374 Y1375 L1376 K1377 T1378 N1379 N1380 I1383 A1384 D1385 W1386 L1387 R1388
A1389 P1390 L1396 V1399 K1400 P1401 L1404 L1405 L1406 R1407 T1408 L1409 A1410 R1411 C1412 L1413 W1416 K1424 D1427 N1437 SER ILE SER LEU SER GLU ILE GLU LEU PRO CYS SER GLU ASP L1452 E1455 I1464 G1467 A1468 C1469 L1470 R1475 F1476 A1477 L1482 C1487 L1488
P1502 N1503 N1511 L1512 C1515 L1516 S1517 V1518 V1519 S1522 L1523 A1524 M1525 V1526 M1527 A1528 G1531 N1532 V1535 L1536 G1537 L1538 C1539 R1540 H1543 M1550 N1551 Y1552 G1553 F1554 H1555 L1556 A1557 H1558 H1559 L1562 G1563 L1564 L1565 F1566 L1567 G1568 R1571 Y1572 S1573 L1574 S1579 A1582



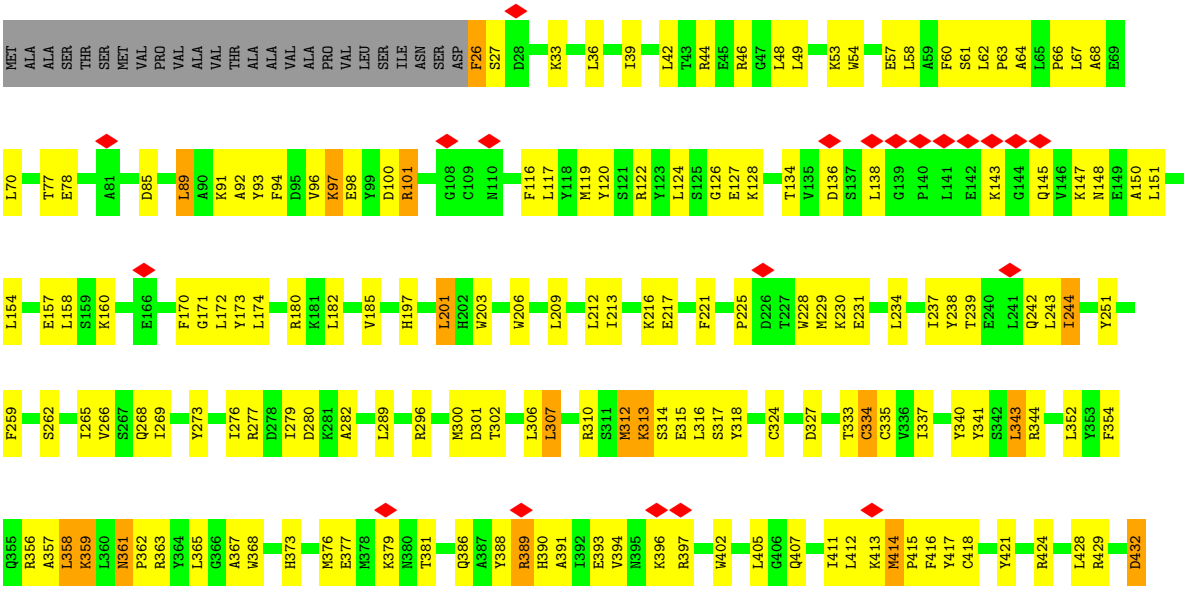
• Molecule 2: Anaphase-promoting complex subunit 11

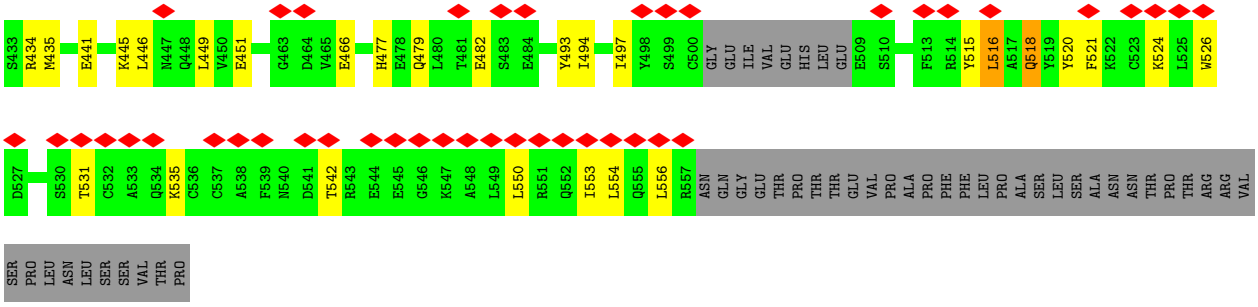
Chain B:



• Molecule 3: Cell division cycle protein 23 homolog

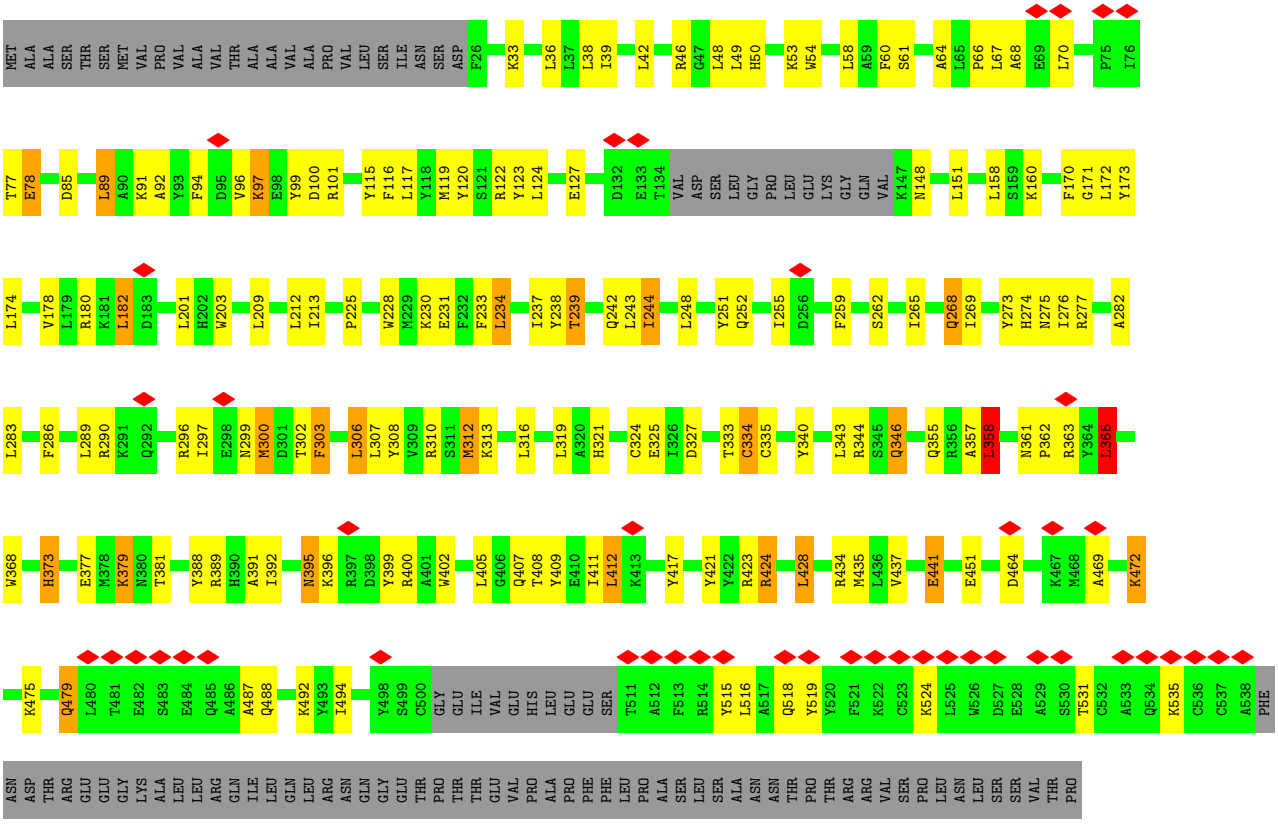
Chain C:





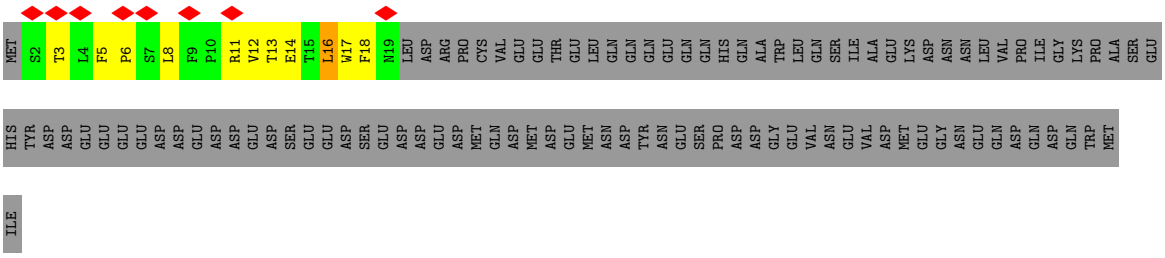
• Molecule 3: Cell division cycle protein 23 homolog

Chain P: 8% 54% 24% • 18%



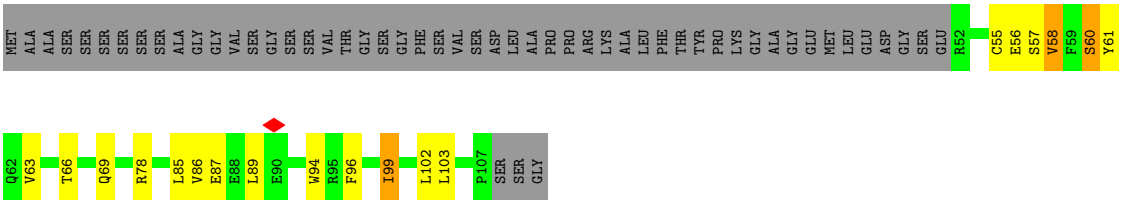
• Molecule 4: Anaphase-promoting complex subunit 15

Chain D: 7% 6% 8% • 85%



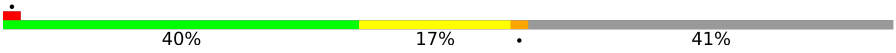
- Molecule 5: Anaphase-promoting complex subunit 16

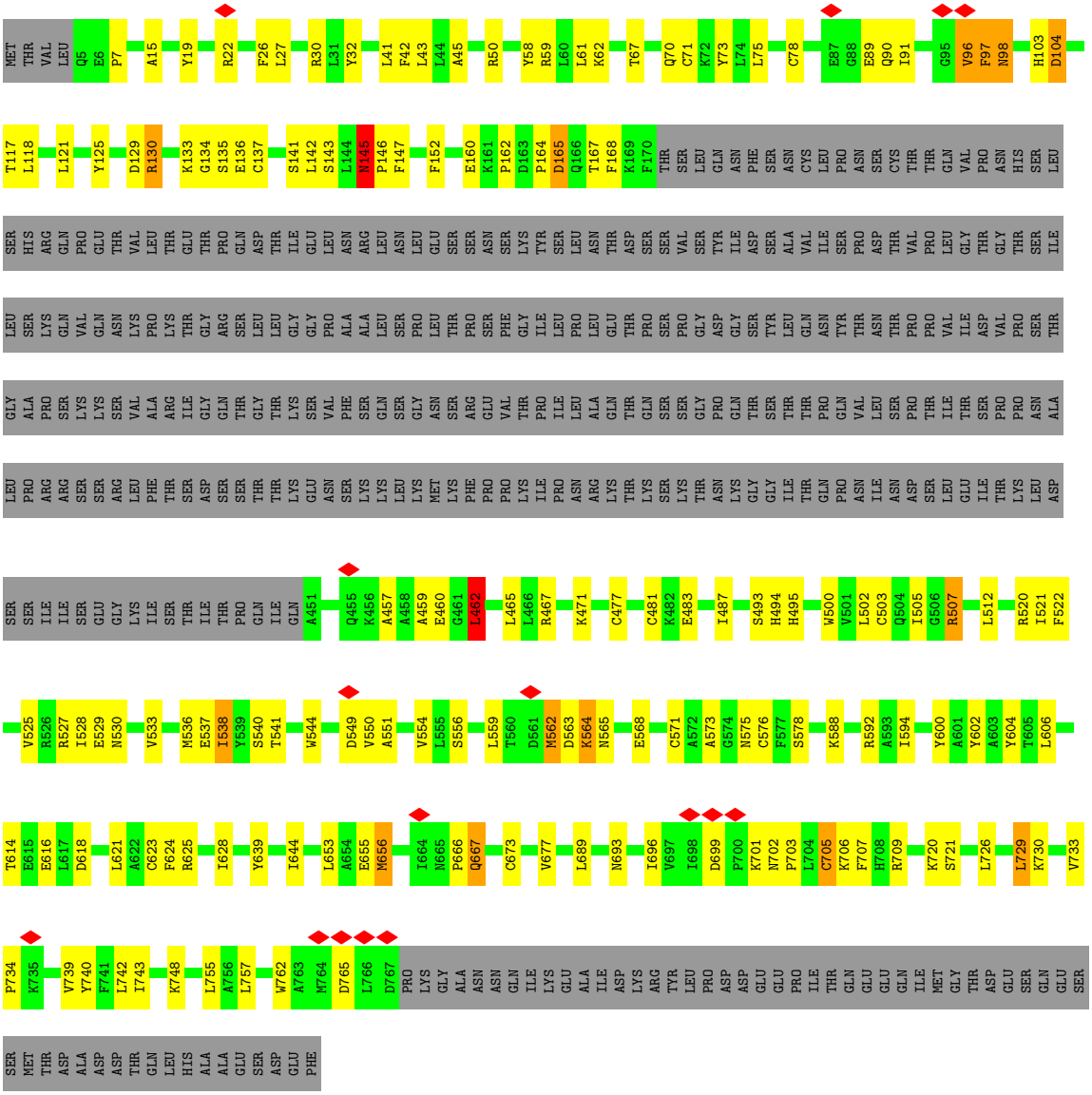
Chain E:



- Molecule 6: Cell division cycle protein 27 homolog

Chain F:





- Molecule 6: Cell division cycle protein 27 homolog

Chain H: 40% 17% • 41%

MET THR VAL LEU Q5 E6 P7 Y19 L27 R30 L31 Y32 L41 F42 L43 Y49 R50 Y58 R59 L60 L61 K62 C71 K72 Y73 C78 L85 Q90 V96 F97 N98 S102 H103 D104 F116 T117 L121 Y125 T128 D129 R130 S141 L142

S143 L144 N145 P146 F147 L148 W149 I158 G159 P162 D163 P164 T167 F168 K169 F170 THR SER LEU GLN ASN PHE SER ASN CYS LEU PRO ASN SER CYS THR THR GLN VAL PRO ASN HIS SER LEU SER HIS ARG GLN PRO GLU THR VAL LEU THR GLU THR PRO GLN ASP THR ILE GLU

LEU ASN ARG LEU ASN LEU GLU SER SER ASN SER LYS TYR SER LEU ASN THR ASP SER SER VAL SER TYR ILE ASP SER ALA VAL ILE SER PRO ASP THR VAL PRO PRO LEU GLY THR GLY THR SER SER ILE LEU SER LYS GLN VAL GLN ASN LYS PRO LYS THR GLY ARG SER LEU LEU GLY

PRO ALA ALA LEU SER PRO LEU THR PRO SER PHE GLY ILE LEU PRO LEU GLU THR PRO SER PRO GLY SER TYR LEU GLN ASN TYR THR ASN THR PRO PRO VAL ILE ASP VAL PRO SER THR GLY ALA PRO SER LYS LYS SER VAL ALA ARG ILE GLY GLN THR GLY THR LYS SER

VAL PHE SER GLN SER GLY ASN SER ARG GLU VAL THR PRO ILE LEU ALA GLN THR GLN SER SER GLY PRO GLN THR SER THR THR PRO GLN VAL LEU SER PRO THR ILE THR SER PRO PRO ASN ALA LEU PRO ARG ARG SER SER ARG LEU PHE THR SER ASP SER SER SER THR THR LYS GLU

ASN SER LYS LYS LEU LYS MET LYS PHE PRO PRO LYS ILE PRO ASN ARG LYS THR LYS SER THR ASN LYS GLY GLY ILE THR GLN PRO ASN ILE ASN ASP SER LEU GLU ILE THR LYS LEU ASP SER SER ILE ILE SER GLU GLY LYS ILE SER THR ILE THR PRO GLN ILE GLN A451

Q455 A459 L462 L465 L466 R467 K471 G472 Y473 L474 C477 S478 Y479 N480 C481 K482 E483 A484 I485 N486 I487 L488 S489 H490 S493 H494 H495 W500 V501 L502 C503 Q504 I505 G506 R507 S513 E514 Y515 R520 I521 F522 V525 R526 R527 I528 E529 N530 E534

G535 M536 E537 S540 T541 H545 L552 S553 V554 L555 S556 K557 M562 D563 K564 N565 E568 A569 W570 C571 A572 A573 G574 N575 C576 E582 H583 D584 K588 F589 R592 A593 I594 Q595 N599 Y600 Y604 D618 L621 A622 C623 F624 R625 I628 R633

Y639 M643 I644 L653 A654 E655 M656 H657 F658 Q659 K660 Q667 S668 S669 C673 V677 S685 L689 N693 I698 D699 N702 P703 L704 F707 H708 R709 N716 K720 L726 L729 K730 V733 E736 V739 Y740 F741 L742 I743 Y747

H754 L755 A756 L757 M758 N759 F760 S761 W762 D765 L766 D767 PRO LYS GLY ALA ASN ASN GLN ILE LYS GLU ALA ILE ASP LYS ARG TYR LEU PRO ASP ASP GLU GLU PRO ILE THR GLN GLU GLU GLN ILE MET GLY THR ASP GLU SER GLN GLU SER SER MET THR ASP ALA ASP ASP THR

GLN LEU HIS ALA ALA GLU SER ASP GLU PHE

• Molecule 7: Anaphase-promoting complex subunit CDC26

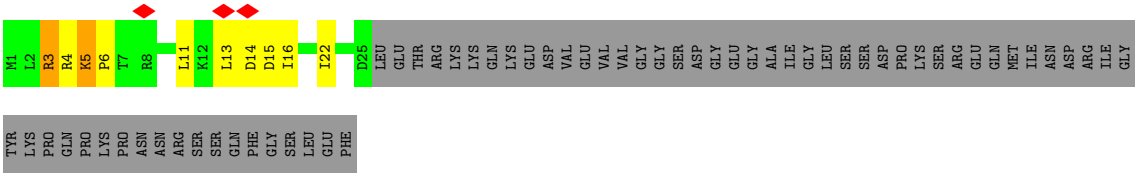
Chain G: 16% 12% • 71%

M1 L2 R3 R4 K5 P6 L11 K12 L13 D14 D15 I16 R23 K24 D25 LEU GLU THR ARG LYS LYS GLN LYS GLU ASP VAL GLU VAL VAL GLY GLY SER ASP GLY GLU GLY ALA ILE GLY LEU SER SER ASP PRO LYS SER ARG GLU GLN MET ILE ASN ASP ARG ILE GLY TYR LYS

PRO GLN PRO LYS PRO ASN ASN ARG SER SER GLN PHE GLY SER LEU GLU PHE

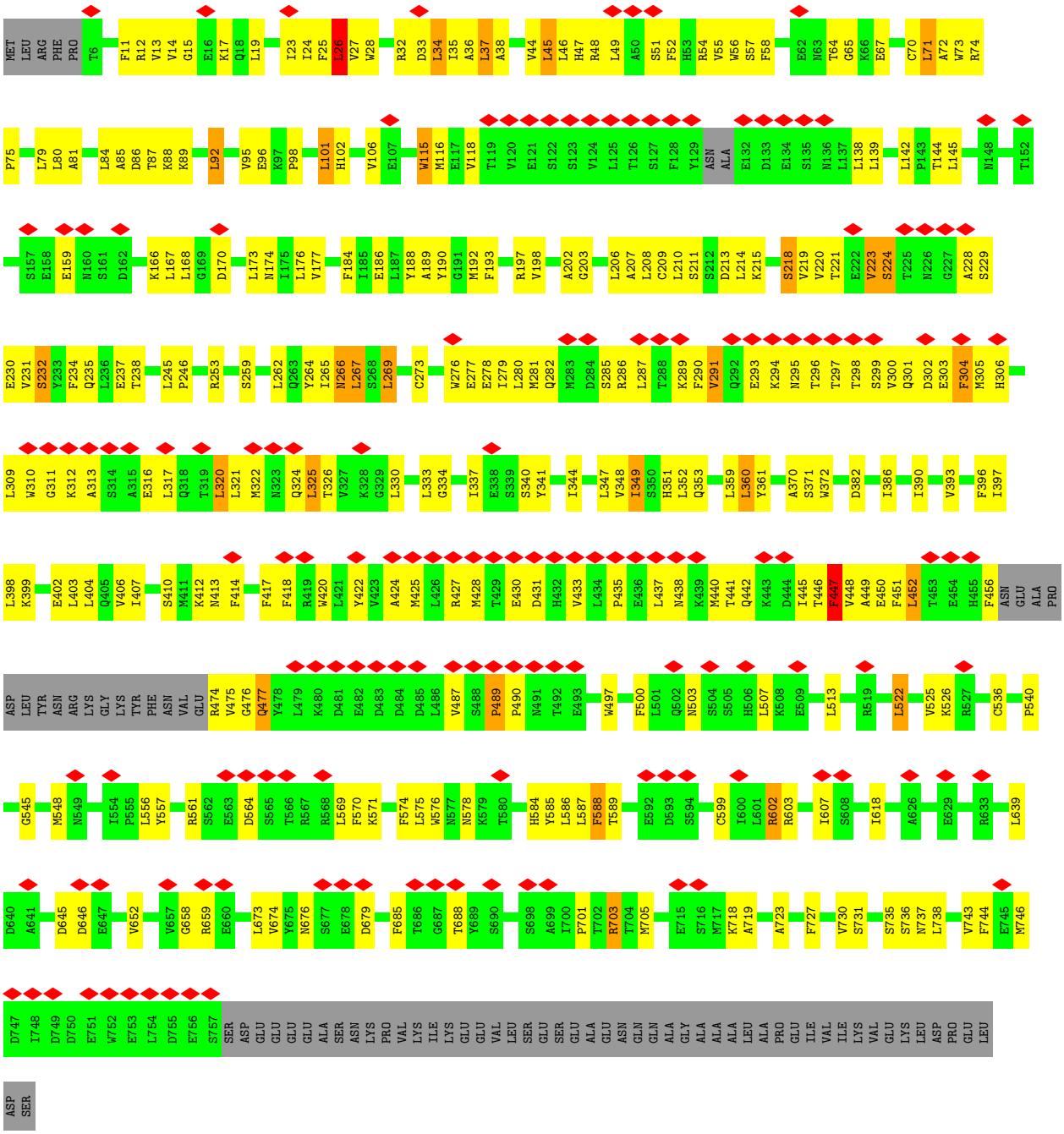
• Molecule 7: Anaphase-promoting complex subunit CDC26

Chain W: • 18% 9% • 71%



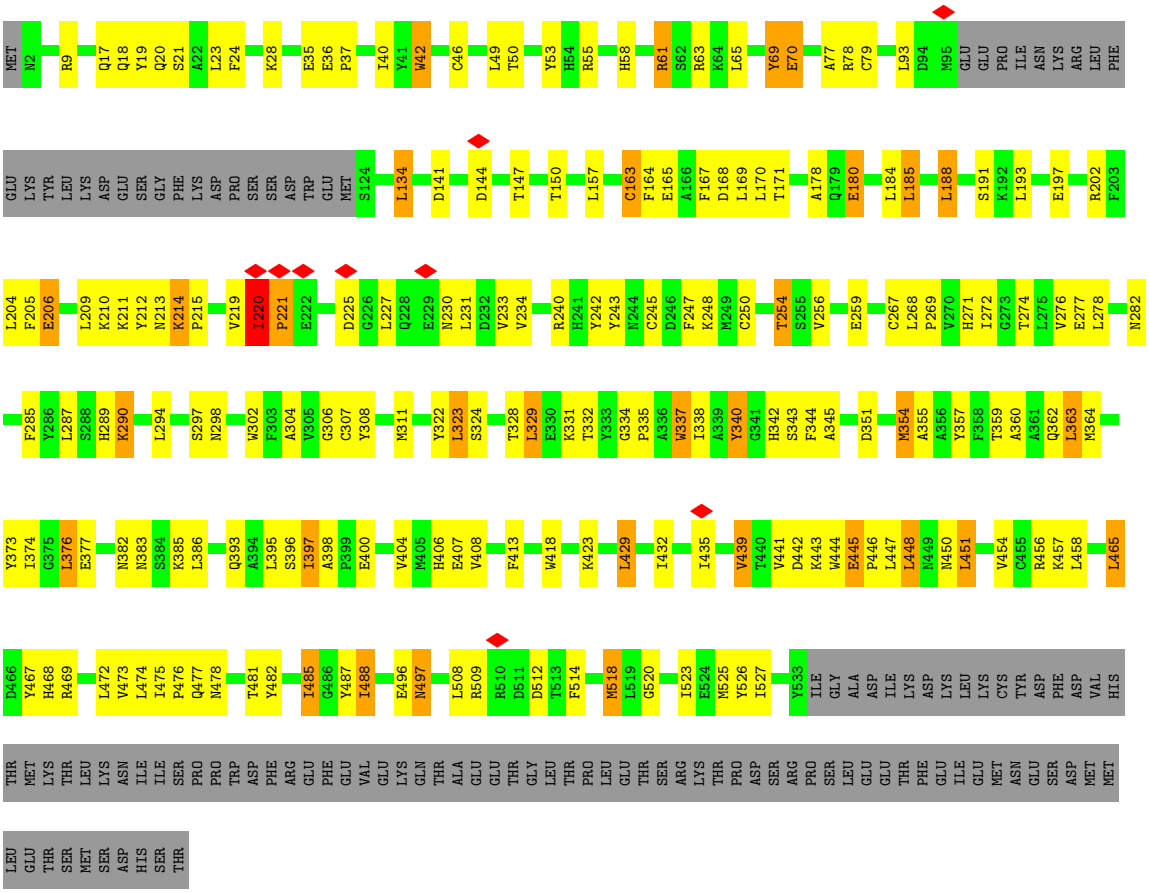
• Molecule 8: Anaphase-promoting complex subunit 4

Chain I:



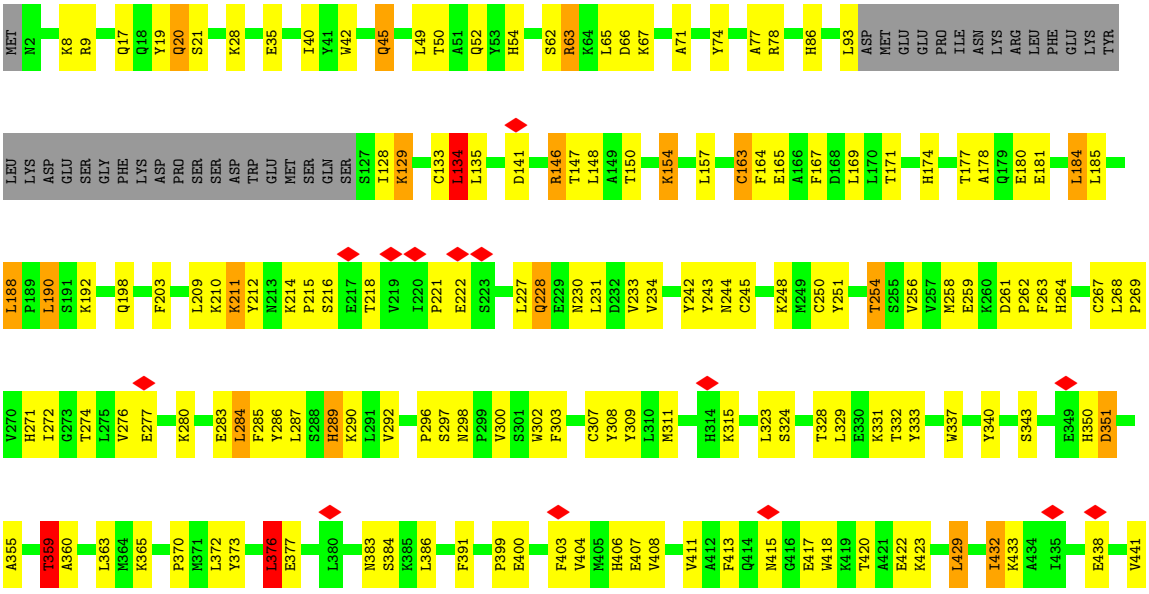
• Molecule 9: Cell division cycle protein 16 homolog

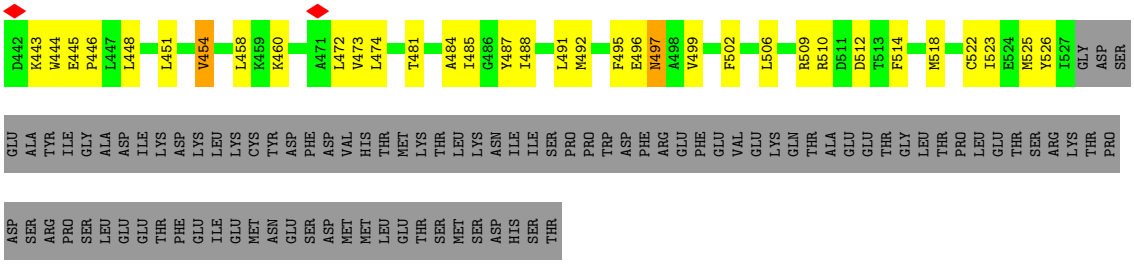
Chain J: 50% 26% 5% 19%



- Molecule 9: Cell division cycle protein 16 homolog

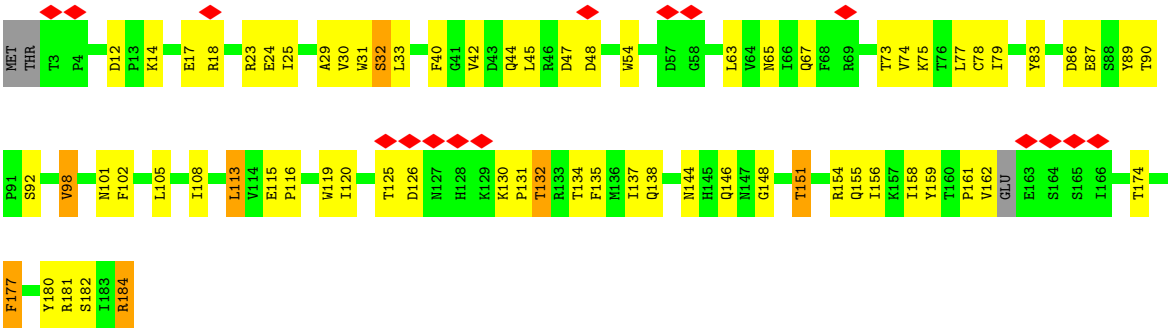
Chain K: 48% 28% • 20%





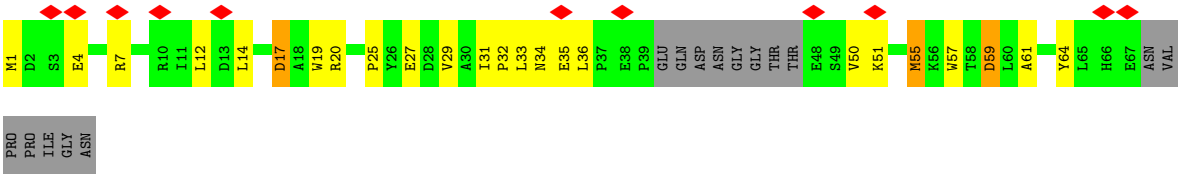
- Molecule 10: Anaphase-promoting complex subunit 10

Chain L:



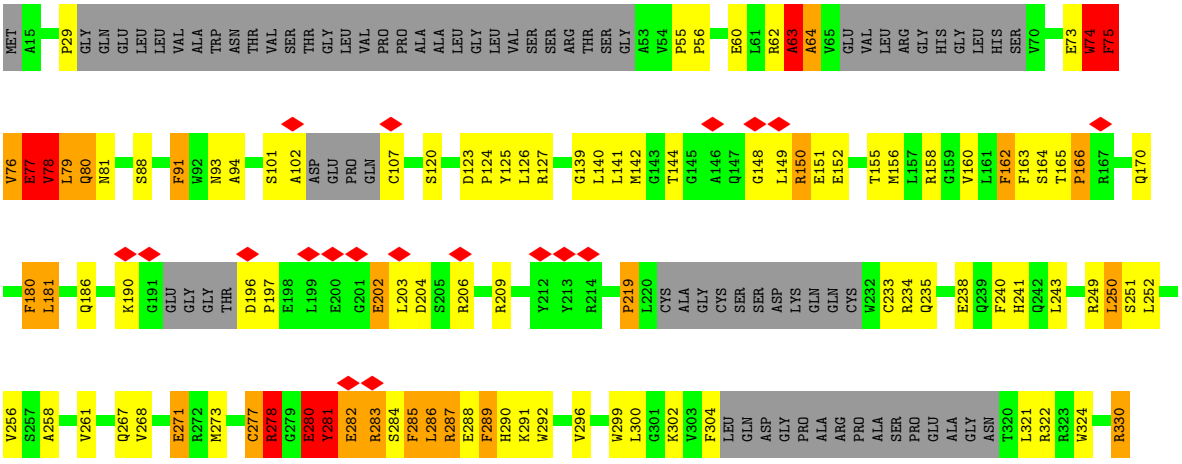
- Molecule 11: Anaphase-promoting complex subunit 13

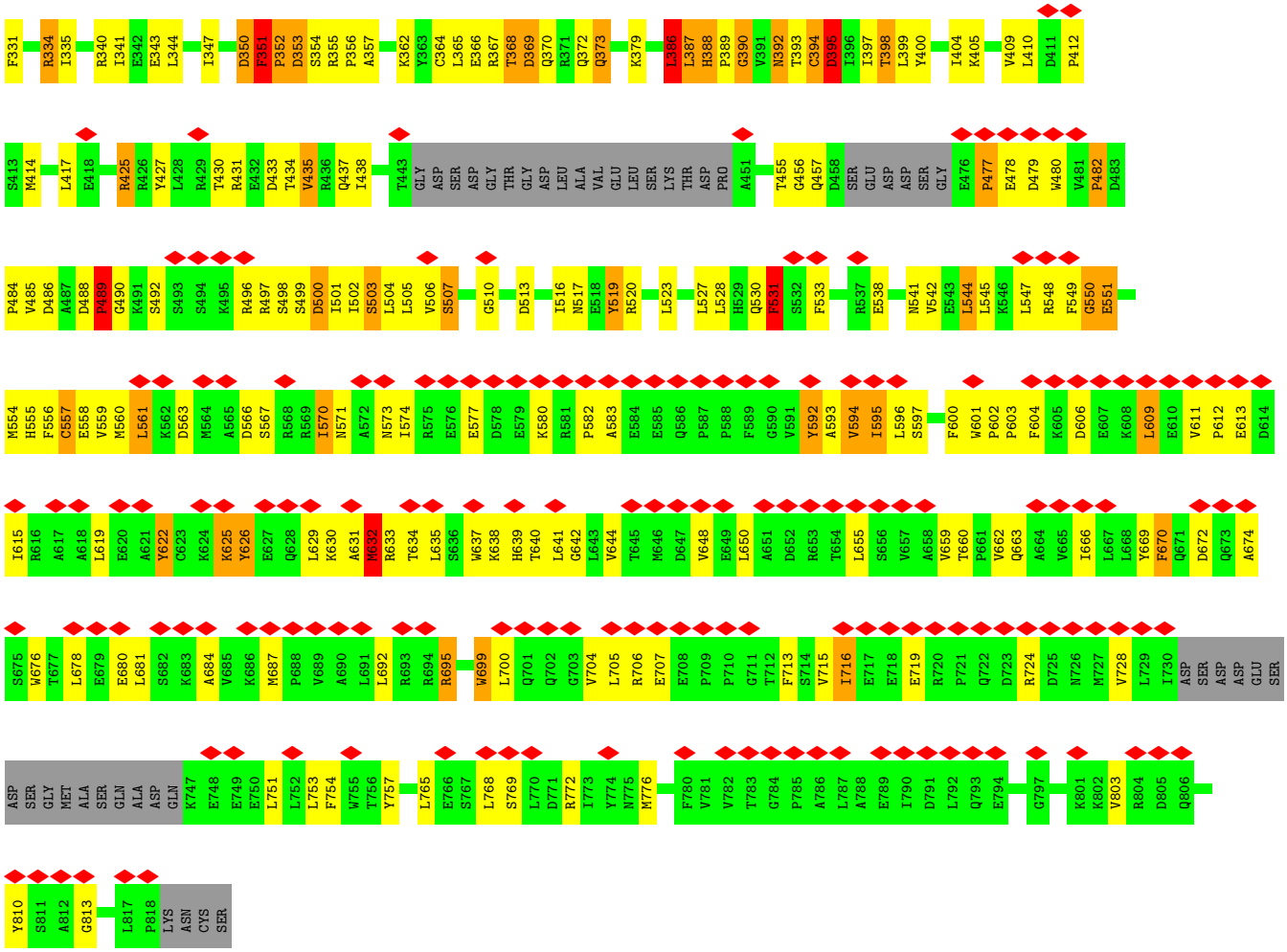
Chain M:



- Molecule 12: Anaphase-promoting complex subunit 2

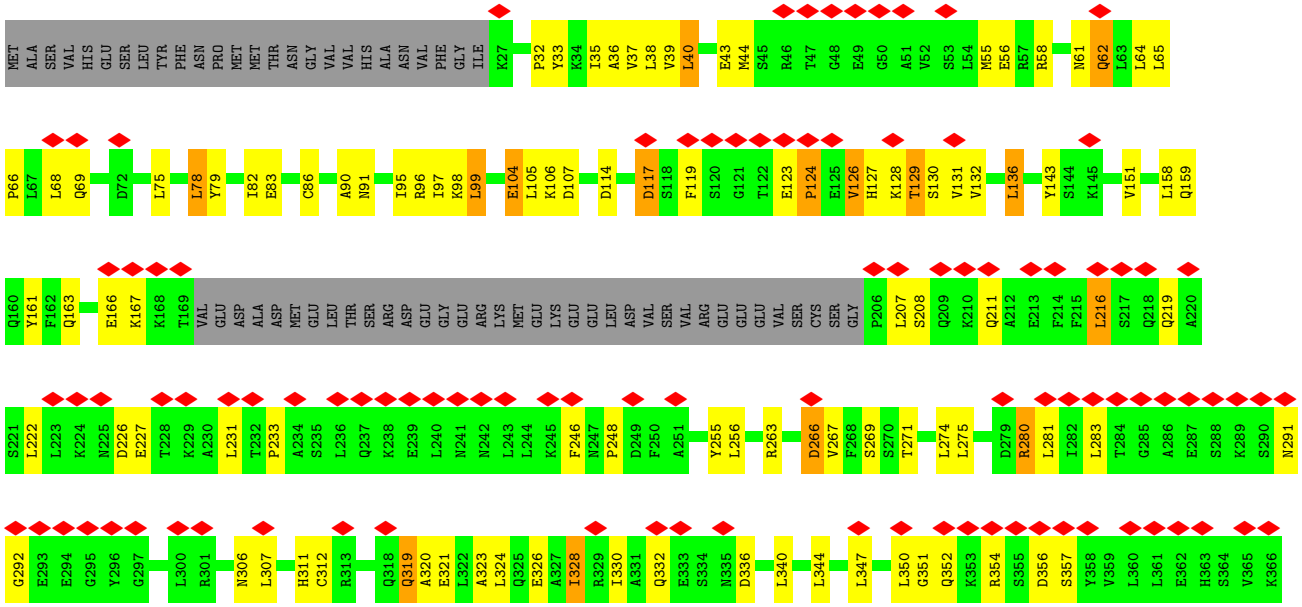
Chain N:

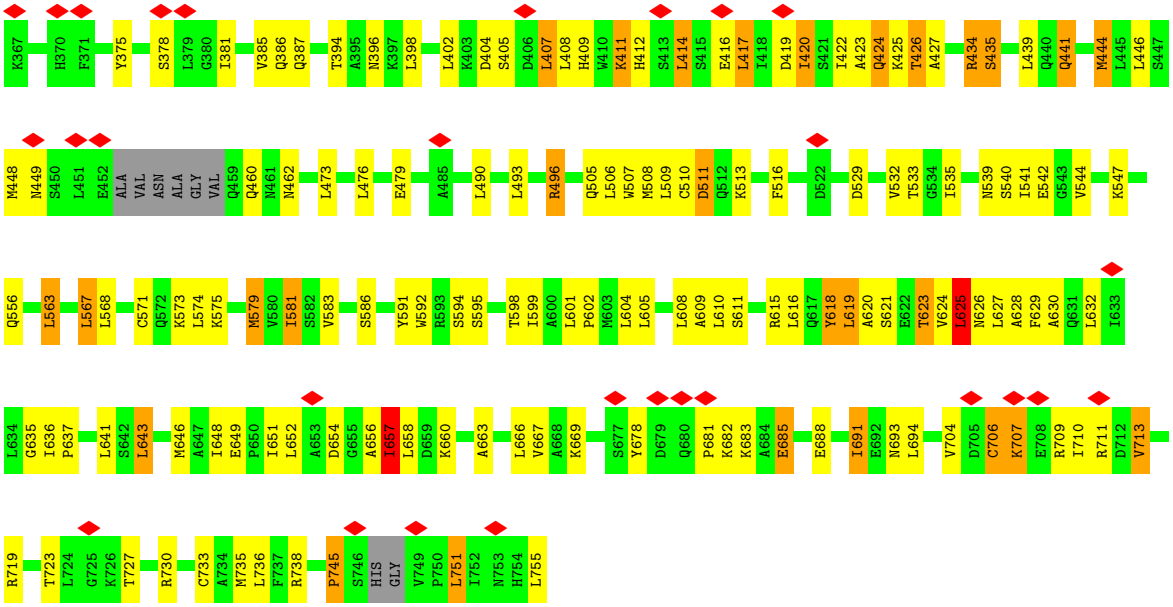




- Molecule 13: Anaphase-promoting complex subunit 5

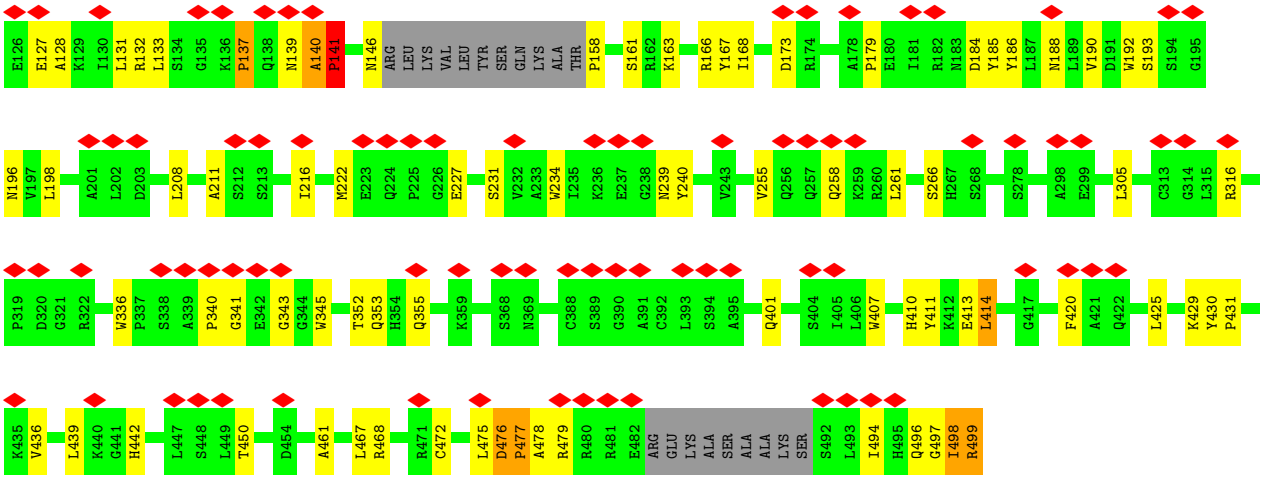
Chain O:





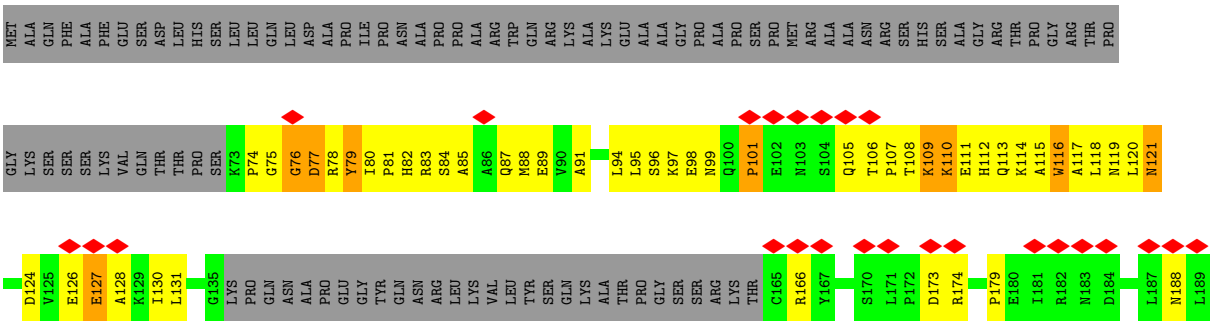
- Molecule 14: Cell division cycle protein 20 homolog

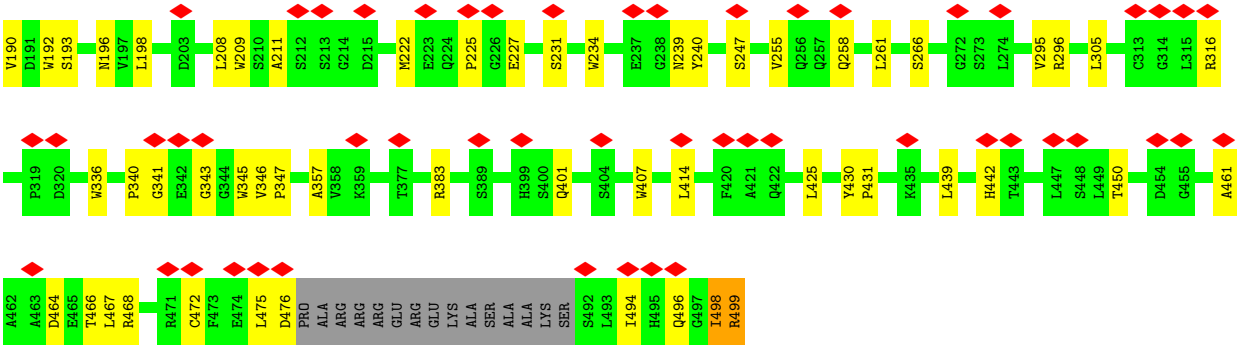
Chain Q:



- Molecule 15: Cell division cycle protein 20 homolog

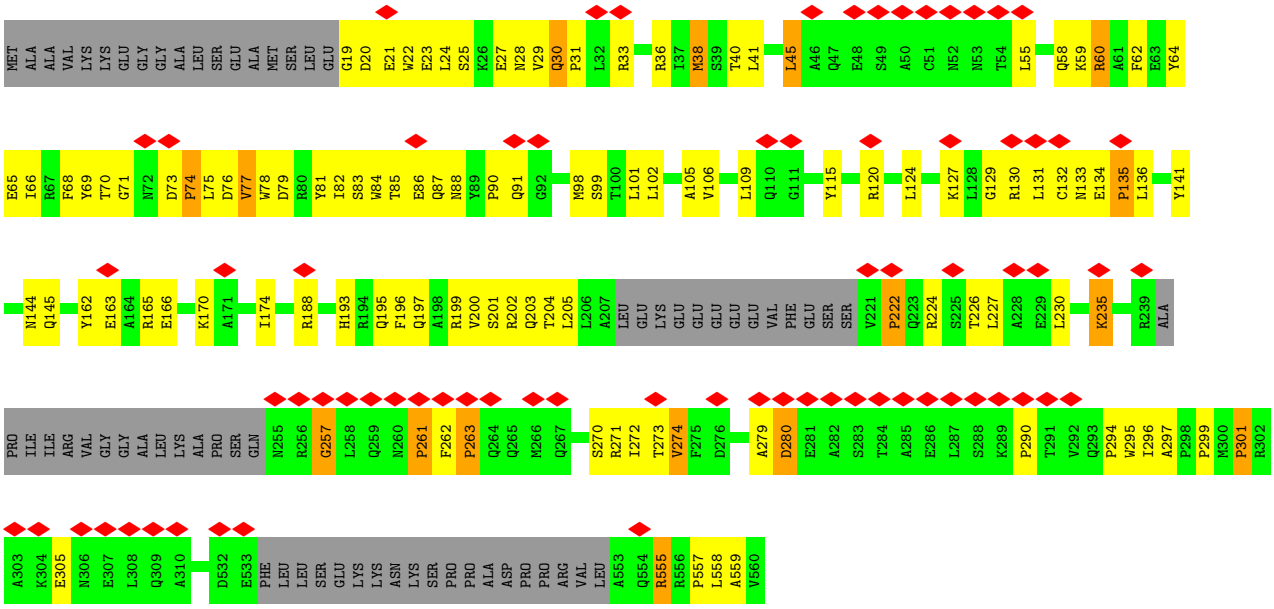
Chain R:





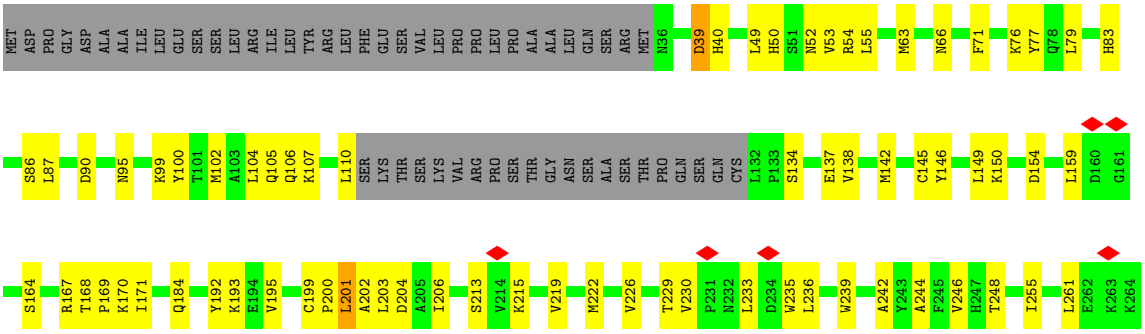
• Molecule 16: Mitotic checkpoint serine/threonine-protein kinase BUB1 beta,Mitotic checkpoint serine/threonine-protein kinase BUB1 beta

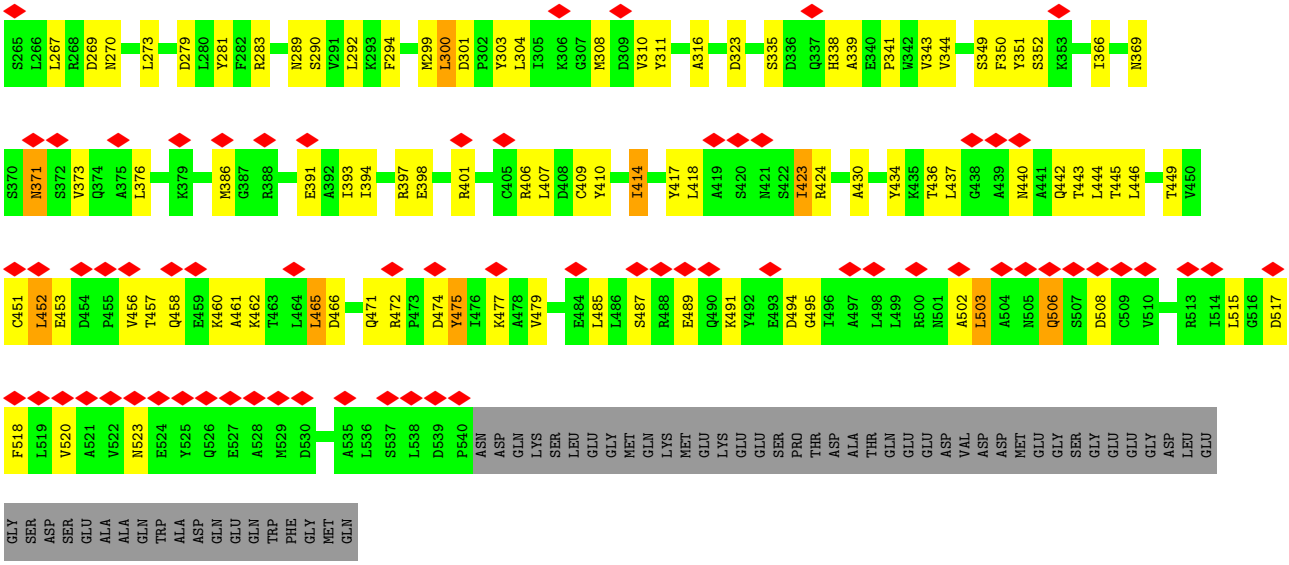
Chain S:



• Molecule 17: Anaphase-promoting complex subunit 7

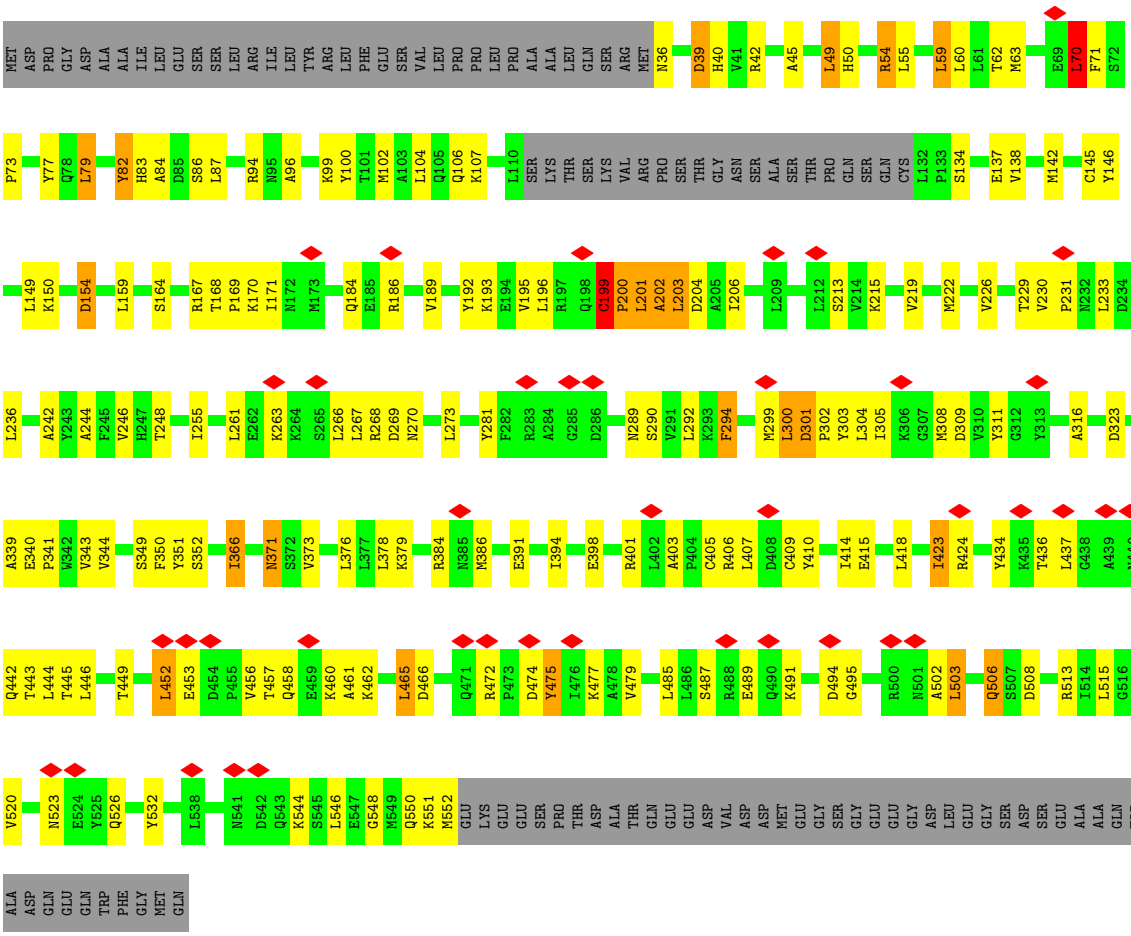
Chain X:





• Molecule 17: Anaphase-promoting complex subunit 7

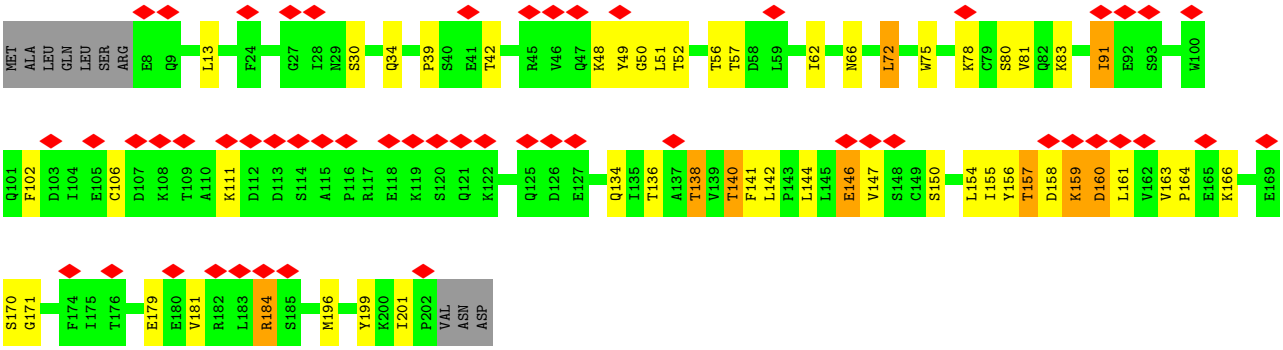
Chain Y: 7% 52% 27% • 17%



• Molecule 18: Mitotic spindle assembly checkpoint protein MAD2A

Chain Z:

26%
69%
21%
5%


MET ALA LEU GLN LEU SER ARG E8 Q9 L13 F24 G27 I28 N29 S30 Q34 P39 S40 E41 T42 R45 V46 Q47 K48 Y49 G50 L51 T52 T56 T57 D58 L59 I62 N66 L72 W75 K78 C79 S80 V81 Q82 K83 I91 E92 S93 W100
Q101 F102 D103 I104 E105 C106 D107 K108 T109 A110 K111 D112 D113 S114 A115 P116 R117 E118 K119 S120 Q121 K122 Q125 D126 E127 Q134 I135 T136 A137 T138 V139 T140 F141 L142 P143 L144 L145 E146 V147 S148 G149 S150 L154 I155 Y156 T157 D158 K159 D160 L161 V162 V163 P164 E165 K166 E169
S170 G171 F174 I175 T176 E179 E180 V181 R182 L183 R184 S185 M196 Y199 K200 I201 P202 VAL ASN ASP

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	155263	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	27	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.292	Depositor
Minimum map value	-0.094	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	359.04, 359.04, 359.04	wwPDB
Map dimensions	264, 264, 264	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.36, 1.36, 1.36	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.67	6/11190 (0.1%)	0.89	23/15236 (0.2%)
2	B	0.81	2/665 (0.3%)	0.98	2/896 (0.2%)
3	C	0.57	0/4404	0.83	4/5945 (0.1%)
3	P	0.60	0/4138	0.86	5/5587 (0.1%)
4	D	0.69	0/159	0.89	0/218
5	E	0.60	0/459	0.80	0/619
6	F	0.58	0/3939	0.82	3/5325 (0.1%)
6	H	0.61	2/3943 (0.1%)	0.82	2/5329 (0.0%)
7	G	0.63	0/214	1.02	1/284 (0.4%)
7	W	0.66	0/214	0.97	1/284 (0.4%)
8	I	0.66	1/5834 (0.0%)	0.92	11/7909 (0.1%)
9	J	0.71	2/4146 (0.0%)	0.95	5/5616 (0.1%)
9	K	0.73	1/4086 (0.0%)	0.93	7/5534 (0.1%)
10	L	0.54	0/1468	0.83	0/1993
11	M	0.66	0/502	0.95	0/680
12	N	0.63	3/5495 (0.1%)	0.94	18/7441 (0.2%)
13	O	0.58	0/5501	0.85	8/7432 (0.1%)
14	Q	0.72	0/2737	0.86	4/3732 (0.1%)
15	R	0.73	0/3029	0.86	2/4124 (0.0%)
16	S	0.66	0/2112	0.88	12/2863 (0.4%)
17	X	0.57	0/3833	0.82	3/5187 (0.1%)
17	Y	0.58	0/3928	0.84	9/5311 (0.2%)
18	Z	0.64	0/1605	0.79	2/2176 (0.1%)
All	All	0.64	17/73601 (0.0%)	0.88	122/99721 (0.1%)

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	1
8	I	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
9	J	0	1
12	N	0	16
16	S	0	1
All	All	0	21

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1030	GLU	CD-OE1	21.93	1.49	1.25
1	A	1030	GLU	CD-OE2	15.62	1.42	1.25
1	A	1199	LYS	CE-NZ	9.92	1.73	1.49
12	N	209	ARG	NE-CZ	9.66	1.45	1.33
1	A	1030	GLU	CG-CD	8.25	1.64	1.51
9	J	302	TRP	CB-CG	-7.73	1.36	1.50
9	K	302	TRP	CB-CG	-6.97	1.37	1.50
1	A	795	ARG	NE-CZ	6.82	1.42	1.33
12	N	330	ARG	CZ-NH2	-6.39	1.24	1.33
9	J	337	TRP	CB-CG	-6.31	1.38	1.50
6	H	730	LYS	CE-NZ	6.22	1.64	1.49
1	A	792	GLN	CG-CD	5.81	1.64	1.51
2	B	16	TRP	CD2-CE2	-5.62	1.34	1.41
8	I	115	TRP	CB-CG	-5.36	1.40	1.50
6	H	570	TRP	CB-CG	-5.25	1.40	1.50
12	N	330	ARG	CD-NE	5.06	1.55	1.46
2	B	14	TRP	CB-CG	5.06	1.59	1.50

All (122) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	N	330	ARG	NE-CZ-NH2	-13.57	113.52	120.30
16	S	60	ARG	NE-CZ-NH1	9.25	124.92	120.30
9	K	351	ASP	CB-CG-OD1	8.97	126.37	118.30
1	A	1235	LEU	CB-CG-CD2	-8.77	96.09	111.00
3	P	358	LEU	CB-CG-CD1	-8.46	96.62	111.00
14	Q	141	PRO	N-CA-CB	8.29	113.25	103.30
12	N	330	ARG	NE-CZ-NH1	8.21	124.41	120.30
16	S	45	LEU	CB-CG-CD2	-7.99	97.42	111.00
16	S	38	MET	CA-CB-CG	7.91	126.75	113.30
13	O	117	ASP	CB-CG-OD1	-7.83	111.25	118.30
9	J	220	ILE	C-N-CD	-7.47	104.17	120.60
3	P	358	LEU	CA-CB-CG	7.47	132.48	115.30
12	N	56	PRO	N-CA-CB	7.46	112.25	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	N	489	PRO	N-CA-CB	7.24	111.98	103.30
12	N	477	PRO	N-CA-CB	7.18	111.92	103.30
16	S	38	MET	CB-CA-C	-7.07	96.26	110.40
17	Y	82	TYR	CB-CG-CD1	7.04	125.22	121.00
9	K	134	LEU	CA-CB-CG	7.04	131.48	115.30
13	O	117	ASP	CB-CG-OD2	7.00	124.60	118.30
1	A	1603	LEU	CA-CB-CG	6.99	131.37	115.30
16	S	60	ARG	NE-CZ-NH2	-6.93	116.83	120.30
9	J	376	LEU	CA-CB-CG	6.91	131.19	115.30
15	R	118	LEU	CA-CB-CG	6.87	131.10	115.30
17	Y	70	LEU	CB-CG-CD1	6.87	122.67	111.00
14	Q	477	PRO	N-CA-CB	6.79	111.44	103.30
17	Y	82	TYR	CB-CG-CD2	-6.76	116.95	121.00
8	I	320	LEU	CB-CG-CD1	-6.69	99.63	111.00
8	I	435	PRO	N-CA-CB	6.60	111.22	103.30
3	C	365	LEU	CA-CB-CG	-6.58	100.18	115.30
1	A	1933	PRO	N-CA-CB	6.57	111.18	103.30
12	N	395	ASP	N-CA-C	6.54	128.65	111.00
9	J	134	LEU	CA-CB-CG	6.44	130.12	115.30
16	S	222	PRO	N-CA-CB	6.40	110.98	103.30
16	S	290	PRO	N-CA-CB	6.40	110.98	103.30
12	N	63	ALA	N-CA-C	6.37	128.21	111.00
14	Q	158	PRO	N-CA-CB	6.37	110.95	103.30
1	A	1030	GLU	CG-CD-OE2	6.35	130.99	118.30
1	A	1168	LEU	CA-CB-CG	6.33	129.86	115.30
1	A	795	ARG	NE-CZ-NH2	-6.24	117.18	120.30
12	N	496	ARG	N-CA-C	6.22	127.80	111.00
9	K	376	LEU	CA-CB-CG	6.16	129.47	115.30
1	A	1924	PRO	N-CA-CB	6.12	110.65	103.30
8	I	223	VAL	CB-CA-C	-6.09	99.82	111.40
12	N	219	PRO	N-CA-CB	6.08	110.60	103.30
3	C	358	LEU	CB-CG-CD2	-6.06	100.69	111.00
9	J	188	LEU	CA-CB-CG	6.03	129.16	115.30
6	H	462	LEU	CA-CB-CG	6.02	129.15	115.30
12	N	29	PRO	N-CA-CB	6.02	110.52	103.30
2	B	14	TRP	CA-CB-CG	5.98	125.06	113.70
13	O	625	LEU	CA-CB-CG	5.95	128.98	115.30
1	A	1882	LEU	CA-CB-CG	5.94	128.95	115.30
12	N	63	ALA	C-N-CA	5.93	136.54	121.70
3	C	306	LEU	CA-CB-CG	5.91	128.90	115.30
18	Z	184	ARG	NE-CZ-NH1	5.91	123.25	120.30
16	S	261	PRO	N-CA-CB	5.90	110.38	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	P	306	LEU	CA-CB-CG	5.88	128.82	115.30
9	K	323	LEU	CA-CB-CG	-5.87	101.80	115.30
1	A	1302	LEU	CA-CB-CG	5.80	128.64	115.30
6	F	462	LEU	CA-CB-CG	5.78	128.59	115.30
1	A	664	LEU	CA-CB-CG	5.78	128.58	115.30
16	S	38	MET	CG-SD-CE	5.76	109.41	100.20
14	Q	137	PRO	N-CA-CB	5.75	110.20	103.30
1	A	1243	LEU	CA-CB-CG	5.75	128.51	115.30
3	C	26	PHE	CB-CG-CD1	5.72	124.80	120.80
16	S	557	PRO	N-CA-CB	5.69	110.13	103.30
13	O	563	LEU	CA-CB-CG	5.68	128.36	115.30
12	N	55	PRO	N-CA-CB	5.67	110.10	103.30
17	X	446	LEU	CA-CB-CG	5.62	128.23	115.30
17	Y	418	LEU	CA-CB-CG	5.61	128.20	115.30
6	F	765	ASP	CB-CG-OD1	5.59	123.33	118.30
12	N	482	PRO	N-CA-CB	5.59	110.00	103.30
1	A	1313	LEU	CA-CB-CG	5.57	128.12	115.30
17	Y	199	CYS	N-CA-C	5.57	126.03	111.00
1	A	1409	LEU	CA-CB-CG	5.56	128.09	115.30
16	S	263	PRO	N-CA-CB	5.56	109.97	103.30
18	Z	140	THR	CA-CB-CG2	-5.56	104.62	112.40
1	A	188	LEU	CA-CB-CG	5.55	128.06	115.30
12	N	125	TYR	C-N-CA	5.53	135.53	121.70
17	X	418	LEU	CA-CB-CG	5.52	127.99	115.30
8	I	45	LEU	CB-CG-CD2	5.49	120.33	111.00
1	A	1030	GLU	CG-CD-OE1	-5.48	107.34	118.30
13	O	751	LEU	CA-CB-CG	5.46	127.85	115.30
6	H	571	CYS	CA-CB-SG	-5.45	104.20	114.00
8	I	645	ASP	CB-CG-OD2	5.43	123.19	118.30
1	A	953	LEU	CA-CB-CG	5.43	127.78	115.30
13	O	216	LEU	CA-CB-CG	5.42	127.76	115.30
2	B	61	LEU	CA-CB-CG	5.40	127.72	115.30
6	F	130	ARG	NE-CZ-NH2	-5.39	117.60	120.30
13	O	64	LEU	CA-CB-CG	5.38	127.67	115.30
17	Y	59	LEU	CA-CB-CG	5.36	127.62	115.30
8	I	602	ARG	NE-CZ-NH1	5.34	122.97	120.30
15	R	383	ARG	NE-CZ-NH1	-5.34	117.63	120.30
1	A	651	PRO	N-CA-CB	5.34	109.70	103.30
8	I	603	ARG	NE-CZ-NH1	5.32	122.96	120.30
9	K	451	LEU	CB-CG-CD2	-5.31	101.97	111.00
17	Y	446	LEU	CA-CB-CG	5.29	127.46	115.30
8	I	447	PHE	N-CA-CB	-5.29	101.09	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1748	LEU	CA-CB-CG	5.28	127.45	115.30
12	N	197	PRO	N-CA-CB	5.25	109.60	103.30
3	P	49	LEU	CA-CB-CG	5.25	127.38	115.30
9	K	448	LEU	CB-CG-CD2	5.25	119.93	111.00
1	A	1032	LEU	CA-CB-CG	5.24	127.35	115.30
3	P	365	LEU	CA-CB-CG	5.23	127.33	115.30
1	A	1405	LEU	CA-CB-CG	5.23	127.32	115.30
1	A	977	LEU	CA-CB-CG	5.21	127.29	115.30
7	G	14	ASP	CB-CG-OD2	5.21	122.99	118.30
9	J	225	ASP	CB-CG-OD2	5.21	122.99	118.30
8	I	26	LEU	CA-CB-CG	5.19	127.24	115.30
9	K	359	THR	N-CA-CB	5.19	120.15	110.30
12	N	386	LEU	CA-CB-CG	5.18	127.22	115.30
17	X	466	ASP	CB-CG-OD2	5.18	122.96	118.30
7	W	3	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	A	1243	LEU	CB-CG-CD2	5.17	119.79	111.00
1	A	1059	ASP	CB-CG-OD2	5.17	122.95	118.30
17	Y	466	ASP	CB-CG-OD2	5.16	122.94	118.30
17	Y	203	LEU	CA-CB-CG	5.11	127.06	115.30
12	N	78	VAL	N-CA-C	-5.05	97.36	111.00
13	O	407	LEU	CA-CB-CG	5.05	126.91	115.30
8	I	703	ARG	NE-CZ-NH1	5.04	122.82	120.30
12	N	547	LEU	CA-CB-CG	5.04	126.89	115.30
8	I	659	ARG	N-CA-C	5.02	124.56	111.00
16	S	301	PRO	N-CA-CB	5.00	109.30	103.30

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1191	LEU	Peptide
8	I	658	GLY	Peptide
8	I	727	PHE	Peptide
9	J	220	ILE	Peptide
12	N	162	PHE	Peptide
12	N	164	SER	Peptide
12	N	280	GLU	Peptide
12	N	281	TYR	Peptide
12	N	351	PHE	Peptide
12	N	352	PRO	Peptide
12	N	353	ASP	Peptide
12	N	367	ARG	Peptide

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Mol	Chain	Res	Type	Group
12	N	369	ASP	Peptide
12	N	387	LEU	Peptide
12	N	390	GLY	Peptide
12	N	394	CYS	Peptide
12	N	395	ASP	Peptide
12	N	485	VAL	Peptide
12	N	62	ARG	Peptide
12	N	77	GLU	Peptide
16	S	235	LYS	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	10949	0	10690	418	0
2	B	643	0	617	80	0
3	C	4306	0	4272	161	0
3	P	4043	0	4000	137	0
4	D	153	0	148	8	0
5	E	450	0	435	10	0
6	F	3849	0	3783	108	0
6	H	3853	0	3794	128	0
7	G	213	0	220	11	0
7	W	213	0	220	12	0
8	I	5716	0	5587	345	0
9	J	4047	0	3949	185	0
9	K	3988	0	3908	174	0
10	L	1435	0	1382	55	0
11	M	493	0	469	24	0
12	N	5403	0	5103	276	0
13	O	5402	0	5436	221	0
14	Q	2671	0	2516	103	0
15	R	2953	0	2839	111	0
16	S	2077	0	1827	327	0
17	X	3773	0	3831	163	0
17	Y	3868	0	3925	169	0
18	Z	1577	0	1592	89	0
All	All	72075	0	70543	2914	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 20.

All (2914) 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)
16:S:38:MET:CE	18:Z:181:VAL:HG23	1.22	1.65
16:S:22:TRP:CZ3	16:S:41:LEU:HB2	1.31	1.64
16:S:19:GLY:CA	18:Z:134:GLN:HE21	1.16	1.54
8:I:413:ASN:HA	8:I:447:PHE:CZ	1.38	1.53
1:A:1199:LYS:NZ	1:A:1199:LYS:CE	1.73	1.45
16:S:19:GLY:CA	18:Z:134:GLN:NE2	1.74	1.43
16:S:68:PHE:CE2	16:S:81:TYR:CD2	2.10	1.40
16:S:38:MET:CE	18:Z:181:VAL:CG2	2.00	1.38
16:S:30:GLN:N	16:S:36:ARG:HH22	1.20	1.38
16:S:19:GLY:C	18:Z:134:GLN:HE21	1.23	1.38
16:S:29:VAL:HG13	16:S:36:ARG:NH1	1.40	1.36
16:S:22:TRP:CZ3	16:S:41:LEU:CB	2.10	1.34
17:X:442:GLN:CD	17:X:472:ARG:NE	1.78	1.34
16:S:36:ARG:NH1	16:S:90:PRO:HB2	1.42	1.33
16:S:58:GLN:HG3	16:S:62:PHE:CE2	1.61	1.32
16:S:38:MET:HE2	18:Z:181:VAL:CG2	1.58	1.32
16:S:19:GLY:HA3	18:Z:134:GLN:NE2	1.34	1.29
12:N:362:LYS:HB2	12:N:410:LEU:CD2	1.62	1.28
2:B:16:TRP:NE1	2:B:44:CYS:CB	1.96	1.26
8:I:413:ASN:HA	8:I:447:PHE:CE1	1.68	1.25
1:A:1332:GLY:O	1:A:1358:ILE:HD12	1.31	1.25
16:S:68:PHE:CZ	16:S:81:TYR:HD2	1.54	1.25
16:S:21:GLU:O	16:S:45:LEU:HD22	1.35	1.24
17:X:442:GLN:OE1	17:X:472:ARG:CZ	1.85	1.22
1:A:1235:LEU:CD2	1:A:1257:ILE:HG13	1.70	1.21
16:S:29:VAL:HG12	18:Z:140:THR:CG2	1.72	1.20
16:S:38:MET:HE3	18:Z:181:VAL:CG2	1.71	1.20
8:I:430:GLU:HG2	14:Q:429:LYS:CG	1.71	1.20
17:Y:42:ARG:HA	17:Y:82:TYR:CE2	1.78	1.17
1:A:1332:GLY:O	1:A:1358:ILE:CD1	1.91	1.17
2:B:16:TRP:CD1	2:B:44:CYS:HB3	1.79	1.16
12:N:362:LYS:CB	12:N:410:LEU:HD23	1.76	1.16
16:S:68:PHE:CE2	16:S:81:TYR:HD2	1.51	1.15
16:S:29:VAL:HA	16:S:36:ARG:HH12	1.11	1.15
16:S:71:GLY:C	16:S:74:PRO:HD2	1.68	1.14
9:K:129:LYS:O	9:K:133:CYS:SG	2.05	1.14
16:S:132:CYS:HB2	16:S:135:PRO:HG3	1.13	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:279:ILE:HD11	8:I:337:ILE:HA	1.23	1.13
13:O:75:LEU:HD11	13:O:161:TYR:CE2	1.82	1.12
17:X:201:LEU:HD11	17:Y:40:HIS:HB3	1.20	1.12
13:O:75:LEU:CD2	13:O:161:TYR:OH	1.98	1.11
8:I:290:PHE:CA	8:I:320:LEU:HD11	1.81	1.11
8:I:413:ASN:CA	8:I:447:PHE:CZ	2.31	1.11
12:N:765:LEU:HD21	16:S:200:VAL:HG21	1.30	1.11
9:K:250:CYS:SG	9:K:274:THR:HG21	1.91	1.11
16:S:29:VAL:CG1	16:S:36:ARG:NH1	2.14	1.11
16:S:29:VAL:HG12	18:Z:140:THR:HG21	1.29	1.10
16:S:76:ASP:O	16:S:77:VAL:HG23	1.49	1.10
16:S:58:GLN:O	16:S:62:PHE:CD2	2.04	1.10
12:N:362:LYS:HB2	12:N:410:LEU:HD23	1.10	1.10
9:J:441:VAL:HG21	9:J:444:TRP:HD1	1.16	1.09
16:S:21:GLU:O	16:S:45:LEU:CD2	1.99	1.09
2:B:16:TRP:NE1	2:B:44:CYS:HB3	1.58	1.09
16:S:22:TRP:CH2	16:S:38:MET:O	2.05	1.09
8:I:313:ALA:HB3	8:I:317:LEU:HB2	1.18	1.08
16:S:132:CYS:HA	16:S:133:ASN:HB2	1.34	1.08
9:J:454:VAL:O	9:J:458:LEU:HD12	1.51	1.08
16:S:20:ASP:OD1	18:Z:184:ARG:HD2	1.53	1.08
8:I:209:CYS:SG	8:I:584:HIS:CE1	2.46	1.07
16:S:30:GLN:H	16:S:91:GLN:HB2	1.18	1.07
16:S:36:ARG:NH1	16:S:90:PRO:CB	2.17	1.07
12:N:180:PHE:CD1	12:N:299:TRP:CZ3	2.43	1.07
13:O:75:LEU:O	13:O:79:TYR:CD2	2.08	1.07
16:S:30:GLN:N	16:S:36:ARG:NH2	2.00	1.07
9:J:332:THR:HA	9:J:363:LEU:HD21	1.37	1.06
16:S:132:CYS:SG	16:S:135:PRO:HA	1.95	1.06
1:A:1235:LEU:HD21	1:A:1257:ILE:CG1	1.85	1.06
8:I:302:ASP:N	8:I:303:GLU:N	2.04	1.06
6:H:656:MET:HE2	6:H:660:LYS:HE2	1.30	1.05
8:I:209:CYS:SG	8:I:584:HIS:ND1	2.30	1.05
17:X:442:GLN:OE1	17:X:472:ARG:NH2	1.87	1.05
12:N:393:THR:O	12:N:395:ASP:HB3	1.54	1.04
6:F:130:ARG:HG2	17:Y:506:GLN:NE2	1.71	1.04
8:I:300:VAL:HA	8:I:303:GLU:OE1	1.55	1.04
17:Y:452:LEU:HD22	17:Y:461:ALA:N	1.73	1.04
17:X:452:LEU:CD2	17:X:457:THR:O	2.06	1.04
8:I:56:TRP:CE3	8:I:98:PRO:HB3	1.93	1.03
16:S:68:PHE:CZ	16:S:81:TYR:CD2	2.37	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:442:GLN:HG2	17:X:472:ARG:CD	1.86	1.03
12:N:362:LYS:CB	12:N:410:LEU:CD2	2.34	1.03
16:S:30:GLN:N	16:S:91:GLN:HB2	1.74	1.03
17:Y:452:LEU:CD2	17:Y:457:THR:O	2.06	1.03
15:R:98:GLU:CG	15:R:101:PRO:HD3	1.88	1.02
16:S:38:MET:HE3	18:Z:181:VAL:HG21	1.40	1.02
14:Q:185:TYR:CD1	16:S:27:GLU:HB3	1.94	1.02
16:S:79:ASP:OD2	16:S:120:ARG:HG2	1.59	1.02
12:N:425:ARG:HG2	12:N:425:ARG:HH11	1.20	1.02
2:B:14:TRP:HA	2:B:15:LEU:HB2	1.41	1.02
16:S:29:VAL:CA	16:S:36:ARG:HH12	1.73	1.02
13:O:581:ILE:HD11	13:O:619:LEU:HB3	1.42	1.01
1:A:1232:ILE:HG13	1:A:1235:LEU:HB2	1.40	1.01
17:X:452:LEU:HD22	17:X:461:ALA:N	1.73	1.01
8:I:295:ASN:O	8:I:316:GLU:HB2	1.61	1.01
14:Q:410:HIS:HB3	14:Q:475:LEU:HD21	1.40	1.01
8:I:289:LYS:HG3	8:I:324:GLN:OE1	1.61	1.00
13:O:75:LEU:CG	13:O:161:TYR:CE2	2.44	1.00
16:S:71:GLY:O	16:S:74:PRO:HD2	1.59	1.00
2:B:16:TRP:HD1	2:B:33:CYS:HA	1.24	1.00
16:S:66:ILE:HA	16:S:69:TYR:HD2	1.24	1.00
8:I:430:GLU:HG2	14:Q:429:LYS:HG3	1.38	1.00
13:O:75:LEU:CD1	13:O:161:TYR:CE2	2.45	0.99
1:A:1162:LYS:HG3	1:A:1163:PRO:HD2	1.44	0.99
17:Y:42:ARG:HG3	17:Y:82:TYR:OH	1.61	0.99
16:S:19:GLY:C	18:Z:134:GLN:NE2	2.04	0.99
8:I:430:GLU:HG2	14:Q:429:LYS:HG2	1.45	0.99
16:S:22:TRP:HH2	16:S:38:MET:CA	1.76	0.99
17:X:442:GLN:HG2	17:X:472:ARG:HD2	1.40	0.99
13:O:435:SER:HB3	13:O:654:ASP:HB2	1.43	0.98
3:C:344:ARG:HH21	11:M:25:PRO:HG2	1.27	0.98
8:I:313:ALA:HB2	8:I:317:LEU:HD12	1.43	0.98
1:A:1235:LEU:HD21	1:A:1257:ILE:HG13	1.00	0.98
14:Q:128:ALA:HB3	18:Z:156:TYR:CZ	1.99	0.98
16:S:29:VAL:HG13	16:S:36:ARG:HH11	1.26	0.98
15:R:225:PRO:HD2	16:S:166:GLU:O	1.64	0.98
9:K:250:CYS:SG	9:K:274:THR:CG2	2.52	0.97
17:X:201:LEU:HD11	17:Y:40:HIS:CB	1.94	0.97
9:J:55:ARG:HH11	9:K:264:HIS:HA	1.24	0.97
16:S:33:ARG:HB2	16:S:130:ARG:HH11	1.30	0.97
8:I:186:GLU:OE1	8:I:197:ARG:NH1	1.97	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:144:THR:HG21	8:I:159:GLU:HA	1.46	0.97
16:S:132:CYS:HB2	16:S:135:PRO:CG	1.93	0.97
8:I:313:ALA:CB	8:I:317:LEU:HD12	1.95	0.96
3:C:134:THR:HG23	3:C:143:LYS:HG3	1.47	0.96
13:O:75:LEU:HD21	13:O:161:TYR:OH	1.62	0.96
16:S:40:THR:HB	16:S:87:GLN:O	1.65	0.96
8:I:313:ALA:HB3	8:I:317:LEU:CB	1.95	0.96
2:B:17:VAL:HG13	2:B:31:ASN:ND2	1.80	0.96
16:S:79:ASP:OD2	16:S:120:ARG:CG	2.13	0.96
8:I:209:CYS:HG	8:I:584:HIS:HD1	1.11	0.95
16:S:79:ASP:OD2	16:S:120:ARG:CB	2.15	0.95
12:N:574:ILE:HD12	12:N:625:LYS:HG2	1.49	0.95
3:P:233:PHE:CZ	3:P:237:ILE:HD11	2.02	0.95
16:S:22:TRP:CH2	16:S:38:MET:HA	2.02	0.95
17:X:442:GLN:CD	17:X:472:ARG:HE	1.61	0.95
13:O:75:LEU:CD2	13:O:161:TYR:CZ	2.50	0.94
16:S:22:TRP:HA	16:S:45:LEU:HD11	1.47	0.94
17:X:442:GLN:NE2	17:X:472:ARG:HE	1.66	0.94
17:Y:305:ILE:HG23	17:Y:340:GLU:OE1	1.68	0.94
1:A:1322:PRO:HG3	1:A:1375:TYR:OH	1.67	0.94
8:I:413:ASN:HA	8:I:447:PHE:HZ	1.24	0.94
9:J:254:THR:HG23	9:J:271:HIS:HD2	1.32	0.94
16:S:86:GLU:HG3	16:S:98:MET:CE	1.98	0.94
13:O:75:LEU:HD21	13:O:161:TYR:CE2	2.03	0.94
16:S:22:TRP:CH2	16:S:41:LEU:HB2	2.02	0.94
13:O:75:LEU:O	13:O:79:TYR:HD2	1.47	0.93
9:K:214:LYS:O	9:K:216:SER:N	2.01	0.93
12:N:538:GLU:HG2	12:N:561:LEU:HG	1.47	0.93
6:H:762:TRP:HA	6:H:765:ASP:HB3	1.48	0.93
8:I:290:PHE:HA	8:I:320:LEU:HD11	1.46	0.93
16:S:38:MET:HE1	18:Z:199:TYR:HE2	1.30	0.93
6:H:656:MET:CE	6:H:660:LYS:HE2	1.98	0.93
2:B:16:TRP:CZ3	12:N:630:LYS:HE2	2.04	0.93
12:N:78:VAL:O	12:N:81:ASN:N	2.01	0.93
2:B:14:TRP:CA	2:B:15:LEU:HB2	1.99	0.92
2:B:16:TRP:HZ2	2:B:45:PRO:N	1.65	0.92
9:J:441:VAL:HG21	9:J:444:TRP:CD1	2.03	0.92
12:N:273:MET:HG3	12:N:277:CYS:SG	2.09	0.92
16:S:22:TRP:HZ3	16:S:41:LEU:CB	1.63	0.92
16:S:163:GLU:CD	16:S:196:PHE:CE1	2.43	0.92
17:X:40:HIS:HB3	17:Y:201:LEU:HD11	1.51	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:S:163:GLU:OE1	16:S:196:PHE:CE1	2.22	0.92
12:N:180:PHE:CD1	12:N:299:TRP:CH2	2.57	0.92
14:Q:352:THR:HG21	18:Z:50:GLY:O	1.70	0.91
1:A:1332:GLY:O	1:A:1358:ILE:CG1	2.18	0.91
13:O:75:LEU:HD21	13:O:161:TYR:CZ	2.04	0.91
16:S:76:ASP:O	16:S:77:VAL:CG2	2.17	0.91
16:S:30:GLN:NE2	16:S:91:GLN:HG3	1.86	0.91
16:S:71:GLY:O	16:S:74:PRO:O	1.86	0.91
16:S:36:ARG:HH12	16:S:90:PRO:HB2	1.18	0.90
16:S:86:GLU:HG3	16:S:98:MET:HE1	1.50	0.90
2:B:46:LEU:HB2	12:N:632:MET:SD	2.09	0.90
8:I:300:VAL:O	8:I:303:GLU:HB2	1.70	0.90
2:B:16:TRP:CD1	2:B:33:CYS:HA	2.05	0.90
13:O:75:LEU:HD23	13:O:161:TYR:OH	1.71	0.90
16:S:163:GLU:OE1	16:S:196:PHE:CD1	2.24	0.90
8:I:26:LEU:HB3	8:I:37:LEU:HB3	1.54	0.90
17:X:267:LEU:HD11	17:Y:59:LEU:CD1	2.01	0.90
16:S:22:TRP:HZ3	16:S:41:LEU:HB2	1.07	0.90
16:S:58:GLN:O	16:S:62:PHE:HD2	1.55	0.90
13:O:75:LEU:HG	13:O:161:TYR:CZ	2.05	0.90
16:S:58:GLN:HG3	16:S:62:PHE:HE2	1.00	0.90
3:C:414:MET:HG2	13:O:330:ILE:CD1	2.02	0.90
14:Q:132:ARG:HG3	18:Z:154:LEU:CD2	2.02	0.90
9:J:211:LYS:O	9:J:212:TYR:CD2	2.24	0.89
17:X:442:GLN:OE1	17:X:472:ARG:NE	1.97	0.89
2:B:14:TRP:HA	2:B:15:LEU:CB	1.99	0.89
8:I:302:ASP:C	8:I:303:GLU:N	2.26	0.89
17:Y:452:LEU:HD23	17:Y:457:THR:O	1.72	0.89
16:S:68:PHE:HE2	16:S:81:TYR:CD2	1.82	0.89
16:S:193:HIS:CE1	16:S:197:GLN:OE1	2.25	0.89
16:S:197:GLN:O	16:S:200:VAL:HG22	1.73	0.89
17:X:452:LEU:HD23	17:X:457:THR:O	1.72	0.89
16:S:132:CYS:CB	16:S:135:PRO:HG3	2.03	0.89
6:F:130:ARG:HG2	17:Y:506:GLN:HE21	1.35	0.89
16:S:66:ILE:HA	16:S:69:TYR:CD2	2.07	0.89
11:M:4:GLU:HG2	3:P:50:HIS:CE1	2.08	0.89
8:I:300:VAL:HG21	8:I:456:PHE:CB	2.03	0.89
17:X:442:GLN:CG	17:X:472:ARG:CD	2.51	0.88
14:Q:185:TYR:CE1	16:S:27:GLU:HG3	2.09	0.88
13:O:55:MET:SD	13:O:58:ARG:NH1	2.47	0.88
17:X:201:LEU:CD1	17:Y:40:HIS:HB3	2.02	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Y:462:LYS:HG2	17:Y:485:LEU:HD13	1.56	0.88
9:J:55:ARG:NH1	9:K:264:HIS:HA	1.89	0.87
13:O:55:MET:SD	13:O:58:ARG:CZ	2.62	0.87
8:I:290:PHE:C	8:I:320:LEU:HD11	1.93	0.87
10:L:83:TYR:CD2	10:L:115:GLU:HA	2.09	0.87
16:S:134:GLU:O	16:S:136:LEU:N	2.08	0.87
12:N:91:PHE:O	12:N:93:ASN:N	2.07	0.87
16:S:41:LEU:CD1	18:Z:141:PHE:HB3	2.05	0.87
1:A:1175:PHE:CZ	1:A:1179:LEU:HD21	2.10	0.87
14:Q:132:ARG:HB2	18:Z:170:SER:HB2	1.55	0.87
16:S:22:TRP:CH2	16:S:38:MET:CA	2.58	0.87
9:J:445:GLU:OE1	9:J:475:ILE:HG21	1.75	0.87
9:J:167:PHE:O	9:J:170:LEU:HD23	1.75	0.86
12:N:362:LYS:HB2	12:N:410:LEU:HD21	1.55	0.86
14:Q:185:TYR:CD1	16:S:27:GLU:CB	2.59	0.86
16:S:22:TRP:HH2	16:S:38:MET:O	1.56	0.86
16:S:83:SER:O	16:S:87:GLN:HG3	1.74	0.86
16:S:199:ARG:O	16:S:202:ARG:HG2	1.73	0.86
16:S:29:VAL:HA	16:S:90:PRO:HB2	1.57	0.86
17:Y:42:ARG:HA	17:Y:82:TYR:CZ	2.10	0.86
2:B:16:TRP:CD1	2:B:44:CYS:CB	2.52	0.86
3:P:276:ILE:HG22	3:P:277:ARG:H	1.40	0.86
16:S:19:GLY:HA3	18:Z:134:GLN:CD	1.96	0.86
16:S:29:VAL:CG1	18:Z:140:THR:HG21	2.05	0.86
6:H:653:LEU:HD22	9:K:523:ILE:HG21	1.58	0.86
12:N:570:ILE:HD13	12:N:633:ARG:HH12	1.41	0.86
12:N:570:ILE:HD13	12:N:633:ARG:NH1	1.91	0.86
16:S:29:VAL:CG1	18:Z:140:THR:CG2	2.54	0.85
16:S:71:GLY:CA	16:S:74:PRO:HD2	2.05	0.85
16:S:82:ILE:CD1	16:S:124:LEU:CD2	2.54	0.85
1:A:1307:LEU:HD11	1:A:1582:ALA:HB2	1.58	0.85
9:K:472:LEU:HG	9:K:481:THR:HG21	1.58	0.85
13:O:75:LEU:HD11	13:O:161:TYR:HE2	1.40	0.85
16:S:83:SER:HB2	16:S:87:GLN:NE2	1.91	0.85
8:I:286:ARG:HE	8:I:333:LEU:HD13	1.40	0.85
8:I:413:ASN:CA	8:I:447:PHE:CE1	2.56	0.85
12:N:180:PHE:CD1	12:N:299:TRP:HZ3	1.90	0.85
1:A:1619:LEU:HD21	1:A:1697:LEU:HD22	1.58	0.85
3:C:259:PHE:HB3	3:C:265:ILE:CD1	2.06	0.85
8:I:73:TRP:CZ2	8:I:80:LEU:HD22	2.11	0.85
17:X:442:GLN:HG2	17:X:472:ARG:CG	2.06	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:16:TRP:HE1	2:B:44:CYS:CB	1.47	0.85
8:I:312:LYS:HG3	8:I:428:MET:SD	2.16	0.85
8:I:301:GLN:C	8:I:303:GLU:N	2.29	0.85
16:S:19:GLY:N	18:Z:134:GLN:NE2	2.25	0.85
8:I:300:VAL:HG21	8:I:456:PHE:HB3	1.59	0.85
10:L:86:ASP:HB3	10:L:89:TYR:HB2	1.58	0.85
17:X:462:LYS:HG2	17:X:485:LEU:HD13	1.57	0.85
13:O:75:LEU:HG	13:O:161:TYR:CE2	2.12	0.84
6:F:571:CYS:SG	6:F:606:LEU:HD12	2.17	0.84
8:I:337:ILE:CG2	8:I:341:TYR:HE2	1.89	0.84
16:S:29:VAL:HG12	18:Z:140:THR:HG22	1.58	0.84
16:S:22:TRP:HH2	16:S:38:MET:C	1.79	0.84
16:S:20:ASP:N	18:Z:134:GLN:NE2	2.25	0.84
17:Y:452:LEU:HD21	17:Y:457:THR:O	1.75	0.84
13:O:114:ASP:O	13:O:117:ASP:OD1	1.93	0.84
16:S:78:TRP:CZ3	16:S:105:ALA:HA	2.13	0.84
17:X:452:LEU:HD21	17:X:457:THR:O	1.75	0.84
9:J:254:THR:HG23	9:J:271:HIS:CD2	2.11	0.84
14:Q:185:TYR:CG	16:S:27:GLU:HB3	2.12	0.84
8:I:262:LEU:HA	8:I:265:ILE:HG22	1.59	0.84
12:N:395:ASP:HB2	12:N:397:ILE:H	1.43	0.83
8:I:310:TRP:HB2	8:I:313:ALA:HA	1.59	0.83
13:O:75:LEU:CD2	13:O:161:TYR:CE2	2.61	0.83
8:I:430:GLU:CG	14:Q:429:LYS:CG	2.55	0.83
8:I:430:GLU:CG	14:Q:429:LYS:HG2	2.08	0.83
16:S:58:GLN:CG	16:S:62:PHE:CE2	2.56	0.83
17:Y:474:ASP:OD1	17:Y:502:ALA:HA	1.78	0.83
9:J:476:PRO:HG2	3:P:182:LEU:HG	1.60	0.83
13:O:75:LEU:HB3	13:O:79:TYR:CE2	2.14	0.83
13:O:539:ASN:HD22	13:O:542:GLU:HB2	1.44	0.83
14:Q:168:ILE:HG23	14:Q:472:CYS:HA	1.61	0.83
13:O:216:LEU:HD22	13:O:256:LEU:HD12	1.59	0.83
17:X:474:ASP:OD1	17:X:502:ALA:HA	1.78	0.83
8:I:295:ASN:O	8:I:316:GLU:CB	2.27	0.82
16:S:38:MET:CE	18:Z:199:TYR:HE2	1.82	0.82
8:I:276:TRP:CH2	8:I:476:GLY:HA3	2.14	0.82
8:I:290:PHE:HE1	8:I:324:GLN:HB3	1.42	0.82
15:R:98:GLU:HG3	15:R:101:PRO:HD3	1.58	0.82
3:C:53:LYS:HD3	3:P:96:VAL:HG21	1.61	0.82
8:I:34:LEU:HD12	8:I:46:LEU:HD21	1.61	0.82
9:K:222:GLU:OE1	9:K:228:GLN:CD	2.17	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:309:LEU:O	13:O:127:HIS:HB2	1.80	0.82
8:I:349:ILE:HD12	13:O:407:LEU:HA	1.62	0.82
16:S:29:VAL:HA	16:S:36:ARG:NH1	1.93	0.82
6:F:537:GLU:OE1	6:F:602:TYR:HB3	1.79	0.82
16:S:30:GLN:H	16:S:36:ARG:HH22	1.23	0.82
3:C:316:LEU:HD21	3:C:340:TYR:HA	1.62	0.81
17:Y:442:GLN:HG2	17:Y:472:ARG:CG	2.07	0.81
3:C:148:ASN:HB3	3:C:151:LEU:HG	1.62	0.81
9:K:192:LYS:HG2	9:K:198:GLN:HG3	1.62	0.81
16:S:132:CYS:HA	16:S:133:ASN:CB	2.10	0.81
17:Y:42:ARG:HA	17:Y:82:TYR:HE2	1.37	0.81
16:S:163:GLU:HB2	16:S:196:PHE:HE1	1.45	0.81
13:O:75:LEU:CG	13:O:161:TYR:CZ	2.63	0.81
16:S:132:CYS:HB3	16:S:135:PRO:CD	2.10	0.81
1:A:1799:ARG:HD3	1:A:1805:MET:HB3	1.63	0.81
14:Q:128:ALA:CB	18:Z:156:TYR:CZ	2.63	0.81
17:X:267:LEU:HD11	17:Y:59:LEU:HD11	1.60	0.81
17:X:442:GLN:CD	17:X:472:ARG:CZ	2.42	0.81
12:N:180:PHE:CE1	12:N:299:TRP:CZ3	2.69	0.80
14:Q:163:LYS:HB2	14:Q:167:TYR:CD2	2.16	0.80
17:Y:305:ILE:CG2	17:Y:340:GLU:OE1	2.29	0.80
17:Y:366:ILE:HD11	17:Y:379:LYS:HD2	1.61	0.80
16:S:86:GLU:CG	16:S:98:MET:HE3	2.11	0.80
8:I:337:ILE:HG23	8:I:341:TYR:HE2	1.45	0.80
17:X:230:VAL:CG2	17:Y:36:ASN:HB3	2.11	0.80
6:H:656:MET:HE2	6:H:660:LYS:CE	2.09	0.80
8:I:32:ARG:HD3	12:N:388:HIS:CE1	2.16	0.80
17:X:230:VAL:HG21	17:Y:36:ASN:HB3	1.62	0.80
14:Q:163:LYS:HB2	14:Q:167:TYR:HD2	1.46	0.80
2:B:16:TRP:O	2:B:32:GLY:HA2	1.82	0.80
9:J:37:PRO:HB3	9:J:69:TYR:CE2	2.16	0.80
2:B:17:VAL:HG13	2:B:31:ASN:HD22	1.47	0.80
2:B:17:VAL:HG11	12:N:632:MET:HB3	1.64	0.80
16:S:65:GLU:O	16:S:69:TYR:CD2	2.34	0.80
2:B:17:VAL:HG21	12:N:634:THR:H	1.46	0.79
1:A:1232:ILE:HD11	1:A:1235:LEU:HD22	1.63	0.79
17:X:442:GLN:CG	17:X:472:ARG:HD2	2.10	0.79
8:I:56:TRP:HZ3	8:I:58:PHE:HB2	1.46	0.79
8:I:312:LYS:N	8:I:428:MET:SD	2.55	0.79
8:I:293:GLU:CB	8:I:324:GLN:NE2	2.46	0.79
16:S:41:LEU:HD11	18:Z:141:PHE:HB3	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:S:145:GLN:HE22	16:S:296:ILE:CB	1.94	0.79
1:A:1209:LEU:HD22	1:A:1228:LEU:HD23	1.64	0.79
13:O:32:PRO:O	13:O:35:ILE:HG22	1.82	0.79
16:S:68:PHE:HZ	16:S:81:TYR:CB	1.95	0.79
16:S:71:GLY:O	16:S:74:PRO:CD	2.29	0.79
17:Y:84:ALA:HB1	17:Y:100:TYR:CE2	2.17	0.79
2:B:43:ASP:HA	12:N:630:LYS:HE3	1.65	0.79
8:I:290:PHE:HD1	8:I:324:GLN:OE1	1.66	0.79
12:N:368:THR:OG1	12:N:369:ASP:HA	1.82	0.78
16:S:30:GLN:O	16:S:36:ARG:NH2	2.16	0.78
6:F:507:ARG:HD3	6:F:538:ILE:HD13	1.65	0.78
8:I:306:HIS:ND1	8:I:317:LEU:HG	1.98	0.78
12:N:577:GLU:HB3	12:N:625:LYS:HE3	1.64	0.78
9:J:185:LEU:HD12	9:J:209:LEU:HD21	1.64	0.78
8:I:276:TRP:CH2	8:I:280:LEU:HD22	2.19	0.78
14:Q:128:ALA:CB	18:Z:156:TYR:CE2	2.67	0.78
8:I:413:ASN:O	8:I:447:PHE:HE1	1.65	0.78
1:A:873:VAL:HG21	1:A:951:ILE:HG21	1.66	0.78
3:C:493:TYR:CE2	3:C:497:ILE:HD11	2.19	0.78
6:H:527:ARG:HB3	17:Y:302:PRO:HB3	1.66	0.78
13:O:581:ILE:HD13	13:O:611:SER:HB3	1.66	0.78
15:R:110:LYS:HE2	15:R:114:LYS:HB2	1.66	0.78
9:J:445:GLU:HG2	9:J:446:PRO:HD3	1.67	0.77
1:A:1656:LEU:H	1:A:1656:LEU:HD12	1.49	0.77
6:H:128:THR:HG21	6:H:130:ARG:NH1	2.00	0.77
8:I:56:TRP:CE3	8:I:98:PRO:CB	2.67	0.77
15:R:115:ALA:O	15:R:119:ASN:HB2	1.84	0.77
16:S:163:GLU:CB	16:S:196:PHE:HE1	1.97	0.77
9:K:487:TYR:OH	7:W:15:ASP:O	2.01	0.77
16:S:82:ILE:HD12	16:S:124:LEU:CD2	2.13	0.77
1:A:1097:THR:HG23	13:O:340:LEU:HB3	1.66	0.77
2:B:14:TRP:CZ2	2:B:42:ASP:OD1	2.38	0.77
2:B:16:TRP:CZ2	2:B:45:PRO:N	2.41	0.77
9:J:383:ASN:HB3	9:J:386:LEU:HD13	1.65	0.77
17:X:442:GLN:CD	17:X:472:ARG:CD	2.52	0.77
8:I:290:PHE:O	8:I:320:LEU:CD1	2.32	0.77
16:S:82:ILE:HD12	16:S:124:LEU:HD23	1.66	0.77
8:I:326:THR:O	8:I:330:LEU:N	2.18	0.77
12:N:281:TYR:CE2	12:N:356:PRO:HB2	2.20	0.77
1:A:1791:ILE:HB	13:O:598:THR:HG21	1.66	0.77
3:C:238:TYR:HD1	3:C:243:LEU:HD12	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:S:163:GLU:HB2	16:S:196:PHE:CE1	2.20	0.77
3:C:373:HIS:CE1	15:R:79:TYR:HA	2.20	0.76
8:I:304:PHE:CZ	8:I:452:LEU:HG	2.19	0.76
12:N:362:LYS:CA	12:N:410:LEU:CD2	2.62	0.76
14:Q:132:ARG:HB2	18:Z:170:SER:CB	2.13	0.76
16:S:201:SER:O	16:S:205:LEU:HG	1.86	0.76
17:X:52:ASN:HD22	17:Y:202:ALA:HB1	1.50	0.76
1:A:1248:ASN:O	1:A:1251:VAL:HG22	1.84	0.76
8:I:297:THR:N	8:I:316:GLU:OE2	2.19	0.76
12:N:289:PHE:O	12:N:291:LYS:N	2.18	0.76
12:N:435:VAL:HA	12:N:438:ILE:HD12	1.67	0.76
2:B:14:TRP:CE2	2:B:42:ASP:OD1	2.39	0.76
8:I:679:ASP:OD1	8:I:703:ARG:NH2	2.18	0.76
12:N:666:ILE:HG12	12:N:681:LEU:HD21	1.66	0.76
16:S:29:VAL:C	16:S:36:ARG:HH22	1.88	0.76
2:B:16:TRP:CZ2	2:B:44:CYS:N	2.53	0.76
8:I:290:PHE:CD1	8:I:324:GLN:OE1	2.38	0.76
10:L:40:PHE:HA	10:L:44:GLN:OE1	1.86	0.76
12:N:670:PHE:CE1	12:N:715:VAL:HB	2.20	0.76
16:S:132:CYS:HB3	16:S:135:PRO:N	2.00	0.76
1:A:1229:SER:HB3	1:A:1236:LEU:HA	1.67	0.76
12:N:425:ARG:HG2	12:N:425:ARG:NH1	1.97	0.76
16:S:82:ILE:CD1	16:S:124:LEU:HD23	2.16	0.76
13:O:411:LYS:HE2	13:O:412:HIS:CE1	2.20	0.76
14:Q:128:ALA:HB3	18:Z:156:TYR:OH	1.85	0.76
15:R:225:PRO:HB2	16:S:166:GLU:HB2	1.68	0.76
1:A:1196:TYR:CB	1:A:1208:LEU:HD11	2.16	0.76
7:G:6:PRO:HB3	9:J:406:HIS:CD2	2.21	0.76
16:S:33:ARG:HB2	16:S:130:ARG:NH1	2.01	0.76
8:I:290:PHE:O	8:I:320:LEU:HD13	1.85	0.75
9:K:174:HIS:HA	9:K:211:LYS:NZ	2.00	0.75
12:N:663:GLN:HE21	12:N:695:ARG:HG3	1.51	0.75
15:R:225:PRO:CB	16:S:166:GLU:HB2	2.16	0.75
1:A:1254:VAL:HG11	1:A:1298:ALA:HA	1.68	0.75
8:I:48:ARG:HG3	8:I:55:VAL:HG22	1.68	0.75
13:O:356:ASP:HA	13:O:357:SER:HB2	1.69	0.75
16:S:132:CYS:SG	16:S:135:PRO:CA	2.74	0.75
3:C:493:TYR:CZ	3:C:497:ILE:HD11	2.21	0.75
8:I:293:GLU:CB	8:I:324:GLN:HE21	1.99	0.75
13:O:163:GLN:O	13:O:167:LYS:HG3	1.85	0.75
3:P:290:ARG:HH21	3:P:319:LEU:HD12	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:332:THR:CA	9:J:363:LEU:HD21	2.15	0.75
10:L:126:ASP:OD2	10:L:130:LYS:O	2.05	0.75
12:N:289:PHE:HA	12:N:292:TRP:HB3	1.68	0.75
6:F:730:LYS:HE2	6:F:740:TYR:HE1	1.50	0.75
12:N:180:PHE:HD1	12:N:299:TRP:HZ3	1.34	0.75
1:A:1375:TYR:HB3	1:A:1378:THR:HG21	1.69	0.75
9:J:19:TYR:CD1	9:J:49:LEU:HD13	2.21	0.75
16:S:76:ASP:O	16:S:77:VAL:CB	2.33	0.75
9:J:406:HIS:CE1	9:J:450:ASN:HD22	2.05	0.75
16:S:30:GLN:H	16:S:91:GLN:CB	1.97	0.75
1:A:873:VAL:HG21	1:A:951:ILE:CG2	2.17	0.74
16:S:86:GLU:HG2	16:S:98:MET:HE3	1.68	0.74
9:K:174:HIS:CE1	9:K:211:LYS:HD3	2.22	0.74
3:C:327:ASP:O	3:C:333:THR:HG21	1.87	0.74
8:I:224:SER:CB	8:I:229:SER:HA	2.17	0.74
8:I:305:MET:HB2	13:O:61:ASN:HD21	1.51	0.74
12:N:120:SER:O	12:N:124:PRO:HD3	1.87	0.74
9:J:451:LEU:HD12	9:J:467:TYR:CE2	2.22	0.74
9:K:184:LEU:O	9:K:188:LEU:HD23	1.87	0.74
13:O:544:VAL:HG23	13:O:567:LEU:HG	1.67	0.74
16:S:22:TRP:CE3	16:S:41:LEU:CB	2.68	0.74
16:S:129:GLY:O	16:S:132:CYS:SG	2.45	0.74
9:J:465:LEU:HA	9:J:488:ILE:HD12	1.67	0.74
16:S:20:ASP:N	18:Z:134:GLN:HE21	1.85	0.74
1:A:629:LEU:HD11	1:A:634:ALA:HB2	1.69	0.74
13:O:312:CYS:SG	13:O:350:LEU:HD21	2.28	0.74
6:F:500:TRP:HB3	6:H:30:ARG:NH2	2.02	0.74
6:F:653:LEU:HA	6:F:656:MET:SD	2.27	0.74
8:I:26:LEU:HB3	8:I:37:LEU:CB	2.17	0.74
8:I:430:GLU:CG	14:Q:429:LYS:HG3	2.17	0.74
16:S:30:GLN:CA	16:S:91:GLN:HB2	2.17	0.74
17:X:52:ASN:ND2	17:Y:202:ALA:HB1	2.01	0.74
8:I:279:ILE:HB	8:I:340:SER:HB2	1.69	0.74
17:Y:452:LEU:HD22	17:Y:461:ALA:H	1.49	0.74
12:N:630:LYS:HD3	12:N:633:ARG:NH1	2.03	0.73
16:S:86:GLU:CG	16:S:98:MET:CE	2.64	0.73
17:X:452:LEU:HD22	17:X:461:ALA:H	1.49	0.73
8:I:417:PHE:HD2	8:I:448:VAL:HG22	1.53	0.73
13:O:75:LEU:HD11	13:O:161:TYR:CD2	2.23	0.73
16:S:41:LEU:O	16:S:45:LEU:HD12	1.88	0.73
3:P:327:ASP:O	3:P:333:THR:HG21	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:S:20:ASP:OD1	18:Z:184:ARG:CD	2.35	0.73
13:O:405:SER:O	13:O:409:HIS:CD2	2.41	0.73
14:Q:186:TYR:CZ	16:S:27:GLU:HB2	2.23	0.73
16:S:163:GLU:CD	16:S:196:PHE:HE1	1.92	0.73
12:N:626:TYR:CD2	12:N:633:ARG:HB3	2.22	0.73
3:P:251:TYR:OH	3:P:268:GLN:HG3	1.88	0.73
6:F:550:VAL:HG21	9:K:289:HIS:HB3	1.70	0.73
10:L:44:GLN:HA	10:L:47:ASP:OD2	1.88	0.73
10:L:74:VAL:HG21	10:L:137:ILE:HD11	1.68	0.73
12:N:542:VAL:HG11	12:N:558:GLU:HG2	1.71	0.73
13:O:539:ASN:HD22	13:O:542:GLU:CB	2.01	0.73
1:A:776:ASN:HD22	1:A:779:MET:HG2	1.54	0.72
8:I:81:ALA:HB2	8:I:92:LEU:HB3	1.71	0.72
8:I:177:VAL:HG12	8:I:208:LEU:HD13	1.70	0.72
12:N:542:VAL:HG11	12:N:558:GLU:CG	2.17	0.72
13:O:291:ASN:O	13:O:336:ASP:HB2	1.89	0.72
16:S:40:THR:HG21	16:S:87:GLN:HB3	1.70	0.72
16:S:193:HIS:NE2	16:S:197:GLN:OE1	2.22	0.72
6:H:707:PHE:HB2	6:H:729:LEU:HD11	1.71	0.72
8:I:26:LEU:CB	8:I:37:LEU:HB3	2.19	0.72
17:X:407:LEU:HD13	17:X:443:THR:HG21	1.72	0.72
8:I:302:ASP:CA	8:I:303:GLU:N	2.51	0.72
9:J:24:PHE:CE1	9:J:28:LYS:HE3	2.24	0.72
16:S:30:GLN:CA	16:S:36:ARG:NH2	2.52	0.72
16:S:163:GLU:CG	16:S:196:PHE:HE1	2.02	0.72
1:A:482:VAL:HG12	1:A:487:THR:O	1.90	0.72
1:A:1138:HIS:HE1	1:A:1604:GLN:HE21	1.37	0.72
9:K:185:LEU:HA	9:K:188:LEU:HD21	1.70	0.72
16:S:22:TRP:HZ3	16:S:41:LEU:CG	2.02	0.72
17:Y:442:GLN:HG2	17:Y:472:ARG:HG3	1.71	0.72
3:C:358:LEU:HD21	3:C:368:TRP:CD2	2.24	0.72
9:J:441:VAL:O	9:J:442:ASP:HB3	1.89	0.72
9:K:63:ARG:HB2	9:K:65:LEU:CD1	2.19	0.72
16:S:132:CYS:CB	16:S:135:PRO:CG	2.64	0.72
1:A:1753:TYR:HD2	13:O:643:LEU:HD12	1.53	0.72
6:F:145:ASN:HB2	6:F:146:PRO:C	2.10	0.72
6:H:754:HIS:CE1	6:H:755:LEU:HD13	2.25	0.72
1:A:1284:GLU:HB2	1:A:1350:TYR:CE2	2.24	0.72
8:I:674:VAL:O	8:I:703:ARG:NH1	2.23	0.72
12:N:520:ARG:HD2	12:N:556:PHE:CD1	2.25	0.72
3:C:238:TYR:CD1	3:C:243:LEU:HD12	2.24	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:72:ALA:O	8:I:80:LEU:HD12	1.89	0.72
11:M:17:ASP:HA	11:M:20:ARG:HG2	1.71	0.72
16:S:30:GLN:HB2	16:S:91:GLN:HA	1.72	0.72
16:S:30:GLN:CD	16:S:91:GLN:HG3	2.10	0.72
8:I:48:ARG:HG3	8:I:55:VAL:CG2	2.20	0.72
13:O:620:ALA:O	13:O:624:VAL:HG23	1.90	0.72
8:I:65:GLY:H	8:I:84:LEU:HG	1.54	0.71
3:C:242:GLN:O	3:C:244:ILE:HG13	1.91	0.71
16:S:163:GLU:CG	16:S:196:PHE:CE1	2.73	0.71
2:B:16:TRP:CH2	12:N:630:LYS:HE2	2.24	0.71
1:A:1786:MET:HA	1:A:1786:MET:CE	2.21	0.71
3:C:36:LEU:HD21	3:C:58:LEU:HB2	1.73	0.71
1:A:1089:LEU:HD11	1:A:1611:VAL:CG2	2.20	0.71
3:C:414:MET:HG2	13:O:330:ILE:HD11	1.73	0.71
8:I:88:LYS:O	8:I:106:VAL:HG22	1.90	0.71
8:I:294:LYS:CB	8:I:320:LEU:HB2	2.20	0.71
9:K:406:HIS:ND1	7:W:6:PRO:HB3	2.05	0.71
12:N:395:ASP:OD1	12:N:398:THR:N	2.24	0.71
17:Y:45:ALA:HB3	17:Y:82:TYR:CE2	2.25	0.71
1:A:116:ALA:O	13:O:266:ASP:HA	1.90	0.71
6:F:656:MET:HG3	17:Y:526:GLN:HB2	1.72	0.71
12:N:60:GLU:O	12:N:63:ALA:HB2	1.91	0.71
3:P:355:GLN:HA	3:P:358:LEU:HD23	1.70	0.71
16:S:30:GLN:HB2	16:S:91:GLN:HB2	1.73	0.71
8:I:116:MET:SD	8:I:210:LEU:HG	2.31	0.71
12:N:120:SER:O	12:N:124:PRO:CD	2.39	0.71
16:S:83:SER:HB2	16:S:87:GLN:HE21	1.56	0.71
1:A:1469:CYS:HB2	1:A:1488:LEU:CD2	2.19	0.71
9:K:45:GLN:HA	9:K:45:GLN:HE21	1.54	0.71
12:N:343:GLU:O	12:N:347:ILE:N	2.23	0.71
16:S:38:MET:HE1	18:Z:199:TYR:CE2	2.21	0.71
1:A:1624:VAL:HG22	1:A:1698:TYR:HD2	1.56	0.71
7:G:6:PRO:HB3	9:J:406:HIS:HD2	1.55	0.71
8:I:300:VAL:HG21	8:I:456:PHE:HB2	1.73	0.71
8:I:500:PHE:HE2	8:I:507:LEU:HD12	1.55	0.71
12:N:362:LYS:CG	12:N:410:LEU:HD23	2.20	0.71
17:Y:42:ARG:CG	17:Y:82:TYR:OH	2.39	0.71
2:B:14:TRP:CB	2:B:15:LEU:HB2	2.21	0.71
17:X:442:GLN:HE21	17:X:472:ARG:HG3	1.55	0.71
9:K:222:GLU:HB3	9:K:228:GLN:OE1	1.90	0.70
12:N:563:ASP:OD2	12:N:597:SER:HB3	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:N:425:ARG:CZ	12:N:507:SER:HB2	2.21	0.70
14:Q:410:HIS:CD2	14:Q:475:LEU:HD11	2.26	0.70
15:R:247:SER:HB2	16:S:170:LYS:NZ	2.05	0.70
16:S:64:TYR:O	16:S:68:PHE:CD2	2.44	0.70
16:S:66:ILE:CA	16:S:69:TYR:HD2	2.02	0.70
16:S:68:PHE:CZ	16:S:81:TYR:CB	2.75	0.70
1:A:1645:GLU:HG3	1:A:1646:GLN:H	1.56	0.70
13:O:706:CYS:HB3	13:O:709:ARG:HB3	1.73	0.70
1:A:801:PRO:HB2	1:A:841:PRO:HG3	1.74	0.70
3:C:39:ILE:HD13	3:C:201:LEU:HB2	1.73	0.70
8:I:269:LEU:CB	8:I:526:LYS:HZ2	2.05	0.70
9:J:254:THR:CG2	9:J:271:HIS:CD2	2.75	0.70
13:O:127:HIS:O	13:O:128:LYS:HB3	1.91	0.70
17:X:442:GLN:NE2	17:X:472:ARG:NE	2.29	0.70
12:N:519:TYR:OH	12:N:541:ASN:HB3	1.90	0.70
16:S:132:CYS:CB	16:S:135:PRO:CD	2.69	0.70
17:X:192:TYR:HA	17:X:195:VAL:HG22	1.73	0.70
8:I:279:ILE:HB	8:I:340:SER:CB	2.22	0.70
9:J:465:LEU:HA	9:J:488:ILE:CD1	2.20	0.70
13:O:479:GLU:O	13:O:656:ALA:O	2.09	0.70
1:A:1390:PRO:HG2	1:A:1396:LEU:HG	1.74	0.70
9:K:417:GLU:HB2	9:K:420:THR:OG1	1.92	0.70
3:P:39:ILE:HD13	3:P:201:LEU:HB2	1.72	0.70
17:X:442:GLN:NE2	17:X:472:ARG:HG3	2.07	0.70
1:A:482:VAL:HG11	1:A:485:ILE:HD12	1.74	0.70
15:R:74:PRO:HB2	15:R:75:GLY:HA2	1.72	0.70
8:I:73:TRP:CG	8:I:80:LEU:HD13	2.26	0.70
8:I:231:VAL:HG21	8:I:557:TYR:CZ	2.27	0.70
8:I:306:HIS:CE1	8:I:313:ALA:O	2.44	0.70
16:S:22:TRP:HH2	16:S:38:MET:HA	1.38	0.70
16:S:25:SER:H	16:S:45:LEU:HD21	1.57	0.70
16:S:78:TRP:CE3	16:S:105:ALA:HB2	2.26	0.70
6:H:761:SER:O	6:H:765:ASP:HB2	1.92	0.70
9:J:475:ILE:HD11	9:J:478:ASN:HD22	1.57	0.70
8:I:312:LYS:HE2	8:I:428:MET:HA	1.72	0.69
3:P:276:ILE:HG22	3:P:277:ARG:N	2.06	0.69
16:S:79:ASP:OD2	16:S:120:ARG:HB3	1.91	0.69
17:Y:186:ARG:HA	17:Y:189:VAL:HG12	1.75	0.69
2:B:16:TRP:HB3	2:B:33:CYS:N	2.08	0.69
3:C:416:PHE:HB2	3:C:446:LEU:HD11	1.74	0.69
8:I:290:PHE:HE1	8:I:324:GLN:CB	2.05	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:252:GLN:O	3:P:255:ILE:HG22	1.92	0.69
17:Y:192:TYR:HA	17:Y:195:VAL:HG22	1.74	0.69
1:A:980:ARG:NH1	1:A:1674:TRP:CD1	2.61	0.69
8:I:289:LYS:CG	8:I:324:GLN:OE1	2.38	0.69
8:I:290:PHE:HA	8:I:320:LEU:CD1	2.22	0.69
3:C:358:LEU:HD13	3:C:367:ALA:HB3	1.75	0.69
8:I:46:LEU:HD22	8:I:56:TRP:HE1	1.58	0.69
9:J:185:LEU:HD13	9:J:206:GLU:OE1	1.92	0.69
9:J:439:VAL:HG21	9:J:448:LEU:HD21	1.73	0.69
13:O:657:ILE:HA	13:O:660:LYS:CB	2.22	0.69
16:S:22:TRP:CH2	16:S:38:MET:C	2.60	0.69
1:A:1332:GLY:O	1:A:1358:ILE:HG13	1.92	0.69
10:L:105:LEU:HD12	10:L:138:GLN:OE1	1.93	0.69
16:S:195:GLN:O	16:S:199:ARG:HG3	1.91	0.69
17:Y:503:LEU:O	17:Y:506:GLN:NE2	2.25	0.69
14:Q:131:LEU:HD13	18:Z:163:VAL:HG11	1.74	0.69
15:R:112:HIS:NE2	15:R:116:TRP:HZ3	1.91	0.69
6:F:554:VAL:HG21	9:K:286:TYR:HD1	1.56	0.69
8:I:574:PHE:HE2	8:I:576:TRP:HB2	1.57	0.69
12:N:350:ASP:CB	12:N:351:PHE:HA	2.23	0.69
4:D:8:LEU:HD23	13:O:420:ILE:HD11	1.73	0.69
6:H:168:PHE:CB	6:H:467:ARG:HD3	2.23	0.69
6:H:653:LEU:CD2	9:K:523:ILE:HG21	2.22	0.69
13:O:539:ASN:ND2	13:O:542:GLU:HB2	2.08	0.69
16:S:22:TRP:HZ3	16:S:41:LEU:CD1	2.04	0.69
6:H:730:LYS:HD3	6:H:740:TYR:HE1	1.56	0.69
8:I:214:LEU:O	8:I:238:THR:OG1	2.11	0.69
14:Q:166:ARG:NH2	14:Q:413:GLU:OE1	2.24	0.69
16:S:22:TRP:CZ3	16:S:41:LEU:HB3	2.25	0.69
1:A:763:PHE:CD1	1:A:793:LEU:HD22	2.29	0.68
2:B:17:VAL:O	2:B:30:PHE:O	2.10	0.68
3:C:434:ARG:HD2	15:R:80:ILE:HD13	1.74	0.68
6:H:685:SER:O	6:H:689:LEU:HD12	1.92	0.68
12:N:597:SER:OG	12:N:600:PHE:HB2	1.93	0.68
16:S:71:GLY:HA2	16:S:74:PRO:HD2	1.75	0.68
4:D:16:LEU:HD23	4:D:16:LEU:H	1.57	0.68
12:N:139:GLY:C	12:N:141:LEU:H	1.97	0.68
17:X:445:THR:O	17:X:449:THR:HG23	1.93	0.68
6:F:133:LYS:HA	6:F:136:GLU:OE1	1.94	0.68
12:N:769:SER:OG	12:N:772:ARG:HD3	1.93	0.68
13:O:274:LEU:HD11	13:O:306:ASN:HB3	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:283:LEU:HD21	3:P:312:MET:CE	2.24	0.68
16:S:29:VAL:CB	16:S:36:ARG:HH12	2.05	0.68
17:Y:270:ASN:HB2	17:Y:273:LEU:HB3	1.74	0.68
1:A:1469:CYS:HB2	1:A:1488:LEU:HD21	1.76	0.68
9:J:35:GLU:CD	9:J:63:ARG:HE	1.96	0.68
9:K:285:PHE:HB2	9:K:308:TYR:CE1	2.28	0.68
9:K:384:SER:HB2	9:K:415:ASN:HD21	1.59	0.68
15:R:107:PRO:O	15:R:109:LYS:HE2	1.93	0.68
17:Y:407:LEU:HD13	17:Y:443:THR:HG21	1.74	0.68
1:A:857:MET:CB	1:A:858:PRO:HD3	2.24	0.68
1:A:1089:LEU:HD11	1:A:1611:VAL:HG23	1.74	0.68
12:N:516:ILE:HG13	12:N:554:MET:HE2	1.75	0.68
17:X:503:LEU:O	17:X:506:GLN:NE2	2.27	0.68
17:Y:371:ASN:H	17:Y:371:ASN:HD22	1.40	0.68
2:B:16:TRP:HH2	12:N:630:LYS:HG2	1.59	0.68
8:I:67:GLU:O	8:I:85:ALA:N	2.19	0.68
8:I:414:PHE:CE1	8:I:451:PHE:CE1	2.82	0.68
9:K:185:LEU:HD13	9:K:209:LEU:HD11	1.75	0.68
9:K:495:PHE:CZ	9:K:525:MET:HG2	2.28	0.68
12:N:285:PHE:O	12:N:289:PHE:HD1	1.76	0.68
12:N:350:ASP:HB3	12:N:351:PHE:HA	1.76	0.68
7:G:4:ARG:HH21	9:J:345:ALA:HB1	1.57	0.68
1:A:980:ARG:NH2	1:A:1674:TRP:O	2.27	0.68
3:C:388:TYR:HB2	3:C:405:LEU:HD13	1.76	0.68
6:F:554:VAL:HG21	9:K:286:TYR:CD1	2.29	0.68
8:I:360:LEU:HD21	8:I:390:ILE:HG23	1.76	0.68
8:I:417:PHE:CD2	8:I:448:VAL:HG22	2.28	0.68
9:J:285:PHE:HB2	9:J:308:TYR:CE1	2.28	0.68
1:A:1470:LEU:HA	1:A:1522:SER:OG	1.93	0.68
2:B:27:ARG:CB	12:N:810:TYR:HE2	2.06	0.68
14:Q:166:ARG:CZ	14:Q:436:VAL:HG11	2.23	0.68
17:Y:407:LEU:CD2	17:Y:437:LEU:HD21	2.24	0.68
1:A:1076:ARG:HE	1:A:1543:HIS:CD2	2.11	0.68
8:I:287:LEU:HG	8:I:456:PHE:CZ	2.29	0.68
3:C:434:ARG:CD	15:R:80:ILE:HG21	2.24	0.67
4:D:13:THR:HG22	13:O:255:TYR:HE2	1.59	0.67
9:J:332:THR:HA	9:J:363:LEU:CD2	2.21	0.67
9:J:397:ILE:HG22	9:J:398:ALA:H	1.59	0.67
8:I:330:LEU:HD23	8:I:425:MET:HE3	1.76	0.67
13:O:75:LEU:HB3	13:O:79:TYR:HE2	1.54	0.67
3:P:358:LEU:HD11	3:P:368:TRP:CE2	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:16:TRP:CD1	2:B:44:CYS:SG	2.88	0.67
2:B:76:CYS:SG	2:B:78:GLN:HG2	2.34	0.67
8:I:317:LEU:HD22	8:I:320:LEU:HD23	1.76	0.67
8:I:574:PHE:CE2	8:I:576:TRP:HB2	2.28	0.67
16:S:78:TRP:CE3	16:S:105:ALA:CB	2.77	0.67
16:S:163:GLU:OE1	16:S:196:PHE:HE1	1.75	0.67
1:A:1329:MET:HE2	1:A:1368:THR:HA	1.77	0.67
8:I:290:PHE:CB	8:I:320:LEU:HD11	2.24	0.67
8:I:306:HIS:ND1	8:I:313:ALA:HB1	2.10	0.67
17:X:442:GLN:HG2	17:X:472:ARG:HG3	1.76	0.67
17:Y:442:GLN:CG	17:Y:472:ARG:HG3	2.24	0.67
17:Y:445:THR:O	17:Y:449:THR:HG23	1.93	0.67
1:A:1153:ILE:HD11	1:A:1184:HIS:HB3	1.76	0.67
3:P:233:PHE:CE1	3:P:237:ILE:HD11	2.28	0.67
1:A:1186:THR:HG23	1:A:1215:ALA:HB1	1.76	0.67
1:A:1470:LEU:HD12	1:A:1518:VAL:HG13	1.75	0.67
10:L:89:TYR:O	10:L:151:THR:HG22	1.95	0.67
15:R:109:LYS:O	15:R:113:GLN:HG3	1.95	0.67
16:S:197:GLN:O	16:S:200:VAL:CG2	2.41	0.67
17:X:442:GLN:CG	17:X:472:ARG:NE	2.58	0.67
18:Z:158:ASP:O	18:Z:160:ASP:N	2.28	0.67
1:A:939:PHE:HZ	1:A:944:LEU:HD13	1.59	0.67
8:I:15:GLY:O	8:I:743:VAL:N	2.26	0.67
9:K:222:GLU:CD	9:K:228:GLN:HG3	2.14	0.67
13:O:657:ILE:HA	13:O:660:LYS:HB3	1.77	0.67
16:S:30:GLN:CB	16:S:91:GLN:HB2	2.24	0.67
16:S:83:SER:O	16:S:87:GLN:N	2.21	0.67
3:C:414:MET:CG	13:O:330:ILE:HD11	2.25	0.67
2:B:14:TRP:HB2	2:B:15:LEU:HB2	1.76	0.66
8:I:28:TRP:NE1	8:I:723:ALA:O	2.28	0.66
8:I:312:LYS:HG2	8:I:428:MET:HB3	1.76	0.66
1:A:1287:TYR:CD1	1:A:1287:TYR:O	2.48	0.66
6:F:168:PHE:CB	6:F:467:ARG:HD3	2.24	0.66
6:H:762:TRP:CA	6:H:765:ASP:HB3	2.25	0.66
16:S:22:TRP:CE3	16:S:41:LEU:HB3	2.30	0.66
17:X:66:ASN:ND2	17:Y:268:ARG:HB3	2.10	0.66
6:F:562:MET:HB2	6:H:59:ARG:HH12	1.58	0.66
13:O:544:VAL:CG2	13:O:567:LEU:HG	2.25	0.66
12:N:165:THR:N	12:N:166:PRO:HA	2.10	0.66
2:B:16:TRP:NE1	2:B:44:CYS:SG	2.67	0.66
8:I:13:VAL:HG22	8:I:744:PHE:CE2	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Q:475:LEU:O	14:Q:476:ASP:HB3	1.94	0.66
17:Y:104:LEU:HD11	17:Y:142:MET:SD	2.36	0.66
1:A:1399:VAL:HG11	1:A:1404:LEU:HG	1.76	0.66
3:C:411:ILE:HG22	15:R:95:LEU:HD23	1.78	0.66
8:I:73:TRP:CD1	8:I:80:LEU:HD13	2.31	0.66
8:I:269:LEU:HB2	8:I:526:LYS:NZ	2.10	0.66
8:I:290:PHE:CE1	8:I:324:GLN:HB3	2.27	0.66
14:Q:131:LEU:CD1	18:Z:163:VAL:HG11	2.26	0.66
16:S:23:GLU:OE2	18:Z:134:GLN:HA	1.96	0.66
16:S:30:GLN:HB2	16:S:91:GLN:CB	2.25	0.66
1:A:1051:VAL:HG21	1:A:1066:LYS:HB3	1.78	0.66
1:A:1138:HIS:HD2	1:A:1608:HIS:NE2	1.94	0.66
1:A:1750:PHE:HD1	13:O:605:LEU:HD11	1.60	0.66
8:I:349:ILE:CD1	13:O:407:LEU:HA	2.26	0.66
8:I:536:CYS:O	8:I:540:PRO:HD3	1.96	0.66
16:S:58:GLN:HG3	16:S:62:PHE:CZ	2.29	0.66
3:C:416:PHE:CE2	13:O:323:ALA:HB2	2.31	0.66
8:I:313:ALA:HB3	8:I:317:LEU:CG	2.26	0.66
13:O:417:LEU:HA	13:O:420:ILE:HG22	1.78	0.66
3:C:251:TYR:HB3	3:C:269:ILE:HD11	1.78	0.66
12:N:74:TRP:CZ2	12:N:77:GLU:HB2	2.31	0.66
1:A:949:PHE:HA	1:A:952:ALA:HB3	1.77	0.66
3:C:521:PHE:CD1	3:C:553:ILE:HG22	2.31	0.66
6:H:743:ILE:CG2	6:H:759:ASN:HD21	2.09	0.66
8:I:24:ILE:O	8:I:569:LEU:HD22	1.96	0.66
17:X:63:MET:HE3	17:Y:266:LEU:HD22	1.78	0.66
6:H:765:ASP:O	17:X:397:ARG:NH2	2.29	0.65
12:N:280:GLU:HA	12:N:281:TYR:HD1	1.61	0.65
1:A:38:GLN:HE21	3:C:396:LYS:H	1.41	0.65
6:F:50:ARG:HE	6:H:19:TYR:HE1	1.44	0.65
9:K:250:CYS:HG	9:K:274:THR:HG21	1.60	0.65
3:P:36:LEU:HD21	3:P:58:LEU:HB2	1.78	0.65
15:R:98:GLU:HG2	15:R:101:PRO:HG3	1.77	0.65
16:S:82:ILE:HD11	16:S:124:LEU:CD2	2.25	0.65
17:X:203:LEU:HD21	17:X:239:TRP:CH2	2.31	0.65
17:X:414:ILE:HD11	17:X:451:CYS:SG	2.36	0.65
1:A:257:MET:HE3	1:A:266:HIS:HB3	1.77	0.65
1:A:1196:TYR:HB2	1:A:1208:LEU:HD11	1.78	0.65
2:B:39:VAL:N	2:B:40:PRO:HD2	2.12	0.65
3:C:314:SER:HB2	9:J:289:HIS:CE1	2.31	0.65
9:J:37:PRO:HB3	9:J:69:TYR:CZ	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:121:LEU:HG	6:H:125:TYR:CE1	2.32	0.65
9:J:429:LEU:HA	9:J:432:ILE:HG22	1.79	0.65
12:N:202:GLU:HB2	12:N:282:GLU:OE2	1.96	0.65
3:C:368:TRP:HB3	3:C:391:ALA:HB2	1.78	0.65
6:F:67:THR:HG21	17:Y:263:LYS:HD3	1.78	0.65
12:N:538:GLU:HG2	12:N:561:LEU:CG	2.25	0.65
16:S:29:VAL:CA	16:S:36:ARG:NH1	2.55	0.65
1:A:150:CYS:HB3	1:A:163:SER:HA	1.78	0.65
1:A:1797:ILE:HG22	1:A:1852:ILE:HD11	1.78	0.65
16:S:163:GLU:OE1	16:S:196:PHE:HD1	1.79	0.65
17:X:40:HIS:HB3	17:Y:201:LEU:CD1	2.24	0.65
1:A:1321:VAL:HG22	1:A:1322:PRO:HD3	1.79	0.65
3:C:477:HIS:HD2	3:C:482:GLU:OE1	1.80	0.65
13:O:658:LEU:HD13	13:O:704:VAL:HG11	1.78	0.65
1:A:175:PHE:CD1	1:A:191:ARG:HG3	2.31	0.65
1:A:1306:CYS:HB2	1:A:1374:ILE:HG12	1.76	0.65
2:B:17:VAL:CG1	12:N:632:MET:HB3	2.26	0.65
8:I:348:VAL:HB	8:I:404:LEU:HD21	1.76	0.65
17:X:371:ASN:HD22	17:X:371:ASN:H	1.43	0.65
1:A:1799:ARG:HD3	1:A:1805:MET:CB	2.26	0.65
3:C:531:THR:O	3:C:535:LYS:HG2	1.97	0.65
8:I:279:ILE:CG1	8:I:340:SER:HB2	2.26	0.65
8:I:295:ASN:O	8:I:316:GLU:CG	2.45	0.65
9:K:376:LEU:HG	9:K:407:GLU:OE1	1.97	0.65
15:R:98:GLU:CB	15:R:101:PRO:HD3	2.26	0.65
1:A:1333:HIS:HB2	1:A:1357:THR:HA	1.78	0.65
13:O:35:ILE:HG21	13:O:158:LEU:HD13	1.78	0.65
16:S:68:PHE:CZ	16:S:81:TYR:HB2	2.32	0.65
16:S:75:LEU:HD13	16:S:75:LEU:C	2.17	0.65
16:S:82:ILE:HD11	16:S:124:LEU:HD22	1.79	0.65
1:A:1405:LEU:HD13	1:A:1467:GLY:HA2	1.78	0.64
8:I:206:LEU:HD22	8:I:570:PHE:CG	2.33	0.64
8:I:337:ILE:HG23	8:I:341:TYR:CE2	2.28	0.64
9:K:254:THR:HG23	9:K:271:HIS:CD2	2.32	0.64
13:O:625:LEU:HD13	13:O:666:LEU:HD22	1.79	0.64
16:S:79:ASP:HB2	16:S:120:ARG:HH11	1.62	0.64
16:S:132:CYS:HB3	16:S:135:PRO:HD3	1.79	0.64
3:P:531:THR:O	3:P:535:LYS:HG2	1.97	0.64
14:Q:146:ASN:C	14:Q:420:PHE:HE1	2.00	0.64
15:R:225:PRO:HB2	16:S:165:ARG:O	1.98	0.64
16:S:144:ASN:HB3	16:S:295:TRP:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:270:ASN:HB2	17:X:273:LEU:CB	2.28	0.64
1:A:611:GLU:O	1:A:645:HIS:NE2	2.30	0.64
8:I:290:PHE:CE1	8:I:324:GLN:CB	2.80	0.64
12:N:74:TRP:CE3	12:N:76:VAL:HG13	2.32	0.64
13:O:460:GLN:HG2	13:O:496:ARG:NH2	2.11	0.64
14:Q:166:ARG:NH1	14:Q:436:VAL:HG11	2.12	0.64
6:F:707:PHE:HB2	6:F:729:LEU:HD11	1.80	0.64
9:K:210:LYS:O	9:K:212:TYR:N	2.28	0.64
17:X:407:LEU:CD2	17:X:437:LEU:HD21	2.26	0.64
1:A:1162:LYS:HG3	1:A:1163:PRO:CD	2.24	0.64
1:A:1475:ARG:HG2	1:A:1476:PHE:CE1	2.32	0.64
8:I:115:TRP:CZ3	8:I:176:LEU:HD22	2.32	0.64
12:N:392:ASN:O	12:N:395:ASP:HA	1.98	0.64
3:P:233:PHE:CZ	3:P:237:ILE:CD1	2.79	0.64
16:S:22:TRP:HA	16:S:45:LEU:CD1	2.26	0.64
17:X:270:ASN:HB2	17:X:273:LEU:HB3	1.79	0.64
1:A:1619:LEU:HD11	1:A:1697:LEU:HB2	1.77	0.64
6:H:703:PRO:HB3	6:H:733:VAL:HG21	1.78	0.64
9:J:40:ILE:HD13	9:J:63:ARG:HD3	1.79	0.64
9:J:294:LEU:HD12	9:K:54:HIS:NE2	2.13	0.64
9:J:454:VAL:C	9:J:458:LEU:HD12	2.17	0.64
12:N:622:TYR:O	12:N:626:TYR:HB2	1.98	0.64
16:S:134:GLU:O	16:S:134:GLU:HG3	1.98	0.64
17:X:442:GLN:CG	17:X:472:ARG:HG3	2.27	0.64
6:H:145:ASN:HB2	6:H:146:PRO:O	1.97	0.64
10:L:45:LEU:O	10:L:155:GLN:OE1	2.16	0.64
1:A:1540:ARG:CZ	12:N:486:ASP:O	2.45	0.64
8:I:265:ILE:HD11	8:I:396:PHE:CE2	2.33	0.64
3:P:441:GLU:HG3	3:P:472:LYS:HZ1	1.63	0.64
17:X:159:LEU:HD22	17:X:171:ILE:HG23	1.80	0.64
17:Y:215:LYS:O	17:Y:219:VAL:HG23	1.98	0.64
12:N:202:GLU:O	12:N:204:ASP:N	2.31	0.63
3:P:368:TRP:HB3	3:P:391:ALA:HB2	1.80	0.63
15:R:475:LEU:O	15:R:476:ASP:HB2	1.98	0.63
17:X:215:LYS:O	17:X:219:VAL:HG23	1.98	0.63
1:A:1100:LEU:HB3	1:A:1101:PRO:HA	1.79	0.63
8:I:73:TRP:CE2	8:I:80:LEU:HD22	2.32	0.63
8:I:290:PHE:C	8:I:320:LEU:CD1	2.67	0.63
9:J:445:GLU:HA	9:J:474:LEU:HD23	1.79	0.63
9:K:372:LEU:HD11	9:K:407:GLU:HG3	1.80	0.63
14:Q:166:ARG:NH1	14:Q:413:GLU:OE1	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:S:84:TRP:O	16:S:88:ASN:ND2	2.31	0.63
2:B:16:TRP:CH2	12:N:630:LYS:HG2	2.34	0.63
8:I:279:ILE:CB	8:I:340:SER:HB2	2.28	0.63
8:I:305:MET:HB2	13:O:61:ASN:ND2	2.14	0.63
9:K:77:ALA:CB	9:K:93:LEU:HD11	2.27	0.63
12:N:78:VAL:O	12:N:80:GLN:N	2.31	0.63
1:A:174:PRO:HA	1:A:360:VAL:O	1.99	0.63
2:B:16:TRP:C	2:B:31:ASN:O	2.28	0.63
6:F:696:ILE:HD11	6:F:709:ARG:HD3	1.81	0.63
8:I:24:ILE:HG22	8:I:38:ALA:O	1.98	0.63
1:A:1229:SER:O	1:A:1236:LEU:HB2	1.98	0.63
1:A:1601:TYR:HH	10:L:102:PHE:HD1	1.45	0.63
3:C:61:SER:HB2	3:C:262:SER:HB2	1.79	0.63
6:H:130:ARG:HH12	9:K:473:VAL:HG22	1.64	0.63
8:I:313:ALA:CB	8:I:317:LEU:CD1	2.72	0.63
3:P:283:LEU:HD21	3:P:312:MET:HE3	1.80	0.63
16:S:38:MET:HE2	18:Z:181:VAL:HG23	0.64	0.63
17:Y:159:LEU:HD22	17:Y:171:ILE:HG23	1.81	0.63
17:Y:373:VAL:HG11	17:Y:403:ALA:HB2	1.79	0.63
1:A:1327:GLN:HA	1:A:1330:VAL:HG12	1.80	0.63
12:N:296:VAL:O	12:N:299:TRP:HB3	1.99	0.63
12:N:765:LEU:HD21	16:S:200:VAL:CG2	2.20	0.63
17:Y:294:PHE:CD1	17:Y:294:PHE:C	2.71	0.63
1:A:1230:ILE:HA	1:A:1236:LEU:HD22	1.81	0.63
1:A:1409:LEU:HG	1:A:1470:LEU:HD22	1.79	0.63
8:I:402:GLU:O	8:I:406:VAL:HG23	1.98	0.63
15:R:225:PRO:HG2	16:S:166:GLU:CB	2.28	0.63
17:X:452:LEU:HB3	17:X:461:ALA:HB2	1.81	0.63
17:Y:270:ASN:HB2	17:Y:273:LEU:CB	2.28	0.63
1:A:1511:ASN:HD22	1:A:1511:ASN:N	1.96	0.63
8:I:321:LEU:HD21	8:I:425:MET:HG2	1.81	0.63
8:I:330:LEU:HD11	8:I:422:TYR:HB2	1.79	0.63
12:N:501:ILE:H	12:N:501:ILE:HD12	1.62	0.63
15:R:208:LEU:CD1	15:R:255:VAL:CG2	2.77	0.63
6:H:478:SER:HA	6:H:633:ARG:HH22	1.63	0.62
13:O:114:ASP:C	13:O:117:ASP:OD1	2.37	0.62
13:O:119:PHE:HE1	13:O:136:LEU:HD21	1.63	0.62
14:Q:208:LEU:CD1	14:Q:255:VAL:CG2	2.77	0.62
17:X:77:TYR:N	17:X:106:GLN:HE21	1.97	0.62
17:X:100:TYR:CD1	17:X:138:VAL:HG13	2.34	0.62
17:X:203:LEU:HD22	17:Y:55:LEU:HB3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Y:452:LEU:HB3	17:Y:461:ALA:HB2	1.81	0.62
8:I:32:ARG:CD	12:N:388:HIS:CE1	2.82	0.62
9:K:429:LEU:HA	9:K:432:ILE:HG22	1.82	0.62
3:P:475:LYS:O	3:P:479:GLN:NE2	2.32	0.62
16:S:21:GLU:C	16:S:45:LEU:HD13	2.18	0.62
16:S:70:THR:O	16:S:74:PRO:HD3	1.98	0.62
1:A:1604:GLN:O	1:A:1607:ARG:HB2	1.99	0.62
8:I:17:LYS:CE	8:I:51:SER:O	2.47	0.62
15:R:95:LEU:HB2	15:R:130:ILE:HD11	1.80	0.62
15:R:192:TRP:CD2	15:R:198:LEU:HD13	2.35	0.62
1:A:1227:LEU:O	1:A:1230:ILE:HG22	1.98	0.62
3:C:341:TYR:OH	11:M:25:PRO:HD3	2.00	0.62
8:I:231:VAL:HG21	8:I:557:TYR:CE1	2.34	0.62
8:I:310:TRP:HB2	8:I:313:ALA:CA	2.29	0.62
8:I:489:PRO:HB2	8:I:490:PRO:C	2.19	0.62
9:K:19:TYR:CD1	9:K:49:LEU:HD13	2.35	0.62
9:K:292:VAL:HG21	11:M:57:TRP:HB3	1.81	0.62
10:L:148:GLY:HA2	16:S:270:SER:HB3	1.79	0.62
12:N:180:PHE:HD1	12:N:299:TRP:CZ3	2.08	0.62
3:P:358:LEU:O	3:P:362:PRO:HA	1.98	0.62
1:A:1351:GLN:O	10:L:42:VAL:HG21	2.00	0.62
9:J:271:HIS:O	9:J:274:THR:HG22	2.00	0.62
9:K:514:PHE:CE2	7:W:11:LEU:HD13	2.34	0.62
10:L:126:ASP:HB2	10:L:132:THR:HG23	1.78	0.62
12:N:619:LEU:HG	12:N:637:TRP:CH2	2.34	0.62
17:X:437:LEU:HB2	17:X:444:LEU:HD11	1.82	0.62
1:A:126:ALA:HA	1:A:152:CYS:O	1.99	0.62
1:A:1677:LEU:HD21	1:A:1687:LEU:HG	1.81	0.62
6:F:89:GLU:OE2	6:F:125:TYR:HE1	1.82	0.62
6:F:500:TRP:HB3	6:H:30:ARG:HH22	1.65	0.62
9:J:520:GLY:O	9:J:523:ILE:HG22	1.99	0.62
16:S:22:TRP:HZ3	16:S:41:LEU:HD12	1.64	0.62
17:Y:196:LEU:O	17:Y:200:PRO:HA	1.99	0.62
17:Y:366:ILE:HD11	17:Y:379:LYS:CD	2.29	0.62
1:A:1555:HIS:O	1:A:1559:HIS:HD2	1.82	0.62
16:S:83:SER:O	16:S:87:GLN:CG	2.47	0.62
17:X:304:LEU:O	17:X:308:MET:HG2	1.99	0.62
1:A:1196:TYR:HB3	1:A:1208:LEU:HD11	1.80	0.62
2:B:16:TRP:CB	2:B:33:CYS:HB3	2.29	0.62
2:B:16:TRP:CE2	2:B:44:CYS:N	2.67	0.62
3:C:434:ARG:HD3	15:R:80:ILE:HG21	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:306:HIS:CG	8:I:313:ALA:HB1	2.34	0.62
9:J:476:PRO:HB3	3:P:182:LEU:HB3	1.82	0.62
1:A:183:THR:HG22	1:A:249:LEU:HG	1.82	0.62
3:C:358:LEU:O	3:C:362:PRO:HA	1.99	0.62
6:H:146:PRO:HG3	6:H:167:THR:HA	1.82	0.62
18:Z:157:THR:OG1	18:Z:158:ASP:N	2.33	0.62
2:B:16:TRP:HD1	2:B:33:CYS:CA	2.04	0.62
3:C:279:ILE:HD11	15:R:76:GLY:O	2.00	0.62
9:J:77:ALA:CB	9:J:93:LEU:HD11	2.29	0.62
9:J:77:ALA:HB1	9:J:93:LEU:HD11	1.81	0.62
1:A:95:VAL:HG22	1:A:100:VAL:HG22	1.81	0.61
6:F:729:LEU:HD13	6:F:739:VAL:HG22	1.81	0.61
8:I:413:ASN:ND2	8:I:450:GLU:OE1	2.33	0.61
9:K:62:SER:C	9:K:63:ARG:HG3	2.19	0.61
16:S:19:GLY:HA2	16:S:22:TRP:HD1	1.65	0.61
1:A:1867:CYS:HB2	1:A:1881:GLN:NE2	2.16	0.61
9:J:445:GLU:HG2	9:J:446:PRO:CD	2.29	0.61
12:N:281:TYR:CZ	12:N:357:ALA:HA	2.35	0.61
12:N:503:SER:O	12:N:507:SER:HB3	1.99	0.61
6:F:146:PRO:HG3	6:F:167:THR:HA	1.82	0.61
8:I:334:GLY:HA2	8:I:418:PHE:CD2	2.36	0.61
12:N:626:TYR:HD2	12:N:633:ARG:HB3	1.63	0.61
13:O:222:LEU:O	13:O:226:ASP:O	2.19	0.61
3:P:344:ARG:NH2	3:P:346:GLN:OE1	2.33	0.61
14:Q:410:HIS:CB	14:Q:475:LEU:HD21	2.22	0.61
17:Y:45:ALA:CB	17:Y:82:TYR:CE2	2.83	0.61
18:Z:39:PRO:O	18:Z:42:THR:HB	1.99	0.61
1:A:1791:ILE:HB	13:O:598:THR:CG2	2.30	0.61
2:B:27:ARG:CD	12:N:813:GLY:HA2	2.29	0.61
16:S:82:ILE:HD13	16:S:102:LEU:CD2	2.29	0.61
17:Y:462:LYS:HG2	17:Y:485:LEU:CD1	2.30	0.61
1:A:844:ILE:O	1:A:848:VAL:HG23	2.00	0.61
1:A:1380:ASN:HD22	1:A:1383:ILE:HD12	1.65	0.61
6:H:515:TYR:HE2	6:H:545:HIS:CD2	2.19	0.61
14:Q:192:TRP:CD2	14:Q:198:LEU:HD13	2.35	0.61
15:R:98:GLU:HG2	15:R:101:PRO:HD3	1.79	0.61
1:A:39:LEU:HD23	1:A:39:LEU:H	1.64	0.61
8:I:56:TRP:CZ3	8:I:58:PHE:HB2	2.34	0.61
8:I:81:ALA:HA	8:I:92:LEU:HA	1.83	0.61
8:I:295:ASN:O	8:I:316:GLU:CD	2.39	0.61
9:K:222:GLU:OE1	9:K:228:GLN:NE2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:529:ASP:O	13:O:532:VAL:HG12	1.99	0.61
1:A:1274:LEU:HG	1:A:1302:LEU:HD11	1.81	0.61
12:N:73:GLU:O	12:N:74:TRP:HB3	2.01	0.61
12:N:362:LYS:HA	12:N:410:LEU:CD2	2.29	0.61
12:N:456:GLY:HA2	12:N:548:ARG:HH21	1.65	0.61
15:R:225:PRO:CD	16:S:166:GLU:O	2.46	0.61
16:S:36:ARG:HH11	16:S:90:PRO:CB	2.11	0.61
9:J:185:LEU:HD11	9:J:205:PHE:CB	2.31	0.61
12:N:331:PHE:CZ	12:N:335:ILE:HD11	2.36	0.61
13:O:354:ARG:HD2	13:O:573:LYS:O	2.01	0.61
16:S:25:SER:N	16:S:45:LEU:HD21	2.15	0.61
3:C:344:ARG:HH21	11:M:25:PRO:CG	2.10	0.61
12:N:769:SER:OG	12:N:772:ARG:CD	2.49	0.61
3:C:344:ARG:NH2	11:M:25:PRO:HG2	2.07	0.61
3:C:414:MET:CG	13:O:330:ILE:CD1	2.77	0.61
12:N:560:MET:CE	12:N:560:MET:HA	2.31	0.61
3:P:94:PHE:O	3:P:97:LYS:HB2	2.01	0.61
16:S:19:GLY:HA2	16:S:22:TRP:CD1	2.35	0.61
17:Y:77:TYR:HB2	17:Y:106:GLN:HG3	1.83	0.61
1:A:1137:PHE:O	1:A:1141:VAL:HG23	2.01	0.60
6:F:699:ASP:HB2	6:F:702:ASN:HD21	1.66	0.60
9:J:37:PRO:HA	9:J:65:LEU:HD11	1.82	0.60
12:N:351:PHE:HE1	12:N:405:LYS:HB2	1.67	0.60
17:X:407:LEU:HD22	17:X:437:LEU:HD21	1.83	0.60
1:A:662:THR:O	1:A:666:ASN:ND2	2.33	0.60
13:O:114:ASP:HA	13:O:117:ASP:OD1	2.00	0.60
14:Q:411:TYR:CE1	14:Q:475:LEU:HD23	2.36	0.60
16:S:58:GLN:CG	16:S:62:PHE:HE2	1.94	0.60
3:P:170:PHE:O	3:P:173:TYR:N	2.33	0.60
14:Q:475:LEU:O	14:Q:476:ASP:CB	2.48	0.60
16:S:22:TRP:CZ3	16:S:41:LEU:HD12	2.36	0.60
13:O:75:LEU:C	13:O:79:TYR:CD2	2.75	0.60
14:Q:127:GLU:O	18:Z:159:LYS:HG2	2.01	0.60
14:Q:341:GLY:O	14:Q:343:GLY:N	2.35	0.60
17:Y:304:LEU:O	17:Y:308:MET:HG2	2.01	0.60
1:A:1640:GLY:N	1:A:1645:GLU:O	2.29	0.60
3:C:94:PHE:O	3:C:97:LYS:HB2	2.01	0.60
8:I:311:GLY:C	8:I:428:MET:SD	2.79	0.60
16:S:41:LEU:CD1	18:Z:141:PHE:CB	2.80	0.60
9:J:167:PHE:HA	9:J:170:LEU:CD2	2.31	0.60
12:N:362:LYS:CA	12:N:410:LEU:HD21	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:R:116:TRP:O	15:R:120:LEU:N	2.32	0.60
15:R:295:VAL:HG23	16:S:274:VAL:HG23	1.84	0.60
6:F:528:ILE:HG22	6:F:529:GLU:HG3	1.82	0.60
17:X:279:ASP:OD1	17:X:310:VAL:HG21	2.00	0.60
17:Y:83:HIS:O	17:Y:86:SER:OG	2.16	0.60
1:A:1153:ILE:HG12	1:A:1184:HIS:CD2	2.37	0.60
2:B:16:TRP:CZ2	2:B:45:PRO:CA	2.85	0.60
6:H:528:ILE:HG22	6:H:529:GLU:HG3	1.82	0.60
12:N:676:TRP:O	12:N:713:PHE:HB2	2.01	0.60
14:Q:140:ALA:O	14:Q:141:PRO:CB	2.49	0.60
1:A:39:LEU:HD12	13:O:248:PRO:HB3	1.84	0.59
9:K:74:TYR:CZ	9:K:78:ARG:HD2	2.37	0.59
16:S:78:TRP:CZ3	16:S:105:ALA:CA	2.85	0.59
1:A:1218:GLY:N	1:A:1259:LEU:O	2.35	0.59
7:G:3:ARG:HB2	9:J:443:LYS:NZ	2.17	0.59
6:H:594:ILE:HD11	6:H:604:TYR:HA	1.84	0.59
8:I:304:PHE:CE2	8:I:452:LEU:HG	2.37	0.59
9:J:17:GLN:CB	9:K:78:ARG:HH12	2.15	0.59
13:O:619:LEU:O	13:O:623:THR:HG22	2.02	0.59
16:S:19:GLY:N	18:Z:134:GLN:HE22	1.97	0.59
8:I:302:ASP:O	8:I:306:HIS:HB2	2.03	0.59
12:N:77:GLU:O	12:N:78:VAL:HG23	2.03	0.59
3:P:389:ARG:O	3:P:392:ILE:HG23	2.02	0.59
17:X:83:HIS:O	17:X:86:SER:OG	2.15	0.59
1:A:1274:LEU:O	1:A:1277:ILE:HG22	2.01	0.59
3:C:145:GLN:HG3	13:O:246:PHE:CD2	2.38	0.59
6:H:73:TYR:CD1	6:H:117:THR:HG22	2.37	0.59
12:N:180:PHE:CD1	12:N:299:TRP:HH2	2.20	0.59
12:N:619:LEU:HG	12:N:637:TRP:CZ2	2.37	0.59
13:O:417:LEU:HA	13:O:420:ILE:CG2	2.32	0.59
16:S:71:GLY:O	16:S:74:PRO:C	2.40	0.59
1:A:1255:VAL:HG11	1:A:1606:LEU:HD21	1.84	0.59
3:C:377:GLU:HA	15:R:130:ILE:CG2	2.33	0.59
8:I:290:PHE:CZ	8:I:325:LEU:HB2	2.37	0.59
1:A:485:ILE:CD1	1:A:609:ILE:HB	2.32	0.59
8:I:334:GLY:HA2	8:I:418:PHE:CE2	2.38	0.59
12:N:609:LEU:HD22	12:N:639:HIS:CD2	2.38	0.59
8:I:32:ARG:HB2	8:I:34:LEU:CD2	2.33	0.59
8:I:337:ILE:HG22	8:I:341:TYR:HE2	1.65	0.59
8:I:337:ILE:HD13	8:I:418:PHE:HZ	1.68	0.59
12:N:341:ILE:O	12:N:344:LEU:HB3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:R:341:GLY:O	15:R:343:GLY:N	2.35	0.59
17:X:229:THR:HG21	17:X:233:LEU:HD12	1.84	0.59
1:A:23:PHE:HB2	1:A:111:LEU:HD22	1.83	0.59
3:C:317:SER:CB	11:M:27:GLU:HG3	2.32	0.59
8:I:17:LYS:NZ	8:I:51:SER:O	2.35	0.59
8:I:299:SER:O	8:I:303:GLU:HG3	2.02	0.59
9:K:403:PHE:O	9:K:407:GLU:HG2	2.02	0.59
10:L:125:THR:HA	10:L:126:ASP:HB3	1.84	0.59
17:Y:434:TYR:HA	17:Y:444:LEU:HD13	1.84	0.59
6:H:656:MET:HE1	9:K:526:TYR:CD2	2.37	0.59
3:P:234:LEU:HD22	3:P:238:TYR:CE2	2.38	0.59
3:P:389:ARG:HA	3:P:392:ILE:CG2	2.32	0.59
16:S:84:TRP:CE2	16:S:88:ASN:OD1	2.55	0.59
1:A:1167:GLU:O	1:A:1168:LEU:HB3	2.03	0.59
2:B:46:LEU:HD23	2:B:47:VAL:N	2.17	0.59
10:L:108:ILE:HB	10:L:125:THR:O	2.03	0.59
17:Y:229:THR:HG21	17:Y:233:LEU:HD12	1.84	0.59
8:I:65:GLY:HA3	8:I:84:LEU:HB3	1.85	0.58
1:A:1194:HIS:HB2	15:R:121:ASN:HD21	1.69	0.58
2:B:64:LEU:HD22	2:B:71:GLN:HA	1.85	0.58
1:A:1060:HIS:O	1:A:1063:ILE:HG22	2.03	0.58
1:A:1599:ASN:HB2	1:A:1603:LEU:HA	1.85	0.58
9:J:193:LEU:O	9:J:197:GLU:HB2	2.03	0.58
9:J:211:LYS:O	9:J:212:TYR:CG	2.55	0.58
3:P:358:LEU:HD11	3:P:368:TRP:CZ2	2.38	0.58
14:Q:222:MET:HB3	14:Q:227:GLU:HG3	1.85	0.58
1:A:880:TYR:O	1:A:926:LEU:HD21	2.02	0.58
3:C:389:ARG:HG3	13:O:280:ARG:HD3	1.85	0.58
6:F:152:PHE:HE1	6:F:162:PRO:HG2	1.69	0.58
8:I:420:TRP:CD1	8:I:440:MET:HE2	2.38	0.58
12:N:148:GLY:HA3	12:N:152:GLU:OE2	2.03	0.58
12:N:520:ARG:HG3	12:N:557:CYS:SG	2.43	0.58
13:O:591:TYR:HA	13:O:594:SER:OG	2.03	0.58
3:P:120:TYR:CZ	3:P:124:LEU:HD11	2.39	0.58
16:S:20:ASP:OD2	18:Z:184:ARG:NH1	2.35	0.58
1:A:436:LEU:H	1:A:501:THR:HG23	1.68	0.58
1:A:1230:ILE:HD12	15:R:116:TRP:CD1	2.39	0.58
9:K:77:ALA:HB1	9:K:93:LEU:HD11	1.85	0.58
13:O:328:ILE:O	13:O:332:GLN:HG3	2.03	0.58
3:P:290:ARG:HH21	3:P:319:LEU:CD1	2.14	0.58
17:Y:45:ALA:HB2	17:Y:82:TYR:CD2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Y:384:ARG:HH22	17:Y:415:GLU:HB3	1.67	0.58
1:A:1404:LEU:HD22	1:A:1464:ILE:HD11	1.85	0.58
2:B:27:ARG:HB2	12:N:810:TYR:HE2	1.67	0.58
3:C:317:SER:HB3	11:M:27:GLU:HG3	1.84	0.58
8:I:413:ASN:O	8:I:447:PHE:CE1	2.52	0.58
9:K:78:ARG:HG3	9:K:135:LEU:HD22	1.84	0.58
17:X:475:TYR:O	17:X:479:VAL:HG23	2.04	0.58
3:C:389:ARG:CG	13:O:280:ARG:HD3	2.34	0.58
6:H:761:SER:O	6:H:765:ASP:CB	2.52	0.58
8:I:500:PHE:CE2	8:I:507:LEU:HD12	2.37	0.58
12:N:278:ARG:HB3	12:N:343:GLU:OE2	2.04	0.58
12:N:699:TRP:CZ3	12:N:728:VAL:HG21	2.39	0.58
17:Y:407:LEU:HD22	17:Y:437:LEU:HD21	1.86	0.58
1:A:1376:LEU:HD23	1:A:1377:LYS:HG3	1.86	0.58
1:A:1405:LEU:HD13	1:A:1467:GLY:CA	2.33	0.58
2:B:27:ARG:HD2	12:N:813:GLY:HA2	1.83	0.58
9:K:386:LEU:H	9:K:386:LEU:HD12	1.68	0.58
14:Q:208:LEU:HD11	14:Q:255:VAL:HG23	1.86	0.58
16:S:99:SER:HB2	16:S:131:LEU:HD13	1.85	0.58
17:Y:437:LEU:HB2	17:Y:444:LEU:HD11	1.86	0.58
8:I:430:GLU:CD	14:Q:429:LYS:HG2	2.24	0.58
9:J:185:LEU:HD11	9:J:205:PHE:HB3	1.86	0.58
3:P:400:ARG:HG3	14:Q:498:ILE:HB	1.85	0.58
3:C:414:MET:HB3	13:O:326:GLU:HB3	1.85	0.57
6:F:26:PHE:CD1	6:H:149:TRP:HB2	2.38	0.57
9:J:178:ALA:HB1	9:J:213:ASN:HD22	1.69	0.57
9:K:355:ALA:O	9:K:359:THR:HG22	2.04	0.57
12:N:300:LEU:O	12:N:304:PHE:HD1	1.87	0.57
17:Y:294:PHE:CD1	17:Y:294:PHE:O	2.57	0.57
6:H:42:PHE:HB2	6:H:71:CYS:SG	2.43	0.57
9:J:219:VAL:C	9:J:221:PRO:HD3	2.24	0.57
12:N:612:PRO:HG2	12:N:615:ILE:HG12	1.85	0.57
12:N:704:VAL:HA	12:N:719:GLU:CD	2.25	0.57
16:S:30:GLN:HB2	16:S:91:GLN:CA	2.33	0.57
17:Y:96:ALA:O	17:Y:100:TYR:HD2	1.86	0.57
9:K:406:HIS:CE1	7:W:6:PRO:HB3	2.39	0.57
10:L:63:LEU:HD13	10:L:138:GLN:NE2	2.18	0.57
13:O:75:LEU:HD21	13:O:161:TYR:HE2	1.62	0.57
3:P:61:SER:HB2	3:P:262:SER:HB2	1.85	0.57
3:P:251:TYR:HB3	3:P:269:ILE:HD11	1.85	0.57
3:P:409:TYR:HA	3:P:412:LEU:HD12	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:R:222:MET:HB3	15:R:227:GLU:HG3	1.86	0.57
1:A:214:LEU:HD21	1:A:407:LEU:HD13	1.87	0.57
1:A:961:HIS:ND1	1:A:964:GLU:OE2	2.37	0.57
3:C:170:PHE:O	3:C:173:TYR:N	2.38	0.57
6:F:544:TRP:CD2	15:R:499:ARG:HD3	2.40	0.57
8:I:27:VAL:C	8:I:35:ILE:HD12	2.25	0.57
12:N:386:LEU:C	12:N:388:HIS:HB3	2.25	0.57
13:O:414:LEU:CD1	13:O:417:LEU:HB2	2.35	0.57
6:H:621:LEU:HB3	6:H:625:ARG:NH2	2.20	0.57
8:I:36:ALA:CB	8:I:80:LEU:HD21	2.35	0.57
6:F:533:VAL:HG13	6:F:568:GLU:OE1	2.03	0.57
8:I:730:VAL:HG22	8:I:731:SER:N	2.19	0.57
16:S:68:PHE:CE2	16:S:81:TYR:CG	2.88	0.57
17:X:55:LEU:HB3	17:Y:203:LEU:HD12	1.86	0.57
17:X:462:LYS:HG2	17:X:485:LEU:CD1	2.31	0.57
1:A:629:LEU:HD22	1:A:633:ILE:HG22	1.86	0.57
2:B:47:VAL:HG11	2:B:60:ILE:HG21	1.85	0.57
3:C:352:LEU:HD21	3:C:356:ARG:CZ	2.35	0.57
3:C:358:LEU:HD21	3:C:368:TRP:CE2	2.40	0.57
8:I:413:ASN:CA	8:I:447:PHE:HZ	1.93	0.57
16:S:29:VAL:CG1	16:S:36:ARG:HH12	2.08	0.57
16:S:60:ARG:O	16:S:64:TYR:HD2	1.88	0.57
17:X:170:LYS:HA	17:Y:49:LEU:HD21	1.86	0.57
18:Z:146:GLU:H	18:Z:146:GLU:CD	2.08	0.57
1:A:215:HIS:CD2	1:A:217:LEU:H	2.23	0.57
3:C:120:TYR:CZ	3:C:124:LEU:HD11	2.40	0.57
8:I:56:TRP:CD2	8:I:98:PRO:HB3	2.38	0.57
12:N:765:LEU:HD11	16:S:200:VAL:HG23	1.87	0.57
16:S:68:PHE:HZ	16:S:81:TYR:HB3	1.69	0.57
6:H:121:LEU:O	6:H:125:TYR:HD1	1.87	0.57
13:O:105:LEU:HD11	13:O:151:VAL:CG1	2.35	0.57
17:Y:475:TYR:O	17:Y:479:VAL:HG23	2.03	0.57
9:J:397:ILE:HG22	9:J:398:ALA:N	2.19	0.57
9:K:296:PRO:HB2	11:M:55:MET:HG3	1.86	0.57
12:N:663:GLN:HB3	12:N:699:TRP:CZ2	2.40	0.57
3:P:244:ILE:C	3:P:244:ILE:HD12	2.26	0.57
16:S:79:ASP:OD2	16:S:120:ARG:CA	2.52	0.57
16:S:145:GLN:NE2	16:S:296:ILE:CB	2.68	0.57
1:A:92:GLU:OE2	1:A:111:LEU:HD21	2.05	0.56
1:A:257:MET:CE	1:A:266:HIS:HB3	2.35	0.56
1:A:1033:ARG:NH1	1:A:1531:GLY:O	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1290:ASP:OD2	1:A:1600:ARG:HA	2.05	0.56
1:A:1532:ASN:HB3	1:A:1535:VAL:HG23	1.86	0.56
2:B:46:LEU:HD21	2:B:54:CYS:HB3	1.86	0.56
6:F:42:PHE:HB2	6:F:71:CYS:SG	2.44	0.56
8:I:276:TRP:NE1	8:I:475:VAL:HB	2.20	0.56
13:O:75:LEU:CB	13:O:79:TYR:HE2	2.18	0.56
15:R:247:SER:HB2	16:S:170:LYS:HZ1	1.69	0.56
16:S:68:PHE:HE1	16:S:78:TRP:CD2	2.23	0.56
1:A:1332:GLY:C	1:A:1358:ILE:HD12	2.21	0.56
6:H:669:SER:HA	6:H:698:ILE:HD11	1.86	0.56
9:J:247:PHE:CD2	9:J:277:GLU:HB3	2.40	0.56
9:J:324:SER:O	9:J:328:THR:HG23	2.05	0.56
12:N:596:LEU:HB3	12:N:601:TRP:NE1	2.19	0.56
13:O:599:ILE:O	13:O:602:PRO:HD2	2.05	0.56
13:O:727:THR:O	13:O:730:ARG:HB2	2.05	0.56
14:Q:208:LEU:HD11	14:Q:255:VAL:CG2	2.35	0.56
1:A:1057:LEU:HA	1:A:1061:GLU:OE1	2.04	0.56
1:A:1086:MET:HG2	1:A:1610:TYR:CZ	2.40	0.56
1:A:1163:PRO:HG3	1:A:1169:ALA:HA	1.86	0.56
1:A:1235:LEU:HD22	1:A:1257:ILE:HG13	1.79	0.56
1:A:1254:VAL:CG1	1:A:1298:ALA:HA	2.36	0.56
3:C:363:ARG:HG2	3:C:363:ARG:O	2.05	0.56
6:F:125:TYR:HD1	6:F:130:ARG:HE	1.49	0.56
8:I:34:LEU:HD13	12:N:389:PRO:O	2.05	0.56
8:I:277:GLU:O	8:I:281:MET:N	2.32	0.56
9:K:472:LEU:HG	9:K:481:THR:CG2	2.33	0.56
12:N:386:LEU:HD21	12:N:399:LEU:HD22	1.86	0.56
12:N:501:ILE:HD12	12:N:501:ILE:N	2.20	0.56
14:Q:410:HIS:CG	14:Q:475:LEU:HD11	2.40	0.56
15:R:208:LEU:HD11	15:R:255:VAL:HG23	1.87	0.56
16:S:88:ASN:HD22	16:S:88:ASN:N	2.02	0.56
17:X:54:ARG:NH2	17:X:90:ASP:OD2	2.39	0.56
12:N:202:GLU:OE2	12:N:283:ARG:HB2	2.05	0.56
12:N:648:VAL:HG13	12:N:650:LEU:HG	1.86	0.56
15:R:225:PRO:HG2	16:S:166:GLU:HB2	1.86	0.56
16:S:132:CYS:CB	16:S:135:PRO:N	2.68	0.56
17:X:66:ASN:HD21	17:Y:268:ARG:HB3	1.71	0.56
8:I:218:SER:HA	8:I:235:GLN:HA	1.88	0.56
9:J:451:LEU:HD12	9:J:467:TYR:CD2	2.40	0.56
12:N:344:LEU:HA	12:N:347:ILE:HB	1.87	0.56
15:R:98:GLU:HB3	15:R:101:PRO:HD3	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:R:208:LEU:HD11	15:R:255:VAL:CG2	2.35	0.56
16:S:38:MET:HB3	18:Z:181:VAL:HG22	1.87	0.56
16:S:271:ARG:HG2	16:S:272:ILE:N	2.21	0.56
17:X:442:GLN:NE2	17:X:472:ARG:CG	2.68	0.56
3:C:89:LEU:HD12	3:P:60:PHE:CG	2.40	0.56
3:C:97:LYS:HG2	3:C:97:LYS:O	2.06	0.56
8:I:269:LEU:CB	8:I:526:LYS:NZ	2.69	0.56
12:N:556:PHE:HA	12:N:600:PHE:CE1	2.41	0.56
13:O:627:LEU:O	13:O:630:ALA:HB3	2.06	0.56
14:Q:216:ILE:HD13	16:S:558:LEU:HB2	1.87	0.56
16:S:68:PHE:CE1	16:S:78:TRP:CD2	2.93	0.56
17:Y:70:LEU:HD12	17:Y:71:PHE:CE2	2.40	0.56
1:A:105:GLY:O	1:A:111:LEU:HG	2.06	0.56
3:C:148:ASN:HB3	3:C:151:LEU:CG	2.34	0.56
12:N:592:TYR:HD1	12:N:593:ALA:N	2.04	0.56
14:Q:146:ASN:C	14:Q:420:PHE:CE1	2.79	0.56
17:X:350:PHE:HB2	17:X:351:TYR:CD1	2.41	0.56
17:Y:350:PHE:HB2	17:Y:351:TYR:CD1	2.40	0.56
1:A:167:LYS:HG2	13:O:319:GLN:HE22	1.70	0.56
1:A:1632:ALA:H	1:A:1653:ALA:HB3	1.70	0.56
6:F:73:TYR:CD1	6:F:117:THR:HG22	2.41	0.56
8:I:231:VAL:HG11	8:I:556:LEU:HD12	1.88	0.56
12:N:704:VAL:HG23	12:N:705:LEU:HD22	1.86	0.56
13:O:104:GLU:N	13:O:107:ASP:OD2	2.39	0.56
15:R:74:PRO:CB	15:R:75:GLY:HA2	2.36	0.56
17:Y:199:CYS:HB3	17:Y:201:LEU:HD12	1.87	0.56
17:Y:475:TYR:CE1	17:Y:477:LYS:HB2	2.41	0.56
2:B:64:LEU:HD11	2:B:80:TRP:CD1	2.41	0.56
3:C:301:ASP:OD2	3:C:335:CYS:HB3	2.06	0.56
4:D:3:THR:O	4:D:5:PHE:CE2	2.58	0.56
8:I:262:LEU:HA	8:I:265:ILE:CG2	2.32	0.56
9:J:212:TYR:HB3	9:J:243:TYR:CD1	2.41	0.56
12:N:502:ILE:HA	12:N:505:LEU:HD12	1.88	0.56
16:S:76:ASP:O	16:S:77:VAL:HB	2.06	0.56
17:X:475:TYR:CE1	17:X:477:LYS:HB2	2.41	0.56
17:Y:100:TYR:HB3	17:Y:142:MET:CG	2.35	0.56
2:B:45:PRO:HB2	12:N:631:ALA:HB3	1.87	0.56
3:C:407:GLN:O	3:C:411:ILE:HG12	2.06	0.56
16:S:41:LEU:CD2	16:S:90:PRO:HB3	2.36	0.56
8:I:167:LEU:HD12	8:I:168:LEU:N	2.21	0.55
9:J:465:LEU:CA	9:J:488:ILE:HD12	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:S:68:PHE:CZ	16:S:81:TYR:CG	2.93	0.55
17:X:63:MET:CE	17:Y:266:LEU:HD22	2.35	0.55
17:X:100:TYR:HD1	17:X:138:VAL:HG13	1.70	0.55
17:X:168:THR:HB	17:X:169:PRO:HD2	1.88	0.55
17:Y:50:HIS:ND1	17:Y:86:SER:HA	2.21	0.55
17:Y:168:THR:HB	17:Y:169:PRO:HD2	1.88	0.55
6:H:121:LEU:O	6:H:125:TYR:CD1	2.59	0.55
8:I:291:VAL:HG13	8:I:303:GLU:OE2	2.07	0.55
13:O:394:THR:HG22	13:O:615:ARG:HH12	1.70	0.55
13:O:490:LEU:HD13	13:O:511:ASP:HB2	1.86	0.55
15:R:105:GLN:C	15:R:107:PRO:HD3	2.26	0.55
17:Y:294:PHE:C	17:Y:294:PHE:HD1	2.10	0.55
1:A:1047:VAL:O	1:A:1109:GLY:HA2	2.06	0.55
1:A:1332:GLY:H	1:A:1358:ILE:HB	1.71	0.55
1:A:1399:VAL:CG1	1:A:1404:LEU:HG	2.36	0.55
1:A:1839:PHE:CE1	1:A:1840:MET:HG3	2.41	0.55
6:F:104:ASP:N	6:F:104:ASP:OD1	2.39	0.55
8:I:64:THR:HG22	8:I:84:LEU:HD11	1.87	0.55
12:N:281:TYR:OH	12:N:357:ALA:HA	2.06	0.55
3:P:441:GLU:HG3	3:P:472:LYS:NZ	2.21	0.55
16:S:22:TRP:CZ3	16:S:41:LEU:CD1	2.86	0.55
1:A:1573:SER:HB2	1:A:1617:ARG:NH2	2.22	0.55
1:A:1786:MET:HA	1:A:1786:MET:HE2	1.89	0.55
6:F:730:LYS:HE2	6:F:740:TYR:CE1	2.38	0.55
8:I:306:HIS:CE1	8:I:316:GLU:HB3	2.41	0.55
9:K:284:LEU:HD13	9:K:308:TYR:HB2	1.88	0.55
14:Q:128:ALA:HB1	18:Z:156:TYR:CE2	2.39	0.55
14:Q:352:THR:HB	18:Z:51:LEU:HA	1.88	0.55
16:S:64:TYR:O	16:S:68:PHE:HD2	1.86	0.55
17:X:76:LYS:CB	17:X:106:GLN:NE2	2.69	0.55
17:Y:203:LEU:HA	17:Y:206:ILE:HD12	1.89	0.55
1:A:1351:GLN:O	10:L:32:SER:HA	2.07	0.55
3:P:407:GLN:O	3:P:411:ILE:HG12	2.06	0.55
16:S:60:ARG:O	16:S:64:TYR:CD2	2.60	0.55
8:I:430:GLU:OE2	14:Q:429:LYS:HB3	2.06	0.55
8:I:497:TRP:CH2	8:I:507:LEU:HD13	2.42	0.55
12:N:676:TRP:HE3	12:N:680:GLU:HB3	1.70	0.55
3:P:180:ARG:HG3	3:P:212:LEU:HD21	1.89	0.55
3:P:441:GLU:HG3	3:P:472:LYS:CE	2.37	0.55
14:Q:185:TYR:CE1	16:S:27:GLU:CG	2.87	0.55
15:R:98:GLU:CG	15:R:101:PRO:CD	2.76	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:52:ASN:HD22	17:Y:202:ALA:CB	2.19	0.55
1:A:1054:TYR:O	1:A:1056:GLU:N	2.40	0.55
1:A:1624:VAL:HG22	1:A:1698:TYR:CD2	2.38	0.55
2:B:42:ASP:O	2:B:43:ASP:HB2	2.07	0.55
8:I:52:PHE:CD1	8:I:743:VAL:HG21	2.42	0.55
8:I:305:MET:CB	13:O:61:ASN:HD21	2.20	0.55
13:O:163:GLN:HB3	13:O:167:LYS:HE3	1.88	0.55
13:O:219:GLN:HE22	13:O:231:LEU:HD13	1.70	0.55
16:S:22:TRP:CZ2	16:S:38:MET:O	2.59	0.55
16:S:79:ASP:OD2	16:S:120:ARG:HA	2.06	0.55
1:A:809:ASP:O	1:A:1807:GLU:O	2.24	0.55
1:A:1531:GLY:HA3	1:A:1566:PHE:CE1	2.42	0.55
6:F:699:ASP:HB3	6:F:702:ASN:OD1	2.06	0.55
9:J:337:TRP:HB3	9:J:360:ALA:HB2	1.88	0.55
13:O:105:LEU:HD11	13:O:151:VAL:HG12	1.89	0.55
13:O:439:LEU:HG	13:O:476:LEU:HD13	1.89	0.55
3:C:259:PHE:HB3	3:C:265:ILE:HD12	1.84	0.55
6:F:594:ILE:HD11	6:F:604:TYR:HA	1.88	0.55
8:I:166:LYS:O	8:I:170:ASP:HB2	2.06	0.55
12:N:165:THR:H	12:N:166:PRO:HA	1.71	0.55
13:O:657:ILE:HA	13:O:660:LYS:HB2	1.89	0.55
17:Y:100:TYR:HD1	17:Y:138:VAL:HG13	1.72	0.55
8:I:213:ASP:OD1	8:I:215:LYS:N	2.24	0.55
9:K:258:MET:HG3	9:K:271:HIS:CD2	2.42	0.55
10:L:75:LYS:HB2	10:L:161:PRO:HG3	1.89	0.55
12:N:520:ARG:HD2	12:N:556:PHE:HD1	1.69	0.55
16:S:68:PHE:CE1	16:S:78:TRP:HA	2.42	0.55
17:X:203:LEU:HA	17:X:206:ILE:HD12	1.89	0.55
1:A:1323:GLU:HG3	1:A:1324:GLN:N	2.22	0.54
1:A:1603:LEU:HD22	1:A:1605:ALA:H	1.72	0.54
3:C:417:TYR:CD2	13:O:307:LEU:HD22	2.42	0.54
9:K:324:SER:O	9:K:328:THR:HG23	2.07	0.54
9:K:373:TYR:CE1	7:W:4:ARG:HG2	2.42	0.54
13:O:119:PHE:CE1	13:O:136:LEU:HD11	2.42	0.54
1:A:1610:TYR:O	1:A:1613:ALA:HB3	2.08	0.54
3:C:429:ARG:HG2	3:C:432:ASP:HB2	1.88	0.54
8:I:46:LEU:HD22	8:I:56:TRP:NE1	2.23	0.54
8:I:497:TRP:CD1	13:O:446:LEU:HB3	2.42	0.54
8:I:607:ILE:HD12	8:I:607:ILE:H	1.72	0.54
9:K:177:THR:HG22	9:K:365:LYS:HB3	1.87	0.54
12:N:681:LEU:HD22	12:N:713:PHE:CZ	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:373:HIS:NE2	14:Q:497:GLY:O	2.39	0.54
15:R:305:LEU:HD23	15:R:336:TRP:CD2	2.43	0.54
1:A:1079:ALA:HB1	1:A:1556:LEU:HA	1.89	0.54
3:C:526:TRP:HE1	3:C:556:LEU:HD23	1.72	0.54
14:Q:305:LEU:HD23	14:Q:336:TRP:CD2	2.42	0.54
15:R:225:PRO:CG	16:S:166:GLU:HB2	2.38	0.54
16:S:78:TRP:CH2	16:S:105:ALA:HA	2.43	0.54
1:A:1189:ALA:HB3	1:A:1192:ASN:HB2	1.89	0.54
2:B:72:HIS:ND1	2:B:77:ARG:HG3	2.21	0.54
3:C:60:PHE:HB2	3:P:89:LEU:HD12	1.90	0.54
8:I:23:ILE:HD12	8:I:37:LEU:HD23	1.88	0.54
8:I:79:LEU:HD11	8:I:168:LEU:HD23	1.88	0.54
12:N:670:PHE:CD1	12:N:715:VAL:HB	2.42	0.54
13:O:354:ARG:HD3	13:O:574:LEU:HA	1.89	0.54
15:R:225:PRO:HG2	16:S:166:GLU:HB3	1.89	0.54
17:X:267:LEU:CD1	17:Y:59:LEU:CD1	2.82	0.54
17:X:294:PHE:C	17:X:294:PHE:CD1	2.80	0.54
1:A:775:LEU:O	1:A:948:PRO:HD3	2.07	0.54
1:A:1037:VAL:HG22	1:A:1562:LEU:HD21	1.89	0.54
3:C:96:VAL:HG21	3:P:53:LYS:HD3	1.89	0.54
17:X:491:LYS:O	17:X:494:ASP:OD1	2.25	0.54
9:J:55:ARG:HD2	9:K:261:ASP:OD1	2.07	0.54
9:J:322:TYR:HE1	11:M:36:LEU:HD11	1.73	0.54
15:R:130:ILE:HG23	15:R:131:LEU:N	2.22	0.54
17:Y:491:LYS:O	17:Y:494:ASP:OD1	2.26	0.54
17:Y:517:ASP:O	17:Y:520:VAL:HG22	2.08	0.54
1:A:612:ILE:O	1:A:641:TRP:CZ3	2.61	0.54
8:I:344:ILE:O	8:I:348:VAL:HG23	2.07	0.54
9:J:277:GLU:OE1	9:J:278:LEU:HD23	2.07	0.54
9:J:406:HIS:HE1	9:J:450:ASN:HD22	1.55	0.54
17:X:394:ILE:HG22	17:X:397:ARG:NH2	2.23	0.54
17:X:517:ASP:O	17:X:520:VAL:HG22	2.08	0.54
6:F:30:ARG:NH2	6:H:500:TRP:HB3	2.22	0.54
8:I:413:ASN:N	8:I:447:PHE:HZ	2.06	0.54
9:J:476:PRO:HB2	3:P:148:ASN:HD21	1.72	0.54
9:K:484:ALA:O	9:K:488:ILE:HG12	2.08	0.54
12:N:395:ASP:HB2	12:N:397:ILE:N	2.18	0.54
13:O:75:LEU:C	13:O:79:TYR:HD2	2.09	0.54
1:A:457:PHE:HB3	1:A:468:PHE:CD1	2.43	0.54
1:A:1378:THR:HG23	1:A:1380:ASN:H	1.72	0.54
2:B:34:CYS:N	2:B:44:CYS:SG	2.79	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:39:VAL:N	2:B:40:PRO:CD	2.71	0.54
8:I:269:LEU:HB3	8:I:526:LYS:HZ2	1.73	0.54
8:I:278:GLU:HA	8:I:281:MET:HG2	1.88	0.54
8:I:287:LEU:HG	8:I:456:PHE:CE2	2.43	0.54
8:I:337:ILE:HD13	8:I:418:PHE:CZ	2.43	0.54
9:J:204:LEU:HD22	9:K:28:LYS:NZ	2.23	0.54
9:K:242:TYR:O	7:W:3:ARG:NH2	2.40	0.54
12:N:331:PHE:CE2	12:N:335:ILE:HD11	2.42	0.54
9:J:53:TYR:O	9:J:79:CYS:SG	2.66	0.54
9:K:71:ALA:HA	9:K:128:ILE:HD13	1.90	0.54
9:K:154:LYS:HE2	9:K:184:LEU:HD22	1.90	0.54
10:L:78:CYS:SG	10:L:119:TRP:CE3	3.01	0.54
12:N:368:THR:CB	12:N:369:ASP:HA	2.38	0.54
16:S:28:ASN:O	16:S:90:PRO:HG2	2.08	0.54
18:Z:30:SER:O	18:Z:34:GLN:HG3	2.08	0.54
1:A:1921:LEU:HA	12:N:78:VAL:HG21	1.90	0.53
6:F:15:ALA:HA	6:H:116:PHE:CE1	2.43	0.53
6:F:130:ARG:CG	17:Y:506:GLN:HB2	2.38	0.53
8:I:218:SER:OG	8:I:584:HIS:ND1	2.41	0.53
9:J:476:PRO:CG	3:P:182:LEU:HG	2.35	0.53
12:N:123:ASP:O	12:N:127:ARG:N	2.41	0.53
1:A:1636:VAL:HG12	1:A:1666:ILE:HG13	1.91	0.53
6:F:145:ASN:HB2	6:F:146:PRO:O	2.08	0.53
8:I:186:GLU:OE1	8:I:197:ARG:CZ	2.53	0.53
8:I:262:LEU:CA	8:I:265:ILE:HG22	2.34	0.53
13:O:68:LEU:HD23	13:O:131:VAL:HG12	1.89	0.53
1:A:45:ALA:O	3:C:180:ARG:NH2	2.42	0.53
1:A:1322:PRO:HG3	1:A:1375:TYR:HH	1.73	0.53
17:X:76:LYS:HB2	17:X:106:GLN:NE2	2.23	0.53
1:A:1797:ILE:HG22	1:A:1852:ILE:CD1	2.39	0.53
8:I:219:VAL:N	8:I:234:PHE:O	2.39	0.53
9:K:174:HIS:CE1	9:K:211:LYS:CD	2.90	0.53
14:Q:132:ARG:HG3	18:Z:154:LEU:HD23	1.90	0.53
17:Y:199:CYS:CB	17:Y:201:LEU:HD12	2.37	0.53
8:I:67:GLU:HB2	8:I:85:ALA:HB3	1.91	0.53
14:Q:132:ARG:HG3	18:Z:154:LEU:HD21	1.86	0.53
17:X:434:TYR:HA	17:X:444:LEU:HD13	1.91	0.53
6:F:7:PRO:HG2	6:H:459:ALA:HB2	1.91	0.53
6:F:89:GLU:OE1	6:F:130:ARG:NH2	2.41	0.53
13:O:733:CYS:HA	13:O:736:LEU:HD12	1.90	0.53
17:X:104:LEU:HD11	17:X:142:MET:SD	2.49	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Y:42:ARG:CA	17:Y:82:TYR:CE2	2.72	0.53
1:A:1568:GLY:O	1:A:1571:ARG:HB3	2.08	0.53
2:B:46:LEU:HD21	2:B:54:CYS:CB	2.39	0.53
3:C:93:TYR:CE1	3:C:98:GLU:OE2	2.61	0.53
8:I:115:TRP:CE3	8:I:176:LEU:HD22	2.44	0.53
8:I:197:ARG:O	8:I:545:GLY:HA3	2.09	0.53
10:L:78:CYS:SG	10:L:119:TRP:HE3	2.32	0.53
12:N:395:ASP:OD2	12:N:397:ILE:HB	2.09	0.53
12:N:501:ILE:O	12:N:505:LEU:HG	2.09	0.53
12:N:596:LEU:HB3	12:N:601:TRP:HE1	1.73	0.53
13:O:33:TYR:CE1	13:O:37:VAL:HG21	2.43	0.53
13:O:707:LYS:HA	13:O:710:ILE:HG22	1.91	0.53
3:P:488:GLN:HE21	3:P:492:LYS:HD2	1.73	0.53
1:A:1100:LEU:HB3	1:A:1101:PRO:CA	2.39	0.53
6:H:762:TRP:HA	6:H:765:ASP:CB	2.29	0.53
8:I:313:ALA:CB	8:I:317:LEU:CG	2.86	0.53
9:K:62:SER:O	9:K:63:ARG:HG3	2.08	0.53
16:S:30:GLN:C	16:S:36:ARG:NH2	2.62	0.53
3:C:415:PRO:HG3	3:C:445:LYS:CB	2.39	0.53
5:E:86:VAL:HG22	6:H:589:PHE:HE1	1.73	0.53
6:F:540:SER:OG	6:F:575:ASN:ND2	2.34	0.53
9:K:300:VAL:HG12	9:K:333:TYR:OH	2.08	0.53
15:R:247:SER:HB2	16:S:170:LYS:HZ3	1.73	0.53
16:S:141:TYR:CE1	16:S:297:ALA:O	2.62	0.53
17:Y:42:ARG:HG3	17:Y:82:TYR:HH	1.72	0.53
1:A:214:LEU:CD2	1:A:407:LEU:HD13	2.39	0.52
1:A:1321:VAL:CG2	1:A:1322:PRO:HD3	2.38	0.52
2:B:47:VAL:HG21	2:B:82:PHE:HD2	1.74	0.52
8:I:286:ARG:NE	8:I:333:LEU:HD13	2.18	0.52
9:J:19:TYR:CE1	9:J:49:LEU:HD13	2.44	0.52
9:J:37:PRO:HB3	9:J:69:TYR:OH	2.08	0.52
9:K:174:HIS:HA	9:K:211:LYS:HZ3	1.74	0.52
14:Q:353:GLN:HA	18:Z:52:THR:HB	1.91	0.52
16:S:71:GLY:C	16:S:74:PRO:CD	2.59	0.52
3:C:377:GLU:HA	15:R:130:ILE:HG21	1.90	0.52
3:C:449:LEU:HD11	3:C:479:GLN:HE22	1.74	0.52
12:N:241:HIS:CE1	12:N:302:LYS:HE3	2.44	0.52
12:N:267:GLN:O	12:N:271:GLU:HG3	2.10	0.52
16:S:25:SER:HB2	16:S:45:LEU:CD2	2.38	0.52
8:I:32:ARG:HG2	12:N:388:HIS:CE1	2.45	0.52
12:N:60:GLU:C	12:N:63:ALA:HB2	2.30	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:N:120:SER:O	12:N:124:PRO:HD2	2.09	0.52
14:Q:128:ALA:HA	18:Z:157:THR:O	2.09	0.52
17:Y:458:GLN:O	17:Y:462:LYS:HG3	2.09	0.52
1:A:159:ILE:HB	1:A:171:ALA:HB3	1.91	0.52
1:A:1307:LEU:CD1	1:A:1582:ALA:HB2	2.36	0.52
9:J:204:LEU:HD22	9:K:28:LYS:HZ2	1.74	0.52
9:K:383:ASN:HB3	9:K:386:LEU:HD13	1.90	0.52
16:S:29:VAL:CB	16:S:36:ARG:NH1	2.64	0.52
1:A:1181:LEU:HB3	1:A:1611:VAL:HG11	1.90	0.52
1:A:1516:LEU:HA	1:A:1519:VAL:HG12	1.91	0.52
8:I:279:ILE:HG12	8:I:340:SER:HB2	1.91	0.52
9:J:481:THR:O	9:J:485:ILE:HG12	2.09	0.52
12:N:596:LEU:HD13	12:N:601:TRP:CE2	2.45	0.52
13:O:378:SER:OG	13:O:417:LEU:HD12	2.09	0.52
3:P:239:THR:O	3:P:275:ASN:ND2	2.43	0.52
15:R:193:SER:HB3	15:R:234:TRP:CE2	2.43	0.52
17:Y:42:ARG:HA	17:Y:82:TYR:OH	2.09	0.52
1:A:72:GLU:HG3	1:A:94:TYR:OH	2.10	0.52
9:K:509:ARG:HG3	9:K:509:ARG:O	2.09	0.52
12:N:190:LYS:O	12:N:196:ASP:N	2.43	0.52
17:Y:100:TYR:CB	17:Y:142:MET:HG2	2.40	0.52
1:A:773:LEU:HD22	1:A:779:MET:HG3	1.92	0.52
3:C:228:TRP:O	3:C:231:GLU:N	2.38	0.52
6:H:656:MET:CE	9:K:526:TYR:CD2	2.92	0.52
8:I:116:MET:SD	8:I:210:LEU:HB3	2.50	0.52
12:N:362:LYS:HA	12:N:410:LEU:HD22	1.91	0.52
13:O:479:GLU:OE1	13:O:618:TYR:OH	2.26	0.52
17:X:397:ARG:HD2	17:X:417:TYR:OH	2.10	0.52
17:X:506:GLN:HG3	17:X:508:ASP:OD1	2.10	0.52
17:Y:54:ARG:HG2	17:Y:54:ARG:HH11	1.73	0.52
1:A:1170:ASN:ND2	1:A:1203:MET:HG3	2.25	0.52
1:A:1639:LYS:HG3	1:A:1664:LYS:HB2	1.91	0.52
2:B:11:VAL:HG13	12:N:642:GLY:HA2	1.91	0.52
3:C:335:CYS:HG	3:C:354:PHE:HE1	1.56	0.52
12:N:362:LYS:CB	12:N:410:LEU:HD21	2.23	0.52
14:Q:184:ASP:HA	16:S:28:ASN:OD1	2.09	0.52
17:Y:84:ALA:HB1	17:Y:100:TYR:CZ	2.45	0.52
1:A:436:LEU:HD13	1:A:638:LEU:HD22	1.91	0.52
1:A:1236:LEU:HD12	1:A:1237:PRO:HD2	1.91	0.52
9:J:276:VAL:HA	9:J:311:MET:SD	2.50	0.52
9:J:469:ARG:O	9:J:473:VAL:HG23	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:33:LEU:HG	10:L:42:VAL:HG22	1.91	0.52
16:S:25:SER:HB2	16:S:45:LEU:HG	1.92	0.52
17:X:423:ILE:HG13	17:X:424:ARG:N	2.25	0.52
17:X:458:GLN:O	17:X:462:LYS:HG3	2.09	0.52
17:Y:506:GLN:HG3	17:Y:508:ASP:OD1	2.09	0.52
1:A:1409:LEU:HD22	1:A:1413:LEU:HG	1.91	0.52
1:A:1502:PRO:O	1:A:1503:ASN:HB3	2.09	0.52
3:C:316:LEU:CD2	3:C:340:TYR:HA	2.35	0.52
6:F:544:TRP:CE3	15:R:499:ARG:HD3	2.45	0.52
6:H:130:ARG:NH1	9:K:473:VAL:HG22	2.24	0.52
8:I:290:PHE:CE1	8:I:324:GLN:HB2	2.44	0.52
9:J:18:GLN:HE22	9:K:134:LEU:CD1	2.23	0.52
13:O:136:LEU:C	13:O:136:LEU:HD12	2.30	0.52
17:X:77:TYR:CE1	17:X:107:LYS:HB2	2.45	0.52
17:X:440:ASN:HA	17:X:471:GLN:HE22	1.75	0.52
6:H:703:PRO:HD2	10:L:180:TYR:CD2	2.45	0.51
9:J:355:ALA:O	9:J:359:THR:HG23	2.11	0.51
13:O:657:ILE:HG13	13:O:704:VAL:HG23	1.92	0.51
3:P:303:PHE:HE1	3:P:307:LEU:HD22	1.75	0.51
16:S:71:GLY:O	16:S:74:PRO:N	2.43	0.51
17:Y:495:GLY:HA3	17:Y:518:PHE:HE2	1.75	0.51
1:A:442:LEU:HG	1:A:444:PHE:CE1	2.44	0.51
1:A:482:VAL:CG2	1:A:593:ASN:HA	2.40	0.51
1:A:1237:PRO:CB	1:A:1238:PRO:HD2	2.40	0.51
1:A:1320:ASN:HB3	1:A:1323:GLU:HG2	1.91	0.51
8:I:27:VAL:O	8:I:35:ILE:HD12	2.09	0.51
8:I:536:CYS:O	8:I:540:PRO:CD	2.58	0.51
9:J:24:PHE:O	9:J:28:LYS:HG2	2.11	0.51
10:L:90:THR:HG21	10:L:116:PRO:HD2	1.91	0.51
15:R:407:TRP:CZ3	15:R:414:LEU:HD11	2.45	0.51
1:A:1385:ASP:O	1:A:1388:ARG:HB2	2.10	0.51
8:I:52:PHE:HD1	8:I:743:VAL:HG21	1.76	0.51
12:N:74:TRP:CH2	12:N:77:GLU:HB2	2.46	0.51
14:Q:407:TRP:CZ3	14:Q:414:LEU:HD11	2.44	0.51
1:A:1138:HIS:HE1	1:A:1604:GLN:NE2	2.06	0.51
1:A:1230:ILE:HD12	15:R:116:TRP:HD1	1.75	0.51
1:A:1869:HIS:O	1:A:1872:LEU:HG	2.10	0.51
2:B:15:LEU:HD21	12:N:635:LEU:HA	1.91	0.51
6:F:755:LEU:HD13	9:J:393:GLN:HE22	1.76	0.51
7:G:1:MET:HE1	9:J:338:ILE:HD12	1.93	0.51
8:I:207:ALA:HB1	8:I:575:LEU:HD12	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:393:VAL:O	8:I:397:ILE:HG13	2.11	0.51
9:J:180:GLU:O	9:J:184:LEU:N	2.35	0.51
9:J:206:GLU:HA	9:J:209:LEU:HG	1.91	0.51
12:N:60:GLU:O	12:N:63:ALA:CB	2.56	0.51
12:N:281:TYR:CE1	12:N:357:ALA:HA	2.46	0.51
12:N:560:MET:SD	12:N:601:TRP:CD1	3.04	0.51
13:O:414:LEU:HD12	13:O:417:LEU:HB2	1.92	0.51
3:P:48:LEU:HD21	3:P:116:PHE:CE2	2.45	0.51
14:Q:193:SER:HB3	14:Q:234:TRP:CE2	2.45	0.51
15:R:110:LYS:O	15:R:114:LYS:N	2.39	0.51
15:R:166:ARG:NH2	15:R:472:CYS:O	2.42	0.51
17:X:281:TYR:CE2	17:X:289:ASN:HB3	2.45	0.51
1:A:42:LEU:HD22	3:C:363:ARG:HB2	1.92	0.51
1:A:766:LEU:HD22	1:A:790:LEU:HD21	1.93	0.51
1:A:1325:LEU:HD21	1:A:1370:ALA:HB1	1.92	0.51
6:F:19:TYR:HE2	6:H:50:ARG:HD3	1.74	0.51
6:F:50:ARG:NE	6:H:19:TYR:HE1	2.09	0.51
9:K:263:PHE:HZ	9:K:290:LYS:HG2	1.76	0.51
12:N:233:CYS:O	12:N:235:GLN:N	2.44	0.51
2:B:15:LEU:HD12	12:N:633:ARG:HG2	1.92	0.51
3:C:117:LEU:HD23	3:C:117:LEU:O	2.11	0.51
3:C:170:PHE:O	3:C:173:TYR:HB3	2.10	0.51
3:C:318:TYR:HD1	9:J:282:ASN:OD1	1.93	0.51
12:N:500:ASP:HB2	12:N:501:ILE:HD12	1.92	0.51
13:O:114:ASP:CA	13:O:117:ASP:OD1	2.58	0.51
17:X:76:LYS:HB3	17:X:106:GLN:HE22	1.76	0.51
17:Y:77:TYR:CE1	17:Y:107:LYS:HB2	2.45	0.51
1:A:661:VAL:HG22	1:A:789:LEU:HD12	1.92	0.51
3:C:216:LYS:HG2	3:C:243:LEU:HD11	1.93	0.51
8:I:290:PHE:HD1	8:I:324:GLN:CD	2.15	0.51
12:N:362:LYS:N	12:N:410:LEU:HD21	2.25	0.51
12:N:765:LEU:HD13	12:N:768:LEU:HD21	1.93	0.51
17:X:54:ARG:CZ	17:X:90:ASP:OD2	2.59	0.51
17:X:226:VAL:HG22	17:X:236:LEU:HD23	1.93	0.51
17:X:430:ALA:CB	17:X:451:CYS:SG	2.99	0.51
1:A:1375:TYR:HB3	1:A:1378:THR:CG2	2.38	0.51
7:G:11:LEU:HD13	9:J:514:PHE:CE2	2.45	0.51
6:H:540:SER:OG	6:H:575:ASN:ND2	2.35	0.51
8:I:588:PHE:CE1	8:I:599:CYS:HB2	2.46	0.51
9:J:245:CYS:HA	9:J:247:PHE:CE1	2.46	0.51
9:K:181:GLU:HB3	9:K:209:LEU:HD13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:222:GLU:CD	9:K:228:GLN:CG	2.79	0.51
12:N:278:ARG:HA	12:N:343:GLU:OE2	2.10	0.51
3:P:170:PHE:O	3:P:173:TYR:HB3	2.11	0.51
1:A:629:LEU:HB2	1:A:630:PRO:HD2	1.92	0.51
1:A:1235:LEU:CD2	1:A:1257:ILE:CG1	2.61	0.51
2:B:16:TRP:HB2	2:B:33:CYS:HB3	1.92	0.51
12:N:662:VAL:CG2	12:N:695:ARG:HG2	2.41	0.51
13:O:119:PHE:CE1	13:O:136:LEU:HD21	2.45	0.51
3:P:303:PHE:CD1	3:P:303:PHE:C	2.83	0.51
14:Q:208:LEU:HD13	14:Q:255:VAL:HG21	1.93	0.51
16:S:79:ASP:CG	16:S:120:ARG:HB3	2.30	0.51
17:Y:309:ASP:HB2	17:Y:340:GLU:HG2	1.93	0.51
1:A:1388:ARG:HA	1:A:1411:ARG:HD2	1.92	0.51
1:A:1556:LEU:HD12	1:A:1556:LEU:O	2.11	0.51
6:H:703:PRO:HD3	10:L:180:TYR:CE2	2.46	0.51
8:I:304:PHE:HZ	8:I:448:VAL:HG13	1.76	0.51
9:K:222:GLU:OE1	9:K:228:GLN:CG	2.59	0.51
11:M:1:MET:HB2	3:P:50:HIS:HB2	1.92	0.51
12:N:181:LEU:HD22	12:N:299:TRP:CE2	2.46	0.51
15:R:192:TRP:CG	15:R:198:LEU:HD13	2.45	0.51
16:S:36:ARG:CZ	16:S:90:PRO:O	2.59	0.51
1:A:1400:LYS:HA	10:L:135:PHE:CZ	2.46	0.50
1:A:1674:TRP:CD1	1:A:1674:TRP:N	2.79	0.50
12:N:570:ILE:HA	12:N:573:ASN:ND2	2.26	0.50
13:O:460:GLN:HG2	13:O:496:ARG:HH22	1.74	0.50
3:P:228:TRP:O	3:P:231:GLU:N	2.38	0.50
3:P:494:ILE:HG21	3:P:516:LEU:HD13	1.92	0.50
17:X:235:TRP:CE3	17:X:236:LEU:HA	2.47	0.50
17:Y:294:PHE:CE2	17:Y:311:TYR:HB2	2.46	0.50
3:C:225:PRO:O	3:C:230:LYS:HD2	2.11	0.50
12:N:555:HIS:O	12:N:559:VAL:HG12	2.11	0.50
13:O:648:ILE:CD1	13:O:663:ALA:HB1	2.41	0.50
15:R:111:GLU:O	15:R:115:ALA:N	2.42	0.50
17:X:495:GLY:HA3	17:X:518:PHE:CE2	2.46	0.50
17:Y:281:TYR:CE2	17:Y:289:ASN:HB3	2.46	0.50
3:C:277:ARG:HB3	15:R:75:GLY:O	2.11	0.50
8:I:138:LEU:HD13	8:I:253:ARG:HG2	1.92	0.50
8:I:413:ASN:N	8:I:447:PHE:CZ	2.78	0.50
9:J:37:PRO:HB3	9:J:69:TYR:HE2	1.75	0.50
9:K:42:TRP:HA	9:K:42:TRP:CE3	2.46	0.50
12:N:102:ALA:HA	12:N:107:CYS:C	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:N:751:LEU:HA	12:N:754:PHE:HD2	1.75	0.50
13:O:75:LEU:CD1	13:O:161:TYR:CD2	2.89	0.50
14:Q:340:PRO:HD3	14:Q:345:TRP:CZ2	2.47	0.50
15:R:98:GLU:HG2	15:R:101:PRO:CD	2.41	0.50
17:Y:73:PRO:O	17:Y:106:GLN:OE1	2.29	0.50
17:Y:196:LEU:O	17:Y:200:PRO:CA	2.59	0.50
17:Y:423:ILE:HG13	17:Y:424:ARG:N	2.25	0.50
17:Y:452:LEU:CD2	17:Y:461:ALA:H	2.23	0.50
2:B:38:LYS:C	2:B:40:PRO:HD2	2.31	0.50
6:H:537:GLU:OE2	6:H:568:GLU:OE1	2.28	0.50
9:J:354:MET:CE	9:J:377:GLU:HB2	2.41	0.50
12:N:75:PHE:O	12:N:78:VAL:N	2.44	0.50
12:N:676:TRP:CE3	12:N:680:GLU:HB3	2.46	0.50
3:P:225:PRO:O	3:P:230:LYS:HD2	2.11	0.50
16:S:21:GLU:O	16:S:45:LEU:HD13	2.10	0.50
17:X:495:GLY:HA3	17:X:518:PHE:HE2	1.75	0.50
1:A:442:LEU:HG	1:A:444:PHE:HE1	1.77	0.50
1:A:873:VAL:CG2	1:A:951:ILE:CG2	2.89	0.50
6:F:26:PHE:CD1	6:H:149:TRP:CB	2.94	0.50
8:I:174:ASN:OD1	8:I:190:TYR:HA	2.12	0.50
8:I:304:PHE:CZ	8:I:448:VAL:CG1	2.95	0.50
12:N:370:GLN:HG2	12:N:373:GLN:HB2	1.93	0.50
3:P:234:LEU:HD22	3:P:238:TYR:CZ	2.46	0.50
14:Q:192:TRP:CG	14:Q:198:LEU:HD13	2.46	0.50
17:X:269:ASP:HB3	17:X:300:LEU:HD21	1.92	0.50
1:A:1234:ALA:HB1	1:A:1272:VAL:HB	1.93	0.50
1:A:1300:LEU:HD13	1:A:1369:LEU:HD13	1.94	0.50
1:A:1601:TYR:OH	10:L:102:PHE:HD1	1.95	0.50
3:C:361:ASN:HB3	3:C:363:ARG:N	2.27	0.50
8:I:245:LEU:HB3	8:I:246:PRO:HD3	1.93	0.50
14:Q:425:LEU:HD12	14:Q:425:LEU:N	2.27	0.50
17:Y:146:TYR:CD1	17:Y:154:ASP:HB2	2.47	0.50
17:Y:495:GLY:HA3	17:Y:518:PHE:CE2	2.46	0.50
18:Z:138:THR:HG23	18:Z:142:LEU:HD12	1.93	0.50
1:A:1523:LEU:O	1:A:1526:VAL:HG22	2.11	0.50
1:A:1840:MET:HE2	1:A:1845:LEU:HG	1.94	0.50
8:I:306:HIS:CE1	8:I:313:ALA:HB1	2.46	0.50
8:I:317:LEU:CD2	8:I:320:LEU:HD23	2.40	0.50
8:I:441:THR:O	8:I:445:ILE:HG12	2.12	0.50
12:N:659:VAL:HG22	12:N:660:THR:N	2.27	0.50
15:R:81:PRO:HG3	15:R:131:LEU:HD21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:S:273:THR:O	16:S:274:VAL:HB	2.12	0.50
18:Z:72:LEU:HD11	18:Z:155:ILE:HD11	1.92	0.50
1:A:39:LEU:HD21	3:C:393:GLU:HG2	1.93	0.50
1:A:489:LEU:HD22	1:A:497:LEU:HD22	1.94	0.50
1:A:852:LEU:HD11	1:A:1819:GLU:HB3	1.93	0.50
3:C:415:PRO:HG3	3:C:445:LYS:HB3	1.92	0.50
6:H:164:PRO:HG3	6:H:471:LYS:HG3	1.93	0.50
6:H:704:LEU:HD22	10:L:181:ARG:HA	1.93	0.50
8:I:47:HIS:CE1	8:I:54:ARG:NH1	2.79	0.50
9:K:185:LEU:HA	9:K:188:LEU:CD2	2.40	0.50
11:M:59:ASP:C	11:M:61:ALA:H	2.14	0.50
12:N:180:PHE:CE2	12:N:240:PHE:HB3	2.47	0.50
15:R:77:ASP:OD1	15:R:77:ASP:N	2.45	0.50
1:A:95:VAL:HG21	1:A:126:ALA:HB3	1.93	0.50
1:A:436:LEU:HB3	1:A:638:LEU:HD13	1.93	0.50
8:I:282:GLN:O	8:I:285:SER:HB3	2.12	0.50
15:R:340:PRO:HD3	15:R:345:TRP:CZ2	2.47	0.50
17:X:294:PHE:CE2	17:X:311:TYR:HB2	2.46	0.50
17:Y:235:TRP:CE3	17:Y:236:LEU:HA	2.47	0.50
1:A:1086:MET:HE1	1:A:1564:LEU:HD13	1.94	0.49
1:A:1325:LEU:HD21	1:A:1370:ALA:CB	2.42	0.49
3:C:273:TYR:HB3	3:C:282:ALA:HB2	1.94	0.49
8:I:266:ASN:HA	8:I:526:LYS:NZ	2.26	0.49
9:J:17:GLN:HB3	9:K:78:ARG:HH12	1.77	0.49
15:R:209:TRP:HB2	16:S:227:LEU:HD13	1.94	0.49
1:A:485:ILE:HD11	1:A:609:ILE:HB	1.94	0.49
1:A:1230:ILE:HA	1:A:1236:LEU:HD13	1.94	0.49
13:O:311:HIS:HB2	13:O:320:ALA:HB2	1.92	0.49
13:O:657:ILE:HG22	13:O:660:LYS:HE2	1.94	0.49
16:S:23:GLU:OE2	18:Z:134:GLN:CA	2.60	0.49
16:S:199:ARG:O	16:S:203:GLN:HG2	2.11	0.49
1:A:480:ALA:HB1	1:A:590:PRO:HG3	1.94	0.49
3:C:251:TYR:HB3	3:C:269:ILE:CD1	2.42	0.49
6:H:465:LEU:HD22	6:H:495:HIS:CE1	2.47	0.49
9:J:213:ASN:OD1	9:J:214:LYS:N	2.45	0.49
9:J:247:PHE:CE2	9:J:277:GLU:CB	2.96	0.49
9:K:227:LEU:O	9:K:230:ASN:HB3	2.13	0.49
9:K:406:HIS:CE1	7:W:6:PRO:CB	2.95	0.49
12:N:393:THR:HG23	12:N:434:THR:HG22	1.94	0.49
12:N:409:VAL:O	12:N:410:LEU:HB2	2.11	0.49
12:N:577:GLU:HB3	12:N:625:LYS:CE	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:R:112:HIS:CD2	15:R:116:TRP:HZ3	2.29	0.49
17:Y:226:VAL:HG22	17:Y:236:LEU:HD23	1.94	0.49
1:A:1229:SER:HA	1:A:1235:LEU:HB3	1.94	0.49
1:A:1401:PRO:HD3	10:L:135:PHE:CE2	2.47	0.49
1:A:1555:HIS:O	1:A:1559:HIS:CD2	2.64	0.49
5:E:94:TRP:CZ2	6:F:592:ARG:HG2	2.46	0.49
6:F:739:VAL:O	6:F:743:ILE:HG13	2.13	0.49
6:H:656:MET:O	6:H:660:LYS:HG3	2.12	0.49
8:I:203:GLY:HA3	8:I:223:VAL:HG22	1.94	0.49
9:J:441:VAL:O	9:J:442:ASP:CB	2.59	0.49
9:K:372:LEU:HD22	9:K:404:VAL:HG22	1.94	0.49
15:R:208:LEU:HD13	15:R:255:VAL:HG21	1.93	0.49
17:Y:269:ASP:HB3	17:Y:300:LEU:HD21	1.94	0.49
1:A:1551:ASN:OD1	1:A:1554:PHE:CD2	2.65	0.49
6:H:743:ILE:HG22	6:H:759:ASN:HD21	1.77	0.49
10:L:63:LEU:HD22	10:L:138:GLN:HE21	1.77	0.49
12:N:249:ARG:HB3	12:N:250:LEU:HD23	1.94	0.49
3:P:117:LEU:HD23	3:P:117:LEU:O	2.11	0.49
14:Q:430:TYR:CD1	14:Q:431:PRO:HA	2.48	0.49
15:R:430:TYR:CD1	15:R:431:PRO:HA	2.48	0.49
3:C:313:LYS:HG2	3:C:343:LEU:HD22	1.95	0.49
8:I:639:LEU:HB2	8:I:652:VAL:HG12	1.93	0.49
13:O:233:PRO:HA	13:O:263:ARG:HH21	1.77	0.49
3:P:303:PHE:C	3:P:303:PHE:HD1	2.14	0.49
15:R:239:ASN:ND2	15:R:240:TYR:CE2	2.81	0.49
16:S:55:LEU:O	16:S:59:LYS:HD3	2.12	0.49
8:I:116:MET:HE1	8:I:211:SER:O	2.13	0.49
9:J:397:ILE:CG2	9:J:398:ALA:H	2.25	0.49
13:O:707:LYS:CA	13:O:710:ILE:HG22	2.42	0.49
15:R:425:LEU:N	15:R:425:LEU:HD12	2.28	0.49
1:A:78:LYS:HD3	1:A:592:HIS:HB2	1.94	0.49
1:A:248:PHE:CZ	1:A:250:ASN:HB2	2.48	0.49
1:A:945:GLU:O	13:O:599:ILE:HD13	2.13	0.49
3:C:48:LEU:HD21	3:C:116:PHE:CZ	2.47	0.49
6:H:739:VAL:O	6:H:743:ILE:HG13	2.13	0.49
8:I:207:ALA:CB	8:I:575:LEU:HD12	2.43	0.49
8:I:337:ILE:O	8:I:341:TYR:CD2	2.66	0.49
9:J:376:LEU:HD23	9:J:407:GLU:HG2	1.93	0.49
9:K:256:VAL:O	9:K:259:GLU:HG2	2.12	0.49
9:K:441:VAL:HG13	9:K:474:LEU:HD22	1.95	0.49
12:N:63:ALA:HB3	12:N:64:ALA:CB	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:402:LEU:HD13	13:O:425:LYS:CG	2.42	0.49
13:O:509:LEU:HG	13:O:513:LYS:HE3	1.95	0.49
17:X:170:LYS:HA	17:Y:49:LEU:CD2	2.42	0.49
17:X:376:LEU:HD11	17:X:398:GLU:OE2	2.13	0.49
17:X:393:ILE:HG22	17:X:397:ARG:HD3	1.94	0.49
1:A:1086:MET:CE	1:A:1564:LEU:HD13	2.42	0.49
1:A:1160:TYR:HB2	13:O:332:GLN:HB3	1.93	0.49
1:A:1770:LEU:HD13	1:A:1798:ARG:HH22	1.78	0.49
7:G:3:ARG:HB2	9:J:443:LYS:HZ1	1.77	0.49
9:J:165:GLU:HB2	9:K:21:SER:HB2	1.94	0.49
10:L:24:GLU:HG3	10:L:159:TYR:CE1	2.48	0.49
12:N:156:MET:O	12:N:160:VAL:HG23	2.12	0.49
12:N:180:PHE:CG	12:N:299:TRP:HH2	2.30	0.49
1:A:455:VAL:HB	1:A:471:VAL:HG12	1.94	0.49
1:A:1157:TRP:HA	13:O:332:GLN:OE1	2.12	0.49
3:C:296:ARG:HD3	3:P:101:ARG:HH22	1.78	0.49
6:H:145:ASN:HB2	6:H:146:PRO:C	2.34	0.49
8:I:36:ALA:HB2	8:I:80:LEU:HD21	1.94	0.49
8:I:412:LYS:C	8:I:447:PHE:HZ	2.15	0.49
10:L:45:LEU:HD11	10:L:156:ILE:HD12	1.95	0.49
12:N:545:LEU:O	12:N:549:PHE:N	2.46	0.49
13:O:36:ALA:CB	13:O:75:LEU:HD21	2.43	0.49
13:O:78:LEU:HD12	13:O:78:LEU:O	2.13	0.49
13:O:669:LYS:HZ1	13:O:751:LEU:HD13	1.78	0.49
3:P:119:MET:HG2	3:P:158:LEU:HD21	1.95	0.49
16:S:21:GLU:O	16:S:45:LEU:HD21	2.06	0.49
1:A:436:LEU:H	1:A:501:THR:CG2	2.26	0.48
8:I:424:ALA:O	8:I:428:MET:HG2	2.13	0.48
12:N:659:VAL:HG22	12:N:660:THR:H	1.77	0.48
3:P:334:CYS:HB3	3:P:357:ALA:HB2	1.94	0.48
6:F:500:TRP:CB	6:H:30:ARG:NH2	2.74	0.48
9:J:294:LEU:HD12	9:K:54:HIS:HE2	1.78	0.48
12:N:286:LEU:O	12:N:288:GLU:N	2.46	0.48
16:S:68:PHE:HE1	16:S:78:TRP:CG	2.31	0.48
17:X:168:THR:OG1	17:X:171:ILE:CD1	2.61	0.48
17:Y:376:LEU:HD11	17:Y:398:GLU:OE2	2.12	0.48
1:A:1644:TYR:O	1:A:1645:GLU:HG2	2.13	0.48
3:C:466:GLU:HG3	15:R:82:HIS:CD2	2.49	0.48
6:F:130:ARG:HG2	17:Y:506:GLN:HB2	1.96	0.48
6:F:537:GLU:CD	6:F:600:TYR:OH	2.52	0.48
8:I:446:THR:O	8:I:449:ALA:HB3	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:20:GLN:OE1	9:J:20:GLN:HA	2.14	0.48
9:J:215:PRO:HB2	9:J:435:ILE:HD11	1.95	0.48
9:J:297:SER:O	9:J:329:LEU:HD11	2.13	0.48
12:N:281:TYR:CZ	12:N:284:SER:HB3	2.48	0.48
12:N:700:LEU:HD13	12:N:707:GLU:HG3	1.95	0.48
13:O:422:ILE:O	13:O:426:THR:HG22	2.14	0.48
14:Q:239:ASN:ND2	14:Q:240:TYR:CE2	2.81	0.48
16:S:38:MET:CE	18:Z:199:TYR:CE2	2.69	0.48
18:Z:91:ILE:HG12	18:Z:150:SER:HB3	1.95	0.48
1:A:612:ILE:O	1:A:641:TRP:HZ3	1.95	0.48
1:A:1082:VAL:HG22	1:A:1138:HIS:CG	2.48	0.48
1:A:1136:SER:O	1:A:1139:ASN:HB3	2.13	0.48
3:C:33:LYS:NZ	3:C:64:ALA:HA	2.29	0.48
6:F:459:ALA:HB2	6:H:7:PRO:HG2	1.95	0.48
6:H:102:SER:OG	6:H:104:ASP:OD1	2.17	0.48
6:H:736:GLU:OE1	10:L:177:PHE:HB2	2.13	0.48
6:H:743:ILE:HG22	6:H:759:ASN:ND2	2.29	0.48
12:N:523:LEU:HD22	12:N:538:GLU:OE1	2.12	0.48
14:Q:208:LEU:CD1	14:Q:255:VAL:HG21	2.43	0.48
3:C:334:CYS:HB3	3:C:357:ALA:HB2	1.95	0.48
3:C:413:LYS:O	3:C:415:PRO:HD3	2.14	0.48
6:F:164:PRO:CG	6:F:471:LYS:HG3	2.43	0.48
8:I:290:PHE:CE2	8:I:325:LEU:HD12	2.47	0.48
8:I:300:VAL:HA	8:I:303:GLU:CD	2.31	0.48
8:I:427:ARG:HB2	8:I:428:MET:CE	2.42	0.48
16:S:58:GLN:C	16:S:62:PHE:CD2	2.84	0.48
16:S:82:ILE:CD1	16:S:102:LEU:HD23	2.43	0.48
1:A:1405:LEU:CD1	1:A:1467:GLY:HA2	2.41	0.48
3:C:265:ILE:O	3:C:269:ILE:HG12	2.14	0.48
6:F:541:THR:HG23	15:R:499:ARG:HG2	1.96	0.48
6:H:564:LYS:O	6:H:565:ASN:HB2	2.14	0.48
8:I:290:PHE:HB3	8:I:320:LEU:HD11	1.95	0.48
9:K:228:GLN:HA	9:K:233:VAL:HG21	1.95	0.48
9:K:458:LEU:HB3	9:K:460:LYS:HG3	1.95	0.48
12:N:88:SER:O	12:N:91:PHE:HB3	2.13	0.48
12:N:91:PHE:CZ	12:N:94:ALA:HB2	2.49	0.48
15:R:208:LEU:CD1	15:R:255:VAL:HG21	2.43	0.48
17:X:393:ILE:HG22	17:X:397:ARG:HH11	1.78	0.48
1:A:772:GLU:HG3	1:A:867:CYS:HA	1.95	0.48
1:A:1080:LEU:N	1:A:1081:PRO:HD2	2.29	0.48
1:A:1602:HIS:O	1:A:1603:LEU:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:49:LEU:HD13	8:I:730:VAL:HG21	1.95	0.48
8:I:269:LEU:HB2	8:I:526:LYS:HZ1	1.77	0.48
12:N:91:PHE:CE1	12:N:94:ALA:HB2	2.48	0.48
13:O:281:LEU:HD21	13:O:283:LEU:HD12	1.95	0.48
13:O:356:ASP:HA	13:O:357:SER:CB	2.42	0.48
15:R:105:GLN:O	15:R:107:PRO:HD3	2.14	0.48
16:S:19:GLY:HA3	18:Z:134:GLN:CG	2.44	0.48
17:X:99:LYS:HD3	17:X:102:MET:CE	2.43	0.48
17:X:339:ALA:O	17:X:343:VAL:HG23	2.14	0.48
17:Y:168:THR:OG1	17:Y:171:ILE:CD1	2.61	0.48
17:Y:338:HIS:O	17:Y:341:PRO:HD2	2.14	0.48
1:A:437:CYS:HA	1:A:626:LYS:HD2	1.96	0.48
1:A:799:LEU:C	1:A:801:PRO:HD2	2.33	0.48
6:F:152:PHE:CE1	6:F:162:PRO:HG2	2.49	0.48
6:H:486:ASN:O	6:H:490:HIS:CD2	2.67	0.48
8:I:410:SER:O	8:I:414:PHE:HD2	1.95	0.48
12:N:519:TYR:CE1	12:N:523:LEU:HD21	2.49	0.48
13:O:635:GLY:O	13:O:637:PRO:HD3	2.14	0.48
17:X:436:THR:HG23	17:X:437:LEU:HD12	1.96	0.48
18:Z:138:THR:HG23	18:Z:142:LEU:CD1	2.44	0.48
1:A:1201:HIS:CE1	1:A:1203:MET:HB2	2.49	0.48
1:A:1573:SER:HB2	1:A:1617:ARG:HH21	1.78	0.48
3:C:521:PHE:HD1	3:C:553:ILE:HG22	1.74	0.48
8:I:188:TYR:HA	8:I:193:PHE:O	2.14	0.48
9:J:413:PHE:CD1	9:J:454:VAL:HG12	2.49	0.48
10:L:144:ASN:ND2	10:L:151:THR:HG23	2.29	0.48
12:N:706:ARG:HB2	12:N:716:ILE:HD13	1.94	0.48
13:O:423:ALA:O	13:O:426:THR:HG23	2.13	0.48
13:O:681:PRO:O	13:O:682:LYS:HB2	2.14	0.48
3:P:437:VAL:HG22	3:P:469:ALA:HB2	1.96	0.48
15:R:98:GLU:HG2	15:R:101:PRO:CG	2.41	0.48
1:A:174:PRO:HG2	1:A:175:PHE:CD2	2.49	0.48
3:C:209:LEU:O	3:C:213:ILE:HG12	2.14	0.48
6:F:130:ARG:HH11	17:Y:506:GLN:CB	2.27	0.48
6:F:564:LYS:O	6:F:565:ASN:HB2	2.13	0.48
8:I:294:LYS:CB	8:I:320:LEU:HD13	2.43	0.48
9:J:230:ASN:OD1	9:J:231:LEU:N	2.47	0.48
17:Y:339:ALA:O	17:Y:343:VAL:HG23	2.13	0.48
18:Z:81:VAL:HG21	18:Z:155:ILE:HD12	1.96	0.48
1:A:1621:PRO:HG3	1:A:1653:ALA:CB	2.44	0.47
3:C:48:LEU:HD21	3:C:116:PHE:CE2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:145:GLN:CG	13:O:246:PHE:HA	2.43	0.47
6:F:59:ARG:HH12	6:H:562:MET:HB2	1.79	0.47
6:F:673:CYS:O	6:F:677:VAL:HG23	2.14	0.47
10:L:75:LYS:HA	10:L:131:PRO:HB3	1.95	0.47
3:P:48:LEU:HD21	3:P:116:PHE:CZ	2.48	0.47
16:S:79:ASP:CB	16:S:120:ARG:HH11	2.27	0.47
17:X:452:LEU:CD2	17:X:461:ALA:H	2.23	0.47
3:C:317:SER:OG	11:M:27:GLU:HG3	2.14	0.47
6:H:121:LEU:HG	6:H:125:TYR:HE1	1.79	0.47
9:J:393:GLN:O	9:J:396:SER:HB3	2.13	0.47
12:N:765:LEU:HD23	12:N:765:LEU:HA	1.70	0.47
3:P:265:ILE:O	3:P:269:ILE:HG12	2.14	0.47
16:S:197:GLN:C	16:S:200:VAL:HG22	2.34	0.47
1:A:1235:LEU:HD21	1:A:1257:ILE:CD1	2.40	0.47
8:I:673:LEU:HA	8:I:676:ASN:HB2	1.95	0.47
12:N:556:PHE:CZ	12:N:600:PHE:HA	2.49	0.47
13:O:39:VAL:HG11	13:O:97:ILE:HG13	1.94	0.47
13:O:411:LYS:HE2	13:O:412:HIS:HE1	1.74	0.47
3:P:308:TYR:CD2	14:Q:499:ARG:HD2	2.49	0.47
16:S:188:ARG:HH12	18:Z:147:VAL:CG1	2.26	0.47
8:I:206:LEU:HD22	8:I:570:PHE:CD2	2.50	0.47
9:K:227:LEU:O	9:K:230:ASN:N	2.48	0.47
9:K:263:PHE:CZ	9:K:290:LYS:HG2	2.49	0.47
12:N:282:GLU:O	12:N:284:SER:N	2.44	0.47
3:P:316:LEU:CD1	3:P:340:TYR:HB2	2.44	0.47
14:Q:166:ARG:CZ	14:Q:413:GLU:OE1	2.62	0.47
15:R:112:HIS:CE1	15:R:116:TRP:HZ3	2.31	0.47
16:S:141:TYR:CE1	16:S:297:ALA:C	2.88	0.47
1:A:1172:TYR:CZ	1:A:1176:LEU:HD23	2.49	0.47
3:C:101:ARG:CZ	3:P:296:ARG:HA	2.44	0.47
6:F:537:GLU:OE1	6:F:600:TYR:CE2	2.67	0.47
9:J:272:ILE:HD11	9:J:304:ALA:HB2	1.97	0.47
9:K:350:HIS:ND1	9:K:377:GLU:OE1	2.47	0.47
10:L:29:ALA:O	10:L:31:TRP:CD1	2.67	0.47
13:O:91:ASN:O	13:O:95:ILE:HG12	2.14	0.47
3:P:209:LEU:O	3:P:213:ILE:HG12	2.15	0.47
1:A:1078:MET:HB2	1:A:1552:TYR:CE1	2.50	0.47
1:A:1511:ASN:HD22	1:A:1511:ASN:H	1.60	0.47
3:C:180:ARG:HG3	3:C:212:LEU:HD21	1.97	0.47
8:I:276:TRP:HA	8:I:279:ILE:HG22	1.96	0.47
9:J:69:TYR:O	9:J:70:GLU:CB	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:456:ARG:CG	9:J:488:ILE:HG22	2.44	0.47
18:Z:80:SER:O	18:Z:157:THR:HB	2.14	0.47
1:A:93:LEU:HD11	1:A:151:ILE:HD12	1.97	0.47
1:A:665:MET:O	1:A:669:GLY:N	2.44	0.47
1:A:1064:GLU:HA	1:A:1125:ILE:HD11	1.97	0.47
1:A:1413:LEU:HD22	1:A:1416:TRP:HZ3	1.80	0.47
3:C:550:LEU:HD22	3:C:553:ILE:HD11	1.97	0.47
8:I:291:VAL:HG12	8:I:298:THR:HA	1.96	0.47
8:I:442:GLN:HE21	13:O:69:GLN:HG2	1.80	0.47
9:J:58:HIS:CD2	9:K:262:PRO:HD3	2.50	0.47
9:J:191:SER:O	9:J:193:LEU:HG	2.14	0.47
13:O:129:THR:O	13:O:130:SER:CB	2.61	0.47
13:O:628:ALA:HB2	13:O:643:LEU:HD22	1.97	0.47
13:O:710:ILE:O	13:O:713:VAL:HG12	2.14	0.47
16:S:21:GLU:O	16:S:45:LEU:CD1	2.62	0.47
16:S:25:SER:HB2	16:S:45:LEU:HD21	1.96	0.47
17:X:349:SER:HA	17:X:352:SER:OG	2.15	0.47
3:C:333:THR:O	3:C:337:ILE:HG12	2.15	0.47
6:F:96:VAL:HG12	6:F:97:PHE:CD1	2.50	0.47
9:J:220:ILE:HG12	9:J:240:ARG:NH1	2.30	0.47
9:J:475:ILE:HD11	9:J:478:ASN:ND2	2.28	0.47
9:K:499:VAL:HG11	9:K:523:ILE:CD1	2.45	0.47
12:N:202:GLU:O	12:N:202:GLU:OE1	2.33	0.47
12:N:542:VAL:HG11	12:N:558:GLU:CD	2.35	0.47
12:N:567:SER:HB2	12:N:594:VAL:O	2.14	0.47
14:Q:196:ASN:ND2	14:Q:211:ALA:HB3	2.30	0.47
17:Y:42:ARG:CB	17:Y:82:TYR:OH	2.63	0.47
2:B:16:TRP:CH2	12:N:630:LYS:CE	2.98	0.47
3:C:119:MET:HG2	3:C:158:LEU:HD21	1.97	0.47
6:H:146:PRO:CG	6:H:167:THR:HA	2.45	0.47
8:I:70:CYS:C	8:I:71:LEU:HD12	2.35	0.47
9:J:78:ARG:NH1	9:K:17:GLN:HB3	2.29	0.47
12:N:73:GLU:O	12:N:74:TRP:CB	2.63	0.47
12:N:273:MET:CG	12:N:277:CYS:SG	2.95	0.47
12:N:577:GLU:HG2	12:N:583:ALA:HB2	1.97	0.47
3:P:274:HIS:O	3:P:276:ILE:O	2.33	0.47
3:P:358:LEU:CD1	3:P:368:TRP:CE2	2.98	0.47
3:P:365:LEU:HB3	3:P:395:ASN:HD21	1.80	0.47
16:S:83:SER:C	16:S:87:GLN:HG3	2.34	0.47
1:A:162:HIS:HD2	1:A:168:ASP:HB3	1.79	0.47
1:A:804:ASP:OD1	1:A:804:ASP:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:845:TYR:HB3	1:A:1812:TRP:CZ3	2.50	0.47
2:B:27:ARG:HD3	12:N:813:GLY:HA2	1.97	0.47
6:H:97:PHE:HA	9:K:433:LYS:HD3	1.97	0.47
8:I:301:GLN:O	8:I:304:PHE:N	2.48	0.47
8:I:578:ASN:ND2	8:I:646:ASP:HB3	2.30	0.47
9:J:496:GLU:HB2	9:J:526:TYR:CE1	2.50	0.47
9:K:248:LYS:N	9:K:438:GLU:OE2	2.48	0.47
9:K:284:LEU:HD12	9:K:311:MET:HE1	1.97	0.47
13:O:36:ALA:O	13:O:39:VAL:HG12	2.15	0.47
13:O:123:GLU:N	13:O:124:PRO:HA	2.30	0.47
13:O:425:LYS:HB2	13:O:441:GLN:HG2	1.96	0.47
14:Q:186:TYR:CE2	16:S:27:GLU:HB2	2.49	0.47
16:S:141:TYR:CE2	16:S:299:PRO:HD3	2.50	0.47
3:C:259:PHE:HB3	3:C:265:ILE:HD13	1.94	0.46
6:F:146:PRO:CG	6:F:167:THR:HA	2.46	0.46
6:F:481:CYS:HB2	6:F:512:LEU:HD13	1.96	0.46
6:H:537:GLU:CD	6:H:600:TYR:OH	2.53	0.46
8:I:287:LEU:O	8:I:291:VAL:HG23	2.15	0.46
8:I:399:LYS:HG2	8:I:525:VAL:HG21	1.98	0.46
9:J:322:TYR:CZ	11:M:31:ILE:HD13	2.50	0.46
9:K:443:LYS:O	9:K:446:PRO:HD2	2.15	0.46
12:N:258:ALA:HA	12:N:261:VAL:HG22	1.97	0.46
3:P:361:ASN:HB3	3:P:363:ARG:N	2.30	0.46
3:P:388:TYR:HB3	3:P:405:LEU:HG	1.98	0.46
14:Q:442:HIS:CE1	14:Q:468:ARG:HD2	2.51	0.46
15:R:461:ALA:HB2	15:R:467:LEU:CD1	2.45	0.46
17:Y:349:SER:HA	17:Y:352:SER:OG	2.15	0.46
1:A:442:LEU:HB3	1:A:455:VAL:HG13	1.96	0.46
2:B:16:TRP:CZ2	2:B:45:PRO:HA	2.50	0.46
5:E:99:ILE:HD11	5:E:103:LEU:HD13	1.98	0.46
6:F:98:ASN:OD1	6:F:98:ASN:N	2.47	0.46
7:G:4:ARG:HB2	9:J:373:TYR:HE1	1.81	0.46
6:H:541:THR:CG2	10:L:184:ARG:HB3	2.45	0.46
6:H:592:ARG:HD3	6:H:592:ARG:HA	1.66	0.46
8:I:25:PHE:CD1	8:I:71:LEU:HD13	2.50	0.46
8:I:440:MET:HB3	8:I:445:ILE:HD11	1.97	0.46
8:I:561:ARG:NH2	8:I:589:THR:O	2.44	0.46
9:K:280:LYS:HB3	9:K:283:GLU:HG2	1.97	0.46
12:N:753:LEU:HG	12:N:757:TYR:HE1	1.81	0.46
3:P:405:LEU:HA	3:P:408:THR:HG22	1.97	0.46
17:X:339:ALA:HB2	17:X:369:ASN:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:494:ASP:OD1	17:X:494:ASP:N	2.48	0.46
17:Y:494:ASP:OD1	17:Y:494:ASP:N	2.48	0.46
1:A:256:VAL:HB	1:A:269:TRP:HB2	1.98	0.46
1:A:957:ASP:CG	1:A:1820:PHE:HZ	2.19	0.46
3:C:477:HIS:CD2	3:C:482:GLU:OE1	2.64	0.46
4:D:5:PHE:CE1	13:O:427:ALA:HB1	2.51	0.46
6:F:533:VAL:HG23	6:F:559:LEU:HD22	1.97	0.46
8:I:145:LEU:HD13	8:I:267:LEU:HD22	1.98	0.46
15:R:130:ILE:HG23	15:R:131:LEU:H	1.78	0.46
17:X:40:HIS:CB	17:Y:201:LEU:HD11	2.36	0.46
1:A:252:ASP:HB2	1:A:253:PRO:HD3	1.98	0.46
1:A:1477:ALA:HA	1:A:1525:MET:O	2.14	0.46
1:A:1621:PRO:HG3	1:A:1653:ALA:HB1	1.97	0.46
5:E:89:LEU:HD11	6:H:592:ARG:HB2	1.97	0.46
6:F:164:PRO:HG3	6:F:471:LYS:HG3	1.98	0.46
6:H:98:ASN:OD1	6:H:98:ASN:N	2.49	0.46
8:I:413:ASN:C	8:I:447:PHE:CE1	2.89	0.46
8:I:414:PHE:CE1	8:I:451:PHE:HE1	2.31	0.46
8:I:437:LEU:HA	8:I:438:ASN:C	2.35	0.46
9:J:219:VAL:O	9:J:221:PRO:HD3	2.14	0.46
9:K:8:LYS:HA	9:K:8:LYS:HD2	1.82	0.46
9:K:93:LEU:HD12	9:K:93:LEU:N	2.31	0.46
9:K:167:PHE:O	9:K:171:THR:HG22	2.15	0.46
9:K:298:ASN:OD1	9:K:300:VAL:HG22	2.15	0.46
9:K:496:GLU:HB2	9:K:526:TYR:CE1	2.50	0.46
15:R:124:ASP:O	15:R:127:GLU:O	2.33	0.46
16:S:36:ARG:NH2	16:S:90:PRO:O	2.48	0.46
17:X:63:MET:SD	17:Y:235:TRP:NE1	2.89	0.46
17:X:146:TYR:CD1	17:X:154:ASP:HB2	2.50	0.46
17:X:373:VAL:O	17:X:376:LEU:N	2.46	0.46
17:X:406:ARG:HB2	17:X:409:CYS:SG	2.56	0.46
1:A:1753:TYR:CD2	13:O:643:LEU:HD12	2.42	0.46
3:C:358:LEU:O	3:C:362:PRO:HB3	2.15	0.46
8:I:28:TRP:CD1	8:I:723:ALA:HB1	2.51	0.46
8:I:139:LEU:HD21	8:I:192:MET:CE	2.45	0.46
8:I:238:THR:HG22	8:I:548:MET:SD	2.55	0.46
9:J:36:GLU:HG2	9:J:37:PRO:HD2	1.98	0.46
9:J:185:LEU:HD11	9:J:205:PHE:HB2	1.96	0.46
9:K:230:ASN:OD1	9:K:231:LEU:N	2.48	0.46
3:P:120:TYR:CE2	3:P:124:LEU:HD11	2.51	0.46
14:Q:163:LYS:HD3	15:R:466:THR:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:R:190:VAL:HG12	15:R:450:THR:HG21	1.98	0.46
17:Y:350:PHE:CZ	17:Y:378:LEU:HD12	2.50	0.46
1:A:1294:TYR:CD1	1:A:1294:TYR:C	2.89	0.46
3:C:101:ARG:NH2	3:P:296:ARG:HA	2.31	0.46
3:C:120:TYR:CE2	3:C:124:LEU:HD11	2.50	0.46
3:C:359:LYS:HG2	11:M:14:LEU:HD22	1.97	0.46
6:H:58:TYR:OH	6:H:62:LYS:HD2	2.16	0.46
8:I:11:PHE:HD1	8:I:746:MET:HA	1.80	0.46
8:I:45:LEU:CD2	8:I:54:ARG:NH1	2.79	0.46
8:I:73:TRP:CD2	8:I:80:LEU:HD13	2.50	0.46
8:I:142:LEU:HD13	8:I:264:TYR:CE2	2.51	0.46
8:I:189:ALA:N	8:I:193:PHE:O	2.48	0.46
8:I:202:ALA:O	8:I:221:THR:OG1	2.30	0.46
8:I:513:LEU:HD23	13:O:473:LEU:HD11	1.98	0.46
8:I:685:PHE:HA	8:I:701:PRO:HD3	1.98	0.46
9:J:42:TRP:CE3	9:J:42:TRP:HA	2.50	0.46
13:O:126:VAL:HG13	13:O:132:VAL:HG12	1.98	0.46
13:O:292:GLY:HA3	13:O:336:ASP:CB	2.45	0.46
13:O:621:SER:HB3	13:O:651:ILE:HG12	1.96	0.46
15:R:196:ASN:ND2	15:R:211:ALA:HB3	2.31	0.46
15:R:296:ARG:CD	16:S:272:ILE:HG12	2.46	0.46
17:X:87:LEU:HD22	17:X:95:ASN:HD22	1.80	0.46
1:A:40:ARG:HG2	13:O:248:PRO:HG2	1.98	0.46
1:A:948:PRO:HB3	1:A:1813:GLN:CD	2.36	0.46
1:A:956:ARG:NH1	1:A:1785:GLU:OE1	2.48	0.46
1:A:1037:VAL:HA	1:A:1040:LEU:HB2	1.98	0.46
9:J:334:GLY:N	9:J:335:PRO:CD	2.79	0.46
17:Y:436:THR:HG23	17:Y:437:LEU:HD12	1.98	0.46
1:A:40:ARG:CZ	13:O:248:PRO:HB2	2.46	0.46
1:A:1079:ALA:HB1	1:A:1556:LEU:CA	2.45	0.46
1:A:1326:TYR:HB2	1:A:1386:TRP:CZ2	2.50	0.46
6:F:58:TYR:OH	6:F:62:LYS:HD2	2.16	0.46
6:H:142:LEU:HA	6:H:146:PRO:HB3	1.97	0.46
6:H:702:ASN:ND2	10:L:180:TYR:CD1	2.84	0.46
9:J:46:CYS:O	9:J:50:THR:OG1	2.22	0.46
9:J:93:LEU:HD12	9:J:93:LEU:N	2.31	0.46
9:J:147:THR:O	9:J:150:THR:HG22	2.16	0.46
9:J:354:MET:CE	9:J:374:ILE:HG23	2.46	0.46
9:K:222:GLU:OE1	9:K:228:GLN:HG3	2.16	0.46
10:L:87:GLU:CD	10:L:146:GLN:HE22	2.19	0.46
13:O:354:ARG:CD	13:O:573:LYS:O	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:290:ARG:NH2	3:P:319:LEU:HD12	2.26	0.46
15:R:85:ALA:O	15:R:88:MET:HB2	2.15	0.46
18:Z:158:ASP:C	18:Z:160:ASP:H	2.19	0.46
18:Z:159:LYS:HE2	18:Z:159:LYS:HB3	1.78	0.46
1:A:1745:PRO:HB3	13:O:609:ALA:HB1	1.97	0.46
3:C:66:PRO:O	3:C:67:LEU:HB3	2.16	0.46
3:C:516:LEU:HD22	3:C:520:TYR:CE2	2.50	0.46
6:H:473:TYR:HD2	6:H:500:TRP:CZ2	2.34	0.46
8:I:45:LEU:HG	8:I:57:SER:HA	1.98	0.46
8:I:286:ARG:O	8:I:290:PHE:CG	2.69	0.46
9:J:445:GLU:CA	9:J:474:LEU:HD23	2.43	0.46
9:J:514:PHE:O	9:J:518:MET:HB2	2.16	0.46
9:K:502:PHE:CZ	9:K:518:MET:HG3	2.51	0.46
13:O:571:CYS:SG	13:O:579:MET:HB3	2.56	0.46
3:P:358:LEU:O	3:P:362:PRO:HB3	2.15	0.46
3:P:365:LEU:HD23	3:P:395:ASN:ND2	2.31	0.46
15:R:127:GLU:HA	15:R:128:ALA:HA	1.70	0.46
16:S:29:VAL:HG11	18:Z:140:THR:HB	1.98	0.46
1:A:776:ASN:HA	1:A:869:ARG:NE	2.31	0.46
1:A:1230:ILE:HG21	15:R:120:LEU:HD23	1.98	0.46
1:A:1246:PRO:HB2	1:A:1249:VAL:HG23	1.98	0.46
3:C:145:GLN:HG3	13:O:246:PHE:CG	2.50	0.46
6:F:563:ASP:OD1	6:F:564:LYS:O	2.34	0.46
6:H:656:MET:SD	9:K:523:ILE:HG23	2.56	0.46
6:H:729:LEU:HD13	6:H:739:VAL:HG22	1.98	0.46
9:K:180:GLU:O	9:K:184:LEU:N	2.35	0.46
12:N:531:PHE:O	12:N:533:PHE:HA	2.15	0.46
13:O:159:GLN:O	13:O:163:GLN:HG2	2.15	0.46
13:O:274:LEU:HD23	13:O:275:LEU:HD12	1.98	0.46
3:P:373:HIS:O	3:P:377:GLU:HG2	2.15	0.46
17:Y:145:CYS:O	17:Y:149:LEU:HG	2.15	0.46
1:A:617:LEU:HD11	1:A:782:GLY:CA	2.46	0.45
3:C:390:HIS:CD2	13:O:280:ARG:NH2	2.84	0.45
8:I:202:ALA:O	8:I:223:VAL:CG2	2.64	0.45
9:K:481:THR:O	9:K:485:ILE:HG13	2.16	0.45
10:L:73:THR:HG22	10:L:131:PRO:HB2	1.97	0.45
12:N:155:THR:HA	12:N:158:ARG:HD2	1.99	0.45
3:P:33:LYS:NZ	3:P:64:ALA:HA	2.30	0.45
17:X:145:CYS:O	17:X:149:LEU:HG	2.15	0.45
1:A:94:TYR:O	1:A:100:VAL:HA	2.16	0.45
1:A:94:TYR:HE1	1:A:96:ALA:HB2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1176:LEU:HD22	1:A:1176:LEU:HA	1.67	0.45
1:A:1522:SER:O	1:A:1526:VAL:HG13	2.17	0.45
1:A:1543:HIS:CD2	1:A:1559:HIS:HE1	2.34	0.45
3:C:92:ALA:O	3:C:96:VAL:HG23	2.16	0.45
3:C:93:TYR:CD1	3:C:98:GLU:OE2	2.69	0.45
8:I:72:ALA:C	8:I:80:LEU:HD12	2.37	0.45
8:I:278:GLU:HA	8:I:281:MET:SD	2.55	0.45
9:J:69:TYR:O	9:J:70:GLU:HB3	2.16	0.45
15:R:261:LEU:CD1	15:R:261:LEU:N	2.79	0.45
17:X:283:ARG:O	17:X:407:LEU:HD12	2.16	0.45
1:A:872:LEU:HD11	1:A:939:PHE:CD2	2.52	0.45
1:A:957:ASP:OD2	1:A:1820:PHE:HZ	1.99	0.45
2:B:17:VAL:CG2	12:N:634:THR:H	2.21	0.45
5:E:55:CYS:O	5:E:58:VAL:HG12	2.17	0.45
6:F:19:TYR:HE2	6:H:50:ARG:CD	2.28	0.45
8:I:74:ARG:HD2	8:I:174:ASN:HD22	1.81	0.45
8:I:166:LYS:O	8:I:170:ASP:N	2.45	0.45
9:J:332:THR:H	9:J:363:LEU:HD11	1.82	0.45
9:J:334:GLY:HA3	9:J:364:MET:SD	2.57	0.45
12:N:519:TYR:HE1	12:N:523:LEU:HD21	1.82	0.45
13:O:62:GLN:O	13:O:66:PRO:CD	2.64	0.45
13:O:226:ASP:OD1	13:O:227:GLU:N	2.48	0.45
13:O:738:ARG:CZ	13:O:738:ARG:HB3	2.45	0.45
3:P:515:TYR:HA	3:P:518:GLN:HG2	1.99	0.45
14:Q:188:ASN:O	14:Q:231:SER:HA	2.16	0.45
15:R:442:HIS:CE1	15:R:468:ARG:HD2	2.51	0.45
17:X:338:HIS:O	17:X:341:PRO:HD2	2.16	0.45
1:A:613:ALA:HB1	1:A:619:GLN:HB2	1.98	0.45
1:A:628:ILE:HG12	1:A:765:VAL:HG11	1.98	0.45
1:A:860:TYR:CG	1:A:861:PRO:HD2	2.51	0.45
1:A:1019:MET:HB2	1:A:1021:HIS:CE1	2.52	0.45
1:A:1086:MET:HG2	1:A:1610:TYR:CE1	2.52	0.45
8:I:737:ASN:OD1	8:I:738:LEU:N	2.49	0.45
9:K:248:LYS:HB2	9:K:438:GLU:OE2	2.17	0.45
13:O:402:LEU:HD13	13:O:425:LYS:HE2	1.98	0.45
16:S:58:GLN:O	16:S:62:PHE:CE2	2.65	0.45
16:S:200:VAL:HG23	16:S:201:SER:N	2.32	0.45
16:S:261:PRO:O	16:S:263:PRO:N	2.49	0.45
17:X:87:LEU:HD22	17:X:95:ASN:ND2	2.30	0.45
17:X:168:THR:OG1	17:X:171:ILE:HD12	2.17	0.45
17:Y:316:ALA:HB1	17:Y:351:TYR:CZ	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Z:75:TRP:NE1	18:Z:161:LEU:HD21	2.31	0.45
1:A:1089:LEU:CD1	1:A:1611:VAL:HG23	2.45	0.45
2:B:42:ASP:O	2:B:43:ASP:CB	2.64	0.45
6:F:639:TYR:CD1	15:R:498:ILE:HG21	2.52	0.45
6:H:515:TYR:CE2	6:H:545:HIS:CD2	3.03	0.45
9:K:384:SER:HB3	9:K:415:ASN:OD1	2.16	0.45
10:L:98:VAL:HB	10:L:134:THR:HG21	1.99	0.45
13:O:83:GLU:HG3	13:O:90:ALA:CB	2.47	0.45
3:P:92:ALA:O	3:P:96:VAL:HG23	2.16	0.45
14:Q:179:PRO:HB3	16:S:555:ARG:CZ	2.47	0.45
14:Q:261:LEU:N	14:Q:261:LEU:CD1	2.79	0.45
14:Q:498:ILE:O	14:Q:499:ARG:HB2	2.16	0.45
15:R:88:MET:O	15:R:91:ALA:HB3	2.16	0.45
16:S:29:VAL:CG1	16:S:36:ARG:CZ	2.91	0.45
16:S:41:LEU:HD12	18:Z:141:PHE:CB	2.47	0.45
18:Z:83:LYS:HA	18:Z:102:PHE:O	2.17	0.45
1:A:617:LEU:HD11	1:A:782:GLY:HA3	1.97	0.45
1:A:1540:ARG:NH1	12:N:486:ASP:O	2.50	0.45
5:E:96:PHE:HB2	6:H:595:GLN:HE21	1.82	0.45
8:I:300:VAL:C	8:I:303:GLU:HB2	2.36	0.45
9:J:376:LEU:CD2	9:J:407:GLU:HG2	2.47	0.45
12:N:76:VAL:O	12:N:80:GLN:HB3	2.16	0.45
3:P:379:LYS:HA	3:P:379:LYS:HD2	1.75	0.45
14:Q:190:VAL:HG12	14:Q:450:THR:HG21	1.99	0.45
1:A:42:LEU:HD21	3:C:394:VAL:HG13	1.99	0.45
1:A:1138:HIS:O	1:A:1141:VAL:N	2.50	0.45
8:I:118:VAL:HG12	8:I:173:LEU:O	2.16	0.45
9:J:354:MET:HE2	9:J:374:ILE:HG23	1.98	0.45
9:K:231:LEU:HA	9:K:234:VAL:HG22	1.98	0.45
12:N:281:TYR:HE2	12:N:356:PRO:HB2	1.71	0.45
13:O:119:PHE:CZ	13:O:136:LEU:HD11	2.52	0.45
16:S:85:THR:HB	16:S:98:MET:CE	2.47	0.45
17:X:442:GLN:CG	17:X:472:ARG:CG	2.79	0.45
17:Y:341:PRO:O	17:Y:344:VAL:HG12	2.16	0.45
17:Y:485:LEU:O	17:Y:489:GLU:HG2	2.17	0.45
18:Z:56:THR:HG23	18:Z:62:ILE:HG13	1.99	0.45
1:A:239:VAL:HG21	1:A:409:ILE:HD12	1.97	0.45
1:A:1145:LEU:HD22	1:A:1611:VAL:HG21	1.99	0.45
5:E:89:LEU:HD21	6:H:588:LYS:HB3	1.98	0.45
6:H:639:TYR:CD1	6:H:658:PHE:HE1	2.35	0.45
8:I:116:MET:SD	8:I:210:LEU:CG	3.02	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:304:PHE:CZ	8:I:448:VAL:HG13	2.51	0.45
9:J:418:TRP:CZ3	9:J:457:LYS:HG3	2.52	0.45
12:N:570:ILE:CD1	12:N:633:ARG:NH1	2.73	0.45
13:O:604:LEU:HB3	13:O:627:LEU:CD2	2.46	0.45
3:P:242:GLN:O	3:P:243:LEU:HB2	2.17	0.45
3:P:312:MET:H	3:P:312:MET:HG2	1.62	0.45
3:P:402:TRP:CH2	3:P:424:ARG:HG2	2.52	0.45
3:P:487:ALA:HB1	3:P:519:TYR:HE1	1.82	0.45
16:S:85:THR:HB	16:S:98:MET:HE2	1.99	0.45
17:X:134:SER:O	17:X:138:VAL:HG23	2.17	0.45
1:A:93:LEU:HD21	1:A:151:ILE:HG13	1.99	0.45
1:A:1279:ARG:HG2	1:A:1280:PRO:HD2	1.98	0.45
2:B:16:TRP:CD1	2:B:33:CYS:CA	2.86	0.45
3:C:494:ILE:HA	3:C:497:ILE:HD12	1.99	0.45
6:H:556:SER:OG	6:H:573:ALA:HA	2.17	0.45
8:I:12:ARG:O	8:I:744:PHE:HA	2.17	0.45
8:I:17:LYS:HE3	8:I:51:SER:O	2.15	0.45
8:I:224:SER:HB2	8:I:230:GLU:H	1.81	0.45
8:I:276:TRP:CZ2	8:I:280:LEU:HD22	2.51	0.45
9:K:277:GLU:OE1	9:K:277:GLU:HA	2.16	0.45
13:O:394:THR:HA	13:O:615:ARG:NH1	2.32	0.45
3:P:273:TYR:HB3	3:P:282:ALA:HB2	1.99	0.45
14:Q:355:GLN:O	18:Z:136:THR:HG21	2.17	0.45
17:Y:532:TYR:CE1	17:Y:548:GLY:HA3	2.52	0.45
1:A:87:VAL:HG12	1:A:88:ASP:N	2.32	0.45
1:A:1189:ALA:HB3	1:A:1192:ASN:HD22	1.81	0.45
3:C:550:LEU:O	3:C:553:ILE:HG12	2.17	0.45
6:F:465:LEU:HD22	6:F:495:HIS:CE1	2.52	0.45
9:J:50:THR:O	9:J:50:THR:HG22	2.16	0.45
9:K:50:THR:HG22	9:K:50:THR:O	2.17	0.45
10:L:24:GLU:HA	10:L:158:ILE:O	2.16	0.45
12:N:268:VAL:HA	12:N:271:GLU:CD	2.38	0.45
12:N:434:THR:O	12:N:437:GLN:N	2.50	0.45
3:P:66:PRO:HD2	3:P:68:ALA:O	2.17	0.45
15:R:84:SER:HB2	15:R:87:GLN:HB3	1.99	0.45
16:S:134:GLU:C	16:S:136:LEU:N	2.68	0.45
17:Y:406:ARG:HB2	17:Y:409:CYS:SG	2.57	0.45
1:A:1781:GLN:HB2	1:A:1783:THR:HG22	1.98	0.44
6:F:130:ARG:HD2	6:F:133:LYS:HD3	1.99	0.44
8:I:347:LEU:O	8:I:351:HIS:HB2	2.17	0.44
9:J:468:HIS:HB3	9:J:485:ILE:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:N:400:TYR:CZ	12:N:404:ILE:HD11	2.52	0.44
12:N:574:ILE:HG13	12:N:625:LYS:HE2	1.99	0.44
12:N:655:LEU:HA	12:N:724:ARG:O	2.17	0.44
14:Q:461:ALA:HB2	14:Q:467:LEU:CD1	2.47	0.44
17:X:87:LEU:HD13	17:X:95:ASN:ND2	2.31	0.44
17:X:134:SER:N	17:X:137:GLU:OE1	2.50	0.44
17:X:235:TRP:NE1	17:Y:63:MET:SD	2.90	0.44
3:C:89:LEU:HD12	3:P:60:PHE:HB2	1.99	0.44
3:C:96:VAL:N	3:C:97:LYS:HA	2.32	0.44
6:H:689:LEU:HD11	6:H:716:ASN:HD21	1.81	0.44
12:N:74:TRP:CG	12:N:75:PHE:N	2.85	0.44
13:O:99:LEU:C	13:O:99:LEU:HD12	2.37	0.44
16:S:162:TYR:HD2	16:S:174:ILE:CD1	2.30	0.44
17:Y:168:THR:OG1	17:Y:171:ILE:HD12	2.18	0.44
1:A:173:LEU:HA	1:A:174:PRO:HD2	1.88	0.44
1:A:268:VAL:O	1:A:412:LEU:HD23	2.17	0.44
3:C:126:GLY:C	3:C:148:ASN:OD1	2.55	0.44
7:G:15:ASP:O	9:J:487:TYR:OH	2.34	0.44
6:H:473:TYR:CD2	6:H:500:TRP:HZ2	2.35	0.44
6:H:703:PRO:CD	10:L:180:TYR:CD2	3.00	0.44
8:I:269:LEU:HD11	8:I:522:LEU:HD13	1.99	0.44
8:I:276:TRP:CZ3	8:I:476:GLY:HA3	2.52	0.44
8:I:410:SER:O	8:I:413:ASN:HB2	2.17	0.44
9:J:163:CYS:O	9:J:163:CYS:SG	2.75	0.44
9:J:227:LEU:HD22	9:J:233:VAL:HG11	2.00	0.44
9:J:476:PRO:HB2	3:P:148:ASN:ND2	2.32	0.44
12:N:550:GLY:HA2	12:N:551:GLU:HB2	1.99	0.44
12:N:609:LEU:HD22	12:N:639:HIS:HD2	1.83	0.44
16:S:25:SER:HB2	16:S:45:LEU:CG	2.47	0.44
16:S:30:GLN:CB	16:S:91:GLN:CB	2.92	0.44
17:X:485:LEU:O	17:X:489:GLU:HG2	2.17	0.44
17:Y:87:LEU:HD11	17:Y:99:LYS:HG3	1.99	0.44
17:Y:261:LEU:HD22	17:Y:267:LEU:HD23	1.99	0.44
1:A:482:VAL:HG22	1:A:593:ASN:HA	2.00	0.44
1:A:1790:TYR:O	1:A:1793:MET:HB2	2.17	0.44
7:G:13:LEU:HA	7:G:16:ILE:HD12	1.98	0.44
6:H:545:HIS:HE1	10:L:182:SER:O	2.00	0.44
8:I:65:GLY:O	8:I:84:LEU:HD12	2.18	0.44
9:K:509:ARG:HG3	9:K:512:ASP:HB2	2.00	0.44
12:N:478:GLU:H	12:N:479:ASP:HA	1.82	0.44
12:N:699:TRP:HB3	12:N:705:LEU:HD23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:286:PHE:HB3	3:P:303:PHE:CE2	2.53	0.44
16:S:163:GLU:CD	16:S:196:PHE:CD1	2.80	0.44
17:X:410:TYR:O	17:X:414:ILE:HG22	2.17	0.44
17:Y:546:LEU:O	17:Y:550:GLN:HG2	2.17	0.44
1:A:1216:LYS:HD2	1:A:1216:LYS:N	2.32	0.44
1:A:1279:ARG:NH1	1:A:1287:TYR:OH	2.51	0.44
6:F:734:PRO:HB2	9:J:144:ASP:HB3	1.99	0.44
8:I:224:SER:HB3	8:I:229:SER:HA	1.96	0.44
8:I:430:GLU:HA	14:Q:429:LYS:HE2	1.99	0.44
12:N:186:GLN:O	12:N:190:LYS:HG3	2.18	0.44
13:O:416:GLU:O	13:O:420:ILE:HG22	2.18	0.44
3:P:283:LEU:HD13	3:P:306:LEU:HD11	2.00	0.44
17:Y:99:LYS:HD3	17:Y:102:MET:CE	2.48	0.44
17:Y:281:TYR:HB3	17:Y:290:SER:OG	2.17	0.44
1:A:872:LEU:HD11	1:A:939:PHE:HB2	1.99	0.44
1:A:1194:HIS:CG	15:R:121:ASN:HD21	2.36	0.44
1:A:1845:LEU:N	1:A:1846:PRO:HD2	2.32	0.44
4:D:14:GLU:HB2	4:D:17:TRP:CZ3	2.53	0.44
6:F:26:PHE:CD1	6:H:149:TRP:CG	3.06	0.44
6:H:483:GLU:O	6:H:487:ILE:HG12	2.17	0.44
6:H:703:PRO:HB3	6:H:733:VAL:CG2	2.47	0.44
8:I:360:LEU:HD12	8:I:397:ILE:CD1	2.47	0.44
9:K:147:THR:O	9:K:150:THR:HG22	2.18	0.44
9:K:163:CYS:O	9:K:163:CYS:SG	2.76	0.44
9:K:404:VAL:O	9:K:408:VAL:HG23	2.18	0.44
14:Q:185:TYR:CD1	16:S:27:GLU:CG	3.01	0.44
14:Q:425:LEU:HB2	14:Q:439:LEU:HB2	1.99	0.44
17:X:149:LEU:O	17:X:150:LYS:HB2	2.17	0.44
17:X:199:CYS:HA	17:X:200:PRO:HD2	1.81	0.44
17:X:371:ASN:HD22	17:X:371:ASN:N	2.09	0.44
17:Y:305:ILE:HG22	17:Y:340:GLU:OE1	2.17	0.44
1:A:454:CYS:O	1:A:471:VAL:HA	2.18	0.44
1:A:1136:SER:OG	1:A:1171:GLU:HB3	2.17	0.44
1:A:1599:ASN:HB2	1:A:1603:LEU:H	1.83	0.44
6:H:522:PHE:O	6:H:525:VAL:HB	2.18	0.44
8:I:44:VAL:C	8:I:45:LEU:HD12	2.37	0.44
9:J:306:GLY:HA3	9:J:323:LEU:HD13	1.99	0.44
9:K:222:GLU:OE2	9:K:228:GLN:HG3	2.18	0.44
9:K:337:TRP:HB3	9:K:360:ALA:HB2	1.98	0.44
12:N:648:VAL:CG1	12:N:650:LEU:HG	2.47	0.44
16:S:30:GLN:CB	16:S:36:ARG:HH21	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:S:41:LEU:HD21	16:S:90:PRO:HB3	1.98	0.44
16:S:59:LYS:HA	16:S:62:PHE:HD2	1.82	0.44
16:S:83:SER:O	16:S:87:GLN:CB	2.65	0.44
17:X:270:ASN:HA	17:Y:62:THR:HG21	1.99	0.44
17:X:281:TYR:HB3	17:X:290:SER:OG	2.17	0.44
1:A:42:LEU:HD13	3:C:363:ARG:HG3	2.00	0.44
1:A:174:PRO:HG3	1:A:356:PHE:CE2	2.53	0.44
1:A:1671:PRO:HB2	1:A:1705:GLN:HE22	1.82	0.44
3:C:60:PHE:CG	3:P:89:LEU:HD12	2.52	0.44
3:C:61:SER:CB	3:C:262:SER:HB2	2.46	0.44
3:C:66:PRO:HD2	3:C:68:ALA:O	2.17	0.44
3:C:296:ARG:HA	3:P:101:ARG:NH2	2.33	0.44
6:F:89:GLU:CD	6:F:130:ARG:NH2	2.71	0.44
6:F:483:GLU:O	6:F:487:ILE:HG12	2.17	0.44
6:H:621:LEU:HG	6:H:644:ILE:HG21	1.99	0.44
8:I:96:GLU:OE1	12:N:427:TYR:HE1	2.01	0.44
8:I:420:TRP:HB2	8:I:440:MET:HE1	1.99	0.44
9:J:477:GLN:O	9:J:508:LEU:HD13	2.17	0.44
9:J:509:ARG:HD2	9:J:512:ASP:HB2	1.99	0.44
10:L:113:LEU:HD13	10:L:120:ILE:HD13	1.99	0.44
3:P:48:LEU:N	3:P:48:LEU:HD23	2.33	0.44
3:P:96:VAL:N	3:P:97:LYS:HA	2.33	0.44
3:P:402:TRP:HZ3	3:P:421:TYR:HD1	1.66	0.44
14:Q:411:TYR:CE1	14:Q:475:LEU:CD2	3.01	0.44
16:S:75:LEU:O	16:S:75:LEU:HD22	2.18	0.44
17:Y:100:TYR:HB2	17:Y:142:MET:HG2	2.00	0.44
1:A:1194:HIS:CD2	15:R:121:ASN:HD21	2.36	0.44
1:A:1552:TYR:OH	1:A:1604:GLN:NE2	2.51	0.44
1:A:1571:ARG:NH1	1:A:1694:ASP:O	2.51	0.44
6:F:522:PHE:O	6:F:525:VAL:HB	2.18	0.44
9:K:391:PHE:CE2	9:K:411:VAL:HG21	2.53	0.44
12:N:165:THR:N	12:N:166:PRO:CA	2.79	0.44
17:X:316:ALA:HB1	17:X:351:TYR:CZ	2.53	0.44
17:Y:39:ASP:OD1	17:Y:39:ASP:N	2.50	0.44
1:A:1621:PRO:HA	1:A:1697:LEU:O	2.18	0.43
2:B:36:ASP:O	2:B:38:LYS:N	2.51	0.43
3:C:148:ASN:HB3	3:C:151:LEU:CD1	2.48	0.43
3:C:358:LEU:O	3:C:362:PRO:CA	2.65	0.43
5:E:78:ARG:NH2	6:H:554:VAL:HG22	2.33	0.43
6:F:556:SER:OG	6:F:573:ALA:HA	2.18	0.43
6:H:489:SER:O	17:X:105:GLN:NE2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:552:LEU:HG	6:H:576:CYS:SG	2.57	0.43
9:K:74:TYR:OH	9:K:78:ARG:HD2	2.17	0.43
9:K:272:ILE:HG21	9:K:303:PHE:CE2	2.53	0.43
9:K:289:HIS:CD2	11:M:57:TRP:CE3	3.06	0.43
9:K:372:LEU:HD11	9:K:407:GLU:CG	2.47	0.43
12:N:574:ILE:HA	12:N:625:LYS:HE2	2.00	0.43
13:O:386:GLN:HB2	13:O:424:GLN:NE2	2.32	0.43
15:R:96:SER:O	15:R:99:ASN:HB2	2.18	0.43
16:S:58:GLN:NE2	16:S:62:PHE:CZ	2.75	0.43
16:S:134:GLU:N	16:S:135:PRO:HD3	2.33	0.43
1:A:119:VAL:HG11	1:A:153:ILE:HG21	2.00	0.43
1:A:1041:LEU:HD13	1:A:1084:ARG:HA	2.00	0.43
1:A:1254:VAL:HG11	1:A:1298:ALA:CA	2.44	0.43
1:A:1634:LEU:O	1:A:1650:GLU:HA	2.18	0.43
1:A:1637:THR:OG1	1:A:1665:GLN:HG3	2.18	0.43
3:C:36:LEU:O	3:C:39:ILE:HG22	2.19	0.43
8:I:294:LYS:CB	8:I:320:LEU:HD22	2.49	0.43
9:J:432:ILE:HD11	9:J:444:TRP:CD1	2.53	0.43
9:K:146:ARG:CZ	9:K:332:THR:HG22	2.48	0.43
9:K:167:PHE:CE1	9:K:171:THR:HG21	2.53	0.43
9:K:178:ALA:HA	9:K:181:GLU:CD	2.38	0.43
12:N:404:ILE:HA	12:N:417:LEU:HD11	2.00	0.43
3:P:158:LEU:HD11	3:P:174:LEU:CD1	2.48	0.43
15:R:188:ASN:O	15:R:231:SER:HA	2.17	0.43
15:R:425:LEU:HB2	15:R:439:LEU:HB2	1.99	0.43
16:S:84:TRP:O	16:S:88:ASN:CG	2.57	0.43
17:Y:134:SER:N	17:Y:137:GLU:OE1	2.51	0.43
1:A:161:MET:HG3	1:A:216:PRO:HB3	2.00	0.43
1:A:790:LEU:HD13	1:A:806:TYR:OH	2.18	0.43
2:B:16:TRP:HB3	2:B:33:CYS:HB3	1.99	0.43
3:C:89:LEU:HD12	3:P:60:PHE:CB	2.49	0.43
3:C:145:GLN:HG2	13:O:246:PHE:HA	1.99	0.43
6:H:657:HIS:HA	6:H:660:LYS:HE3	2.00	0.43
6:H:747:TYR:CD2	6:H:755:LEU:HB3	2.53	0.43
9:J:441:VAL:HG23	9:J:442:ASP:N	2.33	0.43
12:N:560:MET:HA	12:N:560:MET:HE2	2.01	0.43
12:N:602:PRO:N	12:N:603:PRO:HD2	2.32	0.43
3:P:242:GLN:NE2	3:P:428:LEU:O	2.51	0.43
14:Q:185:TYR:CD1	16:S:27:GLU:HG3	2.53	0.43
15:R:84:SER:O	15:R:88:MET:N	2.51	0.43
16:S:38:MET:HB3	18:Z:181:VAL:CG2	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:39:ASP:OD1	17:X:39:ASP:N	2.51	0.43
17:Y:100:TYR:CB	17:Y:142:MET:CG	2.96	0.43
18:Z:170:SER:OG	18:Z:171:GLY:N	2.51	0.43
1:A:409:ILE:HG22	1:A:410:ASP:N	2.33	0.43
2:B:38:LYS:HG2	2:B:40:PRO:HG2	1.99	0.43
2:B:62:LYS:O	2:B:69:VAL:HG21	2.17	0.43
8:I:430:GLU:CD	14:Q:429:LYS:CG	2.86	0.43
9:J:167:PHE:HA	9:J:170:LEU:HD21	1.99	0.43
9:J:242:TYR:HB2	9:J:250:CYS:SG	2.59	0.43
10:L:33:LEU:HD13	10:L:54:TRP:CD2	2.53	0.43
12:N:527:LEU:HD11	12:N:561:LEU:HD22	2.00	0.43
13:O:402:LEU:HD13	13:O:425:LYS:HG2	1.99	0.43
3:P:209:LEU:HB3	3:P:233:PHE:HE1	1.82	0.43
16:S:162:TYR:CD2	16:S:174:ILE:CD1	3.01	0.43
17:X:341:PRO:O	17:X:344:VAL:HG12	2.18	0.43
17:Y:149:LEU:O	17:Y:150:LYS:HB2	2.18	0.43
17:Y:437:LEU:CB	17:Y:444:LEU:HD11	2.48	0.43
1:A:777:THR:HB	1:A:946:THR:O	2.18	0.43
1:A:1138:HIS:CE1	1:A:1604:GLN:HE21	2.26	0.43
1:A:1194:HIS:CB	15:R:121:ASN:HD21	2.31	0.43
1:A:1230:ILE:CA	1:A:1236:LEU:HD13	2.49	0.43
1:A:1404:LEU:CD2	1:A:1464:ILE:HD11	2.46	0.43
1:A:1839:PHE:CD1	1:A:1840:MET:HG3	2.53	0.43
3:C:356:ARG:NH2	11:M:19:TRP:HA	2.33	0.43
4:D:6:PRO:HB2	13:O:420:ILE:HG13	2.01	0.43
4:D:18:PHE:O	4:D:18:PHE:CG	2.71	0.43
8:I:202:ALA:C	8:I:223:VAL:HG22	2.38	0.43
8:I:312:LYS:CG	8:I:428:MET:HB3	2.45	0.43
9:J:247:PHE:CE2	9:J:277:GLU:HG3	2.54	0.43
13:O:663:ALA:O	13:O:667:VAL:HG23	2.18	0.43
1:A:845:TYR:CE1	1:A:951:ILE:HD11	2.52	0.43
1:A:1512:LEU:HA	1:A:1515:CYS:SG	2.58	0.43
1:A:1618:LEU:HA	1:A:1656:LEU:HA	2.01	0.43
1:A:1666:ILE:HG21	1:A:1687:LEU:HD11	2.01	0.43
2:B:16:TRP:HB3	2:B:33:CYS:CA	2.48	0.43
6:F:75:LEU:HG	6:F:91:ILE:HD13	2.00	0.43
8:I:95:VAL:HG12	12:N:389:PRO:HG2	2.01	0.43
8:I:231:VAL:CG1	8:I:556:LEU:HD12	2.48	0.43
9:K:276:VAL:HA	9:K:311:MET:CE	2.49	0.43
10:L:125:THR:CA	10:L:126:ASP:HB3	2.49	0.43
12:N:560:MET:HA	12:N:560:MET:HE3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:601:LEU:HB2	13:O:602:PRO:HD3	2.00	0.43
15:R:179:PRO:HG2	16:S:226:THR:HG22	2.00	0.43
16:S:88:ASN:ND2	16:S:88:ASN:N	2.67	0.43
17:X:50:HIS:HA	17:X:53:VAL:HG22	1.99	0.43
1:A:501:THR:HB	1:A:504:VAL:HG22	2.01	0.43
1:A:871:ARG:HG3	1:A:872:LEU:N	2.34	0.43
1:A:1024:MET:HG2	1:A:1034:VAL:HG11	2.00	0.43
1:A:1110:ARG:HG2	1:A:1117:THR:HG22	2.00	0.43
1:A:1166:ALA:HA	1:A:1169:ALA:HB2	1.99	0.43
1:A:1170:ASN:HD21	1:A:1203:MET:HG3	1.83	0.43
1:A:1304:MET:O	1:A:1307:LEU:HB2	2.18	0.43
1:A:1610:TYR:CD1	1:A:1610:TYR:C	2.92	0.43
2:B:27:ARG:CB	12:N:810:TYR:CE2	2.96	0.43
6:F:130:ARG:HD3	17:Y:506:GLN:HB2	2.00	0.43
6:H:513:SER:HA	6:H:515:TYR:CE1	2.54	0.43
6:H:537:GLU:CD	6:H:568:GLU:OE1	2.57	0.43
9:J:404:VAL:O	9:J:408:VAL:HG23	2.19	0.43
9:J:465:LEU:HD22	9:J:469:ARG:HH11	1.83	0.43
9:K:268:LEU:N	9:K:269:PRO:HD2	2.34	0.43
9:K:432:ILE:HD11	9:K:444:TRP:CD1	2.54	0.43
10:L:14:LYS:HA	10:L:17:GLU:OE1	2.19	0.43
13:O:324:LEU:HD22	13:O:350:LEU:HD12	2.00	0.43
13:O:385:VAL:HG11	13:O:402:LEU:HG	2.01	0.43
3:P:170:PHE:O	3:P:171:GLY:C	2.56	0.43
14:Q:163:LYS:NZ	16:S:224:ARG:HH22	2.16	0.43
16:S:64:TYR:HH	16:S:84:TRP:HD1	1.63	0.43
1:A:457:PHE:HB3	1:A:468:PHE:CE1	2.53	0.43
3:C:67:LEU:HD22	3:P:78:GLU:HA	2.01	0.43
6:H:761:SER:O	6:H:765:ASP:N	2.51	0.43
8:I:207:ALA:HB3	8:I:220:VAL:HB	2.00	0.43
8:I:320:LEU:HA	8:I:320:LEU:HD12	1.75	0.43
8:I:497:TRP:HH2	8:I:507:LEU:HD13	1.81	0.43
9:K:230:ASN:O	9:K:233:VAL:HG22	2.18	0.43
9:K:272:ILE:HG23	9:K:307:CYS:SG	2.59	0.43
9:K:309:TYR:HD2	9:K:315:LYS:HB3	1.83	0.43
3:P:209:LEU:HB3	3:P:233:PHE:CE1	2.53	0.43
15:R:357:ALA:CB	16:S:305:GLU:HG3	2.48	0.43
15:R:498:ILE:O	15:R:499:ARG:HB2	2.19	0.43
16:S:78:TRP:CD1	16:S:109:LEU:HD11	2.54	0.43
17:X:267:LEU:CD1	17:Y:59:LEU:HD11	2.39	0.43
2:B:47:VAL:HG21	2:B:82:PHE:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:46:ARG:HB3	3:C:116:PHE:CE2	2.53	0.43
3:C:414:MET:HG2	13:O:330:ILE:HD13	1.95	0.43
6:F:96:VAL:O	6:F:97:PHE:HB2	2.18	0.43
6:H:515:TYR:HD1	6:H:515:TYR:H	1.66	0.43
6:H:673:CYS:O	6:H:677:VAL:HG23	2.19	0.43
8:I:290:PHE:HE2	8:I:325:LEU:HD12	1.84	0.43
8:I:306:HIS:HE1	8:I:316:GLU:HB3	1.83	0.43
9:J:268:LEU:N	9:J:269:PRO:HD2	2.33	0.43
12:N:501:ILE:HD13	12:N:548:ARG:NH2	2.34	0.43
13:O:648:ILE:O	13:O:652:LEU:HG	2.19	0.43
16:S:38:MET:HE2	18:Z:181:VAL:CB	2.38	0.43
16:S:66:ILE:O	16:S:69:TYR:HB2	2.19	0.43
16:S:68:PHE:HE1	16:S:78:TRP:HA	1.82	0.43
17:X:222:MET:O	17:X:226:VAL:HG23	2.19	0.43
1:A:1165:HIS:HD2	1:A:1167:GLU:H	1.67	0.43
1:A:1550:MET:SD	1:A:1558:HIS:HE1	2.42	0.43
1:A:1595:HIS:NE2	1:A:1598:ASP:HB2	2.34	0.43
2:B:8:TRP:NE1	12:N:644:VAL:HG12	2.34	0.43
2:B:26:CYS:HB3	2:B:59:CYS:SG	2.59	0.43
3:C:54:TRP:CE3	3:C:203:TRP:HB2	2.54	0.43
6:F:142:LEU:HA	6:F:146:PRO:HB3	2.00	0.43
6:H:702:ASN:HA	6:H:703:PRO:HD3	1.91	0.43
8:I:74:ARG:HD2	8:I:174:ASN:ND2	2.34	0.43
8:I:313:ALA:HB3	8:I:317:LEU:CD1	2.47	0.43
8:I:427:ARG:HB2	8:I:428:MET:HE3	2.01	0.43
12:N:556:PHE:CE1	12:N:600:PHE:HA	2.54	0.43
13:O:56:GLU:HB3	13:O:86:CYS:SG	2.59	0.43
15:R:258:GLN:O	15:R:258:GLN:HG2	2.19	0.43
16:S:70:THR:O	16:S:74:PRO:CD	2.65	0.43
16:S:200:VAL:O	16:S:204:THR:HG23	2.19	0.43
7:W:5:LYS:HB3	7:W:5:LYS:HE3	1.76	0.43
17:Y:134:SER:O	17:Y:138:VAL:HG23	2.18	0.43
1:A:1036:ASP:O	1:A:1040:LEU:HD13	2.19	0.42
1:A:1250:GLN:O	1:A:1254:VAL:HG23	2.19	0.42
8:I:19:LEU:HD13	8:I:23:ILE:HG13	2.00	0.42
12:N:151:GLU:O	12:N:155:THR:HG23	2.19	0.42
15:R:112:HIS:NE2	15:R:116:TRP:CZ3	2.80	0.42
16:S:33:ARG:HA	18:Z:144:LEU:HG	2.01	0.42
7:W:13:LEU:HA	7:W:16:ILE:HD12	2.01	0.42
17:X:430:ALA:HB2	17:X:451:CYS:SG	2.59	0.42
17:Y:170:LYS:HG2	17:Y:171:ILE:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Y:222:MET:O	17:Y:226:VAL:HG23	2.18	0.42
17:Y:410:TYR:O	17:Y:414:ILE:HG22	2.19	0.42
1:A:131:PHE:HE1	1:A:187:LEU:HB2	1.84	0.42
1:A:487:THR:HG22	1:A:501:THR:HA	2.00	0.42
1:A:1162:LYS:HZ2	1:A:1196:TYR:HE1	1.65	0.42
1:A:1190:THR:O	1:A:1193:ILE:HB	2.19	0.42
1:A:1813:GLN:O	1:A:1817:VAL:HG23	2.19	0.42
3:C:414:MET:HG3	13:O:330:ILE:HD11	1.99	0.42
8:I:280:LEU:O	8:I:280:LEU:HG	2.19	0.42
9:J:42:TRP:HA	9:J:42:TRP:HE3	1.83	0.42
9:J:482:TYR:CD1	9:J:485:ILE:HD11	2.54	0.42
9:K:386:LEU:HD12	9:K:386:LEU:N	2.34	0.42
12:N:395:ASP:OD1	12:N:398:THR:HG23	2.18	0.42
12:N:455:THR:CB	12:N:501:ILE:HD11	2.49	0.42
13:O:40:LEU:HD22	13:O:82:ILE:HD12	2.00	0.42
16:S:75:LEU:CB	16:S:115:TYR:OH	2.62	0.42
18:Z:163:VAL:HA	18:Z:164:PRO:HD3	1.85	0.42
1:A:250:ASN:HD22	1:A:251:THR:N	2.17	0.42
1:A:1360:VAL:HB	1:A:1364:CYS:HB2	2.00	0.42
6:F:61:LEU:HD23	6:F:61:LEU:HA	1.94	0.42
6:F:135:SER:OG	6:F:160:GLU:HG3	2.18	0.42
6:H:49:TYR:HD1	6:H:78:CYS:HG	1.67	0.42
9:J:210:LYS:HE3	9:J:212:TYR:CZ	2.54	0.42
9:K:289:HIS:ND1	11:M:57:TRP:CZ3	2.87	0.42
12:N:570:ILE:CD1	12:N:633:ARG:HH12	2.22	0.42
12:N:662:VAL:HB	12:N:687:MET:SD	2.58	0.42
3:P:399:TYR:CE2	14:Q:498:ILE:CG2	3.02	0.42
14:Q:258:GLN:HG2	14:Q:258:GLN:O	2.19	0.42
16:S:82:ILE:HG21	16:S:127:LYS:HD3	2.02	0.42
17:Y:465:LEU:HD23	17:Y:485:LEU:HD11	2.01	0.42
1:A:280:ASN:C	1:A:346:ASN:N	2.71	0.42
1:A:877:ILE:HG23	1:A:881:ILE:HD12	2.00	0.42
3:C:60:PHE:CB	3:P:89:LEU:HD12	2.49	0.42
3:C:402:TRP:HZ3	3:C:421:TYR:HD1	1.66	0.42
6:F:621:LEU:HG	6:F:644:ILE:HG21	2.00	0.42
6:H:703:PRO:CD	10:L:180:TYR:CE2	3.02	0.42
8:I:285:SER:O	8:I:289:LYS:HG2	2.19	0.42
8:I:474:ARG:O	8:I:477:GLN:HG3	2.19	0.42
10:L:83:TYR:N	10:L:116:PRO:O	2.53	0.42
12:N:574:ILE:CD1	12:N:625:LYS:HG2	2.34	0.42
12:N:669:TYR:CZ	12:N:684:ALA:HB1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:151:LEU:HB3	3:P:182:LEU:HD11	2.02	0.42
17:X:270:ASN:HB2	17:X:273:LEU:HB2	2.01	0.42
1:A:802:TYR:CZ	1:A:841:PRO:HA	2.54	0.42
1:A:1194:HIS:NE2	15:R:117:ALA:HA	2.35	0.42
1:A:1316:MET:O	1:A:1319:LEU:O	2.38	0.42
1:A:1322:PRO:CG	1:A:1375:TYR:OH	2.54	0.42
6:F:134:GLY:O	6:F:137:CYS:HB3	2.19	0.42
6:H:473:TYR:CD2	6:H:500:TRP:CZ2	3.08	0.42
9:J:18:GLN:NE2	9:K:134:LEU:CD1	2.83	0.42
9:K:251:TYR:HA	9:K:254:THR:HG22	2.01	0.42
11:M:32:PRO:C	11:M:34:ASN:H	2.22	0.42
12:N:506:VAL:O	12:N:510:GLY:HA3	2.19	0.42
12:N:772:ARG:HB3	12:N:776:MET:HE1	2.01	0.42
13:O:594:SER:O	13:O:595:SER:HB3	2.19	0.42
3:P:417:TYR:O	3:P:421:TYR:CD2	2.72	0.42
14:Q:420:PHE:HB3	16:S:31:PRO:HD2	2.02	0.42
17:X:465:LEU:HD23	17:X:485:LEU:HD11	2.02	0.42
1:A:93:LEU:HB2	1:A:128:TRP:CH2	2.54	0.42
1:A:1249:VAL:O	1:A:1252:ALA:HB3	2.20	0.42
1:A:1307:LEU:HD21	1:A:1579:SER:HA	2.01	0.42
3:C:158:LEU:HD11	3:C:174:LEU:CD1	2.49	0.42
9:J:61:ARG:HG2	9:J:61:ARG:NH1	2.34	0.42
9:J:497:ASN:N	9:J:497:ASN:OD1	2.53	0.42
11:M:31:ILE:HG22	11:M:33:LEU:HD22	2.02	0.42
12:N:523:LEU:O	12:N:527:LEU:HG	2.20	0.42
13:O:434:ARG:HA	13:O:434:ARG:HD2	1.75	0.42
13:O:493:LEU:HD13	13:O:507:TRP:HB2	2.01	0.42
3:P:244:ILE:HD11	3:P:276:ILE:HD11	2.02	0.42
3:P:297:ILE:HD11	3:P:333:THR:HB	2.01	0.42
15:R:193:SER:HB3	15:R:234:TRP:CD2	2.55	0.42
16:S:30:GLN:CB	16:S:36:ARG:NH2	2.83	0.42
17:Y:391:GLU:O	17:Y:394:ILE:HG12	2.19	0.42
1:A:971:PRO:HG2	1:A:974:VAL:HG23	2.01	0.42
3:C:515:TYR:HA	3:C:518:GLN:HG2	2.00	0.42
3:C:554:LEU:HD12	9:K:386:LEU:HD11	2.01	0.42
6:F:762:TRP:NE1	9:J:362:GLN:HB2	2.35	0.42
8:I:398:LEU:HD23	13:O:444:MET:HG3	2.01	0.42
9:J:482:TYR:HD1	9:J:485:ILE:HD11	1.85	0.42
12:N:180:PHE:CG	12:N:299:TRP:CH2	3.05	0.42
13:O:256:LEU:HD23	13:O:256:LEU:HA	1.85	0.42
13:O:508:MET:HA	13:O:511:ASP:OD2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:547:LYS:HG3	13:O:563:LEU:HD21	2.02	0.42
3:P:151:LEU:HD22	3:P:178:VAL:HG13	2.01	0.42
3:P:424:ARG:NH1	3:P:424:ARG:HG3	2.33	0.42
14:Q:193:SER:HB3	14:Q:234:TRP:CD2	2.55	0.42
17:X:452:LEU:HD22	17:X:461:ALA:CA	2.47	0.42
18:Z:13:LEU:HD22	18:Z:111:LYS:HB3	2.00	0.42
1:A:857:MET:CB	1:A:858:PRO:CD	2.95	0.42
3:C:262:SER:O	3:C:266:VAL:HG23	2.20	0.42
6:H:481:CYS:O	6:H:485:ILE:HG12	2.19	0.42
8:I:370:ALA:HB2	8:I:386:ILE:HD12	2.01	0.42
8:I:586:LEU:HD12	8:I:587:LEU:N	2.34	0.42
12:N:556:PHE:HA	12:N:600:PHE:CD1	2.55	0.42
13:O:350:LEU:HA	13:O:350:LEU:HD23	1.86	0.42
13:O:568:LEU:HD13	13:O:583:VAL:HG13	2.02	0.42
13:O:711:ARG:HH12	13:O:745:PRO:HB3	1.84	0.42
3:P:127:GLU:HA	3:P:127:GLU:OE2	2.20	0.42
17:Y:230:VAL:HA	17:Y:231:PRO:HD2	1.88	0.42
18:Z:48:LYS:HG3	18:Z:49:TYR:CD2	2.55	0.42
18:Z:81:VAL:CG2	18:Z:155:ILE:HD12	2.49	0.42
1:A:1638:TYR:N	1:A:1638:TYR:CD1	2.88	0.42
1:A:1739:SER:N	1:A:1740:ALA:HB3	2.35	0.42
3:C:434:ARG:HH11	15:R:80:ILE:HD13	1.85	0.42
5:E:102:LEU:HD13	6:H:594:ILE:HG22	2.01	0.42
6:F:699:ASP:CB	6:F:702:ASN:HD21	2.31	0.42
6:H:515:TYR:CD1	6:H:515:TYR:N	2.88	0.42
8:I:403:LEU:HG	8:I:407:ILE:HD11	2.02	0.42
9:J:19:TYR:CD1	9:J:49:LEU:CD1	2.97	0.42
9:J:230:ASN:O	9:J:233:VAL:HG22	2.20	0.42
9:K:289:HIS:CG	11:M:57:TRP:CZ3	3.08	0.42
9:K:497:ASN:OD1	9:K:497:ASN:N	2.52	0.42
9:K:499:VAL:HG11	9:K:523:ILE:HD11	2.02	0.42
12:N:414:MET:SD	12:N:498:SER:N	2.93	0.42
13:O:648:ILE:HA	13:O:651:ILE:HD12	2.02	0.42
16:S:272:ILE:HG13	16:S:273:THR:N	2.35	0.42
17:X:242:ALA:O	17:X:246:VAL:HG23	2.20	0.42
3:C:89:LEU:HD21	3:C:93:TYR:CE2	2.55	0.42
3:C:170:PHE:O	3:C:171:GLY:C	2.57	0.42
6:H:130:ARG:NH1	9:K:473:VAL:CG2	2.82	0.42
8:I:556:LEU:HD11	8:I:586:LEU:HD21	2.02	0.42
9:J:17:GLN:HB3	9:K:78:ARG:NH1	2.34	0.42
9:K:284:LEU:HD11	9:K:307:CYS:SG	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:422:GLU:OE1	9:K:458:LEU:HD22	2.20	0.42
9:K:491:LEU:HA	7:W:22:ILE:HG21	2.02	0.42
10:L:14:LYS:HB3	10:L:18:ARG:CZ	2.50	0.42
12:N:152:GLU:O	12:N:156:MET:HG2	2.19	0.42
13:O:707:LYS:HA	13:O:710:ILE:CG2	2.49	0.42
3:P:123:TYR:CE1	3:P:151:LEU:HD21	2.55	0.42
3:P:303:PHE:CE1	3:P:307:LEU:HD22	2.54	0.42
17:X:261:LEU:HD22	17:X:267:LEU:HD23	2.02	0.42
17:Y:513:ARG:NH1	17:Y:544:LYS:HB3	2.34	0.42
1:A:1191:LEU:HD23	1:A:1191:LEU:H	1.84	0.41
1:A:1424:LYS:HA	1:A:1427:ASP:OD2	2.20	0.41
6:F:130:ARG:NH1	17:Y:506:GLN:HB3	2.35	0.41
6:F:550:VAL:HG21	9:K:289:HIS:CB	2.43	0.41
6:F:726:LEU:HD21	6:F:742:LEU:HD22	2.02	0.41
8:I:86:ASP:OD1	8:I:87:THR:N	2.53	0.41
9:K:20:GLN:CA	9:K:20:GLN:HE21	2.32	0.41
9:K:258:MET:HA	9:K:261:ASP:O	2.20	0.41
9:K:444:TRP:CZ3	7:W:6:PRO:HG2	2.54	0.41
11:M:32:PRO:O	11:M:33:LEU:HB2	2.20	0.41
3:P:251:TYR:HH	3:P:268:GLN:HG3	1.81	0.41
1:A:269:TRP:CZ3	1:A:411:HIS:HB2	2.55	0.41
3:C:48:LEU:N	3:C:48:LEU:HD23	2.35	0.41
9:J:24:PHE:CE1	9:J:28:LYS:CE	3.00	0.41
9:J:354:MET:HE1	9:J:377:GLU:HB2	2.01	0.41
9:J:397:ILE:O	9:J:398:ALA:C	2.59	0.41
10:L:40:PHE:CA	10:L:44:GLN:OE1	2.64	0.41
12:N:286:LEU:O	12:N:287:ARG:C	2.57	0.41
12:N:528:LEU:HD11	12:N:641:LEU:HD13	2.01	0.41
12:N:681:LEU:HD23	12:N:692:LEU:HD21	2.01	0.41
13:O:629:PHE:CE1	13:O:755:LEU:C	2.94	0.41
3:P:290:ARG:HD3	3:P:300:MET:HE2	2.02	0.41
17:X:391:GLU:O	17:X:394:ILE:HG12	2.20	0.41
1:A:129:CYS:SG	1:A:187:LEU:HD13	2.60	0.41
1:A:860:TYR:CD1	1:A:861:PRO:HD2	2.55	0.41
1:A:1371:LEU:HD23	1:A:1371:LEU:HA	1.86	0.41
1:A:1574:LEU:H	1:A:1574:LEU:HG	1.61	0.41
1:A:1814:ILE:O	1:A:1818:LEU:HD12	2.19	0.41
6:H:32:TYR:CE1	6:H:41:LEU:HB2	2.55	0.41
6:H:624:PHE:O	6:H:628:ILE:HG12	2.21	0.41
8:I:28:TRP:HZ3	8:I:33:ASP:O	2.04	0.41
9:J:21:SER:HB2	9:K:165:GLU:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:290:LYS:O	9:J:294:LEU:HD23	2.19	0.41
9:J:323:LEU:HD12	9:J:323:LEU:HA	1.88	0.41
9:J:340:TYR:HE1	9:J:344:PHE:CE2	2.38	0.41
12:N:149:LEU:HB3	12:N:150:ARG:H	1.60	0.41
14:Q:163:LYS:HE2	15:R:464:ASP:O	2.21	0.41
17:Y:244:ALA:O	17:Y:248:THR:HG23	2.20	0.41
1:A:616:GLU:HB2	13:O:556:GLN:HA	2.03	0.41
1:A:780:GLY:C	1:A:782:GLY:H	2.23	0.41
1:A:1236:LEU:HA	1:A:1237:PRO:HD3	1.89	0.41
3:C:415:PRO:HG3	3:C:445:LYS:HB2	2.03	0.41
6:F:457:ALA:HA	6:F:460:GLU:OE1	2.21	0.41
6:F:502:LEU:HA	6:F:505:ILE:HD12	2.02	0.41
6:H:502:LEU:HA	6:H:505:ILE:HD12	2.03	0.41
6:H:689:LEU:O	6:H:693:ASN:HB2	2.20	0.41
8:I:73:TRP:CH2	8:I:80:LEU:HD22	2.55	0.41
8:I:330:LEU:HD13	8:I:330:LEU:C	2.41	0.41
9:J:28:LYS:HD3	9:K:230:ASN:ND2	2.35	0.41
9:J:231:LEU:HA	9:J:234:VAL:HG22	2.01	0.41
9:J:322:TYR:CE1	11:M:36:LEU:HD11	2.54	0.41
9:J:386:LEU:HD12	9:J:386:LEU:H	1.85	0.41
9:K:203:PHE:HE1	9:K:218:THR:HB	1.85	0.41
9:K:203:PHE:CD1	9:K:221:PRO:CG	3.04	0.41
3:P:97:LYS:HG3	3:P:99:TYR:CZ	2.55	0.41
14:Q:498:ILE:O	14:Q:498:ILE:HG22	2.21	0.41
16:S:20:ASP:O	16:S:24:LEU:HG	2.19	0.41
17:X:170:LYS:HG2	17:X:171:ILE:HD12	2.01	0.41
17:X:437:LEU:CB	17:X:444:LEU:HD11	2.48	0.41
18:Z:146:GLU:CD	18:Z:146:GLU:N	2.72	0.41
1:A:811:PRO:HG3	1:A:1806:SER:HB3	2.01	0.41
1:A:1364:CYS:N	1:A:1365:PRO:HD2	2.36	0.41
3:C:389:ARG:HA	3:C:389:ARG:HD3	1.65	0.41
6:F:45:ALA:CB	6:F:61:LEU:HD11	2.51	0.41
7:G:3:ARG:HB2	9:J:443:LYS:HZ3	1.86	0.41
8:I:231:VAL:HG12	8:I:232:SER:N	2.35	0.41
8:I:290:PHE:HB3	8:I:320:LEU:HD21	2.01	0.41
8:I:333:LEU:HG	8:I:337:ILE:HD12	2.02	0.41
9:K:20:GLN:HE21	9:K:20:GLN:HA	1.86	0.41
13:O:541:ILE:O	13:O:544:VAL:HG22	2.20	0.41
3:P:248:LEU:O	3:P:252:GLN:HG2	2.20	0.41
16:S:134:GLU:O	16:S:135:PRO:C	2.57	0.41
17:X:434:TYR:HA	17:X:444:LEU:HD22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Y:70:LEU:O	17:Y:70:LEU:HD13	2.20	0.41
1:A:957:ASP:HA	1:A:1839:PHE:HE2	1.85	0.41
1:A:1251:VAL:HG12	1:A:1294:TYR:HA	2.03	0.41
1:A:1325:LEU:HD23	1:A:1371:LEU:CD2	2.50	0.41
1:A:1387:LEU:HD12	1:A:1407:ARG:HG3	2.03	0.41
2:B:16:TRP:HZ3	12:N:633:ARG:HG3	1.85	0.41
2:B:28:MET:HG2	2:B:33:CYS:O	2.20	0.41
3:C:307:LEU:HD21	3:C:316:LEU:HB2	2.02	0.41
6:F:666:PRO:O	6:F:667:GLN:HG3	2.21	0.41
8:I:34:LEU:HD13	12:N:390:GLY:HA3	2.03	0.41
8:I:306:HIS:NE2	8:I:313:ALA:O	2.53	0.41
9:J:447:LEU:O	9:J:451:LEU:HD23	2.20	0.41
12:N:386:LEU:HD12	12:N:387:LEU:HG	2.02	0.41
12:N:389:PRO:HA	12:N:431:ARG:HH22	1.85	0.41
12:N:501:ILE:H	12:N:501:ILE:CD1	2.29	0.41
13:O:604:LEU:HB3	13:O:627:LEU:HD21	2.02	0.41
3:P:389:ARG:HA	3:P:392:ILE:HG22	2.02	0.41
3:P:396:LYS:HA	3:P:396:LYS:HD3	1.88	0.41
1:A:107:LYS:HB2	1:A:110:ALA:HB3	2.03	0.41
1:A:773:LEU:HB2	1:A:783:ILE:HD12	2.01	0.41
1:A:1750:PHE:HD2	1:A:1775:LEU:HD12	1.86	0.41
3:C:206:TRP:O	3:C:209:LEU:HB2	2.21	0.41
6:F:705:CYS:SG	6:F:706:LYS:N	2.93	0.41
8:I:237:GLU:CG	8:I:607:ILE:HD13	2.51	0.41
9:K:35:GLU:HB3	9:K:40:ILE:HD11	2.03	0.41
9:K:66:ASP:OD1	9:K:67:LYS:N	2.54	0.41
9:K:297:SER:O	9:K:329:LEU:HD21	2.20	0.41
12:N:321:LEU:HD22	12:N:324:TRP:CD2	2.56	0.41
13:O:143:TYR:CD1	13:O:143:TYR:C	2.94	0.41
13:O:266:ASP:CB	13:O:269:SER:HB3	2.51	0.41
13:O:592:TRP:CH2	13:O:630:ALA:HA	2.55	0.41
3:P:358:LEU:O	3:P:362:PRO:CA	2.65	0.41
15:R:430:TYR:CG	15:R:431:PRO:HA	2.56	0.41
1:A:1645:GLU:CG	1:A:1646:GLN:H	2.27	0.41
1:A:1702:ARG:HD3	1:A:1782:GLU:CD	2.41	0.41
3:C:276:ILE:O	3:C:276:ILE:HG22	2.21	0.41
6:F:559:LEU:O	6:F:562:MET:HG3	2.21	0.41
8:I:32:ARG:HD2	8:I:34:LEU:HD21	2.03	0.41
8:I:101:LEU:HD23	8:I:102:HIS:N	2.36	0.41
8:I:184:PHE:HB2	8:I:198:VAL:O	2.20	0.41
8:I:231:VAL:HG21	8:I:557:TYR:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:719:ALA:HA	8:I:735:SER:HA	2.02	0.41
9:J:485:ILE:O	9:J:488:ILE:HG12	2.21	0.41
12:N:235:GLN:HA	12:N:238:GLU:CD	2.41	0.41
12:N:427:TYR:O	12:N:430:THR:HB	2.21	0.41
13:O:208:SER:HB3	13:O:211:GLN:NE2	2.36	0.41
3:P:434:ARG:NH1	14:Q:498:ILE:HD13	2.35	0.41
14:Q:139:ASN:O	14:Q:140:ALA:CB	2.68	0.41
15:R:461:ALA:CA	15:R:467:LEU:HD12	2.51	0.41
16:S:73:ASP:HB3	16:S:74:PRO:HD3	2.02	0.41
17:X:442:GLN:CD	17:X:472:ARG:CG	2.89	0.41
1:A:154:LEU:HD13	1:A:159:ILE:HG12	2.02	0.41
1:A:439:GLN:NE2	1:A:456:LYS:HG3	2.35	0.41
1:A:628:ILE:HD11	1:A:762:ILE:HD13	2.03	0.41
1:A:767:HIS:O	1:A:770:TYR:HB3	2.20	0.41
1:A:1036:ASP:O	1:A:1039:ARG:HB3	2.20	0.41
1:A:1039:ARG:O	1:A:1042:GLN:HG3	2.21	0.41
1:A:1525:MET:HA	1:A:1528:ALA:HB2	2.03	0.41
1:A:1658:PRO:HG2	1:A:1663:LEU:HD13	2.03	0.41
2:B:13:THR:O	2:B:15:LEU:HD23	2.20	0.41
3:C:150:ALA:O	3:C:154:LEU:HD13	2.21	0.41
6:F:462:LEU:HD13	6:F:465:LEU:HD23	2.02	0.41
6:F:703:PRO:HB3	6:F:733:VAL:CG2	2.50	0.41
8:I:224:SER:OG	8:I:228:ALA:O	2.29	0.41
8:I:440:MET:HE3	8:I:440:MET:HA	2.03	0.41
9:J:180:GLU:CA	9:J:180:GLU:OE1	2.69	0.41
9:J:441:VAL:CG2	9:J:444:TRP:CD1	2.91	0.41
9:K:243:TYR:HA	7:W:3:ARG:HH22	1.85	0.41
9:K:418:TRP:HB3	9:K:458:LEU:HD12	2.02	0.41
9:K:445:GLU:HA	9:K:474:LEU:HD12	2.03	0.41
12:N:63:ALA:HB3	12:N:64:ALA:HB3	2.02	0.41
12:N:139:GLY:C	12:N:141:LEU:N	2.70	0.41
12:N:330:ARG:HB2	12:N:334:ARG:NH2	2.36	0.41
12:N:457:GLN:HA	12:N:544:LEU:HD11	2.02	0.41
12:N:550:GLY:HA2	12:N:551:GLU:CB	2.51	0.41
13:O:62:GLN:O	13:O:66:PRO:HD2	2.21	0.41
13:O:678:TYR:O	13:O:683:LYS:HB2	2.20	0.41
13:O:682:LYS:O	13:O:685:GLU:HB3	2.20	0.41
3:P:46:ARG:HG3	3:P:116:PHE:CD2	2.55	0.41
3:P:91:LYS:O	3:P:94:PHE:HB3	2.21	0.41
14:Q:496:GLN:HA	14:Q:497:GLY:HA2	1.78	0.41
15:R:174:ARG:HH11	16:S:257:GLY:N	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:S:279:ALA:N	16:S:280:ASP:HA	2.36	0.41
17:X:244:ALA:O	17:X:248:THR:HG23	2.21	0.41
17:X:335:SER:HB2	17:X:338:HIS:CD2	2.56	0.41
17:Y:45:ALA:HB3	17:Y:82:TYR:HE2	1.79	0.41
17:Y:100:TYR:CD1	17:Y:138:VAL:HG13	2.55	0.41
17:Y:242:ALA:O	17:Y:246:VAL:HG23	2.20	0.41
17:Y:434:TYR:HA	17:Y:444:LEU:HD22	2.03	0.41
1:A:629:LEU:C	1:A:629:LEU:HD12	2.42	0.41
1:A:845:TYR:HB3	1:A:1812:TRP:CE3	2.56	0.41
1:A:1787:LEU:O	1:A:1791:ILE:HG12	2.21	0.41
3:C:185:VAL:HG13	3:C:212:LEU:HD22	2.02	0.41
6:F:507:ARG:HD3	6:F:538:ILE:CD1	2.42	0.41
9:J:165:GLU:OE2	9:K:20:GLN:HB2	2.21	0.41
9:J:168:ASP:HA	9:J:171:THR:HG22	2.03	0.41
12:N:580:LYS:HB3	12:N:582:PRO:HD2	2.03	0.41
12:N:595:ILE:CD1	12:N:626:TYR:OH	2.69	0.41
13:O:321:GLU:HA	13:O:350:LEU:HD13	2.02	0.41
13:O:592:TRP:HH2	13:O:630:ALA:HA	1.86	0.41
13:O:688:GLU:O	13:O:691:ILE:HG22	2.21	0.41
3:P:251:TYR:CZ	3:P:268:GLN:HG3	2.55	0.41
14:Q:352:THR:CB	18:Z:51:LEU:HA	2.51	0.41
14:Q:461:ALA:CA	14:Q:467:LEU:HD12	2.51	0.41
17:X:316:ALA:HB1	17:X:351:TYR:CE1	2.56	0.41
1:A:1031:ASP:OD1	12:N:489:PRO:N	2.54	0.40
1:A:1131:MET:O	1:A:1132:THR:HB	2.21	0.40
1:A:1619:LEU:HD23	1:A:1634:LEU:HD11	2.02	0.40
3:C:217:GLU:O	3:C:221:PHE:HD1	2.03	0.40
3:C:416:PHE:CB	3:C:446:LEU:HD11	2.47	0.40
6:F:702:ASN:HB2	6:F:705:CYS:SG	2.61	0.40
6:H:163:ASP:HA	6:H:164:PRO:HD2	1.98	0.40
6:H:639:TYR:CZ	6:H:643:MET:HG3	2.57	0.40
8:I:209:CYS:HG	8:I:584:HIS:CG	2.22	0.40
8:I:578:ASN:C	8:I:578:ASN:OD1	2.60	0.40
8:I:585:TYR:CE1	8:I:602:ARG:HD3	2.56	0.40
9:K:276:VAL:HA	9:K:311:MET:HE2	2.03	0.40
10:L:79:ILE:HG13	10:L:156:ILE:HG12	2.03	0.40
10:L:119:TRP:HH2	10:L:155:GLN:HG2	1.86	0.40
12:N:595:ILE:HD12	12:N:626:TYR:OH	2.21	0.40
13:O:127:HIS:O	13:O:128:LYS:CB	2.61	0.40
13:O:375:TYR:CE1	13:O:417:LEU:HD23	2.56	0.40
3:P:58:LEU:HD13	3:P:259:PHE:HE2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:276:ILE:CG2	3:P:277:ARG:H	2.22	0.40
16:S:75:LEU:HA	16:S:115:TYR:OH	2.21	0.40
16:S:82:ILE:HD13	16:S:102:LEU:HD21	2.02	0.40
17:X:442:GLN:CD	17:X:472:ARG:HG3	2.41	0.40
18:Z:78:LYS:HB2	18:Z:78:LYS:HE3	1.96	0.40
1:A:799:LEU:O	1:A:801:PRO:HD2	2.21	0.40
1:A:1071:LEU:O	1:A:1074:CYS:HB2	2.22	0.40
1:A:1208:LEU:O	1:A:1212:VAL:HG23	2.21	0.40
1:A:1227:LEU:O	1:A:1231:HIS:ND1	2.55	0.40
1:A:1359:ASN:HB3	10:L:30:VAL:HG11	2.04	0.40
1:A:1694:ASP:OD1	1:A:1696:VAL:HB	2.21	0.40
1:A:1867:CYS:CB	1:A:1881:GLN:NE2	2.83	0.40
3:C:412:LEU:O	3:C:413:LYS:HB2	2.20	0.40
6:F:32:TYR:CE1	6:F:41:LEU:HB2	2.56	0.40
6:H:158:ILE:HG22	6:H:159:GLY:N	2.36	0.40
6:H:162:PRO:HD2	6:H:474:LEU:HD13	2.03	0.40
6:H:557:LYS:HE2	6:H:557:LYS:HB3	1.93	0.40
8:I:618:ILE:HD12	8:I:705:MET:HE1	2.02	0.40
9:J:289:HIS:CD2	9:J:289:HIS:C	2.94	0.40
9:J:337:TRP:O	9:J:340:TYR:HB3	2.21	0.40
9:J:397:ILE:CG2	9:J:398:ALA:N	2.84	0.40
9:K:244:ASN:O	9:K:245:CYS:HB2	2.21	0.40
12:N:596:LEU:HD13	12:N:601:TRP:CZ2	2.56	0.40
12:N:611:VAL:HG11	12:N:637:TRP:CH2	2.56	0.40
13:O:65:LEU:HB3	13:O:66:PRO:HD3	2.03	0.40
13:O:351:GLY:O	13:O:352:GLN:HG3	2.21	0.40
13:O:516:PHE:HB2	13:O:535:ILE:HD11	2.02	0.40
16:S:19:GLY:O	16:S:23:GLU:HG3	2.20	0.40
17:X:164:SER:HA	17:X:167:ARG:NE	2.37	0.40
17:Y:301:ASP:HA	17:Y:302:PRO:HD2	1.95	0.40
17:Y:350:PHE:CE2	17:Y:378:LEU:HD12	2.56	0.40
3:C:116:PHE:HE1	3:C:174:LEU:HB2	1.86	0.40
3:C:312:MET:H	3:C:312:MET:HG2	1.60	0.40
6:F:624:PHE:O	6:F:628:ILE:HG12	2.21	0.40
6:H:698:ILE:HG13	6:H:699:ASP:N	2.36	0.40
6:H:765:ASP:O	17:X:397:ARG:CZ	2.68	0.40
8:I:266:ASN:HA	8:I:526:LYS:HZ3	1.85	0.40
8:I:279:ILE:HD12	8:I:279:ILE:HA	1.92	0.40
9:K:19:TYR:CE1	9:K:49:LEU:HD13	2.56	0.40
9:K:413:PHE:HD1	9:K:454:VAL:HG23	1.86	0.40
12:N:803:VAL:HG21	12:N:810:TYR:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:340:LEU:HD23	13:O:340:LEU:HA	1.93	0.40
3:P:66:PRO:O	3:P:67:LEU:HB3	2.20	0.40
3:P:464:ASP:OD2	3:P:469:ALA:HB3	2.20	0.40
14:Q:128:ALA:HB1	18:Z:156:TYR:CZ	2.50	0.40
14:Q:163:LYS:HD3	15:R:466:THR:CG2	2.51	0.40
14:Q:430:TYR:CG	14:Q:431:PRO:HA	2.56	0.40
15:R:346:VAL:HA	15:R:347:PRO:HD3	1.98	0.40
16:S:41:LEU:HD11	18:Z:141:PHE:CB	2.44	0.40
17:Y:60:LEU:HB3	17:Y:79:LEU:HD11	2.04	0.40
17:Y:452:LEU:HD22	17:Y:461:ALA:CA	2.47	0.40
1:A:181:TRP:HA	1:A:182:PRO:HD3	2.01	0.40
1:A:941:LEU:HB2	1:A:977:LEU:HA	2.03	0.40
3:C:62:LEU:HB3	3:C:63:PRO:HD2	2.03	0.40
5:E:60:SER:O	5:E:63:VAL:HG12	2.21	0.40
6:F:550:VAL:HG13	6:F:551:ALA:N	2.37	0.40
9:J:342:HIS:CD2	9:J:357:TYR:OH	2.74	0.40
9:K:63:ARG:HB2	9:K:65:LEU:HD13	2.01	0.40
9:K:190:LEU:O	9:K:198:GLN:NE2	2.54	0.40
12:N:354:SER:O	12:N:357:ALA:HB3	2.22	0.40
12:N:556:PHE:CG	12:N:600:PHE:HD1	2.39	0.40
12:N:596:LEU:HD22	12:N:601:TRP:CZ2	2.56	0.40
3:P:54:TRP:CE3	3:P:203:TRP:HB2	2.56	0.40
14:Q:128:ALA:HB3	18:Z:156:TYR:CE2	2.39	0.40
17:X:71:PHE:O	17:X:76:LYS:HE3	2.22	0.40
17:X:154:ASP:OD1	17:X:154:ASP:N	2.54	0.40
17:Y:164:SER:HA	17:Y:167:ARG:NE	2.36	0.40
1:A:223:LEU:HD12	1:A:223:LEU:HA	1.98	0.40
1:A:474:ILE:HD11	1:A:490:VAL:HG21	2.03	0.40
1:A:808:ARG:NH2	1:A:1894:VAL:O	2.54	0.40
1:A:1800:LEU:HD11	1:A:1811:LEU:HD21	2.03	0.40
2:B:16:TRP:O	2:B:31:ASN:O	2.39	0.40
3:C:91:LYS:O	3:C:94:PHE:HB3	2.22	0.40
6:F:689:LEU:O	6:F:693:ASN:HB2	2.22	0.40
6:H:726:LEU:HD21	6:H:742:LEU:HD22	2.03	0.40
6:H:765:ASP:O	17:X:397:ARG:NE	2.54	0.40
8:I:14:VAL:N	8:I:743:VAL:O	2.54	0.40
9:K:250:CYS:SG	9:K:274:THR:HG23	2.55	0.40
10:L:86:ASP:HB3	10:L:89:TYR:CB	2.40	0.40
12:N:202:GLU:HB2	12:N:282:GLU:CD	2.40	0.40
12:N:370:GLN:HE21	12:N:373:GLN:HB3	1.87	0.40
13:O:267:VAL:O	13:O:271:THR:HG22	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:544:VAL:HG23	13:O:567:LEU:CG	2.45	0.40
3:P:115:TYR:CD1	3:P:115:TYR:C	2.95	0.40
16:S:20:ASP:H	18:Z:134:GLN:NE2	2.12	0.40
16:S:20:ASP:CG	18:Z:184:ARG:HD2	2.32	0.40
16:S:29:VAL:C	16:S:36:ARG:NH2	2.62	0.40
16:S:65:GLU:C	16:S:69:TYR:CD2	2.94	0.40
18:Z:179:GLU:HG2	18:Z:201:ILE:HG12	2.02	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	1397/1944 (72%)	1267 (91%)	106 (8%)	24 (2%)	7	37
2	B	75/84 (89%)	62 (83%)	8 (11%)	5 (7%)	1	15
3	C	520/597 (87%)	498 (96%)	20 (4%)	2 (0%)	30	67
3	P	485/597 (81%)	465 (96%)	20 (4%)	0	100	100
4	D	16/121 (13%)	14 (88%)	2 (12%)	0	100	100
5	E	54/110 (49%)	53 (98%)	1 (2%)	0	100	100
6	F	479/824 (58%)	458 (96%)	13 (3%)	8 (2%)	7	37
6	H	479/824 (58%)	459 (96%)	14 (3%)	6 (1%)	10	42
7	G	23/85 (27%)	23 (100%)	0	0	100	100
7	W	23/85 (27%)	23 (100%)	0	0	100	100
8	I	725/808 (90%)	683 (94%)	35 (5%)	7 (1%)	13	48
9	J	500/620 (81%)	467 (93%)	29 (6%)	4 (1%)	16	54
9	K	489/620 (79%)	456 (93%)	27 (6%)	6 (1%)	11	44
10	L	180/185 (97%)	165 (92%)	14 (8%)	1 (1%)	22	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	M	55/74 (74%)	46 (84%)	9 (16%)	0	100	100
12	N	679/822 (83%)	557 (82%)	68 (10%)	54 (8%)	1	11
13	O	677/755 (90%)	640 (94%)	29 (4%)	8 (1%)	11	44
14	Q	348/374 (93%)	317 (91%)	21 (6%)	10 (3%)	3	26
15	R	377/499 (76%)	344 (91%)	26 (7%)	7 (2%)	6	35
16	S	267/342 (78%)	237 (89%)	18 (7%)	12 (4%)	2	20
17	X	480/599 (80%)	464 (97%)	13 (3%)	3 (1%)	22	59
17	Y	492/599 (82%)	474 (96%)	13 (3%)	5 (1%)	13	48
18	Z	193/205 (94%)	186 (96%)	6 (3%)	1 (0%)	25	62
All	All	9013/11773 (77%)	8358 (93%)	492 (6%)	163 (2%)	9	36

All (163) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	274	VAL
1	A	630	PRO
1	A	857	MET
1	A	1125	ILE
1	A	1358	ILE
2	B	15	LEU
2	B	37	CYS
2	B	43	ASP
2	B	67	GLN
8	I	431	ASP
8	I	489	PRO
8	I	503	ASN
9	J	221	PRO
9	K	211	LYS
9	K	215	PRO
12	N	74	TRP
12	N	75	PHE
12	N	78	VAL
12	N	79	LEU
12	N	91	PHE
12	N	126	LEU
12	N	140	LEU
12	N	203	LEU
12	N	234	ARG
12	N	252	LEU

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Mol	Chain	Res	Type
12	N	286	LEU
12	N	287	ARG
12	N	290	HIS
12	N	350	ASP
12	N	368	THR
12	N	395	ASP
12	N	412	PRO
12	N	477	PRO
12	N	488	ASP
12	N	489	PRO
12	N	492	SER
12	N	497	ARG
12	N	530	GLN
12	N	606	ASP
12	N	632	MET
12	N	674	ALA
12	N	716	ILE
14	Q	140	ALA
14	Q	141	PRO
14	Q	476	ASP
14	Q	477	PRO
14	Q	478	ALA
14	Q	479	ARG
15	R	106	THR
16	S	77	VAL
16	S	135	PRO
16	S	222	PRO
16	S	230	LEU
16	S	262	PHE
16	S	274	VAL
17	X	213	SER
17	Y	201	LEU
17	Y	213	SER
18	Z	159	LYS
1	A	87	VAL
1	A	860	TYR
1	A	1099	PRO
1	A	1164	LYS
1	A	1307	LEU
1	A	1925	VAL
3	C	27	SER
6	F	129	ASP

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Mol	Chain	Res	Type
6	F	147	PHE
6	F	165	ASP
6	F	493	SER
6	H	129	ASP
6	H	147	PHE
6	H	493	SER
8	I	296	THR
8	I	433	VAL
9	J	70	GLU
12	N	63	ALA
12	N	64	ALA
12	N	101	SER
12	N	278	ARG
12	N	289	PHE
12	N	531	PHE
12	N	550	GLY
13	O	505	GLN
14	Q	137	PRO
14	Q	266	SER
15	R	101	PRO
15	R	266	SER
15	R	494	ILE
16	S	74	PRO
16	S	235	LYS
17	X	202	ALA
17	Y	202	ALA
1	A	1100	LEU
1	A	1283	PRO
1	A	1314	ILE
6	F	103	HIS
8	I	487	VAL
9	J	397	ILE
9	K	129	LYS
9	K	228	GLN
10	L	174	THR
12	N	77	GLU
12	N	144	THR
12	N	280	GLU
12	N	480	TRP
12	N	500	ASP
12	N	629	LEU
12	N	672	ASP

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Mol	Chain	Res	Type
13	O	707	LYS
15	R	108	THR
16	S	559	ALA
17	Y	456	VAL
1	A	253	PRO
1	A	1055	PRO
1	A	1822	SER
2	B	65	HIS
6	F	145	ASN
6	H	145	ASN
9	J	382	ASN
9	K	86	HIS
12	N	219	PRO
12	N	283	ARG
12	N	352	PRO
12	N	353	ASP
12	N	482	PRO
12	N	484	PRO
12	N	595	ILE
13	O	462	ASN
13	O	540	SER
13	O	657	ILE
13	O	745	PRO
17	X	456	VAL
1	A	1356	ASP
1	A	1603	LEU
6	F	96	VAL
6	H	97	PHE
12	N	282	GLU
12	N	499	SER
13	O	126	VAL
15	R	498	ILE
16	S	301	PRO
1	A	502	GLY
1	A	590	PRO
1	A	781	GLU
1	A	1239	THR
3	C	229	MET
6	F	97	PHE
6	H	96	VAL
12	N	142	MET
12	N	551	GLU

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Mol	Chain	Res	Type
14	Q	161	SER
15	R	76	GLY
9	K	399	PRO
16	S	257	GLY
8	I	291	VAL
16	S	294	PRO
1	A	858	PRO
12	N	490	GLY
14	Q	498	ILE
17	Y	200	PRO
12	N	166	PRO
13	O	124	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	1151/1720 (67%)	1011 (88%)	140 (12%)	4	18
2	B	71/75 (95%)	59 (83%)	12 (17%)	1	11
3	C	452/520 (87%)	390 (86%)	62 (14%)	3	16
3	P	422/520 (81%)	374 (89%)	48 (11%)	4	19
4	D	18/115 (16%)	15 (83%)	3 (17%)	2	11
5	E	47/89 (53%)	37 (79%)	10 (21%)	1	5
6	F	407/727 (56%)	361 (89%)	46 (11%)	4	19
6	H	408/727 (56%)	368 (90%)	40 (10%)	6	23
7	G	23/77 (30%)	20 (87%)	3 (13%)	3	16
7	W	23/77 (30%)	21 (91%)	2 (9%)	8	28
8	I	617/730 (84%)	579 (94%)	38 (6%)	15	39
9	J	424/548 (77%)	373 (88%)	51 (12%)	4	18
9	K	423/548 (77%)	383 (90%)	40 (10%)	7	24
10	L	155/170 (91%)	137 (88%)	18 (12%)	4	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	M	55/67 (82%)	45 (82%)	10 (18%)	1	9
12	N	518/724 (72%)	448 (86%)	70 (14%)	3	16
13	O	577/650 (89%)	503 (87%)	74 (13%)	3	17
14	Q	271/310 (87%)	264 (97%)	7 (3%)	41	61
15	R	311/411 (76%)	293 (94%)	18 (6%)	17	40
16	S	186/293 (64%)	181 (97%)	5 (3%)	40	60
17	X	407/513 (79%)	376 (92%)	31 (8%)	11	33
17	Y	418/513 (82%)	381 (91%)	37 (9%)	8	27
18	Z	181/190 (95%)	170 (94%)	11 (6%)	15	39
All	All	7565/10314 (73%)	6789 (90%)	776 (10%)	8	22

All (776) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	HIS
1	A	36	ASN
1	A	37	LEU
1	A	39	LEU
1	A	47	GLU
1	A	88	ASP
1	A	90	ASP
1	A	92	GLU
1	A	98	ASN
1	A	99	MET
1	A	118	THR
1	A	120	ASP
1	A	127	LEU
1	A	128	TRP
1	A	133	ILE
1	A	151	ILE
1	A	159	ILE
1	A	172	SER
1	A	180	VAL
1	A	210	MET
1	A	212	SER
1	A	216	PRO
1	A	249	LEU
1	A	250	ASN
1	A	271	LEU

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Mol	Chain	Res	Type
1	A	429	LYS
1	A	430	VAL
1	A	437	CYS
1	A	439	GLN
1	A	444	PHE
1	A	449	GLN
1	A	450	LEU
1	A	459	GLU
1	A	474	ILE
1	A	491	LEU
1	A	497	LEU
1	A	508	LYS
1	A	583	TYR
1	A	584	ILE
1	A	614	THR
1	A	638	LEU
1	A	640	LYS
1	A	664	LEU
1	A	766	LEU
1	A	772	GLU
1	A	774	LYS
1	A	781	GLU
1	A	796	ASP
1	A	808	ARG
1	A	871	ARG
1	A	934	MET
1	A	953	LEU
1	A	962	CYS
1	A	964	GLU
1	A	980	ARG
1	A	1016	MET
1	A	1043	SER
1	A	1075	GLN
1	A	1076	ARG
1	A	1089	LEU
1	A	1100	LEU
1	A	1107	LEU
1	A	1118	VAL
1	A	1120	LEU
1	A	1146	LYS
1	A	1168	LEU
1	A	1170	ASN

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Mol	Chain	Res	Type
1	A	1176	LEU
1	A	1177	MET
1	A	1179	LEU
1	A	1181	LEU
1	A	1184	HIS
1	A	1202	GLU
1	A	1216	LYS
1	A	1217	LEU
1	A	1220	MET
1	A	1230	ILE
1	A	1232	ILE
1	A	1235	LEU
1	A	1243	LEU
1	A	1273	LEU
1	A	1279	ARG
1	A	1292	GLU
1	A	1312	ASN
1	A	1313	LEU
1	A	1319	LEU
1	A	1323	GLU
1	A	1325	LEU
1	A	1327	GLN
1	A	1359	ASN
1	A	1369	LEU
1	A	1386	TRP
1	A	1400	LYS
1	A	1404	LEU
1	A	1405	LEU
1	A	1409	LEU
1	A	1424	LYS
1	A	1455	GLU
1	A	1482	LEU
1	A	1487	CYS
1	A	1511	ASN
1	A	1536	LEU
1	A	1538	LEU
1	A	1539	CYS
1	A	1540	ARG
1	A	1562	LEU
1	A	1564	LEU
1	A	1573	SER
1	A	1574	LEU

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Mol	Chain	Res	Type
1	A	1586	CYS
1	A	1588	LEU
1	A	1597	THR
1	A	1603	LEU
1	A	1607	ARG
1	A	1611	VAL
1	A	1638	TYR
1	A	1646	GLN
1	A	1650	GLU
1	A	1656	LEU
1	A	1662	LEU
1	A	1667	LYS
1	A	1672	ARG
1	A	1674	TRP
1	A	1687	LEU
1	A	1693	LYS
1	A	1694	ASP
1	A	1706	LEU
1	A	1731	ARG
1	A	1742	THR
1	A	1748	LEU
1	A	1749	SER
1	A	1770	LEU
1	A	1785	GLU
1	A	1798	ARG
1	A	1805	MET
1	A	1851	THR
1	A	1854	ASN
1	A	1858	GLN
1	A	1869	HIS
1	A	1882	LEU
2	B	11	VAL
2	B	14	TRP
2	B	15	LEU
2	B	16	TRP
2	B	23	CYS
2	B	34	CYS
2	B	40	PRO
2	B	42	ASP
2	B	62	LYS
2	B	63	TRP
2	B	71	GLN

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Mol	Chain	Res	Type
2	B	79	GLU
3	C	26	PHE
3	C	42	LEU
3	C	44	ARG
3	C	49	LEU
3	C	57	GLU
3	C	70	LEU
3	C	77	THR
3	C	78	GLU
3	C	85	ASP
3	C	89	LEU
3	C	97	LYS
3	C	100	ASP
3	C	101	ARG
3	C	122	ARG
3	C	127	GLU
3	C	128	LYS
3	C	136	ASP
3	C	138	LEU
3	C	147	LYS
3	C	157	GLU
3	C	160	LYS
3	C	172	LEU
3	C	182	LEU
3	C	197	HIS
3	C	201	LEU
3	C	234	LEU
3	C	237	ILE
3	C	239	THR
3	C	244	ILE
3	C	268	GLN
3	C	280	ASP
3	C	289	LEU
3	C	300	MET
3	C	302	THR
3	C	307	LEU
3	C	310	ARG
3	C	312	MET
3	C	313	LYS
3	C	315	GLU
3	C	324	CYS
3	C	334	CYS

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Mol	Chain	Res	Type
3	C	343	LEU
3	C	359	LYS
3	C	361	ASN
3	C	376	MET
3	C	379	LYS
3	C	381	THR
3	C	386	GLN
3	C	389	ARG
3	C	397	ARG
3	C	414	MET
3	C	418	CYS
3	C	424	ARG
3	C	428	LEU
3	C	432	ASP
3	C	435	MET
3	C	441	GLU
3	C	451	GLU
3	C	516	LEU
3	C	518	GLN
3	C	524	LYS
3	C	542	THR
4	D	11	ARG
4	D	12	VAL
4	D	16	LEU
5	E	56	GLU
5	E	57	SER
5	E	58	VAL
5	E	60	SER
5	E	61	TYR
5	E	66	THR
5	E	69	GLN
5	E	85	LEU
5	E	87	GLU
5	E	99	ILE
6	F	22	ARG
6	F	27	LEU
6	F	43	LEU
6	F	70	GLN
6	F	78	CYS
6	F	90	GLN
6	F	98	ASN
6	F	104	ASP

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Mol	Chain	Res	Type
6	F	118	LEU
6	F	121	LEU
6	F	141	SER
6	F	143	SER
6	F	145	ASN
6	F	165	ASP
6	F	462	LEU
6	F	477	CYS
6	F	494	HIS
6	F	503	CYS
6	F	507	ARG
6	F	520	ARG
6	F	521	ILE
6	F	527	ARG
6	F	530	ASN
6	F	536	MET
6	F	538	ILE
6	F	549	ASP
6	F	562	MET
6	F	564	LYS
6	F	576	CYS
6	F	578	SER
6	F	588	LYS
6	F	614	THR
6	F	616	GLU
6	F	618	ASP
6	F	623	CYS
6	F	625	ARG
6	F	655	GLU
6	F	656	MET
6	F	667	GLN
6	F	701	LYS
6	F	705	CYS
6	F	720	LYS
6	F	721	SER
6	F	729	LEU
6	F	748	LYS
6	F	757	LEU
7	G	4	ARG
7	G	5	LYS
7	G	23	ARG
6	H	27	LEU

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Mol	Chain	Res	Type
6	H	43	LEU
6	H	61	LEU
6	H	78	CYS
6	H	90	GLN
6	H	98	ASN
6	H	141	SER
6	H	143	SER
6	H	462	LEU
6	H	477	CYS
6	H	480	ASN
6	H	494	HIS
6	H	503	CYS
6	H	507	ARG
6	H	515	TYR
6	H	520	ARG
6	H	521	ILE
6	H	530	ASN
6	H	536	MET
6	H	562	MET
6	H	563	ASP
6	H	564	LYS
6	H	571	CYS
6	H	582	GLU
6	H	584	ASP
6	H	588	LYS
6	H	592	ARG
6	H	599	ASN
6	H	618	ASP
6	H	623	CYS
6	H	655	GLU
6	H	667	GLN
6	H	702	ASN
6	H	709	ARG
6	H	720	LYS
6	H	729	LEU
6	H	755	LEU
6	H	757	LEU
6	H	761	SER
6	H	762	TRP
8	I	26	LEU
8	I	34	LEU
8	I	37	LEU

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Mol	Chain	Res	Type
8	I	71	LEU
8	I	75	PRO
8	I	89	LYS
8	I	92	LEU
8	I	101	LEU
8	I	218	SER
8	I	224	SER
8	I	232	SER
8	I	259	SER
8	I	266	ASN
8	I	267	LEU
8	I	269	LEU
8	I	273	CYS
8	I	304	PHE
8	I	322	MET
8	I	325	LEU
8	I	349	ILE
8	I	352	LEU
8	I	353	GLN
8	I	359	LEU
8	I	360	LEU
8	I	361	TYR
8	I	371	SER
8	I	372	TRP
8	I	382	ASP
8	I	447	PHE
8	I	452	LEU
8	I	477	GLN
8	I	522	LEU
8	I	564	ASP
8	I	571	LYS
8	I	588	PHE
8	I	688	THR
8	I	718	LYS
8	I	736	SER
9	J	9	ARG
9	J	23	LEU
9	J	42	TRP
9	J	61	ARG
9	J	69	TYR
9	J	134	LEU
9	J	141	ASP

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Mol	Chain	Res	Type
9	J	157	LEU
9	J	163	CYS
9	J	164	PHE
9	J	169	LEU
9	J	180	GLU
9	J	185	LEU
9	J	188	LEU
9	J	202	ARG
9	J	206	GLU
9	J	214	LYS
9	J	248	LYS
9	J	254	THR
9	J	256	VAL
9	J	259	GLU
9	J	267	CYS
9	J	287	LEU
9	J	290	LYS
9	J	298	ASN
9	J	307	CYS
9	J	323	LEU
9	J	329	LEU
9	J	331	LYS
9	J	340	TYR
9	J	343	SER
9	J	351	ASP
9	J	354	MET
9	J	363	LEU
9	J	385	LYS
9	J	395	LEU
9	J	400	GLU
9	J	423	LYS
9	J	429	LEU
9	J	439	VAL
9	J	445	GLU
9	J	448	LEU
9	J	451	LEU
9	J	465	LEU
9	J	472	LEU
9	J	485	ILE
9	J	488	ILE
9	J	497	ASN
9	J	518	MET

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Mol	Chain	Res	Type
9	J	525	MET
9	J	527	ILE
9	K	9	ARG
9	K	20	GLN
9	K	45	GLN
9	K	52	GLN
9	K	63	ARG
9	K	134	LEU
9	K	141	ASP
9	K	146	ARG
9	K	148	LEU
9	K	154	LYS
9	K	157	LEU
9	K	163	CYS
9	K	164	PHE
9	K	169	LEU
9	K	184	LEU
9	K	188	LEU
9	K	190	LEU
9	K	254	THR
9	K	267	CYS
9	K	284	LEU
9	K	287	LEU
9	K	289	HIS
9	K	331	LYS
9	K	340	TYR
9	K	343	SER
9	K	351	ASP
9	K	359	THR
9	K	363	LEU
9	K	370	PRO
9	K	376	LEU
9	K	400	GLU
9	K	423	LYS
9	K	429	LEU
9	K	432	ILE
9	K	454	VAL
9	K	492	MET
9	K	497	ASN
9	K	506	LEU
9	K	510	ARG
9	K	522	CYS

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Mol	Chain	Res	Type
10	L	12	ASP
10	L	23	ARG
10	L	25	ILE
10	L	32	SER
10	L	48	ASP
10	L	65	ASN
10	L	67	GLN
10	L	77	LEU
10	L	92	SER
10	L	98	VAL
10	L	101	ASN
10	L	113	LEU
10	L	132	THR
10	L	151	THR
10	L	154	ARG
10	L	162	VAL
10	L	177	PHE
10	L	184	ARG
11	M	7	ARG
11	M	12	LEU
11	M	17	ASP
11	M	29	VAL
11	M	35	GLU
11	M	50	VAL
11	M	51	LYS
11	M	55	MET
11	M	59	ASP
11	M	64	TYR
12	N	74	TRP
12	N	75	PHE
12	N	76	VAL
12	N	77	GLU
12	N	79	LEU
12	N	80	GLN
12	N	150	ARG
12	N	162	PHE
12	N	163	PHE
12	N	170	GLN
12	N	180	PHE
12	N	181	LEU
12	N	202	GLU
12	N	206	ARG

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Mol	Chain	Res	Type
12	N	243	LEU
12	N	250	LEU
12	N	251	SER
12	N	256	VAL
12	N	271	GLU
12	N	277	CYS
12	N	278	ARG
12	N	281	TYR
12	N	285	PHE
12	N	322	ARG
12	N	334	ARG
12	N	340	ARG
12	N	351	PHE
12	N	355	ARG
12	N	364	CYS
12	N	365	LEU
12	N	366	GLU
12	N	372	GLN
12	N	373	GLN
12	N	379	LYS
12	N	386	LEU
12	N	388	HIS
12	N	392	ASN
12	N	394	CYS
12	N	398	THR
12	N	425	ARG
12	N	433	ASP
12	N	435	VAL
12	N	503	SER
12	N	504	LEU
12	N	507	SER
12	N	513	ASP
12	N	517	ASN
12	N	519	TYR
12	N	531	PHE
12	N	544	LEU
12	N	557	CYS
12	N	561	LEU
12	N	566	ASP
12	N	570	ILE
12	N	571	ASN
12	N	592	TYR

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Mol	Chain	Res	Type
12	N	594	VAL
12	N	604	PHE
12	N	609	LEU
12	N	613	GLU
12	N	622	TYR
12	N	625	LYS
12	N	626	TYR
12	N	632	MET
12	N	638	LYS
12	N	640	THR
12	N	670	PHE
12	N	678	LEU
12	N	695	ARG
12	N	699	TRP
13	O	38	LEU
13	O	40	LEU
13	O	43	GLU
13	O	44	MET
13	O	62	GLN
13	O	78	LEU
13	O	96	ARG
13	O	98	LYS
13	O	99	LEU
13	O	104	GLU
13	O	106	LYS
13	O	129	THR
13	O	136	LEU
13	O	166	GLU
13	O	207	LEU
13	O	266	ASP
13	O	280	ARG
13	O	319	GLN
13	O	328	ILE
13	O	344	LEU
13	O	347	LEU
13	O	381	ILE
13	O	387	GLN
13	O	396	ASN
13	O	398	LEU
13	O	404	ASP
13	O	408	LEU
13	O	411	LYS

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Mol	Chain	Res	Type
13	O	414	LEU
13	O	417	LEU
13	O	419	ASP
13	O	420	ILE
13	O	424	GLN
13	O	426	THR
13	O	434	ARG
13	O	435	SER
13	O	441	GLN
13	O	444	MET
13	O	448	MET
13	O	449	ASN
13	O	496	ARG
13	O	506	LEU
13	O	510	CYS
13	O	511	ASP
13	O	533	THR
13	O	567	LEU
13	O	575	LYS
13	O	579	MET
13	O	581	ILE
13	O	586	SER
13	O	608	LEU
13	O	610	LEU
13	O	616	LEU
13	O	618	TYR
13	O	619	LEU
13	O	623	THR
13	O	625	LEU
13	O	626	ASN
13	O	632	LEU
13	O	636	ILE
13	O	641	LEU
13	O	643	LEU
13	O	646	MET
13	O	649	GLU
13	O	657	ILE
13	O	685	GLU
13	O	691	ILE
13	O	693	ASN
13	O	694	LEU
13	O	706	CYS

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Mol	Chain	Res	Type
13	O	713	VAL
13	O	719	ARG
13	O	723	THR
13	O	735	MET
3	P	38	LEU
3	P	42	LEU
3	P	70	LEU
3	P	77	THR
3	P	78	GLU
3	P	85	ASP
3	P	89	LEU
3	P	97	LYS
3	P	100	ASP
3	P	122	ARG
3	P	160	LYS
3	P	172	LEU
3	P	182	LEU
3	P	234	LEU
3	P	239	THR
3	P	244	ILE
3	P	268	GLN
3	P	289	LEU
3	P	299	ASN
3	P	300	MET
3	P	302	THR
3	P	303	PHE
3	P	310	ARG
3	P	312	MET
3	P	313	LYS
3	P	321	HIS
3	P	324	CYS
3	P	325	GLU
3	P	334	CYS
3	P	335	CYS
3	P	343	LEU
3	P	346	GLN
3	P	358	LEU
3	P	365	LEU
3	P	373	HIS
3	P	379	LYS
3	P	381	THR
3	P	395	ASN

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Mol	Chain	Res	Type
3	P	412	LEU
3	P	423	ARG
3	P	424	ARG
3	P	428	LEU
3	P	435	MET
3	P	441	GLU
3	P	451	GLU
3	P	472	LYS
3	P	479	GLN
3	P	524	LYS
14	Q	133	LEU
14	Q	173	ASP
14	Q	316	ARG
14	Q	401	GLN
14	Q	414	LEU
14	Q	494	ILE
14	Q	499	ARG
15	R	77	ASP
15	R	78	ARG
15	R	79	TYR
15	R	83	ARG
15	R	89	GLU
15	R	94	LEU
15	R	97	LYS
15	R	109	LYS
15	R	110	LYS
15	R	116	TRP
15	R	121	ASN
15	R	126	GLU
15	R	127	GLU
15	R	173	ASP
15	R	316	ARG
15	R	401	GLN
15	R	496	GLN
15	R	499	ARG
16	S	30	GLN
16	S	101	LEU
16	S	106	VAL
16	S	280	ASP
16	S	555	ARG
7	W	5	LYS
7	W	14	ASP

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Mol	Chain	Res	Type
17	X	39	ASP
17	X	49	LEU
17	X	79	LEU
17	X	110	LEU
17	X	184	GLN
17	X	193	LYS
17	X	201	LEU
17	X	204	ASP
17	X	255	ILE
17	X	292	LEU
17	X	299	MET
17	X	300	LEU
17	X	301	ASP
17	X	303	TYR
17	X	323	ASP
17	X	366	ILE
17	X	371	ASN
17	X	386	MET
17	X	401	ARG
17	X	414	ILE
17	X	423	ILE
17	X	452	LEU
17	X	453	GLU
17	X	460	LYS
17	X	465	LEU
17	X	475	TYR
17	X	487	SER
17	X	503	LEU
17	X	506	GLN
17	X	515	LEU
17	X	523	ASN
17	Y	39	ASP
17	Y	49	LEU
17	Y	54	ARG
17	Y	70	LEU
17	Y	79	LEU
17	Y	94	ARG
17	Y	154	ASP
17	Y	184	GLN
17	Y	193	LYS
17	Y	199	CYS
17	Y	204	ASP

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Mol	Chain	Res	Type
17	Y	255	ILE
17	Y	292	LEU
17	Y	294	PHE
17	Y	299	MET
17	Y	300	LEU
17	Y	301	ASP
17	Y	303	TYR
17	Y	323	ASP
17	Y	366	ILE
17	Y	371	ASN
17	Y	386	MET
17	Y	401	ARG
17	Y	405	CYS
17	Y	423	ILE
17	Y	452	LEU
17	Y	453	GLU
17	Y	460	LYS
17	Y	465	LEU
17	Y	475	TYR
17	Y	487	SER
17	Y	503	LEU
17	Y	506	GLN
17	Y	515	LEU
17	Y	523	ASN
17	Y	551	LYS
17	Y	552	MET
18	Z	57	THR
18	Z	66	ASN
18	Z	72	LEU
18	Z	91	ILE
18	Z	106	CYS
18	Z	138	THR
18	Z	146	GLU
18	Z	157	THR
18	Z	160	ASP
18	Z	166	LYS
18	Z	196	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (162) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN

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Mol	Chain	Res	Type
1	A	124	GLN
1	A	125	GLN
1	A	162	HIS
1	A	176	GLN
1	A	179	ASN
1	A	215	HIS
1	A	242	HIS
1	A	250	ASN
1	A	266	HIS
1	A	439	GLN
1	A	593	ASN
1	A	776	ASN
1	A	792	GLN
1	A	965	GLN
1	A	1138	HIS
1	A	1161	ASN
1	A	1165	HIS
1	A	1170	ASN
1	A	1184	HIS
1	A	1192	ASN
1	A	1266	HIS
1	A	1380	ASN
1	A	1511	ASN
1	A	1543	HIS
1	A	1558	HIS
1	A	1559	HIS
1	A	1591	HIS
1	A	1604	GLN
1	A	1813	GLN
1	A	1892	HIS
2	B	9	ASN
2	B	31	ASN
2	B	50	GLN
2	B	71	GLN
3	C	71	GLN
3	C	163	GLN
3	C	202	HIS
3	C	287	ASN
3	C	299	ASN
3	C	305	ASN
3	C	373	HIS
3	C	386	GLN

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Mol	Chain	Res	Type
3	C	390	HIS
3	C	477	HIS
3	C	479	GLN
5	E	75	GLN
6	F	70	GLN
6	F	495	HIS
6	F	634	HIS
6	F	636	ASN
6	F	667	GLN
6	H	480	ASN
6	H	494	HIS
6	H	495	HIS
6	H	545	HIS
6	H	595	GLN
6	H	634	HIS
6	H	648	GLN
6	H	657	HIS
6	H	716	ASN
6	H	754	HIS
6	H	759	ASN
8	I	18	GLN
8	I	257	HIS
8	I	266	ASN
8	I	323	ASN
8	I	345	GLN
8	I	362	HIS
8	I	442	GLN
8	I	496	GLN
8	I	535	GLN
9	J	16	GLN
9	J	17	GLN
9	J	18	GLN
9	J	58	HIS
9	J	173	HIS
9	J	271	HIS
9	J	289	HIS
9	J	316	ASN
9	J	342	HIS
9	J	382	ASN
9	J	393	GLN
9	J	406	HIS
9	J	503	HIS

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Mol	Chain	Res	Type
9	K	20	GLN
9	K	45	GLN
9	K	86	HIS
9	K	264	HIS
9	K	271	HIS
9	K	316	ASN
9	K	352	GLN
9	K	449	ASN
9	K	477	GLN
10	L	49	ASN
10	L	146	GLN
10	L	152	HIS
12	N	370	GLN
12	N	388	HIS
12	N	571	ASN
12	N	639	HIS
12	N	663	GLN
12	N	671	GLN
12	N	702	GLN
12	N	726	ASN
13	O	61	ASN
13	O	69	GLN
13	O	91	ASN
13	O	211	GLN
13	O	219	GLN
13	O	242	ASN
13	O	247	ASN
13	O	318	GLN
13	O	319	GLN
13	O	387	GLN
13	O	412	HIS
13	O	441	GLN
13	O	449	ASN
13	O	462	ASN
13	O	472	HIS
13	O	539	ASN
13	O	693	ASN
13	O	717	GLN
3	P	50	HIS
3	P	71	GLN
3	P	148	ASN
3	P	287	ASN

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Mol	Chain	Res	Type
3	P	305	ASN
3	P	321	HIS
3	P	361	ASN
3	P	488	GLN
3	P	495	GLN
15	R	99	ASN
15	R	121	ASN
16	S	87	GLN
16	S	88	ASN
16	S	133	ASN
16	S	145	GLN
16	S	192	GLN
16	S	195	GLN
16	S	278	ASN
16	S	306	ASN
17	X	50	HIS
17	X	78	GLN
17	X	89	HIS
17	X	95	ASN
17	X	106	GLN
17	X	151	GLN
17	X	337	GLN
17	X	338	HIS
17	X	371	ASN
17	X	471	GLN
17	X	506	GLN
17	Y	296	GLN
17	Y	337	GLN
17	Y	371	ASN
17	Y	506	GLN
17	Y	541	ASN
18	Z	66	ASN
18	Z	125	GLN
18	Z	134	GLN
18	Z	173	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
12	N	2
16	S	1
8	I	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S	310:ALA	C	529:SER	N	39.42
1	N	92:TRP	C	93:ASN	N	3.29
1	N	563:ASP	C	564:MET	N	2.78
1	I	302:ASP	C	303:GLU	N	2.26

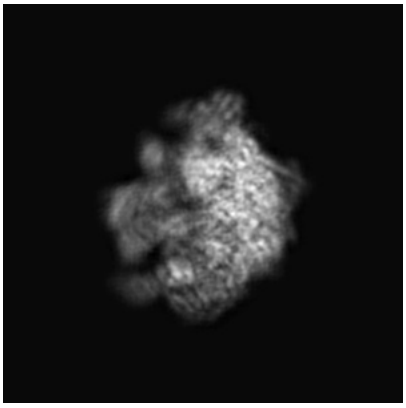
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-4037. These allow visual inspection of the internal detail of the map and identification of artifacts.

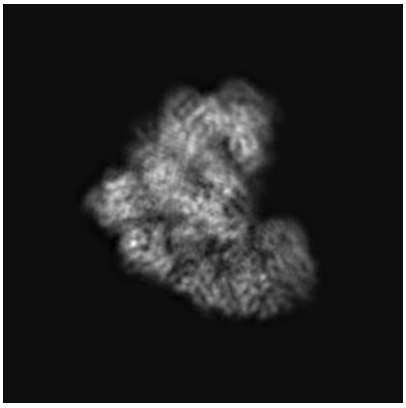
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

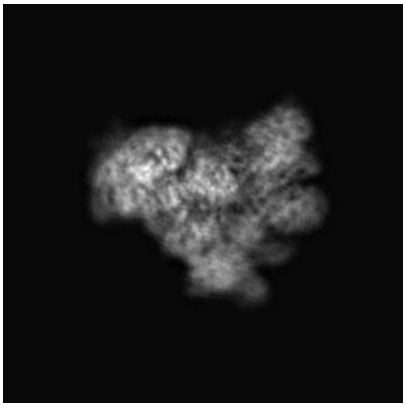
6.1.1 Primary map



X



Y

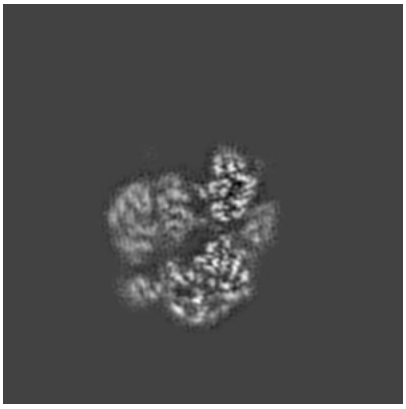


Z

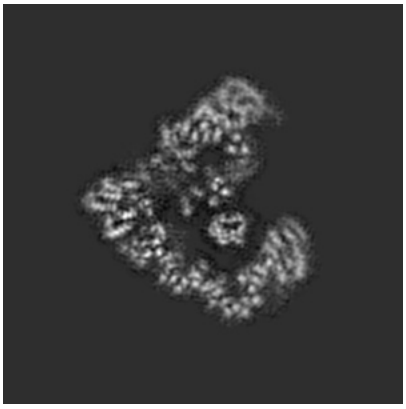
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

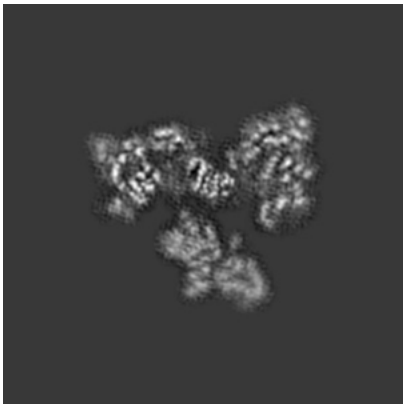
6.2.1 Primary map



X Index: 132



Y Index: 132

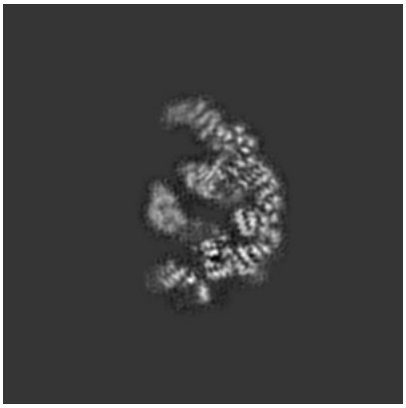


Z Index: 132

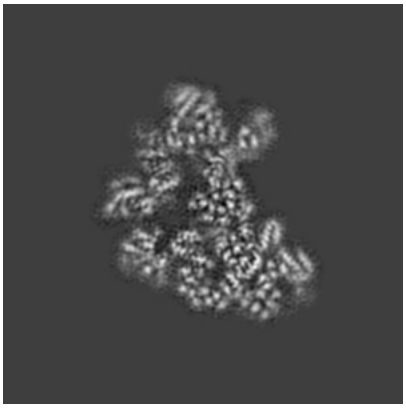
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

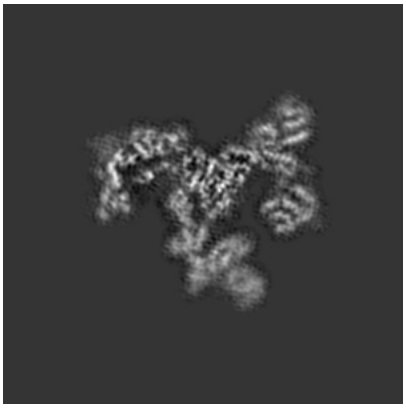
6.3.1 Primary map



X Index: 112



Y Index: 155

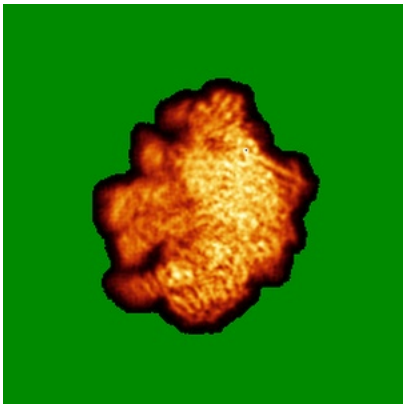


Z Index: 140

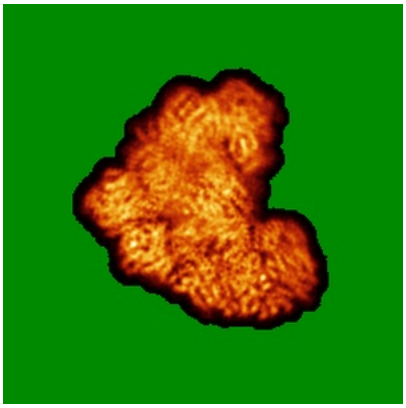
The images above show the largest variance slices of the map in three orthogonal directions.

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

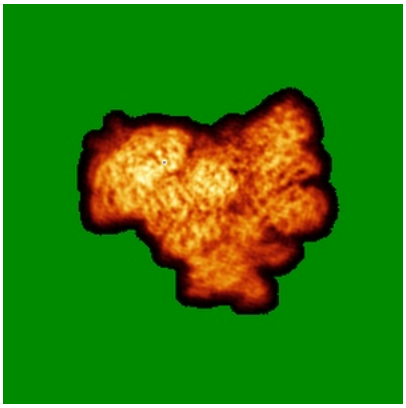
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

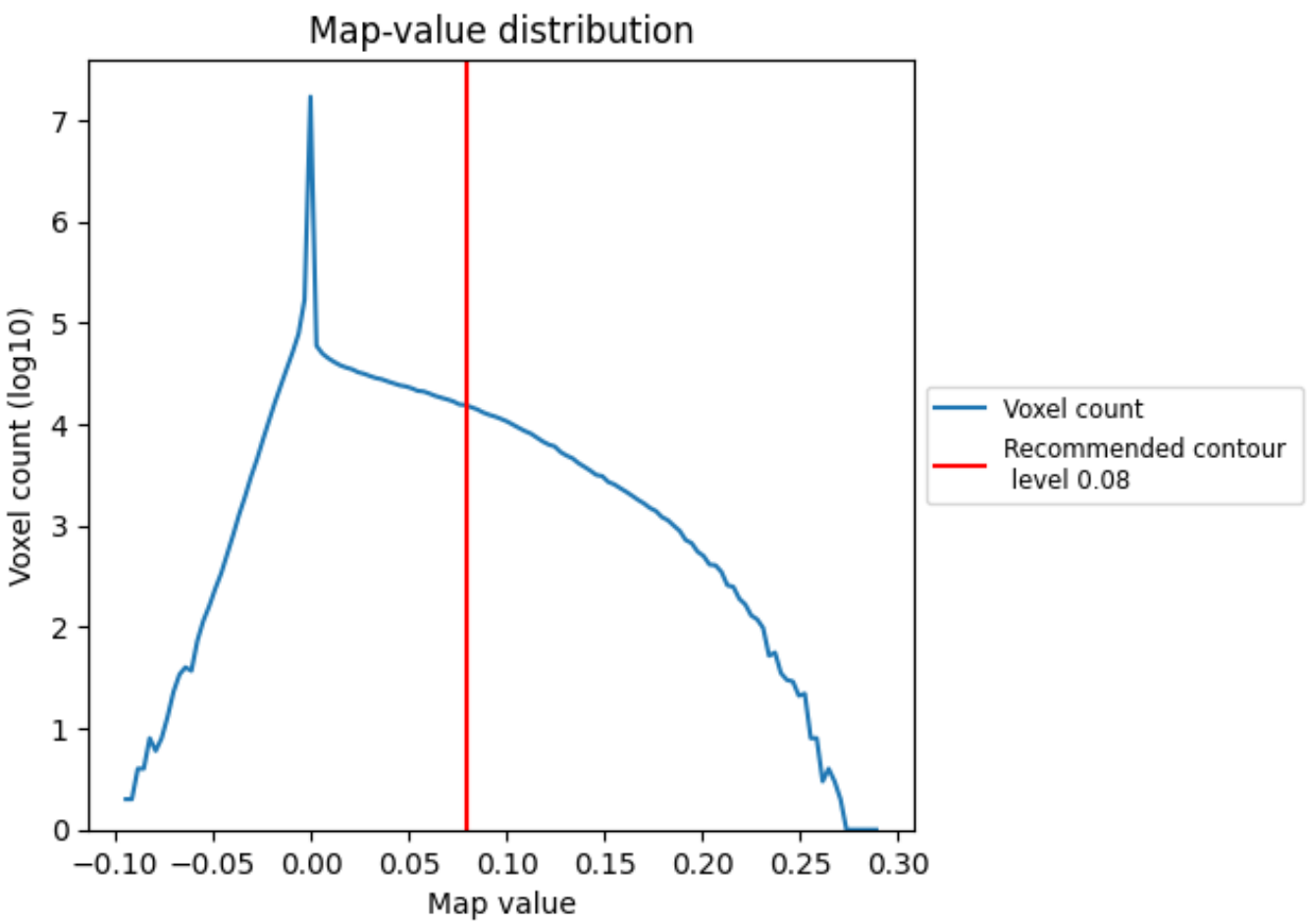
6.6 Mask visualisation (i)

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

7 Map analysis (i)

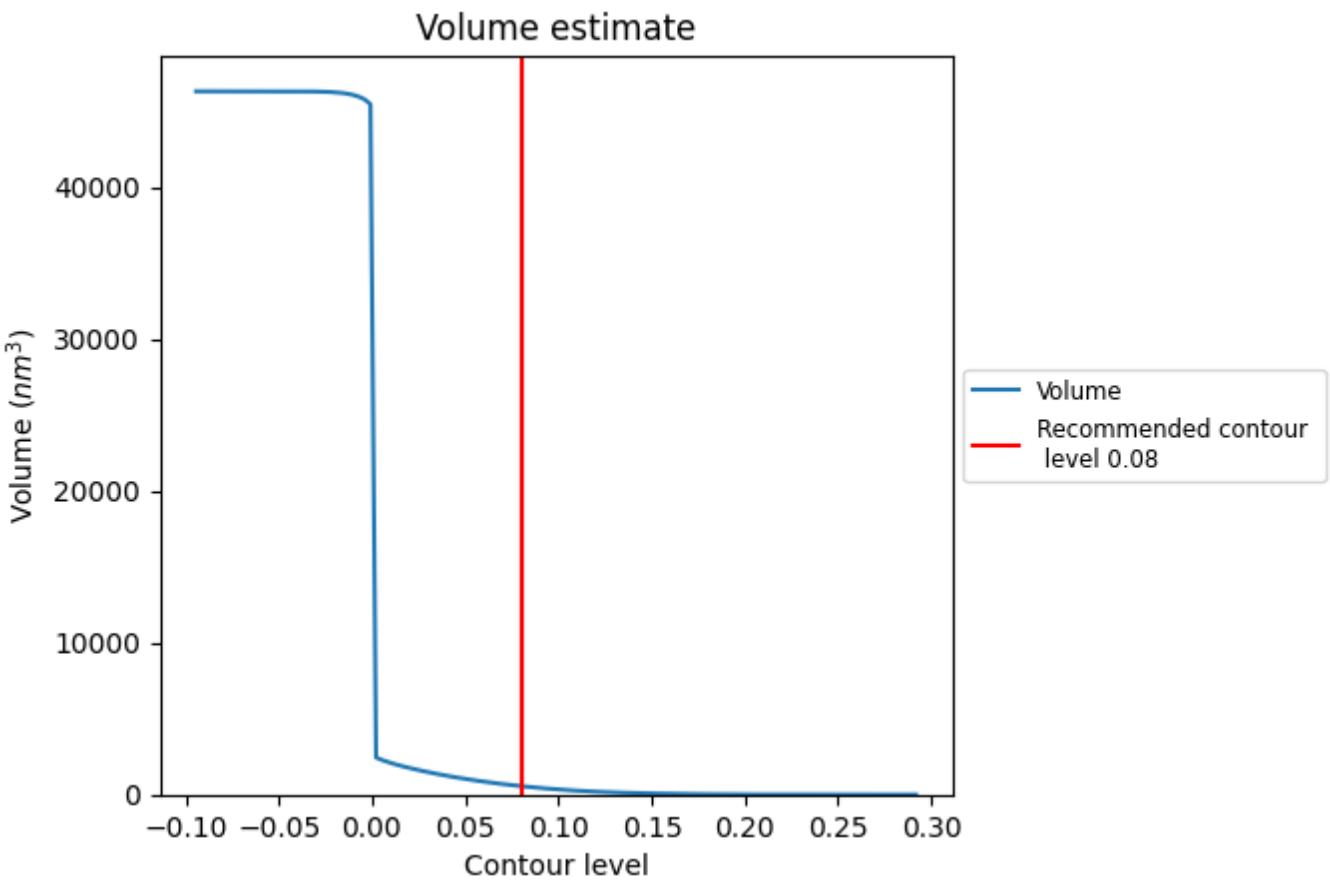
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

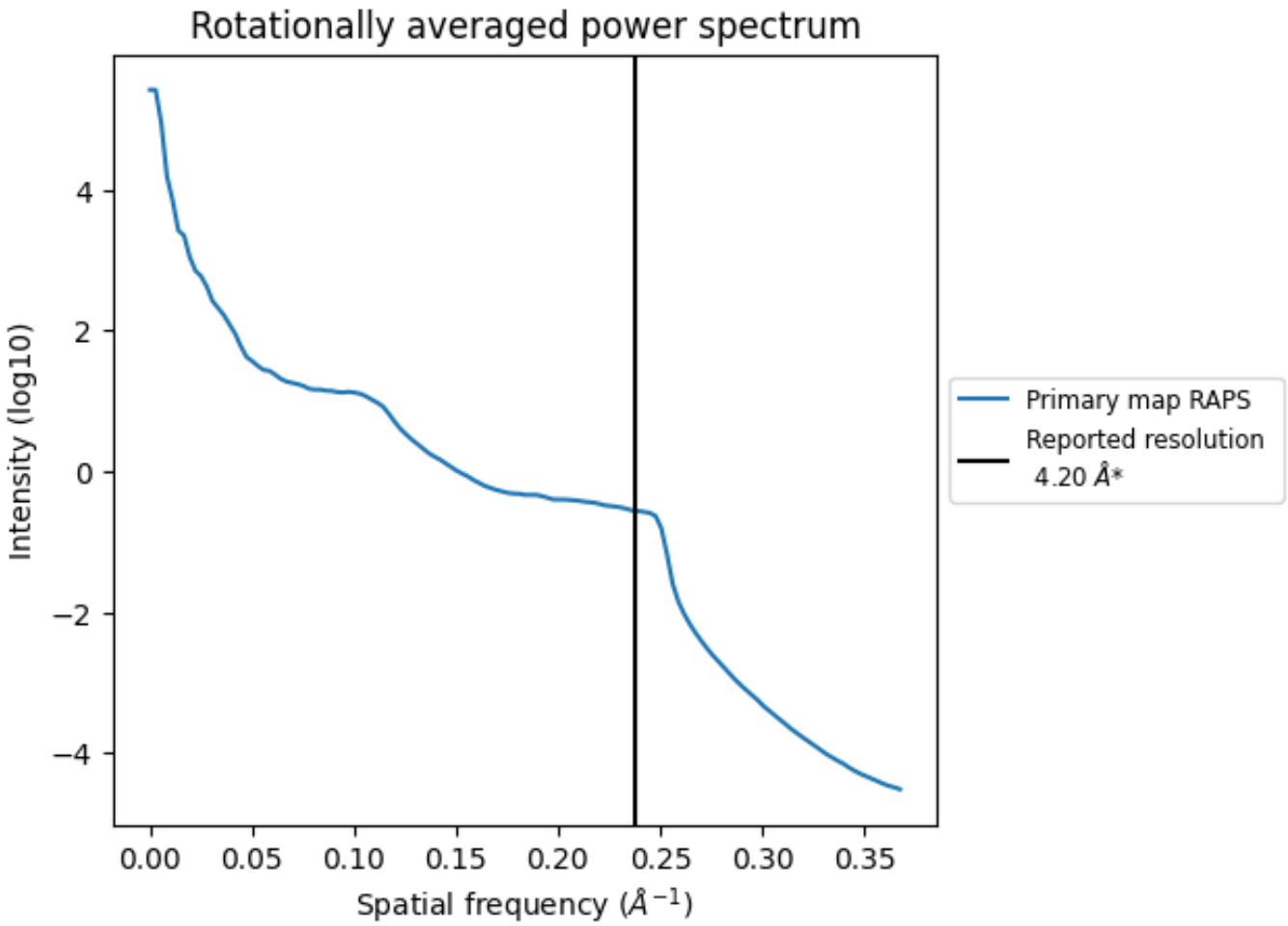
7.2 Volume estimate (i)



The volume at the recommended contour level is 554 nm^3; this corresponds to an approximate mass of 501 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 0.238 Å^{-1}

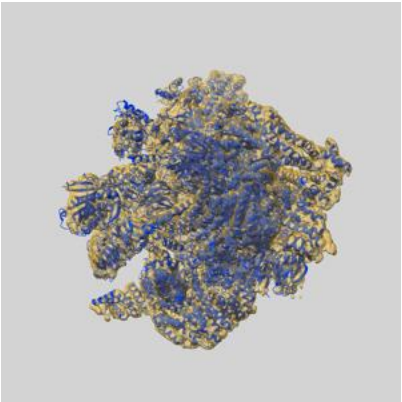
8 Fourier-Shell correlation (i)

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

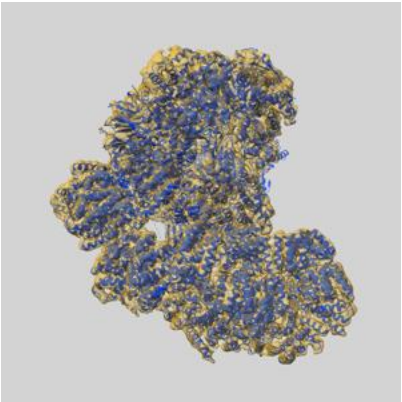
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-4037 and PDB model 5LCW. Per-residue inclusion information can be found in section 3 on page 7.

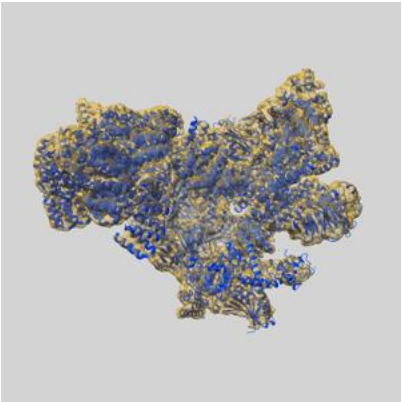
9.1 Map-model overlay (i)



X



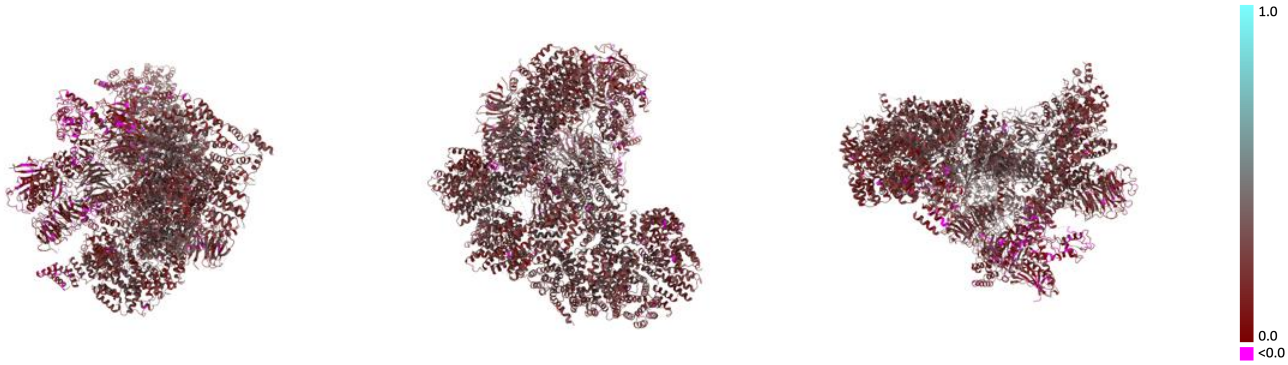
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.08 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.

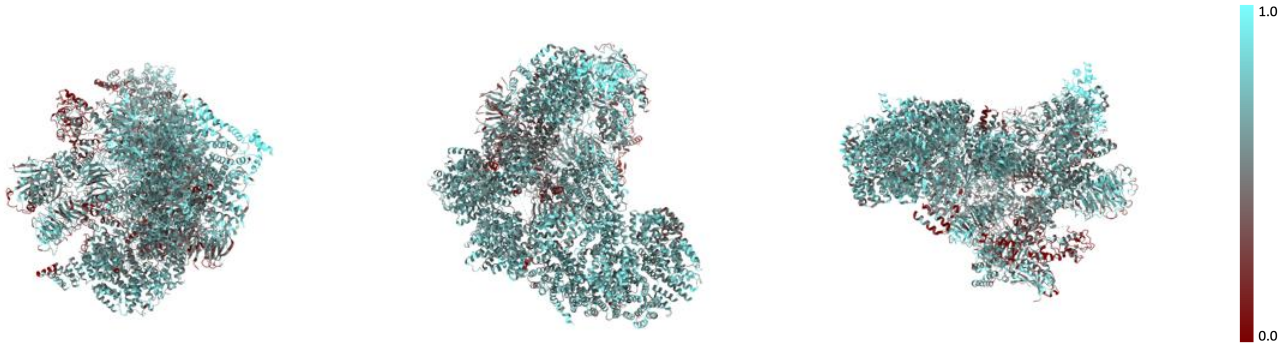
9.2 Q-score mapped to coordinate model (i)



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.

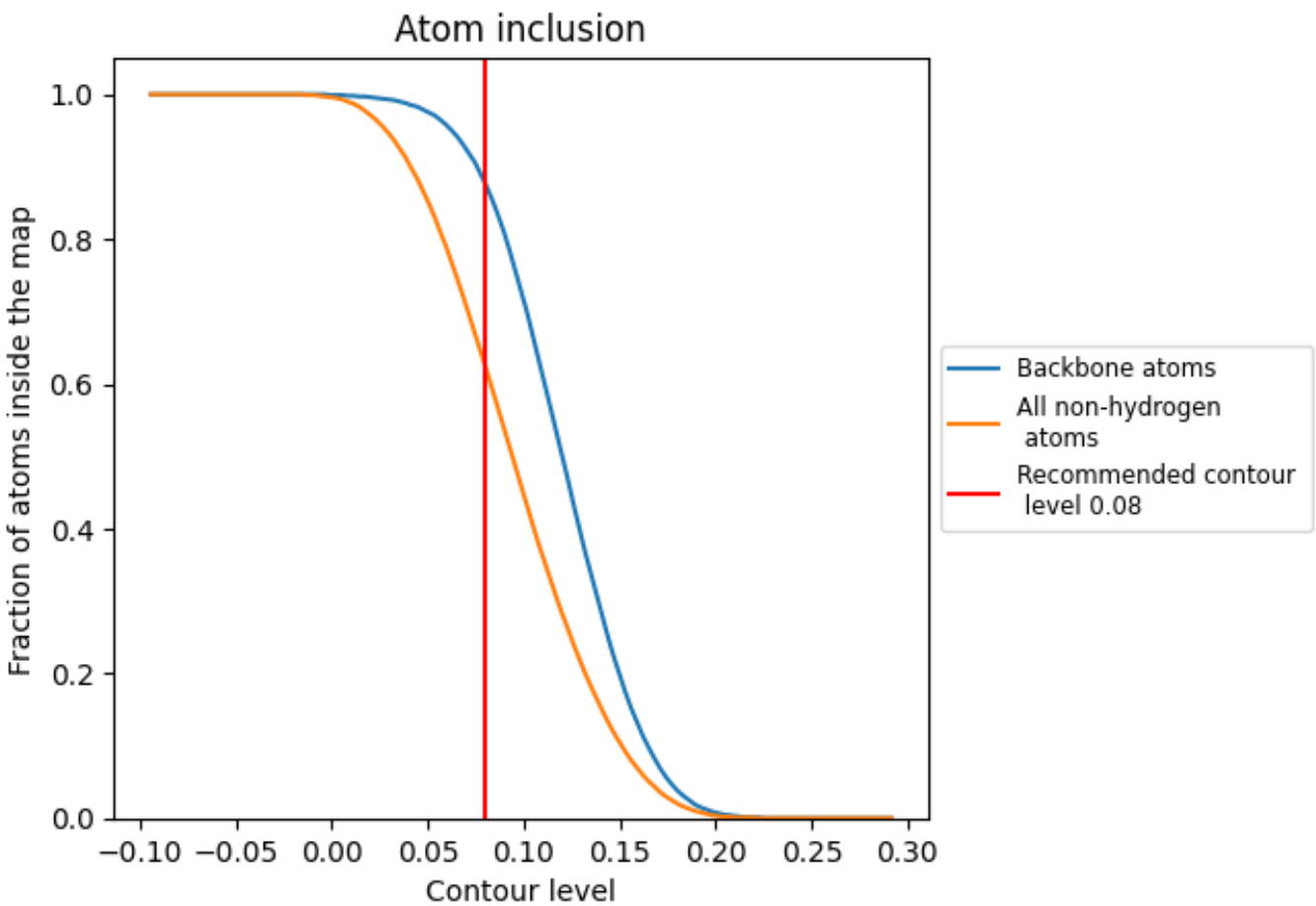
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.08).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 62% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6250	0.2520
A	0.6230	0.3020
B	0.1260	0.0340
C	0.6190	0.2630
D	0.4400	0.3690
E	0.6760	0.3320
F	0.6860	0.2920
G	0.6240	0.3050
H	0.7130	0.3030
I	0.6010	0.2160
J	0.7110	0.2910
K	0.6910	0.2680
L	0.6840	0.3260
M	0.5570	0.3280
N	0.5600	0.1860
O	0.5680	0.2670
P	0.6460	0.2500
Q	0.6250	0.2000
R	0.6390	0.2310
S	0.5830	0.1970
W	0.5900	0.2950
X	0.6020	0.2040
Y	0.6430	0.2340
Z	0.5440	0.1520