Full wwPDB EM Validation Report ⓘ

Jul 7, 2024 – 01:05 AM JST

PDB ID	:	8ZJK
EMDB ID	:	EMD-60148
Title	:	Structure of DOCK5/ELMO1/Rac1 core (RhoG/DOCK5/ELMO1/Rac1 dataset, class 3)
Authors	:	Kukimoto-Niino, M.; Katsura, K.; Ishizuka-Katsura, Y.; Mishima-Tsumagari, C.; Yonemochi, M.; Inoue, M.; Nakagawa, R.; Kaushik, R.; Zhang, K.Y.J.; Shirouzu, M.
Deposited on	:	2024-05-15
Resolution	:	4.23 Å(reported)
Based on initial model	:	7DPA

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

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

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

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

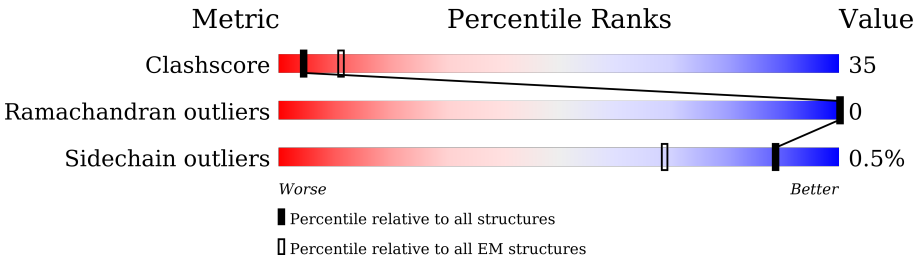
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance

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

The reported resolution of this entry is 4.23 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	733	11% 16% 73%
1	D	733	11% 16% 73%
2	B	1648	7% 41% 58%
2	E	1648	6% 40% 59%
3	C	184	34% 62%
3	F	184	32% 64%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 32858 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 Engulfment and cell motility protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	198	Total	C	N	O	S	0	0
			1608	1018	277	303	10		
1	D	198	Total	C	N	O	S	0	0
			1608	1018	277	303	10		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP Q92556
A	-4	GLY	-	expression tag	UNP Q92556
A	-3	SER	-	expression tag	UNP Q92556
A	-2	GLY	-	expression tag	UNP Q92556
A	-1	GLY	-	expression tag	UNP Q92556
A	0	SER	-	expression tag	UNP Q92556
D	-5	GLY	-	expression tag	UNP Q92556
D	-4	GLY	-	expression tag	UNP Q92556
D	-3	SER	-	expression tag	UNP Q92556
D	-2	GLY	-	expression tag	UNP Q92556
D	-1	GLY	-	expression tag	UNP Q92556
D	0	SER	-	expression tag	UNP Q92556

- Molecule 2 is a protein called Dedicator of cytokinesis protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1642	Total	C	N	O	S	0	0
			13436	8618	2264	2484	70		
2	E	1642	Total	C	N	O	S	0	0
			13436	8618	2264	2484	70		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	GLY	-	expression tag	UNP Q9H7D0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	GLY	-	expression tag	UNP Q9H7D0
B	-3	SER	-	expression tag	UNP Q9H7D0
B	-2	GLY	-	expression tag	UNP Q9H7D0
B	-1	GLY	-	expression tag	UNP Q9H7D0
B	0	SER	-	expression tag	UNP Q9H7D0
B	1285	ARG	LYS	variant	UNP Q9H7D0
E	-5	GLY	-	expression tag	UNP Q9H7D0
E	-4	GLY	-	expression tag	UNP Q9H7D0
E	-3	SER	-	expression tag	UNP Q9H7D0
E	-2	GLY	-	expression tag	UNP Q9H7D0
E	-1	GLY	-	expression tag	UNP Q9H7D0
E	0	SER	-	expression tag	UNP Q9H7D0
E	1285	ARG	LYS	variant	UNP Q9H7D0

- Molecule 3 is a protein called Ras-related C3 botulinum toxin substrate 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	177	Total	C	N	O	S	0	0
			1385	890	228	259	8		
3	F	177	Total	C	N	O	S	0	0
			1385	890	228	259	8		

There are 16 discrepancies between the modelled and reference sequences:

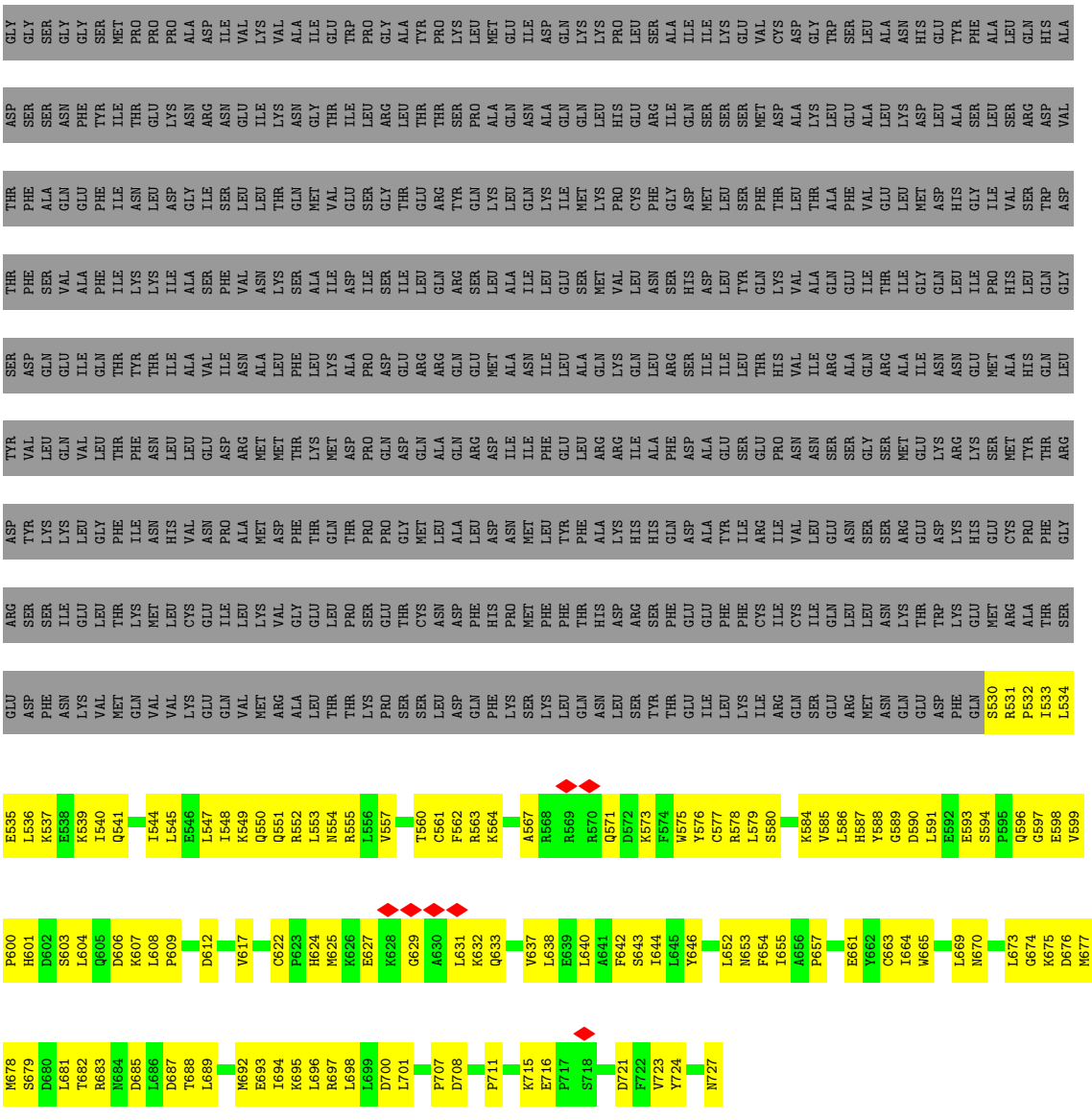
Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	GLY	-	expression tag	UNP P63000
C	-5	SER	-	expression tag	UNP P63000
C	-4	SER	-	expression tag	UNP P63000
C	-3	GLY	-	expression tag	UNP P63000
C	-2	SER	-	expression tag	UNP P63000
C	-1	SER	-	expression tag	UNP P63000
C	0	GLY	-	expression tag	UNP P63000
C	15	ALA	GLY	engineered mutation	UNP P63000
F	-6	GLY	-	expression tag	UNP P63000
F	-5	SER	-	expression tag	UNP P63000
F	-4	SER	-	expression tag	UNP P63000
F	-3	GLY	-	expression tag	UNP P63000
F	-2	SER	-	expression tag	UNP P63000
F	-1	SER	-	expression tag	UNP P63000
F	0	GLY	-	expression tag	UNP P63000
F	15	ALA	GLY	engineered mutation	UNP P63000

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.

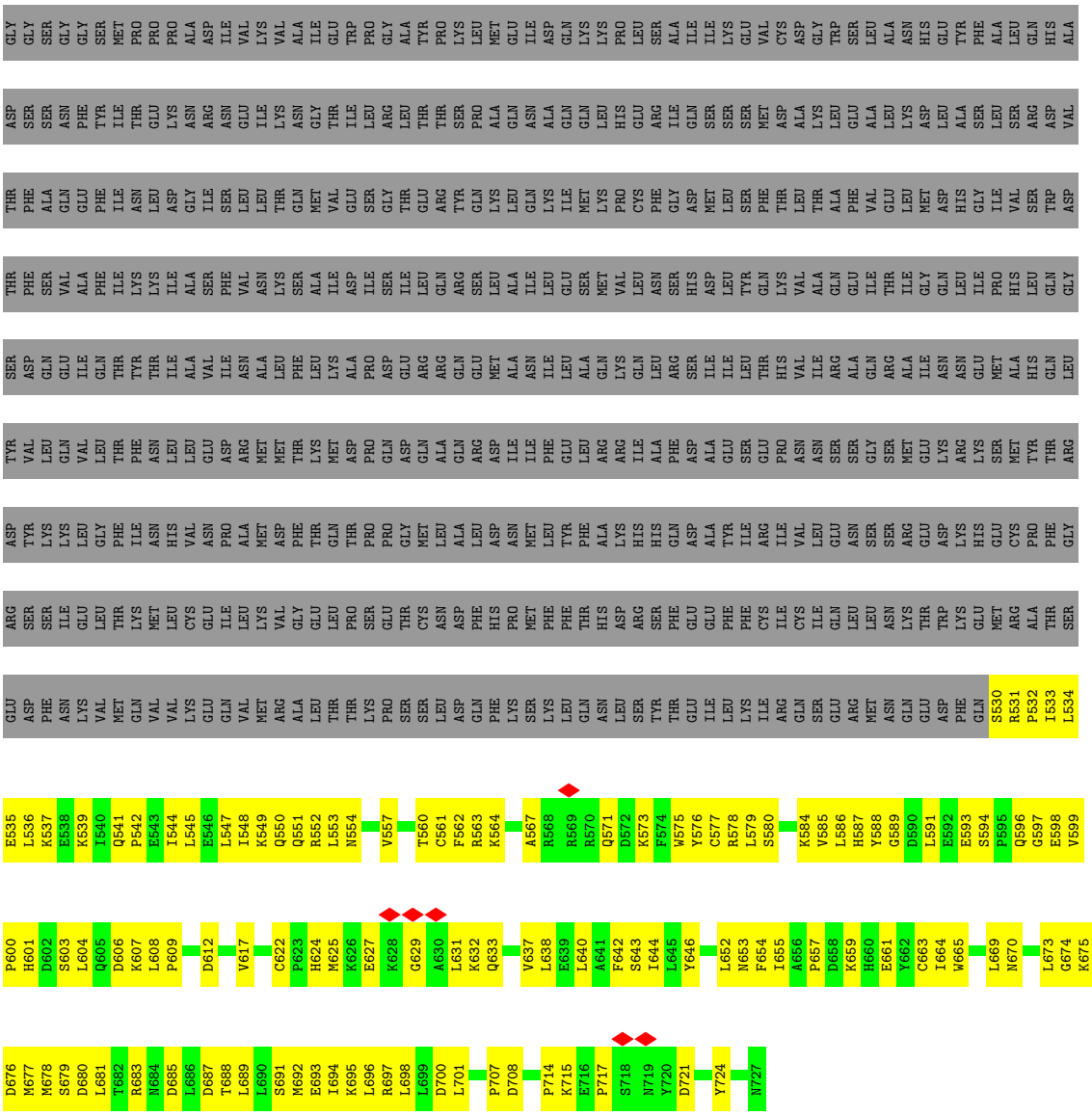
- Molecule 1: Engulfment and cell motility protein 1

Chain A:



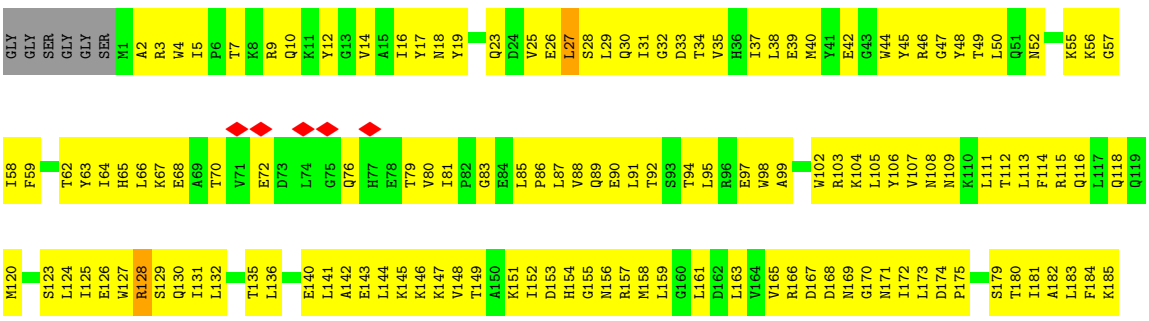
• Molecule 1: Engulfment and cell motility protein 1

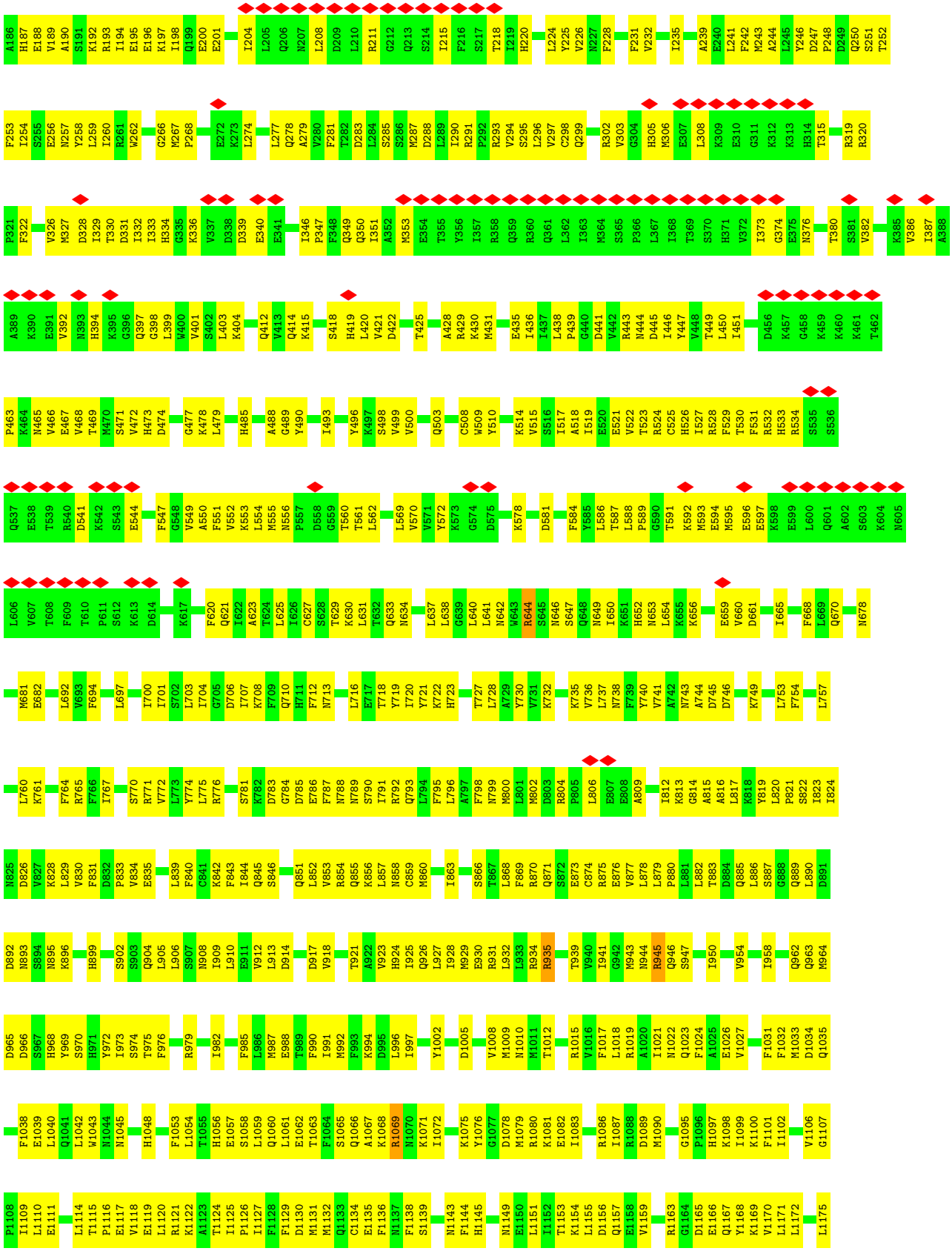
Chain D:



• Molecule 2: Dedicator of cytokinesis protein 5

Chain B:

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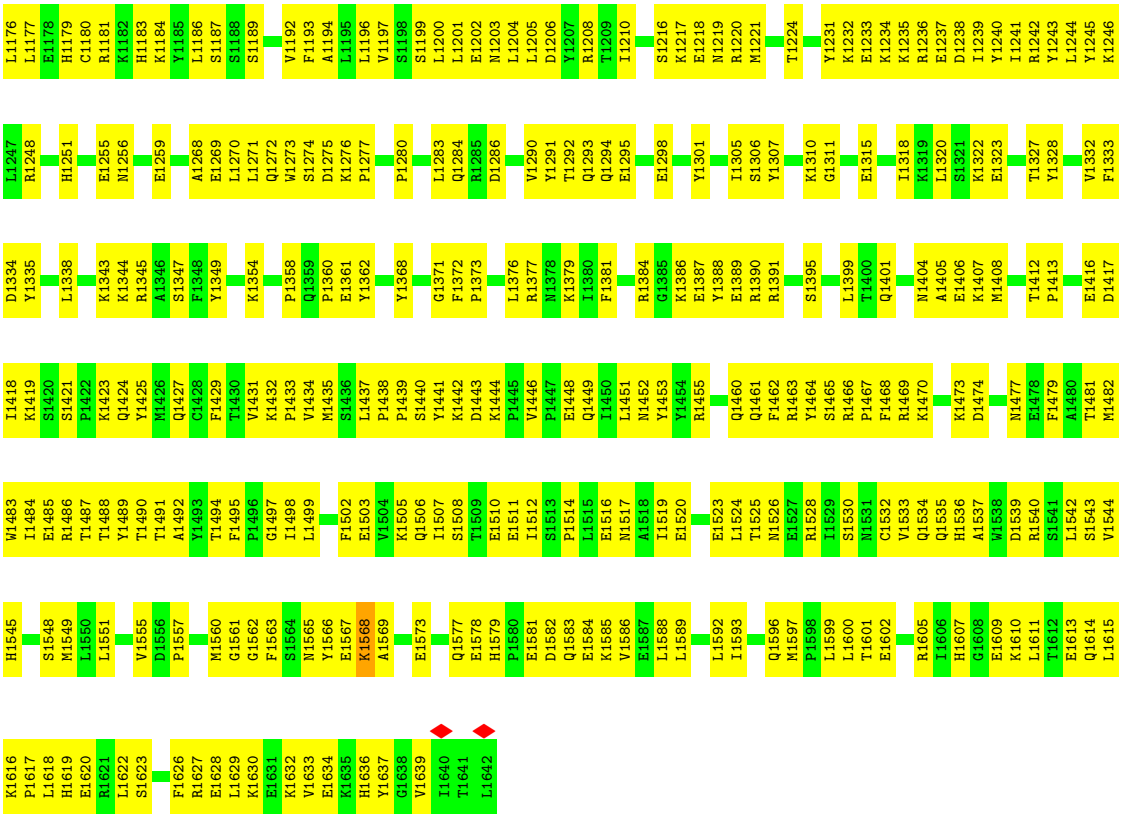
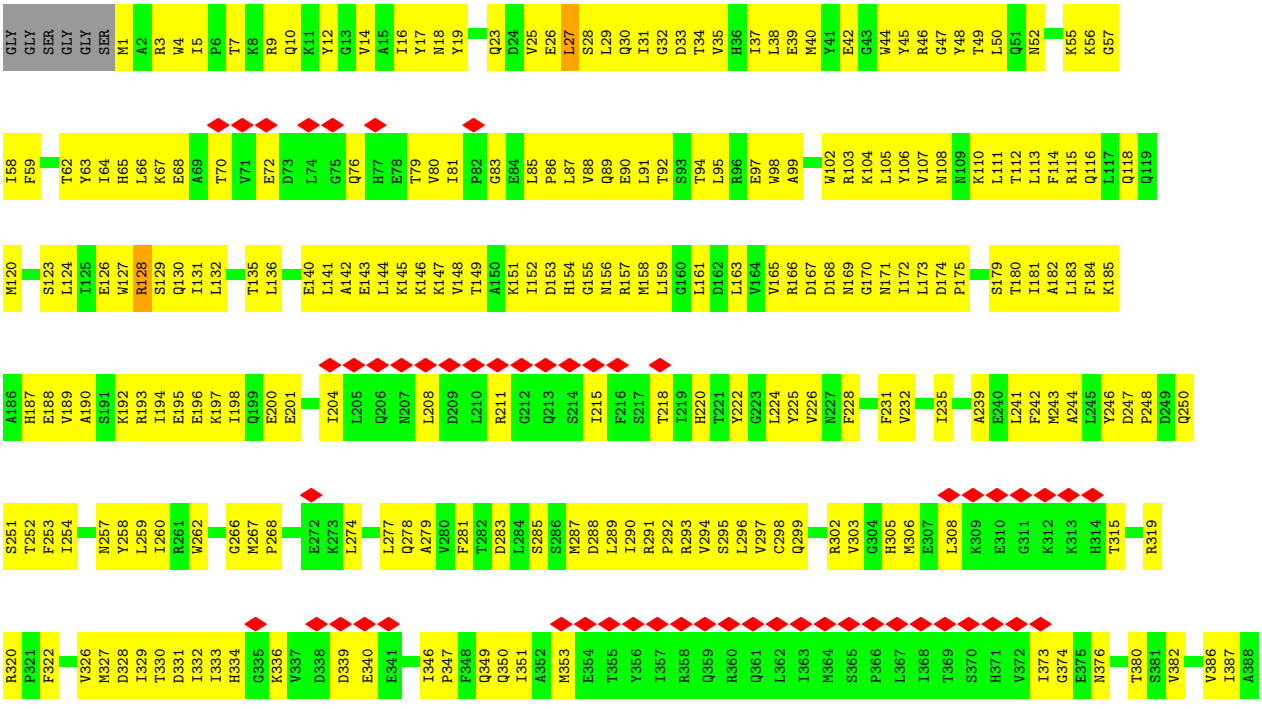
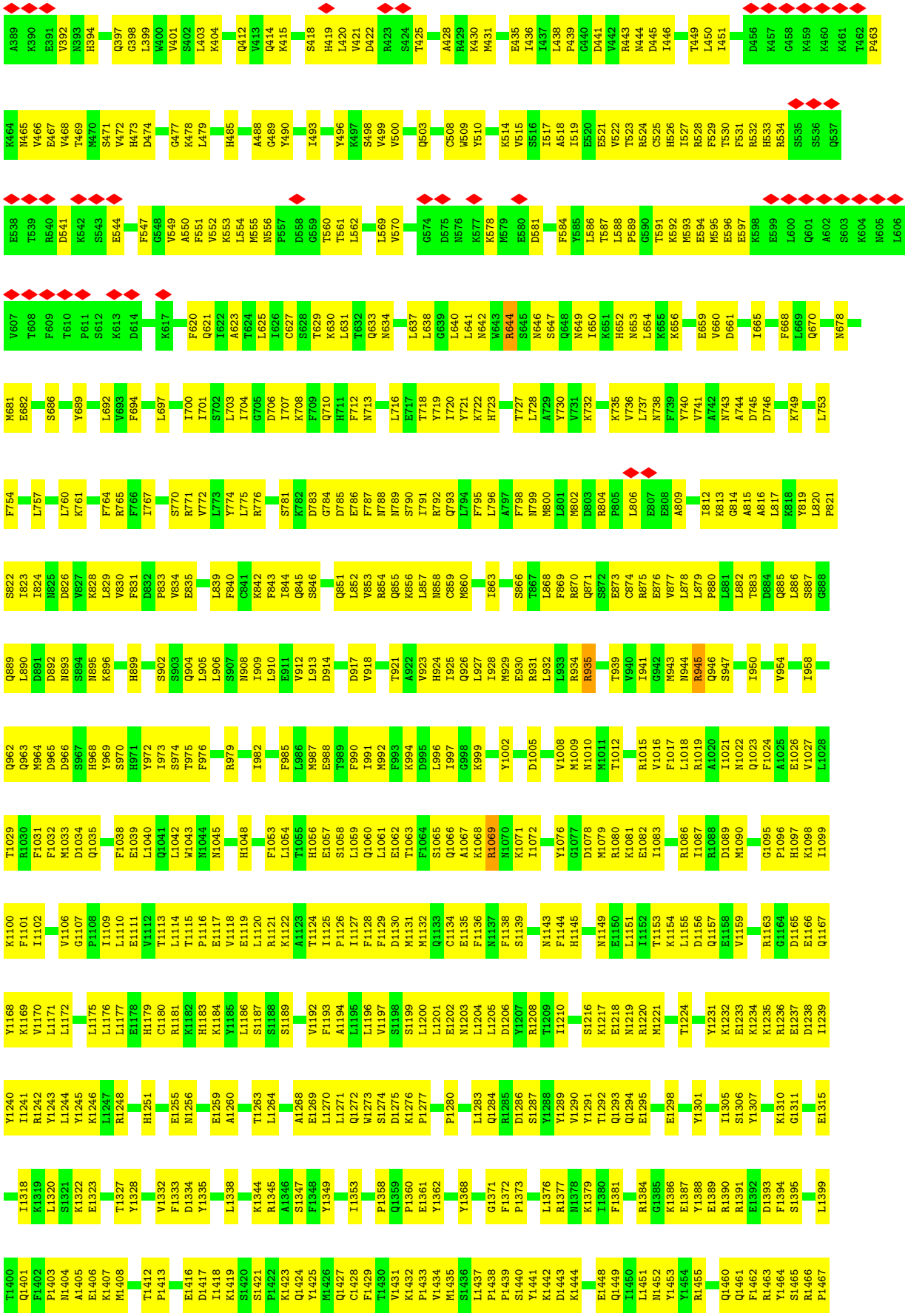
F253 I254 S255 E256 N257 Y258 L259 I260 R261 W262 G266 M267 P268 E272 K273 L274 L277 Q278 A279 V280 F281 T282 D283 L284 S285 S286 M287 D288 L289 I290 R291 P292 R293 V294 S295 L296 V297 C298 Q299 R302 V303 G304 H305 M306 E307 L308 K309 E310 G311 K312 K313 H314 T315 R319 R320
P321 F322 V326 M327 D328 I329 T330 D331 I332 I333 H334 G335 K336 V337 D338 D339 E340 E341 I346 P347 F348 Q349 Q350 I351 A352 M353 E354 T355 Y356 I357 R358 Q359 R360 Q361 L362 I363 M364 S365 P366 L367 I368 T369 S370 H371 V372 I373 G374 E375 N376 T380 S381 V382 K385 V386 I387 A388
A389 K390 E391 V392 N393 H394 K395 G396 Q397 G398 L399 W400 V401 S402 L403 K404 Q412 V413 Q414 K415 S418 H419 L420 V421 D422 T425 A428 R429 K430 M431 E435 I436 I437 L438 P439 G440 D441 V442 R443 N444 D445 I446 Y447 V448 T449 L450 I451 D456 K457 G458 K459 K460 K461 T462
P463 K464 N465 V466 E467 V468 T469 M470 S471 V472 H473 D474 G477 K478 L479 H485 A488 G489 Y490 I493 Y496 K497 S498 V499 V500 Q503 C508 W509 Y510 K514 V515 S516 I517 A518 I519 E520 E521 V522 T523 R524 C525 H526 I527 R528 F529 T530 F531 R532 H533 R534 S535 S536
Q537 E538 T539 R540 D541 K542 S543 E544 F547 G548 V549 A550 F551 V552 K553 L554 M555 N556 P557 D558 G559 T560 T561 L562 L569 V570 V571 Y572 K573 G574 D575 K578 D581 F584 Y585 L586 T587 L588 P589 G590 T591 K592 M593 E594 M595 E596 E597 K598 E599 L600 Q601 A602 S603 K604 N605
L606 V607 T608 F609 T610 P611 S612 K613 D614 K617 F620 Q621 I622 A623 T624 L625 L626 C627 S628 T629 K630 L631 T632 Q633 N634 L637 L638 G639 L640 L641 N642 W643 R644 S645 N646 S647 Q648 N649 I650 K651 H652 N653 L654 K655 K656 E659 V660 D661 I665 F668 L669 Q670 N678
M681 E682 L692 V693 F694 L697 I700 T701 S702 L703 T704 G705 D706 T707 K708 F709 Q710 H711 F712 N713 L716 E717 T718 Y719 I720 Y721 K722 H723 T727 L728 A729 Y730 V731 K732 K735 V736 L737 N738 F739 Y740 V741 A742 N743 A744 D745 D746 K749 L753 F754 L757
L760 K761 F764 R765 F766 I767 S770 R771 V772 L773 Y774 L775 R776 S781 K782 D783 G784 D785 E786 F787 N788 N789 S790 I791 R792 Q793 L794 F795 L796 A797 F798 N799 M800 L801 M802 D803 R804 P805 L806 E807 E808 A809 I812 K813 G814 A815 A816 L817 K818 Y819 L820 P821 S822 I823 I824
N825 D826 V827 K828 L829 V830 F831 D832 P833 V834 E835 L839 F840 C841 K842 F843 I844 Q845 S846 Q851 L852 V853 R854 Q855 K856 L857 N858 C859 M860 I863 S866 T867 L868 F869 R870 Q871 S872 E873 C874 R875 E876 V877 L878 L879 P880 L881 L882 T883 D884 Q885 L886 S887 G888 Q889 L890 D891
D892 N893 S894 N895 K896 H899 S902 S903 Q904 L905 L906 S907 N908 I909 L910 E911 V912 L913 D914 D917 V918 T921 A922 V923 H924 I925 Q926 L927 I928 M929 E930 R931 L932 L933 R934 R935 T939 V940 I941 G942 M943 N944 R945 Q946 S947 I950 V954 I958 Q962 Q963 M964
D965 D966 S967 H968 Y969 S970 H971 Y972 I973 S974 T975 F976 R979 I982 F985 L986 M987 E988 T989 F990 I991 M992 F993 K994 D995 L996 I997 Y1002 D1005 V1008 M1009 N1010 M1011 T1012 R1015 V1016 F1017 L1018 R1019 A1020 I1021 N1022 Q1023 F1024 A1025 E1026 V1027 F1031 F1032 M1033 D1034 Q1035
F1038 E1039 L1040 Q1041 L1042 W1043 N1044 N1045 H1048 F1053 L1054 T1055 H1056 E1057 S1058 L1059 Q1060 L1061 E1062 T1063 F1064 S1065 Q1066 A1067 K1068 R1069 N1070 K1071 I1072 K1075 Y1076 G1077 D1078 M1079 R1080 K1081 E1082 I1083 R1086 I1087 R1088 D1089 M1090 G1095 P1096 H1097 R1098 I1099 K1100 F1101 I1102 V1106 G1107
P1108 I1109 L1110 E1111 L1114 T1115 P1116 E1117 V1118 E1119 L1120 R1121 K1122 A1123 T1124 I1125 P1126 I1127 F1128 F1129 D1130 M1131 M1132 Q1133 C1134 E1135 F1136 N1137 F1138 S1139 N1143 F1144 H1145 N1149 E1150 L1151 I1152 T1153 K1154 L1155 D1156 Q1157 E1158 V1159 R1163 G1164 D1165 E1166 Q1167 Y1168 K1169 V1170 L1171 L1172 L1175



• Molecule 2: Dedicator of cytokinesis protein 5

Chain E:

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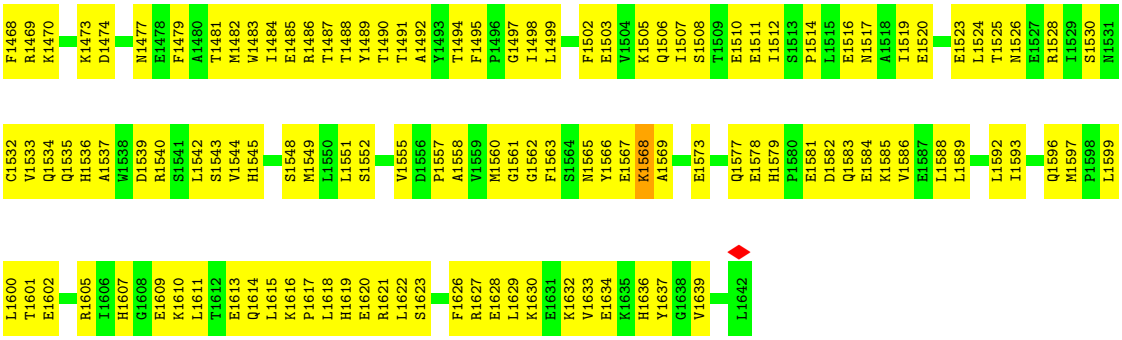
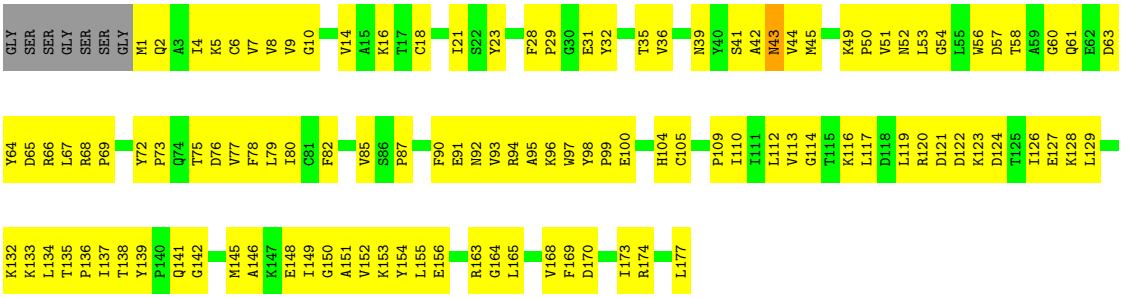
K464 M465 V466 E467 V468 T469 M470 S471 V472 H473 D474 G477 K478 L479 H485 A488 G489 Y490 I493 Y496 K497 S498 V499 V500 Q503 C508 W509 Y510 K514 V515 S516 I517 A518 I519 E520 E521 V522 T523 R524 C525 H526 I527 R528 F529 T530 F531 R532 H533 R534 S535 S536 Q537
E538 T539 R540 D541 K542 S543 E544 F547 G548 V549 A550 F551 V552 K553 L554 M555 N556 P557 D558 G559 T560 T561 L562 L569 V570 G574 D575 N576 K577 K578 M579 E580 D581 F584 Y585 L586 T587 L588 P589 G590 T591 K592 M593 E594 M595 E596 E597 K598 E599 L600 Q601 A602 S603 K604 N605 L606
V607 T608 F609 T610 P611 S612 K613 D614 K617 F620 Q621 I622 A623 T624 L625 I626 C627 S628 T629 K630 L631 T632 Q633 N634 L637 L638 G639 L640 L641 N642 W643 R644 S645 N646 S647 Q648 N649 I650 K651 H652 N653 L654 K655 K656 E659 V660 D661 I665 F668 L669 Q670 M678
M681 E682 S686 Y689 L692 V693 F694 L697 I700 I701 S702 L703 I704 G705 D706 I707 K708 F709 Q710 H711 F712 N713 L716 E717 T718 Y719 I720 Y721 K722 H723 T727 L728 A729 Y730 V731 K732 K735 V736 L737 N738 F739 Y740 V741 A742 N743 A744 D745 D746 K749 L753
F754 L757 L760 K761 F764 R765 F766 I767 S770 R771 V772 L773 Y774 L775 R776 S781 K782 D783 G784 D785 E786 F787 N788 N789 S790 I791 R792 Q793 L794 F795 L796 A797 F798 N799 M800 L801 M802 D803 R804 P805 L806 E807 E808 A809 I812 K813 G814 A815 A816 L817 K818 Y819 L820 P821
S822 I823 I824 N825 D826 V827 K828 L829 V830 F831 D832 P833 V834 E835 L839 F840 C841 K842 F843 I844 Q845 S846 Q851 L852 V853 R854 Q855 K856 L857 N858 C859 M860 I863 S866 T867 L868 F869 R870 Q871 S872 E873 C874 R875 E876 V877 L878 L879 P880 L881 L882 T883 D884 Q885 L886 S887 G888
Q889 L890 D891 D892 N893 S894 N895 K896 H899 S902 S903 Q904 L905 L906 S907 N908 I909 L910 E911 V912 L913 D914 D917 V918 T921 A922 V923 H924 I925 Q926 L927 I928 M929 E930 R931 L932 L933 R934 R935 T939 V940 I941 G942 M943 N944 R945 Q946 S947 I950 V954 I958
Q962 Q963 M964 D965 D966 S967 H968 Y969 S970 H971 Y972 I973 S974 T975 F976 R979 I982 F985 L986 M987 E988 T989 F990 I991 M992 F993 K994 D995 L996 I997 G998 K999 Y1002 D1005 V1008 M1009 N1010 M1011 T1012 R1015 V1016 F1017 L1018 R1019 A1020 I1021 N1022 Q1023 F1024 A1025 E1026 V1027 L1028
T1029 R1030 F1031 F1032 M1033 D1034 Q1035 F1038 E1039 L1040 Q1041 L1042 W1043 N1044 N1045 H1048 F1053 L1054 T1055 H1056 E1057 S1058 L1059 Q1060 L1061 E1062 T1063 F1064 S1065 Q1066 A1067 K1068 R1069 N1070 K1071 I1072 Y1076 G1077 D1078 M1079 R1080 K1081 E1082 I1083 R1086 I1087 R1088 D1089 M1090 G1095 P1096 H1097 K1098 I1099
K1100 F1101 I1102 V1106 G1107 P1108 I1109 L1110 E1111 V1112 T1113 L1114 T1115 P1116 E1117 V1118 E1119 L1120 R1121 K1122 A1123 T1124 I1125 P1126 I1127 F1128 F1129 D1130 M1131 M1132 Q1133 C1134 E1135 F1136 N1137 F1138 S1139 N1143 F1144 H1145 N1149 E1150 L1151 I1152 T1153 K1154 L1155 D1156 Q1157 E1158 V1159 R1163 G1164 D1165 E1166 Q1167
Y1168 K1169 V1170 L1171 L1172 L1175 L1176 L1177 E1178 H1179 C1180 R1181 K1182 H1183 K1184 Y1185 L1186 S1187 S1188 S1189 V1192 F1193 A1194 L1195 L1196 V1197 S1198 S1199 L1200 L1201 E1202 N1203 L1204 L1205 D1206 Y1207 R1208 T1209 I1210 S1216 K1217 E1218 N1219 R1220 M1221 T1224 Y1231 K1232 E1233 K1234 K1235 R1236 E1237 D1238 I1239
Y1240 I1241 R1242 Y1243 L1244 Y1245 K1246 L1247 R1248 H1251 E1255 N1256 E1259 A1260 T1263 L1264 A1268 E1269 L1270 L1271 Q1272 W1273 S1274 D1275 K1276 P1277 P1280 L1283 Q1284 R1285 D1286 S1287 Y1288 Y1289 V1290 Y1291 T1292 Q1293 Q1294 E1295 E1298 Y1301 I1305 S1306 Y1307 K1310 G1311 E1315
I1318 K1319 L1320 S1321 K1322 E1323 T1327 Y1328 V1332 F1333 D1334 Y1335 L1338 K1344 R1345 A1346 S1347 F1348 Y1349 I1353 P1358 Q1359 P1360 E1361 Y1362 Y1368 G1371 F1372 P1373 L1376 R1377 N1378 K1379 I1380 F1381 R1384 G1385 K1386 E1387 Y1388 E1389 R1390 R1391 E1392 D1393 F1394 S1395 L1399
T1400 Q1401 F1402 P1403 N1404 A1405 E1406 K1407 M1408 T1412 P1413 E1416 D1417 I1418 K1419 S1420 S1421 P1422 K1423 Q1424 Y1425 M1426 Q1427 C1428 F1429 T1430 V1431 K1432 P1433 V1434 M1435 S1436 L1437 P1438 P1439 S1440 Y1441 K1442 D1443 K1444 E1448 Q1449 I1450 L1451 N1452 Y1453 Y1454 R1455 Q1460 Q1461 F1462 R1463 Y1464 S1465 R1466 P1467



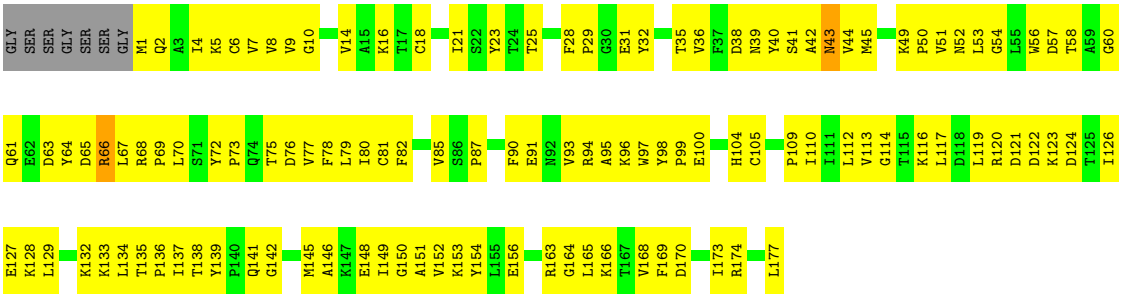
• Molecule 3: Ras-related C3 botulinum toxin substrate 1

Chain C:



• Molecule 3: Ras-related C3 botulinum toxin substrate 1

Chain F:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	120707	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.060	Depositor
Minimum map value	-0.022	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	452.2, 452.2, 452.2	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.33, 1.33, 1.33	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.30	0/1641	0.52	0/2218
1	D	0.30	0/1641	0.52	0/2218
2	B	0.37	1/13722 (0.0%)	0.54	5/18514 (0.0%)
2	E	0.37	1/13722 (0.0%)	0.54	5/18514 (0.0%)
3	C	0.34	0/1415	0.49	0/1924
3	F	0.34	0/1415	0.49	0/1924
All	All	0.36	2/33556 (0.0%)	0.53	10/45312 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	463	PRO	CG-CD	-14.33	1.03	1.50
2	B	463	PRO	CG-CD	-14.29	1.03	1.50

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	463	PRO	N-CD-CG	-17.32	77.21	103.20
2	E	463	PRO	N-CD-CG	-17.30	77.25	103.20
2	B	463	PRO	CA-CB-CG	-11.62	81.93	104.00
2	E	463	PRO	CA-CB-CG	-11.60	81.96	104.00
2	B	463	PRO	CA-N-CD	-7.71	100.70	111.50
2	E	463	PRO	CA-N-CD	-7.69	100.73	111.50
2	B	463	PRO	CB-CG-CD	6.62	132.31	106.50
2	E	463	PRO	CB-CG-CD	6.61	132.28	106.50
2	B	27	LEU	CA-CB-CG	5.24	127.35	115.30
2	E	27	LEU	CA-CB-CG	5.23	127.32	115.30

There are no chirality outliers.

There are no planarity outliers.

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	1608	0	1617	133	0
1	D	1608	0	1617	138	0
2	B	13436	0	13516	927	0
2	E	13436	0	13516	952	0
3	C	1385	0	1407	106	0
3	F	1385	0	1407	120	0
All	All	32858	0	33080	2301	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 35.

All (2301) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:697:ARG:HH21	2:E:30:GLN:HB2	1.33	0.91
1:D:670:ASN:ND2	1:D:676:ASP:O	2.06	0.88
2:E:1579:HIS:HB3	2:E:1582:ASP:HB2	1.56	0.88
1:A:670:ASN:ND2	1:A:676:ASP:O	2.06	0.87
1:D:625:MET:HE1	1:D:638:LEU:HA	1.57	0.86
1:A:697:ARG:HH21	2:B:30:GLN:HB2	1.42	0.85
2:B:1579:HIS:HB3	2:B:1582:ASP:HB2	1.56	0.85
2:B:904:GLN:O	2:B:908:ASN:ND2	2.10	0.84
2:E:144:LEU:HD13	2:E:147:LYS:HE2	1.60	0.84
2:E:241:LEU:HB2	2:E:260:ILE:HB	1.59	0.84
1:A:625:MET:HE1	1:A:638:LEU:HA	1.59	0.83
2:B:144:LEU:HD13	2:B:147:LYS:HE2	1.60	0.83
2:E:904:GLN:O	2:E:908:ASN:ND2	2.10	0.83
2:E:1393:ASP:OD1	3:F:166:LYS:NZ	2.11	0.83
2:E:115:ARG:HA	2:E:118:GLN:HG3	1.62	0.82
2:B:589:PRO:HB3	2:B:594:GLU:HB3	1.62	0.82
2:E:589:PRO:HB3	2:E:594:GLU:HB3	1.62	0.82
2:B:241:LEU:HB2	2:B:260:ILE:HB	1.59	0.81
2:B:115:ARG:HA	2:B:118:GLN:HG3	1.61	0.81
2:B:530:THR:HA	2:B:549:VAL:HG22	1.63	0.80
2:E:1372:PHE:O	2:E:1377:ARG:NH2	2.15	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1372:PHE:O	2:B:1377:ARG:NH2	2.15	0.79
2:B:104:LYS:O	2:B:108:ASN:ND2	2.16	0.79
2:E:104:LYS:O	2:E:108:ASN:ND2	2.16	0.79
2:E:530:THR:HA	2:E:549:VAL:HG22	1.63	0.79
2:E:1536:HIS:O	2:E:1540:ARG:NH2	2.16	0.79
2:B:890:LEU:HD22	2:B:935:ARG:HG3	1.65	0.79
3:C:87:PRO:HD2	3:C:134:LEU:HD13	1.65	0.79
2:E:890:LEU:HD22	2:E:935:ARG:HG3	1.65	0.78
2:B:1536:HIS:O	2:B:1540:ARG:NH2	2.16	0.78
2:E:556:ASN:N	2:E:560:THR:O	2.15	0.78
2:B:556:ASN:N	2:B:560:THR:O	2.15	0.78
2:B:153:ASP:HA	2:B:156:ASN:HD22	1.49	0.77
2:E:1543:SER:OG	2:E:1545:HIS:ND1	2.17	0.77
3:F:87:PRO:HD2	3:F:134:LEU:HD13	1.65	0.77
3:F:93:VAL:HA	3:F:97:TRP:HB2	1.66	0.77
2:B:1390:ARG:NH2	3:C:23:TYR:O	2.18	0.77
2:B:278:GLN:HB2	2:B:425:THR:HG23	1.66	0.77
1:A:563:ARG:HB3	1:A:573:LYS:HE3	1.66	0.77
2:B:879:LEU:HD23	2:B:931:ARG:HH22	1.50	0.77
2:E:4:TRP:HB3	2:E:39:GLU:HB3	1.68	0.76
1:D:563:ARG:HB3	1:D:573:LYS:HE3	1.66	0.76
2:B:749:LYS:HG2	2:B:753:LEU:HD23	1.67	0.76
2:B:902:SER:HA	2:B:905:LEU:HD12	1.66	0.76
2:E:351:ILE:HG12	2:E:382:VAL:HG21	1.66	0.76
2:E:278:GLN:HB2	2:E:425:THR:HG23	1.66	0.76
2:E:749:LYS:HG2	2:E:753:LEU:HD23	1.67	0.76
3:C:93:VAL:HA	3:C:97:TRP:HB2	1.67	0.76
2:E:153:ASP:HA	2:E:156:ASN:HD22	1.49	0.75
2:E:1165:ASP:OD2	2:E:1168:TYR:N	2.20	0.75
2:B:4:TRP:HB3	2:B:39:GLU:HB3	1.68	0.75
2:E:879:LEU:HD23	2:E:931:ARG:HH22	1.50	0.75
2:E:46:ARG:HB3	2:E:58:ILE:HG13	1.69	0.75
2:B:351:ILE:HG12	2:B:382:VAL:HG21	1.66	0.75
2:B:740:TYR:HA	2:B:749:LYS:HD3	1.69	0.75
1:D:701:LEU:HD23	2:E:31:ILE:HG23	1.69	0.75
2:E:740:TYR:HA	2:E:749:LYS:HD3	1.69	0.75
1:A:589:GLY:HA3	1:A:604:LEU:HB2	1.69	0.75
2:B:1328:TYR:HA	2:B:1332:VAL:HG12	1.69	0.75
2:E:902:SER:HA	2:E:905:LEU:HD12	1.66	0.74
2:B:166:ARG:NH1	2:B:167:ASP:OD1	2.20	0.74
2:B:1117:GLU:OE1	2:B:1119:GLU:N	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1465:SER:HA	2:E:1486:ARG:HG2	1.69	0.74
2:E:166:ARG:NH1	2:E:167:ASP:OD1	2.20	0.74
1:A:576:TYR:HB2	1:A:598:GLU:HG2	1.69	0.74
2:B:964:MET:O	2:B:1019:ARG:NH2	2.20	0.74
2:B:242:PHE:HB2	2:B:299:GLN:HB2	1.69	0.74
2:B:1165:ASP:OD2	2:B:1168:TYR:N	2.20	0.73
2:E:1117:GLU:OE1	2:E:1119:GLU:N	2.20	0.73
2:B:23:GLN:HG2	2:B:58:ILE:HB	1.70	0.73
2:B:851:GLN:O	2:B:856:LYS:NZ	2.21	0.73
2:E:964:MET:O	2:E:1019:ARG:NH2	2.20	0.73
1:A:530:SER:HA	1:A:533:ILE:HD12	1.69	0.73
2:B:46:ARG:HB3	2:B:58:ILE:HG13	1.69	0.73
2:E:242:PHE:HB2	2:E:299:GLN:HB2	1.69	0.73
2:B:244:ALA:HB2	2:B:257:ASN:HA	1.69	0.73
2:B:828:LYS:HE2	2:B:833:PRO:HG3	1.70	0.73
1:D:530:SER:HA	1:D:533:ILE:HD12	1.69	0.73
3:F:7:VAL:HG23	3:F:75:THR:HG21	1.70	0.73
2:B:1543:SER:OG	2:B:1545:HIS:ND1	2.17	0.73
2:E:244:ALA:HB2	2:E:257:ASN:HA	1.69	0.73
2:E:1328:TYR:HA	2:E:1332:VAL:HG12	1.69	0.73
2:B:1466:ARG:NH1	2:B:1467:PRO:O	2.22	0.73
1:D:589:GLY:HA3	1:D:604:LEU:HB2	1.69	0.73
2:E:1277:PRO:HG3	2:E:1292:THR:HA	1.70	0.73
2:B:12:TYR:HB2	2:B:67:LYS:HB2	1.70	0.73
2:B:941:ILE:O	2:B:944:ASN:ND2	2.20	0.73
2:B:1277:PRO:HG3	2:B:1292:THR:HA	1.70	0.73
2:E:1466:ARG:NH1	2:E:1467:PRO:O	2.21	0.73
2:B:1465:SER:HA	2:B:1486:ARG:HG2	1.70	0.73
2:E:851:GLN:O	2:E:856:LYS:NZ	2.21	0.73
2:E:828:LYS:HE2	2:E:833:PRO:HG3	1.70	0.73
2:E:1562:GLY:HA3	3:F:36:VAL:HB	1.70	0.73
2:E:1245:TYR:HD2	2:E:1248:ARG:HH21	1.37	0.72
2:B:444:ASN:ND2	2:B:517:ILE:O	2.22	0.72
2:B:1034:ASP:OD1	2:B:1097:HIS:NE2	2.21	0.72
1:D:576:TYR:HB2	1:D:598:GLU:HG2	1.69	0.72
2:E:23:GLN:HG2	2:E:58:ILE:HB	1.70	0.72
3:F:61:GLN:O	3:F:68:ARG:NH2	2.22	0.72
2:E:893:ASN:O	2:E:896:LYS:NZ	2.22	0.72
2:E:1549:MET:SD	3:F:54:GLY:HA3	2.30	0.72
2:B:95:LEU:HD23	2:B:98:TRP:HD1	1.55	0.72
2:E:441:ASP:O	2:E:629:THR:OG1	2.07	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:444:ASN:ND2	2:E:517:ILE:O	2.23	0.72
3:C:7:VAL:HG23	3:C:75:THR:HG21	1.70	0.72
2:E:1292:THR:HG23	2:E:1295:GLU:H	1.54	0.72
2:B:1462:PHE:O	2:B:1489:TYR:N	2.23	0.72
2:B:1292:THR:HG23	2:B:1295:GLU:H	1.54	0.72
2:E:941:ILE:O	2:E:944:ASN:ND2	2.20	0.72
2:B:1245:TYR:HD2	2:B:1248:ARG:HH21	1.37	0.71
3:C:61:GLN:O	3:C:68:ARG:NH2	2.22	0.71
1:D:637:VAL:HG12	1:D:640:LEU:HD12	1.72	0.71
1:A:637:VAL:HG12	1:A:640:LEU:HD12	1.72	0.71
2:E:12:TYR:HB2	2:E:67:LYS:HB2	1.70	0.71
3:F:23:TYR:HB2	3:F:165:LEU:HD21	1.70	0.71
2:B:441:ASP:O	2:B:629:THR:OG1	2.07	0.71
2:B:893:ASN:O	2:B:896:LYS:NZ	2.23	0.71
2:B:1216:SER:OG	2:B:1401:GLN:NE2	2.24	0.71
1:A:550:GLN:HE22	2:B:107:VAL:HG12	1.56	0.71
3:C:23:TYR:HB2	3:C:165:LEU:HD21	1.70	0.71
2:E:1462:PHE:O	2:E:1489:TYR:N	2.23	0.71
2:E:1034:ASP:OD1	2:E:1097:HIS:NE2	2.21	0.71
2:B:970:SER:O	2:B:974:SER:OG	2.09	0.70
1:D:550:GLN:HE22	2:E:107:VAL:HG12	1.55	0.70
2:E:472:VAL:HG22	2:E:527:ILE:HG12	1.73	0.70
2:B:1015:ARG:HH21	2:B:1076:TYR:HE1	1.38	0.70
1:D:561:CYS:SG	1:D:594:SER:OG	2.49	0.70
2:E:95:LEU:HD23	2:E:98:TRP:HD1	1.55	0.70
2:B:1143:ASN:OD1	2:B:1145:HIS:ND1	2.25	0.70
1:A:561:CYS:SG	1:A:594:SER:OG	2.49	0.70
2:B:1078:ASP:OD1	2:B:1081:LYS:N	2.25	0.70
2:E:1057:GLU:HA	2:E:1061:LEU:HD23	1.74	0.70
2:E:1062:GLU:OE2	2:E:1080:ARG:NH1	2.25	0.70
2:B:1432:LYS:HZ1	2:B:1464:TYR:HA	1.57	0.69
2:E:1272:GLN:OE1	2:E:1293:GLN:NE2	2.25	0.69
2:B:1272:GLN:OE1	2:B:1293:GLN:NE2	2.25	0.69
2:B:472:VAL:HG22	2:B:527:ILE:HG12	1.73	0.69
2:B:1259:GLU:OE1	2:B:1259:GLU:N	2.23	0.69
2:E:1216:SER:OG	2:E:1401:GLN:NE2	2.24	0.69
2:E:1432:LYS:HZ1	2:E:1464:TYR:HA	1.58	0.69
3:C:98:TYR:HE1	3:C:149:ILE:HD13	1.57	0.69
2:E:1143:ASN:OD1	2:E:1145:HIS:ND1	2.25	0.69
3:F:116:LYS:HB3	3:F:119:LEU:HB2	1.74	0.69
2:B:518:ALA:HB3	2:B:521:GLU:HB2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1067:ALA:O	2:B:1071:LYS:N	2.17	0.69
3:C:116:LYS:HB3	3:C:119:LEU:HB2	1.74	0.69
2:E:883:THR:HG21	2:E:931:ARG:HB3	1.75	0.69
2:B:1062:GLU:OE2	2:B:1080:ARG:NH1	2.25	0.69
2:E:49:THR:OG1	2:E:52:ASN:OD1	2.11	0.69
2:E:1276:LYS:NZ	2:E:1277:PRO:O	2.26	0.69
2:E:879:LEU:HD12	2:E:882:LEU:HB2	1.74	0.69
2:E:939:THR:O	2:E:943:MET:N	2.17	0.69
2:E:970:SER:O	2:E:974:SER:OG	2.09	0.69
2:E:1335:TYR:HA	2:E:1338:LEU:HD23	1.75	0.69
1:A:724:TYR:HB3	2:B:4:TRP:HB2	1.74	0.69
2:E:1015:ARG:HH21	2:E:1076:TYR:HE1	1.38	0.69
2:E:1391:ARG:NH2	3:F:29:PRO:HD3	2.08	0.69
2:B:1057:GLU:HA	2:B:1061:LEU:HD23	1.74	0.69
2:B:1284:GLN:HE21	2:B:1286:ASP:HB2	1.58	0.69
2:B:49:THR:OG1	2:B:52:ASN:OD1	2.11	0.68
2:B:1149:ASN:HA	2:B:1236:ARG:HH12	1.58	0.68
1:D:551:GLN:HA	1:D:554:ASN:HD22	1.58	0.68
1:D:700:ASP:HB2	2:E:32:GLY:HA2	1.75	0.68
2:E:518:ALA:HB3	2:E:521:GLU:HB2	1.74	0.68
2:B:879:LEU:HD12	2:B:882:LEU:HB2	1.74	0.68
1:D:580:SER:HB2	1:D:585:VAL:HG22	1.76	0.68
1:A:607:LYS:NZ	1:A:608:LEU:O	2.26	0.68
2:B:473:HIS:ND1	2:B:477:GLY:O	2.26	0.68
2:E:1018:LEU:HD21	2:E:1083:ILE:HG12	1.74	0.68
2:B:154:HIS:HE1	2:B:201:GLU:OE2	1.76	0.68
2:B:226:VAL:HB	2:B:279:ALA:HB3	1.76	0.68
2:E:473:HIS:ND1	2:E:477:GLY:O	2.26	0.68
2:E:1284:GLN:HE21	2:E:1286:ASP:HB2	1.58	0.68
3:F:98:TYR:HE1	3:F:149:ILE:HD13	1.57	0.68
2:B:834:VAL:HB	2:B:873:GLU:HG2	1.74	0.68
2:B:883:THR:HG21	2:B:931:ARG:HB3	1.75	0.68
2:E:154:HIS:HE1	2:E:201:GLU:OE2	1.76	0.68
2:E:226:VAL:HB	2:E:279:ALA:HB3	1.75	0.68
2:B:1241:ILE:HA	2:B:1244:LEU:HD12	1.75	0.68
2:E:7:THR:HG22	2:E:9:ARG:H	1.59	0.68
2:B:469:THR:O	2:B:530:THR:OG1	2.12	0.68
2:B:1018:LEU:HD21	2:B:1083:ILE:HG12	1.74	0.68
2:B:1276:LYS:NZ	2:B:1277:PRO:O	2.26	0.68
2:B:70:THR:HG23	2:B:72:GLU:H	1.58	0.68
2:E:1552:SER:HB3	3:F:39:ASN:HD22	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1615:LEU:O	2:E:1619:HIS:N	2.24	0.68
2:E:7:THR:O	2:E:10:GLN:NE2	2.20	0.67
2:E:38:LEU:H	2:E:47:GLY:HA3	1.58	0.67
2:E:70:THR:HG23	2:E:72:GLU:H	1.58	0.67
2:B:7:THR:HG22	2:B:9:ARG:H	1.59	0.67
2:B:562:LEU:O	2:B:633:GLN:NE2	2.27	0.67
2:B:1120:LEU:O	2:B:1124:THR:OG1	2.06	0.67
2:E:445:ASP:HB2	2:E:627:CYS:HB2	1.76	0.67
2:B:1335:TYR:HA	2:B:1338:LEU:HD23	1.75	0.67
1:A:551:GLN:HA	1:A:554:ASN:HD22	1.58	0.67
2:E:1078:ASP:OD1	2:E:1081:LYS:N	2.25	0.67
2:E:1241:ILE:HA	2:E:1244:LEU:HD12	1.75	0.67
1:D:596:GLN:NE2	1:D:597:GLY:O	2.28	0.67
2:E:1032:PHE:HB3	2:E:1043:TRP:HH2	1.59	0.67
2:E:1120:LEU:O	2:E:1124:THR:OG1	2.06	0.67
2:B:38:LEU:H	2:B:47:GLY:HA3	1.58	0.67
2:E:1390:ARG:NH2	3:F:23:TYR:O	2.26	0.67
2:B:1630:LYS:O	2:B:1634:GLU:HG2	1.95	0.67
1:A:580:SER:HB2	1:A:585:VAL:HG22	1.76	0.67
2:B:283:ASP:HB2	2:B:430:LYS:HB3	1.77	0.67
2:B:1043:TRP:H	2:B:1043:TRP:HE3	1.42	0.67
2:E:283:ASP:HB2	2:E:430:LYS:HB3	1.77	0.67
2:E:834:VAL:HB	2:E:873:GLU:HG2	1.74	0.67
2:B:445:ASP:HB2	2:B:627:CYS:HB2	1.76	0.66
3:C:45:MET:HA	3:C:50:PRO:HA	1.77	0.66
2:E:1043:TRP:H	2:E:1043:TRP:HE3	1.42	0.66
2:E:1149:ASN:HA	2:E:1236:ARG:HH12	1.58	0.66
2:E:1630:LYS:O	2:E:1634:GLU:HG2	1.95	0.66
1:A:550:GLN:O	1:A:554:ASN:ND2	2.28	0.66
1:A:596:GLN:NE2	1:A:597:GLY:O	2.28	0.66
2:B:939:THR:O	2:B:943:MET:N	2.17	0.66
2:E:449:THR:HB	2:E:623:ALA:HB3	1.78	0.66
2:B:1516:GLU:HA	2:B:1519:ILE:HD12	1.77	0.66
3:C:170:ASP:HB3	3:C:174:ARG:HH21	1.61	0.66
2:E:562:LEU:O	2:E:633:GLN:NE2	2.27	0.66
2:E:1628:GLU:O	2:E:1632:LYS:HG2	1.95	0.66
3:F:170:ASP:HB3	3:F:174:ARG:HH21	1.61	0.66
1:A:535:GLU:O	1:A:539:LYS:HB3	1.96	0.66
2:E:1516:GLU:HA	2:E:1519:ILE:HD12	1.77	0.66
2:B:87:LEU:HD23	2:B:91:LEU:HD23	1.78	0.66
2:B:1111:GLU:OE1	2:B:1111:GLU:N	2.27	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1218:GLU:OE1	2:B:1218:GLU:N	2.26	0.66
2:B:1536:HIS:HA	2:B:1542:LEU:HD13	1.78	0.66
2:B:1615:LEU:O	2:B:1619:HIS:N	2.24	0.66
2:B:1628:GLU:O	2:B:1632:LYS:HG2	1.95	0.66
3:C:120:ARG:HH12	3:C:139:TYR:HB2	1.61	0.66
1:D:535:GLU:O	1:D:539:LYS:HB3	1.96	0.66
1:A:573:LYS:N	1:A:593:GLU:OE2	2.29	0.66
1:D:607:LYS:NZ	1:D:608:LEU:O	2.26	0.66
2:B:1539:ASP:HB3	2:B:1542:LEU:HD12	1.78	0.66
3:F:45:MET:HA	3:F:50:PRO:HA	1.77	0.66
3:F:120:ARG:HH12	3:F:139:TYR:HB2	1.61	0.66
2:B:842:LYS:O	2:B:845:GLN:NE2	2.30	0.66
2:B:1032:PHE:HB3	2:B:1043:TRP:HH2	1.59	0.66
2:E:1259:GLU:OE1	2:E:1259:GLU:N	2.23	0.66
2:B:163:LEU:HD23	2:B:1005:ASP:HB3	1.78	0.65
2:B:973:ILE:HA	2:B:976:PHE:CE1	2.31	0.65
2:E:469:THR:O	2:E:530:THR:OG1	2.12	0.65
2:E:883:THR:OG1	2:E:931:ARG:NH1	2.29	0.65
2:E:842:LYS:O	2:E:845:GLN:NE2	2.29	0.65
2:E:1216:SER:OG	2:E:1219:ASN:OD1	2.15	0.65
2:E:1536:HIS:HA	2:E:1542:LEU:HD13	1.78	0.65
1:D:550:GLN:O	1:D:554:ASN:ND2	2.28	0.65
2:E:166:ARG:O	2:E:171:ASN:HA	1.97	0.65
2:E:228:PHE:HB3	2:E:277:LEU:HB3	1.79	0.65
1:A:551:GLN:OE1	1:A:552:ARG:NH2	2.26	0.65
2:E:966:ASP:HA	2:E:969:TYR:HD2	1.62	0.65
2:E:1539:ASP:HB3	2:E:1542:LEU:HD12	1.78	0.65
2:B:228:PHE:HB3	2:B:277:LEU:HB3	1.79	0.65
1:D:573:LYS:N	1:D:593:GLU:OE2	2.29	0.65
2:E:246:TYR:HA	2:E:253:PHE:HA	1.79	0.65
2:B:819:TYR:O	2:B:822:SER:OG	2.10	0.65
2:B:883:THR:OG1	2:B:931:ARG:NH1	2.29	0.65
2:B:1219:ASN:OD1	2:B:1401:GLN:NE2	2.30	0.65
1:D:707:PRO:HD2	2:E:16:ILE:HG21	1.79	0.65
2:E:973:ILE:HA	2:E:976:PHE:CE1	2.31	0.65
1:A:575:TRP:HZ3	1:A:588:TYR:HB2	1.61	0.65
2:E:678:ASN:HA	2:E:681:MET:HE3	1.79	0.65
3:F:100:GLU:O	3:F:104:HIS:ND1	2.25	0.65
2:B:129:SER:HA	2:B:132:LEU:HD12	1.79	0.65
2:B:1328:TYR:HB3	2:B:1338:LEU:HD22	1.79	0.65
1:D:551:GLN:OE1	1:D:552:ARG:NH2	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1107:GLY:HA2	2:E:1110:LEU:HD13	1.79	0.65
2:E:1399:LEU:HD22	2:E:1405:ALA:HB1	1.79	0.65
2:B:166:ARG:O	2:B:171:ASN:HA	1.97	0.65
2:B:678:ASN:HA	2:B:681:MET:HE3	1.79	0.65
2:E:204:ILE:HG13	2:E:211:ARG:HB3	1.79	0.65
2:E:1633:VAL:HA	2:E:1637:TYR:HB2	1.79	0.65
3:F:129:LEU:HA	3:F:132:LYS:HG2	1.79	0.65
2:B:204:ILE:HG13	2:B:211:ARG:HB3	1.79	0.64
2:B:966:ASP:HA	2:B:969:TYR:HD2	1.62	0.64
2:E:1328:TYR:HB3	2:E:1338:LEU:HD22	1.79	0.64
2:B:18:ASN:HB3	2:B:28:SER:HB2	1.79	0.64
2:B:569:LEU:N	2:B:620:PHE:O	2.30	0.64
2:E:87:LEU:HD23	2:E:91:LEU:HD23	1.78	0.64
2:E:910:LEU:HA	2:E:913:LEU:HD12	1.79	0.64
2:E:1368:TYR:O	2:E:1425:TYR:N	2.22	0.64
2:B:1107:GLY:HA2	2:B:1110:LEU:HD13	1.79	0.64
3:C:100:GLU:O	3:C:104:HIS:ND1	2.25	0.64
2:E:876:GLU:OE1	2:E:876:GLU:N	2.31	0.64
2:E:1067:ALA:O	2:E:1071:LYS:N	2.18	0.64
2:B:1434:VAL:HB	2:B:1461:GLN:HB2	1.78	0.64
3:C:129:LEU:HA	3:C:132:LYS:HG2	1.79	0.64
2:E:1219:ASN:OD1	2:E:1401:GLN:NE2	2.30	0.64
3:F:8:VAL:O	3:F:58:THR:OG1	2.15	0.64
2:B:555:MET:HA	2:B:561:THR:HA	1.79	0.64
2:B:569:LEU:O	2:B:592:LYS:NZ	2.30	0.64
2:B:1216:SER:OG	2:B:1219:ASN:OD1	2.15	0.64
1:D:575:TRP:HZ3	1:D:588:TYR:HB2	1.61	0.64
2:E:1434:VAL:HB	2:E:1461:GLN:HB2	1.78	0.64
2:B:843:PHE:O	2:B:846:SER:OG	2.16	0.64
2:E:1618:LEU:O	2:E:1622:LEU:HG	1.98	0.64
2:B:1368:TYR:O	2:B:1425:TYR:N	2.22	0.64
2:B:1399:LEU:HD22	2:B:1405:ALA:HB1	1.79	0.64
1:D:578:ARG:HH22	1:D:601:HIS:H	1.46	0.64
2:E:163:LEU:HD23	2:E:1005:ASP:HB3	1.78	0.64
2:E:634:ASN:OD1	2:E:637:LEU:N	2.26	0.64
2:E:819:TYR:O	2:E:822:SER:OG	2.10	0.64
3:F:77:VAL:HG12	3:F:109:PRO:HG2	1.78	0.64
2:B:449:THR:HB	2:B:623:ALA:HB3	1.78	0.64
2:B:554:LEU:O	2:B:562:LEU:N	2.28	0.64
2:B:1059:LEU:O	2:B:1063:THR:OG1	2.12	0.64
2:B:1284:GLN:HG2	2:B:1286:ASP:H	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1506:GLN:NE2	2:E:1507:ILE:O	2.31	0.64
1:A:532:PRO:HG3	1:A:708:ASP:HA	1.80	0.64
2:B:1506:GLN:NE2	2:B:1507:ILE:O	2.31	0.64
3:C:77:VAL:HG12	3:C:109:PRO:HG2	1.78	0.64
2:E:1115:THR:O	2:E:1121:ARG:NH2	2.31	0.64
1:A:670:ASN:HA	1:A:673:LEU:HB2	1.79	0.64
2:B:30:GLN:N	2:B:33:ASP:OD2	2.31	0.64
2:B:1618:LEU:O	2:B:1622:LEU:HG	1.98	0.64
1:D:532:PRO:HG3	1:D:708:ASP:HA	1.80	0.64
1:D:670:ASN:HA	1:D:673:LEU:HB2	1.80	0.64
2:E:485:HIS:HB2	2:E:514:LYS:HB3	1.79	0.64
2:E:569:LEU:O	2:E:592:LYS:NZ	2.30	0.64
2:E:1059:LEU:O	2:E:1063:THR:OG1	2.12	0.64
2:B:239:ALA:HB3	2:B:262:TRP:HB3	1.80	0.63
2:B:246:TYR:HA	2:B:253:PHE:HA	1.79	0.63
1:D:697:ARG:NH2	2:E:30:GLN:HB2	2.10	0.63
2:E:18:ASN:HB3	2:E:28:SER:HB2	1.79	0.63
2:E:129:SER:HA	2:E:132:LEU:HD12	1.79	0.63
2:E:555:MET:HA	2:E:561:THR:HA	1.79	0.63
2:E:1111:GLU:OE1	2:E:1111:GLU:N	2.27	0.63
2:B:910:LEU:HA	2:B:913:LEU:HD12	1.79	0.63
2:B:1115:THR:O	2:B:1121:ARG:NH2	2.31	0.63
1:D:536:LEU:HD11	2:E:17:TYR:HD2	1.63	0.63
2:E:1159:VAL:O	2:E:1208:ARG:NH1	2.32	0.63
2:E:1307:TYR:O	2:E:1311:GLY:N	2.31	0.63
2:B:1633:VAL:HA	2:B:1637:TYR:HB2	1.79	0.63
3:C:8:VAL:O	3:C:58:THR:OG1	2.15	0.63
2:E:843:PHE:O	2:E:846:SER:OG	2.16	0.63
2:E:1602:GLU:HA	2:E:1605:ARG:HG2	1.81	0.63
2:B:932:LEU:HA	2:B:935:ARG:HE	1.64	0.63
2:B:1307:TYR:O	2:B:1311:GLY:N	2.31	0.63
2:B:373:ILE:HG23	2:B:376:ASN:HD22	1.64	0.63
2:B:1280:PRO:HA	2:B:1283:LEU:HD23	1.80	0.63
2:B:1440:SER:H	2:B:1442:LYS:NZ	1.97	0.63
2:B:1460:GLN:NE2	2:B:1491:THR:O	2.28	0.63
2:B:1388:TYR:OH	2:B:1390:ARG:NH1	2.29	0.63
3:C:9:VAL:HG22	3:C:78:PHE:HZ	1.64	0.63
2:E:239:ALA:HB3	2:E:262:TRP:HB3	1.80	0.63
2:E:569:LEU:N	2:E:620:PHE:O	2.30	0.63
2:E:1284:GLN:HG2	2:E:1286:ASP:H	1.63	0.63
2:B:485:HIS:HB2	2:B:514:LYS:HB3	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1388:TYR:OH	3:C:44:VAL:HG22	1.99	0.62
2:E:741:VAL:HG21	2:E:798:PHE:HD1	1.64	0.62
3:F:9:VAL:HG22	3:F:78:PHE:HZ	1.65	0.62
2:B:165:VAL:HG23	2:B:175:PRO:HD3	1.81	0.62
2:B:193:ARG:NH1	2:B:196:GLU:OE2	2.31	0.62
2:B:1159:VAL:O	2:B:1208:ARG:NH1	2.32	0.62
2:E:932:LEU:N	2:E:935:ARG:HH21	1.97	0.62
2:E:1623:SER:HB3	2:E:1627:ARG:HH12	1.64	0.62
2:B:556:ASN:ND2	2:B:561:THR:O	2.33	0.62
2:B:1623:SER:HB3	2:B:1627:ARG:HH12	1.64	0.62
2:E:1388:TYR:OH	2:E:1390:ARG:NH1	2.29	0.62
1:A:578:ARG:HH22	1:A:601:HIS:H	1.46	0.62
1:D:561:CYS:HA	1:D:576:TYR:HA	1.82	0.62
2:E:154:HIS:HA	2:E:157:ARG:HG2	1.82	0.62
2:E:373:ILE:HG23	2:E:376:ASN:HD22	1.64	0.62
2:E:554:LEU:O	2:E:562:LEU:N	2.28	0.62
2:E:1440:SER:H	2:E:1442:LYS:NZ	1.97	0.62
2:B:3:ARG:HH22	2:B:42:GLU:H	1.46	0.62
2:B:1117:GLU:OE2	2:B:1121:ARG:N	2.26	0.62
2:E:1280:PRO:HA	2:E:1283:LEU:HD23	1.80	0.62
3:F:98:TYR:CE1	3:F:149:ILE:HD13	2.35	0.62
2:B:523:THR:OG1	2:B:524:ARG:NH1	2.33	0.62
2:B:932:LEU:N	2:B:935:ARG:HH21	1.97	0.62
3:C:98:TYR:CE1	3:C:149:ILE:HD13	2.35	0.62
2:E:30:GLN:N	2:E:33:ASP:OD2	2.31	0.62
2:E:193:ARG:NH1	2:E:196:GLU:OE2	2.31	0.62
2:E:556:ASN:ND2	2:E:561:THR:O	2.33	0.62
2:E:1117:GLU:OE2	2:E:1121:ARG:N	2.26	0.62
2:E:1460:GLN:NE2	2:E:1491:THR:O	2.28	0.62
2:B:154:HIS:HA	2:B:157:ARG:HG2	1.82	0.62
2:B:1404:ASN:OD1	2:B:1424:GLN:HB2	2.00	0.62
2:E:879:LEU:HG	2:E:931:ARG:HH12	1.65	0.62
2:B:85:LEU:O	2:B:88:VAL:HG22	1.99	0.62
2:B:879:LEU:HG	2:B:931:ARG:HH12	1.65	0.62
2:E:431:MET:HE3	2:E:625:LEU:HD23	1.80	0.62
2:E:1391:ARG:HH22	3:F:29:PRO:HD3	1.65	0.62
2:E:932:LEU:HA	2:E:935:ARG:HE	1.64	0.61
2:E:1404:ASN:OD1	2:E:1424:GLN:HB2	2.00	0.61
2:B:1231:TYR:O	2:B:1235:LYS:N	2.33	0.61
2:E:1479:PHE:HE2	2:E:1560:MET:HE1	1.65	0.61
2:E:1548:SER:HB2	3:F:56:TRP:HH2	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:536:LEU:HD21	2:B:17:TYR:HB2	1.80	0.61
2:B:1602:GLU:HA	2:B:1605:ARG:HG2	1.81	0.61
2:E:569:LEU:HB2	2:E:620:PHE:HB3	1.82	0.61
2:E:1218:GLU:OE1	2:E:1218:GLU:N	2.26	0.61
2:E:1231:TYR:O	2:E:1235:LYS:N	2.33	0.61
2:E:3:ARG:HH22	2:E:42:GLU:H	1.46	0.61
2:E:85:LEU:O	2:E:88:VAL:HG22	1.99	0.61
2:E:523:THR:OG1	2:E:524:ARG:NH1	2.33	0.61
1:A:561:CYS:HA	1:A:576:TYR:HA	1.82	0.61
2:B:80:VAL:HG22	2:B:85:LEU:HD11	1.83	0.61
2:B:443:ARG:NH2	2:B:445:ASP:OD2	2.34	0.61
2:B:853:VAL:O	2:B:857:LEU:HG	2.01	0.61
2:E:876:GLU:HG2	2:E:877:VAL:HG13	1.83	0.61
2:E:1545:HIS:O	2:E:1548:SER:OG	2.14	0.61
1:D:701:LEU:HD11	2:E:16:ILE:HA	1.83	0.61
2:E:165:VAL:HG23	2:E:175:PRO:HD3	1.81	0.61
2:B:254:ILE:HD12	2:B:294:VAL:HG13	1.83	0.61
2:B:741:VAL:HG21	2:B:798:PHE:HD1	1.64	0.61
2:B:771:ARG:NH2	2:B:781:SER:OG	2.34	0.61
2:B:1488:THR:N	2:B:1508:SER:O	2.33	0.61
1:D:724:TYR:HB3	2:E:4:TRP:HB2	1.82	0.61
2:E:37:ILE:HG21	2:E:45:TYR:HB3	1.83	0.61
2:E:925:ILE:HA	2:E:928:ILE:HD12	1.82	0.61
2:E:892:ASP:OD1	2:E:895:ASN:ND2	2.34	0.61
2:E:1315:GLU:OE1	2:E:1315:GLU:N	2.28	0.61
2:B:1294:GLN:O	2:B:1298:GLU:HG3	2.01	0.60
2:E:197:LYS:HA	2:E:200:GLU:HG2	1.83	0.60
2:E:771:ARG:NH2	2:E:781:SER:OG	2.34	0.60
2:E:772:VAL:HA	2:E:775:LEU:HD12	1.83	0.60
3:F:141:GLN:OE1	3:F:141:GLN:N	2.27	0.60
1:A:599:VAL:HG23	1:A:601:HIS:CD2	2.37	0.60
2:B:1135:GLU:O	2:B:1139:SER:N	2.34	0.60
2:B:1448:GLU:OE1	2:B:1452:ASN:ND2	2.33	0.60
2:E:1589:LEU:HA	2:E:1592:LEU:HD12	1.83	0.60
2:B:166:ARG:HH22	2:B:168:ASP:HB2	1.65	0.60
2:B:569:LEU:HB2	2:B:620:PHE:HB3	1.82	0.60
2:B:892:ASP:OD1	2:B:895:ASN:ND2	2.34	0.60
2:B:1479:PHE:CZ	3:C:36:VAL:HG12	2.35	0.60
2:E:1283:LEU:HD11	2:E:1291:TYR:HB2	1.83	0.60
2:B:534:ARG:NE	2:B:541:ASP:OD1	2.27	0.60
2:E:166:ARG:HH22	2:E:168:ASP:HB2	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:853:VAL:O	2:E:857:LEU:HG	2.01	0.60
2:E:1135:GLU:O	2:E:1139:SER:N	2.34	0.60
2:E:1448:GLU:OE1	2:E:1452:ASN:ND2	2.33	0.60
2:B:1315:GLU:OE1	2:B:1315:GLU:N	2.28	0.60
2:E:1066:GLN:HA	2:E:1069:ARG:NH1	2.17	0.60
1:A:562:PHE:N	1:A:575:TRP:O	2.34	0.60
2:B:37:ILE:HG21	2:B:45:TYR:HB3	1.83	0.60
2:E:254:ILE:HD12	2:E:294:VAL:HG13	1.83	0.60
3:F:39:ASN:H	3:F:57:ASP:HB3	1.66	0.60
2:B:7:THR:O	2:B:10:GLN:NE2	2.20	0.60
2:B:772:VAL:HA	2:B:775:LEU:HD12	1.83	0.60
3:C:126:ILE:HG23	3:C:136:PRO:HG2	1.84	0.60
1:D:599:VAL:HG23	1:D:601:HIS:CD2	2.37	0.60
2:E:1099:ILE:HD13	2:E:1138:PHE:HB2	1.83	0.60
2:E:1063:THR:HA	2:E:1069:ARG:HH11	1.67	0.60
2:E:1294:GLN:O	2:E:1298:GLU:HG3	2.01	0.60
1:A:576:TYR:CD1	1:A:591:LEU:HG	2.36	0.60
2:B:730:TYR:OH	2:B:771:ARG:NH1	2.35	0.60
1:D:576:TYR:CD1	1:D:591:LEU:HG	2.36	0.60
2:B:1283:LEU:HD11	2:B:1291:TYR:HB2	1.83	0.59
2:E:809:ALA:HB1	2:E:812:ILE:HB	1.84	0.59
1:A:695:LYS:HD2	2:B:125:ILE:HD12	1.83	0.59
2:E:649:ASN:O	2:E:653:ASN:N	2.24	0.59
2:B:232:VAL:O	2:B:398:GLY:N	2.35	0.59
2:B:925:ILE:HA	2:B:928:ILE:HD12	1.82	0.59
2:B:1563:PHE:HA	2:B:1566:TYR:CD2	2.37	0.59
2:E:14:VAL:HB	2:E:65:HIS:HB3	1.84	0.59
2:E:1549:MET:HA	3:F:39:ASN:ND2	2.16	0.59
2:B:197:LYS:HA	2:B:200:GLU:HG2	1.83	0.59
2:B:1063:THR:HA	2:B:1069:ARG:HH11	1.67	0.59
2:B:1589:LEU:HA	2:B:1592:LEU:HD12	1.83	0.59
3:C:39:ASN:H	3:C:57:ASP:HB3	1.66	0.59
2:E:80:VAL:HG22	2:E:85:LEU:HD11	1.83	0.59
2:E:443:ARG:NH2	2:E:445:ASP:OD2	2.34	0.59
3:F:126:ILE:HG23	3:F:136:PRO:HG2	1.84	0.59
2:B:1066:GLN:HA	2:B:1069:ARG:NH1	2.17	0.59
2:B:1099:ILE:HD13	2:B:1138:PHE:HB2	1.83	0.59
2:E:887:SER:O	2:E:890:LEU:HB3	2.02	0.59
2:E:1460:GLN:HB2	2:E:1494:THR:HG22	1.84	0.59
2:B:37:ILE:HD13	2:B:45:TYR:HB3	1.85	0.59
2:B:809:ALA:HB1	2:B:812:ILE:HB	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:876:GLU:HG2	2:B:877:VAL:HG13	1.83	0.59
2:E:147:LYS:O	2:E:151:LYS:HG2	2.03	0.59
2:E:465:ASN:OD1	2:E:503:GLN:N	2.27	0.59
1:A:608:LEU:HD23	1:A:609:PRO:HD2	1.85	0.59
2:B:1460:GLN:HB2	2:B:1494:THR:HG22	1.84	0.59
2:E:27:LEU:HD23	2:E:28:SER:H	1.68	0.59
1:A:588:TYR:HE1	1:A:608:LEU:HB2	1.68	0.59
2:B:1196:LEU:O	2:B:1199:SER:OG	2.19	0.59
2:B:1446:VAL:HG12	2:E:1333:PHE:CZ	2.37	0.59
2:B:1479:PHE:HE2	2:B:1560:MET:HE1	1.68	0.59
2:E:297:VAL:HG22	2:E:326:VAL:HG22	1.85	0.59
1:A:643:SER:OG	1:A:653:ASN:ND2	2.35	0.59
3:C:21:ILE:HD11	3:C:35:THR:HG23	1.85	0.59
2:E:156:ASN:HA	2:E:161:LEU:HD12	1.85	0.59
2:E:730:TYR:OH	2:E:771:ARG:NH1	2.35	0.59
2:E:1328:TYR:HB3	2:E:1338:LEU:CD2	2.33	0.59
2:E:1563:PHE:HA	2:E:1566:TYR:CD2	2.37	0.59
2:B:1328:TYR:HB3	2:B:1338:LEU:CD2	2.33	0.59
3:C:174:ARG:HA	3:C:177:LEU:HB2	1.85	0.59
1:D:673:LEU:HB3	1:D:675:LYS:NZ	2.18	0.59
2:E:641:LEU:O	2:E:644:ARG:NH1	2.36	0.59
2:E:1196:LEU:O	2:E:1199:SER:OG	2.19	0.59
2:E:1462:PHE:HB2	2:E:1489:TYR:HB2	1.85	0.59
2:B:757:LEU:HD11	2:B:812:ILE:HG23	1.85	0.58
2:B:1080:ARG:HA	2:B:1083:ILE:HD12	1.85	0.58
1:D:643:SER:OG	1:D:653:ASN:ND2	2.35	0.58
2:E:1002:TYR:HB2	2:E:1010:ASN:HD21	1.68	0.58
3:F:174:ARG:HA	3:F:177:LEU:HB2	1.85	0.58
2:B:1545:HIS:O	2:B:1548:SER:OG	2.14	0.58
3:C:5:LYS:N	3:C:76:ASP:OD2	2.29	0.58
1:D:562:PHE:N	1:D:575:TRP:O	2.34	0.58
2:B:887:SER:O	2:B:890:LEU:HB3	2.02	0.58
2:E:19:TYR:O	2:E:28:SER:HA	2.03	0.58
3:C:138:THR:H	3:C:141:GLN:NE2	2.01	0.58
2:B:641:LEU:O	2:B:644:ARG:NH1	2.36	0.58
2:B:876:GLU:N	2:B:876:GLU:OE1	2.31	0.58
2:E:1080:ARG:HA	2:E:1083:ILE:HD12	1.85	0.58
1:A:723:VAL:HB	2:B:3:ARG:H	1.68	0.58
2:B:19:TYR:O	2:B:28:SER:HA	2.03	0.58
2:B:156:ASN:HA	2:B:161:LEU:HD12	1.85	0.58
3:F:21:ILE:HD11	3:F:35:THR:HG23	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:14:VAL:HB	2:B:65:HIS:HB3	1.84	0.58
2:B:569:LEU:HD12	2:B:620:PHE:HD2	1.67	0.58
2:B:637:LEU:HD12	2:B:665:ILE:HD13	1.86	0.58
2:B:719:TYR:HA	2:B:723:HIS:ND1	2.19	0.58
2:B:814:GLY:HA2	2:B:855:GLN:HG2	1.86	0.58
2:B:860:MET:SD	2:B:885:GLN:NE2	2.77	0.58
1:D:588:TYR:HE1	1:D:608:LEU:HB2	1.67	0.58
1:D:608:LEU:HD23	1:D:609:PRO:HD2	1.85	0.58
2:E:569:LEU:HD12	2:E:620:PHE:HD2	1.67	0.58
2:E:1607:HIS:O	2:E:1611:LEU:N	2.36	0.58
2:B:166:ARG:NH2	2:B:168:ASP:HB2	2.19	0.58
2:B:730:TYR:HB2	2:B:767:ILE:HG23	1.85	0.58
2:B:934:ARG:NH2	2:B:988:GLU:OE1	2.37	0.58
2:B:1106:VAL:O	2:B:1109:ILE:HG22	2.04	0.58
2:B:1417:ASP:O	2:B:1421:SER:N	2.37	0.58
2:B:1607:HIS:O	2:B:1611:LEU:N	2.36	0.58
1:D:544:ILE:HG23	1:D:545:LEU:HD22	1.86	0.58
1:D:548:ILE:O	1:D:552:ARG:HG2	2.04	0.58
2:E:59:PHE:HD2	2:E:64:ILE:HG12	1.67	0.58
2:E:730:TYR:HB2	2:E:767:ILE:HG23	1.84	0.58
1:A:548:ILE:O	1:A:552:ARG:HG2	2.04	0.58
2:B:27:LEU:HD23	2:B:28:SER:H	1.68	0.58
2:B:297:VAL:HG22	2:B:326:VAL:HG22	1.85	0.58
2:B:730:TYR:CE1	2:B:771:ARG:HD3	2.39	0.58
2:E:232:VAL:O	2:E:398:GLY:N	2.35	0.58
2:E:262:TRP:HA	2:E:268:PRO:HA	1.86	0.58
2:E:860:MET:SD	2:E:885:GLN:NE2	2.77	0.58
2:E:1106:VAL:O	2:E:1109:ILE:HG22	2.04	0.58
2:E:1121:ARG:O	2:E:1125:ILE:HD12	2.04	0.58
2:B:27:LEU:HD23	2:B:28:SER:N	2.18	0.58
2:B:992:MET:O	2:B:996:LEU:HD23	2.04	0.58
2:E:27:LEU:HD23	2:E:28:SER:N	2.18	0.58
2:E:1231:TYR:HE2	2:E:1243:TYR:CE1	2.22	0.58
2:B:59:PHE:HD2	2:B:64:ILE:HG12	1.67	0.57
2:B:288:ASP:HA	2:B:291:ARG:HE	1.69	0.57
2:B:721:TYR:OH	2:B:765:ARG:NH1	2.37	0.57
2:B:994:LYS:NZ	2:B:1048:HIS:HB3	2.19	0.57
2:E:37:ILE:HD13	2:E:45:TYR:HB3	1.85	0.57
2:E:246:TYR:N	2:E:295:SER:O	2.37	0.57
2:E:787:PHE:O	2:E:791:ILE:HG12	2.04	0.57
2:E:994:LYS:NZ	2:E:1048:HIS:HB3	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:697:ARG:NH2	2:B:30:GLN:HB2	2.14	0.57
2:B:147:LYS:O	2:B:151:LYS:HG2	2.03	0.57
2:B:787:PHE:O	2:B:791:ILE:HG12	2.04	0.57
2:E:721:TYR:OH	2:E:765:ARG:NH1	2.37	0.57
3:F:138:THR:H	3:F:141:GLN:NE2	2.01	0.57
1:A:544:ILE:HG23	1:A:545:LEU:HD22	1.86	0.57
2:B:1002:TYR:HB2	2:B:1010:ASN:HD21	1.68	0.57
2:B:1514:PRO:HA	2:B:1517:ASN:HD22	1.70	0.57
2:E:934:ARG:NH2	2:E:988:GLU:OE1	2.37	0.57
2:B:1121:ARG:O	2:B:1125:ILE:HD12	2.04	0.57
2:B:1231:TYR:HE2	2:B:1243:TYR:CE1	2.22	0.57
2:E:1177:LEU:O	2:E:1181:ARG:HG2	2.05	0.57
1:A:673:LEU:HB3	1:A:675:LYS:NZ	2.18	0.57
2:B:226:VAL:O	2:B:279:ALA:N	2.30	0.57
2:B:465:ASN:OD1	2:B:503:GLN:N	2.27	0.57
2:B:550:ALA:HB1	2:B:569:LEU:HB3	1.86	0.57
2:B:1332:VAL:HG13	2:B:1334:ASP:H	1.69	0.57
2:E:166:ARG:NH2	2:E:168:ASP:HB2	2.19	0.57
2:B:630:LYS:HG2	2:B:668:PHE:HZ	1.70	0.57
2:E:94:THR:HG22	2:E:98:TRP:NE1	2.20	0.57
2:E:550:ALA:HB1	2:E:569:LEU:HB3	1.86	0.57
2:E:630:LYS:HG2	2:E:668:PHE:HZ	1.70	0.57
2:E:1545:HIS:CD2	3:F:5:LYS:HE3	2.40	0.57
2:B:1462:PHE:HB2	2:B:1489:TYR:HB2	1.85	0.57
2:E:792:ARG:NE	2:E:835:GLU:OE1	2.31	0.57
2:E:992:MET:O	2:E:996:LEU:HD23	2.04	0.57
2:B:965:ASP:HB3	2:B:968:HIS:CG	2.40	0.57
2:E:637:LEU:HD12	2:E:665:ILE:HD13	1.86	0.57
2:E:814:GLY:HA2	2:E:855:GLN:HG2	1.86	0.57
1:A:670:ASN:HB3	1:A:677:MET:HE2	1.87	0.57
2:B:1607:HIS:NE2	2:B:1619:HIS:HB2	2.20	0.57
3:C:91:GLU:O	3:C:95:ALA:HB3	2.05	0.57
1:D:643:SER:HA	1:D:652:LEU:O	2.05	0.57
1:A:551:GLN:HG2	2:B:107:VAL:HA	1.85	0.56
2:B:422:ASP:OD1	2:B:425:THR:OG1	2.23	0.56
2:B:1275:ASP:O	2:B:1292:THR:OG1	2.23	0.56
2:E:72:GLU:O	2:E:76:GLN:NE2	2.38	0.56
2:E:757:LEU:HD11	2:E:812:ILE:HG23	1.85	0.56
2:E:1607:HIS:NE2	2:E:1619:HIS:HB2	2.20	0.56
2:B:1135:GLU:OE1	2:B:1139:SER:OG	2.22	0.56
2:E:534:ARG:NE	2:E:541:ASP:OD1	2.27	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:730:TYR:CE1	2:E:771:ARG:HD3	2.39	0.56
2:B:246:TYR:N	2:B:295:SER:O	2.37	0.56
2:B:262:TRP:HA	2:B:268:PRO:HA	1.86	0.56
2:B:792:ARG:NE	2:B:835:GLU:OE1	2.31	0.56
2:E:526:HIS:CE1	2:E:586:LEU:HD21	2.41	0.56
2:E:719:TYR:HA	2:E:723:HIS:ND1	2.19	0.56
2:E:1135:GLU:OE1	2:E:1139:SER:OG	2.22	0.56
3:F:5:LYS:N	3:F:76:ASP:OD2	2.29	0.56
2:B:130:GLN:NE2	2:B:144:LEU:HD11	2.21	0.56
2:B:1177:LEU:O	2:B:1181:ARG:HG2	2.05	0.56
3:C:69:PRO:HB3	3:C:104:HIS:CD2	2.41	0.56
2:E:131:ILE:HD11	2:E:144:LEU:HG	1.88	0.56
2:E:1102:ILE:HD11	2:E:1134:CYS:HB2	1.88	0.56
2:E:1432:LYS:NZ	2:E:1465:SER:H	2.03	0.56
1:A:643:SER:HA	1:A:652:LEU:O	2.05	0.56
2:B:522:VAL:HG11	2:B:631:LEU:HD21	1.88	0.56
2:B:1432:LYS:NZ	2:B:1465:SER:H	2.03	0.56
2:B:1449:GLN:OE1	2:B:1449:GLN:N	2.25	0.56
2:E:35:VAL:HG23	2:E:37:ILE:HG13	1.88	0.56
2:E:1117:GLU:OE2	2:E:1120:LEU:HG	2.06	0.56
2:E:1332:VAL:HG13	2:E:1334:ASP:H	1.69	0.56
2:E:1613:GLU:OE2	2:E:1614:GLN:HG3	2.06	0.56
2:B:820:LEU:O	2:B:823:ILE:HG12	2.04	0.56
2:B:1416:GLU:HA	2:B:1419:LYS:HG2	1.88	0.56
2:B:94:THR:HG22	2:B:98:TRP:NE1	2.20	0.56
2:B:640:LEU:HB2	2:B:653:ASN:HB3	1.88	0.56
1:D:670:ASN:O	1:D:674:GLY:N	2.39	0.56
1:D:670:ASN:HB3	1:D:677:MET:HE2	1.88	0.56
2:E:130:GLN:NE2	2:E:144:LEU:HD11	2.21	0.56
2:E:288:ASP:HA	2:E:291:ARG:HE	1.69	0.56
3:F:69:PRO:HB3	3:F:104:HIS:CD2	2.41	0.56
2:B:35:VAL:HG23	2:B:37:ILE:HG13	1.88	0.56
2:B:754:PHE:HA	2:B:757:LEU:HD12	1.87	0.56
2:E:64:ILE:HG22	2:E:66:LEU:HD22	1.88	0.56
2:E:754:PHE:HA	2:E:757:LEU:HD12	1.87	0.56
2:E:1056:HIS:ND1	2:E:1057:GLU:OE2	2.39	0.56
3:F:41:SER:HA	3:F:54:GLY:HA2	1.88	0.56
2:B:131:ILE:HD11	2:B:144:LEU:HG	1.88	0.56
2:B:1613:GLU:OE2	2:B:1614:GLN:HG3	2.06	0.56
1:D:599:VAL:HG23	1:D:601:HIS:HD2	1.71	0.56
2:E:248:PRO:HD2	2:E:293:ARG:HG3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:820:LEU:O	2:E:823:ILE:HG12	2.04	0.56
1:A:670:ASN:O	1:A:674:GLY:N	2.39	0.56
2:B:235:ILE:HB	2:B:262:TRP:HZ3	1.71	0.56
2:B:526:HIS:CE1	2:B:586:LEU:HD21	2.41	0.56
2:B:1102:ILE:HD11	2:B:1134:CYS:HB2	1.88	0.56
2:B:1557:PRO:HB2	2:B:1561:GLY:HA2	1.87	0.56
2:E:793:GLN:HA	2:E:796:LEU:HG	1.87	0.56
2:E:965:ASP:HB3	2:E:968:HIS:CG	2.40	0.56
2:E:1038:PHE:O	2:E:1039:GLU:HG2	2.06	0.56
2:E:1514:PRO:HA	2:E:1517:ASN:HD22	1.70	0.56
2:E:1623:SER:HB3	2:E:1627:ARG:HH22	1.71	0.56
2:B:248:PRO:HD2	2:B:293:ARG:HG3	1.87	0.55
2:B:1167:GLN:CD	2:B:1167:GLN:H	2.09	0.55
3:C:49:LYS:NZ	3:C:50:PRO:O	2.30	0.55
2:E:347:PRO:HB2	2:E:392:VAL:HB	1.88	0.55
2:B:72:GLU:O	2:B:76:GLN:NE2	2.38	0.55
2:B:634:ASN:OD1	2:B:637:LEU:N	2.26	0.55
2:E:422:ASP:OD1	2:E:425:THR:OG1	2.23	0.55
3:F:119:LEU:HA	3:F:122:ASP:HB2	1.88	0.55
2:B:1451:LEU:O	2:B:1455:ARG:N	2.39	0.55
2:B:1623:SER:HB3	2:B:1627:ARG:NH1	2.22	0.55
2:E:790:SER:O	2:E:793:GLN:HG2	2.06	0.55
2:E:1416:GLU:HA	2:E:1419:LYS:HG2	1.88	0.55
2:E:1451:LEU:O	2:E:1455:ARG:N	2.39	0.55
2:E:1488:THR:N	2:E:1508:SER:O	2.33	0.55
2:B:64:ILE:HG22	2:B:66:LEU:HD22	1.88	0.55
2:B:225:TYR:HE1	2:B:278:GLN:HB3	1.71	0.55
2:B:556:ASN:HD22	2:B:560:THR:HG1	1.54	0.55
2:B:1056:HIS:ND1	2:B:1057:GLU:OE2	2.39	0.55
2:B:1464:TYR:HB3	2:B:1487:THR:OG1	2.07	0.55
2:E:52:ASN:HD21	2:E:55:LYS:HD2	1.71	0.55
2:E:235:ILE:HB	2:E:262:TRP:HZ3	1.71	0.55
2:E:1417:ASP:O	2:E:1421:SER:N	2.37	0.55
3:F:91:GLU:O	3:F:95:ALA:HB3	2.05	0.55
2:B:95:LEU:HA	2:B:98:TRP:CD1	2.42	0.55
3:C:141:GLN:OE1	3:C:141:GLN:N	2.27	0.55
2:E:281:PHE:HD1	2:E:428:ALA:HB3	1.71	0.55
2:E:640:LEU:HB2	2:E:653:ASN:HB3	1.88	0.55
3:F:87:PRO:HA	3:F:90:PHE:HD2	1.72	0.55
1:A:727:ASN:N	2:B:46:ARG:HH22	2.04	0.55
2:B:52:ASN:HD21	2:B:55:LYS:HD2	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:281:PHE:HD1	2:B:428:ALA:HB3	1.71	0.55
2:B:793:GLN:HA	2:B:796:LEU:HG	1.87	0.55
2:E:25:VAL:HG23	2:E:57:GLY:HA2	1.89	0.55
1:A:599:VAL:HG23	1:A:601:HIS:HD2	1.70	0.55
3:C:119:LEU:HA	3:C:122:ASP:HB2	1.88	0.55
2:E:192:LYS:O	2:E:195:GLU:HG2	2.07	0.55
2:E:225:TYR:HE1	2:E:278:GLN:HB3	1.71	0.55
2:E:1557:PRO:HB2	2:E:1561:GLY:HA2	1.87	0.55
2:B:972:TYR:O	2:B:975:THR:N	2.39	0.55
2:B:1038:PHE:O	2:B:1039:GLU:HG2	2.06	0.55
2:E:962:GLN:O	2:E:1019:ARG:NH1	2.37	0.55
2:E:1117:GLU:OE1	2:E:1118:VAL:N	2.40	0.55
2:B:257:ASN:O	2:B:488:ALA:N	2.31	0.55
2:B:1117:GLU:OE2	2:B:1120:LEU:HG	2.06	0.55
2:E:1032:PHE:HB3	2:E:1043:TRP:CH2	2.42	0.55
2:E:1205:LEU:HA	2:E:1208:ARG:HD3	1.89	0.55
2:E:1275:ASP:O	2:E:1292:THR:OG1	2.23	0.55
2:E:1584:GLU:HG3	2:E:1585:LYS:HD3	1.88	0.55
2:E:522:VAL:HG11	2:E:631:LEU:HD21	1.88	0.55
2:B:854:ARG:NH2	2:B:858:ASN:OD1	2.39	0.54
2:B:945:ARG:HD3	2:B:947:SER:H	1.71	0.54
2:B:1082:GLU:OE2	2:B:1086:ARG:NE	2.24	0.54
2:B:1584:GLU:HG3	2:B:1585:LYS:HD3	1.88	0.54
3:C:87:PRO:HA	3:C:90:PHE:HD2	1.72	0.54
1:D:584:LYS:HZ2	2:E:1403:PRO:HA	1.72	0.54
2:E:879:LEU:HA	2:E:882:LEU:HD12	1.90	0.54
2:E:945:ARG:HD3	2:E:947:SER:H	1.72	0.54
2:B:572:TYR:OH	2:B:589:PRO:O	2.17	0.54
3:C:90:PHE:CE2	3:C:137:ILE:HB	2.42	0.54
2:E:95:LEU:HA	2:E:98:TRP:CD1	2.42	0.54
2:E:412:GLN:HA	2:E:415:LYS:HE2	1.90	0.54
2:E:869:PHE:O	2:E:918:VAL:HG13	2.08	0.54
1:A:567:ALA:HA	1:A:571:GLN:HB2	1.89	0.54
2:B:89:GLN:O	2:B:92:THR:OG1	2.23	0.54
2:B:591:THR:H	2:B:594:GLU:HB2	1.72	0.54
2:B:1585:LYS:HA	2:B:1588:LEU:HD12	1.90	0.54
2:E:1167:GLN:CD	2:E:1167:GLN:H	2.09	0.54
2:E:1516:GLU:O	2:E:1519:ILE:N	2.41	0.54
3:F:49:LYS:NZ	3:F:50:PRO:O	2.30	0.54
3:F:90:PHE:CE2	3:F:137:ILE:HB	2.42	0.54
1:A:548:ILE:HB	1:A:549:LYS:NZ	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:446:ILE:HB	2:B:515:VAL:HB	1.90	0.54
2:B:790:SER:O	2:B:793:GLN:HG2	2.06	0.54
3:C:41:SER:HA	3:C:54:GLY:HA2	1.88	0.54
2:E:81:ILE:HD13	2:E:141:LEU:HD21	1.90	0.54
2:E:226:VAL:O	2:E:279:ALA:N	2.30	0.54
2:E:287:MET:HA	2:E:290:ILE:HG12	1.89	0.54
2:B:945:ARG:HH11	2:B:946:GLN:H	1.56	0.54
2:B:962:GLN:O	2:B:1019:ARG:NH1	2.37	0.54
2:B:1095:GLY:H	2:B:1098:LYS:HE3	1.72	0.54
2:B:1626:PHE:HD2	2:B:1627:ARG:HD3	1.72	0.54
1:A:544:ILE:HD11	1:A:689:LEU:HB2	1.90	0.54
1:A:693:GLU:O	1:A:696:LEU:HG	2.08	0.54
2:B:854:ARG:HH11	2:B:854:ARG:HA	1.73	0.54
2:B:1205:LEU:HA	2:B:1208:ARG:HD3	1.89	0.54
2:B:1516:GLU:O	2:B:1519:ILE:N	2.40	0.54
2:B:1563:PHE:HA	2:B:1566:TYR:HD2	1.72	0.54
3:C:5:LYS:HB3	3:C:75:THR:HG23	1.89	0.54
3:C:7:VAL:HB	3:C:78:PHE:HD2	1.73	0.54
2:E:1435:MET:SD	2:E:1455:ARG:HA	2.48	0.54
2:B:646:ASN:ND2	2:B:653:ASN:HD21	2.06	0.54
2:B:1623:SER:HB3	2:B:1627:ARG:HH22	1.71	0.54
2:E:155:GLY:HA2	2:E:158:MET:SD	2.48	0.54
2:E:854:ARG:HH11	2:E:854:ARG:HA	1.73	0.54
2:E:917:ASP:N	2:E:917:ASP:OD1	2.41	0.54
2:B:155:GLY:HA2	2:B:158:MET:SD	2.48	0.54
2:B:192:LYS:O	2:B:195:GLU:HG2	2.07	0.54
3:C:1:MET:HE3	3:C:2:GLN:H	1.72	0.54
3:C:64:TYR:HD2	3:C:67:LEU:HD12	1.73	0.54
1:D:548:ILE:HB	1:D:549:LYS:NZ	2.23	0.54
2:E:771:ARG:HH21	2:E:784:GLY:HA2	1.72	0.54
2:E:854:ARG:NH2	2:E:858:ASN:OD1	2.39	0.54
2:E:1563:PHE:HA	2:E:1566:TYR:HD2	1.73	0.54
1:A:555:ARG:NH2	2:B:109:ASN:OD1	2.40	0.54
2:B:1387:GLU:HG2	2:B:1388:TYR:N	2.22	0.54
2:B:1435:MET:SD	2:B:1455:ARG:HA	2.48	0.54
1:D:544:ILE:HD11	1:D:689:LEU:HB2	1.90	0.54
1:D:567:ALA:HA	1:D:571:GLN:HB2	1.89	0.54
2:E:19:TYR:HB2	2:E:59:PHE:HE1	1.73	0.54
2:E:294:VAL:H	2:E:330:THR:HG1	1.54	0.54
2:E:561:THR:HG21	2:E:631:LEU:HB3	1.90	0.54
2:E:1464:TYR:HB3	2:E:1487:THR:OG1	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:603:SER:N	1:A:606:ASP:OD1	2.41	0.54
2:B:81:ILE:HD13	2:B:141:LEU:HD21	1.90	0.54
2:B:287:MET:HA	2:B:290:ILE:HG12	1.89	0.54
2:B:1202:GLU:OE2	2:B:1203:ASN:ND2	2.41	0.54
2:B:1440:SER:H	2:B:1442:LYS:HZ1	1.56	0.54
2:E:584:PHE:O	2:E:587:THR:OG1	2.22	0.54
3:F:5:LYS:HB3	3:F:75:THR:HG23	1.89	0.54
2:B:589:PRO:CB	2:B:594:GLU:HB3	2.36	0.53
2:E:1344:LYS:O	2:E:1347:SER:OG	2.21	0.53
2:E:1623:SER:HB3	2:E:1627:ARG:NH1	2.22	0.53
1:A:673:LEU:HB3	1:A:675:LYS:HZ1	1.73	0.53
2:B:172:ILE:HG13	2:B:173:LEU:HD12	1.90	0.53
2:B:353:MET:HG3	2:B:374:GLY:O	2.08	0.53
2:B:471:SER:N	2:B:528:ARG:O	2.36	0.53
1:D:552:ARG:NH1	1:D:664:ILE:HG12	2.23	0.53
2:E:172:ILE:HG13	2:E:173:LEU:HD12	1.90	0.53
2:E:302:ARG:HD3	2:E:322:PHE:HD1	1.72	0.53
2:E:1040:LEU:HD12	2:E:1097:HIS:CE1	2.44	0.53
2:E:1601:THR:HG1	2:E:1626:PHE:HZ	1.54	0.53
1:A:544:ILE:CD1	1:A:689:LEU:HB2	2.38	0.53
2:B:25:VAL:HG23	2:B:57:GLY:HA2	1.89	0.53
2:B:181:ILE:HG22	2:B:185:LYS:NZ	2.23	0.53
2:B:347:PRO:HB2	2:B:392:VAL:HB	1.88	0.53
2:B:412:GLN:HA	2:B:415:LYS:HE2	1.90	0.53
2:B:732:LYS:HA	2:B:735:LYS:HD3	1.91	0.53
2:B:1060:GLN:OE1	2:B:1060:GLN:N	2.32	0.53
1:D:603:SER:N	1:D:606:ASP:OD1	2.41	0.53
2:B:771:ARG:HH21	2:B:784:GLY:HA2	1.72	0.53
2:B:869:PHE:O	2:B:918:VAL:HG13	2.08	0.53
2:B:1117:GLU:OE1	2:B:1118:VAL:N	2.40	0.53
2:B:1168:TYR:O	2:B:1172:LEU:HD23	2.08	0.53
2:B:1470:LYS:HB3	2:B:1483:TRP:CD1	2.43	0.53
2:B:1536:HIS:CG	2:B:1542:LEU:HD22	2.44	0.53
2:E:446:ILE:HB	2:E:515:VAL:HB	1.90	0.53
2:E:945:ARG:HH11	2:E:946:GLN:H	1.55	0.53
2:E:1202:GLU:OE2	2:E:1203:ASN:ND2	2.41	0.53
2:E:1387:GLU:HG2	2:E:1388:TYR:N	2.23	0.53
2:E:1418:ILE:HA	2:E:1421:SER:HB3	1.91	0.53
1:A:557:VAL:HA	1:A:579:LEU:HB3	1.91	0.53
2:B:972:TYR:HA	2:B:975:THR:OG1	2.09	0.53
2:B:1418:ILE:HA	2:B:1421:SER:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1449:GLN:HA	2:B:1452:ASN:ND2	2.24	0.53
1:D:693:GLU:O	1:D:696:LEU:HG	2.08	0.53
2:E:130:GLN:HE21	2:E:144:LEU:HD11	1.73	0.53
2:E:471:SER:N	2:E:528:ARG:O	2.36	0.53
2:E:646:ASN:ND2	2:E:653:ASN:HD21	2.06	0.53
2:E:973:ILE:HA	2:E:976:PHE:CZ	2.43	0.53
2:E:1205:LEU:HD13	2:E:1208:ARG:HD3	1.91	0.53
2:E:1477:ASN:HB3	2:E:1568:LYS:NZ	2.23	0.53
2:B:302:ARG:HD3	2:B:322:PHE:HD1	1.72	0.53
2:B:1031:PHE:C	2:B:1035:GLN:HE22	2.11	0.53
2:B:1232:LYS:HB2	2:B:1240:TYR:CE2	2.44	0.53
2:B:1477:ASN:HB3	2:B:1568:LYS:NZ	2.24	0.53
2:E:591:THR:H	2:E:594:GLU:HB2	1.72	0.53
2:E:972:TYR:HA	2:E:975:THR:OG1	2.09	0.53
2:E:1585:LYS:HA	2:E:1588:LEU:HD12	1.90	0.53
2:B:52:ASN:ND2	2:B:55:LYS:HD2	2.24	0.53
2:B:327:MET:HB2	2:B:346:ILE:HG23	1.91	0.53
2:B:529:PHE:HE2	2:B:552:VAL:HG12	1.73	0.53
2:B:883:THR:CG2	2:B:931:ARG:HB3	2.39	0.53
2:B:917:ASP:N	2:B:917:ASP:OD1	2.41	0.53
2:E:353:MET:HG3	2:E:374:GLY:O	2.08	0.53
2:E:529:PHE:HE2	2:E:552:VAL:HG12	1.73	0.53
2:E:589:PRO:CB	2:E:594:GLU:HB3	2.36	0.53
2:E:670:GLN:HG3	2:E:719:TYR:CD1	2.44	0.53
2:E:1024:PHE:HA	2:E:1027:VAL:HG22	1.91	0.53
3:F:1:MET:HE3	3:F:2:GLN:H	1.73	0.53
1:A:541:GLN:O	1:A:544:ILE:HG22	2.09	0.53
1:A:552:ARG:NH1	1:A:664:ILE:HG12	2.23	0.53
1:A:679:SER:HB3	1:A:681:LEU:HG	1.91	0.53
2:B:561:THR:HG21	2:B:631:LEU:HB3	1.90	0.53
2:B:670:GLN:HG3	2:B:719:TYR:CD1	2.44	0.53
2:B:882:LEU:HA	2:B:885:GLN:HE21	1.73	0.53
2:B:973:ILE:HA	2:B:976:PHE:CZ	2.44	0.53
2:B:1017:PHE:O	2:B:1021:ILE:HG12	2.09	0.53
2:B:1551:LEU:HB3	2:B:1622:LEU:HD13	1.91	0.53
2:E:89:GLN:O	2:E:92:THR:OG1	2.23	0.53
2:E:181:ILE:HG22	2:E:185:LYS:NZ	2.23	0.53
2:E:906:LEU:HD12	2:E:909:ILE:HD11	1.91	0.53
2:E:1232:LYS:HB2	2:E:1240:TYR:CE2	2.44	0.53
1:A:578:ARG:HB3	1:A:587:HIS:HB2	1.91	0.53
1:D:536:LEU:HD21	2:E:17:TYR:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1391:ARG:HD2	2:E:1429:PHE:HA	1.91	0.53
2:E:1440:SER:H	2:E:1442:LYS:HZ1	1.57	0.53
3:F:7:VAL:HB	3:F:78:PHE:HD2	1.73	0.53
2:B:649:ASN:O	2:B:653:ASN:N	2.24	0.53
1:D:544:ILE:CD1	1:D:689:LEU:HB2	2.38	0.53
2:E:327:MET:HB2	2:E:346:ILE:HG23	1.91	0.53
2:E:875:ARG:HE	2:E:924:HIS:CD2	2.26	0.53
2:E:882:LEU:HA	2:E:885:GLN:HE21	1.73	0.53
2:E:1059:LEU:HD12	2:E:1116:PRO:HB2	1.90	0.53
2:E:1189:SER:O	2:E:1192:VAL:HG22	2.09	0.53
2:E:1237:GLU:O	2:E:1240:TYR:HB3	2.09	0.53
2:E:1536:HIS:CG	2:E:1542:LEU:HD22	2.44	0.53
2:E:1558:ALA:N	3:F:38:ASP:OD2	2.42	0.53
2:E:1626:PHE:HD2	2:E:1627:ARG:HD3	1.72	0.53
3:F:28:PHE:HB3	3:F:31:GLU:HG3	1.91	0.53
3:F:64:TYR:HD2	3:F:67:LEU:HD12	1.73	0.53
2:B:630:LYS:HG2	2:B:668:PHE:CZ	2.44	0.52
2:B:1205:LEU:HD13	2:B:1208:ARG:HD3	1.91	0.52
2:B:1601:THR:HG1	2:B:1626:PHE:HZ	1.56	0.52
2:E:52:ASN:ND2	2:E:55:LYS:HD2	2.24	0.52
2:E:1031:PHE:C	2:E:1035:GLN:HE22	2.11	0.52
2:E:1168:TYR:O	2:E:1172:LEU:HD23	2.08	0.52
2:E:1362:TYR:CE1	2:E:1384:ARG:HG3	2.44	0.52
2:E:1449:GLN:HA	2:E:1452:ASN:ND2	2.24	0.52
2:E:1470:LYS:HB3	2:E:1483:TRP:CD1	2.43	0.52
2:B:431:MET:HE3	2:B:625:LEU:HD23	1.92	0.52
2:B:710:GLN:HA	2:B:713:ASN:OD1	2.09	0.52
2:B:879:LEU:HA	2:B:882:LEU:HD12	1.90	0.52
2:B:1059:LEU:HD12	2:B:1116:PRO:HB2	1.90	0.52
2:B:1175:LEU:O	2:B:1179:HIS:ND1	2.43	0.52
1:D:557:VAL:HA	1:D:579:LEU:HB3	1.91	0.52
2:E:630:LYS:HG2	2:E:668:PHE:CZ	2.44	0.52
2:E:1095:GLY:H	2:E:1098:LYS:HE3	1.72	0.52
2:B:1322:LYS:HG2	2:B:1345:ARG:NH1	2.24	0.52
2:B:1470:LYS:HD3	2:B:1483:TRP:CG	2.45	0.52
2:E:826:ASP:HA	2:E:829:LEU:HB2	1.91	0.52
2:E:1238:ASP:HA	2:E:1241:ILE:HD12	1.92	0.52
2:E:1277:PRO:HA	2:E:1293:GLN:HG3	1.91	0.52
2:E:1322:LYS:HG2	2:E:1345:ARG:NH1	2.24	0.52
2:E:1551:LEU:HB3	2:E:1622:LEU:HD13	1.91	0.52
3:F:87:PRO:HA	3:F:90:PHE:CD2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:294:VAL:H	2:B:330:THR:HG1	1.52	0.52
2:B:473:HIS:HB2	2:B:526:HIS:CE1	2.45	0.52
2:B:875:ARG:HE	2:B:924:HIS:CD2	2.26	0.52
2:B:1032:PHE:HB3	2:B:1043:TRP:CH2	2.42	0.52
1:D:536:LEU:HD21	2:E:18:ASN:H	1.73	0.52
1:D:714:PRO:HG2	2:E:44:TRP:CZ2	2.44	0.52
1:D:717:PRO:HD2	2:E:1:MET:HE2	1.92	0.52
2:E:852:LEU:HB3	2:E:855:GLN:HB3	1.91	0.52
2:E:1449:GLN:OE1	2:E:1449:GLN:N	2.25	0.52
1:A:665:TRP:O	1:A:669:LEU:HG	2.09	0.52
2:B:19:TYR:HB2	2:B:59:PHE:HE1	1.73	0.52
2:B:906:LEU:HD12	2:B:909:ILE:HD11	1.91	0.52
2:B:923:VAL:O	2:B:927:LEU:HG	2.10	0.52
2:B:1362:TYR:HD2	2:B:1462:PHE:CE2	2.27	0.52
3:C:28:PHE:HB3	3:C:31:GLU:HG3	1.91	0.52
1:D:679:SER:HB3	1:D:681:LEU:HG	1.91	0.52
2:E:226:VAL:N	2:E:279:ALA:O	2.34	0.52
2:E:883:THR:CG2	2:E:931:ARG:HB3	2.39	0.52
2:E:923:VAL:O	2:E:927:LEU:HG	2.10	0.52
2:E:1017:PHE:O	2:E:1021:ILE:HG12	2.09	0.52
2:B:220:HIS:CE1	2:B:436:ILE:HD12	2.45	0.52
2:B:800:MET:O	2:B:804:ARG:HG3	2.10	0.52
2:B:914:ASP:HB2	2:B:963:GLN:NE2	2.25	0.52
2:B:1040:LEU:HD12	2:B:1097:HIS:CE1	2.44	0.52
2:B:1361:GLU:OE2	2:B:1388:TYR:HA	2.10	0.52
3:C:90:PHE:CD2	3:C:137:ILE:HD12	2.44	0.52
2:E:220:HIS:CE1	2:E:436:ILE:HD12	2.45	0.52
2:E:450:LEU:HB3	2:E:620:PHE:HZ	1.75	0.52
2:E:1395:SER:O	2:E:1399:LEU:HG	2.10	0.52
2:B:654:LEU:HB3	2:B:692:LEU:HB3	1.92	0.52
2:B:826:ASP:HA	2:B:829:LEU:HB2	1.91	0.52
2:E:800:MET:O	2:E:804:ARG:HG3	2.10	0.52
2:B:267:MET:SD	2:B:274:LEU:HD22	2.50	0.52
2:B:1238:ASP:HA	2:B:1241:ILE:HD12	1.92	0.52
2:E:267:MET:SD	2:E:274:LEU:HD22	2.50	0.52
2:E:654:LEU:HB3	2:E:692:LEU:HB3	1.92	0.52
2:E:710:GLN:HA	2:E:713:ASN:OD1	2.09	0.52
2:E:965:ASP:OD1	2:E:966:ASP:N	2.42	0.52
2:E:1145:HIS:O	2:E:1149:ASN:ND2	2.43	0.52
2:E:1439:PRO:HA	2:E:1442:LYS:HZ3	1.75	0.52
3:F:43:ASN:HA	3:F:52:ASN:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:37:ILE:HA	2:B:47:GLY:HA3	1.92	0.52
2:B:115:ARG:HE	2:B:118:GLN:HE21	1.57	0.52
2:B:771:ARG:O	2:B:775:LEU:HG	2.09	0.52
2:B:1024:PHE:HA	2:B:1027:VAL:HG22	1.91	0.52
2:B:1217:LYS:HG2	2:B:1220:ARG:NH2	2.25	0.52
2:B:1391:ARG:HH22	3:C:29:PRO:HD3	1.74	0.52
2:B:1578:GLU:HG3	2:B:1579:HIS:ND1	2.25	0.52
3:C:87:PRO:HA	3:C:90:PHE:CD2	2.44	0.52
1:D:564:LYS:HG3	1:D:575:TRP:NE1	2.25	0.52
2:E:532:ARG:NE	2:E:544:GLU:O	2.42	0.52
2:E:732:LYS:HA	2:E:735:LYS:HD3	1.91	0.52
2:E:771:ARG:O	2:E:775:LEU:HG	2.08	0.52
3:F:90:PHE:CD2	3:F:137:ILE:HD12	2.44	0.52
1:A:539:LYS:HZ1	1:A:540:ILE:HD11	1.75	0.52
1:A:609:PRO:HB2	1:A:612:ASP:OD1	2.10	0.52
2:B:285:SER:N	2:B:288:ASP:OD2	2.38	0.52
2:B:965:ASP:OD1	2:B:966:ASP:N	2.42	0.52
2:B:1277:PRO:HA	2:B:1293:GLN:HG3	1.91	0.52
2:B:1362:TYR:CE1	2:B:1384:ARG:HG3	2.44	0.52
2:E:62:THR:HG23	2:E:63:TYR:HD1	1.74	0.52
2:E:257:ASN:O	2:E:488:ALA:N	2.31	0.52
2:E:554:LEU:HA	2:E:562:LEU:HB2	1.91	0.52
2:E:914:ASP:HB2	2:E:963:GLN:NE2	2.25	0.52
2:E:1362:TYR:HD2	2:E:1462:PHE:CE2	2.27	0.52
1:A:564:LYS:HG3	1:A:575:TRP:NE1	2.25	0.51
2:B:474:ASP:OD1	2:B:478:LYS:N	2.43	0.51
2:B:1023:GLN:O	2:B:1027:VAL:HG13	2.11	0.51
2:B:1145:HIS:O	2:B:1149:ASN:ND2	2.43	0.51
3:C:137:ILE:HG23	3:C:141:GLN:HE21	1.75	0.51
2:E:1290:VAL:HG23	2:E:1291:TYR:H	1.76	0.51
2:E:1632:LYS:O	2:E:1637:TYR:N	2.27	0.51
2:B:34:THR:O	2:B:50:LEU:HB2	2.10	0.51
2:B:1189:SER:O	2:B:1192:VAL:HG22	2.09	0.51
3:C:69:PRO:HA	3:C:72:TYR:CD2	2.45	0.51
2:E:115:ARG:HE	2:E:118:GLN:HE21	1.58	0.51
2:E:1217:LYS:O	2:E:1221:MET:HG3	2.11	0.51
2:E:1305:ILE:HD11	2:E:1320:LEU:HB2	1.92	0.51
2:E:1406:GLU:OE1	2:E:1423:LYS:NZ	2.43	0.51
2:E:1470:LYS:HD3	2:E:1483:TRP:CG	2.45	0.51
2:B:130:GLN:HE21	2:B:144:LEU:HD11	1.73	0.51
2:B:853:VAL:HA	2:B:856:LYS:HG2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1301:TYR:HE2	2:B:1320:LEU:HD22	1.74	0.51
1:D:563:ARG:HA	1:D:573:LYS:O	2.11	0.51
2:E:474:ASP:OD1	2:E:478:LYS:N	2.43	0.51
2:E:853:VAL:HA	2:E:856:LYS:HG2	1.93	0.51
2:E:1361:GLU:OE2	2:E:1388:TYR:HA	2.10	0.51
3:F:146:ALA:O	3:F:150:GLY:N	2.43	0.51
2:E:972:TYR:O	2:E:975:THR:N	2.39	0.51
2:E:1217:LYS:HG2	2:E:1220:ARG:NH2	2.25	0.51
3:F:69:PRO:HA	3:F:72:TYR:CD2	2.45	0.51
3:F:137:ILE:HG23	3:F:141:GLN:HE21	1.75	0.51
2:B:62:THR:HG23	2:B:63:TYR:HD1	1.74	0.51
2:B:450:LEU:HB3	2:B:620:PHE:HZ	1.75	0.51
2:B:1391:ARG:HD2	2:B:1429:PHE:HA	1.91	0.51
2:B:1468:PHE:CE2	2:B:1470:LYS:HB2	2.45	0.51
3:C:146:ALA:O	3:C:150:GLY:N	2.43	0.51
1:D:541:GLN:O	1:D:544:ILE:HG22	2.09	0.51
1:D:665:TRP:O	1:D:669:LEU:HG	2.09	0.51
1:D:714:PRO:HG2	2:E:44:TRP:CE2	2.46	0.51
2:E:473:HIS:HB2	2:E:526:HIS:CE1	2.45	0.51
2:E:795:PHE:O	2:E:798:PHE:HB2	2.10	0.51
2:E:1175:LEU:O	2:E:1179:HIS:ND1	2.43	0.51
2:E:1468:PHE:HB3	2:E:1483:TRP:O	2.10	0.51
2:E:1578:GLU:HG3	2:E:1579:HIS:ND1	2.25	0.51
2:B:678:ASN:O	2:B:682:GLU:HG2	2.11	0.51
2:B:1065:SER:OG	2:B:1068:LYS:HB2	2.10	0.51
2:B:1237:GLU:O	2:B:1240:TYR:HB3	2.09	0.51
2:B:1562:GLY:HA3	3:C:36:VAL:HB	1.92	0.51
2:B:1586:VAL:HA	2:B:1589:LEU:HD12	1.93	0.51
1:D:578:ARG:HB3	1:D:587:HIS:HB2	1.91	0.51
2:E:157:ARG:HH21	2:E:194:ILE:HD13	1.76	0.51
2:E:1301:TYR:HE2	2:E:1320:LEU:HD22	1.74	0.51
2:B:1439:PRO:HA	2:B:1442:LYS:HZ3	1.75	0.51
3:C:43:ASN:HA	3:C:52:ASN:HA	1.91	0.51
2:E:288:ASP:OD1	2:E:291:ARG:NH2	2.33	0.51
2:E:493:ILE:HD11	2:E:496:TYR:HD1	1.75	0.51
2:E:882:LEU:O	2:E:886:LEU:HD23	2.11	0.51
2:E:1358:PRO:HB2	2:E:1387:GLU:HB2	1.93	0.51
2:E:1627:ARG:HA	2:E:1630:LYS:HB2	1.93	0.51
1:A:563:ARG:HA	1:A:573:LYS:O	2.11	0.51
2:B:380:THR:HG21	2:B:510:TYR:CD2	2.46	0.51
2:B:554:LEU:HA	2:B:562:LEU:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:719:TYR:CD1	2:B:723:HIS:HB2	2.45	0.51
1:D:588:TYR:N	1:D:603:SER:OG	2.44	0.51
2:E:215:ILE:O	2:E:218:THR:OG1	2.27	0.51
2:E:285:SER:N	2:E:288:ASP:OD2	2.38	0.51
2:E:1197:VAL:O	2:E:1201:LEU:HD23	2.11	0.51
1:A:723:VAL:HG23	2:B:2:ALA:HB1	1.93	0.51
2:B:46:ARG:HA	2:B:57:GLY:O	2.11	0.51
2:B:226:VAL:N	2:B:279:ALA:O	2.34	0.51
2:B:764:PHE:HA	2:B:767:ILE:HB	1.93	0.51
2:B:1358:PRO:HB2	2:B:1387:GLU:HB2	1.93	0.51
2:B:1406:GLU:OE1	2:B:1423:LYS:NZ	2.43	0.51
2:E:380:THR:HG21	2:E:510:TYR:CD2	2.46	0.51
2:E:1066:GLN:OE1	2:E:1069:ARG:NH1	2.40	0.51
2:E:1468:PHE:CE2	2:E:1470:LYS:HB2	2.45	0.51
2:E:1492:ALA:HB2	2:E:1505:LYS:HE3	1.93	0.51
1:A:596:GLN:NE2	1:A:599:VAL:HG13	2.26	0.51
2:B:157:ARG:HH21	2:B:194:ILE:HD13	1.76	0.51
2:B:288:ASP:OD1	2:B:291:ARG:NH2	2.33	0.51
2:B:493:ILE:HD11	2:B:496:TYR:HD1	1.75	0.51
2:B:965:ASP:O	2:B:969:TYR:N	2.42	0.51
2:B:1395:SER:O	2:B:1399:LEU:HG	2.10	0.51
3:C:164:GLY:O	3:C:168:VAL:N	2.39	0.51
1:D:609:PRO:HB2	1:D:612:ASP:OD1	2.10	0.51
1:D:688:THR:O	1:D:692:MET:HG2	2.11	0.51
2:E:1586:VAL:HA	2:E:1589:LEU:HD12	1.93	0.51
2:B:795:PHE:O	2:B:798:PHE:HB2	2.10	0.50
2:B:1305:ILE:HD11	2:B:1320:LEU:HB2	1.92	0.50
1:D:536:LEU:HG	2:E:18:ASN:OD1	2.10	0.50
1:D:596:GLN:NE2	1:D:599:VAL:HG13	2.26	0.50
2:E:760:LEU:HD22	2:E:764:PHE:CZ	2.46	0.50
2:E:1065:SER:OG	2:E:1068:LYS:HB2	2.10	0.50
1:A:588:TYR:CE1	1:A:608:LEU:HB2	2.46	0.50
2:B:180:THR:O	2:B:183:LEU:HB2	2.11	0.50
2:B:1217:LYS:O	2:B:1221:MET:HG3	2.11	0.50
2:B:1492:ALA:HB2	2:B:1505:LYS:HE3	1.93	0.50
2:E:37:ILE:HA	2:E:47:GLY:HA3	1.92	0.50
2:E:259:LEU:HD23	2:E:490:TYR:CG	2.46	0.50
2:E:262:TRP:CZ2	2:E:266:GLY:HA2	2.46	0.50
2:E:990:PHE:CD2	2:E:1042:LEU:HD11	2.47	0.50
2:E:1466:ARG:O	2:E:1484:ILE:HA	2.11	0.50
2:B:215:ILE:O	2:B:218:THR:OG1	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:450:LEU:O	2:B:510:TYR:N	2.44	0.50
2:B:584:PHE:O	2:B:587:THR:OG1	2.22	0.50
2:B:760:LEU:HD22	2:B:764:PHE:CZ	2.46	0.50
2:B:852:LEU:HB3	2:B:855:GLN:HB3	1.92	0.50
2:E:180:THR:O	2:E:183:LEU:HB2	2.11	0.50
2:E:308:LEU:HG	2:E:320:ARG:HH22	1.77	0.50
2:E:678:ASN:O	2:E:682:GLU:HG2	2.11	0.50
2:E:1023:GLN:O	2:E:1027:VAL:HG13	2.11	0.50
3:F:80:ILE:HG23	3:F:112:LEU:HD12	1.93	0.50
1:A:688:THR:O	1:A:692:MET:HG2	2.11	0.50
1:A:701:LEU:HD23	2:B:31:ILE:HG23	1.93	0.50
2:B:308:LEU:HG	2:B:320:ARG:HH22	1.77	0.50
2:B:532:ARG:NE	2:B:544:GLU:O	2.42	0.50
2:B:656:LYS:O	2:B:659:GLU:HG2	2.12	0.50
2:E:46:ARG:HA	2:E:57:GLY:O	2.11	0.50
2:E:719:TYR:CD1	2:E:723:HIS:HB2	2.45	0.50
1:A:578:ARG:NH2	1:A:601:HIS:H	2.09	0.50
1:A:695:LYS:O	1:A:698:LEU:HG	2.12	0.50
2:B:259:LEU:HD23	2:B:490:TYR:CG	2.46	0.50
2:B:471:SER:HB2	2:B:479:LEU:HD13	1.93	0.50
2:B:809:ALA:HB3	2:B:813:LYS:HZ2	1.77	0.50
2:B:1468:PHE:HB3	2:B:1483:TRP:O	2.10	0.50
2:E:225:TYR:N	2:E:404:LYS:O	2.43	0.50
2:E:796:LEU:HA	2:E:799:ASN:ND2	2.27	0.50
2:E:991:ILE:HG22	2:E:1045:ASN:HD21	1.77	0.50
2:E:1484:ILE:HB	2:E:1512:ILE:HD12	1.94	0.50
1:A:588:TYR:N	1:A:603:SER:OG	2.44	0.50
2:B:1098:LYS:O	2:B:1102:ILE:HG13	2.12	0.50
2:B:1197:VAL:O	2:B:1201:LEU:HD23	2.11	0.50
2:B:1239:ILE:O	2:B:1243:TYR:HD1	1.95	0.50
2:B:1290:VAL:HG23	2:B:1291:TYR:H	1.76	0.50
2:B:1484:ILE:HB	2:B:1512:ILE:HD12	1.94	0.50
2:B:1627:ARG:HA	2:B:1630:LYS:HB2	1.92	0.50
1:D:707:PRO:HD2	2:E:16:ILE:CG2	2.41	0.50
2:E:741:VAL:HG21	2:E:798:PHE:CD1	2.46	0.50
2:B:157:ARG:HH12	2:B:197:LYS:HD3	1.77	0.50
2:B:296:LEU:HB2	2:B:329:ILE:HD13	1.94	0.50
2:B:997:ILE:HD13	2:B:1053:PHE:HB2	1.94	0.50
2:E:656:LYS:O	2:E:659:GLU:HG2	2.12	0.50
2:E:997:ILE:HD13	2:E:1053:PHE:HB2	1.94	0.50
3:F:169:PHE:O	3:F:173:ILE:HG12	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:499:VAL:O	2:B:509:TRP:NE1	2.43	0.50
2:B:796:LEU:HA	2:B:799:ASN:ND2	2.27	0.50
2:B:921:THR:OG1	2:B:924:HIS:HB3	2.12	0.50
2:B:1042:LEU:HD12	2:B:1045:ASN:HB3	1.94	0.50
2:B:1183:HIS:CG	2:B:1184:LYS:H	2.30	0.50
2:B:1388:TYR:CE2	3:C:44:VAL:HA	2.47	0.50
1:D:584:LYS:O	1:D:607:LYS:NZ	2.42	0.50
2:E:414:GLN:O	2:E:418:SER:OG	2.19	0.50
2:E:450:LEU:O	2:E:510:TYR:N	2.44	0.50
2:E:471:SER:HB2	2:E:479:LEU:HD13	1.93	0.50
2:E:570:VAL:HG22	2:E:592:LYS:HD3	1.94	0.50
2:E:1066:GLN:HA	2:E:1069:ARG:CZ	2.42	0.50
1:A:617:VAL:O	1:A:642:PHE:HA	2.12	0.50
2:B:1156:ASP:OD1	2:B:1243:TYR:OH	2.30	0.50
2:B:1408:MET:SD	2:B:1427:GLN:HB3	2.52	0.50
2:B:1464:TYR:N	2:B:1487:THR:O	2.45	0.50
2:E:189:VAL:HG13	2:E:193:ARG:NH2	2.27	0.50
2:E:466:VAL:HG22	2:E:547:PHE:HZ	1.77	0.50
2:E:474:ASP:O	2:E:526:HIS:NE2	2.45	0.50
2:E:994:LYS:HZ2	2:E:1048:HIS:HB3	1.75	0.50
2:E:1042:LEU:HD12	2:E:1045:ASN:HB3	1.94	0.50
2:E:1561:GLY:O	2:E:1565:ASN:ND2	2.31	0.50
2:B:99:ALA:O	2:B:103:ARG:HG2	2.12	0.49
2:B:225:TYR:N	2:B:404:LYS:O	2.43	0.49
2:B:1012:THR:HG22	2:B:1015:ARG:NH2	2.27	0.49
2:B:1066:GLN:HA	2:B:1069:ARG:CZ	2.42	0.49
3:C:80:ILE:HG23	3:C:112:LEU:HD12	1.93	0.49
2:E:840:PHE:O	2:E:844:ILE:HG12	2.12	0.49
2:E:1183:HIS:CG	2:E:1184:LYS:H	2.30	0.49
2:E:1408:MET:SD	2:E:1427:GLN:HB3	2.52	0.49
2:E:1464:TYR:N	2:E:1487:THR:O	2.45	0.49
2:E:1479:PHE:HA	2:E:1482:MET:HG2	1.94	0.49
2:B:882:LEU:O	2:B:886:LEU:HD23	2.11	0.49
2:B:990:PHE:CD2	2:B:1042:LEU:HD11	2.47	0.49
2:B:1466:ARG:O	2:B:1484:ILE:HA	2.11	0.49
1:D:548:ILE:HB	1:D:549:LYS:HZ2	1.76	0.49
2:E:34:THR:O	2:E:50:LEU:HB2	2.10	0.49
2:E:99:ALA:O	2:E:103:ARG:HG2	2.12	0.49
2:E:1388:TYR:CE2	3:F:44:VAL:HG13	2.46	0.49
1:A:657:PRO:HB2	1:A:661:GLU:OE2	2.12	0.49
2:B:4:TRP:CE3	2:B:46:ARG:HG2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:474:ASP:O	2:B:526:HIS:NE2	2.45	0.49
2:B:1372:PHE:CZ	2:B:1424:GLN:HB3	2.48	0.49
2:B:1597:MET:HA	2:B:1600:LEU:HD12	1.95	0.49
2:E:921:THR:OG1	2:E:924:HIS:HB3	2.12	0.49
2:E:1372:PHE:CZ	2:E:1424:GLN:HB3	2.48	0.49
2:E:1386:LYS:HG3	2:E:1387:GLU:OE1	2.12	0.49
3:F:52:ASN:OD1	3:F:53:LEU:N	2.45	0.49
1:A:531:ARG:HH21	1:A:534:LEU:HD12	1.77	0.49
2:B:189:VAL:HG13	2:B:193:ARG:NH2	2.27	0.49
2:B:262:TRP:CZ2	2:B:266:GLY:HA2	2.47	0.49
2:B:1623:SER:HB3	2:B:1627:ARG:NH2	2.27	0.49
3:C:170:ASP:HB3	3:C:174:ARG:NH2	2.26	0.49
1:D:586:LEU:HB2	1:D:608:LEU:HB2	1.94	0.49
2:E:4:TRP:CE3	2:E:46:ARG:HG2	2.47	0.49
2:E:764:PHE:HA	2:E:767:ILE:HB	1.93	0.49
2:E:1098:LYS:O	2:E:1102:ILE:HG13	2.12	0.49
3:F:137:ILE:HG23	3:F:141:GLN:HG3	1.94	0.49
1:A:586:LEU:HB2	1:A:608:LEU:HB2	1.94	0.49
2:B:840:PHE:O	2:B:844:ILE:HG12	2.12	0.49
2:B:882:LEU:HD23	2:B:885:GLN:NE2	2.27	0.49
2:B:943:MET:HG3	2:B:950:ILE:HD13	1.94	0.49
2:B:1581:GLU:OE1	2:B:1581:GLU:N	2.44	0.49
1:D:541:GLN:HG3	1:D:545:LEU:HD23	1.94	0.49
2:E:190:ALA:O	2:E:194:ILE:HG12	2.13	0.49
2:E:296:LEU:HB2	2:E:329:ILE:HD13	1.94	0.49
2:E:414:GLN:HG2	2:E:421:VAL:HG12	1.95	0.49
2:E:882:LEU:HD23	2:E:885:GLN:NE2	2.28	0.49
2:E:1082:GLU:OE2	2:E:1086:ARG:NE	2.24	0.49
2:E:1221:MET:HA	2:E:1224:THR:HG22	1.95	0.49
2:B:570:VAL:HG22	2:B:592:LYS:HD3	1.94	0.49
2:B:694:PHE:HZ	2:B:737:LEU:HD13	1.77	0.49
2:B:730:TYR:HB3	2:B:770:SER:HB3	1.95	0.49
2:B:741:VAL:HG21	2:B:798:PHE:CD1	2.46	0.49
1:D:531:ARG:HH21	1:D:534:LEU:HD12	1.77	0.49
1:D:548:ILE:HD13	2:E:106:TYR:CE1	2.48	0.49
1:D:617:VAL:O	1:D:642:PHE:HA	2.12	0.49
1:D:657:PRO:HB2	1:D:661:GLU:OE2	2.12	0.49
2:E:157:ARG:HH12	2:E:197:LYS:HD3	1.77	0.49
3:F:35:THR:OG1	3:F:40:TYR:OH	2.28	0.49
1:A:541:GLN:HG3	1:A:545:LEU:HD23	1.94	0.49
2:B:414:GLN:HG2	2:B:421:VAL:HG12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:508:CYS:HB3	2:B:510:TYR:HE2	1.78	0.49
2:B:788:ASN:HA	2:B:831:PHE:HE1	1.78	0.49
2:B:1534:GLN:HA	2:B:1537:ALA:HB3	1.95	0.49
2:E:4:TRP:CZ3	2:E:46:ARG:HG2	2.48	0.49
2:E:18:ASN:HA	2:E:29:LEU:O	2.13	0.49
2:E:166:ARG:HB3	2:E:171:ASN:HA	1.95	0.49
2:E:467:GLU:HB2	2:E:500:VAL:HG22	1.95	0.49
2:E:753:LEU:HD11	2:E:812:ILE:HG12	1.93	0.49
2:E:1068:LYS:O	2:E:1072:ILE:HG12	2.13	0.49
2:E:1110:LEU:HD21	2:E:1151:LEU:HD12	1.94	0.49
2:E:1156:ASP:OD1	2:E:1243:TYR:OH	2.30	0.49
3:F:139:TYR:O	3:F:142:GLY:N	2.46	0.49
2:B:414:GLN:O	2:B:418:SER:OG	2.19	0.49
2:B:941:ILE:HD13	2:B:988:GLU:HB3	1.95	0.49
2:B:1068:LYS:O	2:B:1072:ILE:HG12	2.13	0.49
2:B:1386:LYS:HG3	2:B:1387:GLU:OE1	2.12	0.49
2:B:1479:PHE:HA	2:B:1482:MET:HG2	1.94	0.49
3:C:2:GLN:O	3:C:52:ASN:N	2.40	0.49
3:C:18:CYS:SG	3:C:32:TYR:OH	2.68	0.49
3:C:124:ASP:O	3:C:127:GLU:HG2	2.13	0.49
2:E:508:CYS:HB3	2:E:510:TYR:HE2	1.77	0.49
2:E:1623:SER:HB3	2:E:1627:ARG:NH2	2.27	0.49
2:B:4:TRP:CZ3	2:B:46:ARG:HG2	2.48	0.49
2:B:190:ALA:O	2:B:194:ILE:HG12	2.13	0.49
2:B:466:VAL:HG22	2:B:547:PHE:HZ	1.77	0.49
2:B:753:LEU:HD11	2:B:812:ILE:HG12	1.93	0.49
1:D:551:GLN:HG2	2:E:107:VAL:HA	1.95	0.49
2:E:868:LEU:HD23	2:E:912:VAL:HG11	1.94	0.49
2:E:943:MET:HG3	2:E:950:ILE:HD13	1.93	0.49
1:A:537:LYS:HG3	1:A:694:ILE:HG21	1.95	0.49
2:B:991:ILE:HG22	2:B:1045:ASN:HD21	1.77	0.49
2:B:1495:PHE:HE1	2:B:1502:PHE:HD2	1.60	0.49
2:E:788:ASN:HA	2:E:831:PHE:HE1	1.78	0.49
2:E:1242:ARG:O	2:E:1246:LYS:HG2	2.13	0.49
2:B:181:ILE:HG22	2:B:185:LYS:HZ1	1.76	0.48
2:B:529:PHE:CE2	2:B:552:VAL:HG12	2.48	0.48
2:B:1485:GLU:HG3	2:B:1511:GLU:OE1	2.13	0.48
1:D:695:LYS:O	1:D:698:LEU:HG	2.12	0.48
2:E:349:GLN:NE2	2:E:350:GLN:O	2.43	0.48
2:E:1544:VAL:HG12	2:E:1610:LYS:HB3	1.95	0.48
2:E:1633:VAL:O	2:E:1639:VAL:HG22	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:579:LEU:HA	1:A:586:LEU:HD13	1.96	0.48
2:B:18:ASN:HA	2:B:29:LEU:O	2.13	0.48
2:B:467:GLU:HB2	2:B:500:VAL:HG22	1.95	0.48
2:B:1242:ARG:O	2:B:1246:LYS:HG2	2.13	0.48
3:C:61:GLN:HB2	3:C:64:TYR:HD1	1.78	0.48
1:D:587:HIS:HA	1:D:606:ASP:HA	1.94	0.48
1:D:588:TYR:CE1	1:D:608:LEU:HB2	2.46	0.48
1:D:659:LYS:NZ	1:D:680:ASP:OD2	2.39	0.48
2:E:718:THR:O	2:E:722:LYS:HE2	2.13	0.48
2:E:1063:THR:HA	2:E:1069:ARG:CD	2.43	0.48
2:E:1486:ARG:NE	2:E:1510:GLU:OE1	2.46	0.48
2:B:288:ASP:HA	2:B:291:ARG:NE	2.27	0.48
2:B:467:GLU:OE2	2:B:534:ARG:NH1	2.46	0.48
2:B:718:THR:O	2:B:722:LYS:HE2	2.13	0.48
2:B:1344:LYS:O	2:B:1347:SER:OG	2.21	0.48
2:B:1544:VAL:HG12	2:B:1610:LYS:HB3	1.95	0.48
2:B:1626:PHE:CD2	2:B:1627:ARG:HD3	2.48	0.48
2:E:467:GLU:OE2	2:E:534:ARG:NH1	2.46	0.48
2:E:694:PHE:HZ	2:E:737:LEU:HD13	1.77	0.48
2:E:1012:THR:HG22	2:E:1015:ARG:NH2	2.28	0.48
2:E:1514:PRO:HA	2:E:1517:ASN:HB2	1.94	0.48
2:E:1534:GLN:HA	2:E:1537:ALA:HB3	1.95	0.48
2:B:792:ARG:HA	2:B:795:PHE:HD2	1.79	0.48
2:B:868:LEU:HD23	2:B:912:VAL:HG11	1.94	0.48
2:B:1062:GLU:O	2:B:1069:ARG:HD3	2.13	0.48
2:B:1066:GLN:OE1	2:B:1069:ARG:NH1	2.41	0.48
3:C:53:LEU:HD22	3:C:173:ILE:HD11	1.95	0.48
2:E:288:ASP:HA	2:E:291:ARG:NE	2.27	0.48
2:E:303:VAL:HG22	2:E:319:ARG:HG2	1.95	0.48
2:E:451:ILE:HD12	2:E:621:GLN:HG2	1.96	0.48
2:E:529:PHE:CE2	2:E:552:VAL:HG12	2.48	0.48
2:E:785:ASP:N	2:E:785:ASP:OD1	2.47	0.48
1:A:536:LEU:HD11	2:B:17:TYR:HD2	1.78	0.48
2:B:12:TYR:HB3	2:B:67:LYS:HD3	1.95	0.48
2:B:143:GLU:HG3	2:B:147:LYS:NZ	2.28	0.48
2:B:187:HIS:CE1	2:B:1009:MET:HB2	2.49	0.48
2:B:1072:ILE:O	2:B:1076:TYR:N	2.40	0.48
3:C:137:ILE:HG23	3:C:141:GLN:HG3	1.94	0.48
2:E:1256:ASN:HB3	2:E:1259:GLU:OE1	2.14	0.48
2:E:1495:PHE:HE1	2:E:1502:PHE:HD2	1.60	0.48
1:A:548:ILE:HD13	2:B:106:TYR:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:135:THR:HG23	2:B:136:LEU:HD22	1.95	0.48
2:B:1033:MET:HG3	2:B:1034:ASP:H	1.78	0.48
2:B:1166:GLU:O	2:B:1170:VAL:HG23	2.14	0.48
2:B:1514:PRO:HA	2:B:1517:ASN:HB2	1.94	0.48
2:E:143:GLU:HG3	2:E:147:LYS:NZ	2.28	0.48
2:E:1239:ILE:O	2:E:1243:TYR:HD1	1.95	0.48
2:E:1418:ILE:HG21	2:E:1425:TYR:HB2	1.95	0.48
2:E:1597:MET:HA	2:E:1600:LEU:HD12	1.95	0.48
3:F:124:ASP:O	3:F:127:GLU:HG2	2.13	0.48
3:F:129:LEU:HB3	3:F:134:LEU:O	2.14	0.48
2:B:208:LEU:HD23	2:B:211:ARG:HH21	1.78	0.48
2:B:1012:THR:HG22	2:B:1015:ARG:HH22	1.79	0.48
2:B:1102:ILE:O	2:B:1106:VAL:HG23	2.14	0.48
2:B:1633:VAL:O	2:B:1639:VAL:HG22	2.13	0.48
3:C:129:LEU:HB3	3:C:134:LEU:O	2.14	0.48
2:E:208:LEU:HD23	2:E:211:ARG:HH21	1.78	0.48
2:E:824:ILE:HD13	2:E:863:ILE:HD13	1.96	0.48
2:E:1012:THR:HG22	2:E:1015:ARG:HH22	1.79	0.48
2:E:1485:GLU:HG3	2:E:1511:GLU:OE1	2.13	0.48
2:E:1588:LEU:O	2:E:1592:LEU:HG	2.14	0.48
3:F:61:GLN:HB2	3:F:64:TYR:HD1	1.78	0.48
3:F:72:TYR:HD2	3:F:104:HIS:HB3	1.79	0.48
2:B:1110:LEU:HD21	2:B:1151:LEU:HD12	1.94	0.48
2:B:1632:LYS:O	2:B:1637:TYR:N	2.27	0.48
3:C:72:TYR:HD2	3:C:104:HIS:HB3	1.79	0.48
3:C:129:LEU:HA	3:C:132:LYS:HE3	1.96	0.48
2:E:187:HIS:CE1	2:E:1009:MET:HB2	2.49	0.48
2:E:228:PHE:HE2	2:E:399:LEU:HD12	1.78	0.48
2:E:660:VAL:HB	2:E:665:ILE:HD11	1.96	0.48
2:E:809:ALA:HB3	2:E:813:LYS:HZ2	1.78	0.48
2:E:1062:GLU:O	2:E:1069:ARG:HD3	2.13	0.48
1:A:545:LEU:O	1:A:549:LYS:HG2	2.14	0.48
1:A:587:HIS:HA	1:A:606:ASP:HA	1.94	0.48
2:B:744:ALA:HA	2:B:753:LEU:HD22	1.96	0.48
2:B:987:MET:CE	2:B:1042:LEU:HD13	2.44	0.48
2:B:994:LYS:HZ3	2:B:1048:HIS:HB3	1.78	0.48
2:B:1129:PHE:HA	2:B:1132:MET:HG3	1.96	0.48
2:B:1199:SER:O	2:B:1202:GLU:HG3	2.14	0.48
2:E:112:THR:OG1	2:E:113:LEU:N	2.45	0.48
2:E:744:ALA:HA	2:E:753:LEU:HD22	1.96	0.48
2:E:1060:GLN:OE1	2:E:1060:GLN:N	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1301:TYR:O	2:E:1305:ILE:HG12	2.14	0.48
2:E:1373:PRO:HD2	2:E:1376:LEU:HD12	1.95	0.48
2:E:1474:ASP:N	2:E:1474:ASP:OD1	2.47	0.48
2:E:1632:LYS:HA	2:E:1636:HIS:HB3	1.96	0.48
3:F:5:LYS:HE2	3:F:56:TRP:HZ2	1.79	0.48
2:B:112:THR:OG1	2:B:113:LEU:N	2.45	0.48
2:B:166:ARG:HB3	2:B:171:ASN:HA	1.95	0.48
2:B:1221:MET:HA	2:B:1224:THR:HG22	1.95	0.48
2:B:1251:HIS:O	2:B:1255:GLU:N	2.47	0.48
2:B:1273:TRP:CE2	2:B:1327:THR:HG21	2.49	0.48
2:E:135:THR:HG23	2:E:136:LEU:HD22	1.95	0.48
2:E:1129:PHE:HA	2:E:1132:MET:HG3	1.96	0.48
2:E:1486:ARG:O	2:E:1510:GLU:N	2.47	0.48
2:E:1621:ARG:CZ	3:F:70:LEU:HD13	2.44	0.48
3:F:129:LEU:HA	3:F:132:LYS:HE3	1.96	0.48
2:B:419:HIS:CD2	2:B:420:LEU:HG	2.50	0.47
2:B:824:ILE:HD13	2:B:863:ILE:HD13	1.96	0.47
2:B:1256:ASN:HB3	2:B:1259:GLU:OE1	2.14	0.47
2:B:1486:ARG:NE	2:B:1510:GLU:OE1	2.46	0.47
3:C:65:ASP:HA	3:C:68:ARG:HG2	1.96	0.47
3:C:139:TYR:O	3:C:142:GLY:N	2.46	0.47
1:D:545:LEU:O	1:D:549:LYS:HG2	2.14	0.47
1:D:578:ARG:NH2	1:D:601:HIS:H	2.09	0.47
2:E:730:TYR:HB3	2:E:770:SER:HB3	1.95	0.47
3:F:65:ASP:HA	3:F:68:ARG:HG2	1.96	0.47
3:F:170:ASP:HB3	3:F:174:ARG:NH2	2.26	0.47
2:B:88:VAL:O	2:B:91:LEU:HG	2.14	0.47
2:B:1200:LEU:O	2:B:1204:LEU:HD23	2.14	0.47
2:B:1301:TYR:O	2:B:1305:ILE:HG12	2.14	0.47
2:B:1470:LYS:HD3	2:B:1483:TRP:CD1	2.49	0.47
3:C:5:LYS:HE2	3:C:56:TRP:HZ2	1.79	0.47
1:D:537:LYS:HG3	1:D:694:ILE:HG21	1.95	0.47
2:E:987:MET:CE	2:E:1042:LEU:HD13	2.44	0.47
2:B:166:ARG:HG2	2:B:173:LEU:HB2	1.96	0.47
2:B:228:PHE:HE2	2:B:399:LEU:HD12	1.78	0.47
2:B:785:ASP:OD1	2:B:785:ASP:N	2.47	0.47
2:B:990:PHE:CE2	2:B:1042:LEU:HD21	2.49	0.47
2:B:1063:THR:HA	2:B:1069:ARG:CD	2.43	0.47
2:B:1418:ILE:HG21	2:B:1425:TYR:HB2	1.95	0.47
1:D:584:LYS:NZ	2:E:1403:PRO:HA	2.29	0.47
2:E:941:ILE:HD13	2:E:988:GLU:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1062:GLU:O	2:E:1068:LYS:HB3	2.15	0.47
2:E:1102:ILE:O	2:E:1106:VAL:HG23	2.14	0.47
2:E:1251:HIS:O	2:E:1255:GLU:N	2.47	0.47
2:E:1273:TRP:CE2	2:E:1327:THR:HG21	2.49	0.47
2:E:1621:ARG:HD3	3:F:67:LEU:HD22	1.95	0.47
3:F:2:GLN:O	3:F:52:ASN:N	2.40	0.47
3:F:164:GLY:O	3:F:168:VAL:HG23	2.14	0.47
1:A:564:LYS:O	1:A:573:LYS:NZ	2.32	0.47
3:C:169:PHE:O	3:C:173:ILE:HG12	2.12	0.47
2:E:792:ARG:HA	2:E:795:PHE:HD2	1.79	0.47
2:E:868:LEU:HD13	2:E:878:LEU:HD21	1.96	0.47
2:E:965:ASP:O	2:E:969:TYR:N	2.42	0.47
2:E:1166:GLU:O	2:E:1170:VAL:HG23	2.14	0.47
2:E:1452:ASN:HA	2:E:1455:ARG:HB2	1.96	0.47
2:E:1485:GLU:OE1	2:E:1485:GLU:N	2.47	0.47
2:B:154:HIS:O	2:B:157:ARG:HG2	2.14	0.47
2:B:303:VAL:HG22	2:B:319:ARG:HG2	1.95	0.47
2:B:436:ILE:HG22	2:B:438:LEU:HD22	1.97	0.47
2:B:661:ASP:O	2:B:665:ILE:HG12	2.15	0.47
2:B:859:CYS:O	2:B:863:ILE:HG12	2.13	0.47
2:B:1060:GLN:HG2	2:B:1061:LEU:N	2.30	0.47
2:B:1485:GLU:OE1	2:B:1485:GLU:N	2.47	0.47
3:C:164:GLY:O	3:C:168:VAL:HG23	2.14	0.47
1:D:578:ARG:O	1:D:587:HIS:N	2.24	0.47
1:D:698:LEU:HA	2:E:31:ILE:HG21	1.95	0.47
2:E:154:HIS:O	2:E:157:ARG:HG2	2.14	0.47
2:E:661:ASP:O	2:E:665:ILE:HG12	2.15	0.47
2:E:1060:GLN:HG2	2:E:1061:LEU:N	2.30	0.47
2:E:1200:LEU:O	2:E:1204:LEU:HD23	2.14	0.47
2:E:1470:LYS:HD3	2:E:1483:TRP:CD1	2.49	0.47
2:B:578:LYS:HB3	2:B:584:PHE:CE2	2.49	0.47
2:B:1083:ILE:O	2:B:1087:ILE:HG12	2.15	0.47
2:B:1127:ILE:O	2:B:1131:MET:HG3	2.15	0.47
2:B:1474:ASP:N	2:B:1474:ASP:OD1	2.47	0.47
1:D:579:LEU:HA	1:D:586:LEU:HD13	1.96	0.47
2:E:170:GLY:O	2:E:172:ILE:HG23	2.14	0.47
2:E:809:ALA:HB3	2:E:813:LYS:NZ	2.30	0.47
2:E:882:LEU:HA	2:E:885:GLN:NE2	2.30	0.47
3:F:121:ASP:HA	3:F:126:ILE:HD11	1.97	0.47
1:A:700:ASP:HB2	2:B:32:GLY:HA2	1.96	0.47
2:B:328:ASP:OD1	2:B:328:ASP:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:382:VAL:O	2:B:386:VAL:HG23	2.15	0.47
2:B:451:ILE:HD12	2:B:621:GLN:HG2	1.96	0.47
2:B:743:ASN:HB3	2:B:749:LYS:HD2	1.95	0.47
2:B:783:ASP:HB3	2:B:786:GLU:HB2	1.97	0.47
2:B:816:ALA:O	2:B:820:LEU:HD23	2.15	0.47
2:B:1121:ARG:HG2	2:B:1125:ILE:HD11	1.96	0.47
2:B:1452:ASN:OD1	2:B:1453:TYR:N	2.48	0.47
2:B:1530:SER:O	2:B:1534:GLN:OE1	2.33	0.47
2:B:1555:VAL:HG21	2:B:1622:LEU:HD22	1.97	0.47
2:B:1588:LEU:O	2:B:1592:LEU:HG	2.14	0.47
3:C:6:CYS:SG	3:C:79:LEU:HD23	2.55	0.47
2:E:12:TYR:HB3	2:E:67:LYS:HD3	1.95	0.47
2:E:105:LEU:HD23	2:E:105:LEU:HA	1.73	0.47
2:E:382:VAL:O	2:E:386:VAL:HG23	2.15	0.47
2:E:471:SER:OG	2:E:528:ARG:HB3	2.15	0.47
2:E:499:VAL:O	2:E:509:TRP:NE1	2.43	0.47
2:E:783:ASP:HB3	2:E:786:GLU:HB2	1.97	0.47
2:E:859:CYS:O	2:E:863:ILE:HG12	2.13	0.47
2:E:1033:MET:HG3	2:E:1034:ASP:H	1.78	0.47
2:E:1199:SER:O	2:E:1202:GLU:HG3	2.14	0.47
2:E:1231:TYR:CE2	2:E:1239:ILE:HD12	2.49	0.47
2:E:1432:LYS:HZ1	2:E:1465:SER:H	1.61	0.47
3:F:153:LYS:NZ	3:F:154:TYR:O	2.44	0.47
2:B:533:HIS:HB3	2:B:544:GLU:HG2	1.96	0.47
2:B:1099:ILE:C	2:B:1101:PHE:H	2.18	0.47
2:B:1125:ILE:N	2:B:1126:PRO:HD2	2.29	0.47
1:D:547:LEU:O	1:D:550:GLN:NE2	2.48	0.47
1:D:687:ASP:OD1	1:D:688:THR:N	2.47	0.47
2:E:38:LEU:HD23	2:E:48:TYR:H	1.80	0.47
2:E:88:VAL:O	2:E:91:LEU:HG	2.14	0.47
2:E:468:VAL:HB	2:E:498:SER:HB3	1.97	0.47
2:E:533:HIS:HB3	2:E:544:GLU:HG2	1.96	0.47
2:E:1042:LEU:O	2:E:1045:ASN:N	2.48	0.47
2:E:1127:ILE:O	2:E:1131:MET:HG3	2.15	0.47
2:E:1154:LYS:HA	2:E:1157:GLN:OE1	2.15	0.47
2:E:1483:TRP:NE1	2:E:1514:PRO:HD3	2.30	0.47
2:E:1626:PHE:CD2	2:E:1627:ARG:HD3	2.48	0.47
3:F:64:TYR:HB2	3:F:68:ARG:NH2	2.30	0.47
1:A:687:ASP:OD1	1:A:688:THR:N	2.48	0.47
2:B:170:GLY:O	2:B:172:ILE:HG23	2.14	0.47
2:B:287:MET:SD	2:B:291:ARG:NH2	2.88	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1386:LYS:HB3	2:B:1389:GLU:HG3	1.97	0.47
2:B:1632:LYS:HA	2:B:1636:HIS:HB3	1.96	0.47
1:D:697:ARG:HH21	2:E:30:GLN:CB	2.16	0.47
2:E:287:MET:SD	2:E:291:ARG:NH2	2.88	0.47
2:E:419:HIS:CD2	2:E:420:LEU:HG	2.49	0.47
2:E:578:LYS:HB3	2:E:584:PHE:CE2	2.49	0.47
2:E:816:ALA:O	2:E:820:LEU:HD23	2.15	0.47
2:E:987:MET:SD	2:E:1042:LEU:HD13	2.54	0.47
2:E:1125:ILE:N	2:E:1126:PRO:HD2	2.29	0.47
2:B:166:ARG:NH1	2:B:168:ASP:H	2.13	0.47
2:B:868:LEU:HD13	2:B:878:LEU:HD21	1.96	0.47
2:B:1042:LEU:O	2:B:1045:ASN:N	2.48	0.47
2:B:1075:LYS:HE3	2:B:1075:LYS:HB3	1.58	0.47
2:B:1406:GLU:HG3	2:B:1425:TYR:CE1	2.50	0.47
2:B:1452:ASN:HA	2:B:1455:ARG:HB2	1.96	0.47
2:B:1486:ARG:O	2:B:1510:GLU:N	2.47	0.47
2:E:305:HIS:HA	2:E:315:THR:O	2.15	0.47
3:F:53:LEU:HD22	3:F:173:ILE:HD11	1.95	0.47
2:B:706:ASP:O	2:B:710:GLN:N	2.48	0.46
2:B:871:GLN:HB3	2:B:875:ARG:HB2	1.97	0.46
2:B:1373:PRO:HD2	2:B:1376:LEU:HD12	1.95	0.46
1:D:688:THR:O	1:D:691:SER:OG	2.30	0.46
2:E:1394:PHE:HD2	2:E:1428:CYS:HG	1.63	0.46
2:E:1557:PRO:HB2	2:E:1560:MET:O	2.15	0.46
2:B:660:VAL:HB	2:B:665:ILE:HD11	1.96	0.46
2:B:1129:PHE:HE1	2:B:1180:CYS:HG	1.62	0.46
2:B:1388:TYR:HE2	3:C:44:VAL:HG13	1.80	0.46
2:E:59:PHE:CD2	2:E:64:ILE:HG12	2.50	0.46
2:E:79:THR:HA	2:E:85:LEU:HD22	1.98	0.46
2:E:706:ASP:O	2:E:710:GLN:N	2.48	0.46
2:E:743:ASN:HB3	2:E:749:LYS:HD2	1.95	0.46
2:E:990:PHE:CE2	2:E:1042:LEU:HD21	2.49	0.46
2:E:1452:ASN:OD1	2:E:1453:TYR:N	2.48	0.46
2:E:1573:GLU:O	2:E:1577:GLN:NE2	2.48	0.46
3:F:14:VAL:HB	3:F:16:LYS:HZ2	1.80	0.46
2:B:258:TYR:HA	2:B:488:ALA:HB3	1.98	0.46
2:B:349:GLN:NE2	2:B:350:GLN:O	2.43	0.46
2:B:1231:TYR:CE2	2:B:1239:ILE:HD12	2.49	0.46
1:D:724:TYR:HB2	2:E:4:TRP:O	2.15	0.46
2:E:59:PHE:CE2	2:E:63:TYR:HB3	2.50	0.46
2:E:166:ARG:HG2	2:E:173:LEU:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:700:ILE:O	2:E:703:LEU:HG	2.16	0.46
2:E:1233:GLU:HG3	2:E:1234:LYS:HD2	1.97	0.46
3:F:132:LYS:HD2	3:F:134:LEU:HD12	1.98	0.46
2:B:59:PHE:CE2	2:B:63:TYR:HB3	2.50	0.46
2:B:806:LEU:HD12	2:B:813:LYS:HE3	1.97	0.46
2:B:817:LEU:HB2	2:B:855:GLN:HG3	1.98	0.46
2:B:882:LEU:HA	2:B:885:GLN:NE2	2.30	0.46
2:B:1154:LYS:HA	2:B:1157:GLN:OE1	2.15	0.46
2:B:1470:LYS:O	2:B:1481:THR:HA	2.15	0.46
2:B:1536:HIS:CD2	2:B:1542:LEU:HB3	2.50	0.46
2:B:1557:PRO:HB2	2:B:1560:MET:O	2.15	0.46
2:B:1573:GLU:O	2:B:1577:GLN:NE2	2.48	0.46
3:C:153:LYS:NZ	3:C:154:TYR:O	2.44	0.46
2:E:436:ILE:HG22	2:E:438:LEU:HD22	1.97	0.46
2:E:594:GLU:HA	2:E:597:GLU:HG3	1.97	0.46
2:E:871:GLN:HB3	2:E:875:ARG:HB2	1.97	0.46
2:E:879:LEU:O	2:E:882:LEU:N	2.49	0.46
2:E:1386:LYS:HB3	2:E:1389:GLU:HG3	1.97	0.46
2:E:1406:GLU:HG3	2:E:1425:TYR:CE1	2.50	0.46
2:E:1470:LYS:O	2:E:1481:THR:HA	2.15	0.46
2:E:1470:LYS:N	2:E:1481:THR:O	2.46	0.46
2:E:1530:SER:O	2:E:1534:GLN:OE1	2.33	0.46
1:A:693:GLU:O	1:A:697:ARG:HG2	2.15	0.46
2:B:111:LEU:O	2:B:115:ARG:HG2	2.16	0.46
2:B:127:TRP:O	2:B:130:GLN:HG2	2.16	0.46
2:B:809:ALA:HB3	2:B:813:LYS:NZ	2.30	0.46
2:B:1125:ILE:HD13	2:B:1171:LEU:HD22	1.98	0.46
2:B:1483:TRP:NE1	2:B:1514:PRO:HD3	2.30	0.46
3:C:64:TYR:HB2	3:C:68:ARG:NH2	2.30	0.46
1:D:536:LEU:HA	1:D:539:LYS:HE3	1.98	0.46
1:D:544:ILE:O	1:D:548:ILE:HG12	2.15	0.46
2:E:932:LEU:CA	2:E:935:ARG:HE	2.28	0.46
2:E:1083:ILE:O	2:E:1087:ILE:HG12	2.15	0.46
3:F:82:PHE:HE1	3:F:112:LEU:HG	1.80	0.46
1:A:544:ILE:O	1:A:548:ILE:HG12	2.15	0.46
2:B:38:LEU:HD23	2:B:48:TYR:H	1.80	0.46
2:B:189:VAL:O	2:B:193:ARG:HG2	2.16	0.46
2:B:647:SER:HA	2:B:650:ILE:HG13	1.97	0.46
2:B:700:ILE:O	2:B:703:LEU:HG	2.16	0.46
2:B:1561:GLY:O	2:B:1565:ASN:ND2	2.31	0.46
2:E:328:ASP:N	2:E:328:ASP:OD1	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:547:LEU:O	1:A:550:GLN:NE2	2.48	0.46
1:A:727:ASN:H	2:B:46:ARG:HH22	1.62	0.46
2:B:987:MET:SD	2:B:1042:LEU:HD13	2.54	0.46
2:B:1530:SER:O	2:B:1533:VAL:HB	2.15	0.46
3:C:52:ASN:OD1	3:C:53:LEU:N	2.45	0.46
2:E:10:GLN:HG3	2:E:37:ILE:HB	1.98	0.46
3:F:164:GLY:O	3:F:168:VAL:N	2.39	0.46
1:A:584:LYS:O	1:A:607:LYS:NZ	2.42	0.46
1:A:622:CYS:HB3	1:A:624:HIS:ND1	2.31	0.46
2:B:127:TRP:O	2:B:131:ILE:HG12	2.16	0.46
2:B:790:SER:HA	2:B:793:GLN:CD	2.36	0.46
2:B:979:ARG:O	2:B:982:ILE:HG22	2.16	0.46
2:B:1611:LEU:HD12	2:B:1615:LEU:HB2	1.96	0.46
2:E:267:MET:SD	2:E:268:PRO:HD2	2.56	0.46
2:E:757:LEU:HD13	2:E:815:ALA:HB3	1.98	0.46
2:E:966:ASP:HA	2:E:969:TYR:CD2	2.48	0.46
2:E:1536:HIS:CD2	2:E:1542:LEU:HB3	2.50	0.46
2:E:1582:ASP:HA	2:E:1585:LYS:HZ3	1.81	0.46
3:F:6:CYS:SG	3:F:79:LEU:HD23	2.55	0.46
2:B:79:THR:HA	2:B:85:LEU:HD22	1.98	0.46
2:B:195:GLU:HA	2:B:198:ILE:HG12	1.97	0.46
2:B:1062:GLU:O	2:B:1068:LYS:HB3	2.15	0.46
1:D:562:PHE:CE1	1:D:577:CYS:HB3	2.51	0.46
2:E:127:TRP:O	2:E:130:GLN:HG2	2.16	0.46
2:E:127:TRP:O	2:E:131:ILE:HG12	2.16	0.46
2:E:979:ARG:O	2:E:982:ILE:HG22	2.16	0.46
2:E:1555:VAL:HG21	2:E:1622:LEU:HD22	1.97	0.46
2:B:319:ARG:HB2	2:B:499:VAL:HA	1.98	0.46
2:B:441:ASP:C	2:B:629:THR:HG1	2.18	0.46
2:B:468:VAL:HB	2:B:498:SER:HB3	1.97	0.46
1:D:591:LEU:HD22	1:D:604:LEU:HD13	1.98	0.46
2:E:166:ARG:NH1	2:E:168:ASP:H	2.13	0.46
2:E:732:LYS:O	2:E:736:VAL:HG23	2.15	0.46
2:E:817:LEU:HB2	2:E:855:GLN:HG3	1.98	0.46
2:E:1306:SER:O	2:E:1310:LYS:HG2	2.16	0.46
2:E:1530:SER:O	2:E:1533:VAL:HB	2.15	0.46
2:E:1611:LEU:HD12	2:E:1615:LEU:HB2	1.96	0.46
2:B:115:ARG:HE	2:B:118:GLN:NE2	2.14	0.45
2:B:306:MET:HA	2:B:306:MET:HE3	1.98	0.45
2:B:1306:SER:O	2:B:1310:LYS:HG2	2.16	0.45
3:C:14:VAL:HB	3:C:16:LYS:HZ2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:121:ASP:HA	3:C:126:ILE:HD11	1.97	0.45
3:C:135:THR:HB	3:C:137:ILE:HG13	1.98	0.45
1:D:629:GLY:O	1:D:632:LYS:HG3	2.16	0.45
2:E:195:GLU:HA	2:E:198:ILE:HG12	1.97	0.45
2:E:258:TYR:HA	2:E:488:ALA:HB3	1.97	0.45
2:E:473:HIS:CE1	2:E:479:LEU:HB2	2.51	0.45
2:E:647:SER:HA	2:E:650:ILE:HG13	1.97	0.45
2:E:806:LEU:HD12	2:E:813:LYS:HE3	1.97	0.45
2:E:908:ASN:O	2:E:912:VAL:HG23	2.16	0.45
2:E:964:MET:SD	2:E:965:ASP:N	2.87	0.45
2:E:1545:HIS:HD2	3:F:5:LYS:HE3	1.79	0.45
2:E:1549:MET:HA	3:F:39:ASN:HD21	1.79	0.45
3:F:135:THR:HB	3:F:137:ILE:HG13	1.98	0.45
1:A:536:LEU:HA	1:A:539:LYS:HE3	1.98	0.45
1:A:550:GLN:HA	1:A:553:LEU:HD12	1.98	0.45
1:A:562:PHE:CE1	1:A:577:CYS:HB3	2.51	0.45
2:B:10:GLN:HG3	2:B:37:ILE:HB	1.97	0.45
2:B:188:GLU:O	2:B:192:LYS:HG3	2.16	0.45
2:B:594:GLU:HA	2:B:597:GLU:HG3	1.97	0.45
2:B:879:LEU:O	2:B:882:LEU:N	2.49	0.45
2:B:964:MET:SD	2:B:965:ASP:N	2.87	0.45
2:B:1233:GLU:HG3	2:B:1234:LYS:HD2	1.97	0.45
3:C:82:PHE:HE1	3:C:112:LEU:HG	1.81	0.45
3:C:132:LYS:HD2	3:C:134:LEU:HD12	1.98	0.45
2:E:26:GLU:OE1	2:E:29:LEU:HD11	2.16	0.45
2:E:188:GLU:O	2:E:192:LYS:HG3	2.16	0.45
2:E:243:MET:HA	2:E:298:CYS:HA	1.99	0.45
2:E:790:SER:HA	2:E:793:GLN:CD	2.36	0.45
2:E:1099:ILE:C	2:E:1101:PHE:H	2.18	0.45
2:E:1153:THR:HG22	2:E:1157:GLN:HE22	1.81	0.45
2:E:1251:HIS:NE2	2:E:1498:ILE:O	2.49	0.45
2:E:1268:ALA:HA	2:E:1271:LEU:HD13	1.98	0.45
2:E:1371:GLY:C	2:E:1424:GLN:HE21	2.20	0.45
2:E:1581:GLU:OE1	2:E:1581:GLU:N	2.44	0.45
2:B:243:MET:HA	2:B:298:CYS:HA	1.99	0.45
2:B:305:HIS:HA	2:B:315:THR:O	2.16	0.45
2:B:431:MET:HE3	2:B:447:TYR:CD2	2.51	0.45
2:B:471:SER:OG	2:B:528:ARG:HB3	2.15	0.45
2:B:732:LYS:O	2:B:736:VAL:HG23	2.15	0.45
2:B:795:PHE:CE2	2:B:839:LEU:HD13	2.52	0.45
2:B:1111:GLU:O	2:B:1163:ARG:NH1	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1183:HIS:HB3	2:B:1187:SER:OG	2.16	0.45
3:C:49:LYS:HZ2	3:C:51:VAL:HG12	1.81	0.45
2:E:896:LYS:HA	2:E:899:HIS:CE1	2.51	0.45
2:E:945:ARG:HH11	2:E:946:GLN:N	2.14	0.45
2:E:1125:ILE:HD13	2:E:1171:LEU:HD22	1.98	0.45
1:A:557:VAL:O	1:A:578:ARG:HG3	2.16	0.45
1:A:591:LEU:HD22	1:A:604:LEU:HD13	1.98	0.45
2:B:267:MET:SD	2:B:268:PRO:HD2	2.56	0.45
2:B:927:LEU:CB	2:B:931:ARG:HH21	2.29	0.45
2:B:1153:THR:HG22	2:B:1157:GLN:HE22	1.81	0.45
2:B:1463:ARG:HA	2:B:1488:THR:HA	1.98	0.45
2:E:474:ASP:OD2	2:E:478:LYS:HE3	2.17	0.45
2:E:772:VAL:O	2:E:776:ARG:HG2	2.16	0.45
2:E:1201:LEU:O	2:E:1205:LEU:HD23	2.17	0.45
1:A:640:LEU:O	1:A:655:ILE:HA	2.16	0.45
2:B:757:LEU:HD13	2:B:815:ALA:HB3	1.98	0.45
2:B:896:LYS:HA	2:B:899:HIS:CE1	2.51	0.45
2:B:929:MET:HB2	2:B:964:MET:HE1	1.99	0.45
2:B:1032:PHE:O	2:B:1040:LEU:HD22	2.17	0.45
2:B:1201:LEU:O	2:B:1205:LEU:HD23	2.17	0.45
3:C:95:ALA:O	3:C:99:PRO:HG2	2.16	0.45
1:D:693:GLU:O	1:D:697:ARG:HG2	2.15	0.45
1:D:701:LEU:HD23	2:E:31:ILE:CG2	2.43	0.45
2:E:115:ARG:HE	2:E:118:GLN:NE2	2.14	0.45
2:E:1033:MET:N	2:E:1035:GLN:HE21	2.14	0.45
2:E:1121:ARG:HG2	2:E:1125:ILE:HD11	1.96	0.45
2:B:145:LYS:O	2:B:149:THR:OG1	2.26	0.45
2:B:184:PHE:O	2:B:188:GLU:OE1	2.35	0.45
2:B:473:HIS:CE1	2:B:479:LEU:HB2	2.51	0.45
3:C:18:CYS:HG	3:C:32:TYR:HH	1.56	0.45
1:D:550:GLN:HA	1:D:553:LEU:HD12	1.98	0.45
1:D:663:CYS:HB3	1:D:679:SER:HA	1.99	0.45
2:E:302:ARG:HD3	2:E:322:PHE:CD1	2.52	0.45
2:E:727:THR:O	2:E:774:TYR:HB2	2.17	0.45
2:E:1473:LYS:HD3	2:E:1481:THR:HG21	1.99	0.45
2:B:930:GLU:O	2:B:935:ARG:NH2	2.50	0.45
2:B:1117:GLU:CD	2:B:1120:LEU:HG	2.37	0.45
2:B:1193:PHE:O	2:B:1196:LEU:HB3	2.17	0.45
2:B:1251:HIS:NE2	2:B:1498:ILE:O	2.49	0.45
1:D:532:PRO:O	1:D:536:LEU:HD13	2.17	0.45
2:E:111:LEU:O	2:E:115:ARG:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:166:ARG:HB2	2:E:174:ASP:H	1.82	0.45
2:E:189:VAL:O	2:E:193:ARG:HG2	2.16	0.45
2:E:1072:ILE:O	2:E:1076:TYR:N	2.40	0.45
2:E:1183:HIS:HB3	2:E:1187:SER:OG	2.16	0.45
3:F:95:ALA:O	3:F:99:PRO:HG2	2.16	0.45
2:B:332:ILE:HD13	2:B:403:LEU:HD12	1.99	0.45
2:B:697:LEU:O	2:B:701:ILE:HG12	2.17	0.45
2:B:945:ARG:HH11	2:B:946:GLN:N	2.14	0.45
2:E:927:LEU:CB	2:E:931:ARG:HH21	2.29	0.45
2:E:930:GLU:O	2:E:935:ARG:NH2	2.50	0.45
2:E:1193:PHE:O	2:E:1196:LEU:HB3	2.17	0.45
1:A:646:TYR:CE1	1:A:652:LEU:HG	2.52	0.45
1:A:716:GLU:HG3	2:B:44:TRP:CZ2	2.52	0.45
2:B:142:ALA:O	2:B:146:LYS:HG3	2.16	0.45
2:B:339:ASP:OD1	2:B:339:ASP:N	2.50	0.45
2:B:908:ASN:O	2:B:912:VAL:HG23	2.16	0.45
2:B:1611:LEU:HD13	2:B:1619:HIS:HB2	1.99	0.45
1:D:622:CYS:HB3	1:D:624:HIS:ND1	2.31	0.45
2:E:102:TRP:CH2	2:E:118:GLN:HG2	2.52	0.45
2:E:179:SER:OG	2:E:182:ALA:HB3	2.17	0.45
2:E:584:PHE:CE2	2:E:588:LEU:HD11	2.51	0.45
2:E:764:PHE:HD2	2:E:767:ILE:HD12	1.82	0.45
2:E:870:ARG:HH12	2:E:874:CYS:N	2.15	0.45
2:E:929:MET:HB2	2:E:964:MET:HE1	1.99	0.45
2:E:1117:GLU:CD	2:E:1120:LEU:HG	2.37	0.45
2:E:1412:THR:HB	2:E:1413:PRO:HD3	1.99	0.45
1:A:629:GLY:O	1:A:632:LYS:HG3	2.16	0.45
1:A:663:CYS:HB3	1:A:679:SER:HA	1.99	0.45
1:A:708:ASP:N	1:A:708:ASP:OD1	2.50	0.45
2:B:26:GLU:HG3	2:B:58:ILE:O	2.17	0.45
2:B:98:TRP:HZ3	2:B:159:LEU:HD12	1.82	0.45
2:B:166:ARG:HB2	2:B:174:ASP:H	1.82	0.45
2:B:294:VAL:N	2:B:330:THR:OG1	2.26	0.45
2:B:727:THR:O	2:B:774:TYR:HB2	2.17	0.45
2:B:789:ASN:HA	2:B:792:ARG:HD2	1.98	0.45
2:B:1033:MET:N	2:B:1035:GLN:HE21	2.14	0.45
2:B:1043:TRP:CE3	2:B:1043:TRP:N	2.83	0.45
2:B:1058:SER:HA	2:B:1080:ARG:NH1	2.32	0.45
2:B:1122:LYS:HD2	2:B:1171:LEU:HD11	1.99	0.45
2:B:1417:ASP:N	2:B:1417:ASP:OD1	2.50	0.45
2:B:1469:ARG:NH1	2:B:1473:LYS:HG3	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:149:ILE:HG23	3:C:151:ALA:H	1.82	0.45
2:E:877:VAL:O	2:E:880:PRO:HD2	2.17	0.45
2:E:1058:SER:HA	2:E:1080:ARG:NH1	2.32	0.45
2:E:1087:ILE:HA	2:E:1090:MET:HG2	1.99	0.45
3:F:149:ILE:HG23	3:F:151:ALA:H	1.82	0.45
2:B:146:LYS:HE2	2:B:146:LYS:HB2	1.78	0.44
2:B:854:ARG:HA	2:B:854:ARG:HD2	1.72	0.44
1:D:640:LEU:O	1:D:655:ILE:HA	2.16	0.44
2:E:37:ILE:HD13	2:E:45:TYR:CB	2.48	0.44
2:E:87:LEU:O	2:E:90:GLU:HG3	2.17	0.44
2:E:332:ILE:HD13	2:E:403:LEU:HD12	1.99	0.44
2:E:1391:ARG:CD	2:E:1429:PHE:HA	2.47	0.44
2:B:772:VAL:O	2:B:776:ARG:HG2	2.16	0.44
2:B:870:ARG:NH1	2:B:874:CYS:SG	2.91	0.44
2:B:1206:ASP:O	2:B:1210:ILE:HG12	2.17	0.44
2:B:1473:LYS:HD3	2:B:1481:THR:HG21	1.99	0.44
2:B:1617:PRO:O	2:B:1620:GLU:HG3	2.18	0.44
1:D:557:VAL:O	1:D:578:ARG:HG3	2.16	0.44
1:D:708:ASP:OD1	1:D:708:ASP:N	2.50	0.44
1:D:721:ASP:OD1	1:D:721:ASP:N	2.50	0.44
2:E:1022:ASN:HB3	2:E:1086:ARG:HH12	1.83	0.44
2:E:1054:LEU:HD11	2:E:1080:ARG:HB3	1.99	0.44
3:F:110:ILE:O	3:F:152:VAL:HG12	2.17	0.44
1:A:549:LYS:HE3	1:A:677:MET:HG2	2.00	0.44
2:B:204:ILE:CG1	2:B:211:ARG:HB3	2.46	0.44
2:B:870:ARG:HH12	2:B:874:CYS:N	2.15	0.44
2:B:875:ARG:HG2	2:B:924:HIS:CE1	2.52	0.44
2:B:923:VAL:O	2:B:926:GLN:HB2	2.17	0.44
2:B:1371:GLY:C	2:B:1424:GLN:HE21	2.20	0.44
2:B:1372:PHE:N	2:B:1424:GLN:HG2	2.33	0.44
2:B:1391:ARG:CD	2:B:1429:PHE:HA	2.47	0.44
3:C:72:TYR:HB3	3:C:105:CYS:SG	2.58	0.44
3:C:85:VAL:O	3:C:129:LEU:HD21	2.17	0.44
2:E:10:GLN:NE2	2:E:37:ILE:O	2.34	0.44
2:E:25:VAL:HB	2:E:56:LYS:O	2.18	0.44
2:E:204:ILE:CG1	2:E:211:ARG:HB3	2.46	0.44
2:E:761:LYS:HE2	2:E:765:ARG:NE	2.32	0.44
2:E:795:PHE:CE2	2:E:839:LEU:HD13	2.52	0.44
2:E:854:ARG:HA	2:E:854:ARG:HD2	1.72	0.44
2:E:857:LEU:HD13	2:E:905:LEU:HD11	2.00	0.44
2:E:870:ARG:NH1	2:E:874:CYS:SG	2.91	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:875:ARG:HG2	2:E:924:HIS:CE1	2.52	0.44
2:E:1125:ILE:HD12	2:E:1125:ILE:H	1.82	0.44
2:E:1129:PHE:HE1	2:E:1180:CYS:HG	1.66	0.44
2:E:1259:GLU:HG3	2:E:1497:GLY:O	2.17	0.44
2:B:140:GLU:O	2:B:144:LEU:HD23	2.17	0.44
2:B:652:HIS:CD2	2:B:656:LYS:HD3	2.53	0.44
2:B:761:LYS:HE2	2:B:765:ARG:NE	2.32	0.44
2:B:764:PHE:HD2	2:B:767:ILE:HD12	1.82	0.44
2:B:1236:ARG:HD3	2:B:1236:ARG:HA	1.80	0.44
2:E:142:ALA:O	2:E:146:LYS:HG3	2.16	0.44
2:E:306:MET:HA	2:E:306:MET:HE3	1.99	0.44
2:E:642:ASN:HA	2:E:644:ARG:NH1	2.32	0.44
2:E:775:LEU:CD2	2:E:781:SER:HB2	2.48	0.44
2:E:1469:ARG:NH1	2:E:1473:LYS:HG3	2.32	0.44
3:F:49:LYS:HZ2	3:F:51:VAL:HG12	1.82	0.44
2:B:87:LEU:O	2:B:90:GLU:HG3	2.17	0.44
2:B:166:ARG:HA	2:B:166:ARG:HD2	1.80	0.44
2:B:179:SER:OG	2:B:182:ALA:HB3	2.16	0.44
2:B:877:VAL:O	2:B:880:PRO:HD2	2.17	0.44
2:B:1125:ILE:HD12	2:B:1125:ILE:H	1.82	0.44
2:B:1582:ASP:HA	2:B:1585:LYS:HZ3	1.82	0.44
2:E:184:PHE:O	2:E:188:GLU:OE1	2.35	0.44
2:E:697:LEU:O	2:E:701:ILE:HG12	2.17	0.44
2:E:1320:LEU:HA	2:E:1323:GLU:OE1	2.17	0.44
2:E:1360:PRO:HG2	2:E:1362:TYR:HE1	1.83	0.44
2:E:1535:GLN:OE1	2:E:1542:LEU:HD11	2.18	0.44
3:F:72:TYR:HB3	3:F:105:CYS:SG	2.58	0.44
1:A:721:ASP:N	1:A:721:ASP:OD1	2.50	0.44
2:B:120:MET:SD	2:B:151:LYS:HE3	2.58	0.44
2:B:519:ILE:HG22	2:B:630:LYS:HE3	2.00	0.44
2:B:642:ASN:HA	2:B:644:ARG:NH1	2.32	0.44
2:B:775:LEU:CD2	2:B:781:SER:HB2	2.48	0.44
2:B:821:PRO:O	2:B:824:ILE:HG12	2.18	0.44
2:B:1114:LEU:HB3	2:B:1163:ARG:HG2	2.00	0.44
2:B:1412:THR:HB	2:B:1413:PRO:HD3	2.00	0.44
3:C:90:PHE:HA	3:C:93:VAL:HG12	2.00	0.44
3:C:110:ILE:O	3:C:152:VAL:HG12	2.17	0.44
2:E:581:ASP:HB3	2:E:584:PHE:HB3	2.00	0.44
2:E:589:PRO:HB2	2:E:595:MET:CE	2.48	0.44
2:E:738:ASN:HA	2:E:741:VAL:HG12	2.00	0.44
2:E:1032:PHE:O	2:E:1040:LEU:HD22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1328:TYR:O	2:E:1333:PHE:N	2.43	0.44
2:E:1372:PHE:N	2:E:1424:GLN:HG2	2.33	0.44
2:E:1490:THR:OG1	2:E:1506:GLN:HB3	2.18	0.44
2:E:1532:CYS:HA	2:E:1535:GLN:CG	2.48	0.44
2:E:1617:PRO:O	2:E:1620:GLU:HG3	2.18	0.44
3:F:63:ASP:OD1	3:F:64:TYR:N	2.51	0.44
1:A:627:GLU:HG2	1:A:631:LEU:HB2	2.00	0.44
2:B:102:TRP:CH2	2:B:118:GLN:HG2	2.52	0.44
2:B:102:TRP:HH2	2:B:118:GLN:HA	1.83	0.44
2:B:584:PHE:CE2	2:B:588:LEU:HD11	2.52	0.44
2:B:589:PRO:HB2	2:B:595:MET:CE	2.48	0.44
2:B:1232:LYS:HB2	2:B:1240:TYR:HE2	1.82	0.44
2:B:1268:ALA:HA	2:B:1271:LEU:HD13	1.98	0.44
2:B:1320:LEU:HA	2:B:1323:GLU:OE1	2.17	0.44
2:B:1535:GLN:OE1	2:B:1542:LEU:HD11	2.18	0.44
1:D:646:TYR:CE1	1:D:652:LEU:HG	2.52	0.44
1:D:678:MET:HA	1:D:683:ARG:HH12	1.83	0.44
2:E:319:ARG:HB2	2:E:499:VAL:HA	1.98	0.44
2:E:745:ASP:OD1	2:E:745:ASP:N	2.49	0.44
2:E:1024:PHE:O	2:E:1027:VAL:HG22	2.18	0.44
2:E:1232:LYS:HB2	2:E:1240:TYR:HE2	1.82	0.44
2:E:1599:LEU:HA	2:E:1602:GLU:OE1	2.18	0.44
2:B:129:SER:O	2:B:132:LEU:HB2	2.18	0.44
2:B:746:ASP:HB3	2:B:749:LYS:HB3	2.00	0.44
2:B:799:ASN:HA	2:B:802:MET:HG3	2.00	0.44
2:B:904:GLN:OE1	2:B:908:ASN:ND2	2.26	0.44
2:B:1087:ILE:HA	2:B:1090:MET:HG2	1.99	0.44
2:B:1175:LEU:HB3	2:B:1179:HIS:CE1	2.53	0.44
2:B:1532:CYS:HA	2:B:1535:GLN:HG3	1.99	0.44
2:E:1125:ILE:HG12	2:E:1172:LEU:HD22	2.00	0.44
2:E:1240:TYR:CE1	2:E:1244:LEU:HD11	2.53	0.44
2:E:1264:LEU:HD12	2:E:1264:LEU:HA	1.81	0.44
2:E:1463:ARG:HA	2:E:1488:THR:HA	1.98	0.44
2:E:1532:CYS:HA	2:E:1535:GLN:HG3	1.99	0.44
3:F:18:CYS:HG	3:F:32:TYR:HH	1.56	0.44
2:B:26:GLU:OE1	2:B:29:LEU:HD11	2.16	0.44
2:B:228:PHE:HA	2:B:401:VAL:HG12	2.00	0.44
2:B:306:MET:HE3	2:B:320:ARG:HD3	1.98	0.44
2:B:738:ASN:HA	2:B:741:VAL:HG12	2.00	0.44
2:B:1024:PHE:O	2:B:1027:VAL:HG22	2.18	0.44
2:B:1545:HIS:O	2:B:1549:MET:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:93:VAL:O	3:C:98:TYR:HB3	2.18	0.44
1:D:549:LYS:HE3	1:D:677:MET:HG2	2.00	0.44
2:E:26:GLU:HG3	2:E:58:ILE:O	2.17	0.44
2:E:98:TRP:HZ3	2:E:159:LEU:HD12	1.82	0.44
2:E:102:TRP:HH2	2:E:118:GLN:HA	1.83	0.44
2:E:152:ILE:O	2:E:156:ASN:ND2	2.51	0.44
2:E:166:ARG:HB2	2:E:174:ASP:HB2	1.99	0.44
2:E:738:ASN:ND2	2:E:793:GLN:HG3	2.33	0.44
2:E:799:ASN:HA	2:E:802:MET:HG3	2.00	0.44
2:E:923:VAL:O	2:E:926:GLN:HB2	2.17	0.44
2:E:1114:LEU:HB3	2:E:1163:ARG:HG2	2.00	0.44
2:E:1417:ASP:N	2:E:1417:ASP:OD1	2.50	0.44
2:E:1516:GLU:O	2:E:1520:GLU:OE1	2.36	0.44
2:B:123:SER:O	2:B:126:GLU:HG3	2.18	0.43
2:B:166:ARG:HB2	2:B:174:ASP:HB2	1.99	0.43
2:B:474:ASP:OD2	2:B:478:LYS:HE3	2.16	0.43
2:B:654:LEU:HB2	2:B:692:LEU:HD13	2.00	0.43
2:B:874:CYS:HA	2:B:877:VAL:HG22	2.00	0.43
2:B:932:LEU:CA	2:B:935:ARG:HE	2.28	0.43
2:B:991:ILE:HG13	2:B:992:MET:N	2.33	0.43
2:B:1155:LEU:HD21	2:B:1201:LEU:HD21	2.00	0.43
1:D:567:ALA:HB3	1:D:573:LYS:HD3	2.00	0.43
2:E:120:MET:SD	2:E:151:LYS:HE3	2.58	0.43
2:E:123:SER:O	2:E:126:GLU:HG3	2.18	0.43
2:E:331:ASP:HB3	2:E:336:LYS:HD2	2.00	0.43
2:E:556:ASN:HD22	2:E:560:THR:HG1	1.59	0.43
2:E:1097:HIS:HA	2:E:1100:LYS:NZ	2.33	0.43
2:E:1111:GLU:O	2:E:1163:ARG:NH1	2.42	0.43
2:E:1122:LYS:HD2	2:E:1171:LEU:HD11	2.00	0.43
2:E:1206:ASP:O	2:E:1210:ILE:HG12	2.17	0.43
2:E:1231:TYR:CZ	2:E:1239:ILE:HD12	2.53	0.43
2:E:1611:LEU:HD13	2:E:1619:HIS:HB2	1.99	0.43
1:A:678:MET:HA	1:A:683:ARG:HH12	1.83	0.43
2:B:439:PRO:HA	2:B:712:PHE:CE2	2.53	0.43
2:B:466:VAL:HG13	2:B:531:PHE:HB3	2.00	0.43
2:B:1022:ASN:HB3	2:B:1086:ARG:HH12	1.83	0.43
2:B:1432:LYS:HZ2	2:B:1465:SER:H	1.65	0.43
2:B:1523:GLU:O	2:B:1526:ASN:N	2.51	0.43
2:E:339:ASP:N	2:E:339:ASP:OD1	2.50	0.43
2:E:746:ASP:HB3	2:E:749:LYS:HB3	2.00	0.43
2:E:826:ASP:O	2:E:830:VAL:HG22	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:874:CYS:HA	2:E:877:VAL:HG22	2.00	0.43
2:E:1545:HIS:O	2:E:1549:MET:HG2	2.18	0.43
1:A:562:PHE:CD1	1:A:577:CYS:HB3	2.54	0.43
1:A:707:PRO:HD2	2:B:16:ILE:HG21	2.00	0.43
2:B:25:VAL:HB	2:B:56:LYS:O	2.18	0.43
2:B:248:PRO:HB3	2:B:387:ILE:HG21	2.01	0.43
2:B:302:ARG:HD3	2:B:322:PHE:CD1	2.52	0.43
2:B:826:ASP:O	2:B:830:VAL:HG22	2.19	0.43
2:B:857:LEU:HD13	2:B:905:LEU:HD11	2.00	0.43
2:B:979:ARG:NH1	2:B:1031:PHE:O	2.52	0.43
2:B:1063:THR:HA	2:B:1069:ARG:HD3	1.99	0.43
1:D:575:TRP:HB2	1:D:591:LEU:H	1.82	0.43
2:E:248:PRO:HB3	2:E:387:ILE:HG21	2.01	0.43
2:E:789:ASN:HA	2:E:792:ARG:HD2	1.98	0.43
2:E:991:ILE:HG13	2:E:992:MET:N	2.33	0.43
2:E:1512:ILE:HA	2:E:1516:GLU:OE1	2.18	0.43
2:E:1583:GLN:O	2:E:1586:VAL:HG12	2.19	0.43
2:B:451:ILE:HD11	2:B:623:ALA:HB2	2.00	0.43
2:B:738:ASN:ND2	2:B:793:GLN:HG3	2.33	0.43
2:B:745:ASP:OD1	2:B:745:ASP:N	2.49	0.43
2:B:1054:LEU:HD11	2:B:1080:ARG:HB3	1.99	0.43
2:B:1240:TYR:CE1	2:B:1244:LEU:HD11	2.53	0.43
2:B:1259:GLU:HG3	2:B:1497:GLY:O	2.17	0.43
2:B:1490:THR:OG1	2:B:1506:GLN:HB3	2.18	0.43
2:B:1532:CYS:HA	2:B:1535:GLN:CG	2.48	0.43
1:D:652:LEU:HB3	1:D:654:PHE:CZ	2.53	0.43
1:D:661:GLU:HA	1:D:664:ILE:HB	2.00	0.43
1:D:701:LEU:CD2	2:E:31:ILE:HG23	2.44	0.43
2:E:439:PRO:HA	2:E:712:PHE:CE2	2.53	0.43
2:E:716:LEU:O	2:E:720:ILE:HG13	2.19	0.43
2:E:1630:LYS:O	2:E:1633:VAL:HG22	2.18	0.43
1:A:532:PRO:O	1:A:536:LEU:HD13	2.17	0.43
1:A:575:TRP:HB2	1:A:591:LEU:H	1.82	0.43
2:B:163:LEU:HD11	2:B:194:ILE:HD11	2.01	0.43
3:C:63:ASP:OD1	3:C:64:TYR:N	2.51	0.43
1:D:562:PHE:CD1	1:D:577:CYS:HB3	2.54	0.43
2:E:140:GLU:O	2:E:144:LEU:HD23	2.18	0.43
2:E:228:PHE:HA	2:E:401:VAL:HG12	2.00	0.43
2:E:519:ILE:HG22	2:E:630:LYS:HE3	2.00	0.43
2:E:652:HIS:CD2	2:E:656:LYS:HD3	2.53	0.43
1:A:661:GLU:HA	1:A:664:ILE:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:9:ARG:HD2	2:B:68:GLU:HG2	2.01	0.43
2:B:1193:PHE:O	2:B:1197:VAL:HG23	2.18	0.43
2:B:1231:TYR:CE2	2:B:1243:TYR:CE1	3.06	0.43
2:B:1381:PHE:CZ	2:B:1503:GLU:HB3	2.53	0.43
2:B:1486:ARG:NE	2:B:1512:ILE:HD11	2.34	0.43
2:B:1512:ILE:HA	2:B:1516:GLU:OE1	2.18	0.43
1:D:678:MET:SD	1:D:678:MET:N	2.92	0.43
2:E:5:ILE:O	2:E:40:MET:HG2	2.19	0.43
2:E:294:VAL:N	2:E:330:THR:OG1	2.26	0.43
2:E:319:ARG:O	2:E:500:VAL:N	2.52	0.43
2:E:654:LEU:HB2	2:E:692:LEU:HD13	2.00	0.43
2:E:969:TYR:CD2	2:E:1023:GLN:HG3	2.54	0.43
2:E:1165:ASP:O	2:E:1168:TYR:HB3	2.19	0.43
2:E:1621:ARG:NH1	3:F:70:LEU:HD13	2.34	0.43
1:A:567:ALA:HB3	1:A:573:LYS:HD3	1.99	0.43
1:A:578:ARG:HB2	1:A:598:GLU:OE1	2.19	0.43
1:A:678:MET:N	1:A:678:MET:SD	2.92	0.43
2:B:127:TRP:HD1	2:B:130:GLN:NE2	2.17	0.43
2:B:152:ILE:O	2:B:156:ASN:ND2	2.51	0.43
2:B:319:ARG:O	2:B:500:VAL:N	2.52	0.43
1:D:578:ARG:HB2	1:D:598:GLU:OE1	2.19	0.43
1:D:627:GLU:HG2	1:D:631:LEU:HB2	2.00	0.43
1:A:552:ARG:HH12	1:A:664:ILE:HG12	1.84	0.43
2:B:331:ASP:HA	2:B:334:HIS:HB2	2.01	0.43
2:B:340:GLU:CD	2:B:420:LEU:HD21	2.39	0.43
2:B:394:HIS:HB2	2:B:397:GLN:O	2.19	0.43
2:B:985:PHE:HA	2:B:988:GLU:OE1	2.19	0.43
2:B:1118:VAL:O	2:B:1122:LYS:HG2	2.19	0.43
2:B:1231:TYR:CZ	2:B:1239:ILE:HD12	2.53	0.43
3:C:129:LEU:O	3:C:133:LYS:N	2.52	0.43
2:E:9:ARG:HD3	2:E:9:ARG:HA	1.70	0.43
2:E:145:LYS:O	2:E:149:THR:OG1	2.26	0.43
2:E:950:ILE:O	2:E:954:VAL:HG23	2.19	0.43
2:E:1175:LEU:HB3	2:E:1179:HIS:CE1	2.53	0.43
2:E:1438:PRO:HB2	2:E:1441:TYR:CD2	2.54	0.43
2:E:1566:TYR:OH	3:F:36:VAL:HG11	2.18	0.43
3:F:69:PRO:HA	3:F:72:TYR:CG	2.54	0.43
3:F:69:PRO:O	3:F:73:PRO:HD3	2.19	0.43
3:F:93:VAL:O	3:F:98:TYR:HB3	2.18	0.43
2:B:5:ILE:O	2:B:40:MET:HG2	2.19	0.43
2:B:59:PHE:CD2	2:B:64:ILE:HG12	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:102:TRP:CH2	2:B:118:GLN:HA	2.54	0.43
2:B:761:LYS:HE2	2:B:765:ARG:HE	1.83	0.43
2:B:1136:PHE:HB2	2:B:1186:LEU:HD23	2.00	0.43
2:B:1613:GLU:HA	2:B:1616:LYS:HD2	2.01	0.43
2:E:340:GLU:CD	2:E:420:LEU:HD21	2.39	0.43
2:E:591:THR:N	2:E:594:GLU:OE2	2.51	0.43
2:E:1381:PHE:CZ	2:E:1503:GLU:HB3	2.53	0.43
2:E:1516:GLU:O	2:E:1517:ASN:C	2.57	0.43
3:F:91:GLU:O	3:F:95:ALA:CB	2.66	0.43
2:B:86:PRO:HA	2:B:89:GLN:OE1	2.19	0.43
2:B:700:ILE:O	2:B:704:ILE:HG13	2.19	0.43
3:C:124:ASP:O	3:C:128:LYS:HD3	2.19	0.43
2:E:94:THR:HG22	2:E:98:TRP:CE2	2.54	0.43
2:E:111:LEU:HA	2:E:114:PHE:HB3	2.01	0.43
2:E:129:SER:O	2:E:132:LEU:HB2	2.18	0.43
2:E:728:LEU:HA	2:E:730:TYR:CE2	2.54	0.43
2:E:821:PRO:O	2:E:824:ILE:HG12	2.18	0.43
2:E:985:PHE:HA	2:E:988:GLU:OE1	2.19	0.43
2:E:1136:PHE:HB2	2:E:1186:LEU:HD23	2.00	0.43
2:E:1379:LYS:HA	2:E:1379:LYS:HD2	1.74	0.43
3:F:85:VAL:O	3:F:129:LEU:HD21	2.17	0.43
3:F:90:PHE:HA	3:F:93:VAL:HG12	2.00	0.43
1:A:689:LEU:HD22	2:B:102:TRP:HE1	1.84	0.42
2:B:91:LEU:HD11	2:B:128:ARG:HG3	2.00	0.42
2:B:250:GLN:HB3	2:B:252:THR:HG22	2.01	0.42
2:B:331:ASP:HB3	2:B:336:LYS:HD2	2.00	0.42
2:B:581:ASP:HB3	2:B:584:PHE:HB3	2.00	0.42
2:B:591:THR:N	2:B:594:GLU:OE2	2.51	0.42
2:B:1022:ASN:O	2:B:1026:GLU:OE1	2.37	0.42
2:B:1360:PRO:HG2	2:B:1362:TYR:HE1	1.83	0.42
2:B:1499:LEU:HD23	2:B:1499:LEU:HA	1.86	0.42
2:B:1516:GLU:O	2:B:1520:GLU:OE1	2.36	0.42
3:C:87:PRO:HG2	3:C:134:LEU:HD22	2.01	0.42
3:C:96:LYS:C	3:C:99:PRO:HD2	2.40	0.42
1:D:563:ARG:HB2	1:D:655:ILE:O	2.18	0.42
2:E:9:ARG:HD2	2:E:68:GLU:HG2	2.01	0.42
2:E:182:ALA:HA	2:E:185:LYS:HG2	2.01	0.42
2:E:451:ILE:HD11	2:E:623:ALA:HB2	2.00	0.42
2:E:1114:LEU:HD22	2:E:1168:TYR:OH	2.19	0.42
2:E:1193:PHE:O	2:E:1197:VAL:HG23	2.18	0.42
2:E:1523:GLU:O	2:E:1526:ASN:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:41:SER:OG	3:F:53:LEU:O	2.29	0.42
1:A:652:LEU:HB3	1:A:654:PHE:CZ	2.53	0.42
2:B:16:ILE:HD12	2:B:63:TYR:HA	2.00	0.42
2:B:37:ILE:HD13	2:B:45:TYR:CB	2.47	0.42
2:B:553:LYS:HE3	2:B:586:LEU:HD22	2.01	0.42
2:B:707:ILE:HD13	2:B:710:GLN:OE1	2.19	0.42
2:B:716:LEU:O	2:B:720:ILE:HG13	2.19	0.42
2:B:1114:LEU:HD22	2:B:1168:TYR:OH	2.19	0.42
2:B:1176:LEU:HD22	2:B:1194:ALA:HB2	2.00	0.42
2:B:1599:LEU:HA	2:B:1602:GLU:OE1	2.18	0.42
2:B:1605:ARG:O	2:B:1609:GLU:HG3	2.19	0.42
3:C:91:GLU:O	3:C:95:ALA:CB	2.66	0.42
2:E:102:TRP:CH2	2:E:118:GLN:HA	2.54	0.42
2:E:231:PHE:HD2	2:E:262:TRP:CG	2.37	0.42
2:E:331:ASP:HA	2:E:334:HIS:HB2	2.01	0.42
2:E:707:ILE:HD13	2:E:710:GLN:OE1	2.19	0.42
2:E:866:SER:C	2:E:868:LEU:H	2.21	0.42
2:E:1008:VAL:O	2:E:1012:THR:HG23	2.19	0.42
2:E:1063:THR:HA	2:E:1069:ARG:HD3	2.00	0.42
2:E:1155:LEU:HD21	2:E:1201:LEU:HD21	2.00	0.42
2:E:1406:GLU:C	2:E:1407:LYS:HD3	2.40	0.42
2:E:1486:ARG:NE	2:E:1512:ILE:HD11	2.34	0.42
2:E:1605:ARG:O	2:E:1609:GLU:HG3	2.19	0.42
2:B:182:ALA:HA	2:B:185:LYS:HG2	2.01	0.42
2:B:594:GLU:O	2:B:597:GLU:HG3	2.19	0.42
2:B:727:THR:O	2:B:730:TYR:HE2	2.03	0.42
2:E:98:TRP:CH2	2:E:155:GLY:HA3	2.55	0.42
2:E:700:ILE:O	2:E:704:ILE:HG13	2.19	0.42
2:E:1022:ASN:O	2:E:1026:GLU:OE1	2.37	0.42
2:E:1499:LEU:HD23	2:E:1499:LEU:HA	1.86	0.42
2:B:94:THR:HG22	2:B:98:TRP:CE2	2.54	0.42
2:B:111:LEU:HA	2:B:114:PHE:HB3	2.01	0.42
2:B:856:LYS:O	2:B:860:MET:HE3	2.20	0.42
2:B:889:GLN:O	2:B:895:ASN:ND2	2.52	0.42
2:B:1125:ILE:HG12	2:B:1172:LEU:HD22	2.00	0.42
3:C:69:PRO:HA	3:C:72:TYR:CG	2.54	0.42
2:E:86:PRO:HA	2:E:89:GLN:OE1	2.19	0.42
2:E:95:LEU:HA	2:E:98:TRP:HD1	1.84	0.42
2:E:144:LEU:O	2:E:148:VAL:HG22	2.20	0.42
2:E:1135:GLU:HG3	2:E:1144:PHE:HA	2.02	0.42
2:E:1613:GLU:HA	2:E:1616:LYS:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:42:ALA:O	3:F:53:LEU:HG	2.20	0.42
3:F:117:LEU:HD13	3:F:156:GLU:HB3	2.01	0.42
1:A:547:LEU:O	1:A:550:GLN:HG3	2.20	0.42
1:A:607:LYS:HE3	1:A:609:PRO:HA	2.00	0.42
2:B:95:LEU:HA	2:B:98:TRP:HD1	1.84	0.42
2:B:1166:GLU:O	2:B:1169:LYS:HG2	2.20	0.42
2:B:1318:ILE:HD13	2:B:1349:TYR:CZ	2.55	0.42
2:B:1516:GLU:O	2:B:1517:ASN:C	2.57	0.42
2:E:127:TRP:HD1	2:E:130:GLN:NE2	2.17	0.42
2:E:761:LYS:HE2	2:E:765:ARG:HE	1.83	0.42
2:E:1176:LEU:HD22	2:E:1194:ALA:HB2	2.00	0.42
3:F:2:GLN:HE22	3:F:4:ILE:HD11	1.84	0.42
3:F:124:ASP:O	3:F:128:LYS:HD3	2.19	0.42
3:F:129:LEU:O	3:F:133:LYS:N	2.52	0.42
2:B:88:VAL:O	2:B:92:THR:HG23	2.20	0.42
2:B:225:TYR:CE1	2:B:278:GLN:HB3	2.54	0.42
2:B:927:LEU:HB3	2:B:931:ARG:HH21	1.85	0.42
2:B:1630:LYS:O	2:B:1633:VAL:HG22	2.18	0.42
3:C:2:GLN:HE22	3:C:4:ILE:HD11	1.84	0.42
3:C:145:MET:O	3:C:148:GLU:HB3	2.20	0.42
3:C:163:ARG:C	3:C:165:LEU:H	2.22	0.42
1:D:563:ARG:NH2	1:D:573:LYS:HE2	2.35	0.42
2:E:551:PHE:CE2	2:E:586:LEU:HD23	2.55	0.42
2:E:979:ARG:NH1	2:E:1031:PHE:O	2.52	0.42
2:E:1166:GLU:O	2:E:1169:LYS:HG2	2.20	0.42
2:E:1488:THR:OG1	2:E:1508:SER:HB2	2.20	0.42
1:A:563:ARG:NH2	1:A:573:LYS:HE2	2.35	0.42
2:B:140:GLU:N	2:B:140:GLU:OE1	2.53	0.42
2:B:950:ILE:O	2:B:954:VAL:HG23	2.19	0.42
2:B:1086:ARG:HA	2:B:1089:ASP:OD2	2.19	0.42
2:B:1165:ASP:O	2:B:1168:TYR:HB3	2.19	0.42
2:B:1168:TYR:CZ	2:B:1172:LEU:HD21	2.55	0.42
2:B:1388:TYR:CE2	3:C:44:VAL:HG13	2.54	0.42
2:B:1438:PRO:HB2	2:B:1441:TYR:CD2	2.54	0.42
3:C:153:LYS:HD2	3:C:153:LYS:HA	1.85	0.42
1:A:563:ARG:HB2	1:A:655:ILE:O	2.19	0.42
2:B:95:LEU:HD23	2:B:98:TRP:CD1	2.45	0.42
2:B:143:GLU:O	2:B:147:LYS:HG2	2.20	0.42
2:B:189:VAL:HA	2:B:192:LYS:HE2	2.02	0.42
2:B:1568:LYS:HD2	2:B:1569:ALA:N	2.35	0.42
1:D:652:LEU:HD23	1:D:652:LEU:HA	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:88:VAL:O	2:E:92:THR:HG23	2.20	0.42
2:E:181:ILE:HG22	2:E:185:LYS:HZ1	1.83	0.42
2:E:466:VAL:HG13	2:E:531:PHE:HB3	2.00	0.42
2:E:1079:MET:O	2:E:1083:ILE:HG13	2.20	0.42
2:E:1168:TYR:CZ	2:E:1172:LEU:HD21	2.55	0.42
2:E:1318:ILE:HD13	2:E:1349:TYR:CZ	2.55	0.42
2:E:1548:SER:HB2	3:F:56:TRP:CH2	2.49	0.42
1:A:624:HIS:CD2	1:A:633:GLN:HG3	2.55	0.42
1:A:627:GLU:HG3	1:A:629:GLY:H	1.84	0.42
1:A:652:LEU:HD23	1:A:652:LEU:HA	1.87	0.42
2:B:113:LEU:HA	2:B:116:GLN:CD	2.41	0.42
2:B:231:PHE:HD2	2:B:262:TRP:CG	2.37	0.42
2:B:728:LEU:HA	2:B:730:TYR:CE2	2.54	0.42
2:B:866:SER:C	2:B:868:LEU:H	2.22	0.42
2:B:1379:LYS:HD2	2:B:1379:LYS:HA	1.74	0.42
3:C:42:ALA:O	3:C:53:LEU:HG	2.20	0.42
1:D:608:LEU:HD21	1:D:644:ILE:HG21	2.02	0.42
2:E:163:LEU:HD11	2:E:194:ILE:HD11	2.00	0.42
2:E:594:GLU:O	2:E:597:GLU:HG3	2.19	0.42
2:E:738:ASN:HD21	2:E:793:GLN:HG3	1.85	0.42
2:E:1059:LEU:HA	2:E:1062:GLU:OE1	2.19	0.42
2:E:1418:ILE:HG21	2:E:1425:TYR:CD2	2.55	0.42
2:E:1524:LEU:HD12	2:E:1528:ARG:HH12	1.85	0.42
2:B:98:TRP:CH2	2:B:155:GLY:HA3	2.55	0.42
2:B:105:LEU:HA	2:B:105:LEU:HD23	1.74	0.42
2:B:522:VAL:HA	2:B:525:CYS:HB2	2.02	0.42
2:B:806:LEU:HD12	2:B:813:LYS:CE	2.49	0.42
2:B:931:ARG:C	2:B:932:LEU:HD22	2.41	0.42
2:B:1269:GLU:OE1	2:B:1270:LEU:HD22	2.20	0.42
2:B:1443:ASP:OD1	2:B:1444:LYS:HD3	2.20	0.42
2:B:1583:GLN:O	2:B:1586:VAL:HG12	2.19	0.42
2:B:1596:GLN:O	2:B:1600:LEU:HG	2.20	0.42
1:D:607:LYS:HE3	1:D:609:PRO:HA	2.00	0.42
1:D:627:GLU:HG3	1:D:629:GLY:H	1.84	0.42
2:E:247:ASP:O	2:E:251:SER:N	2.53	0.42
2:E:1127:ILE:HA	2:E:1130:ASP:OD2	2.20	0.42
3:F:96:LYS:C	3:F:99:PRO:HD2	2.40	0.42
1:A:661:GLU:HA	1:A:664:ILE:HD12	2.01	0.41
2:B:1418:ILE:HG21	2:B:1425:TYR:CD2	2.55	0.41
2:B:1611:LEU:HD11	2:B:1616:LYS:HA	2.02	0.41
3:C:82:PHE:CZ	3:C:114:GLY:HA2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:552:ARG:HH12	1:D:664:ILE:HG12	1.84	0.41
1:D:624:HIS:CD2	1:D:633:GLN:HG3	2.55	0.41
2:E:250:GLN:HB3	2:E:252:THR:HG22	2.01	0.41
2:E:806:LEU:HD12	2:E:813:LYS:CE	2.49	0.41
3:F:82:PHE:CZ	3:F:114:GLY:HA2	2.55	0.41
3:F:87:PRO:HG2	3:F:134:LEU:HD22	2.01	0.41
1:A:715:LYS:HA	1:A:715:LYS:HD3	1.87	0.41
2:B:247:ASP:O	2:B:251:SER:N	2.53	0.41
2:B:435:GLU:O	2:B:708:LYS:HD3	2.20	0.41
2:B:593:MET:O	2:B:596:GLU:HG2	2.20	0.41
2:B:921:THR:O	2:B:925:ILE:N	2.41	0.41
2:B:969:TYR:CD2	2:B:1023:GLN:HG3	2.54	0.41
2:B:1008:VAL:O	2:B:1012:THR:HG23	2.19	0.41
2:B:1097:HIS:HA	2:B:1100:LYS:NZ	2.34	0.41
2:B:1127:ILE:HA	2:B:1130:ASP:OD2	2.20	0.41
2:B:1135:GLU:HG3	2:B:1144:PHE:HA	2.02	0.41
2:B:1432:LYS:HB2	2:B:1463:ARG:HG3	2.02	0.41
3:C:69:PRO:O	3:C:73:PRO:HD3	2.19	0.41
3:C:92:ASN:O	3:C:96:LYS:N	2.40	0.41
3:C:117:LEU:HD13	3:C:156:GLU:HB3	2.01	0.41
2:E:149:THR:HA	2:E:152:ILE:HG12	2.03	0.41
2:E:258:TYR:HE1	2:E:489:GLY:HA3	1.85	0.41
2:E:394:HIS:HB2	2:E:397:GLN:O	2.19	0.41
2:E:879:LEU:O	2:E:882:LEU:HB2	2.20	0.41
2:E:1431:VAL:HG12	2:E:1464:TYR:HB2	2.03	0.41
3:F:163:ARG:C	3:F:165:LEU:H	2.23	0.41
1:A:578:ARG:NH1	1:A:600:PRO:HA	2.35	0.41
2:B:144:LEU:O	2:B:148:VAL:HG22	2.20	0.41
2:B:224:LEU:HD13	2:B:333:ILE:HG12	2.02	0.41
2:B:1406:GLU:C	2:B:1407:LYS:HD3	2.40	0.41
2:B:1628:GLU:HG2	2:B:1629:LEU:HD22	2.02	0.41
2:E:91:LEU:HD11	2:E:128:ARG:HG3	2.01	0.41
2:E:889:GLN:O	2:E:895:ASN:ND2	2.52	0.41
2:E:927:LEU:HB3	2:E:931:ARG:HH21	1.85	0.41
2:E:931:ARG:C	2:E:932:LEU:HD22	2.41	0.41
2:E:1043:TRP:CE3	2:E:1043:TRP:N	2.83	0.41
2:E:1095:GLY:N	2:E:1098:LYS:HE3	2.35	0.41
2:E:1568:LYS:HD2	2:E:1569:ALA:N	2.35	0.41
2:B:9:ARG:HA	2:B:9:ARG:HD3	1.70	0.41
2:B:287:MET:N	2:B:435:GLU:OE2	2.43	0.41
2:B:757:LEU:HA	2:B:760:LEU:HG	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:892:ASP:OD1	2:B:892:ASP:N	2.52	0.41
2:B:1059:LEU:HA	2:B:1062:GLU:OE1	2.19	0.41
2:B:1274:SER:O	2:B:1294:GLN:HG3	2.21	0.41
2:B:1381:PHE:HA	2:B:1503:GLU:HA	2.02	0.41
2:B:1524:LEU:HD12	2:B:1525:THR:N	2.36	0.41
3:C:80:ILE:O	3:C:113:VAL:HG22	2.21	0.41
1:D:661:GLU:HA	1:D:664:ILE:HD12	2.01	0.41
2:E:140:GLU:N	2:E:140:GLU:OE1	2.53	0.41
2:E:740:TYR:HD1	2:E:749:LYS:HG3	1.86	0.41
2:E:757:LEU:HA	2:E:760:LEU:HG	2.01	0.41
2:E:802:MET:HE1	2:E:846:SER:C	2.40	0.41
2:E:1095:GLY:HA3	2:E:1096:PRO:HD3	1.91	0.41
2:E:1118:VAL:O	2:E:1122:LYS:HG2	2.19	0.41
2:E:1381:PHE:HA	2:E:1503:GLU:HA	2.02	0.41
2:E:1443:ASP:OD1	2:E:1444:LYS:HD3	2.20	0.41
3:F:10:GLY:O	3:F:60:GLY:HA3	2.21	0.41
3:F:39:ASN:HA	3:F:57:ASP:H	1.86	0.41
1:A:564:LYS:HZ1	1:A:590:ASP:HA	1.86	0.41
1:A:711:PRO:HG2	2:B:16:ILE:HD12	2.03	0.41
2:B:551:PHE:CE2	2:B:586:LEU:HD23	2.55	0.41
2:B:1079:MET:O	2:B:1083:ILE:HG13	2.20	0.41
2:B:1343:LYS:HE3	2:B:1343:LYS:HB2	1.81	0.41
2:B:1488:THR:OG1	2:B:1508:SER:HB2	2.20	0.41
3:C:10:GLY:O	3:C:60:GLY:HA3	2.21	0.41
1:D:564:LYS:O	1:D:573:LYS:NZ	2.32	0.41
2:E:16:ILE:HD12	2:E:63:TYR:HA	2.00	0.41
2:E:904:GLN:OE1	2:E:908:ASN:ND2	2.26	0.41
2:E:1236:ARG:HD3	2:E:1236:ARG:HA	1.80	0.41
1:A:608:LEU:HD21	1:A:644:ILE:HG21	2.02	0.41
2:B:124:LEU:HD21	2:B:151:LYS:HB2	2.02	0.41
1:D:685:ASP:HA	1:D:688:THR:HG22	2.02	0.41
2:E:113:LEU:HA	2:E:116:GLN:CD	2.40	0.41
2:E:124:LEU:HD21	2:E:151:LYS:HB2	2.02	0.41
2:E:166:ARG:HH21	2:E:169:ASN:HD21	1.69	0.41
2:E:472:VAL:O	2:E:479:LEU:HD12	2.21	0.41
2:E:727:THR:O	2:E:730:TYR:HE2	2.03	0.41
2:E:1086:ARG:HA	2:E:1089:ASP:OD2	2.19	0.41
3:F:80:ILE:O	3:F:113:VAL:HG22	2.21	0.41
2:B:94:THR:O	2:B:97:GLU:HG3	2.21	0.41
2:B:166:ARG:HH21	2:B:169:ASN:HD21	1.69	0.41
2:B:868:LEU:O	2:B:871:GLN:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:965:ASP:O	2:B:968:HIS:HB2	2.21	0.41
2:B:1354:LYS:HE3	2:B:1354:LYS:HB3	1.87	0.41
3:C:39:ASN:HA	3:C:57:ASP:H	1.85	0.41
1:D:578:ARG:NH1	1:D:600:PRO:HA	2.35	0.41
2:E:718:THR:HG22	2:E:723:HIS:HE1	1.86	0.41
2:E:868:LEU:O	2:E:871:GLN:HG3	2.21	0.41
2:E:1276:LYS:HD2	2:E:1277:PRO:HD2	2.03	0.41
3:F:21:ILE:O	3:F:25:THR:OG1	2.32	0.41
3:F:145:MET:O	3:F:148:GLU:HB3	2.20	0.41
1:A:608:LEU:HD23	1:A:609:PRO:CD	2.51	0.41
2:B:1126:PRO:HD3	2:B:1175:LEU:HD13	2.03	0.41
2:B:1328:TYR:O	2:B:1333:PHE:N	2.43	0.41
2:B:1431:VAL:HG12	2:B:1464:TYR:HB2	2.02	0.41
2:B:1536:HIS:NE2	2:B:1542:LEU:HB3	2.36	0.41
2:E:113:LEU:O	2:E:116:GLN:HG2	2.20	0.41
2:E:143:GLU:O	2:E:147:LYS:HG2	2.20	0.41
2:E:220:HIS:O	2:E:285:SER:HA	2.21	0.41
2:E:258:TYR:CE1	2:E:489:GLY:HA3	2.56	0.41
2:E:522:VAL:HA	2:E:525:CYS:HB2	2.02	0.41
2:E:593:MET:O	2:E:596:GLU:HG2	2.20	0.41
1:A:560:THR:O	1:A:576:TYR:HA	2.21	0.41
1:A:685:ASP:HA	1:A:688:THR:HG22	2.02	0.41
2:B:113:LEU:O	2:B:116:GLN:HG2	2.20	0.41
2:B:149:THR:HA	2:B:152:ILE:HG12	2.03	0.41
2:B:258:TYR:HE1	2:B:489:GLY:HA3	1.85	0.41
2:B:472:VAL:O	2:B:479:LEU:HD12	2.21	0.41
2:B:738:ASN:HD21	2:B:793:GLN:HG3	1.85	0.41
2:B:802:MET:HE1	2:B:846:SER:C	2.40	0.41
2:B:1095:GLY:N	2:B:1098:LYS:HE3	2.35	0.41
2:B:1320:LEU:HA	2:B:1320:LEU:HD23	1.85	0.41
2:B:1384:ARG:HD2	2:B:1495:PHE:HB3	2.03	0.41
2:B:1432:LYS:HE2	2:B:1463:ARG:O	2.21	0.41
2:B:1437:LEU:HD21	2:B:1442:LYS:NZ	2.36	0.41
2:B:1464:TYR:O	2:B:1486:ARG:HA	2.21	0.41
2:B:1519:ILE:O	2:B:1523:GLU:HG3	2.21	0.41
2:B:1524:LEU:HD12	2:B:1528:ARG:HH12	1.85	0.41
2:B:1536:HIS:ND1	2:B:1542:LEU:HD22	2.36	0.41
2:B:1563:PHE:O	2:B:1567:GLU:HG2	2.21	0.41
1:D:547:LEU:O	1:D:550:GLN:HG3	2.20	0.41
2:E:70:THR:H	2:E:76:GLN:NE2	2.19	0.41
2:E:189:VAL:HA	2:E:192:LYS:HE2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:225:TYR:CE1	2:E:278:GLN:HB3	2.54	0.41
2:E:905:LEU:O	2:E:909:ILE:HG12	2.21	0.41
2:E:954:VAL:O	2:E:958:ILE:HG12	2.21	0.41
2:E:1260:ALA:O	2:E:1263:THR:OG1	2.35	0.41
2:E:1269:GLU:OE1	2:E:1270:LEU:HD22	2.20	0.41
2:E:1432:LYS:HE2	2:E:1463:ARG:O	2.21	0.41
2:E:1432:LYS:HB2	2:E:1463:ARG:HG3	2.02	0.41
2:E:1433:PRO:HA	2:E:1462:PHE:CD2	2.56	0.41
2:E:1464:TYR:O	2:E:1486:ARG:HA	2.21	0.41
2:E:1524:LEU:HD12	2:E:1525:THR:N	2.36	0.41
2:E:1563:PHE:O	2:E:1567:GLU:HG2	2.21	0.41
2:E:1611:LEU:HD11	2:E:1616:LYS:HA	2.02	0.41
2:E:1628:GLU:HG2	2:E:1629:LEU:HD22	2.02	0.41
3:F:8:VAL:HG13	3:F:81:CYS:SG	2.61	0.41
1:A:579:LEU:HD12	1:A:585:VAL:O	2.21	0.41
1:A:679:SER:HB2	1:A:682:THR:OG1	2.21	0.41
2:B:83:GLY:O	2:B:145:LYS:NZ	2.54	0.41
2:B:220:HIS:NE2	2:B:436:ILE:HB	2.36	0.41
2:B:258:TYR:CE1	2:B:489:GLY:HA3	2.56	0.41
2:B:966:ASP:HA	2:B:969:TYR:CD2	2.48	0.41
2:B:1477:ASN:HB3	2:B:1568:LYS:HZ1	1.85	0.41
2:E:105:LEU:HD22	2:E:110:LYS:HB2	2.03	0.41
2:E:146:LYS:HB2	2:E:146:LYS:HE2	1.78	0.41
2:E:228:PHE:HZ	2:E:231:PHE:HB2	1.86	0.41
2:E:435:GLU:O	2:E:708:LYS:HD3	2.20	0.41
2:E:638:LEU:O	2:E:642:ASN:N	2.54	0.41
2:E:721:TYR:HB2	2:E:722:LYS:NZ	2.36	0.41
2:E:1018:LEU:HD23	2:E:1018:LEU:HA	1.89	0.41
2:E:1026:GLU:O	2:E:1029:THR:OG1	2.33	0.41
2:E:1276:LYS:HD2	2:E:1276:LYS:HA	1.81	0.41
2:E:1287:SER:HG	2:E:1289:TYR:HE1	1.69	0.41
2:E:1437:LEU:HD21	2:E:1442:LYS:HD2	2.02	0.41
2:E:1551:LEU:HD23	2:E:1551:LEU:HA	1.86	0.41
2:E:1596:GLN:O	2:E:1600:LEU:HG	2.20	0.41
2:E:1621:ARG:CD	3:F:67:LEU:HD22	2.50	0.41
2:B:224:LEU:HD23	2:B:281:PHE:CD2	2.56	0.40
2:B:638:LEU:O	2:B:642:ASN:N	2.54	0.40
2:B:905:LEU:O	2:B:909:ILE:HG12	2.21	0.40
2:B:931:ARG:O	2:B:932:LEU:HD22	2.21	0.40
2:B:1386:LYS:CB	2:B:1389:GLU:HG3	2.51	0.40
2:E:80:VAL:H	2:E:85:LEU:HD11	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:166:ARG:HA	2:E:166:ARG:HD2	1.80	0.40
2:E:220:HIS:NE2	2:E:436:ILE:HB	2.36	0.40
2:E:224:LEU:HD23	2:E:281:PHE:CD2	2.56	0.40
2:E:634:ASN:O	2:E:638:LEU:HD23	2.21	0.40
2:E:686:SER:HG	2:E:689:TYR:HD2	1.69	0.40
2:E:931:ARG:O	2:E:932:LEU:HD22	2.21	0.40
2:E:1274:SER:O	2:E:1294:GLN:HG3	2.21	0.40
2:E:1386:LYS:CB	2:E:1389:GLU:HG3	2.51	0.40
2:E:1437:LEU:HD21	2:E:1442:LYS:NZ	2.36	0.40
2:B:1122:LYS:HB3	2:B:1122:LYS:HE2	1.88	0.40
2:B:1437:LEU:HD21	2:B:1442:LYS:HD2	2.02	0.40
2:B:1593:ILE:O	2:B:1596:GLN:HB3	2.22	0.40
2:E:1143:ASN:HD21	2:E:1145:HIS:CE1	2.40	0.40
2:E:1384:ARG:HD2	2:E:1495:PHE:HB3	2.03	0.40
3:F:66:ARG:HG2	3:F:67:LEU:N	2.36	0.40
3:F:153:LYS:HA	3:F:153:LYS:HD2	1.85	0.40
2:B:116:GLN:O	2:B:120:MET:HG2	2.21	0.40
2:B:166:ARG:HH21	2:B:169:ASN:ND2	2.19	0.40
2:B:701:ILE:HD12	2:B:716:LEU:HD21	2.03	0.40
2:B:879:LEU:O	2:B:882:LEU:HB2	2.20	0.40
2:B:924:HIS:HD1	2:B:928:ILE:HD11	1.87	0.40
3:C:113:VAL:HA	3:C:155:LEU:O	2.22	0.40
1:D:541:GLN:N	1:D:542:PRO:HD3	2.36	0.40
2:E:94:THR:O	2:E:97:GLU:HG3	2.21	0.40
2:E:116:GLN:O	2:E:120:MET:HG2	2.21	0.40
2:E:222:TYR:CE2	2:E:289:LEU:HD11	2.57	0.40
2:E:553:LYS:HE3	2:E:586:LEU:HD22	2.01	0.40
2:E:701:ILE:HD12	2:E:716:LEU:HD21	2.03	0.40
2:E:965:ASP:O	2:E:968:HIS:HB2	2.21	0.40
2:E:1486:ARG:HB2	2:E:1510:GLU:HB2	2.04	0.40
2:E:1519:ILE:O	2:E:1523:GLU:HG3	2.21	0.40
2:E:1536:HIS:NE2	2:E:1542:LEU:HB3	2.36	0.40
2:E:1593:ILE:O	2:E:1596:GLN:HB3	2.22	0.40
2:B:10:GLN:CG	2:B:37:ILE:HB	2.52	0.40
2:B:220:HIS:O	2:B:285:SER:HA	2.21	0.40
2:B:256:GLU:OE1	2:B:429:ARG:N	2.47	0.40
2:B:718:THR:HG22	2:B:723:HIS:HE1	1.86	0.40
2:B:1276:LYS:HD2	2:B:1277:PRO:HD2	2.03	0.40
2:B:1483:TRP:CE2	2:B:1514:PRO:HD3	2.56	0.40
3:C:120:ARG:NH2	3:C:139:TYR:H	2.20	0.40
1:D:560:THR:O	1:D:576:TYR:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:698:LEU:HA	2:E:31:ILE:CG2	2.52	0.40
1:D:715:LYS:HA	1:D:715:LYS:HD3	1.87	0.40
2:E:292:PRO:O	2:E:330:THR:HG21	2.21	0.40
2:E:997:ILE:HG21	2:E:1053:PHE:HA	2.04	0.40
2:E:1113:THR:HG21	2:E:1128:PHE:HE2	1.87	0.40
2:E:1126:PRO:HD3	2:E:1175:LEU:HD13	2.03	0.40
2:E:1353:ILE:HD12	2:E:1353:ILE:HA	1.87	0.40
2:E:1466:ARG:H	2:E:1484:ILE:HG23	1.86	0.40
3:F:93:VAL:HG13	3:F:94:ARG:N	2.37	0.40
2:B:80:VAL:H	2:B:85:LEU:HD11	1.86	0.40
2:B:523:THR:HG1	2:B:524:ARG:NH1	2.18	0.40
2:B:740:TYR:HD1	2:B:749:LYS:HG3	1.86	0.40
2:B:954:VAL:O	2:B:958:ILE:HG12	2.21	0.40
2:B:990:PHE:HD2	2:B:1042:LEU:HD11	1.84	0.40
2:B:1433:PRO:HA	2:B:1462:PHE:CD2	2.56	0.40
3:C:93:VAL:HG13	3:C:94:ARG:N	2.37	0.40
2:E:14:VAL:O	2:E:64:ILE:HA	2.22	0.40
2:E:83:GLY:O	2:E:145:LYS:NZ	2.54	0.40
2:E:224:LEU:HD13	2:E:333:ILE:HG12	2.02	0.40
2:E:712:PHE:O	2:E:716:LEU:N	2.52	0.40
2:E:821:PRO:HA	2:E:824:ILE:HG23	2.04	0.40
2:E:870:ARG:NH1	2:E:873:GLU:HB3	2.37	0.40
2:E:958:ILE:HB	2:E:1016:VAL:HG21	2.03	0.40
2:E:999:LYS:HE2	2:E:999:LYS:HB3	1.90	0.40
3:F:21:ILE:HD12	3:F:40:TYR:CZ	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	196/733 (27%)	179 (91%)	17 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	196/733 (27%)	179 (91%)	17 (9%)	0	100	100
2	B	1640/1648 (100%)	1512 (92%)	128 (8%)	0	100	100
2	E	1640/1648 (100%)	1512 (92%)	128 (8%)	0	100	100
3	C	175/184 (95%)	164 (94%)	11 (6%)	0	100	100
3	F	175/184 (95%)	165 (94%)	10 (6%)	0	100	100
All	All	4022/5130 (78%)	3711 (92%)	311 (8%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	183/664 (28%)	183 (100%)	0	100	100
1	D	183/664 (28%)	183 (100%)	0	100	100
2	B	1495/1497 (100%)	1489 (100%)	6 (0%)	91	94
2	E	1495/1497 (100%)	1489 (100%)	6 (0%)	91	94
3	C	153/157 (98%)	150 (98%)	3 (2%)	55	73
3	F	153/157 (98%)	150 (98%)	3 (2%)	55	73
All	All	3662/4636 (79%)	3644 (100%)	18 (0%)	89	93

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	128	ARG
2	B	644	ARG
2	B	935	ARG
2	B	945	ARG
2	B	1069	ARG
2	B	1568	LYS
3	C	43	ASN
3	C	66	ARG

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Mol	Chain	Res	Type
3	C	123	LYS
2	E	128	ARG
2	E	644	ARG
2	E	935	ARG
2	E	945	ARG
2	E	1069	ARG
2	E	1568	LYS
3	F	43	ASN
3	F	66	ARG
3	F	123	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	550	GLN
1	A	554	ASN
1	A	596	GLN
2	B	65	HIS
2	B	130	GLN
2	B	156	ASN
2	B	556	ASN
2	B	653	ASN
2	B	885	GLN
2	B	926	GLN
2	B	968	HIS
2	B	1035	GLN
2	B	1203	ASN
2	B	1401	GLN
2	B	1619	HIS
3	C	2	GLN
1	D	550	GLN
1	D	554	ASN
1	D	596	GLN
2	E	65	HIS
2	E	130	GLN
2	E	156	ASN
2	E	556	ASN
2	E	653	ASN
2	E	885	GLN
2	E	926	GLN
2	E	968	HIS
2	E	1035	GLN

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Mol	Chain	Res	Type
2	E	1203	ASN
2	E	1401	GLN
2	E	1619	HIS
3	F	2	GLN
3	F	39	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

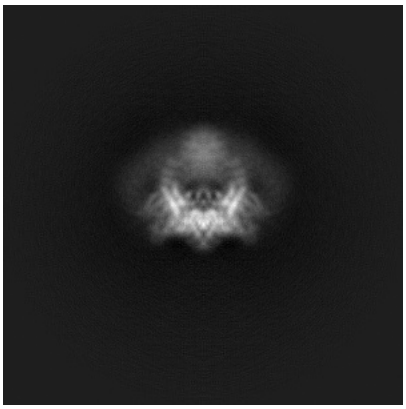
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-60148. These allow visual inspection of the internal detail of the map and identification of artifacts.

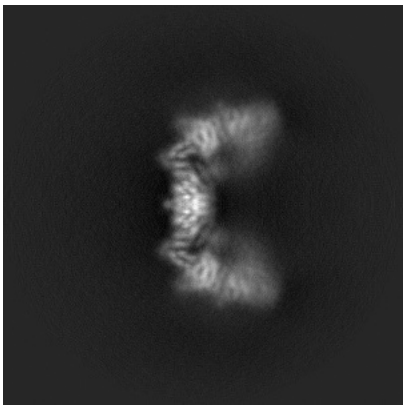
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

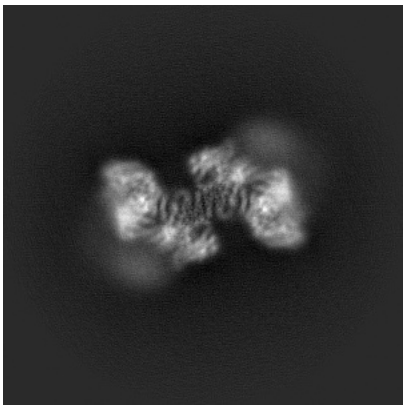
6.1.1 Primary map



X

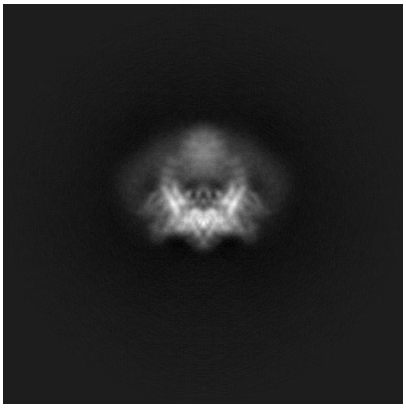


Y

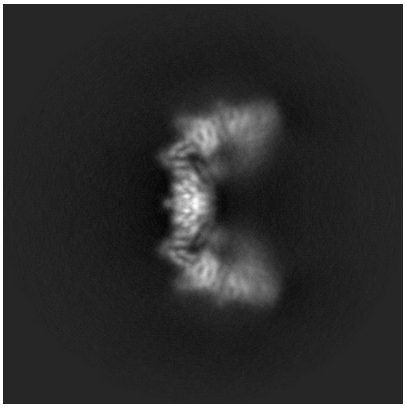


Z

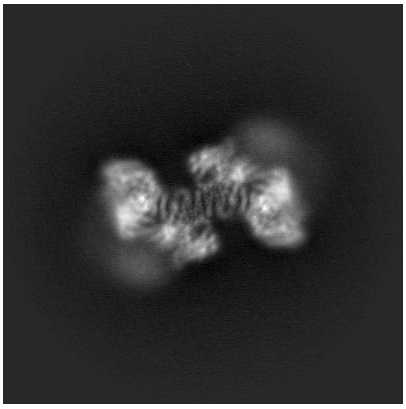
6.1.2 Raw map



X



Y

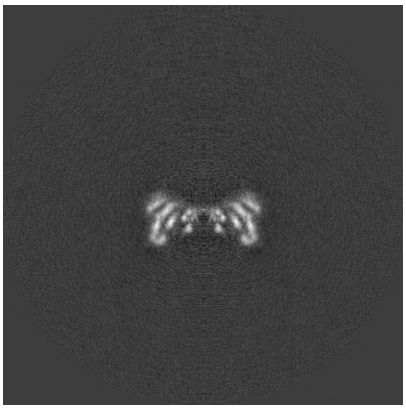


Z

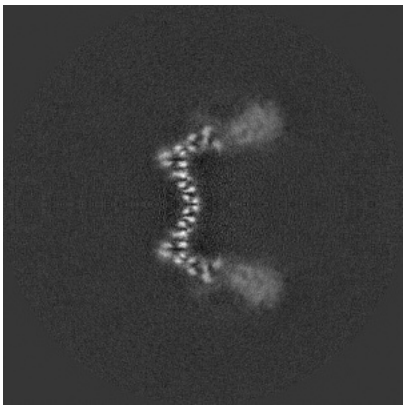
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

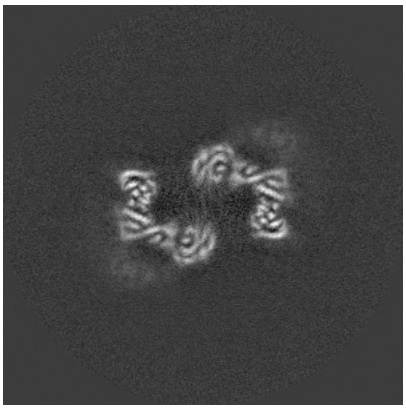
6.2.1 Primary map



X Index: 170

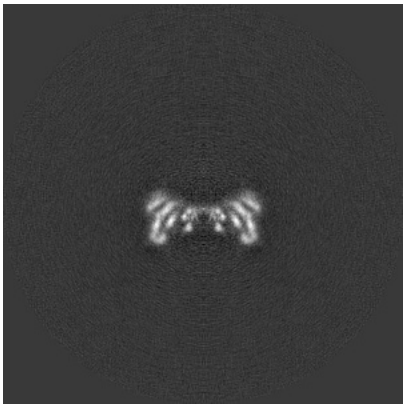


Y Index: 170

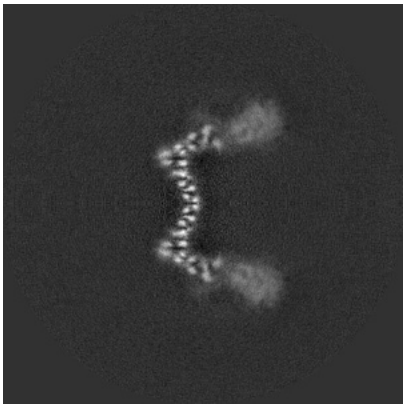


Z Index: 170

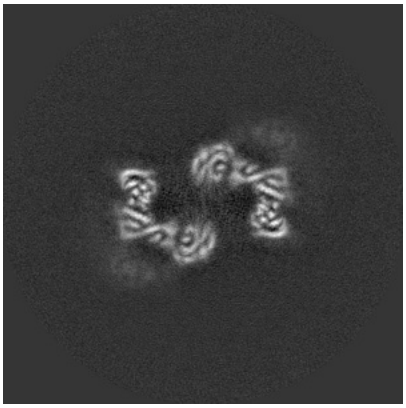
6.2.2 Raw map



X Index: 170



Y Index: 170

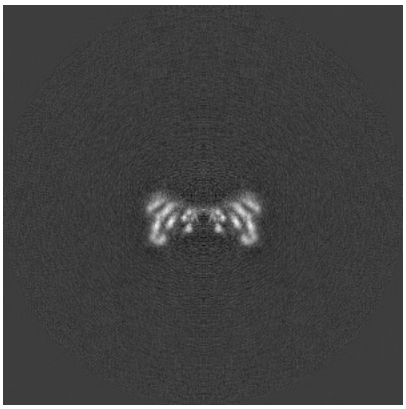


Z Index: 170

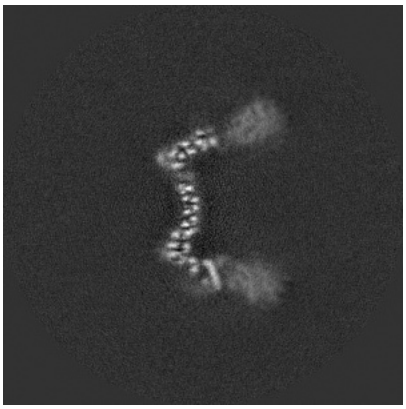
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

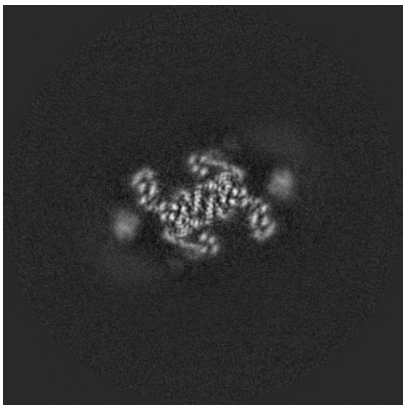
6.3.1 Primary map



X Index: 170

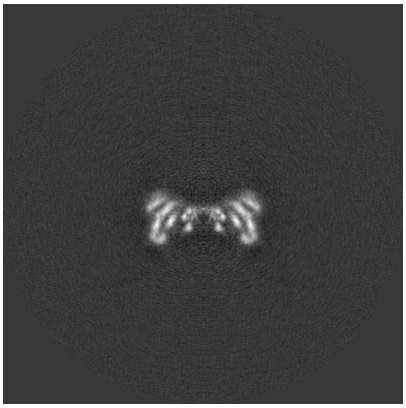


Y Index: 166

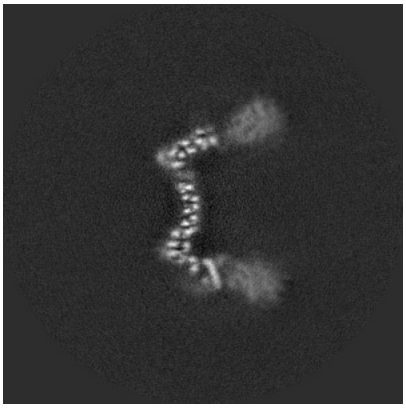


Z Index: 155

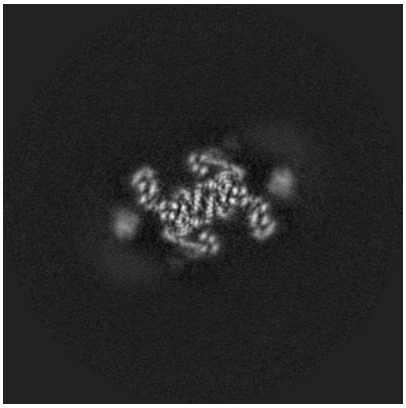
6.3.2 Raw map



X Index: 170



Y Index: 166

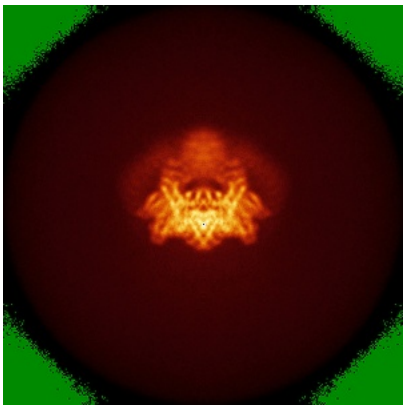


Z Index: 155

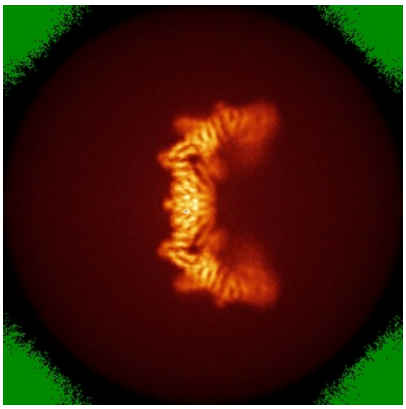
The images above show the largest variance slices of the map in three orthogonal directions.

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

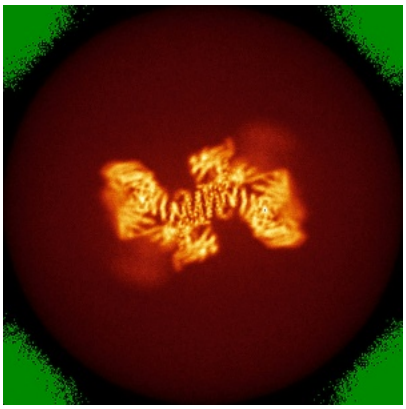
6.4.1 Primary map



X

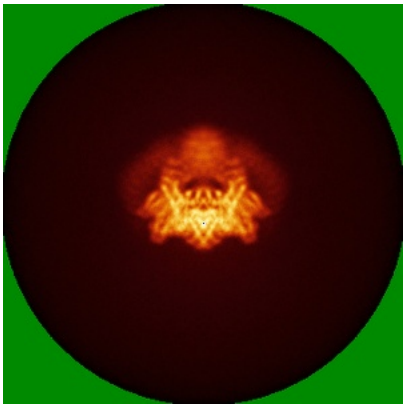


Y



Z

6.4.2 Raw map



X

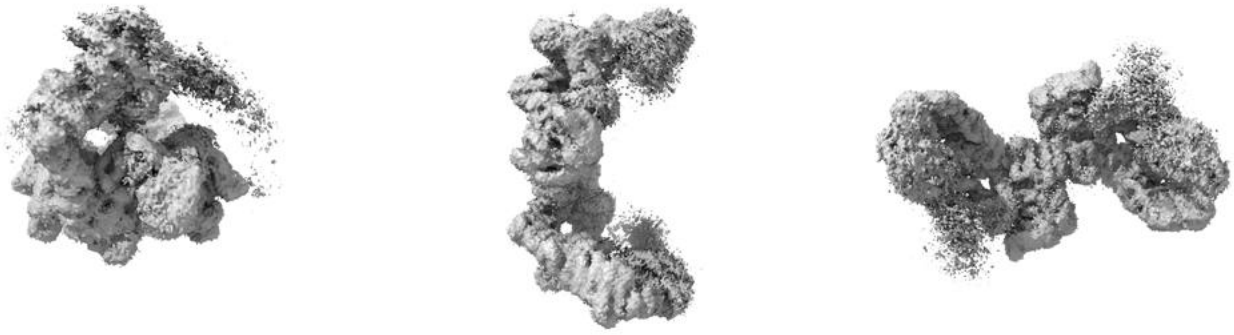
Y

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

6.5.2 Raw map

X Y Z

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

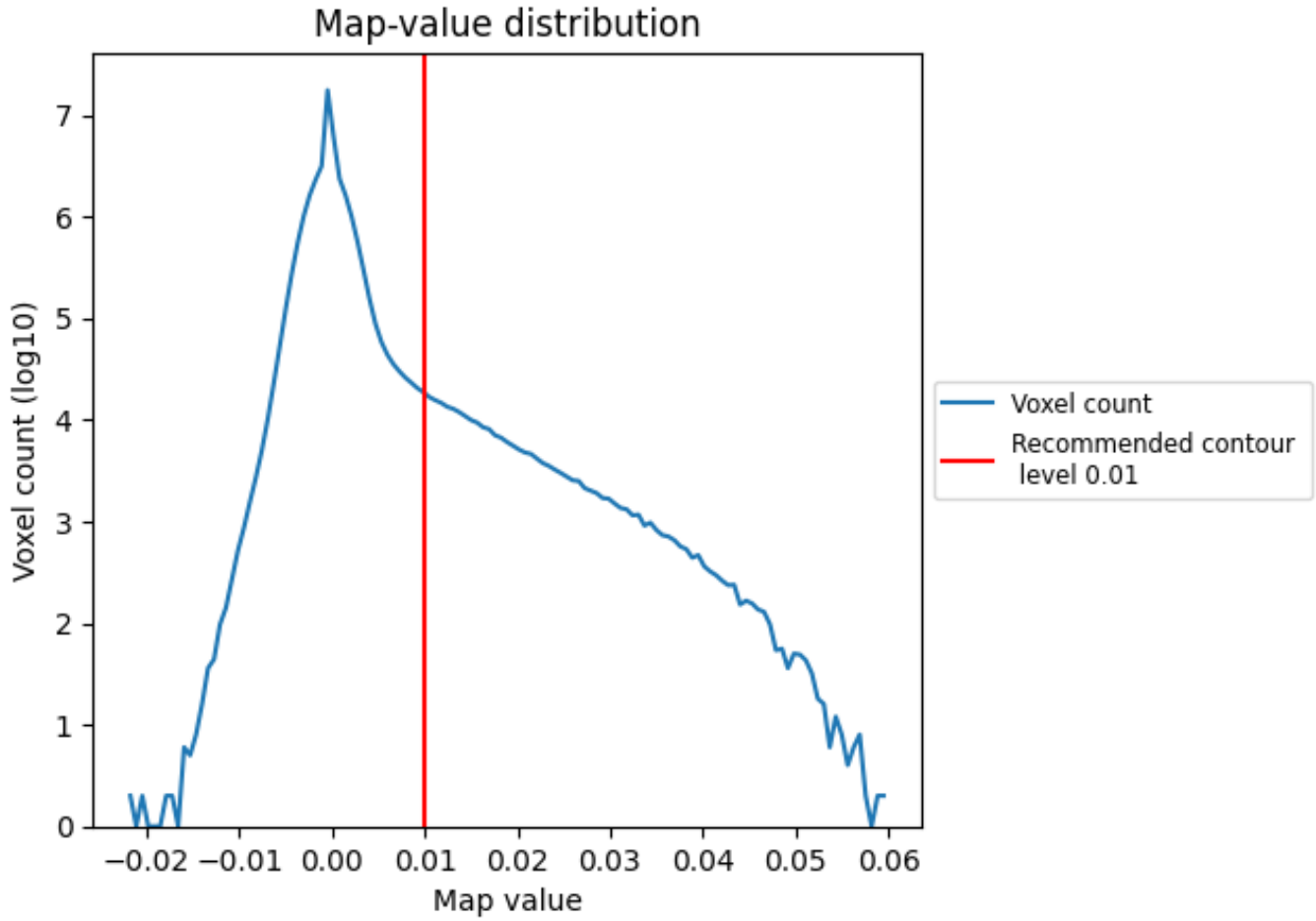
6.6 Mask visualisation (i)

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

7 Map analysis

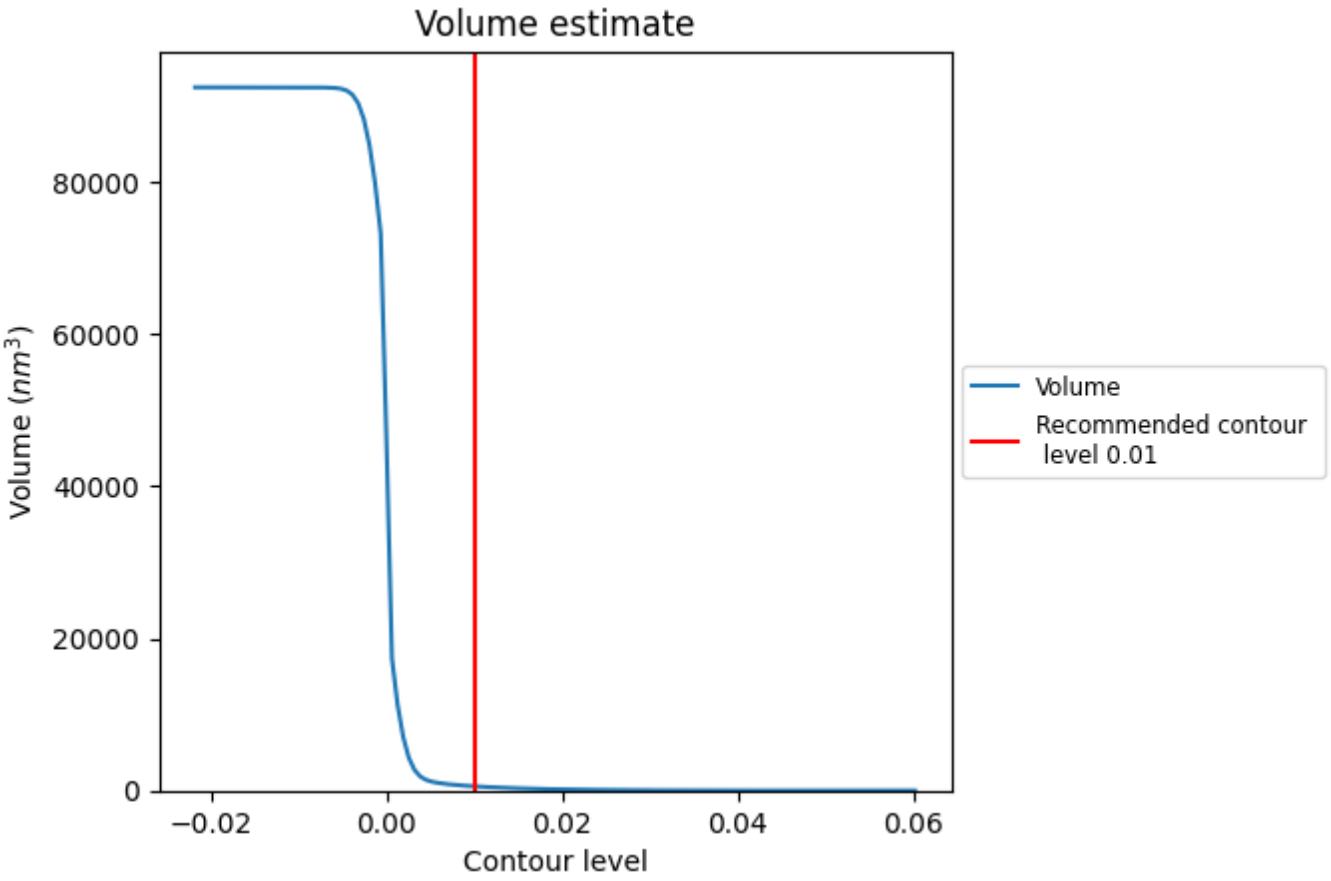
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

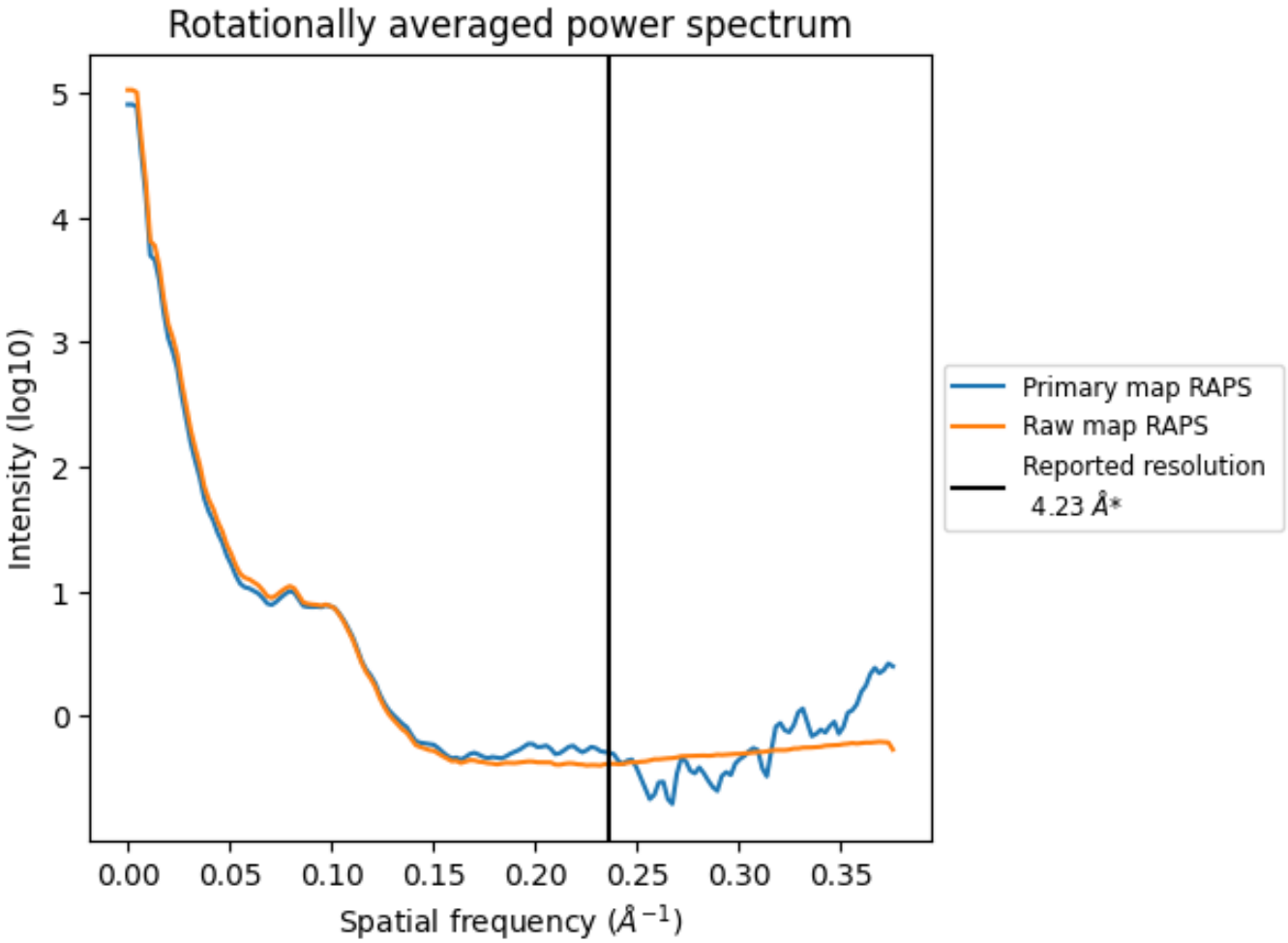
7.2 Volume estimate



The volume at the recommended contour level is 558 nm^3; this corresponds to an approximate mass of 504 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)

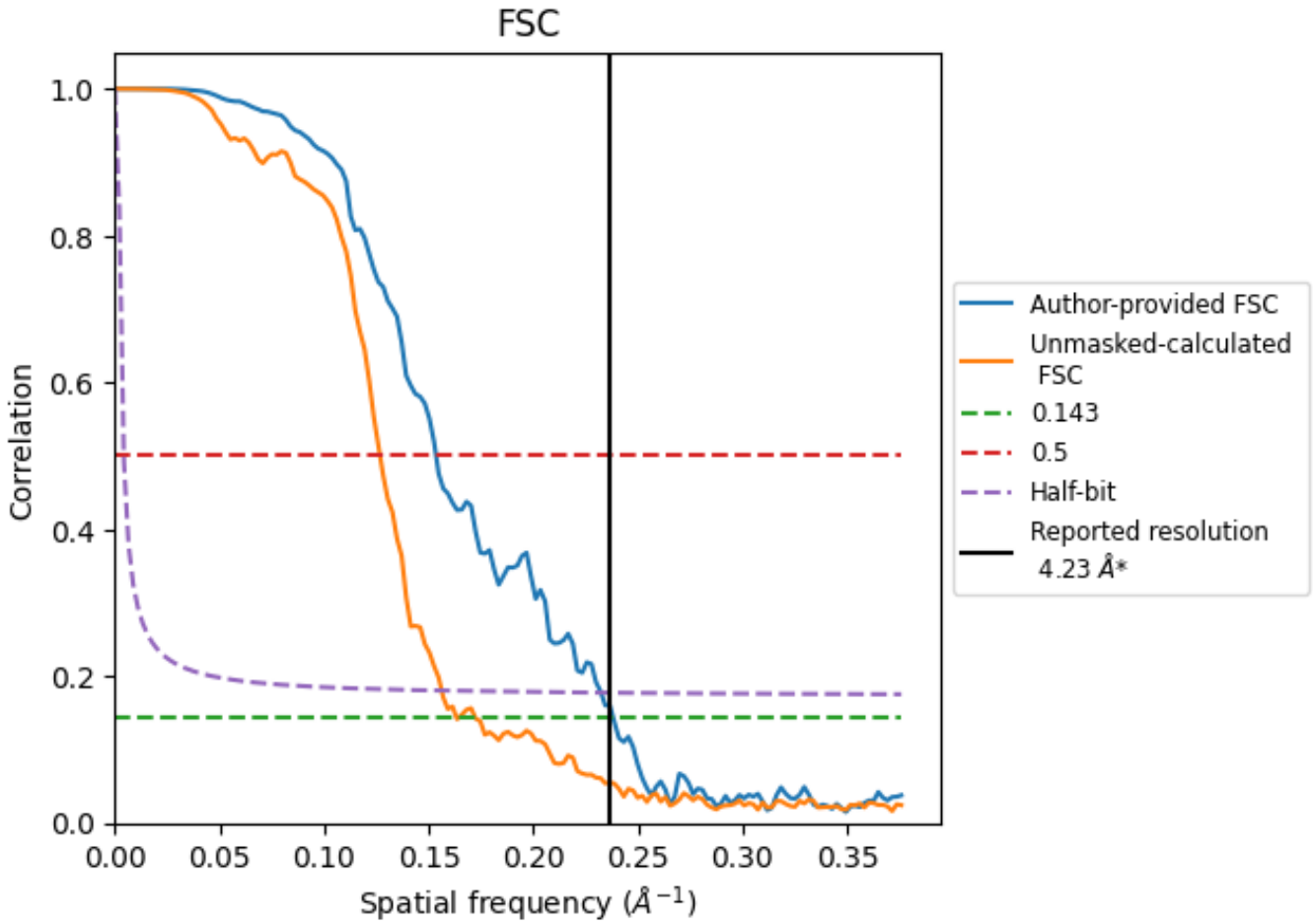


*Reported resolution corresponds to spatial frequency of 0.236 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.236 Å^{-1}

8.2 Resolution estimates (i)

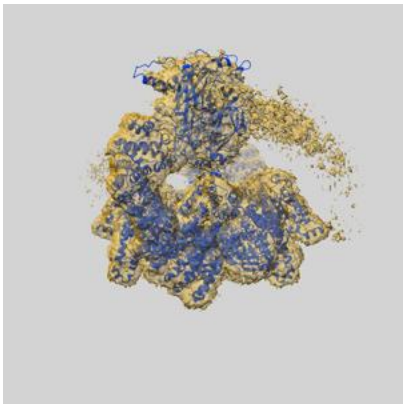
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.23	-	-
Author-provided FSC curve	4.20	6.51	4.30
Unmasked-calculated*	6.12	7.89	6.40

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.12 differs from the reported value 4.23 by more than 10 %

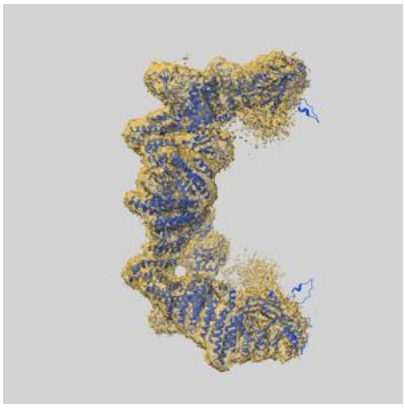
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-60148 and PDB model 8ZJK. Per-residue inclusion information can be found in section 3 on page 5.

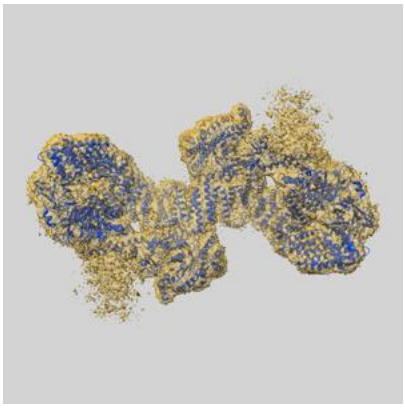
9.1 Map-model overlay



X



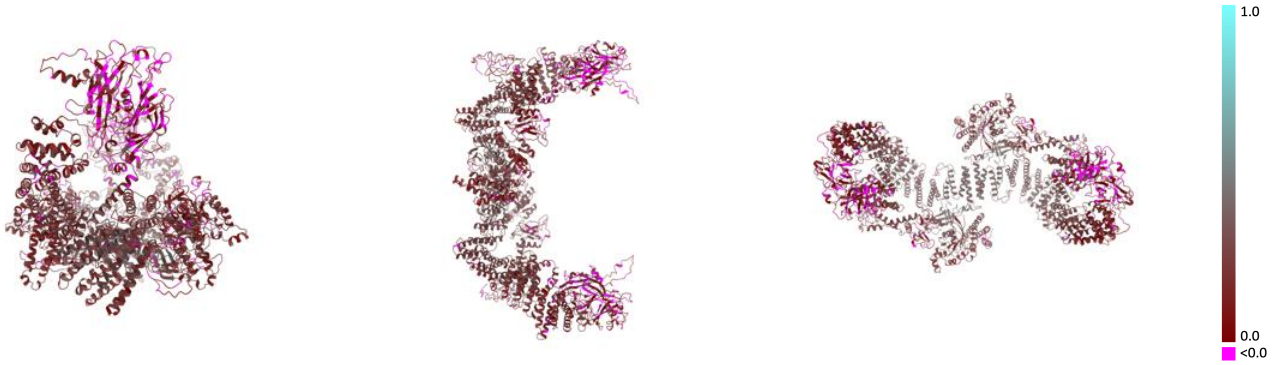
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01 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.

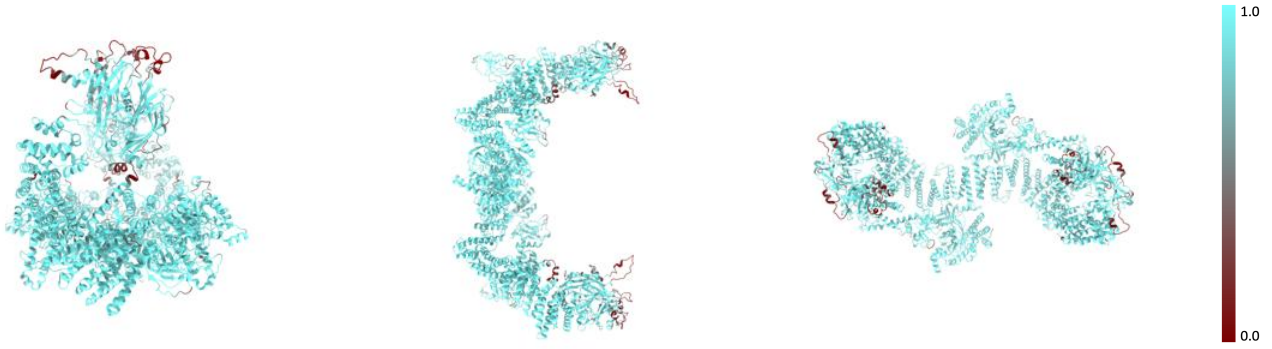
9.2 Q-score mapped to coordinate model (i)



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.

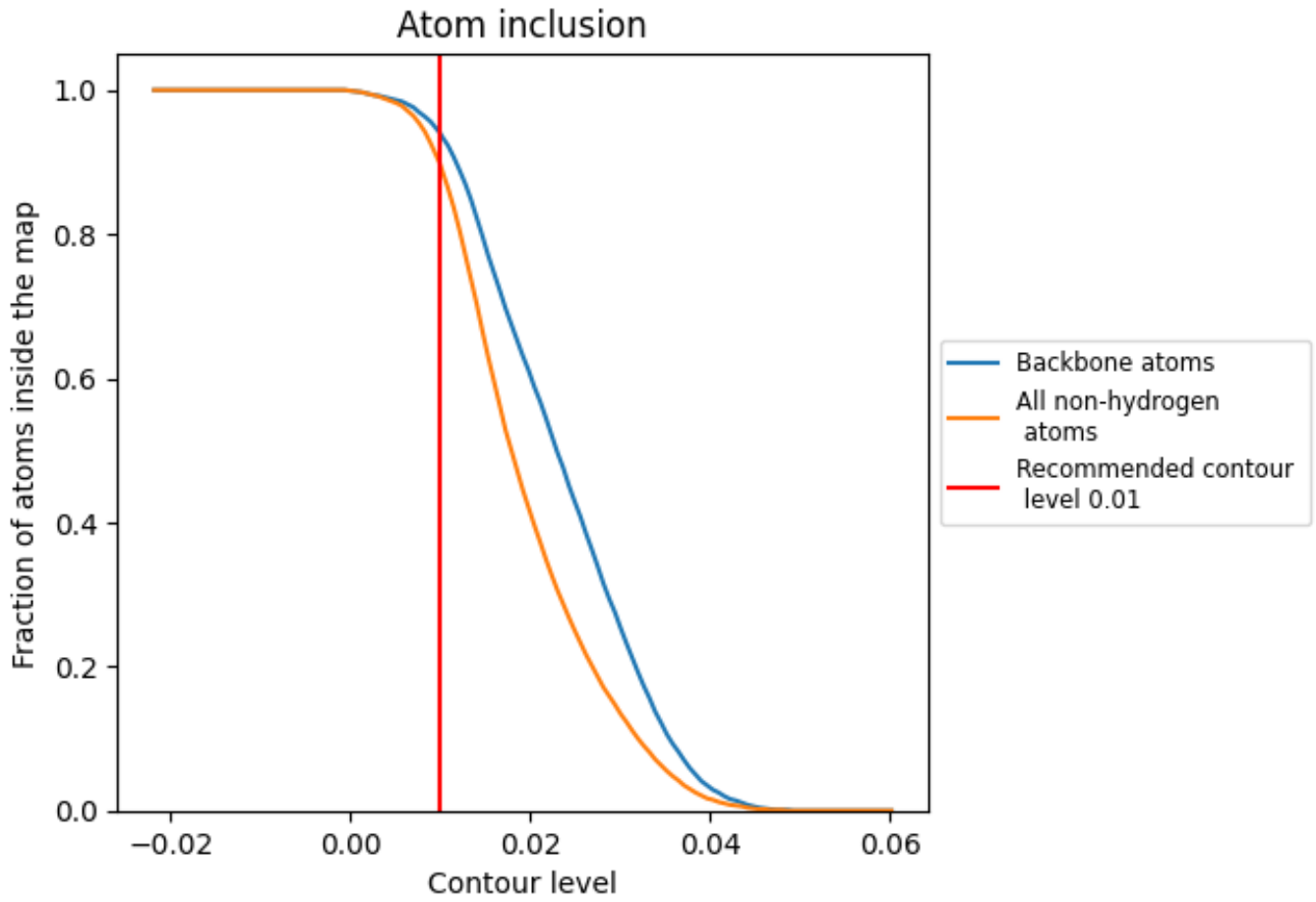
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.01).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8970	0.2030
A	0.8970	0.1680
B	0.8870	0.2030
C	0.9560	0.2450
D	0.9070	0.1610
E	0.8930	0.2040
F	0.9600	0.2420