Full wwPDB EM Validation Report ⓘ

Nov 7, 2022 – 12:10 PM JST

PDB ID	:	5H0S
EMDB ID	:	EMD-9565
Title	:	EM Structure of VP1A and VP1B
Authors	:	Li, X.; Zhou, N.; Xu, B.; Chen, W.; Zhu, B.; Wang, X.; Wang, J.; Liu, H.; Cheng, L.
Deposited on	:	2016-10-06
Resolution	:	3.30 Å(reported)

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

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

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

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

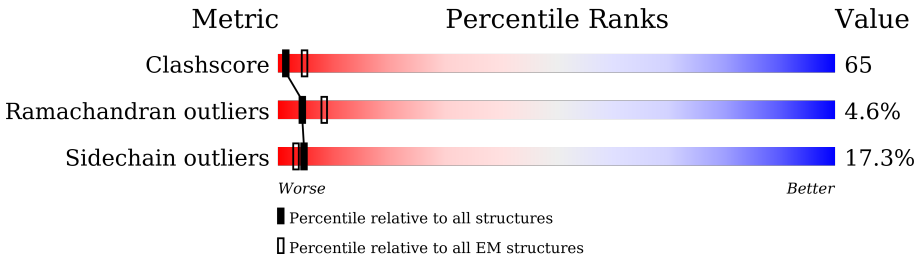
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 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	B	1333	21% 48% 37% · 14%
1	C	1333	25% 19% 39% 27% 8% 6%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 18885 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 VP1.

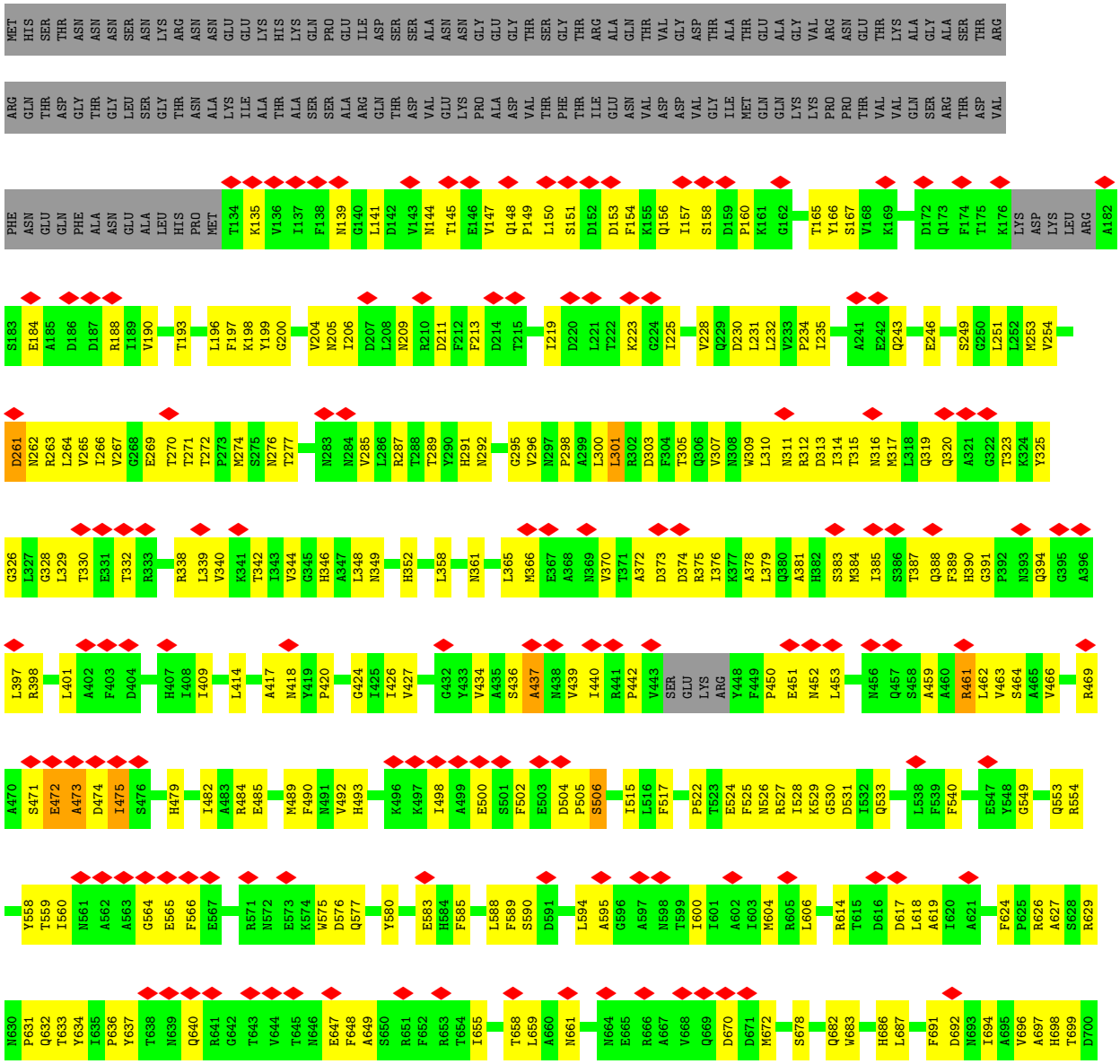
Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	1148	Total	C	N	O	S	0	0
			9058	5731	1574	1718	35		
1	C	1247	Total	C	N	O	S	0	0
			9827	6202	1709	1878	38		

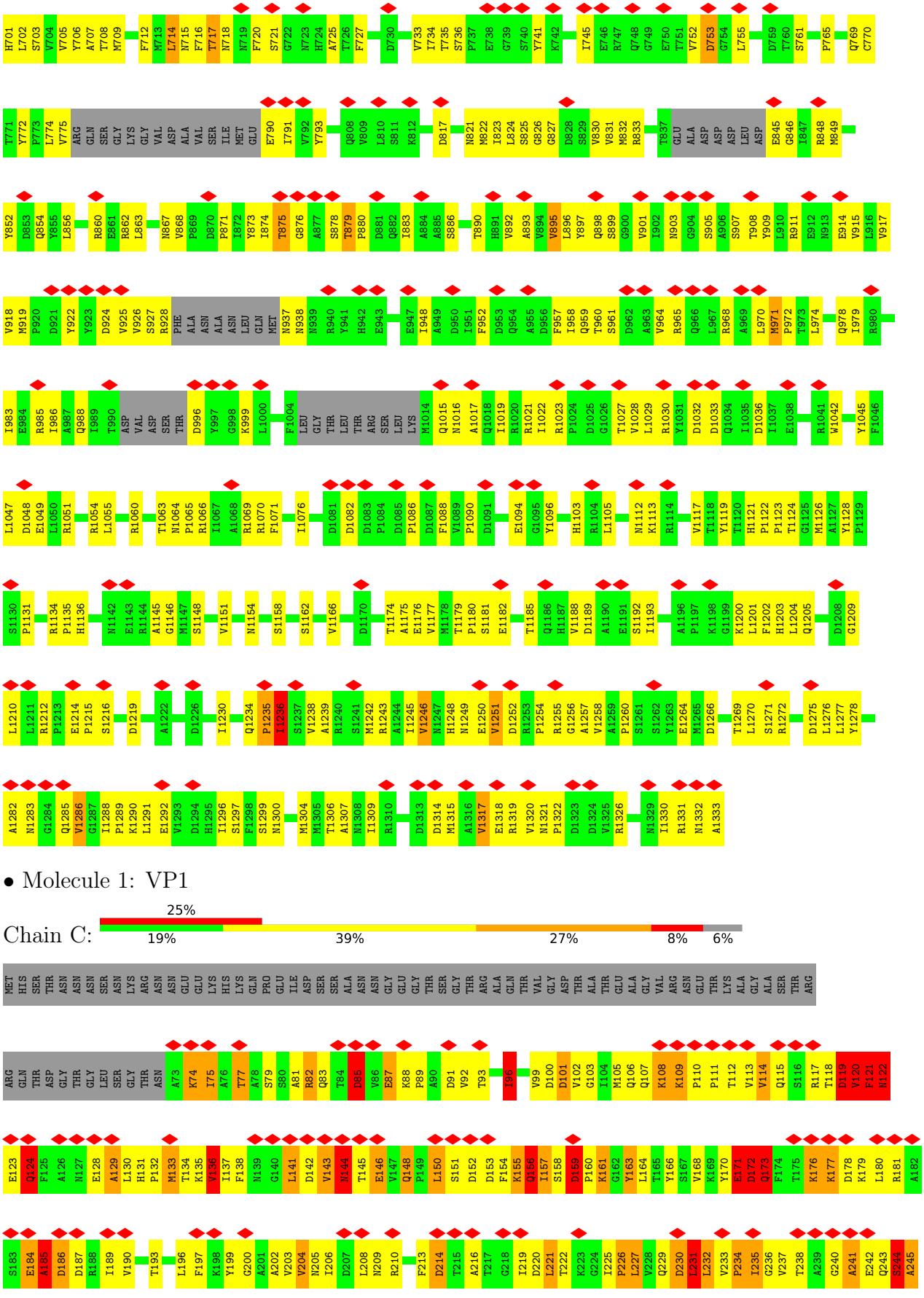
3 Residue-property plots (i)

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.

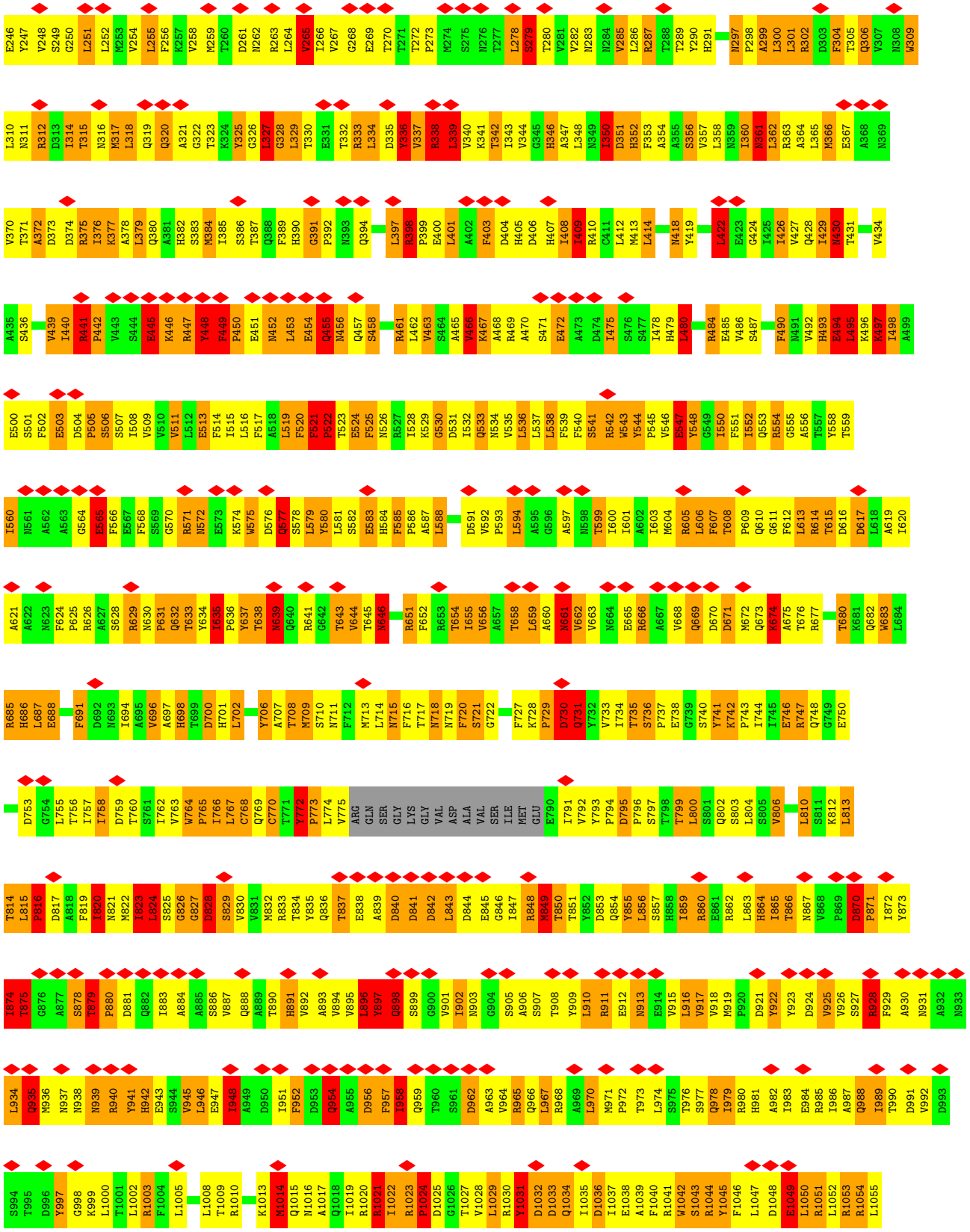
- Molecule 1: VP1

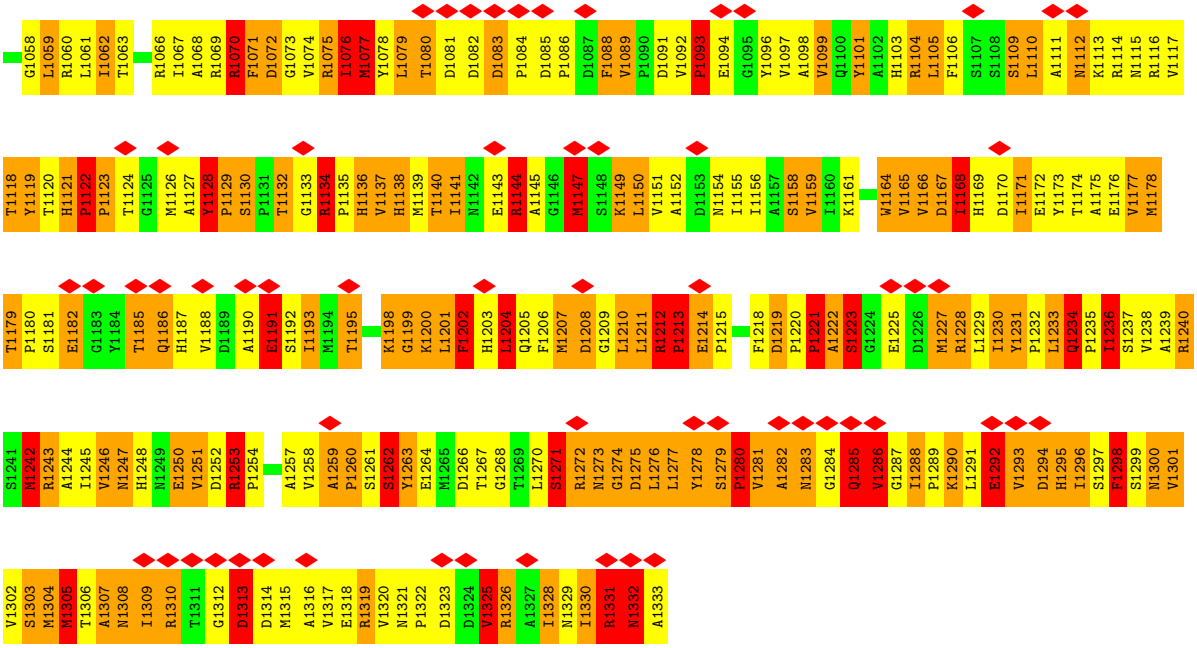
Chain B:





• Molecule 1: VP1


E246 Y247 V248 S249 G250 L251 L252 M253 V254 L255 F256 K257 V258 M259 T260 D261 N262 R263 L264 V265 I266 V267 G268 E269 T270 T271 T272 P273 M274 S275 N276 T277 L278 S279 T280 V281 V282 N283 N284 V285 L286 R287 T288 T289 Y290 H291 N297 P298 A299 L300 L301 R302 D303 F304 T305 Q306 V307 N308 W309
L310 N311 R312 D313 I314 T315 N316 M317 L318 Q319 Q320 A321 G322 T323 K324 Y325 G326 L327 G328 L329 T330 E331 T332 R333 L334 D335 V336 V337 R338 L339 V340 K341 T342 I343 V344 G345 H346 A347 L348 N349 I350 D351 H352 F353 A354 A355 S356 V357 L358 N359 I360 N361 L362 R363 A364 L365 M366 E367 A368 N369
V370 T371 A372 D373 D374 R375 I376 K377 A378 L379 Q380 A381 H382 S383 M384 I385 S386 T387 Q388 F389 H390 G391 P392 N393 Q394 L397 R398 P399 E400 L401 A402 F403 D404 H405 D406 H407 I408 T409 R410 C411 L412 M413 L414 N418 Y419 L422 E423 G424 I425 I426 V427 Q428 I429 M430 T431 V434
A435 S436 V439 I440 R441 P442 V443 S444 E445 K446 R447 Y448 F449 P450 E451 N452 L453 E454 Q455 N456 Q457 S458 R461 L462 V463 S464 A465 V466 K467 A468 R469 A470 S471 E472 A473 D474 I475 S476 S477 I478 H479 L480 R484 E485 V486 S487 F490 N491 V492 H493 E494 L495 K496 K497 I498 A499
E500 S501 F502 E503 D504 P505 S506 S507 I508 V509 V510 V511 L512 E513 F514 I515 L516 F517 A518 L519 F520 F521 P522 T523 E524 F525 N526 R527 I528 K529 G530 D531 I532 Q533 N534 V535 L536 L537 L538 F539 F540 S541 R542 W543 Y544 P545 V546 E547 Y548 G549 I550 F551 I552 Q553 R554 G555 A556 T557 Y558 T559
I560 N561 A562 A563 G564 E565 F566 E567 F568 S569 G570 R571 N572 E573 K574 W575 D576 Q577 S578 L579 Y580 L581 S582 E583 H584 F585 P586 A587 L588 D591 V592 P593 L594 A595 G596 A597 N598 T599 I600 I601 A602 I603 M604 R605 L606 F607 T608 P609 Q610 G611 F612 L613 R614 T615 D616 D617 L618 A619 I620
A621 A622 N623 F624 P625 R626 A627 S628 R629 N630 P631 Q632 T633 Y634 I635 P636 Y637 T638 N639 Q640 R641 G642 T643 V644 T645 N646 R651 F652 R653 T654 I655 V656 A657 T658 L659 A660 N661 V662 V663 N664 E665 R666 A667 V668 Q669 D670 D671 M672 Q673 K674 A675 T676 R677 T680 K681 Q682 W683 L684
R685 H686 L687 E688 F691 D692 N693 I694 A695 V696 A697 H698 T699 D700 H701 L702 Y706 A707 T708 M709 S710 N711 F712 M713 L714 N715 F716 T717 N718 N719 F720 S721 G722 F727 K728 P729 D730 Q731 Y732 V733 I734 T735 S736 P737 E738 G739 S740 Y741 K742 P743 I744 I745 E746 R747 Q748 G749 E750
D753 G754 L755 T756 I757 I758 D759 T760 S761 I762 V763 W764 P765 I766 L767 C768 Q769 C770 T771 Y772 P773 L774 V775 ARG GLN SER GLY LYS GLY VAL ASP ALA VAL SER ILE MET GLU E790 I791 V792 Y793 P794 D795 P796 S797 T798 T799 L800 S801 Q802 S803 L804 S805 V806 L810 S811 K812 L813
T814 L815 P816 D817 A818 F819 I820 N821 M822 I823 L824 S825 G826 G827 D828 S829 V830 V831 M832 R833 T834 Y835 Q836 T837 E838 A839 D840 D841 D842 L843 D844 E845 G846 I847 R848 M849 T850 T851 Y852 D853 Q854 Y855 L856 S857 H858 I859 R860 E861 R862 L863 H864 I865 T866 N867 V868 P869 D870 P871 I872 Y873
I874 T875 G876 A877 S878 T879 P880 D881 Q882 I883 A884 A885 S886 V887 Q888 A889 T890 H891 V892 A893 V894 V895 L896 Y897 Q898 S899 G900 V901 I902 N903 G904 S905 A906 S907 T908 Y909 L910 R911 E912 N913 E914 Y915 L916 V917 Y918 M919 P920 D921 Y922 Y923 D924 V925 V926 S927 R928 F929 A930 N931 A932 N933
L934 Q935 M936 N937 N938 N939 R940 Y941 H942 E943 S944 V945 L946 E947 I948 A949 D950 I951 F952 D953 Q954 A955 D956 Y957 I958 Q959 T960 S961 D962 A963 V964 R965 Q966 L967 R968 A969 L970 M971 P972 T973 L974 S975 T976 S977 Q978 I979 R980 H981 A982 I983 E984 R985 I986 A987 Q988 I989 T990 D991 V992 D993
S994 T995 D996 Y997 G998 K999 L1000 T1001 L1002 R1003 F1004 L1005 L1008 T1009 R1010 K1013 K1014 Q1015 N1016 A1017 Q1018 I1019 R1020 R1021 I1022 R1023 P1024 D1025 G1026 T1027 V1028 L1029 R1030 Y1031 D1032 D1033 Q1034 I1035 D1036 I1037 E1038 A1039 F1040 R1041 W1042 S1043 R1044 Y1045 F1046 L1047 D1048 E1049 L1050 R1051 L1052 R1053 R1054 L1055


G1058 L1059 R1060 L1061 I1062 T1063 R1066 I1067 A1068 R1069 R1070 F1071 D1072 G1073 V1074 R1075 I1076 M1077 Y1078 L1079 T1080 D1081 D1082 D1083 P1084 D1085 P1086 D1087 F1088 V1089 P1090 D1091 V1092 P1093 E1094 G1095 Y1096 V1097 A1098 V1099 Q1100 Y1101 A1102 H1103 R1104 L1105 F1106 S1107 S1108 S1109 L1110 A1111 N1112 K1113 R1114 N1115 R1116 V1117
T1118 Y1119 T1120 H1121 P1122 P1123 T1124 G1125 M1126 A1127 Y1128 P1129 S1130 P1131 T1132 G1133 R1134 P1135 H1136 V1137 H1138 M1139 T1140 I1141 N1142 E1143 R1144 A1145 G1146 M1147 S1148 K1149 L1150 V1151 A1152 D1153 N1154 I1155 I1156 A1157 S1158 V1159 I1160 K1161 W1164 V1165 V1166 D1167 I1168 H1169 D1170 I1171 E1172 Y1173 T1174 A1175 E1176 V1177 M1178
T1179 P1180 S1181 E1182 G1183 Y1184 T1185 Q1186 H1187 V1188 D1189 A1190 E1191 S1192 I1193 M1194 T1195 K1198 G1199 K1200 L1201 F1202 H1203 L1204 Q1205 F1206 M1207 D1208 G1209 L1210 L1211 R1212 P1213 E1214 P1215 F1218 D1219 P1220 P1221 A1222 S1223 G1224 E1225 D1226 M1227 R1228 L1229 I1230 Y1231 P1232 L1233 Q1234 P1235 I1236 S1237 V1238 A1239 R1240
S1241 M1242 R1243 A1244 I1245 V1246 N1247 H1248 N1249 E1250 V1251 D1252 R1253 P1254 A1257 V1258 A1259 P1260 S1261 S1262 Y1263 E1264 M1265 D1266 T1267 G1268 T1269 L1270 S1271 R1272 N1273 G1274 D1275 L1276 L1277 Y1278 S1279 P1280 V1281 A1282 N1283 G1284 Q1285 V1286 G1287 I1288 P1289 K1290 L1291 E1292 V1293 D1294 H1295 I1296 S1297 F1298 S1299 N1300 V1301
V1302 S1303 M1304 M1305 T1306 A1307 N1308 I1309 R1310 T1311 G1312 D1313 D1314 M1315 A1316 V1317 E1318 R1319 V1320 N1321 P1322 D1323 D1324 V1325 R1326 A1327 I1328 N1329 I1330 R1331 N1332 A1333

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	27000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	53.433	Depositor
Minimum map value	-40.259	Depositor
Average map value	0.625	Depositor
Map value standard deviation	5.607	Depositor
Recommended contour level	17.0	Depositor
Map size (Å)	652.39996, 652.39996, 652.39996	wwPDB
Map dimensions	700, 700, 700	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.9319999, 0.9319999, 0.9319999	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	B	0.47	1/9244 (0.0%)	0.65	4/12582 (0.0%)
1	C	1.88	114/10028 (1.1%)	1.75	273/13653 (2.0%)
All	All	1.39	115/19272 (0.6%)	1.34	277/26235 (1.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	9
1	C	0	30
All	All	0	39

All (115) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	543	TRP	CB-CG	-12.16	1.28	1.50
1	C	683	TRP	CB-CG	-11.34	1.29	1.50
1	C	278	LEU	C-N	10.07	1.57	1.34
1	C	449	PHE	C-N	9.81	1.52	1.34
1	C	1167	ASP	CB-CG	-9.25	1.32	1.51
1	C	119	ASP	CB-CG	8.76	1.70	1.51
1	C	543	TRP	CG-CD1	-8.71	1.24	1.36
1	C	325	TYR	CE1-CZ	-8.67	1.27	1.38
1	C	227	LEU	C-N	8.58	1.53	1.34
1	C	244	SER	C-N	7.98	1.52	1.34
1	C	680	THR	CB-CG2	-7.89	1.26	1.52
1	C	764	TRP	CB-CG	-7.63	1.36	1.50
1	C	544	TYR	CB-CG	-7.45	1.40	1.51
1	C	575	TRP	CB-CG	-7.33	1.37	1.50
1	C	803	SER	CB-OG	-7.28	1.32	1.42
1	C	706	TYR	CB-CG	-7.17	1.40	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	683	TRP	CG-CD1	-7.11	1.26	1.36
1	C	741	TYR	CE1-CZ	-6.88	1.29	1.38
1	C	506	SER	CA-CB	-6.82	1.42	1.52
1	C	855	TYR	C-O	-6.75	1.10	1.23
1	C	548	TYR	C-O	-6.64	1.10	1.23
1	C	1158	SER	CB-OG	-6.64	1.33	1.42
1	B	971	MET	C-N	-6.57	1.21	1.34
1	C	1031	TYR	CB-CG	-6.55	1.41	1.51
1	C	1045	TYR	CG-CD1	-6.43	1.30	1.39
1	C	1164	TRP	CG-CD1	-6.29	1.27	1.36
1	C	547	GLU	CD-OE1	-6.25	1.18	1.25
1	C	521	PHE	C-O	-6.22	1.11	1.23
1	C	327	LEU	C-O	-6.14	1.11	1.23
1	C	530	GLY	C-O	-6.12	1.13	1.23
1	C	793	TYR	CE1-CZ	-6.11	1.30	1.38
1	C	585	PHE	C-O	6.10	1.34	1.23
1	C	163	TYR	CE1-CZ	-6.08	1.30	1.38
1	C	637	TYR	CE2-CZ	-6.07	1.30	1.38
1	C	121	PHE	CB-CG	-6.03	1.41	1.51
1	C	1223	SER	CA-CB	-6.01	1.44	1.52
1	C	325	TYR	CZ-OH	-5.99	1.27	1.37
1	C	354	ALA	C-O	-5.98	1.11	1.23
1	C	445	GLU	CG-CD	5.92	1.60	1.51
1	C	1119	TYR	CE1-CZ	-5.92	1.30	1.38
1	C	1045	TYR	CB-CG	-5.90	1.42	1.51
1	C	541	SER	CA-CB	-5.87	1.44	1.52
1	C	857	SER	CB-OG	-5.85	1.34	1.42
1	C	77	THR	C-O	5.83	1.34	1.23
1	C	637	TYR	CG-CD2	-5.82	1.31	1.39
1	C	631	PRO	C-O	-5.81	1.11	1.23
1	C	683	TRP	CD2-CE2	-5.80	1.34	1.41
1	C	75	ILE	C-O	5.79	1.34	1.23
1	C	1101	TYR	CA-C	-5.78	1.38	1.52
1	C	1202	PHE	CB-CG	-5.77	1.41	1.51
1	C	479	HIS	C-O	-5.72	1.12	1.23
1	C	447	ARG	C-N	5.71	1.47	1.34
1	C	1301	VAL	C-O	-5.68	1.12	1.23
1	C	102	VAL	N-CA	-5.67	1.35	1.46
1	C	740	SER	CA-CB	-5.67	1.44	1.52
1	C	956	ASP	CB-CG	5.66	1.63	1.51
1	C	328	GLY	C-O	-5.64	1.14	1.23
1	C	520	PHE	CB-CG	-5.64	1.41	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	544	TYR	CE1-CZ	-5.63	1.31	1.38
1	C	1303	SER	C-O	-5.62	1.12	1.23
1	C	1242	MET	C-O	-5.61	1.12	1.23
1	C	525	PHE	C-O	-5.58	1.12	1.23
1	C	977	SER	CA-CB	-5.56	1.44	1.52
1	C	493	HIS	C-O	-5.53	1.12	1.23
1	C	998	GLY	CA-C	-5.53	1.43	1.51
1	C	346	HIS	N-CA	-5.52	1.35	1.46
1	C	1164	TRP	CD2-CE2	-5.50	1.34	1.41
1	C	430	ASN	CB-CG	-5.47	1.38	1.51
1	C	533	GLN	C-O	-5.46	1.12	1.23
1	C	952	PHE	CB-CG	-5.46	1.42	1.51
1	C	1158	SER	CA-CB	-5.45	1.44	1.52
1	C	1223	SER	CB-OG	-5.44	1.35	1.42
1	C	524	GLU	C-O	-5.43	1.13	1.23
1	C	1077	MET	C-O	-5.42	1.13	1.23
1	C	390	HIS	C-O	-5.40	1.13	1.23
1	C	1201	LEU	CA-C	-5.39	1.39	1.52
1	C	524	GLU	CD-OE1	-5.37	1.19	1.25
1	C	419	TYR	CE1-CZ	-5.35	1.31	1.38
1	C	356	SER	C-O	-5.33	1.13	1.23
1	C	816	PRO	CA-C	-5.32	1.42	1.52
1	C	1231	TYR	CB-CG	-5.32	1.43	1.51
1	C	741	TYR	C-O	-5.32	1.13	1.23
1	C	494	GLU	C-O	-5.30	1.13	1.23
1	C	1076	ILE	C-O	-5.28	1.13	1.23
1	C	547	GLU	CG-CD	-5.27	1.44	1.51
1	C	1042	TRP	CD2-CE2	-5.23	1.35	1.41
1	C	424	GLY	C-O	-5.21	1.15	1.23
1	C	637	TYR	CB-CG	-5.21	1.43	1.51
1	C	691	PHE	C-O	-5.18	1.13	1.23
1	C	938	ASN	N-CA	-5.17	1.36	1.46
1	C	1280	PRO	N-CD	5.17	1.55	1.47
1	C	1071	PHE	C-O	-5.15	1.13	1.23
1	C	769	GLN	N-CA	-5.15	1.36	1.46
1	C	1045	TYR	CE1-CZ	-5.14	1.31	1.38
1	C	1178	MET	C-O	-5.13	1.13	1.23
1	C	683	TRP	C-O	-5.13	1.13	1.23
1	C	735	THR	CA-C	-5.13	1.39	1.52
1	C	74	LYS	C-O	5.13	1.33	1.23
1	C	775	VAL	CA-CB	5.13	1.65	1.54
1	C	1218	PHE	CB-CG	-5.12	1.42	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1164	TRP	CE3-CZ3	-5.12	1.29	1.38
1	C	1165	VAL	C-O	-5.10	1.13	1.23
1	C	490	PHE	C-O	-5.10	1.13	1.23
1	C	506	SER	CB-OG	-5.09	1.35	1.42
1	C	897	TYR	CB-CG	-5.09	1.44	1.51
1	C	580	TYR	CE2-CZ	-5.08	1.31	1.38
1	C	426	ILE	C-O	-5.07	1.13	1.23
1	C	115	GLN	C-O	5.07	1.32	1.23
1	C	706	TYR	CZ-OH	-5.07	1.29	1.37
1	C	1117	VAL	C-O	-5.06	1.13	1.23
1	C	378	ALA	C-O	-5.05	1.13	1.23
1	C	545	PRO	CA-C	-5.04	1.42	1.52
1	C	494	GLU	CD-OE2	-5.03	1.20	1.25
1	C	121	PHE	C-O	-5.02	1.13	1.23
1	C	463	VAL	C-O	-5.00	1.13	1.23

All (277) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	772	TYR	C-N-CD	-26.11	63.15	120.60
1	C	1121	HIS	C-N-CD	-19.15	78.48	120.60
1	C	870	ASP	C-N-CD	-18.50	79.91	120.60
1	C	285	VAL	O-C-N	17.98	151.47	122.70
1	C	173	GLN	O-C-N	-17.55	94.62	122.70
1	C	521	PHE	C-N-CD	-15.71	86.03	120.60
1	C	171	GLU	O-C-N	-15.37	98.10	122.70
1	C	879	THR	C-N-CD	-14.13	89.50	120.60
1	C	285	VAL	CA-C-N	-13.75	86.96	117.20
1	C	279	SER	O-C-N	-13.54	101.03	122.70
1	C	172	ASP	CA-C-N	-13.28	87.98	117.20
1	C	226	PRO	O-C-N	13.07	143.61	122.70
1	C	172	ASP	C-N-CA	-11.88	92.00	121.70
1	C	449	PHE	O-C-N	-11.71	98.85	121.10
1	C	173	GLN	CA-C-N	11.59	142.69	117.20
1	C	285	VAL	C-N-CA	-11.29	93.47	121.70
1	C	119	ASP	CB-CG-OD1	10.98	128.18	118.30
1	C	398	ARG	N-CA-C	10.83	140.24	111.00
1	C	1212	ARG	C-N-CD	-10.53	97.44	120.60
1	C	173	GLN	C-N-CA	10.45	147.83	121.70
1	C	816	PRO	CA-N-CD	-10.39	96.96	111.50
1	C	244	SER	CA-C-N	-10.26	94.63	117.20
1	C	226	PRO	CA-C-N	-10.18	94.81	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	1259	ALA	C-N-CD	-9.96	98.69	120.60
1	C	1178	MET	CB-CG-SD	-9.93	82.61	112.40
1	C	449	PHE	C-N-CD	-9.85	98.92	120.60
1	C	1179	THR	C-N-CD	-9.60	99.49	120.60
1	C	448	TYR	O-C-N	-9.55	107.42	122.70
1	C	827	GLY	N-CA-C	-9.39	89.63	113.10
1	C	773	PRO	N-CA-C	-9.24	88.07	112.10
1	C	767	LEU	CA-CB-CG	9.23	136.53	115.30
1	C	278	LEU	O-C-N	9.13	137.30	122.70
1	C	1285	GLN	N-CA-C	9.12	135.62	111.00
1	C	336	TYR	N-CA-C	9.04	135.41	111.00
1	C	793	TYR	C-N-CD	-8.98	100.84	120.60
1	C	721	SER	N-CA-C	-8.89	87.01	111.00
1	C	244	SER	C-N-CA	-8.88	99.50	121.70
1	C	1122	PRO	C-N-CD	-8.88	101.07	120.60
1	C	172	ASP	O-C-N	8.77	136.73	122.70
1	C	1201	LEU	CA-CB-CG	8.70	135.31	115.30
1	C	1281	VAL	CG1-CB-CG2	8.57	124.61	110.90
1	C	1029	LEU	CB-CG-CD1	-8.56	96.45	111.00
1	C	144	ASN	N-CA-CB	8.51	125.91	110.60
1	C	150	LEU	CB-CG-CD2	-8.45	96.64	111.00
1	C	655	ILE	CB-CA-C	-8.44	94.72	111.60
1	C	1307	ALA	N-CA-C	-8.38	88.36	111.00
1	C	1286	VAL	N-CA-C	8.37	133.61	111.00
1	C	350	ILE	CB-CA-C	-8.24	95.12	111.60
1	C	360	ILE	CB-CA-C	-8.22	95.15	111.60
1	C	361	ASN	O-C-N	-8.20	109.58	122.70
1	C	1291	LEU	CB-CG-CD1	-8.15	97.14	111.00
1	C	674	LYS	CD-CE-NZ	-8.10	93.06	111.70
1	C	226	PRO	C-N-CA	-8.09	101.47	121.70
1	C	1300	ASN	N-CA-C	8.09	132.83	111.00
1	C	418	ASN	CB-CA-C	-8.07	94.25	110.40
1	C	813	LEU	CB-CG-CD2	-8.01	97.39	111.00
1	C	1035	ILE	CG1-CB-CG2	-7.99	93.82	111.40
1	C	1199	GLY	N-CA-C	-7.98	93.16	113.10
1	C	866	THR	N-CA-C	-7.83	89.85	111.00
1	C	1042	TRP	N-CA-C	7.83	132.15	111.00
1	C	896	LEU	CB-CG-CD2	-7.81	97.72	111.00
1	C	185	ALA	O-C-N	-7.70	110.38	122.70
1	C	279	SER	CA-C-N	7.68	134.09	117.20
1	C	938	ASN	CB-CA-C	7.67	125.75	110.40
1	C	661	ASN	CA-C-N	-7.63	100.40	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	849	MET	CB-CG-SD	-7.57	89.69	112.40
1	C	279	SER	C-N-CA	7.57	140.61	121.70
1	C	244	SER	O-C-N	7.56	134.80	122.70
1	B	714	LEU	CA-CB-CG	7.53	132.61	115.30
1	C	687	LEU	CB-CG-CD2	-7.49	98.26	111.00
1	C	1230	ILE	CB-CA-C	-7.47	96.66	111.60
1	C	96	ILE	CG1-CB-CG2	-7.42	95.06	111.40
1	C	480	LEU	CB-CG-CD2	-7.33	98.54	111.00
1	C	1291	LEU	CB-CG-CD2	-7.31	98.57	111.00
1	C	635	ILE	N-CA-C	7.31	130.74	111.00
1	C	1331	ARG	NE-CZ-NH1	7.27	123.94	120.30
1	C	946	LEU	CB-CG-CD1	-7.26	98.66	111.00
1	C	1147	MET	N-CA-C	7.25	130.58	111.00
1	C	1313	ASP	CB-CG-OD2	7.19	124.77	118.30
1	C	1043	SER	N-CA-C	7.18	130.39	111.00
1	C	346	HIS	N-CA-CB	-7.13	97.77	110.60
1	C	391	GLY	C-N-CD	-7.08	105.03	120.60
1	C	456	ASN	O-C-N	-7.07	111.39	122.70
1	C	719	ASN	CB-CA-C	-7.05	96.30	110.40
1	C	278	LEU	CA-C-N	-6.99	101.83	117.20
1	C	1031	TYR	CA-C-N	-6.94	101.92	117.20
1	C	638	THR	N-CA-C	6.93	129.71	111.00
1	C	301	LEU	CA-CB-CG	6.92	131.21	115.30
1	C	536	LEU	CB-CG-CD1	-6.92	99.24	111.00
1	C	1033	ASP	CB-CG-OD2	-6.91	112.08	118.30
1	C	1144	ARG	NE-CZ-NH1	6.91	123.75	120.30
1	C	731	GLN	N-CA-C	6.88	129.59	111.00
1	C	1167	ASP	N-CA-CB	-6.88	98.22	110.60
1	C	75	ILE	O-C-N	6.87	133.69	122.70
1	C	775	VAL	CA-CB-CG2	6.85	121.18	110.90
1	C	409	ILE	CG1-CB-CG2	-6.85	96.34	111.40
1	C	688	GLU	CB-CA-C	6.82	124.05	110.40
1	C	124	GLN	N-CA-C	6.82	129.41	111.00
1	C	606	LEU	CB-CG-CD1	-6.82	99.42	111.00
1	C	100	ASP	N-CA-CB	-6.80	98.36	110.60
1	C	828	ASP	CB-CG-OD1	6.80	124.42	118.30
1	C	863	LEU	CB-CG-CD2	-6.78	99.48	111.00
1	C	758	ILE	CB-CA-C	-6.75	98.09	111.60
1	C	954	GLN	N-CA-C	6.71	129.12	111.00
1	C	1330	ILE	CG1-CB-CG2	-6.69	96.68	111.40
1	C	1271	SER	CB-CA-C	-6.67	97.44	110.10
1	C	1025	ASP	CB-CA-C	-6.66	97.08	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	810	LEU	CA-CB-CG	-6.64	100.02	115.30
1	C	120	VAL	N-CA-C	6.62	128.89	111.00
1	C	448	TYR	CA-C-N	-6.60	102.67	117.20
1	C	946	LEU	CA-CB-CG	-6.60	100.12	115.30
1	C	114	VAL	CB-CA-C	-6.52	99.01	111.40
1	C	700	ASP	N-CA-C	6.51	128.59	111.00
1	C	810	LEU	CB-CG-CD1	6.49	122.03	111.00
1	C	891	HIS	N-CA-C	6.47	128.47	111.00
1	C	700	ASP	O-C-N	6.47	133.05	122.70
1	C	475	ILE	N-CA-C	6.42	128.32	111.00
1	C	119	ASP	N-CA-C	-6.41	93.68	111.00
1	C	768	CYS	N-CA-C	6.39	128.26	111.00
1	C	979	ILE	CG1-CB-CG2	-6.38	97.38	111.40
1	C	1159	VAL	CG1-CB-CG2	-6.37	100.71	110.90
1	C	1204	LEU	CB-CG-CD2	-6.37	100.18	111.00
1	C	875	THR	CA-C-N	6.36	128.92	116.20
1	C	824	LEU	CA-CB-CG	6.32	129.84	115.30
1	C	670	ASP	CB-CA-C	-6.31	97.79	110.40
1	C	635	ILE	C-N-CD	-6.30	106.73	120.60
1	C	1304	MET	CB-CG-SD	-6.30	93.49	112.40
1	C	121	PHE	C-N-CA	6.30	137.45	121.70
1	C	702	LEU	CB-CG-CD2	-6.30	100.29	111.00
1	C	1134	ARG	C-N-CD	6.30	141.62	128.40
1	C	1201	LEU	CB-CG-CD2	-6.28	100.33	111.00
1	C	671	ASP	O-C-N	-6.28	112.66	122.70
1	C	525	PHE	CB-CA-C	-6.25	97.90	110.40
1	C	1043	SER	C-N-CA	6.24	137.30	121.70
1	C	1234	GLN	C-N-CD	6.22	141.47	128.40
1	C	314	ILE	CG1-CB-CG2	-6.22	97.71	111.40
1	C	577	GLN	N-CA-CB	6.22	121.80	110.60
1	C	327	LEU	CA-CB-CG	6.19	129.54	115.30
1	C	1128	TYR	C-N-CD	6.13	141.26	128.40
1	C	588	LEU	CB-CG-CD1	-6.12	100.60	111.00
1	C	1032	ASP	CB-CG-OD1	6.11	123.80	118.30
1	C	1188	VAL	CB-CA-C	-6.06	99.89	111.40
1	C	1331	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	C	272	THR	C-N-CD	6.04	141.08	128.40
1	C	1083	ASP	C-N-CD	6.02	141.05	128.40
1	C	495	LEU	CB-CG-CD1	-6.01	100.78	111.00
1	C	546	VAL	CB-CA-C	-6.01	99.97	111.40
1	C	456	ASN	N-CA-CB	-6.01	99.78	110.60
1	C	401	LEU	CB-CG-CD2	-6.00	100.80	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	767	LEU	CB-CA-C	-5.99	98.83	110.20
1	C	875	THR	C-N-CA	5.97	134.84	122.30
1	C	85	ASP	N-CA-C	5.95	127.05	111.00
1	C	1305	MET	CB-CG-SD	-5.94	94.59	112.40
1	C	1098	ALA	N-CA-C	5.93	127.02	111.00
1	C	864	HIS	CB-CA-C	-5.93	98.53	110.40
1	C	1225	GLU	CA-CB-CG	5.93	126.45	113.40
1	C	329	LEU	CB-CG-CD2	-5.93	100.92	111.00
1	C	1144	ARG	NE-CZ-NH2	-5.89	117.36	120.30
1	C	1221	PRO	N-CA-C	5.89	127.42	112.10
1	C	1225	GLU	N-CA-CB	5.88	121.18	110.60
1	C	159	ASP	CB-CG-OD1	-5.87	113.02	118.30
1	C	715	ASN	N-CA-C	-5.87	95.15	111.00
1	C	461	ARG	N-CA-CB	5.85	121.13	110.60
1	C	661	ASN	C-N-CA	-5.85	107.08	121.70
1	C	1275	ASP	CB-CA-C	-5.83	98.73	110.40
1	C	278	LEU	C-N-CA	-5.80	107.19	121.70
1	C	925	VAL	CB-CA-C	5.80	122.41	111.40
1	C	970	LEU	CB-CG-CD2	-5.79	101.15	111.00
1	C	1191	GLU	O-C-N	5.78	131.95	122.70
1	C	136	VAL	C-N-CA	5.78	136.14	121.70
1	C	630	ASN	N-CA-C	-5.76	95.44	111.00
1	C	730	ASP	CB-CG-OD1	-5.75	113.12	118.30
1	C	1233	LEU	CA-CB-CG	5.75	128.53	115.30
1	C	1168	ILE	CG1-CB-CG2	-5.72	98.81	111.40
1	C	408	ILE	CB-CA-C	-5.72	100.17	111.60
1	C	148	GLN	N-CA-CB	-5.71	100.33	110.60
1	C	1191	GLU	N-CA-C	-5.69	95.64	111.00
1	C	121	PHE	N-CA-CB	-5.68	100.37	110.60
1	B	1317	VAL	C-N-CA	5.65	135.83	121.70
1	C	144	ASN	CB-CA-C	5.65	121.70	110.40
1	C	1286	VAL	CB-CA-C	-5.65	100.67	111.40
1	C	422	LEU	CA-CB-CG	5.64	128.26	115.30
1	C	1070	ARG	N-CA-C	-5.64	95.78	111.00
1	C	1298	PHE	C-N-CA	5.63	135.78	121.70
1	C	1181	SER	C-N-CA	5.62	135.76	121.70
1	C	487	SER	N-CA-CB	-5.62	102.07	110.50
1	C	456	ASN	CA-C-N	5.61	129.54	117.20
1	C	706	TYR	CB-CA-C	-5.60	99.20	110.40
1	C	841	ASP	C-N-CA	5.60	135.71	121.70
1	C	1191	GLU	CA-C-N	-5.59	104.90	117.20
1	C	878	SER	C-N-CA	5.59	135.66	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	82	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	C	413	MET	CB-CG-SD	-5.58	95.67	112.40
1	C	547	GLU	CB-CA-C	-5.57	99.26	110.40
1	C	496	LYS	N-CA-C	-5.56	95.99	111.00
1	C	824	LEU	CB-CG-CD1	-5.56	101.55	111.00
1	C	700	ASP	CA-C-N	-5.51	105.07	117.20
1	C	579	LEU	CB-CG-CD1	-5.51	101.63	111.00
1	C	1230	ILE	N-CA-C	5.50	125.84	111.00
1	C	820	ILE	CG1-CB-CG2	-5.50	99.31	111.40
1	C	156	GLN	CB-CA-C	-5.48	99.43	110.40
1	C	687	LEU	CB-CA-C	5.47	120.59	110.20
1	C	815	LEU	C-N-CD	-5.47	108.57	120.60
1	C	632	GLN	N-CA-C	-5.46	96.25	111.00
1	C	718	ASN	N-CA-C	-5.44	96.31	111.00
1	C	696	VAL	CB-CA-C	-5.41	101.12	111.40
1	C	815	LEU	CB-CG-CD2	-5.39	101.84	111.00
1	C	956	ASP	CB-CA-C	5.39	121.17	110.40
1	C	171	GLU	CA-C-N	5.38	129.04	117.20
1	C	1193	ILE	CG1-CB-CG2	-5.38	99.56	111.40
1	C	844	ASP	N-CA-CB	5.38	120.28	110.60
1	B	1317	VAL	N-CA-C	-5.37	96.50	111.00
1	C	158	SER	N-CA-C	5.35	125.44	111.00
1	C	314	ILE	CB-CA-C	-5.34	100.91	111.60
1	C	1141	ILE	CG1-CB-CG2	-5.34	99.66	111.40
1	C	1253	ARG	C-N-CD	-5.34	108.86	120.60
1	C	447	ARG	O-C-N	5.33	131.23	122.70
1	C	859	ILE	CB-CA-C	5.32	122.23	111.60
1	C	874	ILE	C-N-CA	5.32	134.99	121.70
1	C	1014	MET	N-CA-C	-5.31	96.66	111.00
1	C	654	THR	CB-CA-C	-5.31	97.27	111.60
1	C	299	ALA	N-CA-CB	5.27	117.47	110.10
1	C	956	ASP	CB-CG-OD2	5.27	123.04	118.30
1	C	441	ARG	C-N-CD	-5.26	109.02	120.60
1	C	131	HIS	C-N-CD	-5.26	109.03	120.60
1	C	608	THR	C-N-CD	-5.25	109.04	120.60
1	C	542	ARG	CA-C-N	-5.25	105.66	117.20
1	C	138	PHE	CB-CA-C	-5.24	99.92	110.40
1	C	511	VAL	CB-CA-C	-5.22	101.48	111.40
1	C	928	ARG	CB-CA-C	-5.22	99.96	110.40
1	C	875	THR	N-CA-CB	5.22	120.21	110.30
1	C	458	SER	CA-C-O	5.21	131.05	120.10
1	C	639	ASN	N-CA-CB	5.21	119.97	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	826	GLY	N-CA-C	-5.21	100.08	113.10
1	C	1267	THR	N-CA-C	-5.21	96.94	111.00
1	C	1014	MET	CG-SD-CE	-5.20	91.88	100.20
1	C	1325	VAL	N-CA-C	5.20	125.04	111.00
1	C	534	ASN	CB-CA-C	-5.18	100.04	110.40
1	C	1279	SER	C-N-CD	5.18	139.27	128.40
1	C	1198	LYS	N-CA-C	5.17	124.95	111.00
1	C	543	TRP	N-CA-CB	-5.16	101.31	110.60
1	C	565	GLU	CB-CA-C	5.16	120.72	110.40
1	C	698	HIS	CB-CA-C	-5.15	100.09	110.40
1	B	301	LEU	CA-CB-CG	5.14	127.12	115.30
1	C	96	ILE	CB-CA-C	-5.13	101.34	111.60
1	C	152	ASP	CB-CG-OD2	5.13	122.92	118.30
1	C	1113	LYS	N-CA-C	5.13	124.85	111.00
1	C	152	ASP	N-CA-C	5.12	124.83	111.00
1	C	414	LEU	CB-CG-CD1	-5.12	102.29	111.00
1	C	457	GLN	N-CA-C	5.12	124.83	111.00
1	C	484	ARG	N-CA-C	-5.11	97.19	111.00
1	C	626	ARG	NE-CZ-NH2	-5.11	117.74	120.30
1	C	774	LEU	CA-CB-CG	-5.11	103.55	115.30
1	C	352	HIS	N-CA-C	5.11	124.79	111.00
1	C	645	THR	N-CA-C	5.10	124.77	111.00
1	C	646	ASN	N-CA-C	5.10	124.77	111.00
1	C	495	LEU	CA-CB-CG	5.09	127.02	115.30
1	C	75	ILE	C-N-CA	5.09	134.41	121.70
1	C	922	TYR	N-CA-CB	5.09	119.75	110.60
1	C	537	LEU	CB-CG-CD1	-5.08	102.36	111.00
1	C	1292	GLU	N-CA-CB	5.08	119.75	110.60
1	C	1314	ASP	CB-CG-OD1	5.08	122.87	118.30
1	C	466	VAL	CG1-CB-CG2	-5.07	102.78	110.90
1	C	759	ASP	CB-CG-OD2	5.06	122.85	118.30
1	C	379	LEU	CA-CB-CG	5.05	126.92	115.30
1	C	497	LYS	N-CA-C	5.05	124.63	111.00
1	C	119	ASP	C-N-CA	5.04	134.31	121.70
1	C	1021	ARG	NE-CZ-NH1	-5.04	117.78	120.30
1	C	860	ARG	NE-CZ-NH1	-5.04	117.78	120.30
1	C	700	ASP	CB-CG-OD1	5.04	122.83	118.30
1	C	730	ASP	N-CA-C	5.04	124.59	111.00
1	C	1003	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	C	709	MET	CB-CG-SD	-5.03	97.32	112.40
1	C	1202	PHE	CB-CG-CD2	-5.02	117.28	120.80
1	C	823	ILE	CG1-CB-CG2	-5.01	100.38	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	1166	VAL	CB-CA-C	-5.01	101.88	111.40
1	C	418	ASN	N-CA-C	5.01	124.52	111.00

There are no chirality outliers.

All (39) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1193	ILE	Peptide
1	B	1235	PRO	Peptide
1	B	1236	ILE	Peptide
1	B	261	ASP	Peptide
1	B	506	SER	Peptide
1	B	717	THR	Peptide
1	B	825	SER	Peptide
1	B	875	THR	Peptide
1	B	895	VAL	Peptide
1	C	1031	TYR	Mainchain
1	C	1068	ALA	Mainchain
1	C	1093	PRO	Mainchain
1	C	121	PHE	Mainchain
1	C	171	GLU	Mainchain
1	C	172	ASP	Mainchain
1	C	173	GLN	Mainchain
1	C	185	ALA	Mainchain
1	C	244	SER	Mainchain
1	C	279	SER	Mainchain
1	C	317	MET	Mainchain
1	C	334	LEU	Mainchain
1	C	351	ASP	Mainchain
1	C	361	ASN	Mainchain
1	C	398	ARG	Peptide
1	C	436	SER	Mainchain
1	C	448	TYR	Mainchain
1	C	449	PHE	Mainchain
1	C	456	ASN	Mainchain
1	C	503	GLU	Mainchain
1	C	519	LEU	Mainchain
1	C	533	GLN	Mainchain
1	C	635	ILE	Mainchain,Peptide
1	C	661	ASN	Mainchain
1	C	662	VAL	Mainchain
1	C	697	ALA	Mainchain

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Mol	Chain	Res	Type	Group
1	C	768	CYS	Mainchain
1	C	897	TYR	Mainchain
1	C	997	TYR	Mainchain

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	B	9058	0	8964	531	0
1	C	9827	0	9719	1974	0
All	All	18885	0	18683	2459	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 65.

All (2459) 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:C:835:TYR:CE1	1:C:942:HIS:HB3	1.27	1.68
1:C:1278:TYR:CD2	1:C:1288:ILE:HG13	1.23	1.64
1:C:910:LEU:HD23	1:C:915:VAL:CG2	1.27	1.63
1:C:233:VAL:CG2	1:C:234:PRO:HD2	1.28	1.62
1:C:1093:PRO:HG2	1:C:1096:TYR:CE1	1.30	1.61
1:C:233:VAL:HG11	1:C:981:HIS:CE1	1.31	1.60
1:C:829:SER:CB	1:C:965:ARG:HD2	1.15	1.59
1:C:838:GLU:CB	1:C:934:LEU:HB2	1.12	1.55
1:C:1278:TYR:HD2	1:C:1288:ILE:CG1	1.15	1.55
1:C:910:LEU:CD2	1:C:915:VAL:HG23	1.23	1.55
1:C:835:TYR:CE2	1:C:925:VAL:CG2	1.88	1.53
1:C:835:TYR:CE2	1:C:925:VAL:HG21	1.00	1.52
1:C:838:GLU:HB2	1:C:934:LEU:CB	1.42	1.49
1:C:1080:THR:C	1:C:1227:MET:HG2	1.28	1.48
1:C:835:TYR:CD2	1:C:925:VAL:HG21	1.49	1.47
1:C:301:LEU:HD13	1:C:305:THR:CG2	1.41	1.46
1:C:838:GLU:CG	1:C:934:LEU:C	1.81	1.46
1:C:230:ASP:CB	1:C:985:ARG:NE	1.76	1.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:469:ARG:NH1	1:B:498:ILE:CD1	1.78	1.45
1:C:1080:THR:HA	1:C:1227:MET:CG	0.98	1.45
1:C:829:SER:CB	1:C:965:ARG:CD	1.92	1.45
1:C:843:LEU:HD11	1:C:943:GLU:CG	1.01	1.45
1:C:841:ASP:H	1:C:940:ARG:NH1	1.07	1.44
1:C:180:LEU:HD22	1:C:306:GLN:NE2	1.29	1.44
1:C:449:PHE:HB2	1:C:683:TRP:NE1	1.24	1.44
1:C:1080:THR:CA	1:C:1227:MET:HG2	1.22	1.43
1:C:837:THR:O	1:C:934:LEU:CD1	1.67	1.43
1:C:1080:THR:CA	1:C:1227:MET:CG	1.78	1.43
1:C:233:VAL:HG11	1:C:981:HIS:NE2	1.18	1.43
1:C:843:LEU:CD1	1:C:943:GLU:HG3	0.95	1.42
1:B:442:PRO:HB2	1:B:475:ILE:CD1	1.45	1.42
1:C:838:GLU:HG3	1:C:934:LEU:CA	1.50	1.42
1:C:233:VAL:HG22	1:C:234:PRO:CD	1.49	1.41
1:B:389:PHE:CE1	1:B:1319:ARG:HG3	1.54	1.39
1:C:248:VAL:CG1	1:C:970:LEU:HB3	1.53	1.39
1:C:81:ALA:HB2	1:C:170:TYR:CE2	1.59	1.37
1:C:838:GLU:CB	1:C:934:LEU:CB	1.96	1.36
1:C:1093:PRO:CG	1:C:1096:TYR:CE1	2.08	1.36
1:C:449:PHE:CB	1:C:683:TRP:NE1	1.87	1.35
1:C:1214:GLU:CB	1:C:1215:PRO:CD	1.96	1.34
1:C:835:TYR:CD1	1:C:942:HIS:HB3	1.60	1.34
1:C:233:VAL:CG1	1:C:981:HIS:CE1	2.08	1.33
1:C:449:PHE:CB	1:C:683:TRP:HE1	1.39	1.33
1:C:1219:ASP:OD1	1:C:1220:PRO:HD2	1.16	1.33
1:C:835:TYR:CE1	1:C:942:HIS:CB	2.12	1.32
1:C:338:ARG:CG	1:C:342:THR:HG22	1.57	1.32
1:B:135:LYS:CE	1:C:468:ALA:O	1.77	1.32
1:C:383:SER:OG	1:C:796:PRO:CG	1.78	1.32
1:C:233:VAL:CG1	1:C:981:HIS:NE2	1.91	1.31
1:C:230:ASP:HB3	1:C:985:ARG:CD	1.59	1.31
1:C:864:HIS:CE1	1:C:1030:ARG:NH2	2.01	1.29
1:C:1109:SER:OG	1:C:1118:THR:HG21	1.19	1.29
1:C:835:TYR:CZ	1:C:925:VAL:HG21	1.69	1.28
1:C:151:SER:HB3	1:C:400:GLU:OE1	1.24	1.28
1:C:836:GLN:CB	1:C:940:ARG:HG2	1.62	1.27
1:C:230:ASP:CB	1:C:985:ARG:HE	1.36	1.27
1:C:836:GLN:HB2	1:C:940:ARG:CG	1.62	1.27
1:C:838:GLU:HG3	1:C:934:LEU:C	0.90	1.27
1:C:1089:VAL:HG23	1:C:1232:PRO:O	1.30	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1214:GLU:HB3	1:C:1215:PRO:CD	1.59	1.26
1:C:445:GLU:OE2	1:C:447:ARG:HG2	1.27	1.26
1:C:829:SER:HB2	1:C:965:ARG:CD	1.52	1.26
1:C:230:ASP:OD1	1:C:985:ARG:HD3	1.30	1.26
1:B:442:PRO:CB	1:B:475:ILE:HD11	1.66	1.26
1:C:835:TYR:CZ	1:C:925:VAL:CG2	2.20	1.25
1:C:910:LEU:CD2	1:C:915:VAL:CG2	1.96	1.25
1:C:838:GLU:CG	1:C:935:GLN:N	1.98	1.25
1:C:186:ASP:OD1	1:C:279:SER:N	1.69	1.25
1:C:446:LYS:HD3	1:C:448:TYR:OH	1.34	1.25
1:C:659:LEU:O	1:C:662:VAL:HG23	1.27	1.25
1:C:153:ASP:OD2	1:C:401:LEU:HB2	1.10	1.24
1:C:450:PRO:HA	1:C:454:GLU:CG	1.67	1.24
1:C:180:LEU:CD2	1:C:306:GLN:NE2	2.01	1.23
1:C:830:VAL:CG2	1:C:947:GLU:CB	2.15	1.23
1:C:1191:GLU:O	1:C:1195:THR:OG1	1.55	1.23
1:C:225:ILE:HG21	1:C:247:TYR:CD1	1.73	1.22
1:C:230:ASP:CG	1:C:985:ARG:HD3	1.57	1.22
1:B:135:LYS:HE2	1:C:468:ALA:O	1.30	1.22
1:C:372:ALA:HB1	1:C:1315:MET:CE	1.68	1.22
1:C:449:PHE:HB2	1:C:683:TRP:CD1	1.74	1.22
1:C:230:ASP:CG	1:C:985:ARG:CD	2.07	1.22
1:C:660:ALA:O	1:C:662:VAL:N	1.72	1.22
1:C:1119:TYR:O	1:C:1127:ALA:O	1.54	1.22
1:C:230:ASP:C	1:C:985:ARG:HG2	1.58	1.22
1:C:830:VAL:CG2	1:C:947:GLU:HB2	1.68	1.22
1:C:230:ASP:CB	1:C:985:ARG:CD	2.14	1.21
1:C:230:ASP:HB3	1:C:985:ARG:CG	1.68	1.21
1:C:892:VAL:CG1	1:C:894:VAL:CG1	2.19	1.21
1:C:81:ALA:CB	1:C:170:TYR:CE2	2.24	1.20
1:C:446:LYS:CD	1:C:448:TYR:OH	1.88	1.20
1:C:613:LEU:CD2	1:C:632:GLN:HB3	1.71	1.20
1:C:1079:LEU:CD1	1:C:1231:TYR:OH	1.90	1.20
1:C:1214:GLU:CB	1:C:1215:PRO:HD2	1.60	1.19
1:C:845:GLU:OE2	1:C:911:ARG:NE	1.72	1.19
1:C:449:PHE:CA	1:C:683:TRP:HE1	1.54	1.19
1:C:81:ALA:CB	1:C:170:TYR:HE2	1.55	1.19
1:C:225:ILE:CG2	1:C:247:TYR:HD1	1.56	1.18
1:C:654:THR:O	1:C:658:THR:HG22	1.41	1.18
1:C:1263:TYR:CE1	1:C:1278:TYR:CE1	2.32	1.18
1:C:838:GLU:HG3	1:C:935:GLN:N	1.58	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:213:PHE:CB	1:C:219:ILE:HG21	1.74	1.17
1:C:251:LEU:HD23	1:C:1062:ILE:HG13	1.21	1.17
1:C:1292:GLU:O	1:C:1293:VAL:HG23	1.40	1.17
1:C:230:ASP:CG	1:C:985:ARG:NE	1.95	1.17
1:B:388:GLN:HB2	1:B:1320:VAL:HG11	1.18	1.17
1:B:472:GLU:HB3	1:B:761:SER:OG	1.43	1.17
1:C:841:ASP:N	1:C:940:ARG:NH1	1.93	1.17
1:C:835:TYR:O	1:C:846:GLY:HA2	1.42	1.16
1:C:184:GLU:O	1:C:187:ASP:HB3	1.41	1.16
1:C:232:LEU:CD2	1:C:249:SER:HB3	1.74	1.16
1:C:252:LEU:CD1	1:C:971:MET:HE1	1.76	1.16
1:C:232:LEU:HD21	1:C:249:SER:CB	1.75	1.16
1:C:383:SER:OG	1:C:796:PRO:HG3	1.01	1.16
1:C:240:GLY:O	1:C:242:GLU:N	1.79	1.15
1:C:407:HIS:CD2	1:C:1047:LEU:HA	1.80	1.15
1:C:829:SER:OG	1:C:965:ARG:CD	1.74	1.15
1:C:230:ASP:HB3	1:C:985:ARG:NE	1.38	1.15
1:C:406:ASP:OD1	1:C:1039:ALA:HB2	1.41	1.15
1:C:1306:THR:OG1	1:C:1308:ASN:HA	1.47	1.15
1:C:875:THR:OG1	1:C:899:SER:O	1.61	1.15
1:C:338:ARG:HG3	1:C:342:THR:CG2	1.77	1.15
1:C:1072:ASP:O	1:C:1234:GLN:NE2	1.78	1.15
1:C:837:THR:HG22	1:C:934:LEU:CD1	1.77	1.14
1:B:274:MET:CE	1:C:978:GLN:OE1	1.95	1.14
1:C:638:THR:HG21	1:C:1331:ARG:NH2	1.60	1.14
1:C:838:GLU:OE1	1:C:935:GLN:HB2	1.43	1.14
1:B:469:ARG:NH1	1:B:498:ILE:HD12	0.82	1.14
1:C:1219:ASP:OD1	1:C:1220:PRO:CD	1.94	1.14
1:C:1278:TYR:CD2	1:C:1288:ILE:CG1	1.99	1.14
1:C:233:VAL:CG1	1:C:981:HIS:CD2	2.29	1.13
1:C:362:LEU:HD12	1:C:1302:VAL:CG1	1.79	1.13
1:C:843:LEU:HD11	1:C:943:GLU:HG2	1.29	1.13
1:C:901:VAL:HG22	1:C:930:ALA:HB2	1.30	1.13
1:C:838:GLU:OE1	1:C:935:GLN:N	1.80	1.13
1:C:1000:LEU:CD2	1:C:1010:ARG:HH21	1.62	1.13
1:C:248:VAL:HG13	1:C:970:LEU:HB3	1.15	1.13
1:C:671:ASP:O	1:C:672:MET:HB3	1.49	1.13
1:C:451:GLU:OE1	1:C:685:ARG:HG3	1.46	1.13
1:C:383:SER:HG	1:C:796:PRO:CG	1.55	1.12
1:C:613:LEU:HD21	1:C:632:GLN:CB	1.79	1.12
1:C:230:ASP:CG	1:C:985:ARG:HE	1.49	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:668:VAL:CG2	1:C:673:GLN:HB3	1.78	1.12
1:C:1278:TYR:CE2	1:C:1288:ILE:HG13	1.82	1.12
1:C:1079:LEU:HD11	1:C:1231:TYR:OH	0.97	1.12
1:B:472:GLU:O	1:B:761:SER:HB2	1.47	1.11
1:C:144:ASN:HB3	1:C:1318:GLU:OE1	1.47	1.11
1:C:252:LEU:HD13	1:C:971:MET:CE	1.80	1.11
1:C:323:THR:HB	1:C:1266:ASP:HB2	1.27	1.11
1:C:822:MET:HG3	1:C:1044:ARG:HD3	1.25	1.11
1:B:135:LYS:CD	1:C:468:ALA:O	1.97	1.11
1:C:372:ALA:HB1	1:C:1315:MET:HE1	1.26	1.11
1:C:843:LEU:CG	1:C:943:GLU:HG3	1.79	1.11
1:C:157:ILE:HD11	1:C:263:ARG:CG	1.80	1.11
1:C:338:ARG:HG2	1:C:342:THR:N	1.64	1.11
1:C:362:LEU:CD1	1:C:1302:VAL:CG1	2.29	1.11
1:C:660:ALA:C	1:C:662:VAL:H	1.39	1.11
1:C:701:HIS:HE1	1:C:791:ILE:HG23	1.12	1.10
1:C:1093:PRO:HB2	1:C:1096:TYR:CD1	1.86	1.10
1:B:469:ARG:CZ	1:B:498:ILE:HD12	1.81	1.10
1:C:879:THR:H	1:C:880:PRO:CD	1.63	1.10
1:C:1219:ASP:HB2	1:C:1220:PRO:HD3	1.33	1.10
1:C:252:LEU:HD11	1:C:823:ILE:HG21	1.29	1.09
1:C:410:ARG:NH1	1:C:1048:ASP:OD2	1.85	1.09
1:C:830:VAL:HG21	1:C:947:GLU:CB	1.77	1.09
1:C:1084:PRO:O	1:C:1208:ASP:O	1.68	1.09
1:C:478:ILE:CD1	1:C:762:ILE:HD11	1.82	1.09
1:C:841:ASP:H	1:C:940:ARG:CZ	1.65	1.09
1:C:892:VAL:CG1	1:C:894:VAL:HG13	1.80	1.09
1:B:472:GLU:CB	1:B:761:SER:OG	2.00	1.09
1:C:1171:ILE:HD11	1:C:1202:PHE:CZ	1.86	1.09
1:C:334:LEU:HD21	1:C:366:MET:HE3	1.27	1.08
1:C:338:ARG:HG3	1:C:342:THR:HG22	1.14	1.08
1:C:338:ARG:CD	1:C:342:THR:HG22	1.83	1.08
1:C:1047:LEU:HB2	1:C:1051:ARG:HB2	1.34	1.08
1:B:135:LYS:HE3	1:C:470:ALA:H	1.06	1.08
1:C:864:HIS:CE1	1:C:1030:ARG:HH21	1.66	1.08
1:C:342:THR:O	1:C:1305:MET:SD	2.12	1.08
1:C:528:ILE:HG21	1:C:758:ILE:HD11	1.26	1.08
1:C:1263:TYR:CZ	1:C:1278:TYR:OH	2.06	1.08
1:C:301:LEU:CD1	1:C:305:THR:CG2	2.32	1.07
1:C:362:LEU:CD1	1:C:1302:VAL:HG12	1.80	1.07
1:C:633:THR:HG21	1:C:710:SER:OG	1.53	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:656:VAL:HG11	1:C:688:GLU:HB3	1.27	1.07
1:C:225:ILE:HG21	1:C:247:TYR:HD1	0.97	1.07
1:C:611:GLY:O	1:C:634:TYR:CZ	2.06	1.07
1:C:148:GLN:NE2	1:C:375:ARG:HH12	1.51	1.06
1:C:864:HIS:HE1	1:C:1030:ARG:NH2	1.44	1.06
1:C:929:PHE:HB2	1:C:936:MET:HE1	1.37	1.06
1:C:1289:PRO:O	1:C:1293:VAL:HG21	1.53	1.06
1:C:450:PRO:HA	1:C:454:GLU:HG2	1.34	1.06
1:C:1289:PRO:O	1:C:1293:VAL:CG2	2.02	1.06
1:C:892:VAL:HG12	1:C:894:VAL:HG13	1.32	1.06
1:C:606:LEU:HD13	1:C:655:ILE:HG23	1.25	1.05
1:B:472:GLU:HB3	1:B:761:SER:CB	1.84	1.05
1:C:654:THR:HG22	1:C:658:THR:HG21	1.38	1.05
1:C:1263:TYR:CE1	1:C:1278:TYR:CZ	2.43	1.05
1:C:892:VAL:HG12	1:C:894:VAL:CG1	1.84	1.05
1:C:1000:LEU:CD2	1:C:1010:ARG:NH2	2.20	1.05
1:C:1179:THR:OG1	1:C:1180:PRO:HD2	1.54	1.05
1:B:461:ARG:HB2	1:B:461:ARG:HH11	1.20	1.05
1:B:388:GLN:HB2	1:B:1320:VAL:CG1	1.87	1.04
1:C:153:ASP:OD2	1:C:401:LEU:CB	2.03	1.04
1:C:251:LEU:CD2	1:C:1062:ILE:HG13	1.86	1.04
1:C:838:GLU:CG	1:C:934:LEU:HB2	1.86	1.04
1:C:929:PHE:CB	1:C:936:MET:HE1	1.87	1.04
1:B:459:ALA:O	1:B:463:VAL:HG13	1.56	1.04
1:C:1179:THR:OG1	1:C:1180:PRO:CD	2.05	1.04
1:C:1306:THR:CB	1:C:1308:ASN:H	1.63	1.04
1:C:151:SER:CB	1:C:400:GLU:OE1	2.04	1.04
1:C:736:SER:HB2	1:C:1016:ASN:O	1.57	1.04
1:C:835:TYR:CD1	1:C:942:HIS:CB	2.38	1.04
1:C:887:VAL:HG11	1:C:893:ALA:HB2	1.37	1.03
1:C:1089:VAL:HG21	1:C:1233:LEU:HA	1.38	1.03
1:C:838:GLU:CD	1:C:935:GLN:N	2.11	1.03
1:C:701:HIS:CE1	1:C:791:ILE:HG23	1.94	1.03
1:C:830:VAL:CG2	1:C:947:GLU:HB3	1.83	1.03
1:C:837:THR:HG22	1:C:934:LEU:HD11	1.39	1.03
1:C:839:ALA:O	1:C:940:ARG:NH2	1.91	1.03
1:B:388:GLN:O	1:B:1320:VAL:HG12	1.56	1.03
1:C:233:VAL:CG2	1:C:234:PRO:CD	2.22	1.02
1:C:879:THR:H	1:C:880:PRO:HD3	1.22	1.02
1:C:231:LEU:O	1:C:982:ALA:HA	1.59	1.02
1:C:1280:PRO:HB3	1:C:1287:GLY:HA2	1.41	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:157:ILE:HD11	1:C:263:ARG:HG2	1.39	1.02
1:C:668:VAL:HG21	1:C:673:GLN:HB3	1.05	1.02
1:C:874:ILE:HG21	1:C:902:ILE:HD11	1.42	1.02
1:C:1214:GLU:HB2	1:C:1215:PRO:HD2	1.02	1.02
1:C:248:VAL:HG11	1:C:970:LEU:HB3	1.41	1.02
1:C:1093:PRO:CB	1:C:1096:TYR:CE1	2.41	1.02
1:C:157:ILE:CG1	1:C:263:ARG:HG2	1.90	1.01
1:B:135:LYS:HD3	1:C:468:ALA:O	1.59	1.01
1:C:232:LEU:HD21	1:C:249:SER:HB3	1.03	1.01
1:C:450:PRO:HA	1:C:454:GLU:HG3	1.39	1.01
1:C:611:GLY:N	1:C:636:PRO:O	1.93	1.01
1:C:830:VAL:HG22	1:C:947:GLU:HB3	1.40	1.01
1:C:838:GLU:CG	1:C:934:LEU:CA	2.27	1.01
1:B:274:MET:HE3	1:C:978:GLN:OE1	1.57	1.01
1:B:793:TYR:HD2	1:B:1321:ASN:ND2	1.57	1.00
1:B:135:LYS:HE3	1:C:470:ALA:N	1.76	1.00
1:B:469:ARG:HH12	1:B:498:ILE:HD12	1.21	1.00
1:B:469:ARG:HH11	1:B:498:ILE:CD1	1.52	1.00
1:C:839:ALA:C	1:C:940:ARG:NH1	2.14	1.00
1:C:301:LEU:CD1	1:C:305:THR:HG23	1.92	1.00
1:C:924:ASP:OD1	1:C:927:SER:HB2	1.61	0.99
1:C:384:MET:HA	1:C:708:THR:HG21	1.45	0.99
1:C:1171:ILE:HD11	1:C:1202:PHE:CE1	1.96	0.99
1:C:235:ILE:HD11	1:C:978:GLN:NE2	1.76	0.99
1:C:638:THR:HG21	1:C:1331:ARG:HH21	1.24	0.99
1:C:341:LYS:HG3	1:C:1306:THR:HB	1.43	0.99
1:C:362:LEU:HD12	1:C:1302:VAL:HG12	1.00	0.99
1:C:820:ILE:HG21	1:C:983:ILE:CG1	1.93	0.99
1:C:1093:PRO:CG	1:C:1096:TYR:HE1	1.65	0.99
1:B:389:PHE:HE1	1:B:1319:ARG:CG	1.76	0.99
1:C:301:LEU:HD13	1:C:305:THR:HG23	1.01	0.99
1:C:879:THR:N	1:C:880:PRO:HD3	1.77	0.99
1:C:1079:LEU:HD11	1:C:1231:TYR:HH	1.19	0.99
1:C:157:ILE:CD1	1:C:263:ARG:HG2	1.92	0.99
1:C:896:LEU:HD22	1:C:918:VAL:HG21	1.44	0.99
1:C:1219:ASP:CB	1:C:1220:PRO:HD3	1.89	0.99
1:C:1089:VAL:CG2	1:C:1232:PRO:O	2.11	0.98
1:C:835:TYR:HE2	1:C:925:VAL:HG11	1.28	0.98
1:B:274:MET:HE1	1:C:978:GLN:OE1	1.63	0.98
1:C:243:GLN:O	1:C:246:GLU:HB2	1.61	0.98
1:C:440:ILE:HD13	1:C:478:ILE:HG21	1.43	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:301:LEU:HD13	1:C:305:THR:HG21	1.45	0.98
1:C:654:THR:HG22	1:C:658:THR:CG2	1.93	0.98
1:C:254:VAL:CG1	1:C:1062:ILE:HD11	1.93	0.98
1:C:835:TYR:CZ	1:C:925:VAL:HG22	1.95	0.98
1:C:1173:TYR:CD1	1:C:1204:LEU:HD12	1.98	0.98
1:C:242:GLU:HB3	1:C:1200:LYS:HD2	1.46	0.98
1:C:1109:SER:OG	1:C:1118:THR:CG2	2.12	0.98
1:C:261:ASP:O	1:C:1054:ARG:NH2	1.96	0.98
1:C:840:ASP:N	1:C:940:ARG:HH12	1.60	0.98
1:C:1093:PRO:HG2	1:C:1096:TYR:CZ	1.98	0.98
1:C:213:PHE:HB2	1:C:219:ILE:HG21	1.41	0.98
1:C:815:LEU:HB3	1:C:816:PRO:HD2	1.45	0.98
1:C:1000:LEU:HD22	1:C:1010:ARG:NH2	1.78	0.97
1:C:1214:GLU:HB3	1:C:1215:PRO:HD3	0.98	0.97
1:C:180:LEU:HD22	1:C:306:GLN:HE21	1.23	0.97
1:C:509:VAL:HG23	1:C:683:TRP:CZ3	1.99	0.97
1:C:879:THR:N	1:C:880:PRO:CD	2.23	0.97
1:C:148:GLN:HE21	1:C:375:ARG:NH1	1.62	0.97
1:C:554:ARG:HD2	1:C:594:LEU:HD21	1.47	0.97
1:C:451:GLU:OE1	1:C:685:ARG:CG	2.12	0.97
1:C:1137:VAL:O	1:C:1139:MET:N	1.97	0.97
1:C:452:ASN:O	1:C:453:LEU:HB2	1.64	0.97
1:C:668:VAL:HG21	1:C:673:GLN:CB	1.94	0.97
1:C:638:THR:CG2	1:C:1331:ARG:NH2	2.27	0.96
1:C:1155:ILE:CG2	1:C:1166:VAL:HG11	1.94	0.96
1:C:522:PRO:HG2	1:C:636:PRO:HB3	1.47	0.96
1:C:446:LYS:HD3	1:C:448:TYR:HH	1.24	0.96
1:C:1278:TYR:HD2	1:C:1288:ILE:HG12	1.28	0.96
1:C:841:ASP:N	1:C:940:ARG:CZ	2.28	0.96
1:C:450:PRO:CA	1:C:454:GLU:HG2	1.96	0.96
1:C:963:ALA:HB3	1:C:1059:LEU:HG	1.48	0.96
1:C:862:ARG:HB3	1:C:952:PHE:CZ	2.01	0.95
1:C:1031:TYR:HE2	1:C:1041:ARG:NH1	1.63	0.95
1:C:338:ARG:HG3	1:C:342:THR:CB	1.96	0.95
1:C:371:THR:O	1:C:374:ASP:N	1.98	0.95
1:C:837:THR:O	1:C:934:LEU:HD13	0.78	0.95
1:C:184:GLU:O	1:C:187:ASP:CB	2.15	0.95
1:C:372:ALA:CB	1:C:1315:MET:CE	2.43	0.95
1:C:449:PHE:O	1:C:683:TRP:HD1	1.46	0.95
1:C:659:LEU:O	1:C:662:VAL:CG2	2.15	0.95
1:C:1079:LEU:H	1:C:1079:LEU:HD12	1.27	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:85:ASP:OD2	1:C:161:LYS:HG3	1.65	0.95
1:C:1120:THR:O	1:C:1122:PRO:HD3	1.67	0.95
1:C:910:LEU:HD21	1:C:915:VAL:HG23	1.46	0.95
1:C:321:ALA:HB3	1:C:1283:ASN:ND2	1.81	0.95
1:C:815:LEU:HD13	1:C:1051:ARG:NH2	1.81	0.95
1:C:741:TYR:CE2	1:C:1022:ILE:HD11	2.01	0.94
1:C:1093:PRO:HB2	1:C:1096:TYR:CE1	2.02	0.94
1:C:874:ILE:HD11	1:C:883:ILE:CD1	1.97	0.94
1:C:909:TYR:CE1	1:C:913:ASN:OD1	2.20	0.94
1:C:1121:HIS:CD2	1:C:1135:PRO:CG	2.50	0.94
1:C:1310:ARG:CZ	1:C:1310:ARG:HA	1.96	0.94
1:C:248:VAL:HG11	1:C:970:LEU:C	1.88	0.94
1:C:829:SER:HB3	1:C:965:ARG:HD2	1.49	0.94
1:C:1243:ARG:HB3	1:C:1258:VAL:HG22	1.47	0.94
1:C:148:GLN:NE2	1:C:375:ARG:NH1	2.15	0.94
1:C:838:GLU:OE1	1:C:935:GLN:CB	2.15	0.94
1:C:999:LYS:HB2	1:C:1008:LEU:O	1.67	0.94
1:C:1206:PHE:CD2	1:C:1236:ILE:CD1	2.50	0.94
1:C:1292:GLU:O	1:C:1293:VAL:CG2	2.14	0.94
1:B:472:GLU:CB	1:B:761:SER:CB	2.45	0.94
1:C:1081:ASP:N	1:C:1227:MET:HG2	1.82	0.93
1:C:338:ARG:CG	1:C:342:THR:CG2	2.42	0.93
1:C:176:LYS:HG3	1:C:177:LYS:H	1.32	0.93
1:C:887:VAL:CG1	1:C:893:ALA:HB2	1.97	0.93
1:C:317:MET:SD	1:C:1262:SER:HB2	2.08	0.93
1:C:1134:ARG:HB3	1:C:1135:PRO:HD3	1.51	0.93
1:B:262:ASN:O	1:B:361:ASN:ND2	2.02	0.93
1:C:449:PHE:HA	1:C:683:TRP:HE1	1.32	0.93
1:C:838:GLU:CG	1:C:934:LEU:CB	2.42	0.93
1:B:389:PHE:CE1	1:B:1319:ARG:CG	2.50	0.93
1:C:233:VAL:HG13	1:C:981:HIS:CD2	2.05	0.92
1:C:259:MET:HG3	1:C:1055:LEU:HB2	1.49	0.92
1:C:226:PRO:O	1:C:250:GLY:HA3	1.70	0.92
1:C:311:ASN:O	1:C:315:THR:HG23	1.69	0.92
1:C:892:VAL:HG11	1:C:894:VAL:CG1	1.96	0.92
1:C:445:GLU:OE2	1:C:447:ARG:CG	2.17	0.92
1:B:235:ILE:HG13	1:B:978:GLN:HE21	1.33	0.92
1:C:230:ASP:CB	1:C:985:ARG:CG	2.45	0.92
1:C:822:MET:CG	1:C:1044:ARG:HD3	1.99	0.92
1:C:956:ASP:O	1:C:959:GLN:OE1	1.85	0.92
1:C:701:HIS:CE1	1:C:791:ILE:CG2	2.53	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:839:ALA:O	1:C:940:ARG:CZ	2.18	0.92
1:C:843:LEU:HD12	1:C:943:GLU:HG3	1.46	0.92
1:C:845:GLU:CD	1:C:911:ARG:HE	1.73	0.92
1:C:870:ASP:O	1:C:871:PRO:C	2.06	0.92
1:C:213:PHE:HB3	1:C:219:ILE:HG21	1.47	0.92
1:C:478:ILE:HD12	1:C:762:ILE:HD11	1.50	0.92
1:C:1121:HIS:HD2	1:C:1135:PRO:HG3	1.35	0.92
1:C:405:HIS:CD2	1:C:625:PRO:HA	2.03	0.92
1:B:1249:ASN:OD1	1:C:1115:ASN:OD1	1.88	0.92
1:C:230:ASP:HB2	1:C:985:ARG:HE	1.35	0.92
1:C:841:ASP:H	1:C:940:ARG:HH12	0.97	0.92
1:C:1080:THR:C	1:C:1227:MET:CG	2.25	0.91
1:C:225:ILE:CG2	1:C:247:TYR:CD1	2.41	0.91
1:C:935:GLN:HB3	1:C:939:ASN:HB3	1.51	0.91
1:C:528:ILE:HD13	1:C:758:ILE:HD11	1.53	0.91
1:C:701:HIS:HE1	1:C:791:ILE:CG2	1.83	0.91
1:C:1155:ILE:HG21	1:C:1166:VAL:HG11	1.51	0.91
1:C:495:LEU:HD11	1:C:531:ASP:HB3	1.50	0.90
1:C:838:GLU:O	1:C:940:ARG:NH1	2.04	0.90
1:C:1089:VAL:CG2	1:C:1233:LEU:HA	1.98	0.90
1:C:248:VAL:CG1	1:C:970:LEU:CB	2.47	0.90
1:C:452:ASN:O	1:C:453:LEU:CD2	2.18	0.90
1:C:660:ALA:O	1:C:663:VAL:N	2.05	0.90
1:C:1279:SER:N	1:C:1280:PRO:HA	1.87	0.90
1:C:1084:PRO:HD2	1:C:1085:ASP:OD1	1.72	0.90
1:C:870:ASP:O	1:C:871:PRO:O	1.89	0.90
1:C:446:LYS:HD2	1:C:448:TYR:OH	1.71	0.90
1:C:838:GLU:HB3	1:C:934:LEU:CB	2.02	0.90
1:C:1306:THR:OG1	1:C:1308:ASN:CA	2.19	0.90
1:C:87:GLU:HB2	1:C:159:ASP:O	1.72	0.90
1:C:509:VAL:CG2	1:C:683:TRP:CH2	2.55	0.89
1:C:835:TYR:HE1	1:C:942:HIS:HB3	1.17	0.89
1:C:157:ILE:HD11	1:C:263:ARG:CB	2.01	0.89
1:C:1085:ASP:HB2	1:C:1086:PRO:CD	2.02	0.89
1:C:312:ARG:HG3	1:C:312:ARG:HH21	1.38	0.89
1:C:837:THR:C	1:C:934:LEU:HD13	1.91	0.89
1:C:310:LEU:HD21	1:C:1242:MET:HE3	1.55	0.89
1:C:610:GLN:HA	1:C:610:GLN:HE21	1.36	0.89
1:C:892:VAL:CG1	1:C:894:VAL:HG12	2.00	0.89
1:C:1306:THR:OG1	1:C:1308:ASN:N	2.06	0.89
1:C:671:ASP:O	1:C:672:MET:CB	2.14	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:338:ARG:HA	1:C:342:THR:HA	1.52	0.88
1:C:204:VAL:O	1:C:1240:ARG:O	1.90	0.88
1:C:81:ALA:HB2	1:C:170:TYR:HE2	0.75	0.88
1:B:898:GLN:HE21	1:B:917:VAL:HB	1.38	0.88
1:C:323:THR:HA	1:C:1279:SER:OG	1.72	0.88
1:C:389:PHE:CE1	1:C:1319:ARG:HB3	2.08	0.88
1:C:829:SER:OG	1:C:965:ARG:HD3	1.73	0.88
1:C:843:LEU:CD1	1:C:943:GLU:CG	1.86	0.88
1:C:1134:ARG:HB3	1:C:1135:PRO:CD	2.03	0.88
1:B:276:ASN:HD21	1:C:244:SER:HB3	1.39	0.88
1:C:849:MET:HA	1:C:917:VAL:O	1.74	0.88
1:C:323:THR:HB	1:C:1266:ASP:CB	2.04	0.88
1:C:1322:PRO:HB3	1:C:1328:ILE:HD13	1.54	0.88
1:C:924:ASP:OD1	1:C:927:SER:N	2.06	0.88
1:C:129:ALA:HB3	1:C:133:MET:HG2	1.57	0.87
1:C:77:THR:O	1:C:172:ASP:HB2	1.74	0.87
1:C:334:LEU:HD21	1:C:366:MET:CE	2.04	0.87
1:C:1093:PRO:HB2	1:C:1096:TYR:HD1	1.36	0.87
1:C:735:THR:HG21	1:C:1028:VAL:HG21	1.57	0.87
1:C:610:GLN:OE1	1:C:651:ARG:HG2	1.74	0.87
1:C:910:LEU:CD2	1:C:915:VAL:HG21	2.04	0.87
1:C:96:ILE:CD1	1:C:103:GLY:HA2	2.04	0.87
1:C:266:ILE:HD13	1:C:1304:MET:HB2	1.56	0.87
1:C:449:PHE:CA	1:C:683:TRP:NE1	2.22	0.87
1:C:1271:SER:HA	1:C:1277:LEU:HD13	1.56	0.87
1:C:213:PHE:CB	1:C:219:ILE:CG2	2.53	0.87
1:C:213:PHE:HB3	1:C:219:ILE:CG2	2.05	0.87
1:C:830:VAL:HG22	1:C:947:GLU:CB	2.00	0.87
1:C:838:GLU:HG3	1:C:934:LEU:O	1.75	0.87
1:C:503:GLU:OE2	1:C:542:ARG:HD2	1.75	0.86
1:C:874:ILE:HD11	1:C:883:ILE:HD11	1.57	0.86
1:C:886:SER:O	1:C:890:THR:HG22	1.74	0.86
1:C:248:VAL:HG13	1:C:970:LEU:CB	2.03	0.86
1:C:449:PHE:HA	1:C:683:TRP:NE1	1.89	0.86
1:C:841:ASP:N	1:C:940:ARG:HH12	1.63	0.86
1:C:1093:PRO:CB	1:C:1096:TYR:HE1	1.85	0.86
1:C:122:ASN:O	1:C:122:ASN:ND2	2.07	0.86
1:C:265:VAL:HG21	1:C:1301:VAL:HG23	1.57	0.86
1:C:666:ARG:HG2	1:C:666:ARG:HH11	1.40	0.86
1:C:1093:PRO:CB	1:C:1096:TYR:CD1	2.59	0.86
1:C:1211:LEU:HD11	1:C:1246:VAL:HG23	1.55	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:493:HIS:HB2	1:C:756:THR:O	1.74	0.86
1:C:838:GLU:CD	1:C:935:GLN:H	1.76	0.86
1:C:901:VAL:CG2	1:C:930:ALA:HB2	2.06	0.86
1:C:924:ASP:CG	1:C:927:SER:HB2	1.95	0.86
1:C:1121:HIS:CD2	1:C:1135:PRO:HG3	2.08	0.86
1:B:442:PRO:CB	1:B:475:ILE:CD1	2.39	0.86
1:C:1306:THR:C	1:C:1308:ASN:H	1.56	0.86
1:B:461:ARG:HE	1:B:504:ASP:CB	1.89	0.85
1:C:206:ILE:O	1:C:1239:ALA:HB1	1.76	0.85
1:C:323:THR:CB	1:C:1266:ASP:HB2	2.06	0.85
1:C:530:GLY:HA3	1:C:575:TRP:CD1	2.11	0.85
1:C:375:ARG:HG2	1:C:375:ARG:HH11	1.38	0.85
1:C:213:PHE:HB3	1:C:219:ILE:CB	2.05	0.85
1:C:252:LEU:HD13	1:C:971:MET:HE1	0.89	0.85
1:C:1306:THR:C	1:C:1308:ASN:N	2.21	0.85
1:C:199:TYR:OH	1:C:1247:ASN:ND2	2.09	0.85
1:C:462:LEU:O	1:C:462:LEU:HD22	1.76	0.85
1:C:1219:ASP:CB	1:C:1220:PRO:CD	2.54	0.85
1:B:525:PHE:O	1:B:529:LYS:HB3	1.76	0.85
1:C:163:TYR:CE2	1:C:258:VAL:HG23	2.11	0.85
1:C:148:GLN:HE21	1:C:375:ARG:HH12	1.11	0.85
1:C:338:ARG:HG2	1:C:341:LYS:C	1.97	0.85
1:C:1072:ASP:H	1:C:1234:GLN:HE22	1.25	0.85
1:C:820:ILE:HG21	1:C:983:ILE:HG12	1.58	0.84
1:C:371:THR:O	1:C:373:ASP:N	2.09	0.84
1:C:849:MET:HG2	1:C:919:MET:HE3	1.58	0.84
1:C:552:ILE:HD12	1:C:572:ASN:HB2	1.58	0.84
1:C:929:PHE:CB	1:C:936:MET:CE	2.55	0.84
1:B:919:MET:SD	1:B:928:ARG:NH1	2.51	0.84
1:C:334:LEU:HD11	1:C:366:MET:HE1	1.58	0.84
1:C:405:HIS:NE2	1:C:625:PRO:HA	1.90	0.84
1:C:96:ILE:HD12	1:C:103:GLY:HA2	1.57	0.84
1:C:301:LEU:CD1	1:C:305:THR:HG21	2.05	0.84
1:C:454:GLU:O	1:C:455:GLN:HB3	1.76	0.84
1:C:663:VAL:O	1:C:677:ARG:HD2	1.76	0.84
1:B:269:GLU:HB3	1:B:292:ASN:HD22	1.40	0.84
1:B:461:ARG:HH11	1:B:461:ARG:CB	1.89	0.84
1:C:833:ARG:NH1	1:C:942:HIS:NE2	2.26	0.84
1:B:472:GLU:HA	1:B:473:ALA:HB2	1.57	0.84
1:B:1276:LEU:HB3	1:B:1290:LYS:HD3	1.59	0.84
1:C:154:PHE:CE1	1:C:361:ASN:ND2	2.46	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:700:ASP:OD2	1:C:1326:ARG:HG3	1.77	0.84
1:C:733:VAL:HG21	1:C:1022:ILE:HD12	1.60	0.84
1:C:874:ILE:HG13	1:C:895:VAL:CG1	2.08	0.84
1:C:1263:TYR:HE1	1:C:1278:TYR:CE1	1.95	0.84
1:B:459:ALA:O	1:B:463:VAL:CG1	2.26	0.83
1:C:414:LEU:HD23	1:C:814:THR:OG1	1.77	0.83
1:C:1285:GLN:HE21	1:C:1285:GLN:H	1.24	0.83
1:C:495:LEU:H	1:C:495:LEU:HD12	1.43	0.83
1:C:258:VAL:HG11	1:C:1058:GLY:HA2	1.60	0.83
1:C:656:VAL:HG11	1:C:688:GLU:CB	2.08	0.83
1:C:840:ASP:N	1:C:940:ARG:NH1	2.26	0.83
1:C:887:VAL:HG11	1:C:893:ALA:CB	2.07	0.83
1:B:440:ILE:HG12	1:B:772:TYR:CE2	2.13	0.83
1:C:321:ALA:HB3	1:C:1283:ASN:HD21	1.40	0.83
1:C:1021:ARG:HB2	1:C:1021:ARG:HH11	1.43	0.83
1:C:1322:PRO:HB3	1:C:1328:ILE:CD1	2.06	0.83
1:C:660:ALA:C	1:C:662:VAL:N	2.17	0.83
1:C:839:ALA:C	1:C:940:ARG:CZ	2.46	0.83
1:C:550:ILE:HD12	1:C:550:ILE:O	1.78	0.83
1:C:341:LYS:HG3	1:C:1306:THR:CB	2.09	0.83
1:C:865:ILE:HG21	1:C:957:PHE:HE2	1.41	0.83
1:C:874:ILE:CG2	1:C:902:ILE:HD11	2.08	0.83
1:C:1072:ASP:N	1:C:1234:GLN:HE22	1.75	0.83
1:C:107:GLN:OE1	1:C:107:GLN:N	2.11	0.83
1:C:352:HIS:HD2	1:C:1297:SER:H	1.26	0.83
1:C:448:TYR:C	1:C:450:PRO:HD2	1.98	0.83
1:C:1000:LEU:HD22	1:C:1010:ARG:HH21	1.38	0.83
1:C:230:ASP:CA	1:C:985:ARG:HG2	2.07	0.83
1:C:838:GLU:HG3	1:C:934:LEU:CB	2.06	0.83
1:C:865:ILE:CG2	1:C:957:PHE:HE2	1.91	0.83
1:C:1263:TYR:CE1	1:C:1278:TYR:OH	2.27	0.83
1:B:1249:ASN:O	1:C:1109:SER:HA	1.78	0.83
1:C:265:VAL:HG13	1:C:358:LEU:HD13	1.60	0.83
1:C:1210:LEU:O	1:C:1210:LEU:HG	1.78	0.83
1:C:452:ASN:O	1:C:453:LEU:HD23	1.79	0.82
1:C:896:LEU:HA	1:C:918:VAL:CG2	2.09	0.82
1:C:1263:TYR:CD1	1:C:1278:TYR:HE1	1.97	0.82
1:C:509:VAL:CG2	1:C:683:TRP:CZ3	2.61	0.82
1:C:815:LEU:HB3	1:C:816:PRO:CD	2.08	0.82
1:C:449:PHE:CZ	1:C:463:VAL:HG22	2.14	0.82
1:B:461:ARG:HE	1:B:504:ASP:HB2	1.45	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:494:GLU:N	1:C:494:GLU:OE2	2.13	0.82
1:C:1049:GLU:O	1:C:1053:ARG:HG3	1.80	0.82
1:C:1210:LEU:CD2	1:C:1244:ALA:CB	2.58	0.82
1:B:272:THR:HG22	1:B:289:THR:HG22	1.61	0.82
1:C:180:LEU:CD2	1:C:306:GLN:HE22	1.91	0.82
1:C:333:ARG:HE	1:C:1272:ARG:HA	1.44	0.82
1:C:830:VAL:HG23	1:C:947:GLU:HB2	1.60	0.82
1:C:879:THR:H	1:C:880:PRO:HD2	1.44	0.82
1:C:965:ARG:HH11	1:C:968:ARG:NH1	1.78	0.81
1:C:1179:THR:OG1	1:C:1180:PRO:HD3	1.81	0.81
1:B:135:LYS:HE2	1:C:469:ARG:HA	1.61	0.81
1:C:611:GLY:O	1:C:634:TYR:OH	1.98	0.81
1:C:230:ASP:O	1:C:985:ARG:HG2	1.79	0.81
1:C:446:LYS:HB2	1:C:448:TYR:CE1	2.15	0.81
1:C:929:PHE:CG	1:C:936:MET:CE	2.63	0.81
1:C:654:THR:O	1:C:658:THR:CG2	2.26	0.81
1:C:157:ILE:HD11	1:C:263:ARG:HB3	1.59	0.81
1:C:164:LEU:HD11	1:C:353:PHE:HE2	1.42	0.81
1:C:946:LEU:HD21	1:C:965:ARG:HG2	1.63	0.81
1:C:838:GLU:O	1:C:940:ARG:NE	2.11	0.81
1:C:1289:PRO:O	1:C:1293:VAL:HG23	1.80	0.81
1:B:826:GLY:O	1:B:968:ARG:NH2	2.13	0.81
1:C:233:VAL:HG23	1:C:234:PRO:HD2	1.55	0.81
1:C:493:HIS:CB	1:C:756:THR:O	2.28	0.81
1:C:963:ALA:CB	1:C:1059:LEU:HG	2.09	0.81
1:C:230:ASP:O	1:C:985:ARG:CG	2.29	0.81
1:C:656:VAL:CG1	1:C:688:GLU:HG2	2.11	0.81
1:C:1120:THR:O	1:C:1122:PRO:CD	2.28	0.81
1:C:1210:LEU:HD23	1:C:1244:ALA:CB	2.10	0.81
1:C:87:GLU:CB	1:C:159:ASP:O	2.29	0.81
1:C:495:LEU:HD12	1:C:495:LEU:N	1.93	0.81
1:C:741:TYR:HE2	1:C:1022:ILE:HD11	1.42	0.81
1:C:494:GLU:HB3	1:C:577:GLN:NE2	1.96	0.80
1:C:1273:ASN:O	1:C:1273:ASN:ND2	2.14	0.80
1:C:213:PHE:O	1:C:219:ILE:HB	1.80	0.80
1:C:81:ALA:HB3	1:C:170:TYR:CE2	2.16	0.80
1:C:929:PHE:CG	1:C:936:MET:HE2	2.16	0.80
1:C:1306:THR:HG1	1:C:1308:ASN:HA	1.46	0.80
1:C:629:ARG:HB2	1:C:1037:ILE:HG23	1.61	0.80
1:C:452:ASN:O	1:C:453:LEU:CB	2.29	0.80
1:C:1079:LEU:O	1:C:1227:MET:CB	2.29	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1081:ASP:H	1:C:1227:MET:HB3	1.46	0.80
1:B:793:TYR:CD2	1:B:1321:ASN:ND2	2.48	0.80
1:C:144:ASN:CB	1:C:1318:GLU:OE1	2.28	0.80
1:C:835:TYR:CE2	1:C:925:VAL:HG11	2.17	0.80
1:C:685:ARG:HB3	1:C:685:ARG:HH11	1.45	0.80
1:B:394:GLN:HB2	1:C:1005:LEU:HD21	1.63	0.80
1:C:310:LEU:HD21	1:C:1242:MET:CE	2.11	0.80
1:C:528:ILE:HD13	1:C:758:ILE:CD1	2.11	0.80
1:C:837:THR:HG22	1:C:934:LEU:HD12	1.64	0.79
1:C:1134:ARG:HH22	1:C:1154:ASN:HD21	1.30	0.79
1:C:233:VAL:CG1	1:C:981:HIS:CG	2.65	0.79
1:C:1121:HIS:HD2	1:C:1135:PRO:CG	1.91	0.79
1:C:1281:VAL:O	1:C:1283:ASN:N	2.15	0.79
1:C:332:THR:O	1:C:335:ASP:HB2	1.83	0.79
1:C:847:ILE:HG12	1:C:911:ARG:HB2	1.63	0.79
1:C:1214:GLU:HB2	1:C:1215:PRO:CD	1.80	0.79
1:C:659:LEU:O	1:C:659:LEU:HD22	1.83	0.79
1:C:233:VAL:HG12	1:C:981:HIS:CE1	2.17	0.79
1:C:406:ASP:OD1	1:C:1039:ALA:CB	2.29	0.79
1:C:230:ASP:C	1:C:985:ARG:CG	2.47	0.79
1:C:384:MET:HA	1:C:708:THR:CG2	2.13	0.79
1:C:449:PHE:CD1	1:C:450:PRO:HD3	2.18	0.79
1:C:1076:ILE:HB	1:C:1230:ILE:HG22	1.65	0.79
1:C:252:LEU:CD1	1:C:823:ILE:HG21	2.12	0.78
1:C:230:ASP:CB	1:C:985:ARG:HG2	2.13	0.78
1:C:252:LEU:CD1	1:C:971:MET:CE	2.50	0.78
1:C:1109:SER:HG	1:C:1118:THR:HG21	1.45	0.78
1:C:261:ASP:O	1:C:1054:ARG:CZ	2.30	0.78
1:C:924:ASP:OD1	1:C:927:SER:CB	2.30	0.78
1:C:1263:TYR:CD1	1:C:1278:TYR:CE1	2.71	0.78
1:C:441:ARG:HG2	1:C:441:ARG:HH21	1.48	0.78
1:B:342:THR:HB	1:B:1309:ILE:HD11	1.65	0.78
1:C:449:PHE:C	1:C:686:HIS:HD2	1.87	0.78
1:C:685:ARG:HH11	1:C:685:ARG:CB	1.95	0.78
1:C:985:ARG:O	1:C:985:ARG:NH2	2.15	0.78
1:C:1060:ARG:NH1	1:C:1292:GLU:H	1.82	0.78
1:C:1091:ASP:OD1	1:C:1091:ASP:N	2.15	0.78
1:C:1219:ASP:CG	1:C:1220:PRO:CD	2.52	0.78
1:C:434:VAL:HG23	1:C:709:MET:HE1	1.64	0.78
1:C:821:ASN:HA	1:C:824:LEU:HD22	1.66	0.78
1:C:297:ASN:ND2	1:C:298:PRO:HD2	1.99	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:614:ARG:HD3	1:C:635:ILE:HD12	1.64	0.77
1:C:896:LEU:HD22	1:C:918:VAL:CG2	2.14	0.77
1:C:948:ILE:HG13	1:C:962:ASP:HB3	1.65	0.77
1:C:1290:LYS:HZ1	1:C:1299:SER:HB3	1.49	0.77
1:C:1313:ASP:OD1	1:C:1313:ASP:N	2.12	0.77
1:C:449:PHE:CB	1:C:683:TRP:CD1	2.51	0.77
1:C:901:VAL:HA	1:C:928:ARG:O	1.85	0.77
1:C:986:ILE:O	1:C:989:ILE:HG22	1.83	0.77
1:C:77:THR:O	1:C:172:ASP:CB	2.32	0.77
1:C:615:THR:H	1:C:1333:ALA:C	1.87	0.77
1:C:333:ARG:HG2	1:C:333:ARG:HH21	1.49	0.77
1:C:910:LEU:HD23	1:C:915:VAL:HG22	1.61	0.77
1:C:184:GLU:O	1:C:187:ASP:N	2.16	0.77
1:C:338:ARG:CG	1:C:342:THR:N	2.47	0.77
1:C:449:PHE:O	1:C:683:TRP:CD1	2.34	0.77
1:C:830:VAL:HG21	1:C:947:GLU:HB2	1.43	0.77
1:C:835:TYR:CD2	1:C:925:VAL:CG2	2.40	0.77
1:C:946:LEU:N	1:C:946:LEU:HD12	2.00	0.77
1:B:352:HIS:HA	1:B:1300:ASN:HD21	1.50	0.77
1:C:265:VAL:HG21	1:C:1301:VAL:CG2	2.14	0.77
1:C:407:HIS:NE2	1:C:1047:LEU:HD12	2.00	0.77
1:C:484:ARG:CZ	1:C:758:ILE:HG22	2.15	0.77
1:C:896:LEU:CD2	1:C:918:VAL:HG21	2.14	0.77
1:C:1074:VAL:HB	1:C:1173:TYR:HE2	1.50	0.77
1:C:485:GLU:OE1	1:C:486:VAL:HG13	1.85	0.76
1:C:843:LEU:HD21	1:C:943:GLU:CD	2.04	0.76
1:B:1064:ASN:HD21	1:B:1296:ILE:HD11	1.50	0.76
1:C:516:LEU:HB3	1:C:763:VAL:HG11	1.66	0.76
1:C:492:VAL:HG22	1:C:747:ARG:HA	1.66	0.76
1:C:81:ALA:CB	1:C:170:TYR:CZ	2.69	0.76
1:C:339:LEU:HD21	1:C:366:MET:HA	1.68	0.76
1:C:687:LEU:HD23	1:C:687:LEU:C	2.04	0.76
1:C:129:ALA:CB	1:C:133:MET:HG2	2.16	0.76
1:C:232:LEU:CG	1:C:249:SER:HB3	2.14	0.76
1:C:364:ALA:CB	1:C:1050:LEU:HD21	2.15	0.76
1:C:838:GLU:C	1:C:940:ARG:NE	2.38	0.76
1:C:1104:ARG:HG2	1:C:1104:ARG:HH11	1.49	0.76
1:C:838:GLU:O	1:C:940:ARG:CZ	2.34	0.76
1:B:388:GLN:H	1:B:1320:VAL:CG1	1.98	0.76
1:C:835:TYR:CE2	1:C:925:VAL:CB	2.69	0.76
1:C:613:LEU:HD21	1:C:632:GLN:HB3	0.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:874:ILE:HD11	1:C:883:ILE:HD12	1.67	0.76
1:C:897:TYR:CD1	1:C:898:GLN:N	2.54	0.76
1:C:480:LEU:O	1:C:480:LEU:HD23	1.85	0.76
1:C:1044:ARG:HG3	1:C:1044:ARG:HH11	1.51	0.76
1:B:397:LEU:CD2	1:C:1008:LEU:HD11	2.16	0.75
1:C:321:ALA:CB	1:C:1283:ASN:ND2	2.49	0.75
1:C:556:ALA:C	1:C:587:ALA:HB2	2.07	0.75
1:C:734:ILE:HG23	1:C:1017:ALA:HB1	1.68	0.75
1:B:903:ASN:O	1:B:907:SER:CB	2.34	0.75
1:B:793:TYR:HD2	1:B:1321:ASN:HD21	1.31	0.75
1:C:341:LYS:CG	1:C:1306:THR:HB	2.17	0.75
1:C:910:LEU:HD21	1:C:915:VAL:CG2	2.10	0.75
1:C:449:PHE:CG	1:C:466:VAL:HG11	2.22	0.75
1:C:659:LEU:HD22	1:C:662:VAL:HG21	1.67	0.75
1:C:1285:GLN:HE21	1:C:1285:GLN:N	1.85	0.75
1:C:179:LYS:HE3	1:C:181:ARG:HB3	1.67	0.75
1:C:1031:TYR:HE2	1:C:1041:ARG:HH11	1.31	0.75
1:C:254:VAL:HG13	1:C:1062:ILE:CD1	2.17	0.75
1:C:1093:PRO:HG2	1:C:1096:TYR:CD1	2.17	0.75
1:C:1173:TYR:CE1	1:C:1204:LEU:HD12	2.22	0.75
1:C:910:LEU:HG	1:C:915:VAL:HG21	1.69	0.75
1:C:964:VAL:HG13	1:C:1059:LEU:HD21	1.69	0.75
1:B:873:TYR:HB3	1:B:897:TYR:HB2	1.68	0.75
1:C:333:ARG:HG2	1:C:333:ARG:NH2	2.01	0.75
1:B:1185:THR:O	1:B:1205:GLN:NE2	2.20	0.75
1:C:654:THR:CG2	1:C:658:THR:HG21	2.16	0.75
1:C:865:ILE:CG2	1:C:957:PHE:CE2	2.70	0.75
1:C:1085:ASP:HA	1:C:1208:ASP:O	1.87	0.75
1:C:1144:ARG:HD3	1:C:1168:ILE:HG21	1.68	0.75
1:B:436:SER:O	1:B:437:ALA:HB3	1.86	0.74
1:C:233:VAL:HG12	1:C:981:HIS:CG	2.22	0.74
1:C:525:PHE:CE1	1:C:532:ILE:HD12	2.22	0.74
1:C:495:LEU:HD11	1:C:531:ASP:CB	2.17	0.74
1:C:266:ILE:HD13	1:C:1304:MET:CB	2.16	0.74
1:C:451:GLU:HB2	1:C:686:HIS:HB3	1.68	0.74
1:C:611:GLY:CA	1:C:636:PRO:O	2.35	0.74
1:C:1280:PRO:HG3	1:C:1286:VAL:O	1.87	0.74
1:C:87:GLU:OE1	1:C:157:ILE:HG21	1.88	0.74
1:C:449:PHE:CE2	1:C:463:VAL:HG22	2.22	0.74
1:C:404:ASP:O	1:C:408:ILE:HG12	1.87	0.74
1:C:449:PHE:CA	1:C:683:TRP:CD1	2.71	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:838:GLU:OE1	1:C:935:GLN:CA	2.35	0.74
1:C:910:LEU:CG	1:C:915:VAL:CG2	2.65	0.74
1:C:934:LEU:O	1:C:936:MET:N	2.19	0.74
1:B:196:LEU:HD23	1:B:296:VAL:HG11	1.70	0.74
1:B:442:PRO:HB2	1:B:475:ILE:HD11	0.76	0.74
1:C:213:PHE:HB3	1:C:219:ILE:HG13	1.68	0.74
1:C:1296:ILE:O	1:C:1296:ILE:HD13	1.87	0.74
1:B:439:VAL:O	1:B:440:ILE:HG13	1.87	0.74
1:C:87:GLU:HG3	1:C:87:GLU:O	1.87	0.74
1:B:139:ASN:O	1:C:757:ILE:HB	1.88	0.74
1:B:338:ARG:HH12	1:C:1005:LEU:HD22	1.52	0.74
1:B:699:THR:O	1:B:703:SER:OG	2.04	0.74
1:C:372:ALA:CB	1:C:1315:MET:HE3	2.18	0.74
1:C:422:LEU:CD1	1:C:490:PHE:CE2	2.71	0.73
1:C:449:PHE:HB2	1:C:683:TRP:CE2	2.19	0.73
1:C:509:VAL:HG22	1:C:683:TRP:CH2	2.23	0.73
1:C:1280:PRO:CB	1:C:1287:GLY:HA2	2.18	0.73
1:C:259:MET:CG	1:C:1055:LEU:HB2	2.18	0.73
1:C:265:VAL:HG23	1:C:1303:SER:HA	1.70	0.73
1:C:901:VAL:HG22	1:C:930:ALA:CB	2.15	0.73
1:C:1112:ASN:O	1:C:1112:ASN:ND2	2.15	0.73
1:B:442:PRO:HB2	1:B:475:ILE:HD13	1.64	0.73
1:C:108:LYS:HB2	1:C:108:LYS:NZ	2.03	0.73
1:C:1079:LEU:HD11	1:C:1231:TYR:CZ	2.16	0.73
1:C:1104:ARG:HD2	1:C:1104:ARG:O	1.88	0.73
1:C:338:ARG:O	1:C:340:VAL:N	2.20	0.73
1:C:795:ASP:OD1	1:C:795:ASP:N	2.17	0.73
1:C:1278:TYR:CD2	1:C:1288:ILE:CD1	2.71	0.73
1:C:168:VAL:HG23	1:C:204:VAL:HG13	1.70	0.73
1:C:516:LEU:CB	1:C:763:VAL:HG11	2.17	0.73
1:C:338:ARG:O	1:C:341:LYS:O	2.06	0.73
1:B:903:ASN:O	1:B:907:SER:HB2	1.89	0.73
1:C:146:GLU:N	1:C:146:GLU:OE1	2.21	0.73
1:C:254:VAL:HG13	1:C:1062:ILE:HD11	1.70	0.73
1:C:1081:ASP:N	1:C:1227:MET:HB3	2.03	0.73
1:C:247:TYR:CD2	1:C:1070:ARG:HD3	2.24	0.72
1:C:571:ARG:HB3	1:C:571:ARG:HH11	1.53	0.72
1:C:1259:ALA:HB1	1:C:1260:PRO:CD	2.19	0.72
1:C:81:ALA:HB3	1:C:170:TYR:CZ	2.24	0.72
1:C:327:LEU:HD13	1:C:327:LEU:O	1.88	0.72
1:C:985:ARG:NH1	1:C:989:ILE:HD12	2.05	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1231:TYR:HB3	1:C:1232:PRO:HD2	1.72	0.72
1:C:339:LEU:HD13	1:C:397:LEU:CD2	2.19	0.72
1:C:829:SER:HB2	1:C:965:ARG:HD2	0.72	0.72
1:C:1210:LEU:HD23	1:C:1244:ALA:HB2	1.70	0.72
1:C:713:MET:HE1	1:C:804:LEU:HD21	1.71	0.72
1:C:1306:THR:CA	1:C:1308:ASN:H	2.01	0.72
1:C:120:VAL:O	1:C:121:PHE:O	2.07	0.72
1:C:233:VAL:CG1	1:C:981:HIS:ND1	2.52	0.72
1:C:985:ARG:NH2	1:C:988:GLN:HG3	2.03	0.72
1:C:849:MET:CE	1:C:929:PHE:HE2	2.02	0.72
1:C:1168:ILE:HD13	1:C:1168:ILE:N	2.05	0.72
1:C:265:VAL:HG11	1:C:1301:VAL:HG21	1.70	0.72
1:C:362:LEU:HD13	1:C:1302:VAL:CG1	2.19	0.72
1:C:954:GLN:O	1:C:958:ILE:HD11	1.90	0.72
1:B:372:ALA:O	1:B:375:ARG:HG2	1.89	0.72
1:C:666:ARG:HH11	1:C:666:ARG:CG	2.03	0.72
1:C:733:VAL:CG2	1:C:1022:ILE:HD12	2.19	0.72
1:C:835:TYR:CE1	1:C:942:HIS:CG	2.77	0.72
1:B:394:GLN:CB	1:C:1005:LEU:HD21	2.19	0.72
1:C:864:HIS:CE1	1:C:1030:ARG:CZ	2.73	0.72
1:C:874:ILE:HG13	1:C:895:VAL:HG11	1.71	0.72
1:B:1131:PRO:O	1:B:1162:SER:OG	2.07	0.71
1:C:835:TYR:HE2	1:C:925:VAL:CG1	2.01	0.71
1:C:1176:GLU:OE1	1:C:1203:HIS:CE1	2.43	0.71
1:B:533:GLN:HG3	1:B:588:LEU:HD12	1.72	0.71
1:C:213:PHE:HB2	1:C:219:ILE:CG2	2.16	0.71
1:C:829:SER:CB	1:C:965:ARG:HD3	2.12	0.71
1:C:109:LYS:HD2	1:C:110:PRO:HD3	1.72	0.71
1:C:302:ARG:HD2	1:C:318:LEU:HD23	1.70	0.71
1:C:450:PRO:CA	1:C:454:GLU:CG	2.55	0.71
1:C:554:ARG:HG2	1:C:554:ARG:O	1.91	0.71
1:C:935:GLN:CB	1:C:939:ASN:HB3	2.20	0.71
1:C:108:LYS:HB2	1:C:108:LYS:HZ2	1.56	0.71
1:C:235:ILE:HD11	1:C:978:GLN:HE21	1.55	0.71
1:C:1276:LEU:N	1:C:1276:LEU:HD23	2.05	0.71
1:C:339:LEU:HD13	1:C:397:LEU:HD23	1.72	0.71
1:C:1211:LEU:HD11	1:C:1246:VAL:CG2	2.20	0.71
1:B:272:THR:HG23	1:C:235:ILE:HG21	1.72	0.71
1:C:502:PHE:CD1	1:C:507:SER:HB3	2.24	0.71
1:C:1044:ARG:HH11	1:C:1044:ARG:CG	2.03	0.71
1:C:375:ARG:HH11	1:C:375:ARG:CG	2.04	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:613:LEU:O	1:C:613:LEU:HD13	1.90	0.71
1:C:832:MET:HG3	1:C:832:MET:O	1.88	0.71
1:C:841:ASP:N	1:C:940:ARG:NH2	2.37	0.71
1:B:472:GLU:HB2	1:B:761:SER:OG	1.87	0.71
1:C:96:ILE:HD13	1:C:96:ILE:N	2.05	0.71
1:C:606:LEU:HD11	1:C:659:LEU:HB2	1.72	0.71
1:C:511:VAL:HG21	1:C:539:PHE:CE2	2.26	0.71
1:C:1023:ARG:NH2	1:C:1023:ARG:HB3	2.05	0.71
1:C:1250:GLU:C	1:C:1251:VAL:HG23	2.10	0.71
1:B:316:ASN:O	1:B:320:GLN:NE2	2.24	0.71
1:B:903:ASN:O	1:B:907:SER:OG	2.09	0.71
1:C:225:ILE:HD11	1:C:1069:ARG:C	2.11	0.71
1:C:502:PHE:HD1	1:C:507:SER:HB3	1.55	0.71
1:C:366:MET:HG2	1:C:366:MET:O	1.88	0.70
1:C:265:VAL:CG1	1:C:358:LEU:HD13	2.21	0.70
1:C:862:ARG:HH21	1:C:1042:TRP:HZ2	1.38	0.70
1:C:1000:LEU:HD23	1:C:1010:ARG:NE	2.04	0.70
1:C:1076:ILE:O	1:C:1076:ILE:HG12	1.90	0.70
1:B:313:ASP:O	1:B:317:MET:CB	2.39	0.70
1:C:77:THR:O	1:C:172:ASP:CG	2.29	0.70
1:C:210:ARG:HA	1:C:221:LEU:HD11	1.72	0.70
1:C:213:PHE:HB3	1:C:219:ILE:CG1	2.21	0.70
1:C:258:VAL:HG11	1:C:1058:GLY:CA	2.21	0.70
1:C:611:GLY:HA3	1:C:636:PRO:O	1.91	0.70
1:C:850:THR:OG1	1:C:916:LEU:HD22	1.91	0.70
1:C:897:TYR:CZ	1:C:898:GLN:O	2.43	0.70
1:C:301:LEU:HD12	1:C:301:LEU:O	1.91	0.70
1:C:371:THR:C	1:C:373:ASP:N	2.42	0.70
1:C:835:TYR:CE2	1:C:925:VAL:CG1	2.74	0.70
1:C:383:SER:OG	1:C:796:PRO:HG2	1.88	0.70
1:C:656:VAL:CG1	1:C:688:GLU:HB3	2.15	0.70
1:C:910:LEU:CG	1:C:915:VAL:HG21	2.22	0.70
1:C:1259:ALA:HB1	1:C:1260:PRO:HD3	1.73	0.70
1:C:1263:TYR:CZ	1:C:1278:TYR:CZ	2.74	0.70
1:B:875:THR:H	1:B:878:SER:HB3	1.55	0.70
1:B:1282:ALA:HB1	1:B:1283:ASN:HA	1.73	0.70
1:C:713:MET:HE1	1:C:804:LEU:CD2	2.21	0.70
1:C:1292:GLU:C	1:C:1293:VAL:HG23	2.11	0.70
1:C:141:LEU:O	1:C:141:LEU:HG	1.91	0.70
1:C:204:VAL:HG23	1:C:1242:MET:O	1.92	0.70
1:C:230:ASP:HB2	1:C:985:ARG:NE	1.95	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:896:LEU:HD13	1:C:918:VAL:CG2	2.22	0.70
1:C:897:TYR:CG	1:C:898:GLN:N	2.57	0.70
1:C:1261:SER:O	1:C:1263:TYR:N	2.25	0.70
1:C:154:PHE:HE1	1:C:361:ASN:ND2	1.89	0.70
1:C:659:LEU:HD22	1:C:662:VAL:CG2	2.22	0.70
1:C:1031:TYR:CE2	1:C:1041:ARG:NH1	2.55	0.70
1:C:558:TYR:CZ	1:C:585:PHE:HB2	2.27	0.69
1:C:835:TYR:O	1:C:846:GLY:CA	2.32	0.69
1:C:1122:PRO:HB2	1:C:1123:PRO:HD3	1.74	0.69
1:B:472:GLU:CA	1:B:473:ALA:HB2	2.22	0.69
1:C:206:ILE:HD11	1:C:1066:ARG:HD3	1.74	0.69
1:B:606:LEU:HD11	1:B:658:THR:HG21	1.72	0.69
1:C:233:VAL:HG12	1:C:981:HIS:ND1	2.06	0.69
1:C:407:HIS:CD2	1:C:1047:LEU:CA	2.69	0.69
1:C:1270:LEU:O	1:C:1271:SER:O	2.10	0.69
1:B:139:ASN:O	1:C:757:ILE:O	2.10	0.69
1:B:564:GLY:HA2	1:B:565:GLU:HB3	1.73	0.69
1:B:1189:ASP:O	1:B:1192:SER:N	2.21	0.69
1:C:176:LYS:CG	1:C:177:LYS:H	2.05	0.69
1:C:375:ARG:HD3	1:C:398:ARG:NH2	2.07	0.69
1:C:485:GLU:OE1	1:C:706:TYR:CE1	2.46	0.69
1:C:999:LYS:HE2	1:C:1009:THR:HG22	1.74	0.69
1:C:1047:LEU:HD22	1:C:1051:ARG:HD3	1.71	0.69
1:C:1296:ILE:HD11	1:C:1298:PHE:HE1	1.58	0.69
1:C:180:LEU:CD2	1:C:306:GLN:HE21	1.87	0.69
1:C:429:ILE:C	1:C:429:ILE:HD12	2.13	0.69
1:C:1046:PHE:HD2	1:C:1052:LEU:HD21	1.56	0.69
1:B:388:GLN:CB	1:B:1320:VAL:CG1	2.67	0.69
1:C:449:PHE:C	1:C:686:HIS:CD2	2.65	0.69
1:C:1000:LEU:HD21	1:C:1010:ARG:HH21	1.56	0.69
1:C:1176:GLU:HG2	1:C:1203:HIS:CE1	2.26	0.69
1:B:475:ILE:HD13	1:B:475:ILE:O	1.93	0.69
1:B:640:GLN:HE21	1:B:647:GLU:HB3	1.58	0.69
1:B:1112:ASN:OD1	1:B:1113:LYS:N	2.26	0.69
1:C:371:THR:C	1:C:373:ASP:H	1.94	0.69
1:C:830:VAL:O	1:C:854:GLN:HG2	1.92	0.69
1:C:836:GLN:HB2	1:C:940:ARG:HG2	0.77	0.69
1:C:1322:PRO:CB	1:C:1328:ILE:CD1	2.70	0.69
1:B:469:ARG:HH11	1:B:498:ILE:HD12	0.87	0.69
1:B:926:VAL:HG21	1:B:938:ASN:H	1.56	0.69
1:C:1243:ARG:HG2	1:C:1243:ARG:HH11	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1281:VAL:C	1:C:1283:ASN:H	1.94	0.69
1:B:472:GLU:HB3	1:B:761:SER:HG	1.56	0.69
1:C:77:THR:O	1:C:172:ASP:OD2	2.10	0.69
1:C:251:LEU:HD23	1:C:1062:ILE:CG1	2.12	0.69
1:C:314:ILE:HG22	1:C:318:LEU:CD2	2.22	0.69
1:C:338:ARG:CG	1:C:342:THR:CA	2.70	0.69
1:C:865:ILE:HG21	1:C:957:PHE:CE2	2.26	0.69
1:C:1250:GLU:C	1:C:1251:VAL:CG2	2.61	0.69
1:B:209:ASN:ND2	1:B:211:ASP:OD1	2.25	0.69
1:B:961:SER:HB2	1:B:964:VAL:HG12	1.75	0.69
1:C:333:ARG:O	1:C:335:ASP:N	2.25	0.69
1:C:365:LEU:O	1:C:365:LEU:HD22	1.93	0.69
1:B:699:THR:O	1:B:703:SER:CB	2.41	0.68
1:B:1249:ASN:HB3	1:C:1110:LEU:CB	2.22	0.68
1:C:509:VAL:HG23	1:C:683:TRP:HZ3	1.57	0.68
1:C:837:THR:C	1:C:934:LEU:CD1	2.58	0.68
1:C:232:LEU:HD21	1:C:249:SER:CA	2.23	0.68
1:C:583:GLU:HG3	1:C:583:GLU:O	1.94	0.68
1:C:1085:ASP:OD1	1:C:1085:ASP:N	2.26	0.68
1:C:1173:TYR:CD1	1:C:1204:LEU:CD1	2.74	0.68
1:C:146:GLU:HB2	1:C:1317:VAL:CG1	2.23	0.68
1:C:1093:PRO:CG	1:C:1096:TYR:CD1	2.73	0.68
1:B:1331:ARG:HG2	1:B:1332:ASN:H	1.58	0.68
1:C:180:LEU:HG	1:C:180:LEU:O	1.93	0.68
1:C:320:GLN:O	1:C:321:ALA:HB3	1.93	0.68
1:C:542:ARG:HG3	1:C:542:ARG:O	1.91	0.68
1:C:619:ALA:HB2	1:C:711:ASN:HB2	1.75	0.68
1:C:629:ARG:HG3	1:C:629:ARG:O	1.91	0.68
1:B:472:GLU:HB3	1:B:761:SER:HB2	1.74	0.68
1:C:733:VAL:CB	1:C:1022:ILE:HD12	2.23	0.68
1:C:929:PHE:CG	1:C:936:MET:HE1	2.28	0.68
1:C:1206:PHE:CD2	1:C:1236:ILE:HD11	2.28	0.68
1:B:462:LEU:HD23	1:B:462:LEU:C	2.14	0.68
1:C:168:VAL:HG23	1:C:204:VAL:CG1	2.23	0.68
1:C:448:TYR:C	1:C:450:PRO:CD	2.61	0.68
1:C:168:VAL:HB	1:C:204:VAL:HG12	1.76	0.68
1:C:838:GLU:CB	1:C:934:LEU:HB3	2.16	0.68
1:C:838:GLU:HG2	1:C:935:GLN:C	2.14	0.68
1:C:278:LEU:HD22	1:C:282:VAL:HB	1.76	0.68
1:C:849:MET:CG	1:C:919:MET:CE	2.72	0.68
1:C:1079:LEU:HD12	1:C:1079:LEU:N	2.02	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:259:MET:HG3	1:C:1055:LEU:CB	2.23	0.68
1:C:389:PHE:CE1	1:C:1319:ARG:CB	2.76	0.68
1:C:509:VAL:HG22	1:C:683:TRP:HH2	1.59	0.68
1:C:674:LYS:HB2	1:C:674:LYS:NZ	2.08	0.68
1:C:231:LEU:O	1:C:982:ALA:CA	2.40	0.67
1:C:516:LEU:HB3	1:C:763:VAL:CG1	2.24	0.67
1:C:896:LEU:HD13	1:C:918:VAL:HG21	1.75	0.67
1:C:440:ILE:CD1	1:C:478:ILE:HG21	2.22	0.67
1:C:958:ILE:O	1:C:958:ILE:HG12	1.92	0.67
1:C:1000:LEU:HD23	1:C:1010:ARG:CZ	2.25	0.67
1:B:234:PRO:HB3	1:B:972:PRO:HB3	1.75	0.67
1:B:440:ILE:HG21	1:B:770:CYS:SG	2.34	0.67
1:B:821:ASN:ND2	1:B:1015:GLN:OE1	2.26	0.67
1:C:240:GLY:C	1:C:242:GLU:N	2.47	0.67
1:C:244:SER:C	1:C:246:GLU:N	2.47	0.67
1:C:385:ILE:O	1:C:1328:ILE:HG21	1.95	0.67
1:C:450:PRO:O	1:C:451:GLU:HB3	1.93	0.67
1:C:285:VAL:HG13	1:C:325:TYR:O	1.94	0.67
1:C:791:ILE:HG13	1:C:1325:VAL:CG2	2.25	0.67
1:C:909:TYR:HE1	1:C:913:ASN:OD1	1.77	0.67
1:C:1272:ARG:O	1:C:1272:ARG:HD3	1.93	0.67
1:B:898:GLN:NE2	1:B:917:VAL:HB	2.09	0.67
1:B:409:ILE:HD11	1:B:627:ALA:HA	1.76	0.67
1:C:365:LEU:O	1:C:365:LEU:HD13	1.93	0.67
1:C:820:ILE:CG2	1:C:983:ILE:HG12	2.24	0.67
1:C:1079:LEU:O	1:C:1227:MET:HB2	1.93	0.67
1:C:1149:LYS:O	1:C:1151:VAL:N	2.27	0.67
1:B:397:LEU:O	1:B:398:ARG:NH1	2.24	0.67
1:B:439:VAL:HG23	1:B:440:ILE:H	1.58	0.67
1:C:462:LEU:HD13	1:C:462:LEU:C	2.15	0.67
1:C:702:LEU:HD12	1:C:702:LEU:O	1.93	0.67
1:C:713:MET:CE	1:C:804:LEU:HD23	2.24	0.67
1:C:838:GLU:HB3	1:C:934:LEU:HB3	1.76	0.67
1:C:928:ARG:HH11	1:C:928:ARG:HG3	1.60	0.67
1:B:301:LEU:O	1:B:305:THR:OG1	2.13	0.67
1:C:896:LEU:HA	1:C:918:VAL:HG22	1.76	0.67
1:B:388:GLN:H	1:B:1320:VAL:HG13	1.58	0.67
1:B:388:GLN:C	1:B:1320:VAL:HG12	2.14	0.67
1:B:1119:TYR:HB3	1:B:1134:ARG:HE	1.58	0.67
1:C:607:PHE:O	1:C:608:THR:CG2	2.43	0.66
1:C:659:LEU:C	1:C:659:LEU:HD13	2.15	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:791:ILE:HG13	1:C:1325:VAL:HG21	1.76	0.66
1:C:1105:LEU:H	1:C:1105:LEU:HD12	1.61	0.66
1:C:1206:PHE:HD2	1:C:1236:ILE:CD1	2.04	0.66
1:C:297:ASN:HD22	1:C:298:PRO:HD2	1.58	0.66
1:C:309:TRP:CZ2	1:C:1257:ALA:HB1	2.31	0.66
1:C:394:GLN:HG3	1:C:394:GLN:O	1.96	0.66
1:C:1021:ARG:HH11	1:C:1021:ARG:CB	2.08	0.66
1:C:422:LEU:HD11	1:C:490:PHE:CE2	2.31	0.66
1:C:685:ARG:HB3	1:C:685:ARG:NH1	2.10	0.66
1:B:522:PRO:HG2	1:B:636:PRO:HB3	1.78	0.66
1:C:372:ALA:CB	1:C:1315:MET:HE1	2.12	0.66
1:C:1293:VAL:O	1:C:1294:ASP:HB2	1.95	0.66
1:C:610:GLN:HA	1:C:610:GLN:NE2	2.08	0.66
1:B:147:VAL:HB	1:B:379:LEU:HD22	1.78	0.66
1:B:461:ARG:HB2	1:B:461:ARG:NH1	2.03	0.66
1:B:1066:ARG:HG3	1:B:1239:ALA:HA	1.78	0.66
1:C:822:MET:CE	1:C:1046:PHE:HE2	2.08	0.66
1:C:85:ASP:OD2	1:C:161:LYS:CG	2.41	0.66
1:C:1077:MET:HG3	1:C:1077:MET:O	1.96	0.66
1:C:389:PHE:HZ	1:C:796:PRO:HG2	1.62	0.65
1:C:449:PHE:CG	1:C:450:PRO:N	2.65	0.65
1:B:529:LYS:HB2	1:B:589:PHE:CE2	2.31	0.65
1:B:856:LEU:HD12	1:B:860:ARG:HE	1.60	0.65
1:C:833:ARG:NH1	1:C:942:HIS:CE1	2.63	0.65
1:B:1188:VAL:HG11	1:B:1204:LEU:HD23	1.77	0.65
1:C:179:LYS:HD2	1:C:179:LYS:C	2.16	0.65
1:C:1277:LEU:HD23	1:C:1287:GLY:HA3	1.78	0.65
1:C:225:ILE:HD12	1:C:247:TYR:CE1	2.32	0.65
1:C:766:ILE:HD12	1:C:766:ILE:O	1.97	0.65
1:C:849:MET:CG	1:C:919:MET:HE3	2.27	0.65
1:C:887:VAL:CG1	1:C:893:ALA:CB	2.72	0.65
1:C:1227:MET:O	1:C:1228:ARG:HB3	1.97	0.65
1:C:663:VAL:HG11	1:C:680:THR:HG23	1.77	0.65
1:C:849:MET:HG3	1:C:919:MET:HE2	1.79	0.65
1:C:926:VAL:HG11	1:C:937:ASN:HD22	1.62	0.65
1:B:397:LEU:HD21	1:C:1008:LEU:HD11	1.78	0.65
1:B:1176:GLU:HG2	1:B:1203:HIS:HE1	1.62	0.65
1:C:144:ASN:ND2	1:C:1318:GLU:OE1	2.28	0.65
1:C:157:ILE:HG12	1:C:263:ARG:HG2	1.75	0.65
1:C:317:MET:SD	1:C:1262:SER:CB	2.83	0.65
1:C:612:PHE:HD1	1:C:612:PHE:H	1.45	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:713:MET:CE	1:C:804:LEU:CD2	2.74	0.65
1:C:843:LEU:CD1	1:C:943:GLU:CB	2.73	0.65
1:C:865:ILE:HG22	1:C:957:PHE:CE2	2.30	0.65
1:C:893:ALA:HB1	1:C:915:VAL:HG12	1.77	0.65
1:B:388:GLN:CA	1:B:1320:VAL:HG12	2.27	0.65
1:C:146:GLU:O	1:C:1316:ALA:HA	1.97	0.65
1:C:1060:ARG:HH12	1:C:1292:GLU:H	1.42	0.65
1:B:709:MET:O	1:B:715:ASN:ND2	2.30	0.65
1:C:446:LYS:HD3	1:C:448:TYR:CZ	2.31	0.65
1:C:849:MET:N	1:C:849:MET:SD	2.70	0.65
1:C:180:LEU:HD23	1:C:180:LEU:H	1.62	0.65
1:C:1268:GLY:HA3	1:C:1277:LEU:O	1.97	0.65
1:C:243:GLN:HB2	1:C:246:GLU:HG3	1.77	0.64
1:C:382:HIS:CD2	1:C:800:LEU:HD23	2.31	0.64
1:C:615:THR:HG23	1:C:1333:ALA:C	2.18	0.64
1:C:1074:VAL:CA	1:C:1233:LEU:HD22	2.25	0.64
1:B:588:LEU:HD13	1:B:604:MET:HE3	1.79	0.64
1:C:213:PHE:CZ	1:C:254:VAL:HG23	2.32	0.64
1:C:741:TYR:OH	1:C:1022:ILE:HD13	1.96	0.64
1:C:1135:PRO:HG2	1:C:1137:VAL:HG13	1.78	0.64
1:B:436:SER:O	1:B:437:ALA:CB	2.45	0.64
1:C:117:ARG:HG3	1:C:121:PHE:CZ	2.32	0.64
1:B:1060:ARG:NH1	1:B:1291:LEU:O	2.29	0.64
1:C:840:ASP:CA	1:C:940:ARG:HH12	2.11	0.64
1:C:873:TYR:HD2	1:C:898:GLN:HG3	1.62	0.64
1:C:1127:ALA:O	1:C:1128:TYR:HB2	1.97	0.64
1:C:148:GLN:NE2	1:C:148:GLN:HA	2.12	0.64
1:C:734:ILE:O	1:C:734:ILE:HG22	1.98	0.64
1:C:741:TYR:CE2	1:C:1022:ILE:CD1	2.80	0.64
1:C:1279:SER:HB2	1:C:1280:PRO:O	1.97	0.64
1:C:254:VAL:CG1	1:C:1062:ILE:CD1	2.70	0.64
1:C:547:GLU:HG2	1:C:600:ILE:HG13	1.79	0.64
1:C:750:GLU:HG3	1:C:750:GLU:O	1.96	0.64
1:C:1245:ILE:O	1:C:1245:ILE:HG13	1.98	0.64
1:B:313:ASP:O	1:B:317:MET:HB3	1.97	0.64
1:B:1022:ILE:HG22	1:B:1028:VAL:HA	1.79	0.64
1:C:208:LEU:HB2	1:C:221:LEU:HD22	1.77	0.64
1:C:528:ILE:HG21	1:C:758:ILE:CD1	2.18	0.64
1:C:338:ARG:HG3	1:C:342:THR:CA	2.28	0.64
1:C:362:LEU:HD13	1:C:1302:VAL:HG11	1.79	0.64
1:C:822:MET:HE2	1:C:1046:PHE:HE2	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1020:ARG:NH1	1:C:1041:ARG:O	2.30	0.64
1:C:1210:LEU:CD2	1:C:1244:ALA:HB2	2.28	0.64
1:C:297:ASN:HD22	1:C:298:PRO:CD	2.11	0.64
1:C:753:ASP:N	1:C:753:ASP:OD1	2.30	0.64
1:B:390:HIS:HB2	1:B:1318:GLU:HG2	1.80	0.63
1:C:185:ALA:C	1:C:187:ASP:N	2.50	0.63
1:C:297:ASN:HD22	1:C:297:ASN:C	2.01	0.63
1:C:312:ARG:HH21	1:C:312:ARG:CG	2.09	0.63
1:C:441:ARG:HG2	1:C:441:ARG:NH2	2.12	0.63
1:C:713:MET:HE3	1:C:804:LEU:HD23	1.80	0.63
1:C:909:TYR:CZ	1:C:913:ASN:OD1	2.50	0.63
1:B:135:LYS:CE	1:C:469:ARG:HA	2.28	0.63
1:B:440:ILE:CG2	1:B:770:CYS:SG	2.87	0.63
1:B:1185:THR:H	1:B:1205:GLN:NE2	1.95	0.63
1:C:240:GLY:O	1:C:241:ALA:C	2.37	0.63
1:C:1206:PHE:CE2	1:C:1236:ILE:CD1	2.82	0.63
1:B:1249:ASN:HB3	1:C:1110:LEU:HB2	1.81	0.63
1:C:434:VAL:CG2	1:C:709:MET:HE1	2.29	0.63
1:C:764:TRP:HB2	1:C:765:PRO:HD3	1.79	0.63
1:C:870:ASP:OD1	1:C:870:ASP:N	2.24	0.63
1:C:1080:THR:N	1:C:1227:MET:SD	2.55	0.63
1:B:135:LYS:HE2	1:C:468:ALA:C	2.14	0.63
1:C:258:VAL:CG1	1:C:1058:GLY:CA	2.76	0.63
1:C:1074:VAL:O	1:C:1074:VAL:HG13	1.99	0.63
1:C:1132:THR:O	1:C:1133:GLY:C	2.37	0.63
1:C:422:LEU:HD11	1:C:490:PHE:HE2	1.63	0.63
1:C:616:ASP:OD1	1:C:631:PRO:HB2	1.97	0.63
1:C:836:GLN:O	1:C:838:GLU:N	2.28	0.63
1:C:1137:VAL:CG2	1:C:1164:TRP:CE2	2.81	0.63
1:B:658:THR:HA	1:B:661:ASN:HD22	1.64	0.63
1:C:389:PHE:HD1	1:C:1317:VAL:CG2	2.11	0.63
1:C:655:ILE:O	1:C:659:LEU:HB3	1.98	0.63
1:C:663:VAL:O	1:C:677:ARG:CD	2.45	0.63
1:C:815:LEU:HD13	1:C:1051:ARG:HH21	1.62	0.63
1:C:1049:GLU:O	1:C:1053:ARG:CG	2.46	0.63
1:B:489:MET:SD	1:B:492:VAL:HA	2.39	0.63
1:B:529:LYS:HB2	1:B:589:PHE:HE2	1.64	0.63
1:B:897:TYR:CZ	1:B:899:SER:HB3	2.34	0.63
1:C:1046:PHE:CD2	1:C:1052:LEU:HD21	2.34	0.63
1:C:75:ILE:HG23	1:C:75:ILE:O	1.98	0.63
1:C:154:PHE:CE2	1:C:365:LEU:HB2	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:ASP:O	1:C:985:ARG:HG3	1.98	0.63
1:C:1173:TYR:HB2	1:C:1202:PHE:O	1.99	0.63
1:B:848:ARG:NH1	1:B:914:GLU:O	2.32	0.62
1:B:1048:ASP:OD1	1:B:1049:GLU:N	2.32	0.62
1:C:1054:ARG:CG	1:C:1054:ARG:HH11	2.12	0.62
1:C:143:VAL:HG23	1:C:143:VAL:O	2.00	0.62
1:C:225:ILE:HG23	1:C:226:PRO:HD2	1.81	0.62
1:C:233:VAL:O	1:C:234:PRO:O	2.18	0.62
1:C:259:MET:O	1:C:1054:ARG:NH1	2.31	0.62
1:C:389:PHE:HE1	1:C:1319:ARG:HB3	1.64	0.62
1:B:1047:LEU:HA	1:B:1051:ARG:HH21	1.64	0.62
1:C:156:GLN:NE2	1:C:1309:ILE:HG12	2.13	0.62
1:C:164:LEU:HD11	1:C:353:PHE:CE2	2.31	0.62
1:C:571:ARG:HB3	1:C:571:ARG:NH1	2.14	0.62
1:B:1214:GLU:HG2	1:B:1215:PRO:HD2	1.80	0.62
1:C:81:ALA:CB	1:C:170:TYR:OH	2.47	0.62
1:C:478:ILE:CD1	1:C:762:ILE:CD1	2.68	0.62
1:C:550:ILE:HD12	1:C:550:ILE:C	2.20	0.62
1:C:834:THR:HG22	1:C:848:ARG:HG2	1.81	0.62
1:C:964:VAL:CG1	1:C:1059:LEU:HD21	2.28	0.62
1:C:1173:TYR:CD2	1:C:1204:LEU:HD11	2.35	0.62
1:B:629:ARG:NH2	1:B:1033:ASP:O	2.31	0.62
1:C:333:ARG:HH21	1:C:333:ARG:CG	2.12	0.62
1:C:389:PHE:CD1	1:C:1317:VAL:HG21	2.35	0.62
1:C:428:GLN:OE1	1:C:428:GLN:HA	1.99	0.62
1:C:1135:PRO:HD2	1:C:1164:TRP:HE1	1.64	0.62
1:C:338:ARG:HG2	1:C:342:THR:CA	2.29	0.62
1:C:611:GLY:O	1:C:634:TYR:CE2	2.50	0.62
1:C:827:GLY:HA3	1:C:964:VAL:HG21	1.80	0.62
1:C:830:VAL:HG21	1:C:947:GLU:HB3	1.62	0.62
1:C:985:ARG:NH2	1:C:989:ILE:HB	2.15	0.62
1:B:867:ASN:OD1	1:B:1030:ARG:HD3	2.00	0.62
1:C:656:VAL:HG12	1:C:688:GLU:HG2	1.81	0.62
1:C:945:VAL:C	1:C:946:LEU:HD12	2.20	0.62
1:C:1000:LEU:HD23	1:C:1010:ARG:NH2	2.13	0.62
1:C:1129:PRO:O	1:C:1130:SER:HB3	2.00	0.62
1:C:1296:ILE:HD13	1:C:1296:ILE:C	2.20	0.62
1:C:606:LEU:CD1	1:C:655:ILE:HG23	2.16	0.62
1:C:824:LEU:O	1:C:824:LEU:HD23	1.98	0.62
1:C:849:MET:HE2	1:C:929:PHE:HE2	1.65	0.62
1:C:180:LEU:HD23	1:C:306:GLN:HE22	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:820:ILE:HD13	1:C:820:ILE:O	2.00	0.62
1:C:1060:ARG:HA	1:C:1060:ARG:NE	2.14	0.62
1:B:985:ARG:HH21	1:B:988:GLN:HE21	1.46	0.62
1:C:849:MET:HG3	1:C:919:MET:CE	2.30	0.62
1:B:702:LEU:HA	1:B:705:VAL:HG22	1.82	0.61
1:B:772:TYR:HB2	1:B:775:VAL:HG12	1.81	0.61
1:C:206:ILE:O	1:C:1239:ALA:CB	2.46	0.61
1:C:327:LEU:C	1:C:327:LEU:HD22	2.21	0.61
1:C:733:VAL:HG12	1:C:1020:ARG:O	2.00	0.61
1:C:144:ASN:HD22	1:C:1318:GLU:CD	2.03	0.61
1:C:155:LYS:HD2	1:C:155:LYS:O	2.00	0.61
1:C:718:ASN:OD1	1:C:718:ASN:N	2.29	0.61
1:C:1134:ARG:NH2	1:C:1154:ASN:HD21	1.95	0.61
1:C:1278:TYR:CD2	1:C:1288:ILE:HG12	2.12	0.61
1:B:135:LYS:HE2	1:C:469:ARG:CA	2.30	0.61
1:C:120:VAL:O	1:C:120:VAL:HG22	2.00	0.61
1:C:720:PHE:O	1:C:727:PHE:CE1	2.53	0.61
1:C:1165:VAL:O	1:C:1165:VAL:HG12	2.01	0.61
1:C:1206:PHE:CD2	1:C:1236:ILE:HD12	2.34	0.61
1:C:163:TYR:HE2	1:C:258:VAL:HG23	1.65	0.61
1:C:579:LEU:HB2	1:C:582:SER:OG	2.00	0.61
1:C:1111:ALA:HB2	1:C:1129:PRO:HB2	1.83	0.61
1:C:508:ILE:O	1:C:508:ILE:HG13	2.00	0.61
1:C:820:ILE:CG2	1:C:983:ILE:HD11	2.30	0.61
1:C:1030:ARG:C	1:C:1032:ASP:H	2.02	0.61
1:B:472:GLU:N	1:B:473:ALA:HA	2.16	0.61
1:C:146:GLU:HB2	1:C:1317:VAL:HG12	1.82	0.61
1:C:232:LEU:CD2	1:C:249:SER:CB	2.52	0.61
1:C:674:LYS:HG3	1:C:677:ARG:HH21	1.66	0.61
1:C:1173:TYR:CG	1:C:1204:LEU:HD11	2.36	0.61
1:B:1254:PRO:O	1:B:1256:GLY:N	2.32	0.61
1:C:99:VAL:HG22	1:C:99:VAL:O	2.01	0.61
1:C:255:LEU:HD23	1:C:1058:GLY:C	2.20	0.61
1:C:837:THR:O	1:C:838:GLU:HB2	1.99	0.61
1:C:1036:ASP:OD1	1:C:1036:ASP:N	2.34	0.61
1:C:258:VAL:CG1	1:C:1058:GLY:HA3	2.30	0.61
1:C:849:MET:CE	1:C:929:PHE:CE2	2.84	0.61
1:C:1014:MET:HG3	1:C:1017:ALA:HB2	1.81	0.61
1:C:1277:LEU:O	1:C:1278:TYR:O	2.19	0.61
1:C:348:LEU:CD1	1:C:1301:VAL:HG22	2.30	0.61
1:C:897:TYR:O	1:C:898:GLN:HG2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:THR:HG23	1:C:237:VAL:CG2	2.31	0.61
1:B:629:ARG:NH2	1:B:1036:ASP:O	2.34	0.61
1:C:101:ASP:OD1	1:C:101:ASP:N	2.31	0.61
1:C:309:TRP:CH2	1:C:1257:ALA:HB1	2.36	0.61
1:C:659:LEU:CD2	1:C:662:VAL:HG21	2.31	0.61
1:C:838:GLU:HB2	1:C:934:LEU:CG	2.26	0.61
1:C:965:ARG:NH1	1:C:968:ARG:NH1	2.48	0.61
1:C:1242:MET:SD	1:C:1260:PRO:HG3	2.41	0.61
1:C:114:VAL:HG23	1:C:114:VAL:O	2.00	0.60
1:C:607:PHE:C	1:C:608:THR:HG23	2.20	0.60
1:C:873:TYR:HD2	1:C:898:GLN:CG	2.12	0.60
1:C:1271:SER:HB2	1:C:1275:ASP:O	2.01	0.60
1:B:385:ILE:HG13	1:B:1330:ILE:HG22	1.83	0.60
1:C:466:VAL:HG13	1:C:466:VAL:O	1.99	0.60
1:B:1021:ARG:O	1:B:1029:LEU:HB2	2.01	0.60
1:C:204:VAL:HG21	1:C:1242:MET:HG3	1.81	0.60
1:C:656:VAL:HG13	1:C:656:VAL:O	2.01	0.60
1:C:668:VAL:CG2	1:C:673:GLN:CB	2.66	0.60
1:B:530:GLY:O	1:B:533:GLN:HB3	2.02	0.60
1:B:590:SER:HA	1:B:725:ALA:HB2	1.81	0.60
1:C:843:LEU:HD21	1:C:943:GLU:OE2	2.01	0.60
1:C:1081:ASP:N	1:C:1227:MET:CG	2.57	0.60
1:C:1143:GLU:C	1:C:1145:ALA:H	2.04	0.60
1:C:91:ASP:OD1	1:C:91:ASP:N	2.28	0.60
1:C:123:GLU:O	1:C:123:GLU:HG2	2.00	0.60
1:C:924:ASP:CG	1:C:927:SER:CB	2.69	0.60
1:B:145:THR:HB	1:B:1317:VAL:HG13	1.83	0.60
1:B:453:LEU:HD12	1:B:682:GLN:HE21	1.66	0.60
1:B:1179:THR:OG1	1:B:1181:SER:O	2.18	0.60
1:C:449:PHE:CD1	1:C:450:PRO:CD	2.83	0.60
1:C:874:ILE:HG13	1:C:895:VAL:HG13	1.81	0.60
1:C:1176:GLU:HG3	1:C:1176:GLU:O	2.00	0.60
1:B:427:VAL:HG11	1:B:755:LEU:HD21	1.84	0.60
1:C:184:GLU:O	1:C:187:ASP:CA	2.48	0.60
1:C:929:PHE:CD2	1:C:936:MET:CE	2.84	0.60
1:C:1173:TYR:CG	1:C:1204:LEU:CD1	2.85	0.60
1:C:1271:SER:HB3	1:C:1274:GLY:H	1.66	0.60
1:C:837:THR:CG2	1:C:934:LEU:HD11	2.24	0.60
1:C:874:ILE:CD1	1:C:883:ILE:HD11	2.30	0.60
1:B:475:ILE:O	1:B:475:ILE:HG23	2.01	0.60
1:C:240:GLY:C	1:C:242:GLU:H	2.06	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:446:LYS:CB	1:C:448:TYR:CE1	2.84	0.60
1:B:1234:GLN:HB3	1:B:1235:PRO:HD2	1.82	0.59
1:C:492:VAL:HG23	1:C:492:VAL:O	2.01	0.59
1:C:733:VAL:HG21	1:C:1022:ILE:CD1	2.30	0.59
1:C:862:ARG:HG2	1:C:952:PHE:CE2	2.37	0.59
1:C:929:PHE:CD2	1:C:936:MET:HE2	2.37	0.59
1:B:833:ARG:HD3	1:B:922:TYR:CZ	2.36	0.59
1:B:862:ARG:NH1	1:B:948:ILE:HG21	2.17	0.59
1:C:258:VAL:HG13	1:C:1058:GLY:HA3	1.84	0.59
1:C:980:ARG:O	1:C:984:GLU:HB2	2.02	0.59
1:B:1238:VAL:HG23	1:B:1239:ALA:H	1.67	0.59
1:B:1249:ASN:HB3	1:C:1110:LEU:HB3	1.84	0.59
1:C:1171:ILE:O	1:C:1171:ILE:HG12	2.02	0.59
1:C:1280:PRO:HG3	1:C:1286:VAL:C	2.22	0.59
1:C:146:GLU:HG2	1:C:1317:VAL:HG13	1.84	0.59
1:C:189:ILE:HG12	1:C:286:LEU:CD1	2.32	0.59
1:C:467:LYS:HB3	1:C:467:LYS:NZ	2.16	0.59
1:C:614:ARG:HD3	1:C:635:ILE:CD1	2.32	0.59
1:C:1044:ARG:HG3	1:C:1044:ARG:O	2.02	0.59
1:B:397:LEU:HD21	1:C:1008:LEU:CD1	2.32	0.59
1:C:120:VAL:O	1:C:120:VAL:HG13	2.01	0.59
1:C:176:LYS:HG3	1:C:177:LYS:N	2.11	0.59
1:C:430:ASN:C	1:C:430:ASN:HD22	2.05	0.59
1:C:948:ILE:HG23	1:C:948:ILE:O	2.03	0.59
1:B:637:TYR:HB2	1:B:703:SER:HB3	1.84	0.59
1:C:113:VAL:O	1:C:113:VAL:HG13	2.03	0.59
1:C:154:PHE:HE2	1:C:365:LEU:HB2	1.68	0.59
1:C:208:LEU:CB	1:C:221:LEU:HD22	2.32	0.59
1:C:609:PRO:HB2	1:C:634:TYR:CE2	2.37	0.59
1:C:674:LYS:HB2	1:C:674:LYS:HZ2	1.67	0.59
1:C:989:ILE:HG23	1:C:990:THR:HG23	1.83	0.59
1:C:1094:GLU:HA	1:C:1094:GLU:OE2	2.01	0.59
1:C:1298:PHE:N	1:C:1298:PHE:CD1	2.70	0.59
1:C:1325:VAL:O	1:C:1325:VAL:HG12	2.01	0.59
1:C:493:HIS:HB3	1:C:756:THR:O	2.02	0.59
1:C:494:GLU:O	1:C:494:GLU:HG2	2.02	0.59
1:C:606:LEU:HD13	1:C:655:ILE:CG2	2.17	0.59
1:C:838:GLU:C	1:C:940:ARG:HE	2.01	0.59
1:C:1298:PHE:N	1:C:1298:PHE:HD1	2.00	0.59
1:B:167:SER:OG	1:B:205:ASN:OD1	2.21	0.59
1:B:313:ASP:O	1:B:317:MET:HB2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:GLU:OE1	1:C:133:MET:CE	2.51	0.59
1:C:422:LEU:CD1	1:C:490:PHE:HE2	2.12	0.59
1:C:452:ASN:C	1:C:453:LEU:HD22	2.23	0.59
1:C:1280:PRO:HB3	1:C:1287:GLY:CA	2.27	0.59
1:B:1071:PHE:CZ	1:B:1236:ILE:HD13	2.38	0.59
1:C:928:ARG:H	1:C:928:ARG:CD	2.15	0.59
1:B:231:LEU:HB2	1:B:249:SER:HB2	1.85	0.59
1:C:213:PHE:CE1	1:C:254:VAL:HG23	2.37	0.59
1:C:230:ASP:OD2	1:C:985:ARG:NE	2.27	0.59
1:C:244:SER:O	1:C:247:TYR:HB3	2.03	0.59
1:C:1079:LEU:O	1:C:1227:MET:HB3	2.03	0.59
1:C:1104:ARG:HG2	1:C:1104:ARG:NH1	2.18	0.59
1:B:188:ARG:HH22	1:C:237:VAL:CG1	2.16	0.58
1:B:388:GLN:N	1:B:1320:VAL:CG1	2.64	0.58
1:C:108:LYS:HG3	1:C:108:LYS:O	2.02	0.58
1:C:1060:ARG:HA	1:C:1060:ARG:HE	1.68	0.58
1:B:272:THR:CG2	1:C:235:ILE:HG21	2.33	0.58
1:B:472:GLU:HB2	1:B:761:SER:CB	2.33	0.58
1:B:1285:GLN:O	1:B:1286:VAL:HG23	2.03	0.58
1:C:248:VAL:HG11	1:C:970:LEU:CB	2.21	0.58
1:C:389:PHE:CD1	1:C:1319:ARG:HB3	2.37	0.58
1:C:451:GLU:HB2	1:C:686:HIS:CB	2.33	0.58
1:C:1174:THR:HG23	1:C:1174:THR:O	2.03	0.58
1:C:463:VAL:O	1:C:467:LYS:HG3	2.03	0.58
1:C:654:THR:HG22	1:C:658:THR:HG22	1.82	0.58
1:C:756:THR:O	1:C:756:THR:HG22	2.01	0.58
1:C:185:ALA:C	1:C:187:ASP:H	2.07	0.58
1:C:408:ILE:HG22	1:C:408:ILE:O	2.04	0.58
1:C:1070:ARG:O	1:C:1070:ARG:HG2	2.02	0.58
1:C:81:ALA:HB3	1:C:170:TYR:OH	2.02	0.58
1:C:427:VAL:O	1:C:431:THR:HG22	2.03	0.58
1:C:560:ILE:HG23	1:C:560:ILE:O	2.02	0.58
1:C:820:ILE:HG21	1:C:983:ILE:CD1	2.33	0.58
1:C:850:THR:OG1	1:C:916:LEU:CD2	2.52	0.58
1:C:901:VAL:HG13	1:C:901:VAL:O	2.04	0.58
1:C:963:ALA:HB3	1:C:1059:LEU:CG	2.30	0.58
1:C:1135:PRO:O	1:C:1136:HIS:HB2	2.04	0.58
1:C:1276:LEU:HD23	1:C:1276:LEU:H	1.68	0.58
1:C:256:PHE:HD1	1:C:819:PHE:CE2	2.21	0.58
1:B:699:THR:O	1:B:703:SER:HB3	2.04	0.58
1:B:922:TYR:O	1:B:925:VAL:HG13	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:668:VAL:HG23	1:C:673:GLN:HE21	1.68	0.58
1:C:849:MET:CA	1:C:917:VAL:O	2.50	0.58
1:C:892:VAL:HG11	1:C:894:VAL:HG13	1.63	0.58
1:C:935:GLN:HB3	1:C:939:ASN:CB	2.31	0.58
1:C:957:PHE:CD1	1:C:957:PHE:N	2.72	0.58
1:C:1121:HIS:CD2	1:C:1135:PRO:HG2	2.37	0.58
1:C:1055:LEU:O	1:C:1055:LEU:HG	2.01	0.58
1:B:893:ALA:HB1	1:B:915:VAL:HA	1.86	0.58
1:C:360:ILE:HG22	1:C:360:ILE:O	2.03	0.58
1:C:1198:LYS:O	1:C:1198:LYS:HD3	2.03	0.58
1:B:1250:GLU:O	1:B:1251:VAL:HG13	2.04	0.58
1:C:389:PHE:CD1	1:C:1317:VAL:CG2	2.86	0.58
1:C:452:ASN:O	1:C:453:LEU:HD22	2.03	0.58
1:C:644:VAL:HG13	1:C:644:VAL:O	2.03	0.58
1:C:644:VAL:O	1:C:644:VAL:HG22	2.02	0.58
1:C:918:VAL:HG23	1:C:918:VAL:O	2.02	0.58
1:B:824:LEU:HD22	1:B:979:ILE:HD12	1.86	0.57
1:C:1014:MET:CG	1:C:1017:ALA:HB2	2.34	0.57
1:B:461:ARG:HH11	1:B:461:ARG:CG	2.15	0.57
1:B:1076:ILE:HG12	1:B:1230:ILE:HG22	1.85	0.57
1:C:259:MET:HA	1:C:1054:ARG:HB3	1.86	0.57
1:C:439:VAL:HG22	1:C:439:VAL:O	2.03	0.57
1:C:1079:LEU:CD1	1:C:1231:TYR:HH	1.94	0.57
1:C:1085:ASP:HB2	1:C:1086:PRO:HD2	1.83	0.57
1:B:1064:ASN:ND2	1:B:1296:ILE:HD11	2.18	0.57
1:C:314:ILE:HG22	1:C:318:LEU:HD22	1.87	0.57
1:C:656:VAL:CG1	1:C:688:GLU:CG	2.82	0.57
1:C:668:VAL:CG2	1:C:673:GLN:HE21	2.17	0.57
1:C:747:ARG:HG2	1:C:747:ARG:HH11	1.68	0.57
1:C:965:ARG:HH11	1:C:968:ARG:HH12	1.50	0.57
1:C:1121:HIS:CD2	1:C:1135:PRO:CB	2.87	0.57
1:C:154:PHE:HE1	1:C:361:ASN:HD21	1.50	0.57
1:C:405:HIS:CD2	1:C:625:PRO:CA	2.83	0.57
1:C:610:GLN:HE21	1:C:610:GLN:CA	2.12	0.57
1:C:709:MET:O	1:C:715:ASN:ND2	2.37	0.57
1:C:1140:THR:HA	1:C:1167:ASP:HB3	1.86	0.57
1:B:261:ASP:OD2	1:B:263:ARG:NH2	2.37	0.57
1:B:439:VAL:C	1:B:440:ILE:HG13	2.24	0.57
1:B:577:GLN:O	1:B:580:TYR:N	2.37	0.57
1:C:1023:ARG:HB3	1:C:1023:ARG:HH21	1.68	0.57
1:C:1310:ARG:HA	1:C:1310:ARG:NE	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:LEU:HD11	1:B:1318:GLU:HG2	1.87	0.57
1:B:874:ILE:HG23	1:B:895:VAL:HG21	1.86	0.57
1:C:403:PHE:CZ	1:C:408:ILE:HG13	2.39	0.57
1:C:342:THR:O	1:C:1305:MET:CE	2.52	0.57
1:C:654:THR:CG2	1:C:658:THR:CG2	2.77	0.57
1:C:635:ILE:HD11	1:C:707:ALA:HA	1.85	0.57
1:C:451:GLU:OE1	1:C:685:ARG:HG2	2.03	0.57
1:C:585:PHE:CE1	1:C:728:LYS:HE2	2.40	0.57
1:C:762:ILE:HD12	1:C:762:ILE:O	2.04	0.57
1:C:1147:MET:HE3	1:C:1152:ALA:HB2	1.87	0.57
1:B:469:ARG:NH1	1:B:498:ILE:CG1	2.61	0.57
1:C:255:LEU:CD2	1:C:1058:GLY:C	2.73	0.57
1:C:389:PHE:HD1	1:C:1317:VAL:HG22	1.70	0.57
1:C:434:VAL:HG23	1:C:709:MET:CE	2.33	0.57
1:C:339:LEU:CD1	1:C:397:LEU:HD23	2.34	0.56
1:C:478:ILE:HD13	1:C:762:ILE:HD11	1.80	0.56
1:C:521:PHE:N	1:C:521:PHE:CD1	2.71	0.56
1:C:668:VAL:CG1	1:C:674:LYS:HD3	2.35	0.56
1:C:820:ILE:HG21	1:C:983:ILE:HG13	1.83	0.56
1:C:915:VAL:HG23	1:C:915:VAL:O	2.04	0.56
1:C:939:ASN:HD22	1:C:939:ASN:C	2.00	0.56
1:C:1231:TYR:N	1:C:1231:TYR:CD1	2.72	0.56
1:B:184:GLU:O	1:B:188:ARG:HG2	2.04	0.56
1:B:793:TYR:HD2	1:B:1321:ASN:CG	2.08	0.56
1:B:831:VAL:H	1:B:854:GLN:HE21	1.52	0.56
1:B:957:PHE:HB2	1:B:1042:TRP:CZ3	2.40	0.56
1:B:383:SER:HB3	1:B:387:THR:HG21	1.86	0.56
1:B:461:ARG:NE	1:B:504:ASP:HB2	2.18	0.56
1:B:472:GLU:O	1:B:761:SER:CB	2.38	0.56
1:C:109:LYS:HB3	1:C:109:LYS:NZ	2.21	0.56
1:C:362:LEU:HD23	1:C:362:LEU:O	2.04	0.56
1:C:446:LYS:HB3	1:C:448:TYR:CZ	2.40	0.56
1:C:471:SER:HB3	1:C:765:PRO:HG2	1.87	0.56
1:C:503:GLU:OE2	1:C:542:ARG:CD	2.50	0.56
1:C:747:ARG:HH11	1:C:747:ARG:CG	2.18	0.56
1:C:890:THR:O	1:C:890:THR:OG1	2.21	0.56
1:C:928:ARG:H	1:C:928:ARG:HD3	1.70	0.56
1:C:1054:ARG:NH1	1:C:1054:ARG:HG2	2.19	0.56
1:C:661:ASN:O	1:C:665:GLU:HB3	2.05	0.56
1:C:1000:LEU:CD2	1:C:1010:ARG:CZ	2.81	0.56
1:B:637:TYR:HB3	1:B:699:THR:HA	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:874:ILE:CG2	1:C:902:ILE:CD1	2.82	0.56
1:C:1135:PRO:HG2	1:C:1137:VAL:CG1	2.34	0.56
1:B:1121:HIS:HD2	1:B:1124:THR:HG22	1.69	0.56
1:C:225:ILE:HD11	1:C:1069:ARG:CB	2.36	0.56
1:B:383:SER:HG	1:B:389:PHE:HZ	1.51	0.56
1:C:498:ILE:CD1	1:C:514:PHE:HZ	2.19	0.56
1:C:582:SER:O	1:C:728:LYS:HD2	2.05	0.56
1:C:1317:VAL:HG13	1:C:1317:VAL:O	2.05	0.56
1:B:338:ARG:NH1	1:C:1005:LEU:HD22	2.21	0.56
1:B:366:MET:HE3	1:B:1309:ILE:HD13	1.86	0.56
1:B:558:TYR:CZ	1:B:590:SER:HB3	2.41	0.56
1:C:96:ILE:HD11	1:C:103:GLY:HA2	1.84	0.56
1:C:449:PHE:HZ	1:C:463:VAL:HG22	1.70	0.56
1:C:556:ALA:O	1:C:587:ALA:HB2	2.04	0.56
1:B:489:MET:SD	1:B:527:ARG:HD2	2.46	0.56
1:C:538:LEU:HD21	1:C:542:ARG:HH21	1.70	0.56
1:C:772:TYR:N	1:C:772:TYR:CD1	2.74	0.56
1:B:310:LEU:O	1:B:314:ILE:HG12	2.05	0.56
1:C:554:ARG:CD	1:C:594:LEU:HD21	2.30	0.56
1:C:1111:ALA:HB2	1:C:1129:PRO:CB	2.36	0.56
1:B:287:ARG:HH11	1:B:330:THR:HB	1.71	0.55
1:B:303:ASP:HA	1:B:311:ASN:HD21	1.71	0.55
1:B:1306:THR:HG22	1:B:1307:ALA:H	1.69	0.55
1:C:758:ILE:HG13	1:C:758:ILE:O	2.06	0.55
1:C:987:ALA:O	1:C:992:VAL:HG13	2.06	0.55
1:C:1081:ASP:N	1:C:1227:MET:CB	2.68	0.55
1:C:1332:ASN:O	1:C:1333:ALA:OXT	2.24	0.55
1:B:264:LEU:HD11	1:B:365:LEU:HD11	1.88	0.55
1:B:414:LEU:HA	1:B:734:ILE:HD11	1.88	0.55
1:B:1290:LYS:HE2	1:B:1300:ASN:HB3	1.87	0.55
1:B:198:LYS:O	1:B:200:GLY:HA2	2.06	0.55
1:C:213:PHE:CZ	1:C:254:VAL:CG2	2.88	0.55
1:C:259:MET:O	1:C:1054:ARG:HG2	2.07	0.55
1:C:348:LEU:HD12	1:C:1301:VAL:HG22	1.88	0.55
1:C:838:GLU:HB2	1:C:934:LEU:CD1	2.36	0.55
1:C:874:ILE:HG22	1:C:874:ILE:O	2.06	0.55
1:C:1175:ALA:HA	1:C:1204:LEU:O	2.07	0.55
1:C:1176:GLU:HG2	1:C:1203:HIS:HE1	1.72	0.55
1:B:924:ASP:OD1	1:B:927:SER:HB2	2.07	0.55
1:C:304:PHE:N	1:C:304:PHE:CD1	2.71	0.55
1:C:387:THR:HG23	1:C:387:THR:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:465:ALA:CB	1:C:506:SER:HB3	2.36	0.55
1:C:838:GLU:HG2	1:C:935:GLN:N	2.14	0.55
1:C:845:GLU:CD	1:C:911:ARG:HH21	2.08	0.55
1:C:1074:VAL:HB	1:C:1173:TYR:CE2	2.37	0.55
1:C:117:ARG:CG	1:C:121:PHE:CZ	2.89	0.55
1:C:461:ARG:HG3	1:C:461:ARG:O	2.06	0.55
1:C:607:PHE:O	1:C:608:THR:HG22	2.06	0.55
1:B:309:TRP:CH2	1:B:1257:ALA:HB1	2.42	0.55
1:B:576:ASP:OD1	1:B:577:GLN:N	2.39	0.55
1:C:225:ILE:HD11	1:C:1069:ARG:CA	2.37	0.55
1:C:230:ASP:HB3	1:C:985:ARG:HG3	1.77	0.55
1:C:446:LYS:CD	1:C:448:TYR:CZ	2.89	0.55
1:C:122:ASN:HD22	1:C:122:ASN:C	2.04	0.55
1:C:180:LEU:HD22	1:C:306:GLN:CD	2.15	0.55
1:C:735:THR:HG21	1:C:1028:VAL:CG2	2.34	0.55
1:C:926:VAL:CG1	1:C:937:ASN:HD22	2.19	0.55
1:C:1000:LEU:HD23	1:C:1010:ARG:HE	1.71	0.55
1:B:276:ASN:OD1	1:C:1199:GLY:HA3	2.07	0.55
1:B:315:THR:O	1:B:319:GLN:HB2	2.06	0.55
1:C:254:VAL:HG13	1:C:1062:ILE:HD13	1.89	0.55
1:C:469:ARG:NH2	1:C:498:ILE:HG23	2.21	0.55
1:B:157:ILE:HD11	1:B:265:VAL:HG22	1.88	0.55
1:B:307:VAL:HG13	1:B:310:LEU:HB3	1.88	0.55
1:C:588:LEU:HG	1:C:604:MET:SD	2.47	0.55
1:C:738:GLU:HB3	1:C:1015:GLN:HG3	1.87	0.55
1:C:822:MET:CE	1:C:1046:PHE:CE2	2.89	0.55
1:C:838:GLU:HA	1:C:940:ARG:HD3	1.89	0.55
1:C:1054:ARG:HH11	1:C:1054:ARG:HG2	1.71	0.55
1:C:1116:ARG:NH1	1:C:1130:SER:HB2	2.22	0.55
1:B:332:THR:HG23	1:B:344:VAL:HG12	1.89	0.55
1:C:547:GLU:HG3	1:C:597:ALA:HA	1.90	0.55
1:C:714:LEU:HD11	1:C:806:VAL:HG12	1.89	0.55
1:C:1044:ARG:CG	1:C:1044:ARG:NH1	2.70	0.55
1:B:1124:THR:HG23	1:B:1126:MET:H	1.72	0.54
1:C:146:GLU:CB	1:C:1317:VAL:CG1	2.85	0.54
1:B:235:ILE:HG13	1:B:978:GLN:NE2	2.14	0.54
1:B:832:MET:SD	1:B:848:ARG:HD2	2.47	0.54
1:C:157:ILE:HG13	1:C:263:ARG:HG2	1.86	0.54
1:C:163:TYR:N	1:C:163:TYR:CD1	2.71	0.54
1:C:498:ILE:H	1:C:498:ILE:HD12	1.72	0.54
1:C:1097:VAL:O	1:C:1097:VAL:HG13	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:875:THR:OG1	1:B:876:GLY:HA2	2.07	0.54
1:C:225:ILE:HG23	1:C:247:TYR:CD1	2.40	0.54
1:C:837:THR:CG2	1:C:934:LEU:CD1	2.68	0.54
1:C:892:VAL:HG12	1:C:894:VAL:H	1.72	0.54
1:C:1171:ILE:CD1	1:C:1202:PHE:CZ	2.78	0.54
1:B:926:VAL:CG2	1:B:938:ASN:H	2.20	0.54
1:B:515:ILE:HG21	1:B:655:ILE:HG21	1.90	0.54
1:C:128:GLU:OE1	1:C:133:MET:HE2	2.08	0.54
1:C:495:LEU:N	1:C:495:LEU:CD1	2.70	0.54
1:C:972:PRO:O	1:C:972:PRO:HG2	2.08	0.54
1:C:1310:ARG:HH21	1:C:1312:GLY:H	1.55	0.54
1:B:291:HIS:CD2	1:B:348:LEU:HD21	2.43	0.54
1:B:1276:LEU:HD22	1:B:1300:ASN:HB2	1.89	0.54
1:C:820:ILE:CG2	1:C:983:ILE:CG1	2.77	0.54
1:C:840:ASP:C	1:C:940:ARG:HH22	2.11	0.54
1:C:1310:ARG:NE	1:C:1310:ARG:CA	2.70	0.54
1:C:1319:ARG:HG3	1:C:1319:ARG:O	2.08	0.54
1:C:511:VAL:HG21	1:C:539:PHE:CZ	2.43	0.54
1:C:887:VAL:HG22	1:C:893:ALA:HA	1.90	0.54
1:C:1134:ARG:HH22	1:C:1154:ASN:ND2	2.04	0.54
1:C:1179:THR:HG23	1:C:1179:THR:O	2.07	0.54
1:C:1193:ILE:HG23	1:C:1193:ILE:O	2.06	0.54
1:B:1314:ASP:N	1:B:1314:ASP:OD1	2.40	0.54
1:C:168:VAL:CG2	1:C:204:VAL:CG1	2.85	0.54
1:C:220:ASP:OD1	1:C:222:THR:HG23	2.08	0.54
1:C:265:VAL:O	1:C:1303:SER:HA	2.08	0.54
1:C:364:ALA:CB	1:C:1050:LEU:CD2	2.85	0.54
1:C:446:LYS:CB	1:C:448:TYR:CZ	2.91	0.54
1:C:467:LYS:HB3	1:C:467:LYS:HZ2	1.72	0.54
1:B:225:ILE:HG23	1:B:1069:ARG:HB2	1.90	0.54
1:C:81:ALA:HB3	1:C:168:VAL:CG1	2.38	0.54
1:C:427:VAL:O	1:C:427:VAL:HG12	2.07	0.54
1:C:458:SER:HB3	1:C:675:ALA:HB1	1.90	0.54
1:C:500:GLU:HA	1:C:500:GLU:OE1	2.08	0.54
1:C:515:ILE:HG21	1:C:655:ILE:HG21	1.89	0.54
1:C:559:THR:HG22	1:C:583:GLU:HG3	1.90	0.54
1:C:612:PHE:N	1:C:612:PHE:CD1	2.73	0.54
1:C:736:SER:CB	1:C:1016:ASN:O	2.46	0.54
1:B:206:ILE:HB	1:B:1066:ARG:HD3	1.90	0.53
1:B:267:VAL:HA	1:B:1304:MET:HE1	1.90	0.53
1:B:434:VAL:O	1:B:439:VAL:HG22	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:258:VAL:CG1	1:C:1058:GLY:HA2	2.34	0.53
1:C:449:PHE:N	1:C:450:PRO:HD3	2.22	0.53
1:C:666:ARG:HG2	1:C:666:ARG:NH1	2.18	0.53
1:C:822:MET:HE3	1:C:1046:PHE:CE2	2.43	0.53
1:C:843:LEU:CD2	1:C:943:GLU:HG3	2.38	0.53
1:C:870:ASP:C	1:C:871:PRO:O	2.44	0.53
1:C:297:ASN:ND2	1:C:298:PRO:CD	2.67	0.53
1:C:385:ILE:O	1:C:1328:ILE:CG2	2.56	0.53
1:C:615:THR:N	1:C:1333:ALA:C	2.59	0.53
1:C:985:ARG:HH22	1:C:989:ILE:HB	1.71	0.53
1:B:139:ASN:O	1:C:757:ILE:CB	2.56	0.53
1:B:1282:ALA:HB1	1:B:1283:ASN:CA	2.39	0.53
1:C:146:GLU:HB2	1:C:1317:VAL:HG13	1.90	0.53
1:C:505:PRO:O	1:C:508:ILE:HG22	2.08	0.53
1:C:741:TYR:CZ	1:C:1022:ILE:CD1	2.91	0.53
1:C:1173:TYR:CE1	1:C:1204:LEU:CD1	2.91	0.53
1:B:1250:GLU:OE1	1:B:1250:GLU:N	2.41	0.53
1:C:259:MET:SD	1:C:1055:LEU:HB2	2.48	0.53
1:C:543:TRP:HD1	1:C:544:TYR:HD1	1.54	0.53
1:C:607:PHE:C	1:C:608:THR:CG2	2.77	0.53
1:C:635:ILE:HG23	1:C:635:ILE:O	2.08	0.53
1:C:849:MET:CG	1:C:919:MET:HG3	2.39	0.53
1:C:352:HIS:CD2	1:C:1297:SER:H	2.17	0.53
1:C:462:LEU:HD22	1:C:462:LEU:C	2.23	0.53
1:C:571:ARG:NH1	1:C:571:ARG:CB	2.71	0.53
1:C:1046:PHE:HB2	1:C:1052:LEU:HD21	1.90	0.53
1:C:1118:THR:HB	1:C:1129:PRO:HA	1.91	0.53
1:C:1322:PRO:CB	1:C:1328:ILE:HD11	2.38	0.53
1:B:1242:MET:SD	1:B:1260:PRO:HG3	2.49	0.53
1:C:157:ILE:CD1	1:C:263:ARG:HB3	2.36	0.53
1:C:206:ILE:HD11	1:C:1066:ARG:CD	2.39	0.53
1:C:652:PHE:HE1	1:C:688:GLU:HB3	1.74	0.53
1:B:1158:SER:O	1:B:1162:SER:HB2	2.09	0.53
1:C:154:PHE:HD1	1:C:262:ASN:HB2	1.73	0.53
1:C:651:ARG:HD2	1:C:651:ARG:O	2.08	0.53
1:C:865:ILE:HD13	1:C:865:ILE:N	2.23	0.53
1:C:1307:ALA:O	1:C:1309:ILE:N	2.39	0.53
1:C:1318:GLU:O	1:C:1318:GLU:HG2	2.08	0.53
1:C:144:ASN:HA	1:C:1318:GLU:HB3	1.91	0.53
1:C:1159:VAL:O	1:C:1159:VAL:HG22	2.09	0.53
1:B:373:ASP:O	1:B:376:ILE:HB	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:422:LEU:C	1:C:422:LEU:HD13	2.29	0.53
1:C:840:ASP:CA	1:C:940:ARG:HH22	2.22	0.53
1:C:1014:MET:HG3	1:C:1017:ALA:CB	2.38	0.53
1:C:1022:ILE:HG12	1:C:1027:THR:O	2.08	0.53
1:C:1231:TYR:HB3	1:C:1232:PRO:CD	2.39	0.53
1:B:388:GLN:N	1:B:1320:VAL:HG12	2.24	0.53
1:B:1148:SER:HB2	1:B:1151:VAL:H	1.74	0.53
1:C:256:PHE:HD1	1:C:819:PHE:CD2	2.26	0.53
1:C:910:LEU:HD23	1:C:915:VAL:HG23	0.57	0.53
1:C:1258:VAL:HG23	1:C:1258:VAL:O	2.07	0.53
1:C:1283:ASN:N	1:C:1283:ASN:OD1	2.41	0.53
1:B:309:TRP:HB3	1:B:1252:ASP:O	2.10	0.52
1:C:434:VAL:O	1:C:434:VAL:HG12	2.09	0.52
1:C:466:VAL:O	1:C:466:VAL:HG22	2.07	0.52
1:C:838:GLU:C	1:C:940:ARG:CZ	2.77	0.52
1:C:1002:LEU:HD13	1:C:1005:LEU:HD13	1.91	0.52
1:B:197:PHE:HD2	1:B:301:LEU:HD22	1.74	0.52
1:B:874:ILE:H	1:B:897:TYR:HB3	1.75	0.52
1:B:1071:PHE:HZ	1:B:1236:ILE:HD13	1.74	0.52
1:C:189:ILE:HG12	1:C:286:LEU:HD12	1.91	0.52
1:C:309:TRP:CD1	1:C:309:TRP:C	2.83	0.52
1:C:498:ILE:HD11	1:C:514:PHE:HZ	1.75	0.52
1:C:736:SER:HB2	1:C:1016:ASN:C	2.28	0.52
1:C:1322:PRO:HB2	1:C:1328:ILE:HD11	1.91	0.52
1:B:144:ASN:H	1:B:1318:GLU:H	1.58	0.52
1:C:168:VAL:CB	1:C:204:VAL:HG12	2.38	0.52
1:C:233:VAL:HG22	1:C:234:PRO:HD2	0.57	0.52
1:C:403:PHE:CE1	1:C:408:ILE:HG13	2.44	0.52
1:C:536:LEU:HD11	1:C:607:PHE:CZ	2.44	0.52
1:B:626:ARG:NH2	1:B:712:PHE:O	2.43	0.52
1:C:285:VAL:HG13	1:C:326:GLY:HA2	1.91	0.52
1:C:607:PHE:O	1:C:608:THR:HG23	2.09	0.52
1:C:1046:PHE:CD2	1:C:1052:LEU:CD2	2.93	0.52
1:B:352:HIS:HD2	1:B:1297:SER:H	1.57	0.52
1:C:855:TYR:CD1	1:C:859:ILE:HB	2.44	0.52
1:C:879:THR:N	1:C:880:PRO:HD2	2.09	0.52
1:B:388:GLN:CA	1:B:1320:VAL:CG1	2.87	0.52
1:B:472:GLU:N	1:B:473:ALA:CA	2.73	0.52
1:B:817:ASP:OD1	1:B:983:ILE:HG21	2.09	0.52
1:C:350:ILE:O	1:C:350:ILE:HG13	2.09	0.52
1:C:397:LEU:H	1:C:397:LEU:HD12	1.72	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:603:ILE:HD13	1:C:659:LEU:HD23	1.91	0.52
1:C:838:GLU:HB2	1:C:934:LEU:HB2	0.53	0.52
1:C:1097:VAL:HG12	1:C:1136:HIS:O	2.10	0.52
1:C:1099:VAL:O	1:C:1139:MET:HA	2.10	0.52
1:C:1105:LEU:HD12	1:C:1105:LEU:N	2.20	0.52
1:B:451:GLU:HG2	1:B:452:ASN:N	2.25	0.52
1:B:472:GLU:C	1:B:761:SER:HB2	2.27	0.52
1:C:157:ILE:HD11	1:C:263:ARG:NE	2.24	0.52
1:C:157:ILE:CD1	1:C:263:ARG:CG	2.61	0.52
1:C:341:LYS:CB	1:C:1306:THR:HB	2.39	0.52
1:C:449:PHE:N	1:C:450:PRO:CD	2.72	0.52
1:C:750:GLU:HA	1:C:756:THR:HG21	1.90	0.52
1:C:937:ASN:N	1:C:937:ASN:OD1	2.41	0.52
1:C:1193:ILE:HG13	1:C:1202:PHE:CZ	2.43	0.52
1:B:878:SER:O	1:B:879:THR:HG23	2.09	0.52
1:C:193:THR:HG21	1:C:300:LEU:HB3	1.91	0.52
1:B:559:THR:HG23	1:B:583:GLU:HG3	1.90	0.52
1:C:285:VAL:CG1	1:C:326:GLY:HA2	2.39	0.52
1:C:830:VAL:HG21	1:C:947:GLU:CG	2.38	0.52
1:C:929:PHE:HB3	1:C:936:MET:CE	2.38	0.52
1:C:967:LEU:HD22	1:C:1062:ILE:HG21	1.92	0.52
1:C:1021:ARG:CB	1:C:1021:ARG:NH1	2.72	0.52
1:B:897:TYR:CE2	1:B:899:SER:HB3	2.44	0.52
1:C:146:GLU:CB	1:C:1317:VAL:HG12	2.40	0.52
1:C:442:PRO:HG2	1:C:442:PRO:O	2.09	0.52
1:C:656:VAL:HG11	1:C:688:GLU:CG	2.39	0.52
1:C:835:TYR:CE1	1:C:942:HIS:CD2	2.98	0.52
1:C:924:ASP:OD1	1:C:927:SER:CA	2.57	0.52
1:C:1230:ILE:O	1:C:1230:ILE:HG13	2.09	0.52
1:C:1247:ASN:HD22	1:C:1247:ASN:N	2.07	0.52
1:B:188:ARG:HH22	1:C:237:VAL:HG13	1.75	0.51
1:B:440:ILE:CG2	1:B:770:CYS:HB2	2.41	0.51
1:B:924:ASP:HB3	1:B:928:ARG:CZ	2.40	0.51
1:C:338:ARG:O	1:C:341:LYS:N	2.42	0.51
1:C:579:LEU:C	1:C:579:LEU:HD12	2.31	0.51
1:C:1081:ASP:O	1:C:1227:MET:HB3	2.10	0.51
1:C:1279:SER:H	1:C:1280:PRO:HA	1.70	0.51
1:C:339:LEU:O	1:C:397:LEU:HD21	2.10	0.51
1:C:511:VAL:CG2	1:C:539:PHE:CE2	2.93	0.51
1:C:612:PHE:CE2	1:C:614:ARG:HB3	2.45	0.51
1:C:613:LEU:HD22	1:C:613:LEU:C	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:694:ILE:C	1:C:694:ILE:HD12	2.31	0.51
1:C:928:ARG:CD	1:C:928:ARG:N	2.73	0.51
1:B:1103:HIS:CE1	1:B:1145:ALA:HB3	2.45	0.51
1:C:210:ARG:HA	1:C:221:LEU:CD1	2.39	0.51
1:C:254:VAL:HG11	1:C:1062:ILE:HD11	1.87	0.51
1:B:1306:THR:HG22	1:B:1307:ALA:N	2.25	0.51
1:B:517:PHE:CE2	1:B:528:ILE:HD11	2.46	0.51
1:C:434:VAL:CG2	1:C:709:MET:CE	2.88	0.51
1:C:484:ARG:O	1:C:485:GLU:C	2.47	0.51
1:C:669:GLN:OE1	1:C:669:GLN:N	2.43	0.51
1:C:815:LEU:CB	1:C:816:PRO:CD	2.81	0.51
1:C:1054:ARG:HH11	1:C:1054:ARG:CB	2.23	0.51
1:C:1259:ALA:HB1	1:C:1260:PRO:HD2	1.91	0.51
1:B:150:LEU:HD21	1:B:378:ALA:HB3	1.93	0.51
1:B:489:MET:SD	1:B:493:HIS:ND1	2.81	0.51
1:B:735:THR:HG21	1:B:1028:VAL:HG11	1.92	0.51
1:B:1128:TYR:HB3	1:B:1134:ARG:HG2	1.93	0.51
1:C:264:LEU:O	1:C:266:ILE:HG12	2.11	0.51
1:C:336:TYR:O	1:C:337:VAL:O	2.29	0.51
1:C:502:PHE:HA	1:C:507:SER:CB	2.41	0.51
1:C:1310:ARG:HG3	1:C:1310:ARG:O	2.11	0.51
1:B:461:ARG:NH1	1:B:461:ARG:CG	2.73	0.51
1:B:531:ASP:OD1	1:B:531:ASP:N	2.37	0.51
1:B:974:LEU:HA	1:B:978:GLN:OE1	2.10	0.51
1:B:1066:ARG:HD2	1:B:1296:ILE:HD13	1.92	0.51
1:C:334:LEU:HD11	1:C:366:MET:CE	2.37	0.51
1:C:409:ILE:HG23	1:C:1040:PHE:CZ	2.44	0.51
1:C:849:MET:HG2	1:C:919:MET:HG3	1.92	0.51
1:C:1222:ALA:O	1:C:1223:SER:HB2	2.10	0.51
1:B:1121:HIS:CD2	1:B:1123:PRO:HD2	2.45	0.51
1:B:1134:ARG:NH1	1:B:1158:SER:OG	2.44	0.51
1:C:285:VAL:O	1:C:327:LEU:N	2.39	0.51
1:C:285:VAL:O	1:C:326:GLY:HA2	2.11	0.51
1:C:320:GLN:O	1:C:321:ALA:CB	2.58	0.51
1:C:516:LEU:HB2	1:C:763:VAL:HG11	1.90	0.51
1:C:668:VAL:CG1	1:C:674:LYS:CD	2.88	0.51
1:B:388:GLN:CB	1:B:1320:VAL:HG11	2.12	0.51
1:C:190:VAL:HG11	1:C:304:PHE:CZ	2.46	0.51
1:C:231:LEU:HD13	1:C:982:ALA:HB1	1.93	0.51
1:C:485:GLU:OE1	1:C:486:VAL:CG1	2.56	0.51
1:B:879:THR:O	1:B:883:ILE:HD12	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:672:MET:SD	1:C:672:MET:C	2.89	0.51
1:C:1101:TYR:OH	1:C:1147:MET:HG2	2.10	0.51
1:B:231:LEU:HD23	1:B:985:ARG:HB3	1.93	0.50
1:B:305:THR:HG22	1:B:307:VAL:HG12	1.92	0.50
1:B:526:ASN:HB2	1:B:721:SER:HB3	1.92	0.50
1:C:337:VAL:HG12	1:C:338:ARG:H	1.76	0.50
1:C:741:TYR:CZ	1:C:1022:ILE:HD11	2.45	0.50
1:C:873:TYR:HA	1:C:896:LEU:O	2.11	0.50
1:C:878:SER:HB3	1:C:903:ASN:CG	2.31	0.50
1:C:887:VAL:O	1:C:887:VAL:HG12	2.10	0.50
1:C:954:GLN:CA	1:C:958:ILE:HD13	2.41	0.50
1:C:986:ILE:C	1:C:989:ILE:HG22	2.32	0.50
1:C:1077:MET:HB2	1:C:1165:VAL:HG22	1.91	0.50
1:C:1206:PHE:CE2	1:C:1236:ILE:HD13	2.46	0.50
1:C:1261:SER:C	1:C:1263:TYR:H	2.12	0.50
1:B:524:GLU:O	1:B:528:ILE:HG13	2.12	0.50
1:C:339:LEU:CD1	1:C:397:LEU:CD2	2.87	0.50
1:C:559:THR:CG2	1:C:583:GLU:HG3	2.41	0.50
1:C:568:PHE:N	1:C:568:PHE:CD1	2.77	0.50
1:C:820:ILE:HG22	1:C:983:ILE:HD11	1.92	0.50
1:C:1202:PHE:CD1	1:C:1202:PHE:C	2.84	0.50
1:C:1259:ALA:CB	1:C:1260:PRO:HD3	2.29	0.50
1:B:490:PHE:HA	1:B:745:ILE:HG12	1.92	0.50
1:B:735:THR:O	1:B:1017:ALA:HA	2.11	0.50
1:C:1078:TYR:HD2	1:C:1229:LEU:CD1	2.25	0.50
1:C:638:THR:HG22	1:C:638:THR:O	2.11	0.50
1:C:836:GLN:HB2	1:C:940:ARG:CB	2.38	0.50
1:C:947:GLU:O	1:C:947:GLU:HG3	2.11	0.50
1:C:1119:TYR:HE2	1:C:1135:PRO:HG3	1.76	0.50
1:C:614:ARG:HG3	1:C:614:ARG:O	2.10	0.50
1:C:617:ASP:HA	1:C:620:ILE:HG22	1.93	0.50
1:C:652:PHE:HZ	1:C:687:LEU:HD21	1.76	0.50
1:C:835:TYR:CE1	1:C:925:VAL:CG2	2.89	0.50
1:C:1248:HIS:HB3	1:C:1252:ASP:O	2.11	0.50
1:C:157:ILE:HD11	1:C:263:ARG:CD	2.41	0.50
1:C:204:VAL:CG2	1:C:1242:MET:O	2.58	0.50
1:C:255:LEU:HD23	1:C:1058:GLY:O	2.10	0.50
1:C:338:ARG:HG3	1:C:342:THR:HB	1.88	0.50
1:C:405:HIS:CD2	1:C:624:PHE:O	2.64	0.50
1:C:409:ILE:HD13	1:C:409:ILE:O	2.12	0.50
1:C:881:ASP:O	1:C:884:ALA:HB3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:987:ALA:O	1:C:992:VAL:CG1	2.60	0.50
1:C:1206:PHE:CD2	1:C:1236:ILE:HD13	2.45	0.50
1:B:683:TRP:CH2	1:B:687:LEU:HD11	2.46	0.50
1:C:235:ILE:HG22	1:C:236:GLY:N	2.27	0.50
1:C:304:PHE:N	1:C:304:PHE:HD1	2.10	0.50
1:C:551:PHE:CD1	1:C:551:PHE:C	2.85	0.50
1:C:1071:PHE:HB3	1:C:1234:GLN:OE1	2.12	0.50
1:C:1122:PRO:CB	1:C:1123:PRO:HD3	2.41	0.50
1:C:232:LEU:HD11	1:C:245:ALA:O	2.11	0.50
1:C:251:LEU:HD21	1:C:1062:ILE:HG13	1.87	0.50
1:C:338:ARG:HD3	1:C:342:THR:HG22	1.83	0.50
1:C:109:LYS:HD2	1:C:110:PRO:CD	2.39	0.50
1:C:449:PHE:HA	1:C:683:TRP:CD1	2.45	0.50
1:C:485:GLU:OE1	1:C:706:TYR:CD1	2.65	0.50
1:C:1031:TYR:CE2	1:C:1041:ARG:HG3	2.47	0.50
1:C:1247:ASN:ND2	1:C:1247:ASN:N	2.58	0.50
1:B:461:ARG:NE	1:B:504:ASP:CB	2.69	0.49
1:B:1021:ARG:HH22	1:B:1032:ASP:HB2	1.77	0.49
1:C:176:LYS:CG	1:C:177:LYS:N	2.73	0.49
1:C:270:THR:HG22	1:C:291:HIS:HA	1.94	0.49
1:C:462:LEU:HD23	1:C:506:SER:OG	2.11	0.49
1:C:887:VAL:CG2	1:C:893:ALA:HA	2.42	0.49
1:C:1085:ASP:CB	1:C:1086:PRO:CD	2.79	0.49
1:C:248:VAL:HG11	1:C:970:LEU:O	2.12	0.49
1:C:547:GLU:CD	1:C:599:THR:HG23	2.32	0.49
1:C:1088:PHE:CG	1:C:1088:PHE:O	2.65	0.49
1:B:269:GLU:HB3	1:B:292:ASN:ND2	2.20	0.49
1:C:446:LYS:HE2	1:C:472:GLU:OE2	2.12	0.49
1:C:686:HIS:ND1	1:C:686:HIS:O	2.45	0.49
1:B:526:ASN:HD21	1:B:727:PHE:HD2	1.60	0.49
1:B:1245:ILE:O	1:B:1246:VAL:HG13	2.12	0.49
1:C:157:ILE:CD1	1:C:263:ARG:NE	2.75	0.49
1:C:314:ILE:N	1:C:314:ILE:HD13	2.28	0.49
1:C:347:ALA:CB	1:C:1300:ASN:HB3	2.43	0.49
1:C:820:ILE:CG2	1:C:983:ILE:CD1	2.90	0.49
1:C:1250:GLU:O	1:C:1251:VAL:CG2	2.60	0.49
1:B:206:ILE:O	1:B:1239:ALA:HB1	2.12	0.49
1:C:268:GLY:O	1:C:269:GLU:HB2	2.11	0.49
1:C:409:ILE:HD12	1:C:1040:PHE:CZ	2.47	0.49
1:C:467:LYS:NZ	1:C:467:LYS:CB	2.72	0.49
1:C:606:LEU:HD22	1:C:655:ILE:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:853:ASP:OD1	1:C:854:GLN:N	2.46	0.49
1:C:199:TYR:CZ	1:C:1246:VAL:HG12	2.47	0.49
1:B:427:VAL:HG11	1:B:755:LEU:CD2	2.42	0.49
1:B:845:GLU:N	1:B:846:GLY:HA2	2.26	0.49
1:B:1269:THR:HG22	1:B:1270:LEU:H	1.78	0.49
1:C:555:GLY:HA2	1:C:570:GLY:HA2	1.95	0.49
1:C:639:ASN:HB3	1:C:1330:ILE:CD1	2.43	0.49
1:C:862:ARG:HB3	1:C:952:PHE:HZ	1.70	0.49
1:B:243:GLN:O	1:B:246:GLU:HB2	2.13	0.49
1:B:437:ALA:O	1:B:701:HIS:CE1	2.66	0.49
1:C:441:ARG:NH2	1:C:441:ARG:CG	2.73	0.49
1:C:494:GLU:HB2	1:C:531:ASP:OD2	2.13	0.49
1:C:912:GLU:O	1:C:912:GLU:HG2	2.12	0.49
1:B:271:THR:HG23	1:C:237:VAL:HG23	1.94	0.49
1:C:339:LEU:HD13	1:C:397:LEU:HD21	1.91	0.49
1:B:631:PRO:HA	1:B:718:ASN:HD21	1.78	0.49
1:B:649:ALA:HB1	1:B:692:ASP:OD1	2.12	0.49
1:B:996:ASP:HB2	1:B:999:LYS:HG3	1.94	0.49
1:B:1210:LEU:HD11	1:B:1256:GLY:HA3	1.95	0.49
1:C:225:ILE:HD12	1:C:247:TYR:HE1	1.76	0.49
1:C:312:ARG:CG	1:C:312:ARG:NH2	2.71	0.49
1:C:558:TYR:CZ	1:C:585:PHE:CB	2.96	0.49
1:B:558:TYR:CE1	1:B:590:SER:HB3	2.48	0.48
1:B:893:ALA:HB1	1:B:915:VAL:HG12	1.94	0.48
1:C:1101:TYR:CD1	1:C:1101:TYR:O	2.66	0.48
1:C:1297:SER:C	1:C:1298:PHE:HD1	2.16	0.48
1:B:150:LEU:HD12	1:B:150:LEU:O	2.12	0.48
1:C:565:GLU:HG2	1:C:566:PHE:N	2.29	0.48
1:C:1281:VAL:C	1:C:1283:ASN:N	2.58	0.48
1:B:276:ASN:OD1	1:C:1199:GLY:CA	2.62	0.48
1:B:970:LEU:HD21	1:B:1070:ARG:HH21	1.79	0.48
1:C:348:LEU:HD11	1:C:1301:VAL:HG22	1.95	0.48
1:C:445:GLU:CD	1:C:447:ARG:HG2	2.22	0.48
1:C:833:ARG:HH11	1:C:942:HIS:CE1	2.27	0.48
1:C:892:VAL:HG11	1:C:894:VAL:HG11	1.90	0.48
1:C:987:ALA:O	1:C:992:VAL:O	2.31	0.48
1:C:1186:GLN:H	1:C:1205:GLN:HE22	1.60	0.48
1:C:1290:LYS:NZ	1:C:1299:SER:HB3	2.22	0.48
1:B:439:VAL:HG23	1:B:440:ILE:N	2.27	0.48
1:C:96:ILE:HD12	1:C:96:ILE:HG23	1.62	0.48
1:C:820:ILE:HG21	1:C:983:ILE:HD11	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:836:GLN:C	1:C:838:GLU:H	2.14	0.48
1:C:1210:LEU:HD23	1:C:1244:ALA:HB1	1.92	0.48
1:B:361:ASN:OD1	1:B:1054:ARG:NH2	2.36	0.48
1:C:128:GLU:OE1	1:C:133:MET:HE1	2.13	0.48
1:C:492:VAL:CG1	1:C:580:TYR:HD2	2.26	0.48
1:C:605:ARG:HG3	1:C:605:ARG:O	2.13	0.48
1:C:741:TYR:OH	1:C:1022:ILE:CD1	2.61	0.48
1:C:828:ASP:N	1:C:828:ASP:OD1	2.45	0.48
1:C:849:MET:HG2	1:C:919:MET:CE	2.30	0.48
1:C:985:ARG:NH2	1:C:988:GLN:CG	2.76	0.48
1:C:1276:LEU:HB3	1:C:1290:LYS:HG3	1.95	0.48
1:B:505:PRO:HG3	1:B:670:ASP:OD2	2.14	0.48
1:B:560:ILE:HG23	1:B:564:GLY:HA3	1.96	0.48
1:B:862:ARG:NH1	1:B:948:ILE:HD13	2.29	0.48
1:B:1103:HIS:NE2	1:B:1146:GLY:O	2.46	0.48
1:B:1117:VAL:HB	1:B:1154:ASN:HD22	1.78	0.48
1:C:302:ARG:CD	1:C:318:LEU:HD23	2.43	0.48
1:C:840:ASP:HA	1:C:940:ARG:HH22	1.77	0.48
1:C:1137:VAL:HG22	1:C:1164:TRP:NE1	2.28	0.48
1:C:1259:ALA:CB	1:C:1260:PRO:CD	2.76	0.48
1:B:157:ILE:O	1:B:158:SER:OG	2.26	0.48
1:B:614:ARG:NH1	1:B:707:ALA:HB1	2.29	0.48
1:B:1088:PHE:CE2	1:B:1090:PRO:HG3	2.48	0.48
1:C:592:VAL:HG13	1:C:593:PRO:HD2	1.95	0.48
1:C:843:LEU:HD12	1:C:943:GLU:CG	2.15	0.48
1:C:878:SER:HB2	1:C:880:PRO:HD3	1.95	0.48
1:C:1066:ARG:HG2	1:C:1238:VAL:O	2.14	0.48
1:C:339:LEU:HD12	1:C:399:PRO:HB3	1.94	0.48
1:C:539:PHE:O	1:C:543:TRP:HB3	2.12	0.48
1:B:434:VAL:O	1:B:439:VAL:CG2	2.62	0.48
1:B:549:GLY:O	1:B:553:GLN:HG2	2.14	0.48
1:B:634:TYR:HB2	1:B:720:PHE:HD1	1.79	0.48
1:C:824:LEU:HA	1:C:968:ARG:HD2	1.96	0.48
1:C:892:VAL:HG12	1:C:894:VAL:HG12	1.69	0.48
1:C:1137:VAL:HG21	1:C:1164:TRP:CE2	2.48	0.48
1:B:157:ILE:HG21	1:B:263:ARG:HD2	1.95	0.48
1:B:426:ILE:HG12	1:B:714:LEU:HD21	1.95	0.48
1:C:189:ILE:HG12	1:C:286:LEU:HD11	1.96	0.48
1:C:290:TYR:HA	1:C:328:GLY:HA2	1.96	0.48
1:C:530:GLY:HA3	1:C:575:TRP:NE1	2.29	0.48
1:C:629:ARG:HB2	1:C:1037:ILE:CG2	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1104:ARG:NH1	1:C:1104:ARG:CG	2.71	0.48
1:C:1243:ARG:HG2	1:C:1243:ARG:NH1	2.24	0.48
1:B:868:VAL:HB	1:B:890:THR:HA	1.96	0.47
1:C:408:ILE:N	1:C:408:ILE:HD13	2.29	0.47
1:C:560:ILE:HG22	1:C:585:PHE:HE2	1.79	0.47
1:C:671:ASP:HA	1:C:674:LYS:HZ1	1.78	0.47
1:C:730:ASP:OD1	1:C:731:GLN:N	2.46	0.47
1:C:838:GLU:HG2	1:C:934:LEU:C	2.13	0.47
1:C:1116:ARG:NH1	1:C:1130:SER:CB	2.77	0.47
1:B:199:TYR:CE1	1:B:1246:VAL:HA	2.48	0.47
1:C:82:ARG:HH22	1:C:209:ASN:HD22	1.62	0.47
1:C:121:PHE:HB3	1:C:122:ASN:H	1.34	0.47
1:C:144:ASN:HB3	1:C:1318:GLU:CD	2.27	0.47
1:C:450:PRO:O	1:C:451:GLU:CB	2.60	0.47
1:C:451:GLU:CB	1:C:686:HIS:CB	2.92	0.47
1:C:713:MET:CE	1:C:804:LEU:HD21	2.41	0.47
1:C:1075:ARG:O	1:C:1075:ARG:HG3	2.14	0.47
1:B:148:GLN:HB2	1:B:149:PRO:HD2	1.96	0.47
1:C:247:TYR:CG	1:C:1070:ARG:HD3	2.48	0.47
1:C:259:MET:O	1:C:1054:ARG:HB3	2.14	0.47
1:C:312:ARG:HG3	1:C:312:ARG:NH2	2.18	0.47
1:C:382:HIS:NE2	1:C:800:LEU:HD23	2.28	0.47
1:C:822:MET:C	1:C:822:MET:SD	2.92	0.47
1:C:835:TYR:CD1	1:C:942:HIS:HB2	2.44	0.47
1:C:1105:LEU:HD12	1:C:1105:LEU:C	2.35	0.47
1:C:1250:GLU:O	1:C:1251:VAL:HG22	2.14	0.47
1:B:426:ILE:HG12	1:B:714:LEU:CD2	2.44	0.47
1:B:558:TYR:CZ	1:B:585:PHE:HB2	2.48	0.47
1:C:514:PHE:HE2	1:C:535:VAL:HG13	1.80	0.47
1:C:838:GLU:O	1:C:839:ALA:HB3	2.14	0.47
1:C:1046:PHE:HD2	1:C:1052:LEU:CD2	2.22	0.47
1:C:1155:ILE:CG2	1:C:1166:VAL:CG1	2.81	0.47
1:B:139:ASN:O	1:C:757:ILE:CG2	2.63	0.47
1:B:863:LEU:HD21	1:B:871:PRO:HD3	1.95	0.47
1:B:1131:PRO:HA	1:B:1134:ARG:NH1	2.29	0.47
1:C:227:LEU:HD23	1:C:246:GLU:O	2.14	0.47
1:C:338:ARG:NE	1:C:342:THR:HG22	2.26	0.47
1:C:370:VAL:CG1	1:C:398:ARG:HB2	2.44	0.47
1:C:543:TRP:CD1	1:C:543:TRP:C	2.86	0.47
1:C:1021:ARG:HB2	1:C:1021:ARG:NH1	2.22	0.47
1:C:1105:LEU:O	1:C:1105:LEU:HD13	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:GLN:HG2	1:B:266:ILE:HD11	1.96	0.47
1:B:204:VAL:CG1	1:B:1242:MET:HB2	2.45	0.47
1:B:752:VAL:O	1:B:753:ASP:HB2	2.15	0.47
1:B:971:MET:HA	1:B:972:PRO:HD3	1.60	0.47
1:B:1023:ARG:NE	1:B:1027:THR:OG1	2.48	0.47
1:C:498:ILE:HD11	1:C:514:PHE:CZ	2.50	0.47
1:C:516:LEU:HA	1:C:516:LEU:HD23	1.72	0.47
1:C:552:ILE:CD1	1:C:572:ASN:HB2	2.39	0.47
1:C:826:GLY:H	1:C:968:ARG:CD	2.27	0.47
1:C:896:LEU:CD1	1:C:918:VAL:HG21	2.42	0.47
1:C:928:ARG:HG3	1:C:928:ARG:NH1	2.29	0.47
1:B:154:PHE:CG	1:B:264:LEU:HG	2.50	0.47
1:B:383:SER:O	1:B:708:THR:HG23	2.15	0.47
1:B:528:ILE:HG13	1:B:528:ILE:H	1.56	0.47
1:B:697:ALA:HA	1:B:774:LEU:HD12	1.97	0.47
1:B:1200:LYS:HD3	1:B:1202:PHE:HE1	1.79	0.47
1:C:118:THR:O	1:C:119:ASP:C	2.52	0.47
1:C:203:VAL:HG12	1:C:1243:ARG:HD2	1.97	0.47
1:C:579:LEU:HD12	1:C:579:LEU:O	2.15	0.47
1:C:686:HIS:ND1	1:C:686:HIS:C	2.68	0.47
1:C:843:LEU:HD12	1:C:943:GLU:CB	2.44	0.47
1:B:298:PRO:O	1:B:301:LEU:HB3	2.15	0.47
1:B:694:ILE:HG22	1:B:698:HIS:ND1	2.30	0.47
1:B:733:VAL:HG21	1:B:741:TYR:CD1	2.50	0.47
1:B:960:THR:HG23	1:B:965:ARG:NH1	2.30	0.47
1:B:1066:ARG:HH21	1:B:1296:ILE:HD12	1.79	0.47
1:C:200:GLY:HA2	1:C:1246:VAL:HG22	1.95	0.47
1:C:323:THR:CG2	1:C:1266:ASP:HB2	2.44	0.47
1:C:835:TYR:HE1	1:C:942:HIS:CD2	2.33	0.47
1:C:1206:PHE:HD2	1:C:1236:ILE:HD11	1.73	0.47
1:B:231:LEU:HB2	1:B:249:SER:CB	2.45	0.47
1:B:323:THR:HA	1:B:1266:ASP:OD1	2.15	0.47
1:B:329:LEU:HD21	1:B:332:THR:OG1	2.14	0.47
1:B:482:ILE:HG23	1:B:706:TYR:CE1	2.50	0.47
1:B:530:GLY:HA3	1:B:575:TRP:CD1	2.49	0.47
1:C:153:ASP:OD1	1:C:153:ASP:N	2.48	0.47
1:C:379:LEU:O	1:C:380:GLN:C	2.51	0.47
1:C:525:PHE:O	1:C:525:PHE:CG	2.68	0.47
1:C:1228:ARG:HG3	1:C:1228:ARG:O	2.15	0.47
1:B:154:PHE:HA	1:B:262:ASN:OD1	2.15	0.47
1:B:232:LEU:HD22	1:B:974:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:VAL:HG21	1:B:358:LEU:HD13	1.97	0.47
1:B:957:PHE:CD2	1:B:958:ILE:HG13	2.50	0.47
1:C:652:PHE:HB3	1:C:691:PHE:CD2	2.50	0.47
1:C:1021:ARG:O	1:C:1029:LEU:HB2	2.15	0.47
1:C:1031:TYR:O	1:C:1031:TYR:CG	2.68	0.47
1:C:1062:ILE:HG23	1:C:1062:ILE:O	2.15	0.47
1:C:1205:GLN:O	1:C:1205:GLN:HG3	2.15	0.47
1:C:1254:PRO:HG2	1:C:1257:ALA:HB2	1.97	0.47
1:C:1270:LEU:O	1:C:1271:SER:C	2.52	0.47
1:C:237:VAL:HG12	1:C:238:THR:H	1.80	0.46
1:C:560:ILE:CG2	1:C:585:PHE:HE2	2.28	0.46
1:C:733:VAL:HB	1:C:1022:ILE:HD12	1.94	0.46
1:C:804:LEU:HD23	1:C:804:LEU:HA	1.66	0.46
1:C:873:TYR:CD2	1:C:898:GLN:HG3	2.48	0.46
1:C:946:LEU:N	1:C:946:LEU:CD1	2.73	0.46
1:C:1112:ASN:HD22	1:C:1112:ASN:C	2.01	0.46
1:B:274:MET:HB2	1:B:277:THR:HG23	1.97	0.46
1:B:424:GLY:HA2	1:B:427:VAL:HG12	1.98	0.46
1:B:701:HIS:CD2	1:B:791:ILE:HD11	2.50	0.46
1:C:451:GLU:OE1	1:C:686:HIS:N	2.49	0.46
1:C:451:GLU:OE2	1:C:682:GLN:CB	2.64	0.46
1:C:741:TYR:O	1:C:741:TYR:CD1	2.68	0.46
1:C:1176:GLU:OE1	1:C:1203:HIS:HE1	1.96	0.46
1:B:617:ASP:OD1	1:B:618:LEU:N	2.48	0.46
1:B:880:PRO:HB3	1:B:909:TYR:HB2	1.96	0.46
1:B:1210:LEU:HD13	1:B:1243:ARG:NH1	2.30	0.46
1:B:1271:SER:HB3	1:B:1275:ASP:OD2	2.15	0.46
1:C:163:TYR:CE2	1:C:258:VAL:CG2	2.93	0.46
1:C:171:GLU:OE2	1:C:1179:THR:OG1	2.21	0.46
1:C:370:VAL:HG13	1:C:398:ARG:H	1.79	0.46
1:C:492:VAL:HG22	1:C:747:ARG:CA	2.41	0.46
1:C:838:GLU:CG	1:C:934:LEU:O	2.47	0.46
1:B:793:TYR:CD2	1:B:1321:ASN:CG	2.87	0.46
1:C:841:ASP:N	1:C:940:ARG:HH22	2.13	0.46
1:C:962:ASP:O	1:C:965:ARG:HB3	2.15	0.46
1:B:1064:ASN:OD1	1:B:1065:PRO:HD2	2.16	0.46
1:B:1269:THR:HG22	1:B:1270:LEU:N	2.30	0.46
1:B:1278:TYR:CE2	1:B:1290:LYS:HA	2.50	0.46
1:C:450:PRO:C	1:C:454:GLU:HG2	2.35	0.46
1:C:947:GLU:HA	1:C:947:GLU:OE2	2.16	0.46
1:B:482:ILE:O	1:B:485:GLU:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:926:VAL:HG21	1:B:937:ASN:N	2.30	0.46
1:B:1174:THR:HG23	1:B:1201:LEU:HD21	1.97	0.46
1:C:820:ILE:HD12	1:C:820:ILE:HG23	1.58	0.46
1:C:901:VAL:CG2	1:C:930:ALA:CB	2.85	0.46
1:C:997:TYR:C	1:C:999:LYS:N	2.67	0.46
1:B:219:ILE:HA	1:B:228:VAL:HG22	1.98	0.46
1:C:652:PHE:HE1	1:C:688:GLU:CB	2.29	0.46
1:C:663:VAL:HG11	1:C:680:THR:CG2	2.46	0.46
1:B:231:LEU:HD12	1:B:249:SER:HB2	1.97	0.46
1:B:285:VAL:HG21	1:B:325:TYR:CE2	2.50	0.46
1:C:338:ARG:CG	1:C:342:THR:HA	2.44	0.46
1:C:747:ARG:CG	1:C:747:ARG:NH1	2.72	0.46
1:C:1155:ILE:O	1:C:1155:ILE:HG22	2.16	0.46
1:B:919:MET:SD	1:B:925:VAL:HG12	2.56	0.46
1:B:1216:SER:O	1:B:1219:ASP:HB2	2.16	0.46
1:C:178:ASP:O	1:C:306:GLN:OE1	2.34	0.46
1:C:329:LEU:HA	1:C:329:LEU:HD23	1.67	0.46
1:C:514:PHE:CD2	1:C:532:ILE:HG23	2.51	0.46
1:C:716:PHE:CD1	1:C:716:PHE:C	2.88	0.46
1:C:716:PHE:CD1	1:C:716:PHE:O	2.69	0.46
1:C:872:ILE:HD12	1:C:873:TYR:H	1.81	0.46
1:C:887:VAL:HG13	1:C:893:ALA:HA	1.98	0.46
1:C:1233:LEU:C	1:C:1234:GLN:HG3	2.37	0.46
1:B:822:MET:HG3	1:B:1045:TYR:CD1	2.51	0.46
1:B:845:GLU:HG2	1:B:911:ARG:HD2	1.98	0.46
1:C:81:ALA:HB3	1:C:168:VAL:HG13	1.98	0.46
1:C:322:GLY:O	1:C:1279:SER:CB	2.64	0.46
1:C:455:GLN:HG2	1:C:455:GLN:O	2.15	0.46
1:C:525:PHE:CE1	1:C:532:ILE:CD1	2.96	0.46
1:C:543:TRP:CD1	1:C:543:TRP:O	2.69	0.46
1:C:558:TYR:CE1	1:C:585:PHE:HB2	2.51	0.46
1:C:579:LEU:CB	1:C:582:SER:OG	2.63	0.46
1:C:585:PHE:HA	1:C:586:PRO:HD3	1.56	0.46
1:C:825:SER:O	1:C:825:SER:OG	2.34	0.46
1:C:1078:TYR:O	1:C:1078:TYR:CD1	2.68	0.46
1:C:1132:THR:O	1:C:1133:GLY:O	2.33	0.46
1:C:1275:ASP:OD1	1:C:1275:ASP:N	2.34	0.46
1:B:342:THR:HB	1:B:1309:ILE:CD1	2.42	0.45
1:B:793:TYR:CD2	1:B:1322:PRO:HD2	2.51	0.45
1:B:1204:LEU:HD21	1:B:1230:ILE:HD11	1.98	0.45
1:C:262:ASN:HA	1:C:361:ASN:OD1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:696:VAL:O	1:C:696:VAL:HG12	2.15	0.45
1:C:720:PHE:O	1:C:720:PHE:CD1	2.70	0.45
1:C:1047:LEU:HB2	1:C:1051:ARG:HD3	1.98	0.45
1:C:1105:LEU:C	1:C:1105:LEU:CD1	2.85	0.45
1:B:165:THR:HG22	1:B:166:TYR:N	2.30	0.45
1:B:230:ASP:OD1	1:B:230:ASP:N	2.49	0.45
1:B:231:LEU:CD2	1:B:986:ILE:HG13	2.46	0.45
1:B:554:ARG:CZ	1:B:594:LEU:HD12	2.46	0.45
1:B:1122:PRO:HB2	1:B:1123:PRO:HD3	1.98	0.45
1:C:439:VAL:O	1:C:439:VAL:HG13	2.16	0.45
1:C:603:ILE:HD13	1:C:659:LEU:CD2	2.46	0.45
1:C:874:ILE:HG21	1:C:902:ILE:CD1	2.29	0.45
1:C:928:ARG:HH11	1:C:928:ARG:CG	2.23	0.45
1:B:329:LEU:HD12	1:B:346:HIS:CE1	2.51	0.45
1:B:504:ASP:O	1:B:506:SER:HA	2.16	0.45
1:C:96:ILE:HD13	1:C:96:ILE:H	1.76	0.45
1:C:108:LYS:NZ	1:C:108:LYS:CB	2.72	0.45
1:C:497:LYS:H	1:C:497:LYS:HG2	1.49	0.45
1:C:1127:ALA:O	1:C:1128:TYR:CB	2.64	0.45
1:C:1206:PHE:CE2	1:C:1236:ILE:HD12	2.51	0.45
1:C:1219:ASP:CG	1:C:1220:PRO:HD2	2.08	0.45
1:B:479:HIS:O	1:B:482:ILE:N	2.50	0.45
1:B:1238:VAL:HG23	1:B:1239:ALA:N	2.31	0.45
1:C:160:PRO:HG3	1:C:265:VAL:HG12	1.98	0.45
1:C:213:PHE:HB3	1:C:219:ILE:HB	1.92	0.45
1:C:525:PHE:HE1	1:C:532:ILE:CD1	2.30	0.45
1:C:629:ARG:CB	1:C:1037:ILE:HG23	2.41	0.45
1:C:643:THR:HG22	1:C:644:VAL:HG12	1.97	0.45
1:C:674:LYS:NZ	1:C:674:LYS:CB	2.73	0.45
1:C:1062:ILE:HD12	1:C:1062:ILE:HA	1.53	0.45
1:C:1078:TYR:HB2	1:C:1229:LEU:CD1	2.47	0.45
1:B:307:VAL:HG11	1:B:1245:ILE:HG23	1.98	0.45
1:B:370:VAL:HG23	1:B:374:ASP:OD2	2.17	0.45
1:B:1278:TYR:HD2	1:B:1288:ILE:HG23	1.82	0.45
1:C:285:VAL:O	1:C:326:GLY:CA	2.65	0.45
1:C:341:LYS:HB2	1:C:1306:THR:HB	1.98	0.45
1:C:375:ARG:NH1	1:C:375:ARG:CG	2.69	0.45
1:C:376:ILE:HA	1:C:376:ILE:HD12	1.62	0.45
1:C:407:HIS:HD2	1:C:1047:LEU:HA	1.63	0.45
1:C:407:HIS:CE1	1:C:1047:LEU:HD12	2.52	0.45
1:C:441:ARG:O	1:C:770:CYS:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:742:LYS:HA	1:C:743:PRO:HD3	1.84	0.45
1:C:986:ILE:HA	1:C:989:ILE:HG22	1.97	0.45
1:B:166:TYR:OH	1:B:1264:GLU:OE2	2.31	0.45
1:B:340:VAL:HG21	1:C:1008:LEU:HB3	1.98	0.45
1:B:696:VAL:HG21	1:B:1326:ARG:HH12	1.81	0.45
1:B:716:PHE:O	1:B:717:THR:HB	2.16	0.45
1:C:377:LYS:HE2	1:C:621:ALA:O	2.16	0.45
1:C:746:GLU:N	1:C:746:GLU:OE2	2.49	0.45
1:C:838:GLU:CG	1:C:934:LEU:HA	2.36	0.45
1:C:838:GLU:CG	1:C:935:GLN:CA	2.89	0.45
1:C:1168:ILE:N	1:C:1168:ILE:CD1	2.73	0.45
1:C:1285:GLN:CA	1:C:1285:GLN:NE2	2.80	0.45
1:B:147:VAL:HG13	1:B:375:ARG:HD2	1.99	0.45
1:B:270:THR:HG23	1:B:289:THR:HB	1.99	0.45
1:B:461:ARG:HE	1:B:504:ASP:HB3	1.75	0.45
1:C:484:ARG:NE	1:C:758:ILE:HG22	2.31	0.45
1:C:517:PHE:CE1	1:C:521:PHE:CD2	3.04	0.45
1:C:674:LYS:HB2	1:C:674:LYS:HZ3	1.80	0.45
1:C:829:SER:O	1:C:965:ARG:NH2	2.49	0.45
1:C:240:GLY:O	1:C:242:GLU:CA	2.59	0.45
1:C:270:THR:HB	1:C:289:THR:CG2	2.47	0.45
1:C:849:MET:CG	1:C:919:MET:CG	2.94	0.45
1:C:853:ASP:HA	1:C:856:LEU:HB2	1.98	0.45
1:C:1060:ARG:NH1	1:C:1292:GLU:N	2.59	0.45
1:B:231:LEU:HD21	1:B:986:ILE:HG13	1.99	0.45
1:B:301:LEU:HG	1:B:305:THR:OG1	2.17	0.45
1:B:875:THR:OG1	1:B:901:VAL:O	2.34	0.45
1:B:1096:TYR:CE1	1:B:1136:HIS:HB3	2.51	0.45
1:B:1181:SER:O	1:B:1182:GLU:HB3	2.17	0.45
1:C:180:LEU:HD11	1:C:304:PHE:O	2.16	0.45
1:C:208:LEU:HB3	1:C:221:LEU:CD2	2.47	0.45
1:C:310:LEU:CD2	1:C:1242:MET:HE3	2.37	0.45
1:C:407:HIS:NE2	1:C:1047:LEU:HA	2.22	0.45
1:C:541:SER:C	1:C:543:TRP:H	2.17	0.45
1:C:1212:ARG:HA	1:C:1213:PRO:HD3	1.73	0.45
1:C:1297:SER:C	1:C:1298:PHE:CD1	2.91	0.45
1:B:1176:GLU:HG2	1:B:1203:HIS:CE1	2.46	0.45
1:C:737:PRO:HD2	1:C:1016:ASN:O	2.17	0.45
1:C:840:ASP:C	1:C:940:ARG:HH12	2.18	0.45
1:B:338:ARG:O	1:B:339:LEU:HB2	2.17	0.44
1:B:594:LEU:HD23	1:B:595:ALA:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:863:LEU:HD21	1:B:871:PRO:CD	2.47	0.44
1:C:109:LYS:HB3	1:C:110:PRO:CD	2.48	0.44
1:C:225:ILE:O	1:C:227:LEU:N	2.50	0.44
1:C:504:ASP:OD2	1:C:506:SER:HB2	2.16	0.44
1:C:738:GLU:HG3	1:C:738:GLU:O	2.17	0.44
1:C:839:ALA:CA	1:C:940:ARG:NH1	2.80	0.44
1:C:905:SER:O	1:C:908:THR:HG22	2.16	0.44
1:C:1034:GLN:OE1	1:C:1034:GLN:HA	2.17	0.44
1:C:1111:ALA:HB2	1:C:1129:PRO:CG	2.47	0.44
1:B:462:LEU:HD23	1:B:462:LEU:O	2.17	0.44
1:B:484:ARG:O	1:B:527:ARG:NH1	2.51	0.44
1:B:588:LEU:HD22	1:B:604:MET:HE2	1.99	0.44
1:C:362:LEU:C	1:C:362:LEU:CD2	2.85	0.44
1:C:492:VAL:CG2	1:C:747:ARG:HA	2.42	0.44
1:C:564:GLY:O	1:C:565:GLU:HB3	2.17	0.44
1:C:654:THR:C	1:C:658:THR:HG22	2.25	0.44
1:C:720:PHE:C	1:C:722:GLY:N	2.68	0.44
1:B:1332:ASN:HA	1:B:1333:ALA:HA	1.58	0.44
1:C:310:LEU:HD21	1:C:1242:MET:HE1	1.97	0.44
1:C:449:PHE:C	1:C:683:TRP:CD1	2.89	0.44
1:C:1219:ASP:CG	1:C:1220:PRO:HD3	2.25	0.44
1:C:1263:TYR:CE2	1:C:1278:TYR:OH	2.55	0.44
1:C:1294:ASP:O	1:C:1295:HIS:CG	2.71	0.44
1:B:135:LYS:CE	1:C:469:ARG:CA	2.93	0.44
1:B:575:TRP:CG	1:B:576:ASP:N	2.85	0.44
1:C:252:LEU:HD11	1:C:823:ILE:CG2	2.22	0.44
1:C:429:ILE:HD12	1:C:429:ILE:O	2.16	0.44
1:C:543:TRP:HD1	1:C:544:TYR:CD1	2.34	0.44
1:C:883:ILE:HG23	1:C:895:VAL:HG21	2.00	0.44
1:C:1101:TYR:CD1	1:C:1101:TYR:C	2.91	0.44
1:C:1250:GLU:O	1:C:1250:GLU:HG3	2.18	0.44
1:B:1242:MET:HA	1:B:1258:VAL:O	2.17	0.44
1:C:81:ALA:O	1:C:168:VAL:HG12	2.17	0.44
1:C:176:LYS:HA	1:C:176:LYS:HD3	1.81	0.44
1:C:204:VAL:CG2	1:C:1242:MET:HB2	2.48	0.44
1:C:449:PHE:CE2	1:C:454:GLU:HG3	2.53	0.44
1:C:451:GLU:OE2	1:C:682:GLN:HB3	2.18	0.44
1:C:540:PHE:HE2	1:C:604:MET:HE3	1.82	0.44
1:C:713:MET:HE3	1:C:804:LEU:CD2	2.44	0.44
1:C:836:GLN:O	1:C:940:ARG:HB3	2.17	0.44
1:C:954:GLN:HG2	1:C:957:PHE:CD1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1099:VAL:O	1:C:1099:VAL:CG2	2.66	0.44
1:C:1144:ARG:HE	1:C:1144:ARG:HB3	1.49	0.44
1:B:261:ASP:HA	1:B:262:ASN:HB3	1.99	0.44
1:B:540:PHE:CD1	1:B:600:ILE:HG12	2.53	0.44
1:C:259:MET:HG3	1:C:1055:LEU:CA	2.46	0.44
1:C:375:ARG:HA	1:C:375:ARG:HD2	1.74	0.44
1:C:985:ARG:HH22	1:C:989:ILE:CA	2.31	0.44
1:C:1143:GLU:C	1:C:1145:ALA:N	2.69	0.44
1:B:157:ILE:HD13	1:B:263:ARG:HD2	1.98	0.44
1:B:349:ASN:HA	1:B:1299:SER:HA	1.99	0.44
1:C:146:GLU:CB	1:C:1317:VAL:HG13	2.47	0.44
1:C:256:PHE:CD1	1:C:819:PHE:CD2	3.06	0.44
1:B:733:VAL:HG22	1:B:734:ILE:N	2.33	0.44
1:B:886:SER:O	1:B:890:THR:HG22	2.17	0.44
1:B:1082:ASP:CG	1:B:1212:ARG:HH12	2.21	0.44
1:C:161:LYS:HB2	1:C:161:LYS:HE2	1.79	0.44
1:C:168:VAL:CG2	1:C:204:VAL:HG12	2.47	0.44
1:C:176:LYS:HB2	1:C:199:TYR:CD2	2.53	0.44
1:C:738:GLU:O	1:C:738:GLU:CG	2.66	0.44
1:C:865:ILE:HG22	1:C:865:ILE:O	2.17	0.44
1:C:1073:GLY:HA3	1:C:1233:LEU:HD21	1.78	0.44
1:B:312:ARG:HA	1:B:315:THR:HG22	1.99	0.44
1:B:387:THR:HG22	1:B:1322:PRO:HD3	2.00	0.44
1:B:389:PHE:CD1	1:B:1319:ARG:HG3	2.34	0.44
1:B:895:VAL:HG22	1:B:896:LEU:H	1.83	0.44
1:B:1076:ILE:HB	1:B:1166:VAL:HG13	2.00	0.44
1:C:233:VAL:HG23	1:C:234:PRO:CD	2.28	0.44
1:C:302:ARG:HH11	1:C:302:ARG:CG	2.31	0.44
1:C:426:ILE:HG21	1:C:426:ILE:HD13	1.74	0.44
1:C:714:LEU:HA	1:C:714:LEU:HD23	1.58	0.44
1:C:970:LEU:HA	1:C:970:LEU:HD23	1.64	0.44
1:C:979:ILE:HD13	1:C:979:ILE:HG21	1.77	0.44
1:C:1014:MET:O	1:C:1014:MET:HG2	2.17	0.44
1:C:1138:HIS:CG	1:C:1138:HIS:O	2.68	0.44
1:B:272:THR:HG21	1:C:235:ILE:HD13	1.63	0.43
1:B:833:ARG:O	1:B:849:MET:N	2.49	0.43
1:C:556:ALA:O	1:C:587:ALA:CB	2.64	0.43
1:C:849:MET:CG	1:C:919:MET:HE2	2.40	0.43
1:C:1122:PRO:N	1:C:1123:PRO:CD	2.81	0.43
1:B:285:VAL:HG23	1:B:326:GLY:HA2	1.99	0.43
1:C:314:ILE:HG23	1:C:314:ILE:HD12	1.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1023:ARG:NH1	1:C:1029:LEU:HD21	2.33	0.43
1:C:1050:LEU:HA	1:C:1050:LEU:HD13	1.72	0.43
1:C:1094:GLU:OE2	1:C:1094:GLU:CA	2.66	0.43
1:C:1137:VAL:HG22	1:C:1164:TRP:CE2	2.52	0.43
1:C:1310:ARG:HA	1:C:1310:ARG:NH1	2.31	0.43
1:B:1180:PRO:HB3	1:B:1212:ARG:HB3	1.99	0.43
1:C:144:ASN:CG	1:C:1318:GLU:OE1	2.56	0.43
1:C:153:ASP:OD2	1:C:401:LEU:HD22	2.17	0.43
1:C:614:ARG:O	1:C:614:ARG:CG	2.66	0.43
1:C:652:PHE:CB	1:C:691:PHE:CE2	3.01	0.43
1:C:1078:TYR:HB2	1:C:1229:LEU:HD11	2.00	0.43
1:C:1176:GLU:OE1	1:C:1203:HIS:NE2	2.51	0.43
1:C:1263:TYR:O	1:C:1297:SER:HB2	2.18	0.43
1:B:251:LEU:HA	1:B:254:VAL:HG22	2.01	0.43
1:B:823:ILE:HG23	1:B:964:VAL:HG23	2.00	0.43
1:B:849:MET:SD	1:B:917:VAL:HG23	2.59	0.43
1:B:908:THR:HG23	1:B:911:ARG:NH1	2.33	0.43
1:C:733:VAL:HG23	1:C:743:PRO:HA	2.01	0.43
1:C:880:PRO:HB3	1:C:906:ALA:HA	1.66	0.43
1:B:381:ALA:HB3	1:B:624:PHE:HE2	1.82	0.43
1:B:388:GLN:OE1	1:B:1320:VAL:CG1	2.66	0.43
1:B:515:ILE:HD12	1:B:659:LEU:HD11	2.01	0.43
1:B:733:VAL:HG22	1:B:734:ILE:H	1.84	0.43
1:B:895:VAL:HG12	1:B:917:VAL:HG12	2.00	0.43
1:B:1121:HIS:CD2	1:B:1124:THR:HG22	2.51	0.43
1:C:237:VAL:HG12	1:C:238:THR:N	2.34	0.43
1:C:310:LEU:HA	1:C:310:LEU:HD12	1.51	0.43
1:C:635:ILE:O	1:C:635:ILE:CG2	2.67	0.43
1:C:928:ARG:N	1:C:928:ARG:HD2	2.34	0.43
1:C:954:GLN:HG2	1:C:957:PHE:HD1	1.83	0.43
1:C:1075:ARG:O	1:C:1075:ARG:CG	2.64	0.43
1:C:1120:THR:O	1:C:1122:PRO:HD2	2.12	0.43
1:C:1290:LYS:NZ	1:C:1297:SER:OG	2.44	0.43
1:B:922:TYR:HD1	1:B:925:VAL:HG11	1.82	0.43
1:C:144:ASN:HB3	1:C:1318:GLU:H	1.83	0.43
1:C:674:LYS:CB	1:C:674:LYS:HZ3	2.32	0.43
1:C:716:PHE:O	1:C:716:PHE:HD1	2.00	0.43
1:C:760:THR:O	1:C:760:THR:OG1	2.29	0.43
1:C:923:TYR:N	1:C:923:TYR:CD1	2.86	0.43
1:C:971:MET:HE2	1:C:971:MET:HB3	1.64	0.43
1:C:1023:ARG:HG2	1:C:1024:PRO:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1029:LEU:HA	1:C:1029:LEU:HD23	1.71	0.43
1:C:1202:PHE:O	1:C:1202:PHE:HD1	2.01	0.43
1:B:213:PHE:HB3	1:B:219:ILE:HD12	1.99	0.43
1:B:895:VAL:O	1:B:918:VAL:HG12	2.18	0.43
1:B:1175:ALA:HA	1:B:1204:LEU:O	2.18	0.43
1:B:1209:GLY:O	1:B:1212:ARG:HG2	2.18	0.43
1:C:156:GLN:HE22	1:C:1309:ILE:HG12	1.79	0.43
1:C:548:TYR:CZ	1:C:552:ILE:HG13	2.53	0.43
1:C:1156:ILE:O	1:C:1156:ILE:HG22	2.17	0.43
1:C:1159:VAL:HG23	1:C:1164:TRP:O	2.18	0.43
1:C:1186:GLN:H	1:C:1205:GLN:NE2	2.16	0.43
1:C:1310:ARG:NE	1:C:1310:ARG:C	2.72	0.43
1:B:188:ARG:HH22	1:C:237:VAL:HG11	1.84	0.43
1:B:442:PRO:HB3	1:B:770:CYS:HB3	1.99	0.43
1:C:343:ILE:HD13	1:C:343:ILE:HG21	1.73	0.43
1:C:494:GLU:N	1:C:494:GLU:CD	2.72	0.43
1:C:614:ARG:CD	1:C:635:ILE:HD12	2.42	0.43
1:C:639:ASN:HB3	1:C:1330:ILE:HD13	2.01	0.43
1:C:672:MET:O	1:C:672:MET:HG2	2.18	0.43
1:C:830:VAL:HA	1:C:854:GLN:HG2	2.00	0.43
1:C:1099:VAL:HG11	1:C:1119:TYR:OH	2.19	0.43
1:B:417:ALA:HB3	1:B:734:ILE:HD12	2.00	0.43
1:B:619:ALA:HA	1:B:624:PHE:HD2	1.84	0.43
1:C:233:VAL:HG13	1:C:981:HIS:NE2	2.04	0.43
1:C:550:ILE:HD11	1:C:594:LEU:CD1	2.48	0.43
1:C:1050:LEU:HD12	1:C:1054:ARG:CZ	2.48	0.43
1:C:1060:ARG:HH12	1:C:1292:GLU:N	2.14	0.43
1:C:1074:VAL:HG12	1:C:1171:ILE:CG2	2.48	0.43
1:B:450:PRO:HG3	1:B:686:HIS:HB2	2.00	0.43
1:B:505:PRO:HG2	1:B:672:MET:CE	2.49	0.43
1:B:1236:ILE:HD12	1:B:1238:VAL:N	2.34	0.43
1:C:136:VAL:O	1:C:136:VAL:HG13	2.19	0.43
1:C:601:ILE:HD12	1:C:601:ILE:HG23	1.70	0.43
1:C:887:VAL:HG13	1:C:893:ALA:CA	2.49	0.43
1:C:896:LEU:HD22	1:C:896:LEU:HA	1.76	0.43
1:C:1072:ASP:HB3	1:C:1172:GLU:HG2	2.01	0.43
1:C:1193:ILE:HG13	1:C:1202:PHE:CE2	2.54	0.43
1:C:1193:ILE:HG21	1:C:1193:ILE:HD13	1.65	0.43
1:B:505:PRO:HA	1:B:506:SER:HA	1.59	0.42
1:B:873:TYR:HD1	1:B:896:LEU:HB2	1.83	0.42
1:B:880:PRO:HG3	1:B:905:SER:C	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151:SER:N	1:C:400:GLU:OE1	2.50	0.42
1:C:186:ASP:CG	1:C:279:SER:N	2.62	0.42
1:C:265:VAL:O	1:C:1303:SER:CA	2.67	0.42
1:C:357:VAL:HG22	1:C:1054:ARG:HD2	2.01	0.42
1:C:469:ARG:HD3	1:C:513:GLU:OE1	2.18	0.42
1:C:810:LEU:HD23	1:C:810:LEU:HA	1.42	0.42
1:C:833:ARG:HH11	1:C:942:HIS:CD2	2.37	0.42
1:C:1074:VAL:O	1:C:1074:VAL:CG1	2.67	0.42
1:C:1085:ASP:HB3	1:C:1243:ARG:NH2	2.34	0.42
1:C:1270:LEU:HA	1:C:1270:LEU:HD23	1.57	0.42
1:C:1276:LEU:CB	1:C:1290:LYS:HG3	2.49	0.42
1:B:153:ASP:OD2	1:B:401:LEU:HD21	2.19	0.42
1:B:701:HIS:NE2	1:B:791:ILE:HD11	2.34	0.42
1:B:952:PHE:HB2	1:B:958:ILE:HD12	2.02	0.42
1:B:1128:TYR:CE2	1:B:1135:PRO:HD3	2.53	0.42
1:C:155:LYS:O	1:C:155:LYS:CG	2.67	0.42
1:C:448:TYR:HB2	1:C:449:PHE:H	1.10	0.42
1:C:936:MET:O	1:C:936:MET:SD	2.77	0.42
1:C:1013:LYS:HE3	1:C:1015:GLN:NE2	2.34	0.42
1:C:1022:ILE:O	1:C:1022:ILE:HG22	2.17	0.42
1:C:1059:LEU:HD12	1:C:1059:LEU:HA	1.80	0.42
1:C:1134:ARG:CB	1:C:1135:PRO:CD	2.85	0.42
1:B:228:VAL:HG11	1:B:253:MET:HG3	2.01	0.42
1:B:1066:ARG:HH21	1:B:1296:ILE:CD1	2.32	0.42
1:B:1236:ILE:CD1	1:B:1238:VAL:HG22	2.49	0.42
1:C:197:PHE:HE1	1:C:1242:MET:HG3	1.83	0.42
1:C:225:ILE:CG2	1:C:226:PRO:HD2	2.48	0.42
1:C:454:GLU:OE2	1:C:454:GLU:HA	2.19	0.42
1:C:612:PHE:O	1:C:612:PHE:CG	2.70	0.42
1:C:720:PHE:O	1:C:720:PHE:CG	2.69	0.42
1:C:791:ILE:HG21	1:C:1325:VAL:HG21	2.01	0.42
1:C:845:GLU:HB3	1:C:846:GLY:H	1.54	0.42
1:C:1014:MET:CG	1:C:1014:MET:O	2.67	0.42
1:C:1137:VAL:CG2	1:C:1164:TRP:CD2	3.03	0.42
1:C:1177:VAL:O	1:C:1177:VAL:CG2	2.66	0.42
1:C:1178:MET:HG3	1:C:1178:MET:O	2.20	0.42
1:B:372:ALA:HB3	1:B:1315:MET:CE	2.49	0.42
1:B:500:GLU:CD	1:B:502:PHE:H	2.22	0.42
1:B:720:PHE:HD2	1:B:727:PHE:CD1	2.36	0.42
1:B:1051:ARG:O	1:B:1055:LEU:HB2	2.20	0.42
1:C:267:VAL:HG21	1:C:344:VAL:CG2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:409:ILE:HG23	1:C:409:ILE:HD12	1.58	0.42
1:C:494:GLU:HB3	1:C:577:GLN:HE22	1.79	0.42
1:C:504:ASP:N	1:C:504:ASP:OD1	2.52	0.42
1:C:892:VAL:HG13	1:C:894:VAL:HG12	1.94	0.42
1:C:941:TYR:HD1	1:C:941:TYR:HA	1.72	0.42
1:C:954:GLN:C	1:C:958:ILE:CD1	2.88	0.42
1:C:1193:ILE:HG13	1:C:1202:PHE:HZ	1.84	0.42
1:C:1273:ASN:ND2	1:C:1273:ASN:C	2.72	0.42
1:C:1321:ASN:HB3	1:C:1322:PRO:HD2	2.01	0.42
1:B:188:ARG:NH2	1:C:237:VAL:HG11	2.35	0.42
1:B:287:ARG:HB2	1:B:328:GLY:HA3	2.00	0.42
1:B:434:VAL:HB	1:B:439:VAL:HG11	2.01	0.42
1:B:734:ILE:HG12	1:B:1019:ILE:HD13	2.01	0.42
1:C:144:ASN:CA	1:C:1318:GLU:HB3	2.49	0.42
1:C:389:PHE:CZ	1:C:796:PRO:HG2	2.50	0.42
1:C:560:ILE:HG22	1:C:585:PHE:CE2	2.54	0.42
1:C:830:VAL:HA	1:C:854:GLN:CG	2.50	0.42
1:C:985:ARG:HH21	1:C:988:GLN:HG3	1.79	0.42
1:C:1205:GLN:O	1:C:1205:GLN:CG	2.67	0.42
1:C:1330:ILE:H	1:C:1330:ILE:HD12	1.85	0.42
1:B:135:LYS:CE	1:C:470:ALA:N	2.65	0.42
1:B:139:ASN:O	1:C:757:ILE:HG22	2.20	0.42
1:B:190:VAL:HG12	1:B:300:LEU:HB3	2.01	0.42
1:B:193:THR:HA	1:B:296:VAL:HG13	2.01	0.42
1:C:314:ILE:O	1:C:318:LEU:HD22	2.18	0.42
1:C:519:LEU:HA	1:C:519:LEU:HD23	1.51	0.42
1:C:520:PHE:CZ	1:C:691:PHE:HE1	2.38	0.42
1:C:1079:LEU:O	1:C:1079:LEU:HD13	2.19	0.42
1:C:1084:PRO:O	1:C:1209:GLY:C	2.58	0.42
1:C:1089:VAL:O	1:C:1089:VAL:CG1	2.68	0.42
1:B:390:HIS:HB2	1:B:1318:GLU:CG	2.47	0.42
1:B:440:ILE:CG2	1:B:770:CYS:CB	2.98	0.42
1:C:455:GLN:O	1:C:455:GLN:CG	2.68	0.42
1:C:1046:PHE:C	1:C:1048:ASP:N	2.73	0.42
1:C:1078:TYR:O	1:C:1078:TYR:HD1	2.02	0.42
1:C:1159:VAL:O	1:C:1159:VAL:CG2	2.67	0.42
1:B:265:VAL:HG12	1:B:1304:MET:HE2	2.01	0.42
1:C:208:LEU:CB	1:C:221:LEU:CD2	2.98	0.42
1:C:333:ARG:NE	1:C:1272:ARG:HA	2.24	0.42
1:C:613:LEU:HD22	1:C:614:ARG:N	2.35	0.42
1:C:965:ARG:NH1	1:C:968:ARG:CZ	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:986:ILE:HA	1:C:989:ILE:CG2	2.49	0.42
1:C:1034:GLN:N	1:C:1034:GLN:CD	2.72	0.42
1:C:1278:TYR:CE2	1:C:1288:ILE:CD1	3.01	0.42
1:B:614:ARG:O	1:B:633:THR:HG22	2.19	0.42
1:B:712:PHE:HB2	1:B:715:ASN:ND2	2.34	0.42
1:B:1060:ARG:HA	1:B:1063:THR:HG22	2.02	0.42
1:C:124:GLN:OE1	1:C:124:GLN:CA	2.68	0.42
1:C:923:TYR:N	1:C:923:TYR:HD1	2.17	0.42
1:B:274:MET:O	1:B:277:THR:N	2.49	0.42
1:B:852:TYR:CE2	1:B:856:LEU:HD22	2.54	0.42
1:B:1105:LEU:HD11	1:B:1122:PRO:HD3	2.01	0.42
1:B:1248:HIS:HB2	1:B:1251:VAL:HG22	2.01	0.42
1:C:365:LEU:HD13	1:C:365:LEU:C	2.38	0.42
1:C:839:ALA:C	1:C:940:ARG:NH2	2.66	0.42
1:C:1247:ASN:ND2	1:C:1247:ASN:O	2.51	0.42
1:C:1282:ALA:C	1:C:1284:GLY:N	2.73	0.42
1:B:588:LEU:HD13	1:B:604:MET:CE	2.47	0.41
1:B:632:GLN:H	1:B:718:ASN:ND2	2.18	0.41
1:B:649:ALA:HA	1:B:691:PHE:HE1	1.85	0.41
1:B:1289:PRO:HG2	1:B:1292:GLU:HG2	2.00	0.41
1:C:385:ILE:H	1:C:708:THR:HG22	1.85	0.41
1:C:430:ASN:C	1:C:430:ASN:ND2	2.73	0.41
1:C:503:GLU:OE2	1:C:542:ARG:CG	2.68	0.41
1:C:913:ASN:HD22	1:C:913:ASN:HA	1.72	0.41
1:C:1149:LYS:O	1:C:1150:LEU:C	2.59	0.41
1:C:1212:ARG:O	1:C:1212:ARG:HG3	2.20	0.41
1:B:472:GLU:CB	1:B:761:SER:HB3	2.42	0.41
1:B:1276:LEU:HD13	1:B:1300:ASN:ND2	2.35	0.41
1:C:179:LYS:HD2	1:C:180:LEU:N	2.35	0.41
1:C:480:LEU:C	1:C:480:LEU:CD2	2.88	0.41
1:C:656:VAL:CG1	1:C:688:GLU:CB	2.85	0.41
1:C:743:PRO:HD2	1:C:743:PRO:O	2.19	0.41
1:C:870:ASP:CB	1:C:871:PRO:HD2	2.47	0.41
1:C:1137:VAL:HG22	1:C:1164:TRP:CD1	2.55	0.41
1:C:1278:TYR:CD2	1:C:1288:ILE:HD11	2.53	0.41
1:C:1288:ILE:HG12	1:C:1288:ILE:H	1.55	0.41
1:B:303:ASP:O	1:C:1103:HIS:HE1	2.03	0.41
1:B:451:GLU:HG2	1:B:452:ASN:H	1.85	0.41
1:B:479:HIS:ND1	1:B:479:HIS:N	2.67	0.41
1:B:683:TRP:O	1:B:686:HIS:HB3	2.19	0.41
1:B:862:ARG:HH12	1:B:948:ILE:HG21	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:892:VAL:HG21	1:B:952:PHE:CE1	2.56	0.41
1:B:985:ARG:NH2	1:B:988:GLN:HE21	2.14	0.41
1:B:1119:TYR:HB3	1:B:1134:ARG:NE	2.31	0.41
1:B:1300:ASN:OD1	1:B:1300:ASN:N	2.52	0.41
1:C:202:ALA:O	1:C:1244:ALA:N	2.38	0.41
1:C:289:THR:O	1:C:329:LEU:N	2.54	0.41
1:C:371:THR:O	1:C:372:ALA:C	2.56	0.41
1:C:418:ASN:OD1	1:C:418:ASN:N	2.53	0.41
1:C:676:THR:O	1:C:676:THR:HG22	2.20	0.41
1:C:721:SER:O	1:C:721:SER:OG	2.10	0.41
1:C:1207:MET:HE2	1:C:1207:MET:HB2	1.80	0.41
1:B:305:THR:CG2	1:B:307:VAL:HG12	2.51	0.41
1:B:694:ILE:HD12	1:B:772:TYR:CE1	2.55	0.41
1:C:133:MET:SD	1:C:133:MET:O	2.78	0.41
1:C:136:VAL:O	1:C:136:VAL:CG1	2.68	0.41
1:C:362:LEU:O	1:C:362:LEU:CD2	2.68	0.41
1:C:383:SER:HG	1:C:796:PRO:HG3	0.58	0.41
1:C:385:ILE:HG12	1:C:708:THR:HG22	2.00	0.41
1:C:612:PHE:HE2	1:C:614:ARG:HB3	1.85	0.41
1:C:700:ASP:CG	1:C:1326:ARG:HG3	2.38	0.41
1:C:734:ILE:HD13	1:C:734:ILE:HG21	1.74	0.41
1:C:865:ILE:CG2	1:C:865:ILE:O	2.68	0.41
1:C:883:ILE:HD12	1:C:883:ILE:HG23	1.76	0.41
1:C:77:THR:C	1:C:172:ASP:OD2	2.58	0.41
1:C:214:ASP:C	1:C:216:ALA:N	2.73	0.41
1:C:236:GLY:C	1:C:237:VAL:CG2	2.88	0.41
1:C:407:HIS:HD2	1:C:1047:LEU:CA	2.28	0.41
1:C:427:VAL:O	1:C:427:VAL:CG1	2.69	0.41
1:C:449:PHE:HB3	1:C:683:TRP:HE1	1.61	0.41
1:C:536:LEU:HD23	1:C:536:LEU:HA	1.56	0.41
1:C:934:LEU:H	1:C:934:LEU:HG	1.66	0.41
1:C:971:MET:HB2	1:C:972:PRO:HD2	2.03	0.41
1:C:1072:ASP:N	1:C:1072:ASP:OD1	2.52	0.41
1:C:1078:TYR:HB3	1:C:1159:VAL:O	2.20	0.41
1:C:1215:PRO:CD	1:C:1215:PRO:O	2.68	0.41
1:C:1251:VAL:O	1:C:1251:VAL:HG12	2.21	0.41
1:B:390:HIS:O	1:B:1317:VAL:HG23	2.20	0.41
1:B:437:ALA:O	1:B:701:HIS:HE1	2.04	0.41
1:B:1271:SER:OG	1:B:1272:ARG:N	2.53	0.41
1:C:298:PRO:CG	1:C:298:PRO:O	2.68	0.41
1:C:485:GLU:HB3	1:C:706:TYR:HE1	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:520:PHE:C	1:C:521:PHE:CD1	2.94	0.41
1:C:651:ARG:HD2	1:C:655:ILE:HG12	2.02	0.41
1:C:729:PRO:O	1:C:731:GLN:N	2.53	0.41
1:C:928:ARG:NH1	1:C:928:ARG:CG	2.77	0.41
1:C:1019:ILE:O	1:C:1019:ILE:HG13	2.19	0.41
1:C:1191:GLU:O	1:C:1191:GLU:HG3	2.16	0.41
1:B:560:ILE:HG12	1:B:566:PHE:CD1	2.56	0.41
1:B:733:VAL:HG21	1:B:741:TYR:HD1	1.86	0.41
1:B:873:TYR:CB	1:B:897:TYR:HB2	2.43	0.41
1:B:1236:ILE:HD13	1:B:1238:VAL:HG22	2.02	0.41
1:C:265:VAL:HG23	1:C:1302:VAL:O	2.21	0.41
1:C:287:ARG:CB	1:C:329:LEU:O	2.68	0.41
1:C:370:VAL:HG13	1:C:370:VAL:O	2.21	0.41
1:C:548:TYR:CE2	1:C:552:ILE:HG13	2.55	0.41
1:C:1014:MET:HE3	1:C:1014:MET:HB3	1.96	0.41
1:C:1037:ILE:HD11	1:C:1040:PHE:CD2	2.56	0.41
1:B:765:PRO:O	1:B:769:GLN:HB2	2.20	0.41
1:C:77:THR:OG1	1:C:172:ASP:OD2	2.37	0.41
1:C:367:GLU:OE1	1:C:367:GLU:HA	2.21	0.41
1:C:571:ARG:HH11	1:C:571:ARG:CB	2.26	0.41
1:C:585:PHE:CE1	1:C:728:LYS:HG2	2.56	0.41
1:C:742:LYS:HE2	1:C:742:LYS:HB3	1.32	0.41
1:C:897:TYR:CD1	1:C:897:TYR:C	2.94	0.41
1:C:974:LEU:HA	1:C:974:LEU:HD23	1.83	0.41
1:C:1099:VAL:HG21	1:C:1119:TYR:OH	2.20	0.41
1:B:141:LEU:HD21	1:B:391:GLY:HA2	2.02	0.41
1:B:223:LYS:HD2	1:B:1203:HIS:ND1	2.35	0.41
1:B:262:ASN:H	1:B:1054:ARG:CZ	2.34	0.41
1:B:418:ASN:O	1:B:420:PRO:HD3	2.21	0.41
1:B:694:ILE:HG23	1:B:772:TYR:CE1	2.56	0.41
1:B:752:VAL:O	1:B:752:VAL:HG12	2.20	0.41
1:B:791:ILE:HD12	1:B:791:ILE:HA	1.82	0.41
1:B:826:GLY:HA2	1:B:827:GLY:HA3	1.50	0.41
1:B:890:THR:C	1:B:892:VAL:H	2.24	0.41
1:C:110:PRO:CB	1:C:111:PRO:CD	2.98	0.41
1:C:236:GLY:O	1:C:237:VAL:HG22	2.21	0.41
1:C:429:ILE:HD13	1:C:799:THR:HG22	2.01	0.41
1:C:501:SER:O	1:C:501:SER:OG	2.23	0.41
1:C:601:ILE:N	1:C:601:ILE:HD13	2.36	0.41
1:C:731:GLN:O	1:C:731:GLN:CG	2.69	0.41
1:C:835:TYR:HE1	1:C:942:HIS:CG	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:990:THR:OG1	1:C:992:VAL:HG12	2.20	0.41
1:C:1085:ASP:HB2	1:C:1086:PRO:HD3	1.98	0.41
1:C:1262:SER:O	1:C:1262:SER:OG	2.30	0.41
1:C:1280:PRO:HB2	1:C:1281:VAL:H	1.62	0.41
1:B:157:ILE:HG12	1:B:264:LEU:O	2.21	0.41
1:B:157:ILE:HD12	1:B:160:PRO:HA	2.02	0.41
1:B:648:PHE:CE2	1:B:691:PHE:HZ	2.39	0.41
1:B:1096:TYR:CD1	1:B:1136:HIS:HB3	2.55	0.41
1:C:364:ALA:HB1	1:C:1050:LEU:HD21	2.01	0.41
1:C:471:SER:O	1:C:765:PRO:HG3	2.20	0.41
1:C:837:THR:HA	1:C:936:MET:CG	2.51	0.41
1:C:865:ILE:HD11	1:C:1020:ARG:NH2	2.36	0.41
1:B:261:ASP:OD1	1:B:263:ARG:HB2	2.21	0.40
1:B:394:GLN:O	1:B:394:GLN:HG2	2.21	0.40
1:B:958:ILE:HG22	1:B:959:GLN:N	2.35	0.40
1:C:101:ASP:O	1:C:103:GLY:N	2.54	0.40
1:C:110:PRO:HB2	1:C:111:PRO:HD2	2.03	0.40
1:C:225:ILE:O	1:C:227:LEU:HG	2.21	0.40
1:C:399:PRO:O	1:C:399:PRO:CG	2.69	0.40
1:C:579:LEU:O	1:C:579:LEU:CD1	2.69	0.40
1:C:743:PRO:O	1:C:743:PRO:CD	2.69	0.40
1:C:762:ILE:CD1	1:C:762:ILE:O	2.69	0.40
1:C:979:ILE:O	1:C:983:ILE:HG13	2.21	0.40
1:C:1022:ILE:O	1:C:1022:ILE:CG2	2.68	0.40
1:C:360:ILE:O	1:C:360:ILE:CG2	2.68	0.40
1:C:408:ILE:HG22	1:C:412:LEU:HD12	2.02	0.40
1:C:730:ASP:O	1:C:731:GLN:HG2	2.22	0.40
1:C:897:TYR:OH	1:C:928:ARG:HG3	2.21	0.40
1:C:909:TYR:OH	1:C:913:ASN:OD1	2.32	0.40
1:C:978:GLN:HE21	1:C:978:GLN:HB2	1.75	0.40
1:C:1253:ARG:HA	1:C:1254:PRO:HD3	1.87	0.40
1:B:295:GLY:N	1:B:349:ASN:OD1	2.54	0.40
1:B:558:TYR:CE1	1:B:585:PHE:HB2	2.57	0.40
1:B:736:SER:HA	1:B:1016:ASN:O	2.21	0.40
1:B:830:VAL:HA	1:B:854:GLN:HE21	1.85	0.40
1:B:924:ASP:HB3	1:B:928:ARG:NH2	2.36	0.40
1:C:146:GLU:CG	1:C:1317:VAL:HG13	2.49	0.40
1:C:164:LEU:HD13	1:C:1296:ILE:HG13	2.03	0.40
1:C:166:TYR:HE1	1:C:1298:PHE:CZ	2.38	0.40
1:C:451:GLU:CB	1:C:686:HIS:HB2	2.51	0.40
1:C:750:GLU:HB3	1:C:757:ILE:HG13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1000:LEU:O	1:C:1000:LEU:CG	2.69	0.40
1:C:1185:THR:OG1	1:C:1186:GLN:N	2.55	0.40
1:C:1278:TYR:HB3	1:C:1279:SER:H	1.68	0.40
1:B:678:SER:O	1:B:682:GLN:HG2	2.21	0.40
1:B:1086:PRO:HB3	1:B:1177:VAL:HG22	2.02	0.40
1:B:1277:LEU:HA	1:B:1289:PRO:HA	2.02	0.40
1:C:554:ARG:CZ	1:C:594:LEU:CD2	2.99	0.40
1:C:985:ARG:HH22	1:C:989:ILE:CB	2.33	0.40
1:C:1033:ASP:HB3	1:C:1034:GLN:NE2	2.37	0.40
1:C:1245:ILE:HG21	1:C:1245:ILE:HD13	1.62	0.40
1:C:1254:PRO:O	1:C:1254:PRO:CD	2.69	0.40
1:C:1292:GLU:O	1:C:1292:GLU:CG	2.69	0.40
1:B:462:LEU:O	1:B:466:VAL:HG23	2.22	0.40
1:B:606:LEU:HD21	1:B:658:THR:HG23	2.02	0.40
1:B:874:ILE:HG23	1:B:895:VAL:CG2	2.50	0.40
1:B:898:GLN:O	1:B:928:ARG:HD3	2.21	0.40
1:C:322:GLY:O	1:C:1279:SER:HB2	2.20	0.40
1:C:391:GLY:HA3	1:C:392:PRO:HD3	1.90	0.40
1:C:407:HIS:HE2	1:C:1047:LEU:HD12	1.79	0.40
1:C:841:ASP:CA	1:C:940:ARG:CZ	2.98	0.40
1:C:1034:GLN:OE1	1:C:1034:GLN:CA	2.69	0.40
1:C:1105:LEU:O	1:C:1105:LEU:CD1	2.69	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	B	1132/1333 (85%)	999 (88%)	121 (11%)	12 (1%)	14 45
1	C	1243/1333 (93%)	937 (75%)	209 (17%)	97 (8%)	1 6
All	All	2375/2666 (89%)	1936 (82%)	330 (14%)	109 (5%)	4 15

All (109) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	120	VAL
1	C	121	PHE
1	C	122	ASN
1	C	129	ALA
1	C	144	ASN
1	C	186	ASP
1	C	234	PRO
1	C	241	ALA
1	C	280	THR
1	C	299	ALA
1	C	337	VAL
1	C	338	ARG
1	C	372	ALA
1	C	450	PRO
1	C	455	GLN
1	C	475	ILE
1	C	661	ASN
1	C	730	ASP
1	C	772	TYR
1	C	773	PRO
1	C	871	PRO
1	C	875	THR
1	C	879	THR
1	C	880	PRO
1	C	891	HIS
1	C	935	GLN
1	C	1024	PRO
1	C	1130	SER
1	C	1134	ARG
1	C	1138	HIS
1	C	1147	MET
1	C	1150	LEU
1	C	1182	GLU
1	C	1213	PRO
1	C	1221	PRO
1	C	1262	SER
1	C	1271	SER
1	C	1278	TYR
1	C	1282	ALA
1	C	1293	VAL
1	C	1308	ASN
1	B	437	ALA

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Mol	Chain	Res	Type
1	B	473	ALA
1	B	1251	VAL
1	B	1255	ARG
1	B	1286	VAL
1	C	130	LEU
1	C	184	GLU
1	C	339	LEU
1	C	403	PHE
1	C	453	LEU
1	C	565	GLU
1	C	639	ASN
1	C	837	THR
1	C	842	ASP
1	C	948	ILE
1	C	1049	GLU
1	C	1067	ILE
1	C	1190	ALA
1	C	1228	ARG
1	C	1251	VAL
1	C	1280	PRO
1	C	1295	HIS
1	C	1325	VAL
1	C	1329	ASN
1	C	1332	ASN
1	B	151	SER
1	B	753	ASP
1	C	231	LEU
1	C	235	ILE
1	C	442	PRO
1	C	448	TYR
1	C	522	PRO
1	C	1045	TYR
1	C	1129	PRO
1	C	1222	ALA
1	C	1294	ASP
1	C	265	VAL
1	C	646	ASN
1	C	731	GLN
1	C	1093	PRO
1	C	1136	HIS
1	C	1144	ARG
1	C	1191	GLU

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Mol	Chain	Res	Type
1	C	1223	SER
1	C	1235	PRO
1	B	384	MET
1	B	1094	GLU
1	C	336	TYR
1	C	577	GLN
1	C	898	GLN
1	C	942	HIS
1	C	958	ILE
1	C	1260	PRO
1	B	879	THR
1	C	245	ALA
1	C	644	VAL
1	C	794	PRO
1	C	1109	SER
1	C	1234	GLN
1	C	1137	VAL
1	B	1236	ILE
1	C	273	PRO
1	C	635	ILE
1	B	1246	VAL
1	C	1128	TYR
1	C	1236	ILE
1	C	1274	GLY
1	C	1286	VAL

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	B	1000/1155 (87%)	993 (99%)	7 (1%)	84 90
1	C	1087/1155 (94%)	733 (67%)	354 (33%)	0 1
All	All	2087/2310 (90%)	1726 (83%)	361 (17%)	5 8

All (361) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	461	ARG
1	B	464	SER
1	B	471	SER
1	B	472	GLU
1	B	474	ASP
1	B	475	ILE
1	B	790	GLU
1	C	74	LYS
1	C	79	SER
1	C	83	GLN
1	C	85	ASP
1	C	87	GLU
1	C	88	LYS
1	C	89	PRO
1	C	92	VAL
1	C	93	THR
1	C	96	ILE
1	C	101	ASP
1	C	105	MET
1	C	106	GLN
1	C	108	LYS
1	C	109	LYS
1	C	112	THR
1	C	119	ASP
1	C	120	VAL
1	C	122	ASN
1	C	124	GLN
1	C	132	PRO
1	C	133	MET
1	C	134	THR
1	C	135	LYS
1	C	136	VAL
1	C	137	ILE
1	C	141	LEU
1	C	142	ASP
1	C	143	VAL
1	C	145	THR
1	C	146	GLU
1	C	150	LEU
1	C	155	LYS
1	C	156	GLN
1	C	157	ILE
1	C	159	ASP

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Mol	Chain	Res	Type
1	C	161	LYS
1	C	173	GLN
1	C	176	LYS
1	C	177	LYS
1	C	196	LEU
1	C	204	VAL
1	C	205	ASN
1	C	214	ASP
1	C	221	LEU
1	C	229	GLN
1	C	230	ASP
1	C	231	LEU
1	C	232	LEU
1	C	251	LEU
1	C	255	LEU
1	C	265	VAL
1	C	283	ASN
1	C	287	ARG
1	C	297	ASN
1	C	300	LEU
1	C	302	ARG
1	C	304	PHE
1	C	306	GLN
1	C	309	TRP
1	C	312	ARG
1	C	315	THR
1	C	316	ASN
1	C	318	LEU
1	C	319	GLN
1	C	320	GLN
1	C	327	LEU
1	C	330	THR
1	C	333	ARG
1	C	338	ARG
1	C	339	LEU
1	C	342	THR
1	C	346	HIS
1	C	350	ILE
1	C	351	ASP
1	C	356	SER
1	C	361	ASN
1	C	362	LEU

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Mol	Chain	Res	Type
1	C	363	ARG
1	C	366	MET
1	C	375	ARG
1	C	376	ILE
1	C	377	LYS
1	C	384	MET
1	C	386	SER
1	C	397	LEU
1	C	409	ILE
1	C	422	LEU
1	C	429	ILE
1	C	430	ASN
1	C	439	VAL
1	C	440	ILE
1	C	441	ARG
1	C	445	GLU
1	C	446	LYS
1	C	448	TYR
1	C	452	ASN
1	C	454	GLU
1	C	455	GLN
1	C	466	VAL
1	C	467	LYS
1	C	472	GLU
1	C	480	LEU
1	C	494	GLU
1	C	495	LEU
1	C	497	LYS
1	C	498	ILE
1	C	505	PRO
1	C	513	GLU
1	C	521	PHE
1	C	522	PRO
1	C	523	THR
1	C	524	GLU
1	C	526	ASN
1	C	529	LYS
1	C	538	LEU
1	C	547	GLU
1	C	550	ILE
1	C	552	ILE
1	C	553	GLN

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Mol	Chain	Res	Type
1	C	554	ARG
1	C	560	ILE
1	C	565	GLU
1	C	571	ARG
1	C	572	ASN
1	C	574	LYS
1	C	576	ASP
1	C	578	SER
1	C	581	LEU
1	C	583	GLU
1	C	584	HIS
1	C	591	ASP
1	C	594	LEU
1	C	599	THR
1	C	605	ARG
1	C	607	PHE
1	C	613	LEU
1	C	614	ARG
1	C	615	THR
1	C	617	ASP
1	C	628	SER
1	C	629	ARG
1	C	633	THR
1	C	635	ILE
1	C	637	TYR
1	C	639	ASN
1	C	641	ARG
1	C	643	THR
1	C	646	ASN
1	C	651	ARG
1	C	656	VAL
1	C	658	THR
1	C	659	LEU
1	C	666	ARG
1	C	669	GLN
1	C	674	LYS
1	C	685	ARG
1	C	686	HIS
1	C	698	HIS
1	C	708	THR
1	C	717	THR
1	C	720	PHE

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Mol	Chain	Res	Type
1	C	729	PRO
1	C	736	SER
1	C	742	LYS
1	C	744	ILE
1	C	746	GLU
1	C	747	ARG
1	C	748	GLN
1	C	755	LEU
1	C	765	PRO
1	C	766	ILE
1	C	767	LEU
1	C	770	CYS
1	C	792	VAL
1	C	795	ASP
1	C	797	SER
1	C	799	THR
1	C	800	LEU
1	C	802	GLN
1	C	806	VAL
1	C	812	LYS
1	C	813	LEU
1	C	814	THR
1	C	816	PRO
1	C	817	ASP
1	C	820	ILE
1	C	823	ILE
1	C	824	LEU
1	C	828	ASP
1	C	829	SER
1	C	840	ASP
1	C	842	ASP
1	C	843	LEU
1	C	848	ARG
1	C	849	MET
1	C	850	THR
1	C	851	THR
1	C	856	LEU
1	C	860	ARG
1	C	865	ILE
1	C	866	THR
1	C	867	ASN
1	C	870	ASP

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Mol	Chain	Res	Type
1	C	874	ILE
1	C	888	GLN
1	C	896	LEU
1	C	897	TYR
1	C	898	GLN
1	C	902	ILE
1	C	907	SER
1	C	910	LEU
1	C	911	ARG
1	C	913	ASN
1	C	916	LEU
1	C	917	VAL
1	C	921	ASP
1	C	922	TYR
1	C	928	ARG
1	C	931	ASN
1	C	934	LEU
1	C	935	GLN
1	C	939	ASN
1	C	940	ARG
1	C	941	TYR
1	C	945	VAL
1	C	948	ILE
1	C	951	ILE
1	C	954	GLN
1	C	957	PHE
1	C	958	ILE
1	C	962	ASP
1	C	965	ARG
1	C	966	GLN
1	C	967	LEU
1	C	973	THR
1	C	976	THR
1	C	978	GLN
1	C	988	GLN
1	C	989	ILE
1	C	991	ASP
1	C	1003	ARG
1	C	1014	MET
1	C	1021	ARG
1	C	1022	ILE
1	C	1023	ARG

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Mol	Chain	Res	Type
1	C	1024	PRO
1	C	1034	GLN
1	C	1036	ASP
1	C	1038	GLU
1	C	1043	SER
1	C	1044	ARG
1	C	1049	GLU
1	C	1050	LEU
1	C	1051	ARG
1	C	1053	ARG
1	C	1054	ARG
1	C	1059	LEU
1	C	1061	LEU
1	C	1062	ILE
1	C	1063	THR
1	C	1070	ARG
1	C	1072	ASP
1	C	1075	ARG
1	C	1076	ILE
1	C	1077	MET
1	C	1079	LEU
1	C	1080	THR
1	C	1082	ASP
1	C	1083	ASP
1	C	1088	PHE
1	C	1089	VAL
1	C	1092	VAL
1	C	1099	VAL
1	C	1104	ARG
1	C	1105	LEU
1	C	1106	PHE
1	C	1110	LEU
1	C	1112	ASN
1	C	1114	ARG
1	C	1118	THR
1	C	1122	PRO
1	C	1123	PRO
1	C	1124	THR
1	C	1126	MET
1	C	1132	THR
1	C	1140	THR
1	C	1141	ILE

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Mol	Chain	Res	Type
1	C	1147	MET
1	C	1149	LYS
1	C	1158	SER
1	C	1161	LYS
1	C	1168	ILE
1	C	1169	HIS
1	C	1170	ASP
1	C	1171	ILE
1	C	1177	VAL
1	C	1182	GLU
1	C	1185	THR
1	C	1186	GLN
1	C	1187	HIS
1	C	1191	GLU
1	C	1192	SER
1	C	1195	THR
1	C	1200	LYS
1	C	1201	LEU
1	C	1202	PHE
1	C	1204	LEU
1	C	1207	MET
1	C	1208	ASP
1	C	1210	LEU
1	C	1211	LEU
1	C	1212	ARG
1	C	1213	PRO
1	C	1214	GLU
1	C	1219	ASP
1	C	1221	PRO
1	C	1227	MET
1	C	1236	ILE
1	C	1237	SER
1	C	1240	ARG
1	C	1242	MET
1	C	1243	ARG
1	C	1246	VAL
1	C	1247	ASN
1	C	1250	GLU
1	C	1253	ARG
1	C	1262	SER
1	C	1263	TYR
1	C	1264	GLU

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Mol	Chain	Res	Type
1	C	1272	ARG
1	C	1273	ASN
1	C	1276	LEU
1	C	1277	LEU
1	C	1283	ASN
1	C	1285	GLN
1	C	1286	VAL
1	C	1288	ILE
1	C	1290	LYS
1	C	1292	GLU
1	C	1296	ILE
1	C	1298	PHE
1	C	1305	MET
1	C	1309	ILE
1	C	1310	ARG
1	C	1313	ASP
1	C	1319	ARG
1	C	1320	VAL
1	C	1323	ASP
1	C	1325	VAL
1	C	1326	ARG
1	C	1328	ILE
1	C	1331	ARG
1	C	1332	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	139	ASN
1	B	148	GLN
1	B	291	HIS
1	B	292	ASN
1	B	311	ASN
1	B	346	HIS
1	B	438	ASN
1	B	661	ASN
1	B	682	GLN
1	B	693	ASN
1	B	698	HIS
1	B	701	HIS
1	B	718	ASN
1	B	748	GLN

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Mol	Chain	Res	Type
1	B	854	GLN
1	B	898	GLN
1	B	913	ASN
1	B	942	HIS
1	B	988	GLN
1	B	1064	ASN
1	B	1169	HIS
1	B	1205	GLN
1	B	1300	ASN
1	C	106	GLN
1	C	115	GLN
1	C	144	ASN
1	C	148	GLN
1	C	173	GLN
1	C	195	ASN
1	C	205	ASN
1	C	209	ASN
1	C	229	GLN
1	C	297	ASN
1	C	306	GLN
1	C	311	ASN
1	C	352	HIS
1	C	369	ASN
1	C	430	ASN
1	C	455	GLN
1	C	577	GLN
1	C	610	GLN
1	C	646	ASN
1	C	673	GLN
1	C	690	GLN
1	C	693	ASN
1	C	701	HIS
1	C	748	GLN
1	C	802	GLN
1	C	854	GLN
1	C	864	HIS
1	C	882	GLN
1	C	959	GLN
1	C	966	GLN
1	C	1103	HIS
1	C	1121	HIS
1	C	1154	ASN

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Mol	Chain	Res	Type
1	C	1186	GLN
1	C	1203	HIS
1	C	1205	GLN
1	C	1247	ASN
1	C	1285	GLN
1	C	1308	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.

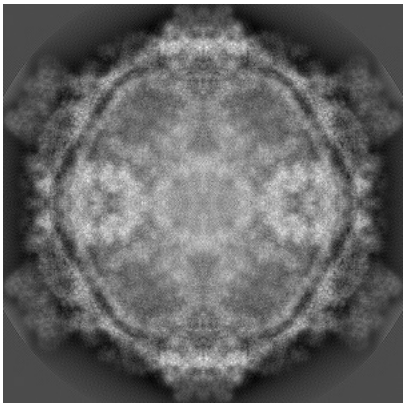
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-9565. These allow visual inspection of the internal detail of the map and identification of artifacts.

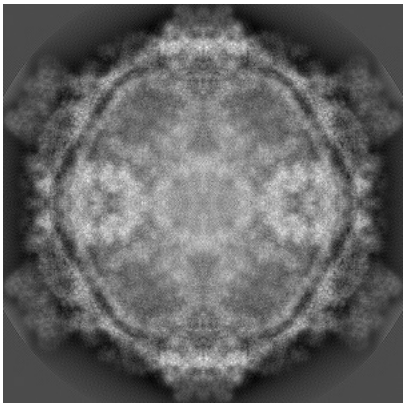
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

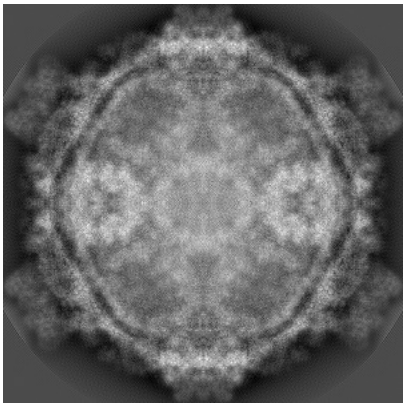
6.1.1 Primary map



X



Y

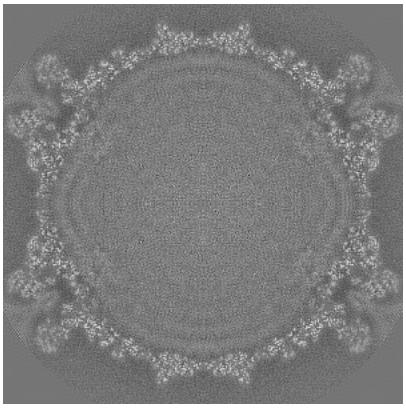


Z

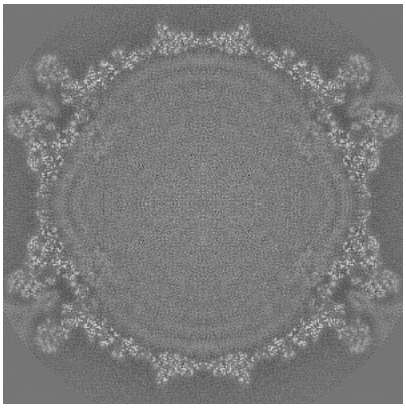
The images above show the map projected in three orthogonal directions.

6.2 Central slices

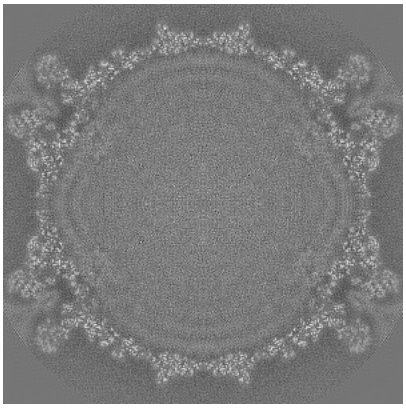
6.2.1 Primary map



X Index: 350



Y Index: 350

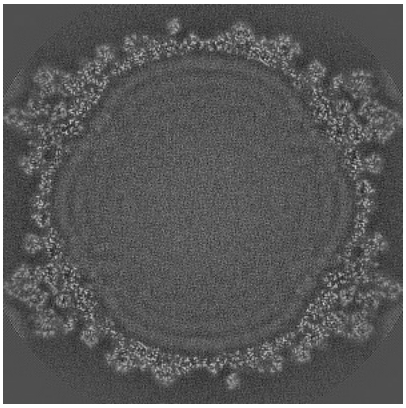


Z Index: 350

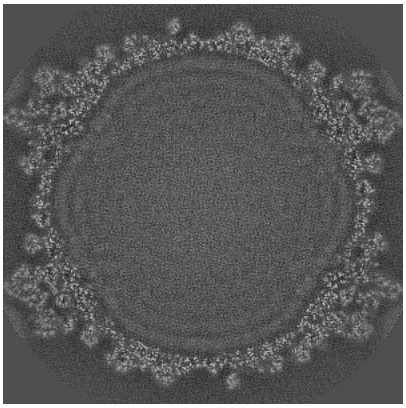
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

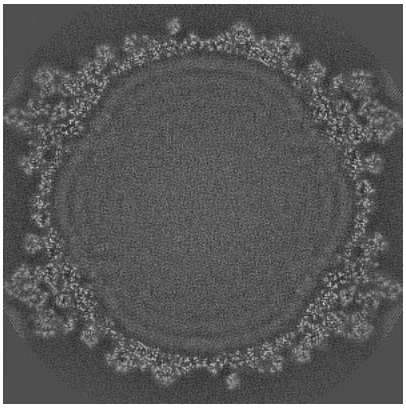
6.3.1 Primary map



X Index: 320



Y Index: 320

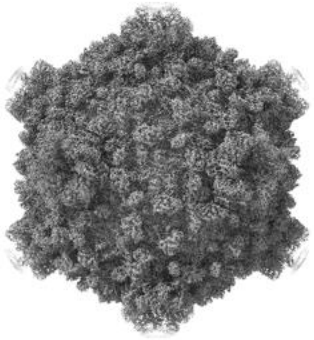


Z Index: 320

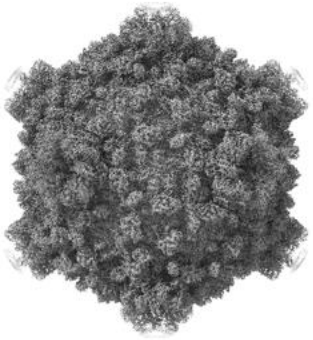
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

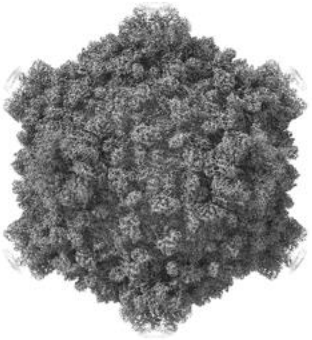
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 17.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

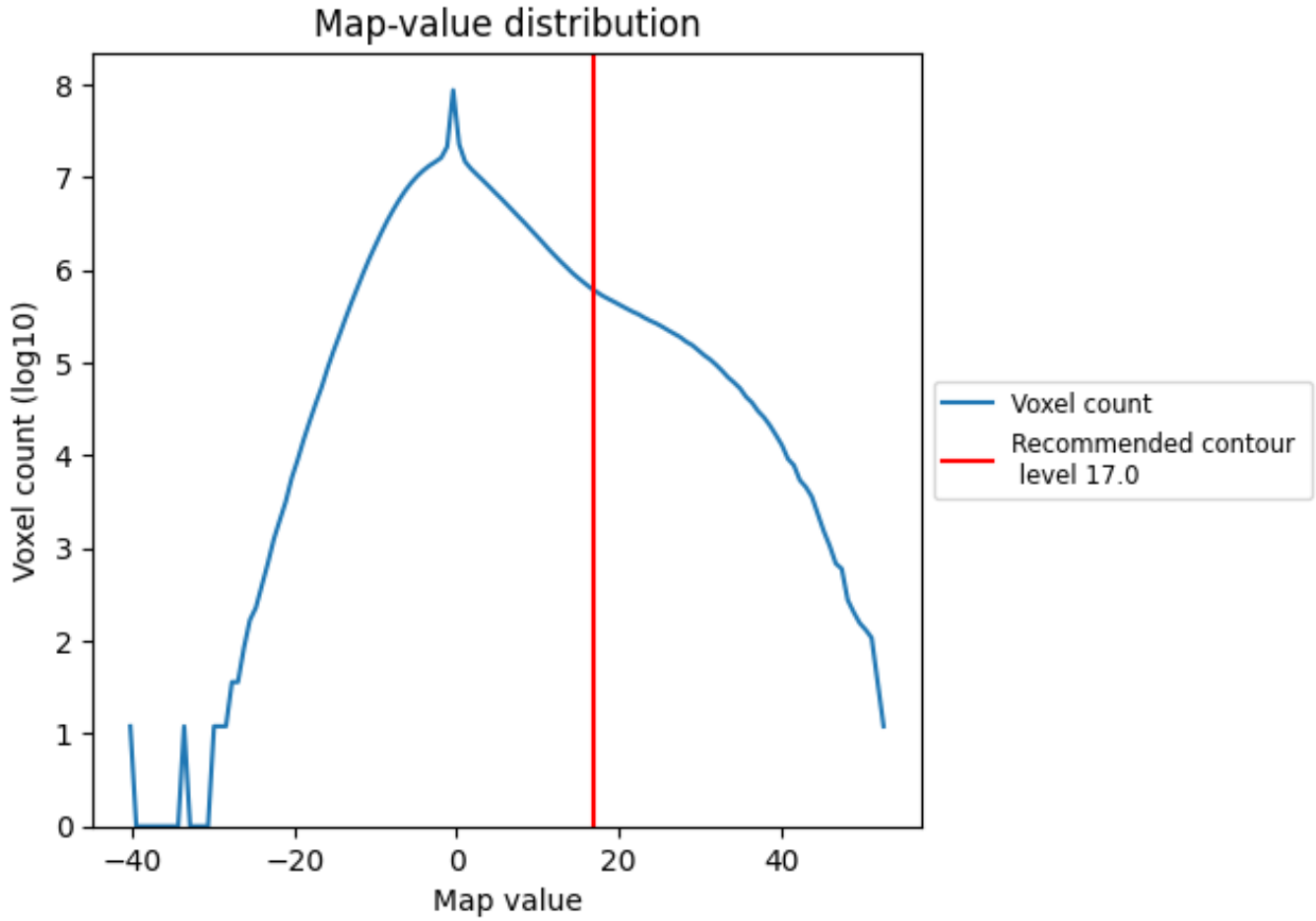
6.5 Mask visualisation (i)

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

7 Map analysis

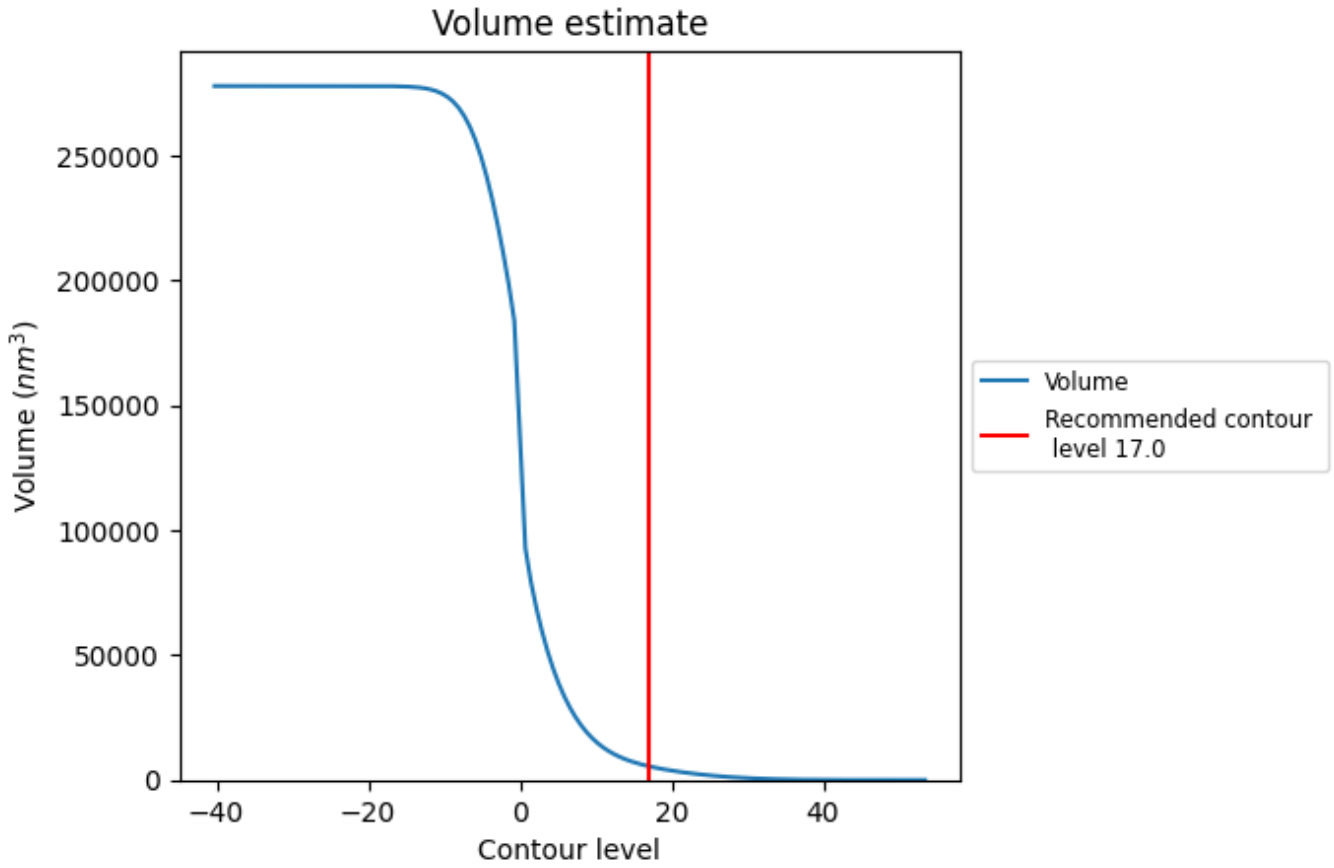
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

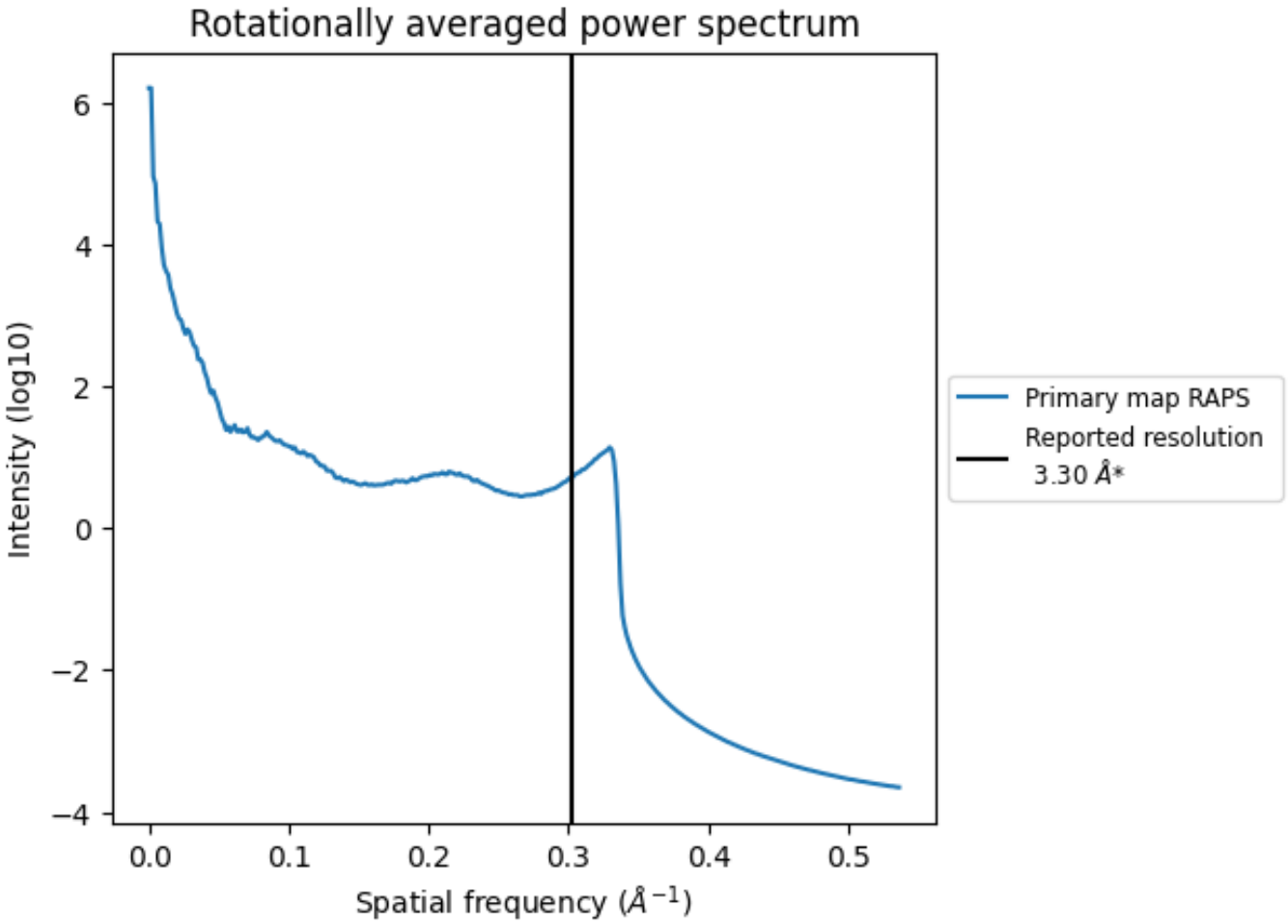
7.2 Volume estimate



The volume at the recommended contour level is 5491 nm^3; this corresponds to an approximate mass of 4961 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 0.303 Å^{-1}

8 Fourier-Shell correlation (i)

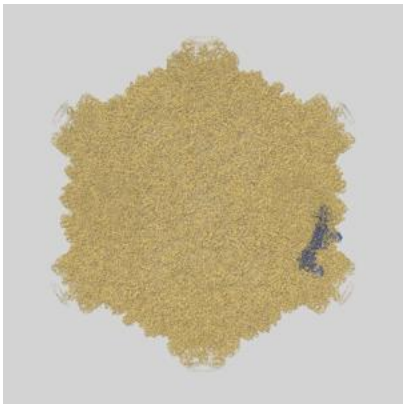
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

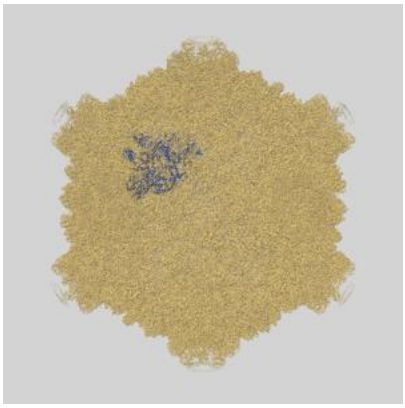
This section contains information regarding the fit between EMDB map EMD-9565 and PDB model 5H0S. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay

X



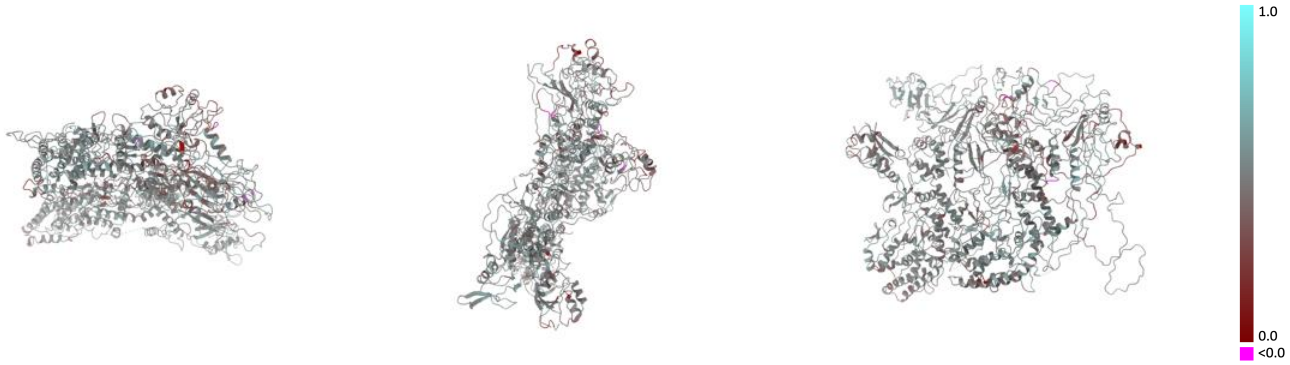
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 17.0 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.

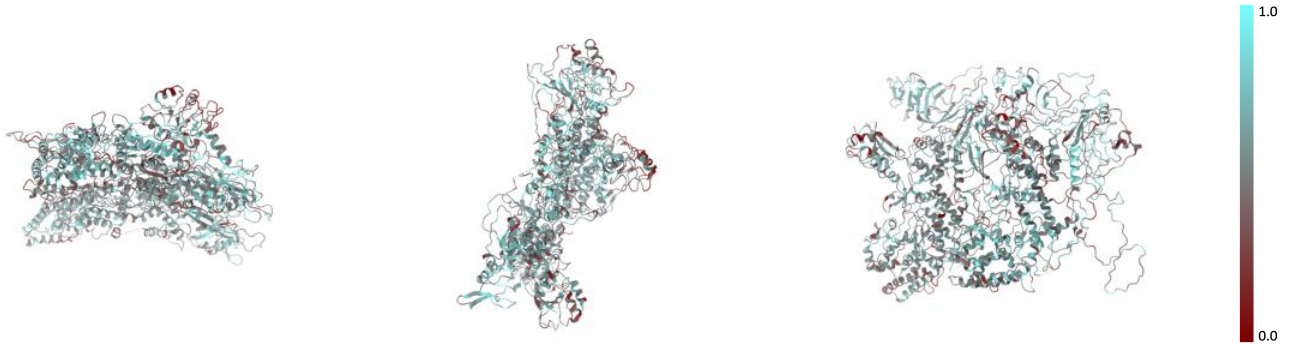
9.2 Q-score mapped to coordinate model (i)



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.

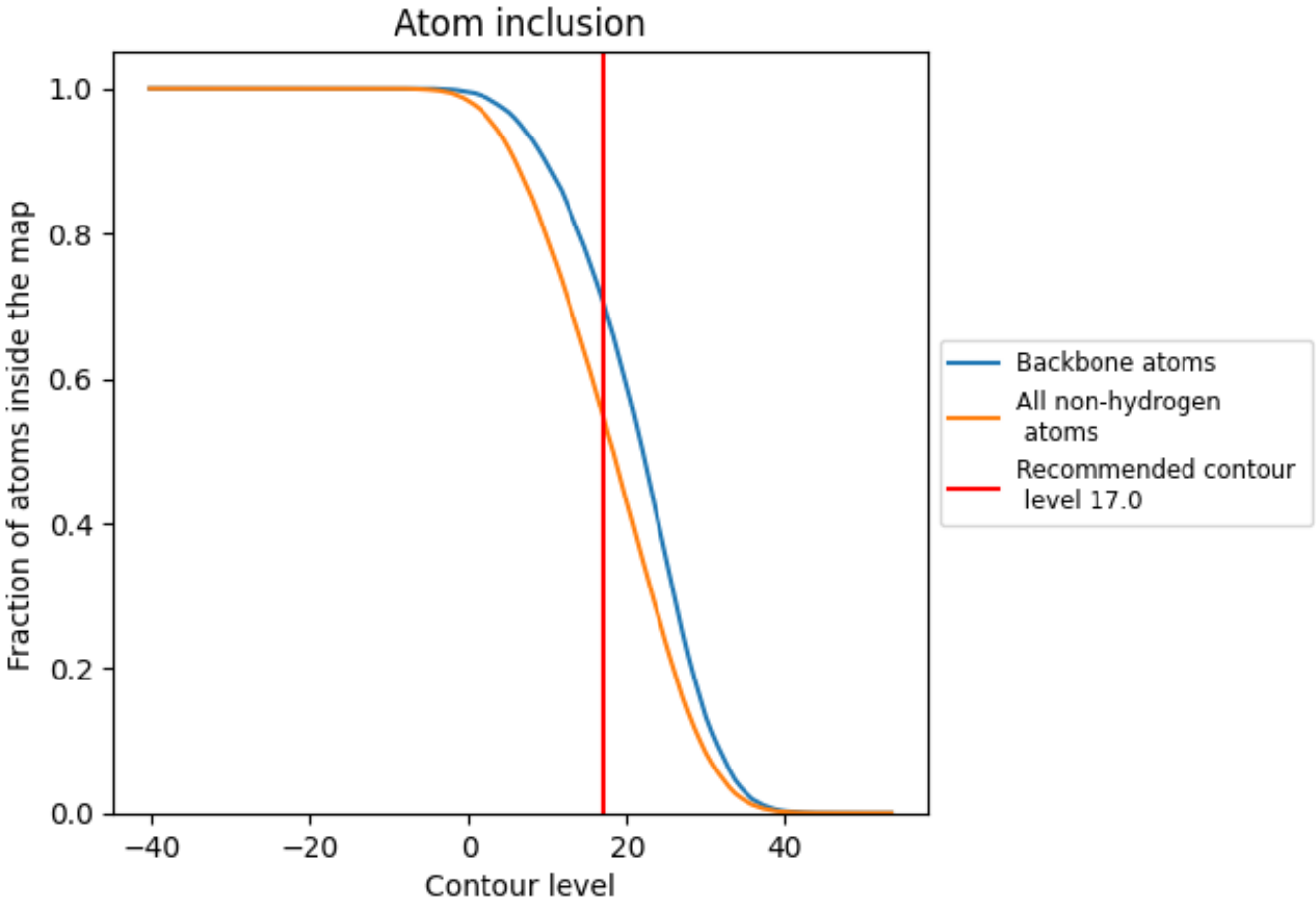
9.3 Atom inclusion mapped to coordinate model (i)



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 (17.0).

9.4 Atom inclusion (i)



At the recommended contour level, 71% of all backbone atoms, 55% 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 (17.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5491	0.4770
B	0.5458	0.4780
C	0.5522	0.4760