Full wwPDB EM Validation Report (i)

Nov 19, 2022 – 03:18 pm GMT

PDB ID	:	5N61
EMDB ID	:	EMD-3593
Title	:	RNA polymerase I initially transcribing complex
Authors	:	Engel, C.; Gubbey, T.; Neyer, S.; Sainsbury, S.; Oberthuer, C.; Baejen, C.; Bernecky, C.; Cramer, P.
Deposited on	:	2017-02-14
Resolution	:	3.40 Å(reported)

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

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

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

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

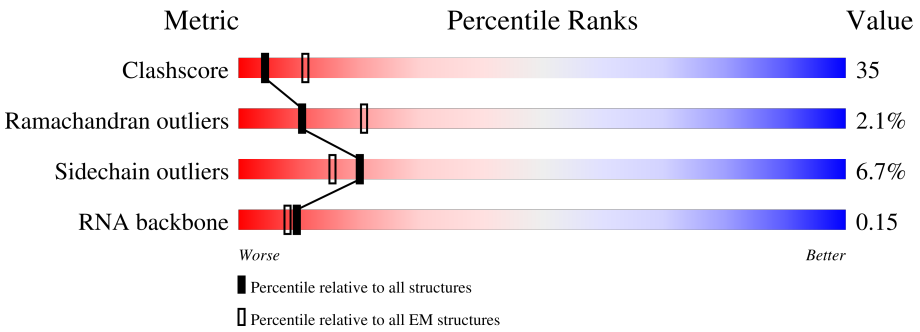
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 3.40 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
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	A	1664	48% 39% • 12%
2	B	1203	50% 46% • •
3	C	335	52% 39% 9%
4	D	137	28% 11% 61%
5	E	215	57% 42% •
6	F	155	41% 24% 35%
7	G	326	5% 32% 27% 41%

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Mol	Chain	Length	Quality of chain
8	H	146	53% 37% 10%
9	I	125	13% 37% 50%
10	J	70	46% 51%
11	K	142	43% 28% 29%
12	L	70	31% 31% 37%
13	M	415	16% 10% 74%
14	N	233	9% 31% 24% 45%
15	O	627	28% 37% 36% 26%
16	P	894	64% 18% 31% 14% 34%
17	Q	514	71% 24% 39% 11% 24%
18	R	507	43% 15% 30% 13% 40%
19	S	5	20% 20% 60% 20%
20	T	47	64% 23% 64% 13%
21	U	47	53% 30% 38% 30%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	SO4	B	1301	-	-	X	-

2 Entry composition (i)

There are 24 unique types of molecules in this entry. The entry contains 48547 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase I subunit RPA190.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1459	11526	7281	2004	2180	61	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase I subunit RPA135.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1177	9350	5913	1639	1747	51	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	305	2423	1539	416	460	8	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase I subunit RPA14.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	D	54	431	270	73	88	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	212	1735	1102	306	316	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	100	823	522	144	154	3	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase I subunit RPA43.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	193	1526	985	262	274	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	131	1052	664	176	208	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	63	466	292	77	93	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	69	569	362	101	100	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	101	793	496	130	162	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	44	352	217	70	61	4	0	0

- Molecule 13 is a protein called DNA-directed RNA polymerase I subunit RPA49.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	M	108	856	543	142	171	0	0

- Molecule 14 is a protein called DNA-directed RNA polymerase I subunit RPA34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	N	129	1029	665	170	191	3	0	0

- Molecule 15 is a protein called RNA polymerase I-specific transcription initiation factor RRN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	O	463	3811	2473	623	694	21	0	0

- Molecule 16 is a protein called RNA polymerase I-specific transcription initiation factor RRN6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	P	587	4764	3030	811	912	11	0	0

- Molecule 17 is a protein called RNA polymerase I-specific transcription initiation factor RRN7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	Q	389	3254	2110	552	572	20	0	0

- Molecule 18 is a protein called RNA polymerase I-specific transcription initiation factor RRN11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	R	303	2535	1634	456	434	11	0	0

- Molecule 19 is a RNA chain called product RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
19	S	5	108	48	21	34	5	0	0

- Molecule 20 is a DNA chain called template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
20	T	41	641	304	66	231	40	0	0

- Molecule 21 is a DNA chain called non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
21	U	33	490	228	55	174	33	0	0

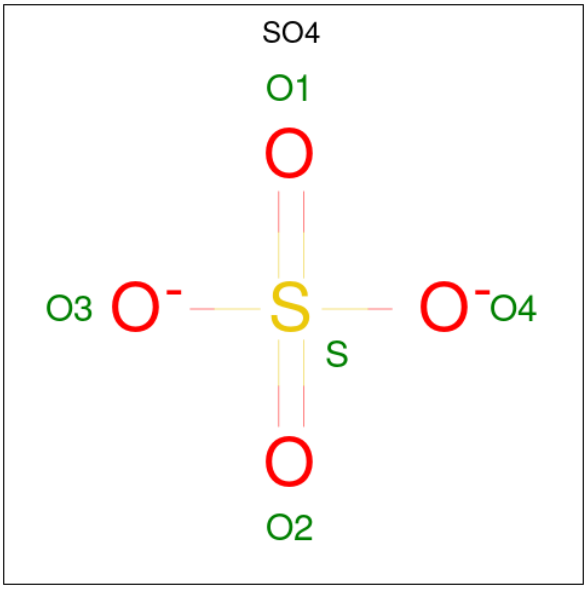
- Molecule 22 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
22	A	2	2	2	0
22	B	1	1	1	0
22	I	1	1	1	0
22	J	1	1	1	0
22	L	1	1	1	0
22	Q	1	1	1	0

- Molecule 23 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
23	A	1	1	1	0

- Molecule 24 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



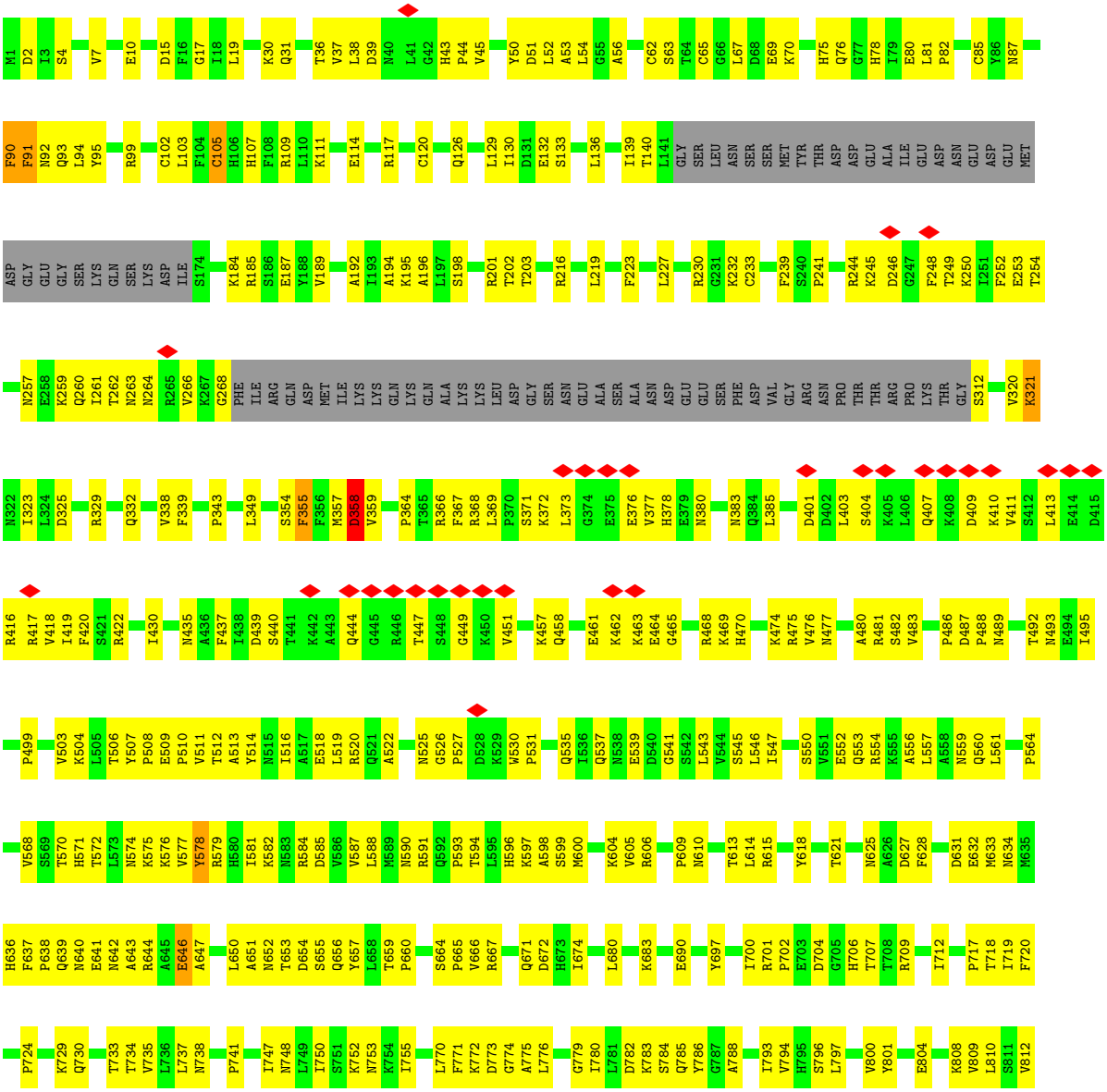
Mol	Chain	Residues	Atoms			AltConf
			Total	O	S	
24	B	1	5	4	1	0

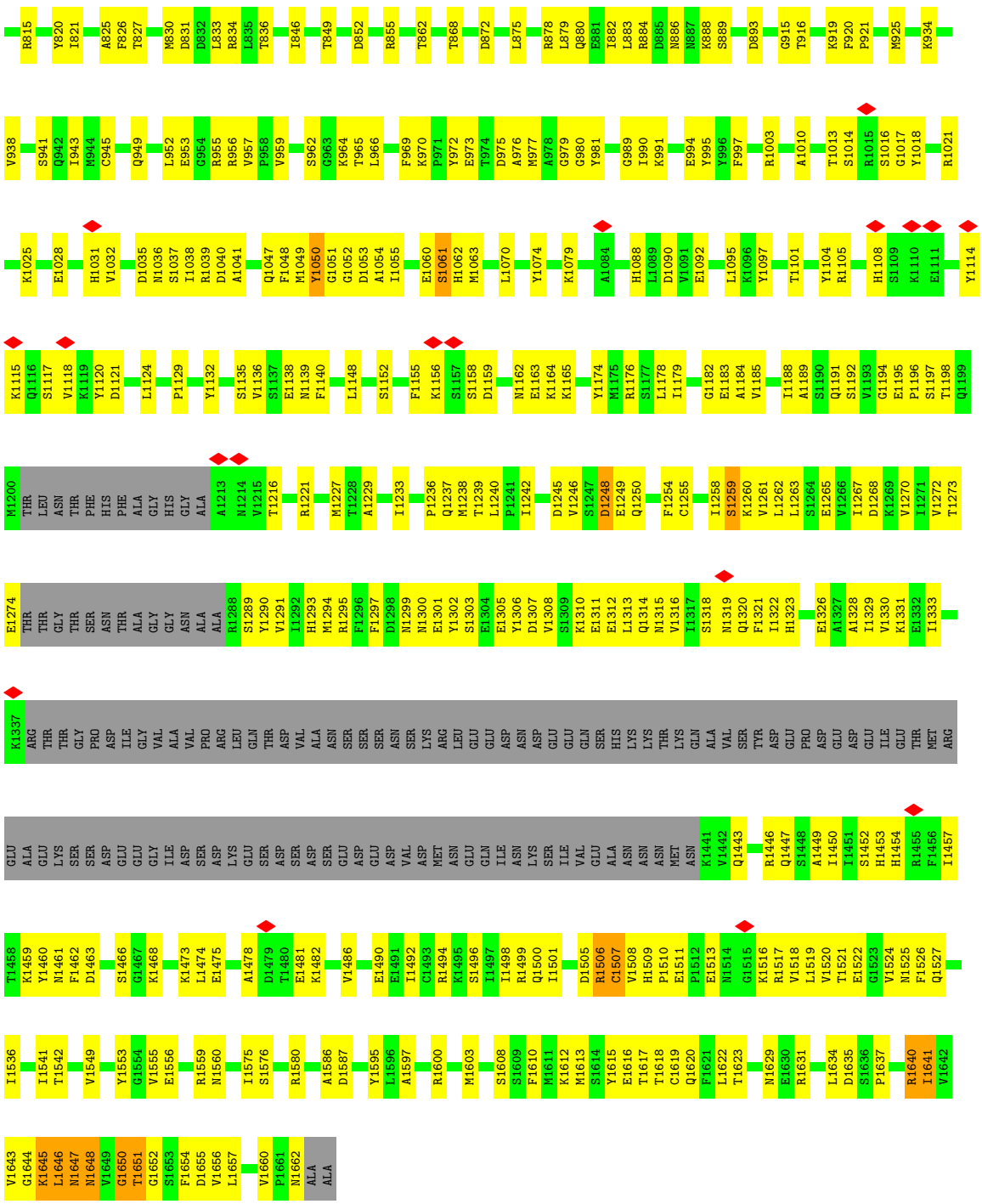
3 Residue-property plots (i)

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

- Molecule 1: DNA-directed RNA polymerase I subunit RPA190

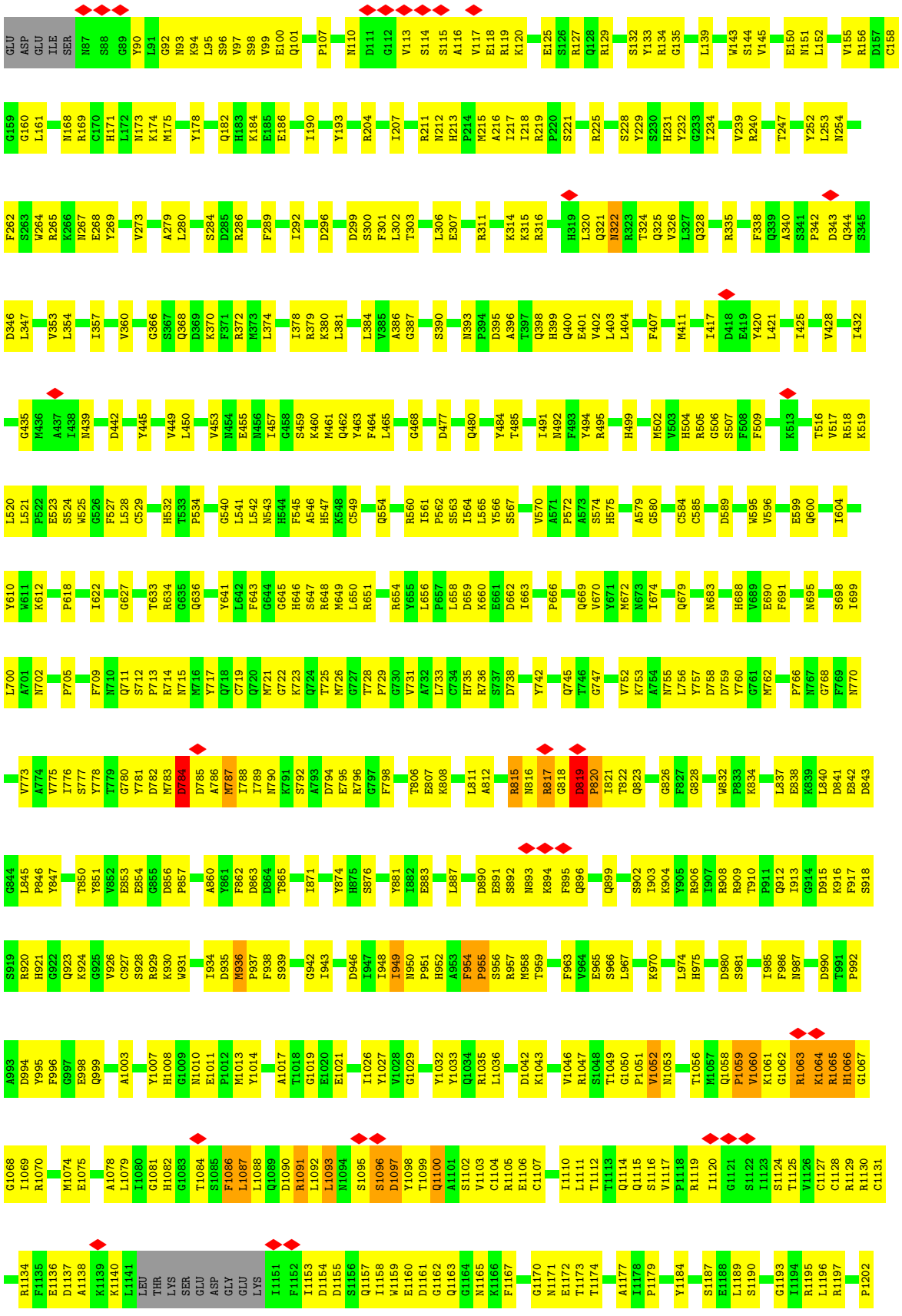
Chain A: 48% 39% 12%





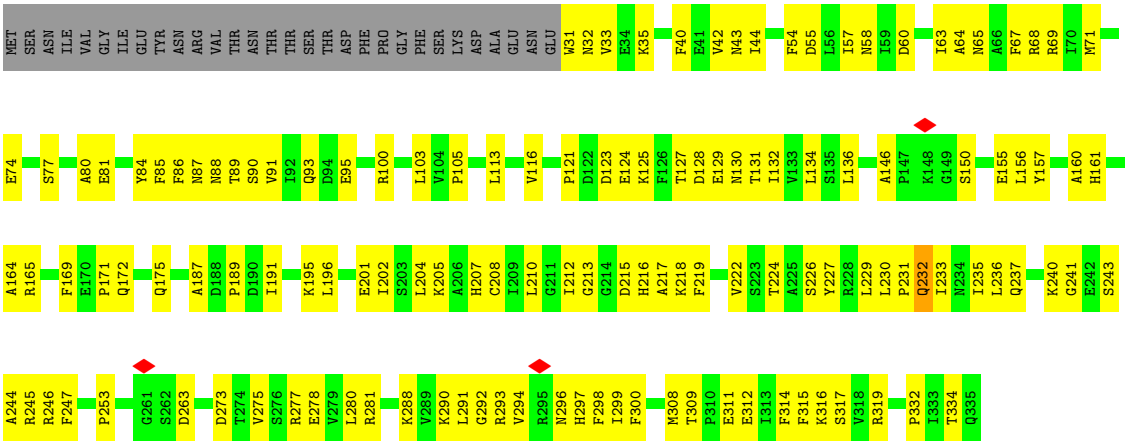
• Molecule 2: DNA-directed RNA polymerase I subunit RPA135

Chain B:


GLU ASP GLU ILE SER N87 S88 G89 Y90 L91 G92 N93 K94 L95 S96 V97 S98 V99 E100 Q101 P107 N110 D111 G112 V113 S114 S115 A116 V117 E118 R119 K120 E125 S126 R127 Q128 R129 S132 Y133 R134 G135 L139 W143 S144 V145 E150 N151 L152 V155 R156 D157 C158
G159 G160 L161 N168 R169 C170 H171 L172 N173 K174 M175 Y178 Q182 H183 K184 E185 E186 I190 Y193 R204 I207 R211 N212 H213 P214 M215 A216 I217 I218 R219 P220 S221 R225 S228 Y229 S230 H231 Y232 G233 I234 V239 R240 T247 Y252 L253 N254
F262 S263 W264 R265 K266 N267 E268 Y269 V273 A279 L280 S284 D285 R286 F289 I292 D296 D299 S300 F301 L302 T303 L306 E307 R311 K314 K315 R316 H319 L320 Q321 N322 R323 T324 Q325 V326 L327 Q328 R335 F338 Q339 A340 S341 P342 D343 Q344 S345
D346 L347 V353 L354 I357 V360 G366 S367 Q368 D369 K370 F371 R372 H373 L374 I378 R379 K380 L381 L384 V385 A386 G387 S390 N393 P394 D395 A396 T397 Q398 H399 Q400 E401 V402 L403 L404 F407 M411 I417 D418 E419 Y420 L421 I425 V428 I432
G435 M436 A437 I438 N439 D442 Y445 V449 L450 V453 N454 E455 N456 I457 G458 S459 K460 M461 Q462 Y463 F464 L465 G468 D477 Q480 Y484 T485 I491 N492 F493 Y494 R495 H499 M502 V503 H504 R505 G506 S507 F508 F509 K513 T516 V517 R518 K519
L520 L521 P522 E523 S524 W525 G526 F527 L528 C529 H532 T533 P534 G540 L541 L542 N543 H544 F545 A546 H547 K548 C549 Q554 R560 I561 P562 S563 I564 L565 Y566 S567 V570 A571 P572 A573 S574 H575 A579 G580 C584 C585 D589 W595 V596 E599 Q600 I604
Y610 W611 K612 P618 I622 G627 T633 R634 G635 Q636 Y641 L642 F643 G644 G645 H646 S647 R648 M649 L650 R651 R654 Y655 L656 P657 L658 D659 K660 E661 D662 I663 P666 Q669 V670 Y671 M672 N673 I674 Q679 N683 H638 V689 E690 F691 N695 S698 I699
L700 A701 N702 P705 F709 N710 Q711 S712 P713 R714 N715 M716 Y717 Q718 C719 Q720 M721 G722 K723 Q724 T725 M726 G727 T728 P729 G730 V731 A732 L733 C734 H735 R736 S737 D738 Y742 Q745 T746 G747 V752 K753 A754 N755 L756 Y757 D758 D759 Y760 G761 M762 P766 N767 G768 F769 N770
V773 A774 V775 I776 S777 Y778 T779 G780 Y781 D782 M783 D784 D785 A786 M787 I788 I789 N790 K791 S792 A793 D794 E795 R796 G797 F798 T806 E807 K808 L811 A812 R815 N816 R817 G818 D819 P820 I821 T822 Q823 G826 F827 G828 W832 P833 K834 L837 E838 K839 L840 D841 E842 D843
G844 L845 P846 Y847 T850 Y851 V852 E853 E854 G855 D856 P857 A860 Y861 F862 D863 D864 T865 I871 Y874 H875 S876 Y881 I882 E883 L887 D890 E891 S892 N893 K894 F895 Q896 Q899 S902 I903 K904 Y905 R906 I907 R908 R909 T910 P911 Q912 I913 G914 D915 K916 F917 S918
S919 R920 H921 G922 Q923 K924 G925 V926 C927 S928 R929 K930 W931 I934 D935 M936 P937 F938 S939 G942 I943 D946 I947 I948 I949 N950 P951 H952 A953 F954 P955 S956 R957 M958 T959 F963 V964 E965 S966 L967 K970 L974 H975 D980 S981 I985 F986 N987 D990 T991 P992
A993 D994 Y995 F996 G997 E998 Q999 A1003 Y1007 H1008 G1009 N1010 E1011 P1012 M1013 Y1014 A1017 T1018 G1019 E1020 E1021 I1026 Y1027 V1028 G1029 Y1032 Y1033 Q1034 R1035 L1036 D1042 K1043 V1046 R1047 S1048 T1049 G1050 P1051 V1052 N1053 T1056 M1057 Q1058 P1059 V1060 K1061 G1062 R1063 K1064 R1065 H1066 G1067
G1068 I1069 R1070 M1074 E1075 A1078 L1079 I1080 G1081 H1082 G1083 T1084 S1085 F1086 L1087 L1088 Q1089 D1090 R1091 L1092 L1093 N1094 S1095 S1096 D1097 Y1098 T1099 Q1100 A1101 S1102 V1103 C1104 R1105 E1106 C1107 I1110 L1111 T1112 T1113 Q1114 Q1115 S1116 V1117 P1118 R1119 I1120 G1121 S1122 I1123 S1124 T1125 V1126 C1127 C1128 R1129 R1130 C1131
R1134 F1135 E1136 D1137 A1138 K1139 K1140 L1141 LEU THR LYS SER GLU ASP GLY GLU LYS T1151 F1152 I1153 D1154 D1155 S1156 Q1157 I1158 W1159 E1160 D1161 G1162 Q1163 G1164 N1165 K1166 F1167 G1170 N1171 E1172 T1173 T1174 A1177 I1178 P1179 Y1184 S1187 E1188 L1189 S1190 G1193 I1194 R1195 L1196 R197 P1202

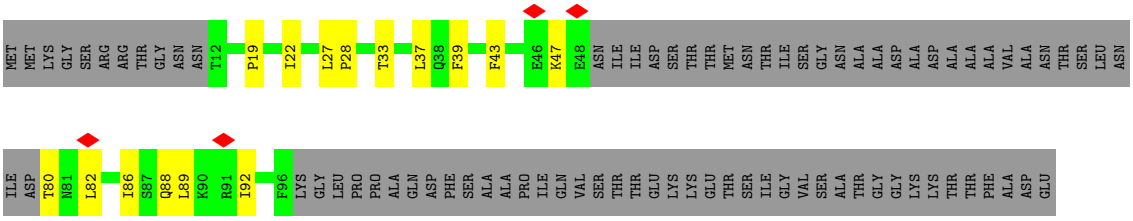
• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1

Chain C:



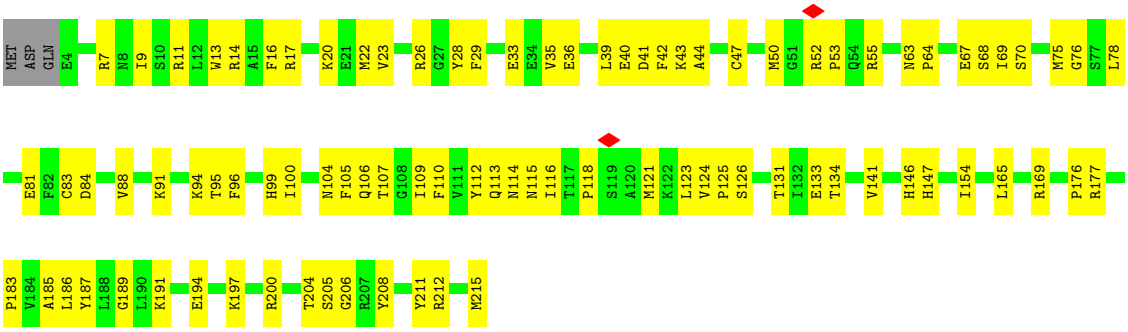
• Molecule 4: DNA-directed RNA polymerase I subunit RPA14

Chain D:



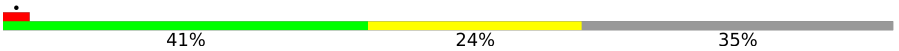
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

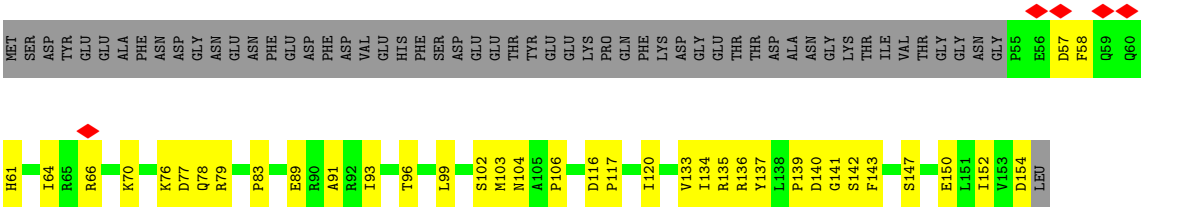
Chain E:



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

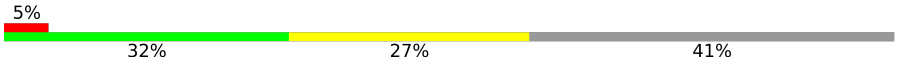
Chain F:

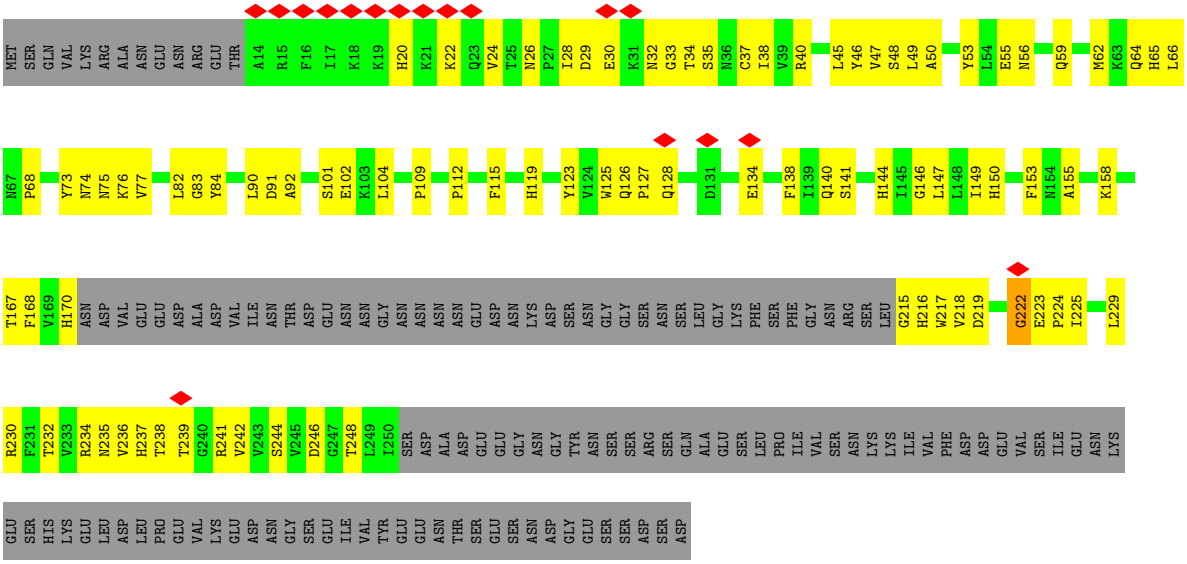




• Molecule 7: DNA-directed RNA polymerase I subunit RPA43

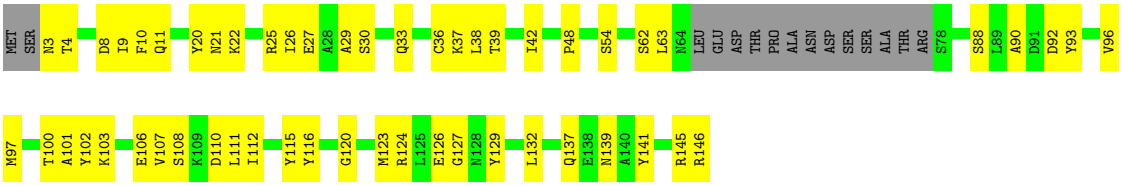
Chain G:





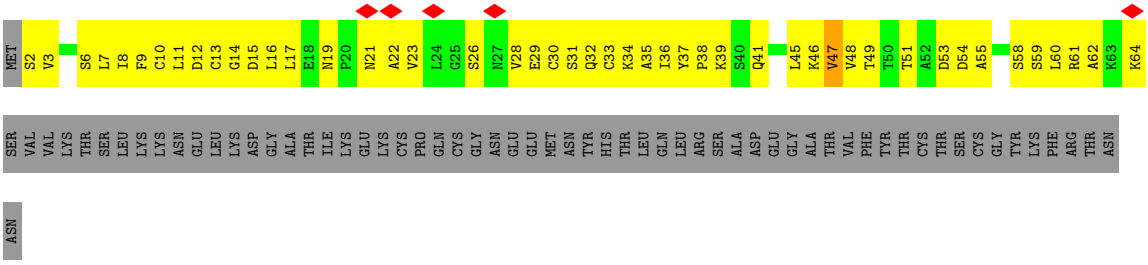
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:



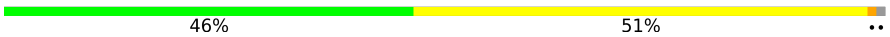
• Molecule 9: DNA-directed RNA polymerase I subunit RPA12

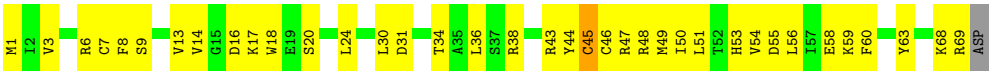
Chain I:



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

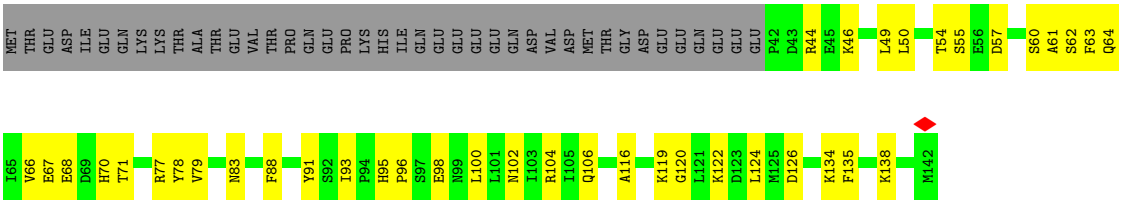
Chain J:





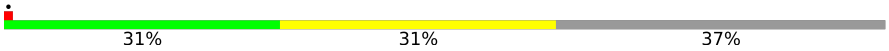
• Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2

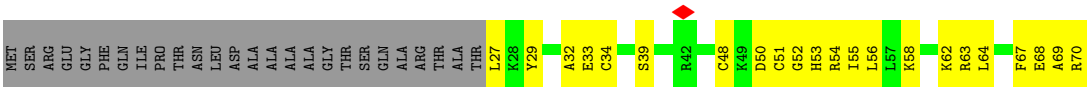
Chain K:



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

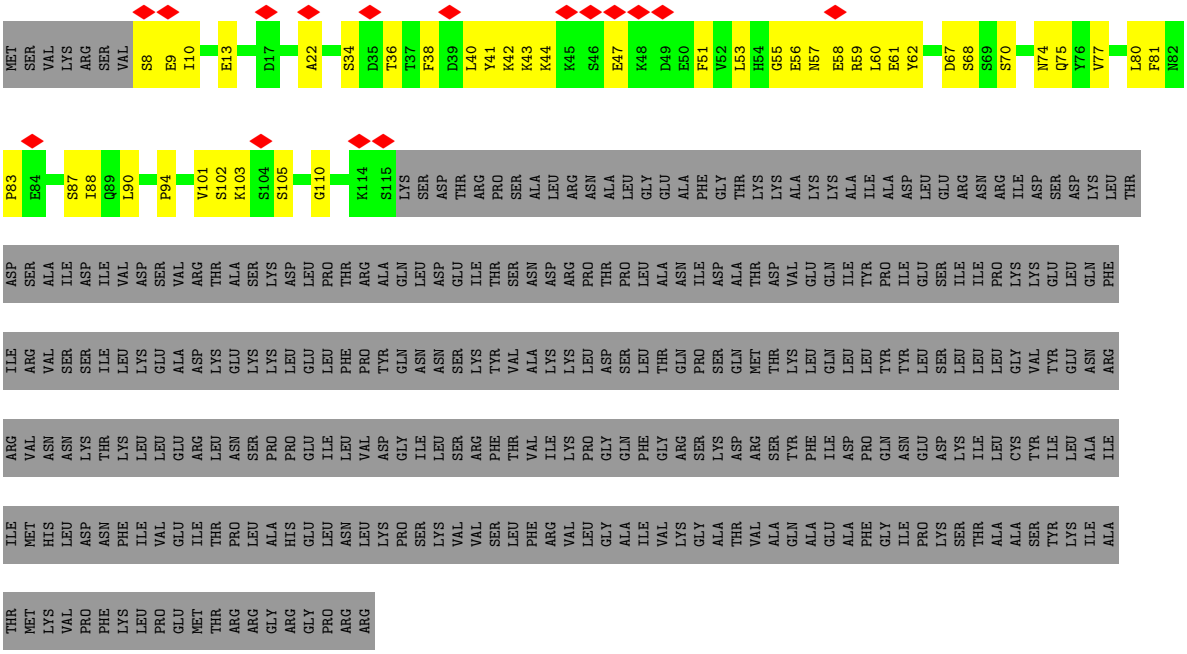
Chain L:





• Molecule 13: DNA-directed RNA polymerase I subunit RPA49

Chain M:



• Molecule 14: DNA-directed RNA polymerase I subunit RPA34

Chain N: 9% 31% 24% 45%

MET SER LYS LEU SER LYS ASP TYR VAL SER ASP SER ASP SER ASP ASP GLU GLU VAL ILE SER ASN GLU PHE S24 I25 P26 D27 G28 F29 K30 K31 C32 K33 H34 L35 F38 P39 L40 N41 GLY ASP ASN LYS LYS LYS ALA K49 Q50 Q51 Q52 V53 W54 L55 I56 K57 F58 P59 S60

D63 I64 S65 K66 L67 K68 S69 L70 P71 V72 ASP PHE GLU SER SER T78 T81 I82 D83 K84 H85 D86 Y87 K88 I89 MET ASP ASP THR ASP ILE GLU SER SER LEU THR GLN ASP ASN LEU SER N106 M107 V111 P112 S113 E114 S115 K116 E117 S118 L119 K120 S123 T124 A125 K126

D127 N128 A129 P130 L131 D134 K135 V136 F137 S138 V139 S140 E141 T142 D149 Y150 V153 R157 K158 D159 L166 D176 A177 E178 D179 F180 HIS VAL ALA GLU GLU VAL LYS GLU ASN LYS LYS GLU PRO LYS LYS ARG SER HIS HIS ASP ASP GLU GLU GLU SER SER GLU LYS

LYS LYS LYS LYS LYS GLU LYS ARG GLU LYS ARG GLU LYS LYS ASP LYS LYS ASP LYS LYS LYS LYS HIS ARG ASP

• Molecule 15: RNA polymerase I-specific transcription initiation factor RRN3

Chain O: 28% 37% 36% • 26%

MET MET ALA PHE GLU ASN THR SER LYS ARG PRO PRO GLN ASP PHE VAL ALA PRO ILE ASP GLN LYS LYS ARG LYS VAL GLN PHE SER ASP SER THR GLY LEU VAL THR LEU GLN PRO GLU GLU ILE LYS ASP GLU VAL PHE S48 A49 A50 M51 Y52 S53 R54 F55 V56 K57 S58 A59 L60

D61 D62 L63 D64 K65 N66 D67 S68 T69 Q70 I71 G72 I73 I74 A75 N76 Q77 V78 A79 L80 P81 S82 K83 N84 P85 E86 R87 I88 K91 N92 L93 L97 D98 I99 L100 S101 S102 N103 I104 N105 R106 I107 E108 S109 S110 R111 G112 T113 F114 L115 I116 Q117 S118 I119 I120 N121 K124

E127 L128 P129 P130 H131 S134 K141 I147 P148 K149 W150 W151 Q152 D153 V154 S155 M156 F162 T169 V170 C171 H172 H173 D174 M175 L176 K177 Y178 F179 L180 R181 M182 I183 P184 S185 S186 F189 T192 Y193 K196 F197 F198 P199 N200 K201 N202 D203 T204 R205 Y211

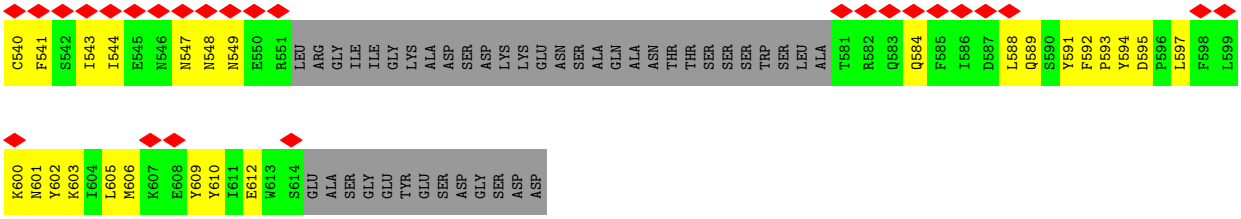
L216 K217 L218 R219 G220 Y221 C222 S223 E224 L225 G226 F227 Q228 I229 W230 S231 I234 E235 K236 I237 I238 S239 I240 D241 V242 Q245 N246 E247 L248 ASP GLU LEU ASP ASP ASP VAL ASP ASP ASP ASP VAL ASP LEU GLU LEU GLU GLU VAL ASP LEU GLU ASP ASP ASP ASP LEU ASP ASP ASP SER GLY

ASP ASP ASP ASP GLU ASN CYS GLY ASN SER ASN GLU GLU LEU ARG SER GLY ALA ALA ASP GLY SER GLN SER ASP SER GLU ASP MET ASP ILE ILE GLU GLY MET ASP GLY THR GLU GLU TYR ASN VAL GLU LEU THR GLN G324 I325 K326 E327 L328 K331 I335 V339 H342

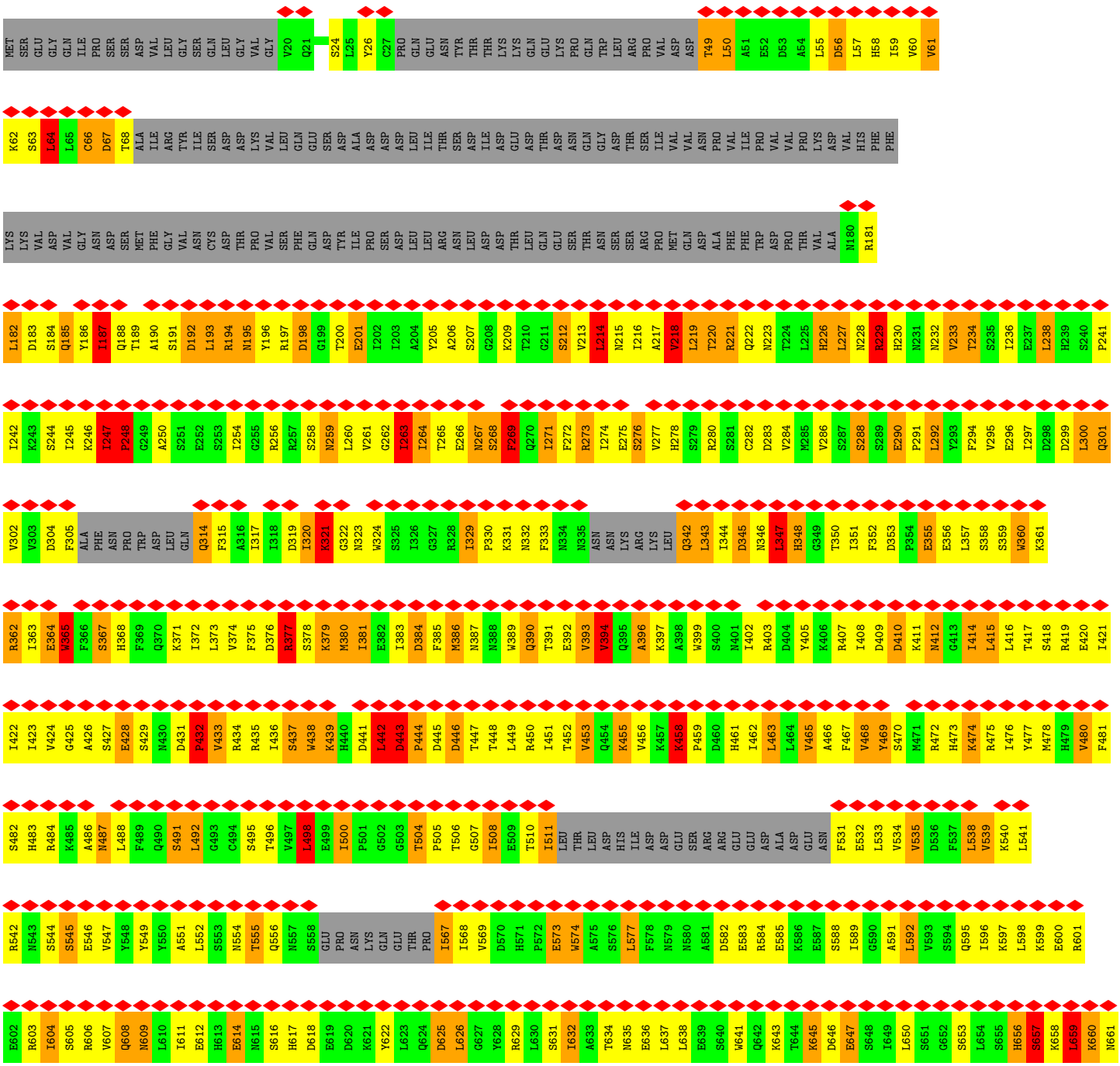
V347 T348 S351 L352 E353 S354 G355 E356 G357 V358 G359 V360 F361 N362 T363 L364 H371 Y376 Y377 T378 R379 S380 I381 Q382 Y383 I384 M385 F386 H387 V388 S389 Q390 Q391 Q392 L393 E394 L395 M396 D397 S398 F399 L403 I404 D405 I406 A409 V410 N411 E412 A413 A414 E415 K416 K417

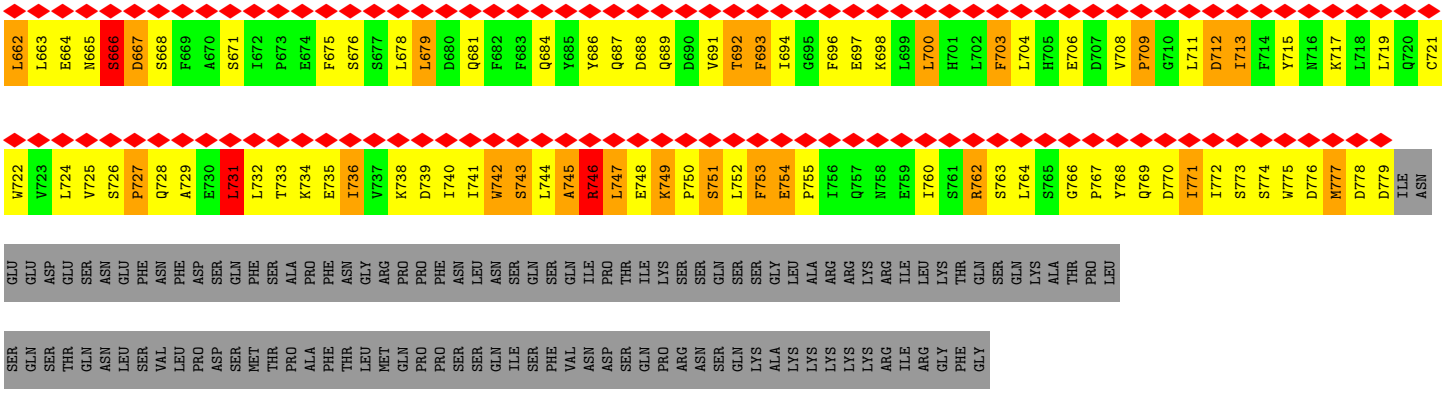
I418 Q422 Y423 L424 G425 S426 Y427 I428 A429 R430 A431 K432 K433 L434 S435 R436 T437 Q438 I439 I440 F441 V442 A443 S444 Y445 L446 T447 S448 W449 L450 N451 R452 Y453 V454 I455 E456 R457 E458 E459 E460 V461 D462 Q463 R464 G465 G466 M467 E468 R469 F470 K471 H472 F473 Y474 A475 A476 F477 Q478 A479

L480 C481 Y482 I483 F484 C485 F486 R487 H488 N489 I490 F491 R492 D493 T494 D495 G496 N497 W498 E499 C500 E501 L502 D503 K504 F505 F506 Q507 R508 M509 V510 I511 S512 K513 F514 N515 P516 L517 K518 F519 C520 N521 E522 N523 V524 M525 I526 M527 F528 A529 R530 I531 A532 Q533 Q534 E535 S536 V537 A538 Y539



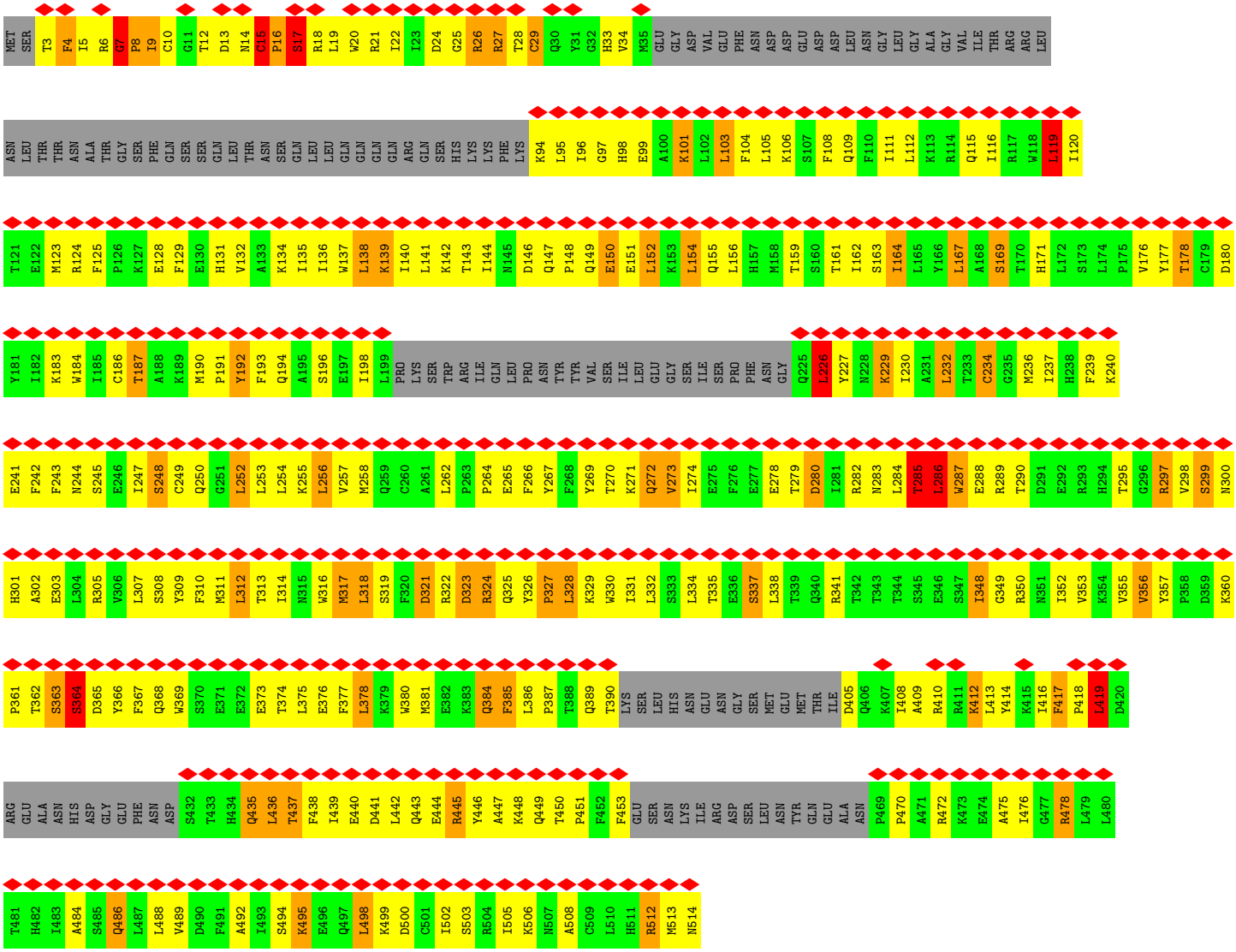
• Molecule 16: RNA polymerase I-specific transcription initiation factor RRN6





- Molecule 17: RNA polymerase I-specific transcription initiation factor RRN7

Chain Q:



- Molecule 18: RNA polymerase I-specific transcription initiation factor RRN11

Chain R: 43% 15% 30% 13% • 40%

M1 F2 E3 V4 P5 I6 T7 L8 T9 N10 R11 K12 F13 A14 Q15 R16 R17 K18 L19 K20 Y21 Q22 Y23 I24 N25 Y26 I27 S28 R29 R30 F31 D32 R33 I34 S35 K36 LYS SER THR THR THR ASP SER LEU PRO THR PRO GLU ASN SER ALA ALA GLU ASN ASN ASP GLU GLU GLU GLY

GLN ASN SER GLU ALA GLY THR TYR ARG ARG SER VAL LEU Q74 Q75 K76 K77 R78 R79 R80 E81 R82 H83 W84 R85 S86 V87 VAL GLY GLU GLU ILE TYR SER THR THR GLU SER GLU THR ASP SER GLN GLU GLU GLU THR GLU GLU GLY GLY GLU HIS ASP THR GLY ILE ASP LYS GLU ASP

SER ASP GLU GLU ARG LYS PHE TRP LYS LYS TYR GLU LYS PRO GLU LYS S137 F138 E139 I140 W141 R142 T143 V144 S145 S146 Q147 N148 K149 Q150 P151 I152 N153 K154 Q155 K156 M157 T158 Y159 H160 N161 F162 K163 K164 I165 E166 K167 I168 P169 L170 R171 K172 M173 E174 I175 P176 L177 L178 H179 C180

T181 K182 E183 N184 K185 L186 Y187 F188 Q189 S190 I191 S192 R193 G194 L195 E196 P197 L198 K199 T200 S201 T202 S203 E204 V205 R206 N207 Y208 R209 T210 R211 H212 I213 V214 T215 L216 T217 D218 L219 L222 N223 V224 S225 R226 H227 N228 W229 S230 L231 A232 Y233 K234 I235 F236 A237 T238 L239 I240 R241

I242 P243 G244 V245 Q246 I247 K248 S249 L250 W251 G252 I253 G254 V255 E256 I257 L258 D259 N260 L261 S262 N263 S264 S265 S266 G267 F270 L271 Q272 W273 M274 C275 Q276 I277 Y278 S279 S280 K281 S282 ARG PHE VAL GLN ASN ILE ASN TYR R291 S292 I293 V294 P295 P296 F297 Q298 T299 G300 S301 R302

T303 H304 T305 A306 K307 F308 A309 L313 W314 N319 C320 Q321 K322 S323 M324 GLU PRO SER SER ASN ILE ILE ASP LYS PRO PHE ASP THR GLU ASN ASP LEU LEU GLN GLU L345 I346 D347 K348 I349 S350 E351 W352 V353 L354 T355 P356 P357 F358 M359 E360 D361 A362 E363 V364 W365 F366 I367

Y368 H372 L373 L374 K375 A376 D377 THR LEU SER ARG GLN PHE VAL ASN ASP ASN LYS ASN ASN ASP LEU ILE GLY LEU ASP ARG ASP ILE LYS I401 N402 Q403 V404 I405 K406 H407 I408 H409 Y410 V411 R412 T413 F414 L415 K416 I417 C418 L419 D420 K421 G422 G423 F424 A425 V426 P427 S428 R429

L430 I431 E432 N433 Q434 L435 K436 S437 F438 E439 S440 ARG LEU TYR GLY GLU ALA GLN ASP ILE GLN GLU ARG ASP VAL ALA ASN VAL TYR ASP SER ILE ASP ASN SER SER VAL GLU ASN SER PHE GLY ASP VAL TYR GLU THR ASN ALA GLU PHE LEU ASP THR GLN LEU MET ASP LEU SER

PRO GLU ASP ASN GLY LEU ASP GLU MET HIS TYR SER ASP GLU ASP SER SER GLU

- Molecule 19: product RNA

Chain S: 20% 20% 60% 20%

C2 G3 C4 G5 A6

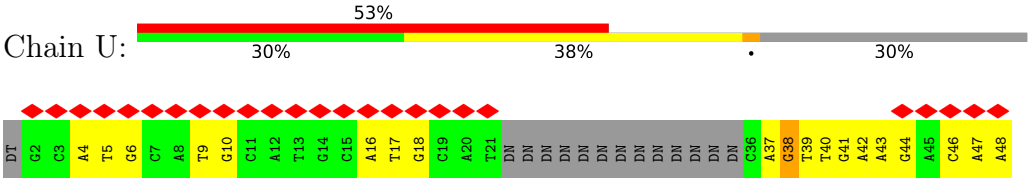
- Molecule 20: template DNA

Chain T: 64% 23% 64% 13%

T2 T3 G4 T5 C6 T7 T8 C9 A10 A11 C12 T13 G14 C15 T16 T17 T18 C19 G20 C21 G22 DN DN DN DN DN A30 T31 G32 C33 A34 T35 G36 C37 A38 T39 G40 C41 A42 T43 G44 C45 A46 T47 G48 C49 DA

- Molecule 21: non-template DNA

Chain U:


53%
30%
38%
30%
DT G2 C3 A4 T5 G6 C7 A8 T9 G10 C11 A12 T13 G14 C15 A16 T17 G18 C19 A20 T21 DN DN DN DN DN DN DN DN DN DN DN DN DN C36 A37 G38 T39 T40 G41 A42 A43 G44 A45 C46 A47 A48

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	345000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.407	Depositor
Minimum map value	-0.199	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.065	Depositor
Map size (Å)	372.9, 372.9, 372.9	wwPDB
Map dimensions	330, 330, 330	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.13, 1.13, 1.13	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SO4, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.48	0/11738	0.53	0/15851
2	B	0.52	0/9557	0.59	1/12918 (0.0%)
3	C	0.53	0/2475	0.54	0/3354
4	D	0.36	0/436	0.45	0/591
5	E	0.45	0/1771	0.49	0/2383
6	F	0.49	0/838	0.54	0/1129
7	G	0.42	0/1564	0.51	1/2127 (0.0%)
8	H	0.54	0/1070	0.55	0/1449
9	I	0.38	0/472	0.56	0/639
10	J	0.56	0/578	0.57	0/775
11	K	0.53	0/804	0.55	0/1083
12	L	0.52	0/354	0.57	0/468
13	M	0.41	0/872	0.51	0/1170
14	N	0.35	0/1049	0.50	0/1411
15	O	0.34	0/3897	0.44	0/5268
16	P	0.61	1/4857 (0.0%)	0.88	12/6572 (0.2%)
17	Q	0.65	2/3330 (0.1%)	0.91	9/4492 (0.2%)
18	R	0.52	0/2591	0.75	2/3483 (0.1%)
19	S	0.28	0/120	0.61	0/185
20	T	0.53	0/707	0.83	0/1076
21	U	0.67	1/543 (0.2%)	0.95	0/823
All	All	0.51	4/49623 (0.0%)	0.63	25/67247 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
16	P	0	18
17	Q	0	11

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Mol	Chain	#Chirality outliers	#Planarity outliers
18	R	0	10
All	All	0	39

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Q	323	ASP	C-N	19.90	1.79	1.34
17	Q	356	VAL	C-N	-7.09	1.17	1.34
21	U	38	DG	C1'-N9	-6.35	1.38	1.47
16	P	247	ILE	C-N	5.97	1.45	1.34

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	819	ASP	C-N-CD	-28.25	58.44	120.60
17	Q	323	ASP	O-C-N	21.78	157.54	122.70
17	Q	323	ASP	CA-C-N	-17.00	79.80	117.20
17	Q	7	GLY	C-N-CD	-15.29	86.97	120.60
17	Q	323	ASP	C-N-CA	-14.08	86.50	121.70
16	P	431	ASP	C-N-CD	-8.77	101.30	120.60
16	P	747	LEU	CA-CB-CG	8.59	135.06	115.30
17	Q	119	LEU	CA-CB-CG	7.56	132.69	115.30
16	P	443	ASP	CB-CG-OD1	6.52	124.17	118.30
17	Q	226	LEU	CA-CB-CG	-6.43	100.51	115.30
17	Q	419	LEU	CA-CB-CG	6.25	129.67	115.30
17	Q	338	LEU	CA-CB-CG	5.67	128.33	115.30
16	P	347	LEU	CA-CB-CG	5.64	128.28	115.30
18	R	198	LEU	CA-CB-CG	5.57	128.11	115.30
16	P	214	LEU	CA-CB-CG	5.47	127.88	115.30
18	R	178	LEU	CA-CB-CG	5.45	127.83	115.30
16	P	415	LEU	CA-CB-CG	5.35	127.60	115.30
16	P	431	ASP	C-N-CA	5.24	144.01	122.00
16	P	64	LEU	CA-CB-CG	5.23	127.33	115.30
16	P	498	LEU	CA-CB-CG	5.21	127.28	115.30
7	G	222	GLY	C-N-CA	-5.13	108.86	121.70
16	P	498	LEU	CB-CG-CD2	5.12	119.70	111.00
17	Q	286	LEU	CA-CB-CG	5.10	127.04	115.30
16	P	347	LEU	CB-CG-CD1	5.04	119.56	111.00
16	P	731	LEU	CA-CB-CG	5.03	126.87	115.30

There are no chirality outliers.

All (39) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	P	218	VAL	Peptide
16	P	234	THR	Peptide
16	P	247	ILE	Peptide
16	P	256	ARG	Peptide
16	P	258	SER	Peptide
16	P	331	LYS	Peptide
16	P	333	PHE	Peptide
16	P	386	MET	Peptide
16	P	396	ALA	Peptide
16	P	432	PRO	Peptide
16	P	442	LEU	Peptide
16	P	498	LEU	Peptide
16	P	661	ASN	Peptide
16	P	666	SER	Peptide
16	P	667	ASP	Peptide
16	P	688	ASP	Peptide
16	P	727	PRO	Peptide
16	P	767	PRO	Peptide
17	Q	15	CYS	Peptide
17	Q	17	SER	Peptide
17	Q	194	GLN	Peptide
17	Q	25	GLY	Peptide
17	Q	285	THR	Peptide
17	Q	287	TRP	Peptide
17	Q	29	CYS	Peptide
17	Q	298	VAL	Peptide
17	Q	385	PHE	Peptide
17	Q	4	PHE	Peptide
17	Q	417	PHE	Peptide
18	R	10	ASN	Peptide
18	R	149	LYS	Peptide
18	R	294	VAL	Peptide
18	R	295	PRO	Peptide
18	R	303	THR	Peptide
18	R	304	HIS	Peptide
18	R	352	TRP	Peptide
18	R	357	PRO	Peptide
18	R	424	PHE	Peptide
18	R	426	VAL	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11526	0	11612	862	0
2	B	9350	0	9231	839	0
3	C	2423	0	2412	122	0
4	D	431	0	428	16	0
5	E	1735	0	1764	70	0
6	F	823	0	841	52	0
7	G	1526	0	1540	73	0
8	H	1052	0	1021	42	0
9	I	466	0	466	55	0
10	J	569	0	585	45	0
11	K	793	0	790	41	0
12	L	352	0	375	22	0
13	M	856	0	855	46	0
14	N	1029	0	1061	57	0
15	O	3811	0	3802	243	0
16	P	4764	0	4711	528	0
17	Q	3254	0	3296	484	0
18	R	2535	0	2594	459	0
19	S	108	0	53	19	0
20	T	641	0	362	130	0
21	U	490	0	267	45	0
22	A	2	0	0	0	0
22	B	1	0	0	0	0
22	I	1	0	0	0	0
22	J	1	0	0	0	0
22	L	1	0	0	0	0
22	Q	1	0	0	0	0
23	A	1	0	0	0	0
24	B	5	0	0	2	0
All	All	48547	0	48066	3403	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 35.

All (3403) 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)
17:Q:20:TRP:CZ3	17:Q:22:ILE:CG2	1.76	1.66
2:B:116:ALA:H	18:R:282:SER:CB	1.05	1.65
17:Q:12:THR:HG21	17:Q:33:HIS:CE1	1.12	1.62
16:P:725:VAL:HG21	17:Q:446:TYR:CD1	1.14	1.60
17:Q:356:VAL:HG21	18:R:208:TYR:CD2	1.09	1.59
17:Q:356:VAL:CG2	18:R:208:TYR:CD2	1.85	1.58
17:Q:356:VAL:HG21	18:R:208:TYR:CE2	1.05	1.55
17:Q:12:THR:CG2	17:Q:33:HIS:HE1	1.10	1.53
17:Q:20:TRP:HZ3	17:Q:22:ILE:CG2	1.10	1.53
1:A:672:ASP:H	2:B:783:MET:CE	1.21	1.50
17:Q:356:VAL:HG11	18:R:208:TYR:CD1	1.43	1.50
17:Q:366:TYR:CD1	18:R:215:THR:HG23	1.43	1.49
2:B:815:ARG:NH2	2:B:821:ILE:CG1	1.72	1.48
1:A:474:LYS:HD3	2:B:1096:SER:CB	1.39	1.47
2:B:101:GLN:NE2	18:R:359:MET:HE1	1.17	1.47
2:B:1084:THR:O	2:B:1088:LEU:CG	1.64	1.45
2:B:116:ALA:H	18:R:282:SER:CA	1.28	1.44
1:A:628:PHE:HD2	2:B:784:ASP:CB	1.32	1.43
1:A:1018:TYR:CD1	20:T:16:DT:H5”	1.55	1.42
1:A:1014:SER:HA	20:T:17:DT:C6	1.54	1.41
2:B:117:VAL:CG2	18:R:276:GLN:HG3	1.49	1.39
1:A:1238:MET:CB	1:A:1521:THR:OG1	1.68	1.39
15:O:492:ARG:CG	15:O:496:GLY:HA2	1.50	1.38
1:A:1654:PHE:CZ	6:F:89:GLU:HA	1.58	1.38
17:Q:386:LEU:HA	18:R:241:ARG:NH2	1.10	1.38
17:Q:186:CYS:HB3	18:R:208:TYR:CE2	1.60	1.36
1:A:672:ASP:OD1	2:B:952:HIS:CD2	1.79	1.36
1:A:1018:TYR:CE1	20:T:16:DT:OP1	1.78	1.36
1:A:672:ASP:N	2:B:783:MET:CE	1.83	1.34
1:A:651:ALA:CB	2:B:1084:THR:HG23	1.54	1.34
17:Q:356:VAL:CG2	18:R:208:TYR:CE2	1.95	1.33
17:Q:360:LYS:NZ	18:R:211:ARG:HH22	1.24	1.33
1:A:651:ALA:HB3	2:B:1084:THR:CG2	1.56	1.32
19:S:5:G:N2	20:T:19:DC:O2	1.60	1.32
17:Q:323:ASP:C	17:Q:324:ARG:N	1.79	1.31
2:B:931:TRP:HB3	2:B:936:MET:CE	1.61	1.31
16:P:389:TRP:HZ2	18:R:146:SER:C	1.32	1.31
16:P:725:VAL:CG2	17:Q:446:TYR:CD1	2.11	1.31
1:A:1238:MET:HB2	1:A:1521:THR:OG1	1.12	1.30
17:Q:26:ARG:HB3	17:Q:34:VAL:CG1	1.61	1.29
17:Q:356:VAL:HG11	18:R:208:TYR:CE1	1.69	1.28
1:A:474:LYS:CD	2:B:1096:SER:CB	2.10	1.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:628:PHE:CD2	2:B:784:ASP:HB2	1.68	1.27
20:T:4:DG:N2	21:U:46:DC:O2	1.67	1.27
2:B:817:ARG:CB	21:U:17:DT:H5'	1.63	1.26
2:B:1096:SER:O	2:B:1097:ASP:CG	1.75	1.25
1:A:672:ASP:N	2:B:783:MET:HE3	1.40	1.25
2:B:101:GLN:NE2	18:R:359:MET:CE	1.99	1.25
2:B:116:ALA:N	18:R:282:SER:CB	1.79	1.24
1:A:474:LYS:CD	2:B:1096:SER:HB3	1.69	1.23
1:A:640:ASN:ND2	2:B:1090:ASP:OD2	1.71	1.23
15:O:200:ASN:CB	17:Q:14:ASN:HB2	1.69	1.23
1:A:1018:TYR:CE1	20:T:16:DT:H5"	1.73	1.23
2:B:113:VAL:CG1	20:T:39:DT:H4'	1.67	1.22
17:Q:366:TYR:CG	18:R:215:THR:HG23	1.73	1.22
2:B:894:LYS:HE3	17:Q:405:ASP:OD2	1.35	1.22
2:B:1079:LEU:CD2	2:B:1088:LEU:HB3	1.69	1.22
17:Q:12:THR:CG2	17:Q:33:HIS:CE1	1.95	1.22
2:B:115:SER:O	18:R:280:SER:HB2	1.38	1.22
2:B:115:SER:C	18:R:280:SER:HB2	1.50	1.21
15:O:200:ASN:CA	17:Q:14:ASN:HB2	1.69	1.21
1:A:1018:TYR:HE1	20:T:16:DT:OP1	0.88	1.20
16:P:443:ASP:HB3	18:R:3:GLU:N	1.57	1.20
16:P:725:VAL:HG21	17:Q:446:TYR:CG	1.77	1.20
2:B:1093:LEU:CD1	2:B:1098:TYR:HB2	1.70	1.20
17:Q:386:LEU:CA	18:R:241:ARG:NH2	2.03	1.19
17:Q:20:TRP:CZ3	17:Q:22:ILE:HG23	1.48	1.19
1:A:511:VAL:HG12	1:A:575:LYS:O	1.04	1.18
1:A:1238:MET:CA	1:A:1521:THR:OG1	1.92	1.18
2:B:117:VAL:HG21	18:R:276:GLN:CB	1.50	1.18
16:P:55:LEU:HB3	18:R:227:HIS:ND1	1.56	1.18
1:A:70:LYS:NZ	17:Q:27:ARG:HH12	1.39	1.18
17:Q:378:LEU:CD1	18:R:231:LEU:HD21	1.74	1.18
1:A:511:VAL:CG1	1:A:575:LYS:O	1.92	1.17
2:B:817:ARG:CB	21:U:17:DT:C5'	2.22	1.17
16:P:389:TRP:NE1	18:R:146:SER:HB2	1.58	1.17
17:Q:356:VAL:HG13	18:R:212:HIS:CE1	1.80	1.17
2:B:117:VAL:CG2	18:R:276:GLN:CG	2.23	1.17
2:B:116:ALA:HB2	18:R:282:SER:O	1.01	1.16
2:B:117:VAL:HG21	18:R:276:GLN:CG	1.75	1.16
2:B:1078:ALA:O	2:B:1082:HIS:N	1.75	1.16
1:A:646:GLU:HG3	1:A:650:LEU:HD12	1.21	1.16
1:A:547:ILE:CD1	17:Q:26:ARG:HH22	1.59	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:817:ARG:HB3	21:U:17:DT:H5'	1.20	1.15
16:P:389:TRP:CE2	18:R:146:SER:HB2	1.82	1.15
20:T:9:DC:N4	21:U:41:DG:H1	1.41	1.15
16:P:389:TRP:CZ2	18:R:146:SER:C	2.19	1.15
20:T:9:DC:N4	21:U:41:DG:N1	1.92	1.15
2:B:1079:LEU:HD23	2:B:1088:LEU:CB	1.77	1.15
2:B:817:ARG:HB3	21:U:17:DT:C5'	1.77	1.15
1:A:628:PHE:CD2	2:B:784:ASP:CB	2.24	1.14
17:Q:22:ILE:CD1	17:Q:24:ASP:OD1	1.96	1.13
2:B:116:ALA:N	18:R:282:SER:CA	2.01	1.13
1:A:476:VAL:HA	2:B:1095:SER:O	1.47	1.12
1:A:1238:MET:HB2	1:A:1521:THR:CB	1.79	1.12
2:B:1079:LEU:HG	2:B:1088:LEU:HD22	1.19	1.12
17:Q:386:LEU:CA	18:R:241:ARG:HH22	1.59	1.12
2:B:113:VAL:O	18:R:282:SER:HA	1.49	1.12
17:Q:366:TYR:CD2	18:R:215:THR:OG1	2.00	1.12
17:Q:360:LYS:NZ	18:R:211:ARG:NH2	1.96	1.12
2:B:931:TRP:HB3	2:B:936:MET:HE3	1.17	1.11
16:P:435:ARG:NH2	18:R:140:ILE:CD1	2.14	1.11
1:A:508:PRO:HA	1:A:577:VAL:O	1.46	1.11
2:B:116:ALA:N	18:R:282:SER:HB3	1.41	1.11
17:Q:20:TRP:CZ3	17:Q:22:ILE:HG22	1.58	1.11
2:B:116:ALA:CB	18:R:282:SER:O	1.97	1.11
17:Q:134:LYS:O	17:Q:138:LEU:HB2	1.50	1.11
16:P:358:SER:OG	18:R:196:GLU:OE1	1.67	1.10
17:Q:356:VAL:HB	18:R:208:TYR:HA	1.22	1.10
2:B:114:SER:HB3	18:R:282:SER:HA	1.34	1.10
15:O:200:ASN:CB	17:Q:14:ASN:CB	2.28	1.10
2:B:815:ARG:NH2	2:B:821:ILE:HG12	0.77	1.10
17:Q:356:VAL:CG1	18:R:208:TYR:CD1	2.33	1.10
17:Q:26:ARG:HB3	17:Q:34:VAL:HG13	1.12	1.09
17:Q:323:ASP:CA	17:Q:324:ARG:N	2.14	1.09
19:S:3:G:N2	20:T:21:DC:O2	1.84	1.09
1:A:597:LYS:HB2	2:B:1082:HIS:HA	1.33	1.09
16:P:420:GLU:OE2	18:R:3:GLU:OE2	1.68	1.09
16:P:477:TYR:CE2	18:R:2:PHE:CE2	2.40	1.09
1:A:543:LEU:CD2	1:A:578:TYR:OH	2.00	1.09
1:A:651:ALA:HB2	2:B:1084:THR:HG23	1.33	1.09
1:A:1014:SER:HB3	20:T:17:DT:C7	1.83	1.08
17:Q:355:VAL:CG1	18:R:212:HIS:HA	1.82	1.08
15:O:200:ASN:HA	17:Q:14:ASN:HB2	1.24	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1240:LEU:HD11	1:A:1521:THR:CG2	1.84	1.08
15:O:241:ASP:OD1	15:O:380:SER:HB2	1.50	1.08
17:Q:9:ILE:HG13	17:Q:10:CYS:H	1.06	1.08
17:Q:258:MET:HE2	17:Q:438:PHE:HE2	1.16	1.08
17:Q:17:SER:O	17:Q:29:CYS:HB2	1.55	1.07
2:B:1093:LEU:HD12	2:B:1098:TYR:HB2	1.36	1.06
1:A:627:ASP:HA	2:B:784:ASP:OD1	1.54	1.06
1:A:1654:PHE:CE2	6:F:89:GLU:HA	1.90	1.06
15:O:491:PHE:HE2	15:O:502:LEU:HD11	1.19	1.06
16:P:477:TYR:HE2	18:R:2:PHE:CE2	1.72	1.06
2:B:113:VAL:HG11	20:T:39:DT:H4'	1.06	1.06
2:B:115:SER:O	18:R:280:SER:CB	2.02	1.06
17:Q:366:TYR:CD1	18:R:215:THR:CG2	2.38	1.06
2:B:320:LEU:HD23	2:B:325:GLN:HB3	1.31	1.06
16:P:189:THR:HG22	16:P:247:ILE:HG23	1.34	1.06
1:A:651:ALA:HB3	2:B:1084:THR:HG21	1.30	1.05
2:B:1084:THR:HB	2:B:1087:LEU:CD2	1.85	1.05
16:P:435:ARG:NH2	18:R:140:ILE:HD13	1.68	1.05
2:B:815:ARG:HH12	2:B:899:GLN:HG3	1.21	1.05
17:Q:366:TYR:CG	18:R:215:THR:CG2	2.38	1.05
1:A:628:PHE:HD2	2:B:784:ASP:HB2	0.91	1.05
16:P:55:LEU:HB3	18:R:227:HIS:CE1	1.90	1.05
16:P:389:TRP:CZ2	18:R:147:GLN:N	2.24	1.05
17:Q:15:CYS:HB3	17:Q:17:SER:N	1.70	1.05
1:A:628:PHE:HB2	2:B:785:ASP:H	1.12	1.05
18:R:350:SER:O	18:R:354:LEU:HB2	1.56	1.05
1:A:543:LEU:HD21	1:A:578:TYR:OH	1.57	1.04
15:O:491:PHE:HB3	15:O:498:TRP:HZ3	1.20	1.04
17:Q:5:ILE:O	17:Q:19:LEU:O	1.74	1.04
2:B:113:VAL:HG11	20:T:39:DT:C4'	1.87	1.04
15:O:492:ARG:HG2	15:O:496:GLY:CA	1.86	1.04
17:Q:186:CYS:CB	18:R:208:TYR:CE2	2.41	1.04
2:B:116:ALA:HB2	18:R:282:SER:C	1.76	1.04
16:P:389:TRP:HZ2	18:R:146:SER:CA	1.68	1.04
17:Q:186:CYS:HB3	18:R:208:TYR:CZ	1.93	1.04
17:Q:323:ASP:C	17:Q:324:ARG:CA	2.24	1.04
2:B:117:VAL:HG22	18:R:276:GLN:HG3	1.08	1.04
15:O:492:ARG:CG	15:O:496:GLY:CA	2.34	1.04
19:S:5:G:N2	20:T:19:DC:C2	2.26	1.03
2:B:1063:ARG:HG3	20:T:22:DG:OP2	1.57	1.03
15:O:492:ARG:HG3	15:O:496:GLY:O	1.57	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:356:VAL:CB	18:R:208:TYR:CD2	2.39	1.03
17:Q:386:LEU:HD12	18:R:241:ARG:NH2	1.73	1.03
17:Q:356:VAL:HG11	18:R:208:TYR:CG	1.94	1.02
2:B:1079:LEU:HG	2:B:1088:LEU:CD2	1.84	1.02
2:B:1096:SER:O	2:B:1097:ASP:CB	2.06	1.02
1:A:651:ALA:CB	2:B:1084:THR:CG2	2.25	1.02
1:A:672:ASP:N	2:B:783:MET:HE1	1.74	1.02
1:A:953:GLU:OE2	2:B:519:LYS:NZ	1.93	1.02
17:Q:357:TYR:CD2	17:Q:489:VAL:HG22	1.93	1.02
2:B:321:GLN:N	2:B:325:GLN:OE1	1.92	1.01
1:A:1014:SER:CA	20:T:17:DT:C6	2.43	1.01
2:B:114:SER:HB3	18:R:282:SER:CA	1.89	1.01
2:B:1084:THR:C	2:B:1088:LEU:HG	1.80	1.01
16:P:435:ARG:HH21	18:R:140:ILE:CD1	1.69	1.01
16:P:443:ASP:HB2	18:R:2:PHE:HB3	1.42	1.01
16:P:389:TRP:CZ2	18:R:146:SER:CB	2.44	1.01
1:A:547:ILE:HD12	17:Q:26:ARG:HH22	1.20	1.00
2:B:1068:GLY:O	2:B:1069:ILE:HD13	1.59	1.00
2:B:116:ALA:N	18:R:282:SER:N	2.07	1.00
2:B:785:ASP:OD2	2:B:926:VAL:HB	1.62	1.00
2:B:817:ARG:HB2	21:U:17:DT:C5'	1.90	1.00
2:B:1084:THR:OG1	2:B:1088:LEU:HD21	1.61	1.00
16:P:443:ASP:CB	18:R:3:GLU:N	2.18	1.00
16:P:625:ASP:O	16:P:629:ARG:HB2	1.61	1.00
17:Q:378:LEU:HD11	18:R:231:LEU:HD21	1.02	1.00
2:B:115:SER:C	18:R:280:SER:CB	2.27	1.00
17:Q:9:ILE:HG13	17:Q:10:CYS:N	1.77	1.00
20:T:11:DA:C2	20:T:12:DC:C2	2.50	1.00
1:A:672:ASP:CB	2:B:783:MET:CE	2.40	1.00
17:Q:22:ILE:CD1	17:Q:26:ARG:NE	2.25	1.00
1:A:1506:ARG:O	1:A:1522:GLU:HG3	1.61	0.99
1:A:672:ASP:HB2	2:B:783:MET:HE1	1.41	0.99
17:Q:12:THR:CB	17:Q:33:HIS:CE1	2.44	0.99
2:B:1079:LEU:HD23	2:B:1088:LEU:HB3	1.00	0.99
17:Q:9:ILE:HB	17:Q:16:PRO:HB2	1.43	0.99
16:P:186:TYR:HB3	18:R:198:LEU:CD2	1.93	0.98
17:Q:360:LYS:HZ3	18:R:211:ARG:NH2	1.56	0.98
1:A:511:VAL:O	1:A:574:ASN:ND2	1.96	0.98
1:A:672:ASP:HB2	2:B:783:MET:CE	1.94	0.97
17:Q:356:VAL:CB	18:R:208:TYR:CG	2.46	0.97
17:Q:366:TYR:CE2	18:R:215:THR:OG1	2.11	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:9:DC:H2"	20:T:10:DA:H8	1.28	0.97
1:A:511:VAL:HG13	1:A:574:ASN:HB2	1.47	0.97
1:A:1654:PHE:HB2	6:F:134:ILE:HG23	1.47	0.97
1:A:1021:ARG:NH2	20:T:16:DT:OP1	1.98	0.96
15:O:491:PHE:HE2	15:O:502:LEU:CD1	1.77	0.96
1:A:1641:ILE:H	1:A:1641:ILE:HD12	1.29	0.96
1:A:463:LYS:NZ	20:T:16:DT:H6	1.63	0.96
17:Q:15:CYS:SG	17:Q:17:SER:HB2	2.05	0.96
1:A:642:ASN:HB3	2:B:1086:PHE:CD2	2.00	0.96
1:A:671:GLN:HB2	2:B:783:MET:HE2	1.47	0.96
1:A:1018:TYR:CE1	20:T:16:DT:C5'	2.48	0.96
2:B:114:SER:CB	18:R:282:SER:CA	2.44	0.96
17:Q:356:VAL:HB	18:R:208:TYR:CA	1.94	0.96
11:K:104:ARG:HH21	11:K:106:GLN:HE21	1.13	0.96
1:A:628:PHE:HB3	2:B:785:ASP:CG	1.86	0.95
2:B:894:LYS:HZ2	17:Q:405:ASP:HB3	1.31	0.95
2:B:817:ARG:HB2	21:U:17:DT:H5"	1.46	0.95
2:B:929:ARG:HH12	11:K:96:PRO:HB2	1.30	0.95
16:P:477:TYR:CE2	18:R:2:PHE:HE2	1.83	0.95
1:A:712:ILE:H	11:K:106:GLN:HE22	1.15	0.95
2:B:101:GLN:HE21	18:R:359:MET:CE	1.70	0.95
17:Q:22:ILE:HD11	17:Q:26:ARG:NE	1.81	0.95
1:A:1014:SER:HB3	20:T:17:DT:C5	2.02	0.94
16:P:389:TRP:CZ2	18:R:146:SER:HB2	2.01	0.94
17:Q:366:TYR:CE1	18:R:215:THR:HA	2.03	0.94
1:A:475:ARG:O	2:B:1095:SER:O	1.86	0.94
1:A:672:ASP:CB	2:B:783:MET:HE1	1.96	0.94
2:B:320:LEU:HD21	2:B:325:GLN:C	1.87	0.94
17:Q:381:MET:HG3	18:R:238:THR:HG21	1.48	0.94
1:A:1240:LEU:CD1	1:A:1521:THR:HG23	1.98	0.94
2:B:320:LEU:CD2	2:B:325:GLN:HB3	1.98	0.94
2:B:1104:CYS:CB	2:B:1107:CYS:SG	2.55	0.93
16:P:725:VAL:CG2	17:Q:446:TYR:CG	2.42	0.93
17:Q:356:VAL:CB	18:R:208:TYR:HA	1.99	0.93
2:B:1058:GLN:HG2	2:B:1096:SER:O	1.67	0.93
17:Q:9:ILE:CG1	17:Q:10:CYS:H	1.79	0.93
1:A:1018:TYR:CD1	20:T:16:DT:C5'	2.51	0.93
2:B:1104:CYS:HB3	2:B:1107:CYS:SG	2.08	0.93
17:Q:386:LEU:HA	18:R:241:ARG:CZ	1.98	0.93
2:B:213:HIS:CD2	2:B:643:PHE:HZ	1.87	0.93
1:A:618:TYR:CE1	2:B:783:MET:HB3	2.03	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:386:LEU:CB	18:R:241:ARG:HH22	1.80	0.92
16:P:389:TRP:CZ2	18:R:146:SER:CA	2.52	0.92
1:A:1654:PHE:CZ	6:F:89:GLU:CA	2.52	0.92
17:Q:15:CYS:CB	17:Q:16:PRO:HA	1.99	0.92
18:R:168:ILE:HG23	18:R:169:PRO:HD3	1.52	0.92
15:O:491:PHE:HB3	15:O:498:TRP:CZ3	2.04	0.92
17:Q:155:GLN:HA	20:T:49:DC:H2"	1.53	0.91
1:A:70:LYS:NZ	17:Q:27:ARG:NH1	2.18	0.91
2:B:320:LEU:CD2	2:B:325:GLN:CB	2.48	0.91
17:Q:356:VAL:HB	18:R:208:TYR:CG	2.05	0.91
17:Q:356:VAL:CG1	18:R:208:TYR:CG	2.52	0.91
17:Q:357:TYR:CD2	17:Q:489:VAL:HA	2.05	0.91
17:Q:378:LEU:HD11	18:R:231:LEU:CD2	1.97	0.91
17:Q:186:CYS:HB3	18:R:208:TYR:HE2	1.29	0.91
2:B:117:VAL:CG1	18:R:277:ILE:HA	2.01	0.91
16:P:389:TRP:HE1	18:R:146:SER:HB2	1.29	0.91
17:Q:15:CYS:HB3	17:Q:16:PRO:CA	2.00	0.91
1:A:672:ASP:OD1	2:B:952:HIS:HD2	1.54	0.91
2:B:115:SER:O	18:R:280:SER:CA	2.17	0.91
2:B:894:LYS:NZ	17:Q:405:ASP:CB	2.34	0.91
16:P:662:LEU:HB3	16:P:665:ASN:HB2	1.52	0.91
1:A:1240:LEU:HD11	1:A:1521:THR:HG21	1.51	0.91
17:Q:22:ILE:HD12	17:Q:24:ASP:OD1	1.68	0.91
17:Q:353:VAL:HG12	17:Q:489:VAL:CG1	2.00	0.91
2:B:101:GLN:HE22	18:R:359:MET:CE	1.80	0.90
17:Q:26:ARG:CB	17:Q:34:VAL:HG13	1.99	0.90
1:A:637:PHE:H	2:B:1091:ARG:HH22	1.14	0.90
2:B:1084:THR:HB	2:B:1087:LEU:HD22	1.49	0.90
1:A:628:PHE:HD2	2:B:784:ASP:HB3	1.35	0.90
2:B:114:SER:HB3	18:R:282:SER:C	1.91	0.90
16:P:477:TYR:CE2	18:R:2:PHE:CZ	2.58	0.90
2:B:950:ASN:OD1	2:B:952:HIS:HD2	1.54	0.90
17:Q:19:LEU:HD11	17:Q:27:ARG:HB3	1.54	0.90
17:Q:262:LEU:O	17:Q:446:TYR:OH	1.90	0.90
16:P:532:GLU:HA	16:P:554:ASN:HD22	1.37	0.89
16:P:358:SER:HB3	16:P:377:ARG:HD3	1.55	0.89
20:T:11:DA:C6	20:T:12:DC:C4	2.60	0.89
1:A:354:SER:OG	1:A:355:PHE:CD1	2.25	0.89
17:Q:350:ARG:CD	17:Q:486:GLN:HG2	2.03	0.89
2:B:1084:THR:HB	2:B:1087:LEU:HD23	1.53	0.89
17:Q:20:TRP:CZ3	17:Q:22:ILE:HG21	2.08	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:350:ARG:NH1	17:Q:486:GLN:OE1	2.05	0.89
2:B:950:ASN:OD1	2:B:952:HIS:CD2	2.26	0.89
15:O:527:MET:SD	15:O:530:ARG:NH2	2.46	0.89
16:P:55:LEU:CB	18:R:227:HIS:CE1	2.55	0.89
17:Q:313:THR:O	17:Q:317:MET:HB2	1.71	0.89
2:B:776:ILE:C	2:B:951:PRO:HD3	1.93	0.89
1:A:1014:SER:CB	20:T:17:DT:C7	2.50	0.88
17:Q:3:THR:HG22	17:Q:20:TRP:HB2	1.53	0.88
17:Q:258:MET:CE	17:Q:438:PHE:HE2	1.85	0.88
2:B:284:SER:HB2	9:I:14:GLY:HA3	1.55	0.88
20:T:9:DC:H2"	20:T:10:DA:C8	2.08	0.88
20:T:9:DC:N4	21:U:41:DG:C6	2.40	0.88
2:B:711:GLN:HG2	2:B:713:PRO:HD2	1.55	0.88
2:B:1084:THR:O	2:B:1088:LEU:HG	0.71	0.88
1:A:1637:PRO:CB	1:A:1647:ASN:HD21	1.87	0.88
2:B:114:SER:CB	18:R:282:SER:C	2.42	0.88
1:A:646:GLU:CG	1:A:650:LEU:HD12	2.02	0.88
15:O:491:PHE:CE2	15:O:502:LEU:HD11	2.08	0.88
1:A:70:LYS:HZ3	17:Q:27:ARG:HH12	0.88	0.87
16:P:186:TYR:HB3	18:R:198:LEU:HD23	1.54	0.87
1:A:1486:VAL:HG23	9:I:51:THR:HG22	1.57	0.87
1:A:1654:PHE:CE2	6:F:89:GLU:CA	2.55	0.87
17:Q:20:TRP:CH2	17:Q:22:ILE:CG2	2.56	0.87
1:A:1506:ARG:O	1:A:1522:GLU:CG	2.23	0.87
2:B:776:ILE:O	2:B:951:PRO:HD3	1.75	0.87
15:O:492:ARG:HG2	15:O:496:GLY:HA2	0.89	0.87
17:Q:360:LYS:HZ1	18:R:211:ARG:NH2	1.69	0.87
1:A:672:ASP:OD1	2:B:952:HIS:NE2	2.07	0.87
17:Q:29:CYS:SG	17:Q:33:HIS:HB2	2.15	0.87
2:B:320:LEU:HD13	2:B:326:VAL:HG22	1.57	0.86
16:P:196:TYR:O	16:P:197:ARG:NH1	2.07	0.86
17:Q:12:THR:CB	17:Q:33:HIS:ND1	2.37	0.86
1:A:672:ASP:CA	2:B:783:MET:HE1	2.04	0.86
1:A:707:THR:HG22	1:A:709:ARG:H	1.40	0.86
1:A:618:TYR:CE1	2:B:783:MET:CB	2.58	0.86
1:A:1014:SER:CB	20:T:17:DT:C5	2.57	0.86
1:A:508:PRO:CA	1:A:577:VAL:O	2.23	0.86
2:B:1096:SER:O	2:B:1097:ASP:OD1	1.91	0.86
13:M:38:PHE:HB3	13:M:53:LEU:HD11	1.55	0.86
2:B:816:ASN:HB3	21:U:18:DG:OP1	1.76	0.86
1:A:637:PHE:N	2:B:1091:ARG:HH22	1.72	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:CYS:HB3	1:A:75:HIS:NE2	1.91	0.85
17:Q:258:MET:HE2	17:Q:438:PHE:CE2	2.09	0.85
16:P:55:LEU:CB	18:R:227:HIS:ND1	2.38	0.85
1:A:672:ASP:CA	2:B:783:MET:CE	2.55	0.85
2:B:320:LEU:HD23	2:B:325:GLN:CB	2.05	0.85
19:S:5:G:N1	20:T:19:DC:N3	2.23	0.85
1:A:700:ILE:O	1:A:706:HIS:ND1	2.09	0.85
16:P:725:VAL:CG2	17:Q:446:TYR:CB	2.54	0.85
1:A:628:PHE:HB2	2:B:785:ASP:N	1.90	0.85
16:P:725:VAL:CG2	17:Q:446:TYR:HB3	2.07	0.85
17:Q:350:ARG:HD3	17:Q:486:GLN:HG2	1.56	0.85
17:Q:385:PHE:O	18:R:241:ARG:CZ	2.25	0.85
16:P:725:VAL:HG21	17:Q:446:TYR:HD1	1.02	0.84
2:B:894:LYS:NZ	17:Q:405:ASP:HB3	1.91	0.84
1:A:70:LYS:HZ3	17:Q:27:ARG:NH1	1.72	0.84
2:B:894:LYS:CE	17:Q:405:ASP:OD2	2.21	0.84
16:P:389:TRP:CE2	18:R:146:SER:CB	2.60	0.84
15:O:200:ASN:CA	17:Q:14:ASN:CB	2.54	0.84
15:O:488:HIS:HB2	15:O:531:ILE:HG21	1.59	0.84
1:A:1637:PRO:CG	1:A:1647:ASN:HD21	1.90	0.84
17:Q:353:VAL:HG12	17:Q:489:VAL:HG13	1.59	0.84
17:Q:381:MET:HG3	18:R:238:THR:CG2	2.07	0.84
1:A:597:LYS:HB2	2:B:1082:HIS:CA	2.07	0.84
16:P:446:ASP:HA	18:R:200:THR:HG22	1.60	0.84
17:Q:15:CYS:HB3	17:Q:16:PRO:C	1.98	0.84
1:A:463:LYS:NZ	20:T:16:DT:C6	2.41	0.84
1:A:1238:MET:O	1:A:1521:THR:OG1	1.96	0.83
1:A:1013:THR:HB	20:T:17:DT:H3	1.42	0.83
1:A:1014:SER:O	20:T:17:DT:H5'	1.78	0.83
2:B:213:HIS:CD2	2:B:643:PHE:CZ	2.67	0.83
15:O:491:PHE:HD2	15:O:498:TRP:HE3	1.25	0.83
16:P:55:LEU:HG	18:R:227:HIS:CB	2.07	0.83
16:P:443:ASP:HB2	18:R:2:PHE:CB	2.08	0.83
20:T:11:DA:C6	20:T:12:DC:N4	2.46	0.83
2:B:1063:ARG:CG	20:T:22:DG:OP2	2.27	0.83
1:A:1637:PRO:HG3	1:A:1647:ASN:ND2	1.93	0.83
2:B:931:TRP:CB	2:B:936:MET:CE	2.53	0.83
16:P:725:VAL:HG23	17:Q:446:TYR:HB3	1.58	0.82
18:R:373:LEU:HD12	18:R:411:VAL:HG21	1.61	0.82
13:M:38:PHE:HB2	14:N:119:LEU:HB2	1.58	0.82
2:B:518:ARG:HB3	2:B:540:GLY:HA3	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:200:ASN:HA	17:Q:14:ASN:CB	2.08	0.82
1:A:486:PRO:HG2	2:B:781:TYR:O	1.78	0.82
1:A:547:ILE:HD12	17:Q:26:ARG:NH2	1.92	0.82
2:B:117:VAL:HG12	18:R:277:ILE:HA	1.59	0.82
17:Q:15:CYS:HB3	17:Q:16:PRO:HA	1.60	0.82
2:B:116:ALA:H	18:R:282:SER:HB3	1.07	0.82
17:Q:20:TRP:CE3	17:Q:22:ILE:HG23	2.15	0.82
2:B:815:ARG:HH12	2:B:899:GLN:CG	1.92	0.82
17:Q:26:ARG:CB	17:Q:34:VAL:CG1	2.53	0.82
1:A:628:PHE:CD2	2:B:784:ASP:HB3	2.09	0.82
17:Q:350:ARG:NE	17:Q:486:GLN:HG2	1.93	0.82
18:R:171:ARG:O	18:R:174:GLU:N	2.11	0.82
1:A:1246:VAL:HG13	1:A:1250:GLN:HB3	1.61	0.82
2:B:894:LYS:HZ1	17:Q:405:ASP:CG	1.81	0.82
1:A:1014:SER:HA	20:T:17:DT:N1	1.94	0.81
2:B:818:GLY:O	2:B:820:PRO:CD	2.28	0.81
17:Q:20:TRP:HZ3	17:Q:22:ILE:HG22	0.65	0.81
16:P:188:GLN:HG2	16:P:360:TRP:HB3	1.61	0.81
16:P:662:LEU:HB2	16:P:665:ASN:HD22	1.45	0.81
17:Q:357:TYR:CG	17:Q:489:VAL:HG22	2.15	0.81
1:A:550:SER:H	1:A:553:GLN:HE22	1.28	0.81
1:A:1637:PRO:HG3	1:A:1647:ASN:HD21	1.42	0.81
16:P:346:ASN:OD1	16:P:347:LEU:N	2.12	0.81
1:A:477:ASN:H	2:B:1095:SER:CB	1.91	0.81
1:A:628:PHE:HB2	2:B:784:ASP:HB3	1.61	0.81
1:A:1654:PHE:CD2	6:F:89:GLU:HG2	2.15	0.81
2:B:817:ARG:CB	21:U:17:DT:H5”	2.04	0.81
15:O:491:PHE:HD2	15:O:498:TRP:CE3	1.98	0.81
17:Q:350:ARG:CZ	17:Q:486:GLN:OE1	2.29	0.81
1:A:597:LYS:O	2:B:1082:HIS:NE2	2.13	0.81
1:A:1031:HIS:N	1:A:1039:ARG:O	2.11	0.81
2:B:1096:SER:C	2:B:1097:ASP:OD1	2.19	0.81
16:P:355:GLU:HB3	18:R:24:ILE:HD12	1.62	0.81
1:A:1014:SER:HA	20:T:17:DT:C5	2.13	0.81
1:A:642:ASN:ND2	2:B:1086:PHE:HE2	1.77	0.80
16:P:487:ASN:HB3	18:R:138:PHE:CZ	2.13	0.80
16:P:245:ILE:HD12	16:P:269:PHE:HD2	1.43	0.80
1:A:597:LYS:CB	2:B:1082:HIS:HA	2.12	0.80
1:A:1240:LEU:CD1	1:A:1521:THR:CG2	2.57	0.80
16:P:435:ARG:HH21	18:R:140:ILE:HD11	1.43	0.80
18:R:250:LEU:HD21	18:R:307:LYS:HG2	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:LEU:HD12	1:A:82:PRO:HD2	1.63	0.80
1:A:600:MET:HB3	2:B:1082:HIS:HD2	1.44	0.80
1:A:1654:PHE:CD2	6:F:89:GLU:CG	2.65	0.80
1:A:1014:SER:CA	20:T:17:DT:C5	2.65	0.80
12:L:48:CYS:HB3	12:L:52:GLY:H	1.45	0.80
19:S:4:C:O2	20:T:20:DG:N2	2.14	0.80
1:A:102:CYS:SG	1:A:105:CYS:N	2.54	0.80
1:A:587:VAL:HG12	1:A:637:PHE:HD1	1.47	0.80
1:A:600:MET:HB3	2:B:1082:HIS:CD2	2.17	0.80
1:A:638:PRO:CG	2:B:1087:LEU:CD1	2.60	0.80
2:B:1093:LEU:HD11	2:B:1098:TYR:HB2	1.64	0.80
15:O:492:ARG:HG3	15:O:496:GLY:C	2.03	0.80
1:A:527:PRO:HD3	1:A:554:ARG:HH12	1.46	0.79
1:A:547:ILE:HD11	17:Q:26:ARG:HH22	1.46	0.79
2:B:1049:THR:OG1	17:Q:24:ASP:HB2	1.82	0.79
6:F:99:LEU:HD23	7:G:112:PRO:HD3	1.64	0.79
18:R:11:ARG:NH1	21:U:4:DA:P	2.51	0.79
1:A:646:GLU:HG3	1:A:650:LEU:CD1	2.08	0.79
2:B:1079:LEU:CG	2:B:1088:LEU:HB3	2.07	0.79
20:T:11:DA:N1	20:T:12:DC:N3	2.31	0.79
1:A:1014:SER:HB3	20:T:17:DT:H73	1.64	0.79
2:B:954:PHE:O	2:B:956:SER:N	2.15	0.79
2:B:1075:GLU:O	2:B:1079:LEU:HD13	1.81	0.79
18:R:78:ARG:NH2	20:T:43:DT:H5"	1.97	0.79
21:U:38:DG:C2	21:U:39:DT:O2	2.35	0.79
16:P:375:PHE:HD2	16:P:402:ILE:HD13	1.48	0.79
16:P:389:TRP:CH2	18:R:147:GLN:N	2.50	0.79
16:P:577:LEU:O	17:Q:506:LYS:NZ	2.15	0.79
18:R:26:TYR:HB3	18:R:169:PRO:HB3	1.63	0.79
1:A:354:SER:OG	1:A:355:PHE:HD1	1.63	0.79
1:A:1322:ILE:HG21	1:A:1457:ILE:HD11	1.62	0.79
16:P:477:TYR:HE2	18:R:2:PHE:CZ	1.98	0.79
1:A:1238:MET:C	1:A:1521:THR:OG1	2.22	0.79
15:O:491:PHE:CE2	15:O:502:LEU:CD1	2.66	0.79
2:B:492:ASN:ND2	2:B:722:GLY:O	2.16	0.78
2:B:816:ASN:CB	21:U:18:DG:OP1	2.31	0.78
17:Q:192:TYR:HD1	17:Q:193:PHE:H	1.29	0.78
1:A:1038:ILE:HB	1:A:1047:GLN:H	1.48	0.78
1:A:1303:SER:HA	1:A:1308:VAL:H	1.48	0.78
15:O:434:LEU:HD22	15:O:439:ILE:HD11	1.65	0.78
17:Q:366:TYR:CZ	18:R:215:THR:HA	2.17	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:VAL:HG12	1:A:575:LYS:C	2.02	0.78
16:P:484:ARG:HB2	16:P:488:LEU:HB3	1.64	0.78
20:T:8:DT:H2'	20:T:9:DC:C6	2.17	0.78
1:A:1013:THR:HB	20:T:17:DT:N3	1.98	0.78
2:B:1086:PHE:HZ	7:G:109:PRO:O	1.67	0.78
17:Q:17:SER:O	17:Q:29:CYS:CB	2.30	0.78
17:Q:323:ASP:C	17:Q:324:ARG:HA	2.04	0.78
18:R:11:ARG:NH1	21:U:4:DA:OP2	2.17	0.78
1:A:321:LYS:HE3	1:A:325:ASP:OD2	1.84	0.78
16:P:245:ILE:HD12	16:P:269:PHE:CD2	2.19	0.78
19:S:4:C:O2	20:T:20:DG:N1	2.17	0.78
1:A:1258:ILE:HD11	1:A:1507:CYS:SG	2.23	0.78
7:G:237:HIS:HB2	7:G:244:SER:HB3	1.66	0.78
1:A:642:ASN:CG	2:B:1086:PHE:HE2	1.87	0.77
16:P:247:ILE:HG22	16:P:248:PRO:HD3	1.64	0.77
16:P:443:ASP:HB3	18:R:3:GLU:HB3	1.66	0.77
16:P:596:ILE:HA	16:P:599:LYS:HB3	1.65	0.77
18:R:158:THR:HG23	18:R:161:ASN:HB3	1.66	0.77
1:A:1014:SER:CB	20:T:17:DT:H71	2.14	0.77
9:I:28:VAL:N	9:I:37:TYR:O	2.16	0.77
2:B:641:TYR:HB3	2:B:643:PHE:CE1	2.19	0.77
2:B:818:GLY:O	2:B:820:PRO:HD3	1.85	0.77
16:P:389:TRP:HH2	18:R:149:LYS:H	1.31	0.77
17:Q:12:THR:OG1	17:Q:33:HIS:ND1	2.17	0.77
7:G:140:GLN:NE2	7:G:225:ILE:O	2.18	0.77
16:P:585:GLU:HA	16:P:588:SER:HB3	1.66	0.77
2:B:818:GLY:O	2:B:820:PRO:N	2.18	0.77
17:Q:355:VAL:C	18:R:212:HIS:CE1	2.58	0.77
15:O:492:ARG:NH2	15:O:535:GLU:OE1	2.17	0.77
18:R:248:LYS:HA	18:R:298:GLN:NE2	2.00	0.77
9:I:53:ASP:O	9:I:61:ARG:NH2	2.18	0.77
16:P:263:ILE:HG21	16:P:276:SER:HA	1.65	0.77
17:Q:378:LEU:CD1	18:R:231:LEU:CD2	2.57	0.77
1:A:638:PRO:HG3	2:B:1087:LEU:HD11	1.67	0.76
20:T:4:DG:N2	21:U:46:DC:C2	2.33	0.76
2:B:113:VAL:O	18:R:282:SER:CA	2.30	0.76
16:P:214:LEU:HB2	16:P:222:GLN:NE2	1.99	0.76
20:T:11:DA:C2	20:T:12:DC:N3	2.52	0.76
17:Q:386:LEU:CD1	18:R:241:ARG:NH2	2.48	0.76
1:A:1506:ARG:O	1:A:1522:GLU:CD	2.24	0.76
1:A:474:LYS:HD2	2:B:1096:SER:CB	2.14	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:26:ILE:HD12	8:H:42:ILE:HD12	1.65	0.76
16:P:218:VAL:HG23	16:P:219:LEU:HB3	1.68	0.76
16:P:477:TYR:CD2	18:R:2:PHE:CZ	2.73	0.76
17:Q:356:VAL:HG13	18:R:212:HIS:NE2	2.01	0.76
1:A:90:PHE:O	1:A:92:ASN:N	2.19	0.76
2:B:883:GLU:OE1	2:B:906:ARG:NH1	2.19	0.76
2:B:954:PHE:O	2:B:957:ARG:N	2.19	0.76
15:O:392:GLN:HB2	15:O:395:LEU:HD13	1.66	0.76
17:Q:331:ILE:HG22	17:Q:475:ALA:HB1	1.68	0.76
1:A:606:ARG:NH2	11:K:98:GLU:OE2	2.19	0.75
7:G:56:ASN:HB3	7:G:59:GLN:HB3	1.68	0.75
2:B:921:HIS:NE2	2:B:965:GLU:OE1	2.19	0.75
7:G:26:ASN:ND2	7:G:37:CYS:SG	2.58	0.75
7:G:140:GLN:HB3	7:G:217:TRP:HD1	1.49	0.75
1:A:543:LEU:HD22	1:A:578:TYR:OH	1.83	0.75
1:A:642:ASN:HB3	2:B:1086:PHE:HD2	1.48	0.75
18:R:9:THR:HG21	18:R:13:PHE:CD2	2.21	0.75
1:A:545:SER:HB2	17:Q:34:VAL:HG21	1.68	0.75
16:P:357:LEU:HB3	18:R:191:ILE:O	1.85	0.75
1:A:618:TYR:OH	2:B:780:GLY:O	2.03	0.75
2:B:320:LEU:CD2	2:B:325:GLN:C	2.55	0.75
17:Q:357:TYR:HD2	17:Q:489:VAL:HA	1.51	0.75
1:A:1237:GLN:HA	1:A:1521:THR:O	1.87	0.75
1:A:1238:MET:N	1:A:1521:THR:OG1	2.19	0.75
8:H:63:LEU:HB3	8:H:88:SER:HB2	1.67	0.75
17:Q:15:CYS:CB	17:Q:16:PRO:CA	2.62	0.75
9:I:33:CYS:O	13:M:59:ARG:NH1	2.20	0.75
15:O:383:TYR:OH	15:O:595:ASP:N	2.20	0.75
16:P:462:ILE:HB	16:P:483:HIS:HB3	1.69	0.75
1:A:509:GLU:CD	1:A:579:ARG:HE	1.90	0.75
17:Q:22:ILE:HD11	17:Q:24:ASP:OD1	1.86	0.75
2:B:816:ASN:OD1	21:U:18:DG:OP1	2.04	0.75
2:B:1060:VAL:O	2:B:1067:GLY:HA3	1.86	0.75
15:O:241:ASP:CG	15:O:380:SER:HB2	2.07	0.75
17:Q:22:ILE:CG1	17:Q:24:ASP:OD1	2.34	0.75
17:Q:386:LEU:HA	18:R:241:ARG:HH22	0.94	0.75
15:O:492:ARG:O	15:O:493:ASP:O	2.05	0.74
16:P:625:ASP:O	16:P:629:ARG:CB	2.34	0.74
1:A:637:PHE:N	2:B:1091:ARG:NH2	2.33	0.74
17:Q:3:THR:O	17:Q:20:TRP:HB3	1.87	0.74
17:Q:357:TYR:CD2	17:Q:489:VAL:CG2	2.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:815:ARG:NH1	2:B:899:GLN:HG3	2.00	0.74
16:P:358:SER:CB	18:R:196:GLU:OE1	2.35	0.74
1:A:1637:PRO:O	1:A:1641:ILE:N	2.18	0.74
2:B:143:TRP:HB3	2:B:152:LEU:HB2	1.68	0.74
17:Q:378:LEU:HD21	18:R:235:ILE:HD13	1.68	0.74
1:A:672:ASP:H	2:B:783:MET:HE3	0.59	0.74
17:Q:355:VAL:O	18:R:211:ARG:HB3	1.86	0.74
1:A:464:GLU:HB3	1:A:469:LYS:HB2	1.70	0.74
2:B:935:ASP:OD1	3:C:69:ARG:NH1	2.21	0.74
9:I:2:SER:O	9:I:9:PHE:N	2.21	0.74
17:Q:22:ILE:CD1	17:Q:26:ARG:CZ	2.65	0.74
1:A:771:PHE:HE1	1:A:776:LEU:HD13	1.53	0.74
2:B:465:LEU:HA	2:B:485:THR:HG21	1.68	0.74
8:H:106:GLU:HG2	8:H:112:ILE:HG12	1.68	0.74
15:O:444:SER:O	15:O:447:THR:OG1	2.06	0.74
16:P:420:GLU:CD	18:R:3:GLU:OE2	2.26	0.74
2:B:891:GLU:HG2	2:B:892:SER:H	1.52	0.73
16:P:597:LYS:HE3	17:Q:323:ASP:HB3	1.68	0.73
17:Q:155:GLN:HA	20:T:49:DC:C2'	2.18	0.73
17:Q:186:CYS:O	18:R:208:TYR:OH	2.03	0.73
17:Q:323:ASP:HA	17:Q:324:ARG:N	2.01	0.73
17:Q:356:VAL:CG1	18:R:208:TYR:CE1	2.61	0.73
1:A:489:ASN:ND2	2:B:781:TYR:OH	2.21	0.73
1:A:526:GLY:HA2	1:A:554:ARG:CZ	2.18	0.73
1:A:618:TYR:CZ	2:B:783:MET:HB2	2.23	0.73
1:A:637:PHE:O	2:B:1091:ARG:NH1	2.21	0.73
2:B:335:ARG:HG3	2:B:340:ALA:HB3	1.70	0.73
2:B:1079:LEU:HD23	2:B:1088:LEU:CA	2.18	0.73
15:O:181:ARG:HH22	15:O:222:CYS:HA	1.52	0.73
16:P:67:ASP:HA	16:P:545:SER:O	1.88	0.73
18:R:253:ILE:O	18:R:256:GLU:N	2.22	0.73
14:N:157:ARG:NH1	14:N:159:ASP:OD1	2.21	0.73
16:P:435:ARG:NH2	18:R:140:ILE:HD11	1.98	0.73
1:A:550:SER:N	1:A:553:GLN:HE22	1.85	0.73
2:B:1084:THR:OG1	2:B:1088:LEU:CD2	2.36	0.73
3:C:229:LEU:HB2	3:C:293:ARG:HD2	1.69	0.73
15:O:200:ASN:CG	17:Q:14:ASN:HB2	2.09	0.73
1:A:94:LEU:HB2	1:A:355:PHE:CD2	2.23	0.73
3:C:91:VAL:HG21	10:J:60:PHE:HB3	1.69	0.73
20:T:14:DG:N2	21:U:37:DA:C2	2.56	0.73
2:B:212:ASN:HB3	2:B:589:ASP:O	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:626:LEU:HD21	16:P:665:ASN:HA	1.70	0.73
1:A:591:ARG:NH2	19:S:6:A:H1'	2.04	0.73
1:A:636:HIS:HB3	2:B:1091:ARG:HH21	1.54	0.73
2:B:114:SER:OG	18:R:282:SER:C	2.26	0.73
2:B:213:HIS:HD2	2:B:643:PHE:HZ	1.33	0.73
16:P:264:ILE:HG22	16:P:275:GLU:HB2	1.71	0.73
17:Q:258:MET:CE	17:Q:438:PHE:CE2	2.70	0.72
1:A:646:GLU:OE1	1:A:1651:THR:HG21	1.89	0.72
2:B:212:ASN:HB3	2:B:589:ASP:C	2.09	0.72
15:O:492:ARG:HG3	15:O:496:GLY:CA	2.10	0.72
14:N:81:THR:HA	14:N:86:ASP:HA	1.72	0.72
3:C:241:GLY:N	3:C:263:ASP:OD2	2.17	0.72
1:A:597:LYS:O	2:B:1082:HIS:CD2	2.42	0.72
1:A:1319:ASN:O	1:A:1323:HIS:ND1	2.18	0.72
1:A:10:GLU:OE2	1:A:1645:LYS:HG3	1.88	0.72
1:A:637:PHE:H	2:B:1091:ARG:NH2	1.85	0.72
1:A:834:ARG:HH12	2:B:1007:TYR:HE2	1.35	0.72
1:A:1541:ILE:O	5:E:147:HIS:NE2	2.23	0.72
2:B:1017:ALA:O	3:C:65:ASN:ND2	2.22	0.72
9:I:23:VAL:O	9:I:39:LYS:NZ	2.22	0.72
16:P:302:VAL:HG11	16:P:362:ARG:HH11	1.55	0.72
16:P:442:LEU:HA	16:P:443:ASP:OD1	1.90	0.72
16:P:446:ASP:CA	18:R:200:THR:HG22	2.19	0.72
17:Q:12:THR:OG1	17:Q:33:HIS:CE1	2.42	0.72
18:R:252:GLY:O	18:R:256:GLU:HB2	1.89	0.72
1:A:1654:PHE:HB2	6:F:134:ILE:CG2	2.19	0.72
2:B:745:GLN:OE1	3:C:93:GLN:NE2	2.23	0.72
2:B:894:LYS:NZ	17:Q:405:ASP:CG	2.42	0.72
17:Q:356:VAL:HB	18:R:208:TYR:CB	2.20	0.72
1:A:1014:SER:HB2	20:T:17:DT:H71	1.69	0.72
2:B:168:ASN:HA	2:B:173:ASN:HD22	1.53	0.72
8:H:48:PRO:O	8:H:146:ARG:NH2	2.22	0.72
16:P:230:HIS:O	16:P:232:ASN:ND2	2.23	0.72
20:T:11:DA:C5	20:T:12:DC:C4	2.77	0.72
1:A:671:GLN:HB2	2:B:783:MET:CE	2.18	0.72
1:A:672:ASP:HB2	2:B:783:MET:SD	2.28	0.72
18:R:162:PHE:HA	18:R:165:ILE:HD12	1.72	0.72
2:B:1050:GLY:HA2	17:Q:24:ASP:HA	1.71	0.71
16:P:659:LEU:H	16:P:659:LEU:HD13	1.54	0.71
18:R:414:PHE:HA	18:R:417:ILE:HG22	1.70	0.71
1:A:1613:MET:HE3	1:A:1622:LEU:HD13	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:939:SER:HA	2:B:1013:MET:HG2	1.72	0.71
3:C:278:GLU:OE2	3:C:281:ARG:NH1	2.22	0.71
17:Q:322:ARG:O	17:Q:324:ARG:N	2.22	0.71
1:A:474:LYS:HD3	2:B:1096:SER:HB3	0.75	0.71
1:A:1306:TYR:O	1:A:1499:ARG:NH2	2.22	0.71
16:P:420:GLU:O	16:P:441:ASP:HA	1.88	0.71
18:R:303:THR:HA	18:R:358:PHE:CZ	2.25	0.71
7:G:32:ASN:ND2	7:G:34:THR:OG1	2.24	0.71
15:O:389:SER:HA	15:O:395:LEU:HB3	1.71	0.71
1:A:706:HIS:CE1	1:A:815:ARG:HH12	2.09	0.71
1:A:80:GLU:HA	1:A:359:VAL:HG12	1.71	0.71
1:A:642:ASN:HB3	2:B:1086:PHE:CE2	2.25	0.71
2:B:134:ARG:HD3	2:B:160:GLY:HA3	1.72	0.71
2:B:1084:THR:CB	2:B:1087:LEU:HD23	2.20	0.71
3:C:60:ASP:OD2	11:K:78:TYR:OH	2.04	0.71
4:D:47:LYS:NZ	7:G:84:TYR:OH	2.23	0.71
16:P:443:ASP:HB3	18:R:3:GLU:CA	2.21	0.71
1:A:1301:GLU:O	1:A:1305:GLU:N	2.21	0.71
2:B:505:ARG:HB3	2:B:509:PHE:HD2	1.54	0.71
16:P:622:TYR:O	16:P:626:LEU:HB2	1.90	0.71
1:A:973:GLU:HG3	1:A:975:ASP:H	1.55	0.71
1:A:1654:PHE:CE2	6:F:89:GLU:CG	2.74	0.71
2:B:184:LYS:HD2	2:B:735:HIS:CD2	2.25	0.71
3:C:65:ASN:OD1	3:C:68:ARG:NH2	2.24	0.71
1:A:1184:ALA:O	1:A:1188:ILE:HG12	1.91	0.70
2:B:547:HIS:HD1	2:B:760:TYR:HH	1.37	0.70
2:B:1084:THR:CB	2:B:1087:LEU:CD2	2.65	0.70
13:M:40:LEU:HD11	13:M:51:PHE:HB3	1.72	0.70
16:P:315:PHE:HB3	16:P:317:ILE:HD11	1.73	0.70
17:Q:386:LEU:CD1	18:R:241:ARG:HH22	2.03	0.70
20:T:11:DA:C4	20:T:12:DC:C5	2.79	0.70
20:T:12:DC:H2"	20:T:13:DT:H5'	1.72	0.70
2:B:894:LYS:HZ2	17:Q:405:ASP:CB	1.96	0.70
7:G:149:ILE:HB	7:G:153:PHE:HB2	1.73	0.70
15:O:225:LEU:HD11	15:O:228:GLN:HB2	1.73	0.70
15:O:379:ARG:HA	15:O:382:GLN:NE2	2.06	0.70
2:B:17:ARG:NH1	2:B:758:ASP:OD2	2.25	0.70
2:B:213:HIS:HD2	2:B:643:PHE:CZ	2.08	0.70
2:B:1127:CYS:SG	2:B:1171:ASN:ND2	2.63	0.70
17:Q:22:ILE:HD12	17:Q:24:ASP:CG	2.11	0.70
17:Q:350:ARG:CZ	17:Q:486:GLN:CD	2.60	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1641:ILE:HD12	1:A:1641:ILE:N	2.05	0.70
2:B:812:ALA:CB	2:B:815:ARG:HH11	2.04	0.70
16:P:435:ARG:HH21	18:R:140:ILE:HD13	1.33	0.70
2:B:817:ARG:NE	21:U:16:DA:O3'	2.24	0.70
2:B:1075:GLU:O	2:B:1079:LEU:CD1	2.39	0.70
3:C:227:TYR:HB3	3:C:300:PHE:CD1	2.27	0.70
17:Q:355:VAL:CG1	18:R:212:HIS:CA	2.64	0.70
1:A:1248:ASP:N	1:A:1248:ASP:OD1	2.23	0.70
16:P:389:TRP:NE1	18:R:146:SER:CB	2.49	0.70
16:P:719:LEU:HD13	16:P:733:THR:HG21	1.73	0.70
15:O:100:LEU:HD22	15:O:107:ILE:HD11	1.72	0.70
16:P:182:LEU:HD13	16:P:184:SER:H	1.56	0.70
16:P:567:ILE:HB	16:P:569:VAL:HG23	1.74	0.70
1:A:512:THR:HG21	1:A:514:TYR:CE2	2.27	0.70
1:A:526:GLY:HA2	1:A:554:ARG:NH2	2.06	0.70
1:A:627:ASP:CA	2:B:784:ASP:OD1	2.35	0.70
15:O:104:ILE:HD12	15:O:107:ILE:HD12	1.72	0.70
1:A:403:LEU:HB2	1:A:419:ILE:HG21	1.74	0.70
16:P:355:GLU:HA	18:R:24:ILE:HD12	1.74	0.70
17:Q:286:LEU:HB3	17:Q:300:ASN:HB3	1.73	0.70
1:A:7:VAL:HG21	2:B:1177:ALA:HB2	1.73	0.69
1:A:1047:GLN:NE2	1:A:1587:ASP:OD2	2.25	0.69
2:B:731:VAL:HA	10:J:60:PHE:HE1	1.55	0.69
2:B:895:PHE:CE2	20:T:39:DT:OP1	2.45	0.69
5:E:17:ARG:HH12	5:E:36:GLU:HA	1.55	0.69
17:Q:245:SER:HB3	17:Q:284:LEU:HD13	1.73	0.69
1:A:1641:ILE:H	1:A:1641:ILE:CD1	1.98	0.69
17:Q:192:TYR:HD1	17:Q:193:PHE:N	1.89	0.69
1:A:30:LYS:NZ	1:A:51:ASP:OD2	2.25	0.69
1:A:647:ALA:O	1:A:652:ASN:ND2	2.26	0.69
17:Q:186:CYS:SG	18:R:208:TYR:CE2	2.85	0.69
17:Q:322:ARG:C	17:Q:324:ARG:N	2.46	0.69
1:A:597:LYS:HD3	2:B:1081:GLY:O	1.92	0.69
2:B:117:VAL:HB	18:R:277:ILE:CA	2.14	0.69
2:B:1065:ARG:O	2:B:1066:HIS:HB2	1.92	0.69
17:Q:22:ILE:HG13	17:Q:24:ASP:OD1	1.92	0.69
1:A:597:LYS:HD2	2:B:1082:HIS:HA	1.74	0.69
2:B:795:GLU:OE1	3:C:217:ALA:N	2.24	0.69
2:B:816:ASN:CG	21:U:18:DG:OP1	2.31	0.69
1:A:527:PRO:HD3	1:A:554:ARG:HH22	1.57	0.69
2:B:116:ALA:N	18:R:282:SER:C	2.45	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:274:ILE:HD13	16:P:305:PHE:HE2	1.58	0.69
1:A:638:PRO:HG3	2:B:1087:LEU:CD1	2.22	0.69
1:A:646:GLU:CD	1:A:1651:THR:HG21	2.13	0.69
1:A:1259:SER:OG	1:A:1260:LYS:N	2.22	0.69
9:I:26:SER:HA	9:I:39:LYS:HE2	1.73	0.69
16:P:405:TYR:HB2	16:P:416:LEU:HD12	1.75	0.69
16:P:487:ASN:HB3	18:R:138:PHE:CE1	2.27	0.69
17:Q:183:LYS:O	17:Q:187:THR:OG1	2.11	0.69
2:B:480:GLN:OE1	2:B:507:SER:N	2.24	0.69
2:B:1060:VAL:O	2:B:1067:GLY:CA	2.41	0.69
16:P:186:TYR:CB	18:R:198:LEU:HD23	2.21	0.69
16:P:446:ASP:N	18:R:200:THR:CG2	2.55	0.69
16:P:473:HIS:NE2	18:R:1:MET:HB2	2.08	0.69
1:A:593:PRO:HD3	19:S:6:A:H2	1.58	0.69
1:A:641:GLU:HB2	6:F:99:LEU:HD12	1.75	0.69
16:P:446:ASP:N	18:R:200:THR:HG22	2.08	0.69
17:Q:360:LYS:HZ3	18:R:211:ARG:HH22	0.71	0.69
16:P:275:GLU:HG3	16:P:288:SER:HA	1.76	0.68
16:P:675:PHE:HE2	16:P:741:ILE:HG21	1.57	0.68
1:A:587:VAL:HG12	1:A:637:PHE:CD1	2.27	0.68
1:A:1619:CYS:O	1:A:1623:THR:N	2.19	0.68
2:B:698:SER:O	2:B:702:ASN:ND2	2.25	0.68
9:I:28:VAL:HG23	9:I:39:LYS:HA	1.74	0.68
16:P:218:VAL:HB	16:P:245:ILE:HG23	1.76	0.68
18:R:349:ILE:O	18:R:353:VAL:HB	1.93	0.68
1:A:628:PHE:CB	2:B:785:ASP:H	2.00	0.68
8:H:8:ASP:OD1	8:H:9:ILE:N	2.25	0.68
16:P:592:LEU:HA	16:P:595:GLN:HB2	1.74	0.68
18:R:264:SER:O	18:R:266:SER:OG	2.09	0.68
18:R:365:TRP:HB3	18:R:418:CYS:HB2	1.76	0.68
2:B:1107:CYS:O	2:B:1195:ARG:NH2	2.25	0.68
3:C:216:HIS:ND1	3:C:218:LYS:HG2	2.09	0.68
3:C:232:GLN:N	3:C:292:GLY:O	2.27	0.68
1:A:65:CYS:CB	1:A:75:HIS:NE2	2.54	0.68
1:A:407:GLN:O	1:A:411:VAL:N	2.25	0.68
1:A:511:VAL:HG11	1:A:575:LYS:N	2.08	0.68
2:B:924:LYS:NZ	19:S:6:A:OP1	2.25	0.68
2:B:934:ILE:HB	3:C:69:ARG:HD2	1.73	0.68
2:B:1189:LEU:HD12	2:B:1196:LEU:HD11	1.74	0.68
6:F:58:PHE:HA	6:F:61:HIS:CE1	2.28	0.68
17:Q:353:VAL:CG1	17:Q:489:VAL:CG1	2.71	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:356:VAL:HG11	18:R:208:TYR:CZ	2.27	0.68
15:O:461:VAL:HG11	15:O:513:LYS:HB3	1.75	0.68
1:A:862:THR:O	1:A:878:ARG:NH1	2.26	0.68
2:B:1093:LEU:CD1	2:B:1098:TYR:CB	2.62	0.68
2:B:1105:ARG:NH1	2:B:1172:GLU:OE1	2.26	0.68
9:I:3:VAL:HG22	9:I:8:ILE:HG23	1.75	0.68
1:A:1003:ARG:NH2	2:B:540:GLY:HA2	2.09	0.68
15:O:487:ARG:HH21	15:O:502:LEU:HD13	1.57	0.68
17:Q:162:ILE:HG21	17:Q:226:LEU:HD11	1.73	0.68
2:B:895:PHE:HE2	20:T:39:DT:OP1	1.75	0.68
16:P:363:ILE:HG23	16:P:374:VAL:HG13	1.76	0.68
16:P:393:VAL:HG23	16:P:394:VAL:H	1.59	0.68
17:Q:8:PRO:HG2	17:Q:19:LEU:HD23	1.75	0.68
20:T:9:DC:C2'	20:T:10:DA:C8	2.76	0.68
2:B:841:ASP:N	2:B:845:LEU:O	2.20	0.68
18:R:361:ASP:O	18:R:364:VAL:HG22	1.94	0.68
1:A:1242:ILE:HG22	1:A:1536:ILE:HG22	1.74	0.67
2:B:1079:LEU:CD2	2:B:1088:LEU:CB	2.55	0.67
3:C:32:ASN:OD1	3:C:33:VAL:N	2.27	0.67
16:P:480:VAL:HG23	16:P:492:LEU:HD21	1.76	0.67
17:Q:22:ILE:CD1	17:Q:26:ARG:HE	2.04	0.67
1:A:672:ASP:OD2	2:B:783:MET:SD	2.53	0.67
1:A:1654:PHE:CD2	6:F:89:GLU:HG3	2.28	0.67
2:B:894:LYS:HZ1	17:Q:405:ASP:CB	2.04	0.67
2:B:1047:ARG:CZ	2:B:1049:THR:HG22	2.24	0.67
2:B:1078:ALA:O	2:B:1082:HIS:HB2	1.93	0.67
14:N:85:HIS:HE1	14:N:141:GLU:HG3	1.58	0.67
16:P:357:LEU:O	18:R:194:GLY:HA2	1.93	0.67
3:C:127:THR:H	3:C:130:ASN:HB2	1.60	0.67
15:O:506:PHE:O	15:O:510:VAL:N	2.23	0.67
17:Q:356:VAL:CG2	18:R:208:TYR:HD2	1.97	0.67
21:U:38:DG:C2	21:U:39:DT:C2	2.82	0.67
1:A:355:PHE:HD1	1:A:355:PHE:H	1.39	0.67
2:B:480:GLN:O	2:B:484:TYR:OH	2.12	0.67
2:B:1096:SER:O	2:B:1097:ASP:HB3	1.93	0.67
1:A:70:LYS:HZ2	17:Q:27:ARG:NH1	1.92	0.67
1:A:1260:LYS:NZ	1:A:1500:GLN:OE1	2.27	0.67
16:P:229:ARG:HG3	16:P:230:HIS:H	1.57	0.67
17:Q:386:LEU:HD12	18:R:241:ARG:HH22	1.58	0.67
1:A:509:GLU:OE2	1:A:584:ARG:NH2	2.28	0.67
1:A:1600:ARG:NH2	1:A:1620:GLN:OE1	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:VAL:CG1	1:A:575:LYS:N	2.58	0.67
1:A:543:LEU:HD21	1:A:578:TYR:HH	1.57	0.67
16:P:238:LEU:HD11	16:P:284:VAL:HB	1.74	0.67
16:P:367:SER:OG	16:P:368:HIS:N	2.28	0.67
16:P:384:ASP:HB3	16:P:389:TRP:HB3	1.76	0.67
2:B:213:HIS:HB2	2:B:643:PHE:HE2	1.58	0.67
15:O:189:PHE:O	15:O:192:THR:OG1	2.11	0.67
1:A:855:ARG:NH1	1:A:868:THR:O	2.26	0.67
2:B:184:LYS:NZ	10:J:69:ARG:HH22	1.92	0.67
1:A:652:ASN:HB2	1:A:655:SER:HB2	1.77	0.67
2:B:113:VAL:C	18:R:282:SER:HA	2.15	0.67
5:E:17:ARG:NH1	5:E:35:VAL:O	2.27	0.67
16:P:468:VAL:HG22	16:P:477:TYR:HB3	1.76	0.67
18:R:236:PHE:O	18:R:240:ILE:HG22	1.94	0.67
18:R:361:ASP:HB2	18:R:364:VAL:HG13	1.77	0.67
15:O:453:TYR:CE2	15:O:473:PHE:HB2	2.29	0.66
16:P:506:THR:HG23	16:P:542:ARG:HD3	1.78	0.66
17:Q:232:LEU:HA	17:Q:287:TRP:CD1	2.30	0.66
1:A:512:THR:HG22	1:A:513:ALA:N	2.10	0.66
2:B:1014:TYR:HD1	2:B:1021:GLU:HA	1.60	0.66
15:O:446:LEU:O	15:O:450:LEU:N	2.26	0.66
16:P:362:ARG:HH22	16:P:364:GLU:HG3	1.61	0.66
16:P:498:LEU:HD13	17:Q:368:GLN:HE21	1.59	0.66
17:Q:361:PRO:O	17:Q:363:SER:N	2.28	0.66
1:A:1148:LEU:HG	1:A:1155:PHE:HE2	1.60	0.66
9:I:26:SER:O	9:I:39:LYS:N	2.27	0.66
15:O:379:ARG:CA	15:O:382:GLN:HE22	2.09	0.66
5:E:88:VAL:HB	5:E:116:ILE:HA	1.78	0.66
1:A:690:GLU:HB3	11:K:77:ARG:HH22	1.61	0.66
2:B:116:ALA:CB	18:R:282:SER:C	2.51	0.66
2:B:564:ILE:O	2:B:567:SER:OG	2.14	0.66
2:B:843:ASP:OD2	12:L:29:TYR:OH	2.13	0.66
17:Q:15:CYS:HB2	17:Q:16:PRO:HA	1.77	0.66
17:Q:355:VAL:CA	18:R:212:HIS:HE1	2.04	0.66
2:B:107:PRO:O	2:B:171:HIS:NE2	2.21	0.66
2:B:1107:CYS:HB2	2:B:1130:ARG:HH11	1.61	0.66
5:E:55:ARG:HG3	5:E:84:ASP:HA	1.77	0.66
17:Q:104:PHE:CZ	17:Q:156:LEU:HB2	2.31	0.66
17:Q:412:LYS:O	17:Q:416:ILE:HG13	1.96	0.66
2:B:974:LEU:O	10:J:47:ARG:NH2	2.29	0.66
11:K:54:THR:HG22	11:K:61:ALA:HA	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:200:ASN:CG	17:Q:14:ASN:CB	2.64	0.66
16:P:355:GLU:CB	18:R:24:ILE:HD12	2.25	0.66
2:B:815:ARG:NH2	2:B:821:ILE:CB	2.58	0.66
2:B:1092:LEU:HD23	2:B:1092:LEU:C	2.16	0.66
9:I:38:PRO:HD2	9:I:41:GLN:HE21	1.61	0.66
14:N:63:ASP:OD2	14:N:66:LYS:NZ	2.25	0.66
16:P:443:ASP:HB3	18:R:3:GLU:CB	2.26	0.66
18:R:250:LEU:HB2	18:R:270:PHE:HE2	1.60	0.66
2:B:144:SER:HA	2:B:151:ASN:HA	1.76	0.66
2:B:916:LYS:HD3	2:B:924:LYS:HD2	1.77	0.66
7:G:28:ILE:HD13	7:G:35:SER:HB3	1.78	0.66
11:K:60:SER:OG	11:K:104:ARG:NH2	2.29	0.65
1:A:1037:SER:OG	1:A:1039:ARG:NE	2.25	0.65
15:O:179:PHE:O	15:O:183:ILE:N	2.22	0.65
16:P:419:ARG:HG2	16:P:420:GLU:N	2.10	0.65
16:P:555:THR:HG22	16:P:556:GLN:HG2	1.78	0.65
16:P:724:LEU:CD1	17:Q:443:GLN:HG2	2.26	0.65
17:Q:15:CYS:SG	17:Q:17:SER:CB	2.83	0.65
1:A:385:LEU:HD23	1:A:437:PHE:HA	1.77	0.65
1:A:504:LYS:O	1:A:506:THR:HG23	1.96	0.65
2:B:115:SER:O	18:R:280:SER:N	2.29	0.65
2:B:731:VAL:HG13	10:J:60:PHE:CD1	2.32	0.65
3:C:64:ALA:O	3:C:68:ARG:N	2.21	0.65
3:C:85:PHE:HE1	3:C:204:LEU:HD22	1.60	0.65
15:O:466:GLY:O	15:O:469:ARG:NE	2.29	0.65
19:S:4:C:O5'	19:S:4:C:H6	1.79	0.65
3:C:212:ILE:HG13	3:C:215:ASP:H	1.61	0.65
17:Q:355:VAL:HG11	18:R:212:HIS:HA	1.76	0.65
1:A:372:LYS:HA	1:A:377:VAL:HA	1.78	0.65
2:B:954:PHE:O	2:B:955:PRO:C	2.33	0.65
9:I:10:CYS:HB3	9:I:13:CYS:SG	2.37	0.65
15:O:487:ARG:HA	15:O:491:PHE:HB2	1.78	0.65
18:R:6:ILE:HG22	18:R:245:VAL:HA	1.78	0.65
18:R:417:ILE:O	18:R:420:ASP:HB2	1.96	0.65
1:A:1302:TYR:HA	1:A:1305:GLU:HB3	1.77	0.65
1:A:1640:ARG:NH1	1:A:1640:ARG:HG2	2.11	0.65
16:P:420:GLU:HB2	16:P:442:LEU:N	2.12	0.65
17:Q:409:ALA:O	17:Q:413:LEU:HB2	1.97	0.65
3:C:222:VAL:C	3:C:224:THR:H	2.00	0.65
15:O:327:GLU:HB3	15:O:331:LYS:HE3	1.77	0.65
1:A:1162:ASN:HB3	1:A:1165:LYS:HG2	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1461:ASN:OD1	1:A:1462:PHE:N	2.29	0.65
2:B:1050:GLY:CA	17:Q:24:ASP:HA	2.27	0.65
16:P:458:LYS:HD3	16:P:459:PRO:HD3	1.78	0.65
16:P:662:LEU:CB	16:P:665:ASN:HB2	2.26	0.65
17:Q:366:TYR:HA	17:Q:369:TRP:NE1	2.12	0.65
1:A:474:LYS:CD	2:B:1096:SER:HB2	2.21	0.65
2:B:115:SER:C	18:R:282:SER:HB3	2.16	0.65
2:B:662:ASP:OD1	2:B:663:ILE:N	2.30	0.65
2:B:1079:LEU:CG	2:B:1088:LEU:HD22	2.12	0.65
16:P:355:GLU:HA	18:R:24:ILE:CD1	2.27	0.65
17:Q:288:GLU:O	17:Q:290:THR:N	2.30	0.65
18:R:217:THR:HG22	18:R:239:LEU:HD21	1.77	0.65
1:A:672:ASP:CA	2:B:783:MET:HE3	2.24	0.65
2:B:143:TRP:O	2:B:152:LEU:N	2.28	0.65
9:I:8:ILE:HG22	9:I:17:LEU:HD12	1.79	0.65
1:A:339:PHE:O	1:A:1629:ASN:ND2	2.30	0.64
1:A:568:VAL:O	1:A:571:HIS:ND1	2.25	0.64
1:A:916:THR:O	1:A:919:LYS:NZ	2.28	0.64
1:A:1185:VAL:HA	1:A:1188:ILE:HB	1.79	0.64
1:A:1258:ILE:HD12	1:A:1258:ILE:O	1.96	0.64
16:P:315:PHE:HB3	16:P:317:ILE:CD1	2.27	0.64
17:Q:104:PHE:CE1	20:T:49:DC:OP1	2.51	0.64
1:A:1326:GLU:HA	1:A:1329:ILE:HD12	1.78	0.64
2:B:817:ARG:CG	21:U:17:DT:H5'	2.25	0.64
2:B:1051:PRO:HD3	2:B:1066:HIS:O	1.97	0.64
2:B:1098:TYR:CE1	2:B:1177:ALA:HB1	2.33	0.64
16:P:446:ASP:HA	18:R:200:THR:CG2	2.27	0.64
1:A:872:ASP:OD2	1:A:875:LEU:N	2.30	0.64
1:A:1104:TYR:HB3	1:A:1120:TYR:HE2	1.63	0.64
2:B:812:ALA:HA	2:B:815:ARG:HD2	1.79	0.64
18:R:206:ARG:C	18:R:207:ASN:HB2	2.17	0.64
18:R:427:PRO:HG2	18:R:429:ARG:HH21	1.63	0.64
17:Q:355:VAL:HG13	18:R:212:HIS:HA	1.79	0.64
17:Q:356:VAL:CG1	18:R:212:HIS:CE1	2.69	0.64
1:A:358:ASP:OD1	1:A:358:ASP:N	2.31	0.64
4:D:39:PHE:HZ	7:G:83:GLY:HA3	1.62	0.64
15:O:600:LYS:HG3	15:O:601:ASN:H	1.62	0.64
16:P:729:ALA:O	16:P:733:THR:HG22	1.96	0.64
1:A:827:THR:HG21	2:B:1026:ILE:HA	1.78	0.64
1:A:1018:TYR:CE1	20:T:16:DT:P	2.89	0.64
1:A:1299:ASN:HA	1:A:1302:TYR:CZ	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:63:LEU:HB2	15:O:71:ILE:HG13	1.79	0.64
16:P:487:ASN:HB3	18:R:138:PHE:HZ	1.60	0.64
16:P:658:LYS:O	16:P:747:LEU:HG	1.97	0.64
16:P:698:LYS:HE2	17:Q:124:ARG:HH21	1.62	0.64
3:C:69:ARG:NE	11:K:71:THR:OG1	2.23	0.64
15:O:186:SER:HA	15:O:189:PHE:CE2	2.33	0.64
16:P:421:ILE:HG22	16:P:423:ILE:HG13	1.79	0.64
2:B:936:MET:CG	2:B:948:ILE:HD11	2.27	0.64
15:O:446:LEU:HD11	15:O:476:ALA:HB1	1.80	0.64
16:P:62:LYS:HG2	16:P:63:SER:N	2.13	0.64
16:P:658:LYS:HB3	16:P:660:LYS:H	1.62	0.64
1:A:95:TYR:OH	1:A:99:ARG:NH1	2.31	0.64
1:A:1654:PHE:CE2	6:F:89:GLU:HG3	2.33	0.64
3:C:89:THR:OG1	3:C:201:GLU:N	2.17	0.64
13:M:36:THR:HG21	13:M:62:TYR:HE2	1.63	0.64
13:M:57:ASN:HD21	13:M:60:LEU:HB2	1.62	0.64
15:O:218:LEU:HD12	15:O:221:TYR:HB2	1.79	0.64
15:O:430:ARG:HG2	15:O:482:TYR:OH	1.97	0.64
16:P:221:ARG:HH12	16:P:264:ILE:HG21	1.63	0.64
1:A:109:ARG:NH1	1:A:230:ARG:O	2.30	0.64
1:A:1651:THR:HG21	2:B:1086:PHE:HB2	1.80	0.64
2:B:709:PHE:HE2	2:B:992:PRO:HG2	1.63	0.64
15:O:440:ILE:O	15:O:444:SER:N	2.31	0.64
1:A:527:PRO:HD3	1:A:554:ARG:NH1	2.13	0.63
1:A:879:LEU:HA	1:A:882:ILE:HG22	1.80	0.63
16:P:380:MET:HB3	16:P:393:VAL:HG21	1.79	0.63
16:P:592:LEU:O	16:P:596:ILE:HG22	1.98	0.63
17:Q:19:LEU:HD11	17:Q:27:ARG:CB	2.27	0.63
17:Q:198:ILE:HD12	17:Q:390:THR:HA	1.81	0.63
17:Q:356:VAL:HG12	18:R:208:TYR:O	1.98	0.63
1:A:368:ARG:HA	1:A:380:ASN:HD22	1.63	0.63
1:A:638:PRO:CG	2:B:1087:LEU:HD11	2.26	0.63
1:A:1013:THR:CB	20:T:17:DT:N3	2.61	0.63
17:Q:22:ILE:HD11	17:Q:26:ARG:HE	1.62	0.63
17:Q:101:LYS:HE3	17:Q:154:LEU:HD12	1.79	0.63
1:A:552:GLU:O	15:O:246:ASN:ND2	2.31	0.63
1:A:628:PHE:HB3	2:B:785:ASP:OD1	1.99	0.63
1:A:880:GLN:NE2	2:B:633:THR:H	1.96	0.63
7:G:167:THR:O	7:G:218:VAL:N	2.29	0.63
13:M:61:GLU:N	13:M:101:VAL:O	2.25	0.63
17:Q:337:SER:HB2	17:Q:448:LYS:HD3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:646:GLU:OE2	6:F:91:ALA:HB1	1.98	0.63
1:A:672:ASP:CG	2:B:783:MET:SD	2.76	0.63
2:B:307:GLU:HB2	9:I:7:LEU:HD11	1.80	0.63
2:B:787:MET:HG3	2:B:928:SER:N	2.12	0.63
1:A:852:ASP:OD1	1:A:855:ARG:NE	2.29	0.63
1:A:882:ILE:O	1:A:889:SER:OG	2.17	0.63
1:A:1139:ASN:ND2	5:E:204:THR:O	2.31	0.63
2:B:674:ILE:HG12	2:B:688:HIS:HB2	1.79	0.63
2:B:1117:VAL:HG21	2:B:1162:GLY:HA2	1.79	0.63
11:K:64:GLN:HE21	11:K:100:LEU:HD22	1.63	0.63
1:A:1105:ARG:NH1	1:A:1138:GLU:HG2	2.14	0.63
2:B:145:VAL:N	2:B:150:GLU:O	2.23	0.63
3:C:150:SER:OG	3:C:155:GLU:OE2	2.17	0.63
6:F:83:PRO:HB2	6:F:152:ILE:HD13	1.80	0.63
16:P:697:GLU:OE1	16:P:697:GLU:N	2.25	0.63
1:A:618:TYR:CE1	2:B:783:MET:HB2	2.33	0.63
2:B:216:ALA:HA	2:B:234:ILE:HD13	1.80	0.63
2:B:366:GLY:O	2:B:370:LYS:N	2.24	0.63
15:O:61:ASP:OD1	15:O:106:ARG:NH2	2.31	0.63
16:P:596:ILE:HD13	17:Q:272:GLN:NE2	2.14	0.63
16:P:760:ILE:HA	16:P:763:SER:HB3	1.81	0.63
1:A:1634:LEU:O	1:A:1640:ARG:NH1	2.31	0.63
1:A:1635:ASP:O	1:A:1640:ARG:HD2	1.99	0.63
2:B:225:ARG:NH2	2:B:268:GLU:OE1	2.24	0.63
2:B:731:VAL:HG13	10:J:60:PHE:HD1	1.63	0.63
17:Q:12:THR:HG1	17:Q:33:HIS:CE1	2.15	0.63
17:Q:278:GLU:O	17:Q:279:THR:OG1	2.14	0.63
19:S:3:G:C2	20:T:21:DC:O2	2.52	0.63
1:A:833:LEU:HD22	1:A:943:ILE:HG21	1.81	0.63
1:A:956:ARG:NH2	1:A:979:GLY:HA3	2.13	0.63
2:B:532:HIS:ND1	24:B:1301:SO4:O4	2.31	0.63
2:B:790:ASN:HA	2:B:936:MET:SD	2.39	0.63
3:C:89:THR:HG1	3:C:201:GLU:H	1.45	0.63
9:I:60:LEU:O	9:I:64:LYS:N	2.31	0.63
17:Q:6:ARG:O	17:Q:7:GLY:O	2.17	0.63
17:Q:8:PRO:HB2	17:Q:19:LEU:HD23	1.79	0.63
18:R:346:ILE:HB	18:R:375:LYS:HE2	1.80	0.63
1:A:1032:VAL:HG22	1:A:1038:ILE:HD13	1.81	0.62
2:B:96:SER:HB2	2:B:144:SER:HB3	1.80	0.62
10:J:18:TRP:NE1	10:J:55:ASP:OD2	2.32	0.62
16:P:384:ASP:OD2	16:P:387:ASN:HB2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:435:ARG:HH22	18:R:140:ILE:CD1	2.09	0.62
1:A:964:LYS:NZ	2:B:672:MET:O	2.32	0.62
2:B:158:CYS:O	2:B:457:ILE:N	2.32	0.62
2:B:320:LEU:HD21	2:B:325:GLN:O	1.98	0.62
2:B:534:PRO:HG3	2:B:542:LEU:HD12	1.81	0.62
2:B:1137:ASP:HA	2:B:1140:LYS:HD2	1.80	0.62
16:P:420:GLU:HA	16:P:442:LEU:O	1.99	0.62
16:P:700:LEU:HD12	16:P:703:PHE:HD2	1.64	0.62
16:P:721:CYS:SG	17:Q:442:LEU:HD23	2.39	0.62
17:Q:355:VAL:HG12	18:R:212:HIS:CA	2.26	0.62
1:A:373:LEU:N	1:A:376:GLU:O	2.32	0.62
1:A:1262:LEU:HB2	1:A:1265:GLU:HG3	1.80	0.62
1:A:1646:LEU:HD11	2:B:1086:PHE:CE1	2.33	0.62
2:B:811:LEU:HD13	2:B:823:GLN:HB2	1.80	0.62
16:P:305:PHE:HE1	16:P:314:GLN:HG3	1.64	0.62
17:Q:10:CYS:CB	17:Q:17:SER:H	2.12	0.62
17:Q:329:LYS:HA	17:Q:332:LEU:HD23	1.80	0.62
17:Q:386:LEU:CG	18:R:241:ARG:HH22	2.11	0.62
2:B:1063:ARG:NE	20:T:22:DG:OP2	2.31	0.62
3:C:58:ASN:HA	3:C:296:ASN:ND2	2.15	0.62
5:E:100:ILE:HG23	5:E:105:PHE:HB2	1.81	0.62
16:P:603:ARG:O	16:P:607:VAL:HG23	1.99	0.62
17:Q:3:THR:HG22	17:Q:20:TRP:CB	2.29	0.62
17:Q:356:VAL:HG22	18:R:208:TYR:CE2	2.24	0.62
17:Q:410:ARG:HA	17:Q:413:LEU:HB3	1.80	0.62
1:A:520:ARG:HH21	1:A:559:ASN:HD21	1.48	0.62
6:F:61:HIS:HA	6:F:64:ILE:HB	1.81	0.62
16:P:209:LYS:NZ	16:P:277:VAL:HG11	2.14	0.62
16:P:405:TYR:HE2	16:P:414:ILE:HG13	1.64	0.62
16:P:722:TRP:CD1	17:Q:264:PRO:HD3	2.34	0.62
20:T:21:DC:O5'	20:T:21:DC:H6	1.81	0.62
1:A:15:ASP:HB2	2:B:1197:ARG:HB3	1.79	0.62
1:A:1603:MET:HG2	1:A:1612:LYS:HG2	1.81	0.62
16:P:345:ASP:OD1	16:P:345:ASP:N	2.32	0.62
16:P:414:ILE:HG12	16:P:425:GLY:H	1.62	0.62
16:P:442:LEU:HB3	16:P:477:TYR:CZ	2.34	0.62
18:R:173:MET:O	18:R:177:LEU:HB2	2.00	0.62
1:A:1258:ILE:HB	1:A:1501:ILE:CD1	2.29	0.62
2:B:314:LYS:O	2:B:315:LYS:HG2	1.99	0.62
2:B:1105:ARG:HH21	2:B:1174:THR:HG22	1.64	0.62
8:H:103:LYS:HB3	8:H:115:TYR:HD2	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:357:TYR:CE2	17:Q:489:VAL:HA	2.34	0.62
1:A:70:LYS:HZ2	17:Q:27:ARG:HH12	1.40	0.62
1:A:512:THR:HG22	1:A:513:ALA:H	1.65	0.62
1:A:782:ASP:OD1	1:A:783:LYS:N	2.33	0.62
1:A:1507:CYS:HB3	1:A:1520:VAL:O	1.99	0.62
5:E:26:ARG:NH1	5:E:133:GLU:OE1	2.29	0.62
8:H:115:TYR:HE1	8:H:124:ARG:HG3	1.65	0.62
17:Q:318:LEU:HB3	17:Q:476:ILE:HD12	1.82	0.62
18:R:273:TRP:O	18:R:277:ILE:HG22	1.99	0.62
2:B:302:LEU:HD13	2:B:379:ARG:NH1	2.14	0.62
16:P:356:GLU:OE1	16:P:377:ARG:NE	2.33	0.62
17:Q:274:ILE:HD13	17:Q:282:ARG:HH12	1.64	0.62
20:T:7:DT:H3	21:U:43:DA:H61	1.46	0.62
1:A:511:VAL:HG13	1:A:574:ASN:CB	2.25	0.62
1:A:1240:LEU:HD12	1:A:1521:THR:HG23	1.78	0.62
2:B:815:ARG:NH1	2:B:899:GLN:CD	2.53	0.62
15:O:393:LEU:HD21	15:O:438:GLN:HE22	1.64	0.62
16:P:631:SER:O	16:P:686:TYR:OH	2.17	0.62
16:P:721:CYS:SG	17:Q:439:ILE:HG22	2.39	0.62
18:R:361:ASP:OD1	18:R:361:ASP:N	2.25	0.62
1:A:17:GLY:O	2:B:1195:ARG:N	2.33	0.61
2:B:70:GLU:HA	2:B:98:SER:HB3	1.82	0.61
2:B:302:LEU:HD13	2:B:379:ARG:HH12	1.65	0.61
16:P:622:TYR:OH	16:P:665:ASN:O	2.16	0.61
17:Q:299:SER:O	17:Q:299:SER:OG	2.11	0.61
18:R:160:HIS:HA	18:R:163:LYS:HE2	1.81	0.61
18:R:242:ILE:HG22	18:R:245:VAL:HG22	1.81	0.61
1:A:547:ILE:CD1	17:Q:26:ARG:NH2	2.45	0.61
1:A:1176:ARG:NH2	6:F:154:ASP:O	2.32	0.61
2:B:1053:ASN:N	2:B:1058:GLN:O	2.29	0.61
7:G:141:SER:O	7:G:217:TRP:NE1	2.34	0.61
16:P:596:ILE:HD13	17:Q:272:GLN:CD	2.20	0.61
1:A:702:PRO:HD3	1:A:712:ILE:HD11	1.82	0.61
1:A:1510:PRO:HG3	1:A:1520:VAL:HG23	1.81	0.61
2:B:368:GLN:HG3	2:B:372:ARG:HH12	1.65	0.61
3:C:69:ARG:HH21	11:K:71:THR:H	1.47	0.61
15:O:403:LEU:HB3	15:O:424:LEU:HB2	1.81	0.61
16:P:434:ARG:HB3	18:R:143:THR:HG21	1.81	0.61
16:P:584:ARG:O	16:P:588:SER:HB2	2.00	0.61
18:R:75:GLN:HA	18:R:78:ARG:HE	1.64	0.61
2:B:796:ARG:HD2	10:J:8:PHE:HA	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:812:ALA:HB1	2:B:815:ARG:HH11	1.66	0.61
3:C:84:TYR:HB3	12:L:64:LEU:HD11	1.82	0.61
16:P:376:ASP:O	16:P:378:SER:N	2.33	0.61
17:Q:324:ARG:NE	17:Q:324:ARG:O	2.33	0.61
1:A:94:LEU:HB2	1:A:355:PHE:HD2	1.63	0.61
2:B:651:ARG:NH2	2:B:690:GLU:OE2	2.23	0.61
12:L:68:GLU:HG2	12:L:70:ARG:H	1.65	0.61
16:P:629:ARG:NH2	16:P:662:LEU:HD21	2.14	0.61
17:Q:230:ILE:O	17:Q:234:CYS:HB2	2.00	0.61
17:Q:265:GLU:OE1	17:Q:265:GLU:N	2.31	0.61
1:A:638:PRO:CG	2:B:1087:LEU:HD12	2.29	0.61
1:A:1300:ASN:OD1	1:A:1301:GLU:N	2.33	0.61
1:A:1307:ASP:HB3	1:A:1499:ARG:HH12	1.64	0.61
2:B:234:ILE:HG12	2:B:381:LEU:HD13	1.81	0.61
2:B:324:THR:HG23	2:B:347:LEU:HD13	1.81	0.61
2:B:547:HIS:ND1	2:B:760:TYR:OH	2.26	0.61
15:O:205:ARG:HD3	15:O:331:LYS:HA	1.82	0.61
15:O:379:ARG:CB	15:O:591:TYR:OH	2.49	0.61
17:Q:115:GLN:NE2	17:Q:191:PRO:O	2.27	0.61
19:S:4:C:O2	20:T:20:DG:C2	2.53	0.61
1:A:1640:ARG:HG2	1:A:1640:ARG:HH11	1.66	0.61
1:A:1650:GLY:C	1:A:1652:GLY:H	2.02	0.61
2:B:114:SER:CB	18:R:282:SER:HA	1.97	0.61
5:E:47:CYS:HA	5:E:53:PRO:HA	1.81	0.61
13:M:34:SER:OG	14:N:128:ASN:ND2	2.33	0.61
15:O:383:TYR:O	15:O:387:HIS:N	2.32	0.61
17:Q:356:VAL:HB	18:R:208:TYR:CD2	2.23	0.61
1:A:952:LEU:HD12	1:A:957:VAL:HA	1.83	0.61
2:B:838:GLU:O	12:L:63:ARG:NH2	2.34	0.61
3:C:164:ALA:HB2	3:C:191:ILE:HB	1.83	0.61
14:N:89:ILE:HG12	14:N:139:VAL:HG22	1.83	0.61
16:P:55:LEU:CA	18:R:227:HIS:CE1	2.84	0.61
20:T:4:DG:H8	20:T:4:DG:O5'	1.82	0.61
1:A:597:LYS:O	2:B:1082:HIS:CE1	2.53	0.61
1:A:729:LYS:HD2	8:H:120:GLY:HA3	1.82	0.61
1:A:1654:PHE:CE2	6:F:89:GLU:N	2.69	0.61
11:K:88:PHE:HB3	11:K:106:GLN:HB2	1.81	0.61
13:M:51:PHE:HD2	13:M:94:PRO:HG3	1.65	0.61
18:R:295:PRO:O	18:R:297:PHE:N	2.33	0.61
2:B:910:THR:O	2:B:1035:ARG:NH2	2.33	0.61
5:E:200:ARG:O	5:E:208:TYR:N	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:113:SER:HG	14:N:115:SER:HG	1.46	0.61
15:O:152:GLN:O	15:O:155:SER:OG	2.16	0.61
15:O:442:VAL:O	15:O:446:LEU:N	2.29	0.61
16:P:290:GLU:O	16:P:343:LEU:HD21	2.00	0.61
16:P:486:ALA:HB1	18:R:137:SER:OG	2.01	0.61
1:A:638:PRO:HG2	2:B:1087:LEU:CD1	2.31	0.60
1:A:1450:ILE:HA	1:A:1453:HIS:HD2	1.65	0.60
16:P:221:ARG:NH1	16:P:264:ILE:HG21	2.16	0.60
16:P:724:LEU:HD12	17:Q:443:GLN:HA	1.83	0.60
1:A:1459:LYS:HD3	1:A:1473:LYS:HD3	1.83	0.60
2:B:931:TRP:CB	2:B:936:MET:HE3	2.11	0.60
3:C:227:TYR:HB3	3:C:300:PHE:HD1	1.66	0.60
15:O:379:ARG:HA	15:O:382:GLN:CD	2.21	0.60
16:P:475:ARG:H	16:P:475:ARG:HD2	1.65	0.60
17:Q:232:LEU:HD22	17:Q:287:TRP:CD1	2.36	0.60
18:R:26:TYR:CB	18:R:169:PRO:HB3	2.31	0.60
1:A:1302:TYR:O	1:A:1306:TYR:N	2.33	0.60
2:B:494:TYR:HB3	2:B:700:LEU:HD11	1.82	0.60
3:C:57:ILE:HG13	3:C:297:HIS:CD2	2.36	0.60
6:F:66:ARG:O	6:F:70:LYS:N	2.32	0.60
15:O:353:GLU:HG3	15:O:354:SER:H	1.65	0.60
16:P:220:THR:HG22	16:P:241:PRO:HB3	1.82	0.60
1:A:925:MET:SD	2:B:955:PRO:HB3	2.41	0.60
1:A:1643:VAL:O	2:B:1179:PRO:HD2	2.00	0.60
2:B:929:ARG:NH1	11:K:96:PRO:HB2	2.10	0.60
15:O:458:GLU:HB3	15:O:513:LYS:HD2	1.82	0.60
16:P:687:GLN:O	16:P:689:GLN:NE2	2.35	0.60
5:E:176:PRO:HB2	5:E:212:ARG:HD3	1.83	0.60
16:P:477:TYR:CE2	18:R:2:PHE:HZ	2.19	0.60
16:P:477:TYR:HE2	18:R:2:PHE:HE2	1.19	0.60
4:D:47:LYS:HB3	4:D:82:LEU:HD21	1.83	0.60
15:O:328:LEU:HA	15:O:331:LYS:HB2	1.82	0.60
18:R:257:ILE:CG2	18:R:267:GLY:H	2.13	0.60
1:A:260:GLN:O	1:A:264:ASN:N	2.27	0.60
3:C:132:ILE:HB	3:C:208:CYS:HB2	1.84	0.60
15:O:62:ASP:O	15:O:67:ASP:N	2.35	0.60
16:P:55:LEU:HA	18:R:227:HIS:CE1	2.36	0.60
17:Q:15:CYS:HB3	17:Q:17:SER:H	1.62	0.60
18:R:412:ARG:NE	18:R:432:GLU:OE2	2.28	0.60
1:A:216:ARG:NH2	1:A:338:VAL:O	2.34	0.60
1:A:709:ARG:NH1	1:A:737:LEU:O	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1640:ARG:HH11	1:A:1640:ARG:CG	2.15	0.60
2:B:320:LEU:CD2	2:B:325:GLN:HB2	2.30	0.60
2:B:815:ARG:NH1	2:B:899:GLN:CG	2.62	0.60
2:B:1087:LEU:HD23	2:B:1088:LEU:HD23	1.83	0.60
3:C:236:LEU:HD11	3:C:290:LYS:HG3	1.83	0.60
7:G:22:LYS:NZ	7:G:77:VAL:O	2.33	0.60
14:N:40:LEU:HA	14:N:51:GLN:HE22	1.66	0.60
16:P:446:ASP:CA	18:R:200:THR:CG2	2.80	0.60
1:A:597:LYS:CD	2:B:1081:GLY:O	2.50	0.60
2:B:987:ASN:OD1	2:B:990:ASP:N	2.24	0.60
3:C:77:SER:OG	3:C:219:PHE:O	2.20	0.60
16:P:608:GLN:HA	16:P:611:ILE:HD12	1.83	0.60
17:Q:154:LEU:H	17:Q:154:LEU:HD22	1.66	0.60
1:A:1188:ILE:O	1:A:1192:SER:N	2.30	0.60
2:B:296:ASP:OD2	2:B:379:ARG:NH2	2.34	0.60
2:B:420:TYR:HE1	2:B:455:GLU:HB3	1.65	0.60
9:I:2:SER:HB2	9:I:11:LEU:HD21	1.83	0.60
16:P:320:ILE:O	16:P:320:ILE:HG12	2.01	0.60
16:P:657:SER:HA	16:P:747:LEU:O	2.02	0.60
2:B:1161:ASP:OD1	2:B:1165:ASN:N	2.28	0.59
5:E:88:VAL:HG21	5:E:116:ILE:HG12	1.82	0.59
16:P:473:HIS:CE1	18:R:1:MET:SD	2.95	0.59
17:Q:378:LEU:HD21	18:R:235:ILE:CD1	2.32	0.59
1:A:719:ILE:O	1:A:724:PRO:HA	2.02	0.59
15:O:447:THR:HB	15:O:505:PHE:CZ	2.37	0.59
17:Q:366:TYR:CB	18:R:215:THR:CG2	2.80	0.59
18:R:177:LEU:HD21	18:R:185:LYS:HA	1.84	0.59
1:A:1194:GLY:O	1:A:1197:SER:OG	2.20	0.59
1:A:1654:PHE:HZ	6:F:89:GLU:HA	1.56	0.59
2:B:311:ARG:HE	9:I:16:LEU:HG	1.66	0.59
9:I:12:ASP:OD2	13:M:59:ARG:NH2	2.36	0.59
15:O:352:LEU:HD11	15:O:392:GLN:HG3	1.84	0.59
1:A:195:LYS:O	1:A:198:SER:OG	2.14	0.59
2:B:790:ASN:HA	2:B:936:MET:CE	2.33	0.59
16:P:60:VAL:O	16:P:61:VAL:HG23	2.02	0.59
16:P:355:GLU:HB3	18:R:24:ILE:HG23	1.83	0.59
17:Q:12:THR:HB	17:Q:33:HIS:ND1	2.18	0.59
17:Q:389:GLN:O	18:R:243:PRO:HG3	2.01	0.59
20:T:19:DC:H2'	20:T:20:DG:C8	2.37	0.59
1:A:91:PHE:O	1:A:95:TYR:N	2.24	0.59
2:B:1058:GLN:CG	2:B:1096:SER:O	2.45	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:136:LEU:HB3	3:C:204:LEU:HG	1.84	0.59
15:O:484:PHE:CE1	15:O:528:PHE:HA	2.36	0.59
1:A:1035:ASP:OD2	1:A:1039:ARG:NH2	2.33	0.59
2:B:396:ALA:HB1	2:B:523:GLU:OE1	2.02	0.59
2:B:931:TRP:HB3	2:B:936:MET:HE2	1.74	0.59
3:C:243:SER:OG	3:C:246:ARG:NH2	2.36	0.59
17:Q:139:LYS:HG2	17:Q:237:ILE:HG12	1.85	0.59
18:R:78:ARG:HH21	20:T:43:DT:H5"	1.64	0.59
1:A:1105:ARG:HH12	1:A:1138:GLU:HG2	1.66	0.59
1:A:1508:VAL:O	1:A:1508:VAL:HG12	2.00	0.59
1:A:1619:CYS:HA	1:A:1622:LEU:HB3	1.85	0.59
1:A:1651:THR:O	1:A:1651:THR:HG22	2.01	0.59
2:B:117:VAL:CB	18:R:277:ILE:HA	2.31	0.59
5:E:9:ILE:HG22	5:E:39:LEU:HD11	1.85	0.59
15:O:61:ASP:HA	15:O:64:ASP:HB2	1.84	0.59
1:A:513:ALA:O	1:A:516:ILE:HG22	2.02	0.59
1:A:552:GLU:HG2	1:A:553:GLN:H	1.67	0.59
1:A:1289:SER:HB3	1:A:1475:GLU:HG2	1.85	0.59
16:P:362:ARG:NH2	16:P:364:GLU:HG3	2.18	0.59
1:A:642:ASN:CB	2:B:1086:PHE:CE2	2.85	0.59
3:C:131:THR:O	3:C:175:GLN:NE2	2.34	0.59
6:F:106:PRO:HG2	7:G:55:GLU:HG2	1.84	0.59
17:Q:186:CYS:CB	18:R:208:TYR:HE2	1.95	0.59
17:Q:227:TYR:O	17:Q:230:ILE:HG13	2.03	0.59
18:R:299:THR:CG2	18:R:305:THR:HA	2.33	0.59
18:R:314:TRP:NE1	18:R:363:GLU:OE2	2.35	0.59
1:A:1013:THR:C	20:T:17:DT:C2	2.76	0.59
2:B:420:TYR:CE1	2:B:455:GLU:HB3	2.37	0.59
2:B:560:ARG:O	2:B:563:SER:OG	2.16	0.59
8:H:93:TYR:HA	8:H:145:ARG:HB3	1.84	0.59
16:P:477:TYR:CD2	18:R:2:PHE:HZ	2.19	0.59
2:B:116:ALA:CA	18:R:282:SER:C	2.71	0.58
2:B:299:ASP:OD1	2:B:301:PHE:N	2.35	0.58
2:B:1074:MET:CE	20:T:18:DT:H4'	2.33	0.58
9:I:19:ASN:HB3	9:I:22:ALA:HB2	1.85	0.58
15:O:422:GLN:NE2	15:O:591:TYR:O	2.36	0.58
1:A:464:GLU:HB2	1:A:465:GLY:HA2	1.85	0.58
1:A:591:ARG:HH21	19:S:6:A:H1'	1.67	0.58
16:P:197:ARG:HD2	16:P:262:GLY:N	2.18	0.58
17:Q:350:ARG:NE	17:Q:486:GLN:CG	2.64	0.58
1:A:596:HIS:CD2	1:A:598:ALA:HB3	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:671:GLN:CB	2:B:783:MET:CE	2.80	0.58
1:A:1316:VAL:HG13	1:A:1320:GLN:HE21	1.68	0.58
3:C:86:PHE:HE2	3:C:205:LYS:HG3	1.69	0.58
15:O:446:LEU:O	15:O:450:LEU:HG	2.03	0.58
16:P:59:ILE:O	16:P:552:LEU:HA	2.04	0.58
17:Q:9:ILE:HB	17:Q:16:PRO:CB	2.26	0.58
17:Q:20:TRP:CH2	17:Q:22:ILE:HG21	2.29	0.58
18:R:11:ARG:HG3	18:R:12:LYS:H	1.68	0.58
2:B:1119:ARG:NH2	2:B:1160:GLU:OE2	2.36	0.58
3:C:311:GLU:OE1	3:C:311:GLU:N	2.34	0.58
7:G:140:GLN:HB3	7:G:217:TRP:CD1	2.36	0.58
15:O:130:PRO:O	15:O:134:SER:N	2.25	0.58
16:P:458:LYS:HZ3	16:P:458:LYS:HA	1.68	0.58
17:Q:22:ILE:HD11	17:Q:26:ARG:CD	2.33	0.58
17:Q:375:LEU:HA	17:Q:378:LEU:HD12	1.84	0.58
18:R:362:ALA:O	18:R:365:TRP:HB2	2.02	0.58
1:A:582:LYS:HE3	1:A:584:ARG:HE	1.67	0.58
1:A:793:ILE:HG23	1:A:794:VAL:H	1.68	0.58
1:A:1258:ILE:HB	1:A:1501:ILE:HD12	1.83	0.58
8:H:110:ASP:O	8:H:129:TYR:N	2.36	0.58
17:Q:10:CYS:HB2	17:Q:17:SER:H	1.67	0.58
17:Q:249:CYS:SG	17:Q:282:ARG:NH1	2.77	0.58
1:A:53:ALA:HA	1:A:63:SER:HB2	1.85	0.58
1:A:65:CYS:HB3	1:A:75:HIS:CE1	2.38	0.58
1:A:411:VAL:HG11	1:A:416:ARG:HE	1.68	0.58
1:A:474:LYS:HD2	2:B:1096:SER:HB2	1.83	0.58
1:A:1637:PRO:CA	1:A:1647:ASN:HD21	2.16	0.58
2:B:1105:ARG:NH2	2:B:1173:THR:O	2.36	0.58
2:B:1134:ARG:HD3	2:B:1167:PHE:HE1	1.67	0.58
4:D:89:LEU:HD23	4:D:92:ILE:HD12	1.86	0.58
16:P:443:ASP:CB	18:R:3:GLU:HB3	2.31	0.58
17:Q:8:PRO:O	17:Q:9:ILE:C	2.42	0.58
17:Q:26:ARG:HB3	17:Q:34:VAL:HG11	1.75	0.58
17:Q:142:LYS:NZ	17:Q:146:ASP:OD2	2.25	0.58
18:R:257:ILE:HG23	18:R:266:SER:HB3	1.86	0.58
1:A:62:CYS:SG	1:A:65:CYS:N	2.75	0.58
2:B:280:LEU:HD23	2:B:354:LEU:HD13	1.85	0.58
2:B:464:PHE:O	2:B:468:GLY:N	2.31	0.58
2:B:1093:LEU:HD13	2:B:1093:LEU:O	2.04	0.58
15:O:445:TYR:O	15:O:449:TRP:N	2.23	0.58
18:R:168:ILE:HG12	18:R:169:PRO:N	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:ALA:O	1:A:196:ALA:N	2.29	0.58
1:A:628:PHE:CB	2:B:784:ASP:HB3	2.34	0.58
1:A:628:PHE:CB	2:B:785:ASP:CG	2.67	0.58
5:E:14:ARG:HD2	5:E:141:VAL:HG13	1.86	0.58
5:E:165:LEU:O	5:E:169:ARG:N	2.36	0.58
16:P:428:GLU:N	16:P:433:VAL:HG11	2.18	0.58
16:P:622:TYR:CZ	16:P:668:SER:HB3	2.38	0.58
20:T:14:DG:H8	20:T:14:DG:O5'	1.85	0.58
1:A:1155:PHE:CD2	1:A:1163:GLU:HG2	2.38	0.58
1:A:1274:GLU:HA	1:A:1290:TYR:HB3	1.85	0.58
2:B:211:ARG:HD2	2:B:239:VAL:HG11	1.85	0.58
2:B:504:HIS:CD2	2:B:506:GLY:H	2.21	0.58
3:C:40:PHE:HA	3:C:58:ASN:HB2	1.85	0.58
16:P:436:ILE:CG2	18:R:141:TRP:O	2.52	0.58
16:P:739:ASP:OD2	17:Q:271:LYS:HE2	2.04	0.58
1:A:469:LYS:O	2:B:1070:ARG:NH1	2.30	0.58
1:A:638:PRO:HB3	2:B:1087:LEU:HD12	1.86	0.58
1:A:672:ASP:CB	2:B:783:MET:SD	2.91	0.58
2:B:841:ASP:HA	2:B:847:TYR:CZ	2.39	0.58
2:B:893:ASN:OD1	20:T:39:DT:OP1	2.21	0.58
15:O:387:HIS:ND1	15:O:606:MET:SD	2.76	0.58
1:A:671:GLN:CB	2:B:783:MET:HE2	2.29	0.57
1:A:1447:GLN:HG3	1:A:1460:TYR:HB3	1.85	0.57
1:A:355:PHE:CD1	1:A:355:PHE:N	2.73	0.57
1:A:537:GLN:HB2	1:A:578:TYR:OH	2.04	0.57
1:A:642:ASN:CG	2:B:1086:PHE:CE2	2.73	0.57
14:N:123:SER:HA	14:N:131:LEU:H	1.69	0.57
15:O:391:GLN:NE2	15:O:609:TYR:OH	2.36	0.57
16:P:535:VAL:HG12	16:P:552:LEU:HB2	1.85	0.57
17:Q:24:ASP:OD2	17:Q:26:ARG:NH1	2.31	0.57
1:A:1258:ILE:HD12	1:A:1258:ILE:C	2.24	0.57
2:B:1063:ARG:CD	20:T:22:DG:OP2	2.51	0.57
2:B:1063:ARG:HD3	20:T:22:DG:OP1	2.04	0.57
13:M:81:PHE:HB2	13:M:88:ILE:HD12	1.85	0.57
16:P:329:ILE:HD12	16:P:330:PRO:HD2	1.86	0.57
17:Q:355:VAL:C	18:R:212:HIS:ND1	2.57	0.57
17:Q:366:TYR:HA	17:Q:369:TRP:CD1	2.39	0.57
17:Q:378:LEU:CD2	18:R:235:ILE:HD13	2.34	0.57
20:T:11:DA:N1	20:T:12:DC:C4	2.71	0.57
1:A:1559:ARG:HD2	1:A:1587:ASP:OD1	2.04	0.57
7:G:232:THR:O	7:G:248:THR:N	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:41:TYR:HB3	14:N:29:PHE:HB3	1.86	0.57
15:O:390:GLN:HE21	15:O:432:LYS:H	1.52	0.57
15:O:480:LEU:HA	15:O:483:ILE:HD12	1.86	0.57
16:P:391:THR:OG1	18:R:146:SER:HB3	2.04	0.57
16:P:419:ARG:CG	16:P:420:GLU:H	2.17	0.57
16:P:422:ILE:HG13	16:P:442:LEU:HD11	1.87	0.57
17:Q:441:ASP:O	17:Q:445:ARG:HG2	2.04	0.57
18:R:175:ILE:O	18:R:178:LEU:HB3	2.04	0.57
20:T:8:DT:H2'	20:T:9:DC:H6	1.68	0.57
1:A:1050:TYR:HB3	1:A:1054:ALA:HA	1.86	0.57
1:A:1311:GLU:OE1	1:A:1311:GLU:N	2.36	0.57
12:L:32:ALA:HB3	12:L:55:ILE:HG23	1.87	0.57
13:M:13:GLU:HG3	13:M:87:SER:HB2	1.86	0.57
15:O:484:PHE:CB	15:O:528:PHE:HD1	2.17	0.57
15:O:484:PHE:HB2	15:O:528:PHE:HD1	1.68	0.57
16:P:186:TYR:CD1	18:R:198:LEU:HB3	2.40	0.57
1:A:579:ARG:NH2	1:A:585:ASP:OD1	2.34	0.57
1:A:755:ILE:HD12	1:A:780:ILE:HD11	1.87	0.57
1:A:1053:ASP:OD2	1:A:1580:ARG:NH2	2.37	0.57
1:A:1246:VAL:O	1:A:1517:ARG:NH2	2.38	0.57
1:A:1310:LYS:HA	1:A:1313:LEU:HB3	1.86	0.57
2:B:117:VAL:HB	18:R:277:ILE:HA	1.86	0.57
2:B:1155:ASP:OD2	7:G:239:THR:N	2.37	0.57
7:G:147:LEU:HB2	7:G:155:ALA:HB3	1.86	0.57
15:O:379:ARG:CB	15:O:382:GLN:HE22	2.17	0.57
17:Q:140:ILE:HG22	17:Q:236:MET:HG2	1.85	0.57
1:A:581:ILE:HD11	1:A:605:VAL:HG21	1.87	0.57
1:A:1010:ALA:O	1:A:1013:THR:OG1	2.23	0.57
16:P:355:GLU:CA	18:R:24:ILE:HD12	2.34	0.57
16:P:422:ILE:CG1	16:P:442:LEU:HD11	2.35	0.57
16:P:732:LEU:O	16:P:735:GLU:N	2.37	0.57
17:Q:22:ILE:HD12	17:Q:24:ASP:OD2	2.04	0.57
17:Q:186:CYS:HB3	18:R:208:TYR:OH	2.05	0.57
18:R:138:PHE:CE2	18:R:140:ILE:HD11	2.38	0.57
1:A:477:ASN:H	2:B:1095:SER:HB2	1.70	0.57
1:A:493:ASN:HA	1:A:653:THR:HG21	1.86	0.57
1:A:1262:LEU:H	1:A:1265:GLU:CD	2.07	0.57
2:B:1084:THR:O	2:B:1088:LEU:CB	2.48	0.57
15:O:422:GLN:NE2	15:O:589:GLN:O	2.38	0.57
16:P:391:THR:HG23	18:R:149:LYS:HD3	1.86	0.57
17:Q:366:TYR:CB	18:R:215:THR:HG21	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:LEU:HD12	1:A:241:PRO:HD2	1.87	0.57
2:B:114:SER:O	18:R:281:LYS:CA	2.25	0.57
2:B:117:VAL:CG1	18:R:277:ILE:CA	2.80	0.57
2:B:627:GLY:N	2:B:641:TYR:O	2.34	0.57
10:J:9:SER:HB2	10:J:45:CYS:SG	2.45	0.57
15:O:385:MET:HA	15:O:388:VAL:HG12	1.87	0.57
16:P:384:ASP:HB3	16:P:389:TRP:CD1	2.39	0.57
18:R:177:LEU:CD2	18:R:185:LYS:HA	2.34	0.57
1:A:87:ASN:N	1:A:355:PHE:O	2.32	0.57
1:A:371:SER:O	1:A:378:HIS:N	2.37	0.57
1:A:747:ILE:HG22	1:A:774:GLY:HA2	1.87	0.57
16:P:376:ASP:C	16:P:378:SER:H	2.09	0.57
16:P:419:ARG:HG2	16:P:420:GLU:H	1.67	0.57
16:P:725:VAL:HG23	17:Q:446:TYR:CG	2.35	0.57
17:Q:286:LEU:HD13	17:Q:286:LEU:H	1.69	0.57
18:R:354:LEU:HG	18:R:368:TYR:OH	2.04	0.57
2:B:156:ARG:HH21	2:B:450:LEU:HD12	1.70	0.56
2:B:709:PHE:CE2	2:B:992:PRO:HG2	2.39	0.56
2:B:817:ARG:HB3	21:U:17:DT:C4'	2.35	0.56
3:C:160:ALA:O	3:C:196:LEU:N	2.36	0.56
17:Q:20:TRP:CE2	17:Q:28:THR:HB	2.39	0.56
17:Q:436:LEU:HD12	17:Q:436:LEU:H	1.70	0.56
1:A:618:TYR:HE1	2:B:783:MET:HB3	1.65	0.56
2:B:117:VAL:HG21	18:R:276:GLN:HB3	1.75	0.56
2:B:379:ARG:HE	2:B:580:GLY:HA2	1.69	0.56
2:B:752:VAL:HG21	2:B:965:GLU:HG3	1.88	0.56
2:B:812:ALA:HB2	2:B:815:ARG:HH11	1.70	0.56
2:B:1099:THR:OG1	2:B:1100:GLN:N	2.38	0.56
8:H:25:ARG:NH1	8:H:27:GLU:OE2	2.32	0.56
9:I:15:ASP:OD2	9:I:32:GLN:N	2.36	0.56
15:O:487:ARG:HE	15:O:502:LEU:HD13	1.69	0.56
17:Q:328:LEU:HD22	17:Q:328:LEU:H	1.69	0.56
17:Q:366:TYR:HB2	18:R:215:THR:HG21	1.87	0.56
18:R:299:THR:HG21	18:R:305:THR:HA	1.86	0.56
1:A:556:ALA:HA	15:O:242:VAL:HG12	1.87	0.56
1:A:831:ASP:OD2	2:B:1010:ASN:ND2	2.37	0.56
1:A:1013:THR:CB	20:T:17:DT:H3	2.15	0.56
2:B:212:ASN:HD22	2:B:212:ASN:N	2.02	0.56
2:B:894:LYS:HE3	17:Q:405:ASP:CG	2.21	0.56
16:P:24:SER:OG	18:R:321:GLN:OE1	2.22	0.56
16:P:68:THR:HB	16:P:545:SER:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:320:ILE:O	16:P:322:GLY:N	2.38	0.56
16:P:629:ARG:HH22	16:P:662:LEU:HD21	1.70	0.56
17:Q:22:ILE:HD12	17:Q:26:ARG:NE	2.18	0.56
1:A:593:PRO:HB3	20:T:18:DT:H1'	1.86	0.56
1:A:1016:SER:OG	1:A:1197:SER:OG	2.19	0.56
1:A:1182:GLY:O	1:A:1650:GLY:CA	2.54	0.56
2:B:60:LEU:O	2:B:64:GLY:N	2.37	0.56
2:B:338:PHE:HZ	2:B:357:ILE:HD11	1.69	0.56
2:B:705:PRO:HG2	2:B:921:HIS:CE1	2.40	0.56
6:F:140:ASP:OD1	6:F:142:SER:N	2.35	0.56
7:G:37:CYS:HB2	7:G:125:TRP:NE1	2.20	0.56
9:I:30:CYS:HB3	9:I:35:ALA:H	1.70	0.56
1:A:509:GLU:CG	1:A:579:ARG:HE	2.18	0.56
2:B:247:THR:OG1	2:B:477:ASP:OD1	2.21	0.56
2:B:320:LEU:HD11	2:B:326:VAL:HA	1.87	0.56
2:B:714:ARG:HG2	2:B:959:THR:HG22	1.86	0.56
2:B:753:LYS:O	2:B:981:SER:N	2.24	0.56
2:B:768:GLY:N	2:B:1032:TYR:OH	2.38	0.56
5:E:40:GLU:O	5:E:44:ALA:N	2.27	0.56
5:E:183:PRO:O	5:E:187:TYR:N	2.34	0.56
15:O:379:ARG:HA	15:O:382:GLN:OE1	2.05	0.56
15:O:457:ARG:O	15:O:460:GLU:N	2.38	0.56
16:P:209:LYS:HZ1	16:P:277:VAL:HG11	1.69	0.56
18:R:309:ALA:O	18:R:313:LEU:HB2	2.05	0.56
1:A:320:VAL:HA	1:A:323:ILE:HD12	1.88	0.56
2:B:264:TRP:CD1	2:B:265:ARG:HG2	2.40	0.56
7:G:29:ASP:OD1	7:G:30:GLU:N	2.36	0.56
8:H:3:ASN:OD1	8:H:4:THR:N	2.38	0.56
16:P:290:GLU:HB3	16:P:342:GLN:HB3	1.86	0.56
19:S:5:G:C2	20:T:19:DC:N3	2.74	0.56
1:A:1088:HIS:CG	6:F:152:ILE:HD11	2.41	0.56
2:B:913:ILE:HD11	2:B:930:LYS:H	1.71	0.56
14:N:85:HIS:CE1	14:N:141:GLU:HG3	2.40	0.56
15:O:442:VAL:HA	15:O:445:TYR:HB3	1.87	0.56
16:P:273:ARG:HG2	16:P:291:PRO:HB3	1.87	0.56
16:P:450:ARG:NH2	16:P:506:THR:O	2.38	0.56
16:P:657:SER:O	16:P:657:SER:OG	2.19	0.56
17:Q:96:ILE:HD12	17:Q:103:LEU:HD12	1.87	0.56
1:A:653:THR:OG1	1:A:654:ASP:N	2.39	0.56
2:B:566:TYR:HB3	13:M:74:ASN:OD1	2.06	0.56
2:B:1074:MET:HE1	20:T:18:DT:C4'	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1084:THR:O	2:B:1088:LEU:CD2	2.49	0.56
7:G:234:ARG:N	7:G:246:ASP:O	2.37	0.56
16:P:428:GLU:HB3	16:P:433:VAL:HG21	1.87	0.56
17:Q:495:LYS:HD2	17:Q:499:LYS:HZ2	1.71	0.56
18:R:222:LEU:O	18:R:226:ARG:HG3	2.06	0.56
18:R:294:VAL:HB	18:R:295:PRO:CD	2.36	0.56
1:A:1463:ASP:OD2	1:A:1468:LYS:N	2.35	0.56
2:B:714:ARG:HG2	2:B:959:THR:CG2	2.36	0.56
7:G:82:LEU:HD11	7:G:125:TRP:HB2	1.87	0.56
10:J:45:CYS:O	10:J:48:ARG:HG2	2.06	0.56
13:M:75:GLN:O	14:N:58:PHE:N	2.39	0.56
1:A:512:THR:HG21	1:A:514:TYR:HE2	1.70	0.56
11:K:50:LEU:HD11	11:K:64:GLN:HB2	1.87	0.56
16:P:666:SER:HB3	16:P:742:TRP:NE1	2.21	0.56
16:P:713:ILE:O	16:P:717:LYS:HG2	2.06	0.56
18:R:171:ARG:O	18:R:174:GLU:HB3	2.05	0.56
1:A:117:ARG:HB3	1:A:185:ARG:NH1	2.20	0.55
1:A:880:GLN:HG3	1:A:972:TYR:OH	2.06	0.55
2:B:1093:LEU:HD11	2:B:1098:TYR:CB	2.33	0.55
6:F:99:LEU:O	6:F:102:SER:OG	2.15	0.55
6:F:147:SER:N	6:F:150:GLU:OE2	2.35	0.55
13:M:36:THR:HG21	13:M:62:TYR:CE2	2.41	0.55
16:P:185:GLN:C	18:R:198:LEU:HD23	2.27	0.55
16:P:300:LEU:HA	16:P:320:ILE:HA	1.87	0.55
16:P:697:GLU:HG2	16:P:698:LYS:H	1.70	0.55
16:P:725:VAL:CG2	17:Q:446:TYR:HD1	1.81	0.55
17:Q:410:ARG:HE	17:Q:413:LEU:HD13	1.71	0.55
1:A:36:THR:HG22	1:A:45:VAL:HG21	1.86	0.55
1:A:37:VAL:HG12	1:A:38:LEU:HG	1.88	0.55
1:A:1179:ILE:HD11	1:A:1183:GLU:OE2	2.07	0.55
2:B:17:ARG:O	2:B:21:ARG:N	2.30	0.55
15:O:491:PHE:CD2	15:O:498:TRP:CE3	2.88	0.55
16:P:724:LEU:HD11	17:Q:443:GLN:HG2	1.88	0.55
1:A:543:LEU:HB2	17:Q:34:VAL:O	2.06	0.55
1:A:666:VAL:HG23	1:A:667:ARG:HG3	1.87	0.55
2:B:20:GLU:OE2	2:B:24:ARG:NH1	2.33	0.55
2:B:321:GLN:O	2:B:322:ASN:HB2	2.06	0.55
2:B:1061:LYS:O	2:B:1067:GLY:HA3	2.05	0.55
2:B:1078:ALA:C	2:B:1082:HIS:HB2	2.26	0.55
8:H:21:ASN:OD1	8:H:22:LYS:N	2.39	0.55
15:O:379:ARG:HA	15:O:382:GLN:HE22	1.69	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:194:ARG:HG2	16:P:538:LEU:HD11	1.87	0.55
16:P:420:GLU:O	16:P:442:LEU:HD22	2.07	0.55
16:P:760:ILE:O	16:P:764:LEU:HG	2.06	0.55
1:A:527:PRO:HD3	1:A:554:ARG:NH2	2.20	0.55
1:A:882:ILE:HG13	1:A:888:LYS:HB3	1.88	0.55
1:A:959:VAL:HG22	1:A:965:THR:HG22	1.88	0.55
2:B:132:SER:OG	2:B:462:GLN:NE2	2.39	0.55
7:G:40:ARG:HB2	7:G:123:TYR:HE1	1.70	0.55
15:O:498:TRP:HB3	15:O:502:LEU:HD12	1.88	0.55
16:P:301:GLN:HG3	16:P:361:LYS:H	1.70	0.55
18:R:408:ILE:HG23	18:R:435:LEU:HD13	1.87	0.55
1:A:1238:MET:HE2	1:A:1525:ASN:N	2.22	0.55
2:B:816:ASN:HB3	21:U:18:DG:P	2.46	0.55
16:P:254:ILE:HD11	16:P:365:TRP:HD1	1.71	0.55
18:R:253:ILE:HA	18:R:256:GLU:HB3	1.89	0.55
1:A:1637:PRO:CB	1:A:1647:ASN:ND2	2.64	0.55
3:C:69:ARG:NH2	11:K:70:HIS:HB2	2.21	0.55
16:P:323:ASN:HA	16:P:350:THR:HA	1.88	0.55
17:Q:131:HIS:O	17:Q:135:ILE:HG12	2.05	0.55
17:Q:308:SER:O	17:Q:312:LEU:HD22	2.05	0.55
17:Q:505:ILE:HA	17:Q:508:ALA:HB3	1.88	0.55
18:R:16:ARG:HG3	18:R:184:ASN:ND2	2.22	0.55
18:R:222:LEU:HD23	18:R:226:ARG:NH2	2.20	0.55
18:R:412:ARG:NH2	18:R:439:GLU:OE2	2.35	0.55
20:T:11:DA:C5	20:T:12:DC:N4	2.75	0.55
1:A:588:LEU:HD22	2:B:1087:LEU:HD21	1.88	0.55
2:B:186:GLU:CD	2:B:731:VAL:H	2.10	0.55
2:B:728:THR:HG21	10:J:56:LEU:HD21	1.88	0.55
2:B:731:VAL:HG11	10:J:59:LYS:HB3	1.88	0.55
2:B:818:GLY:C	2:B:820:PRO:N	2.59	0.55
2:B:851:TYR:HD1	2:B:881:TYR:CE1	2.24	0.55
15:O:173:HIS:HB3	15:O:221:TYR:CE2	2.41	0.55
15:O:359:GLY:HA2	15:O:362:ASN:HD22	1.72	0.55
15:O:383:TYR:OH	15:O:595:ASP:O	2.16	0.55
16:P:353:ASP:OD1	16:P:355:GLU:HG3	2.06	0.55
17:Q:104:PHE:HZ	17:Q:156:LEU:HB2	1.72	0.55
17:Q:310:PHE:O	17:Q:314:ILE:HG13	2.06	0.55
17:Q:331:ILE:CG2	17:Q:475:ALA:HB1	2.36	0.55
18:R:83:HIS:O	18:R:85:ARG:N	2.39	0.55
1:A:463:LYS:HZ1	20:T:16:DT:H2'	1.72	0.55
1:A:938:VAL:O	1:A:941:SER:OG	2.16	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1104:TYR:HB3	1:A:1120:TYR:CE2	2.42	0.55
2:B:74:PHE:HE1	2:B:94:LYS:HG3	1.70	0.55
2:B:894:LYS:CE	17:Q:405:ASP:CG	2.75	0.55
3:C:95:GLU:OE1	3:C:95:GLU:N	2.39	0.55
3:C:172:GLN:H	3:C:175:GLN:HB2	1.70	0.55
16:P:762:ARG:HA	16:P:762:ARG:HE	1.71	0.55
1:A:487:ASP:OD2	11:K:95:HIS:NE2	2.30	0.55
1:A:642:ASN:ND2	2:B:1086:PHE:CE2	2.68	0.55
1:A:1182:GLY:O	1:A:1650:GLY:HA2	2.06	0.55
1:A:1297:PHE:CE2	9:I:58:SER:HB2	2.42	0.55
1:A:1660:VAL:O	7:G:102:GLU:HA	2.07	0.55
2:B:936:MET:HG2	2:B:948:ILE:HD11	1.88	0.55
3:C:218:LYS:HG3	3:C:218:LYS:O	2.06	0.55
5:E:78:LEU:HD12	5:E:107:THR:O	2.07	0.55
8:H:115:TYR:CE1	8:H:124:ARG:HG3	2.42	0.55
16:P:371:LYS:HD2	16:P:432:PRO:HB3	1.89	0.55
20:T:11:DA:C2	20:T:12:DC:C4	2.95	0.55
1:A:553:GLN:N	1:A:553:GLN:OE1	2.40	0.55
3:C:253:PRO:HD2	14:N:180:PHE:HB3	1.88	0.55
4:D:19:PRO:HA	7:G:47:VAL:HG12	1.89	0.55
15:O:443:ALA:O	15:O:446:LEU:HB3	2.07	0.55
16:P:348:HIS:HE1	18:R:154:LYS:HD3	1.72	0.55
16:P:614:GLU:OE2	16:P:734:LYS:NZ	2.26	0.55
17:Q:177:TYR:OH	17:Q:248:SER:O	2.11	0.55
18:R:23:TYR:HD1	18:R:173:MET:HG3	1.71	0.55
1:A:1238:MET:HE3	1:A:1526:PHE:HA	1.90	0.54
7:G:138:PHE:CZ	7:G:146:GLY:HA3	2.42	0.54
16:P:443:ASP:HB2	18:R:2:PHE:CA	2.37	0.54
16:P:486:ALA:O	18:R:138:PHE:CE1	2.59	0.54
2:B:641:TYR:CB	2:B:643:PHE:CE1	2.89	0.54
16:P:182:LEU:CD1	16:P:185:GLN:HG2	2.36	0.54
16:P:348:HIS:HE1	18:R:154:LYS:CD	2.21	0.54
16:P:743:SER:OG	17:Q:250:GLN:HG3	2.07	0.54
17:Q:8:PRO:HB2	17:Q:19:LEU:CD2	2.36	0.54
18:R:301:SER:O	18:R:303:THR:N	2.35	0.54
1:A:527:PRO:CD	1:A:554:ARG:HH12	2.19	0.54
1:A:1018:TYR:HB2	20:T:17:DT:H5”	1.89	0.54
2:B:115:SER:O	18:R:280:SER:C	2.33	0.54
2:B:320:LEU:HD22	2:B:325:GLN:HB2	1.87	0.54
7:G:74:ASN:OD1	7:G:75:ASN:N	2.41	0.54
18:R:246:GLN:NE2	18:R:247:ILE:HD12	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1014:SER:O	20:T:17:DT:O4'	2.25	0.54
2:B:71:LYS:N	2:B:97:VAL:O	2.40	0.54
2:B:265:ARG:O	2:B:267:ASN:ND2	2.39	0.54
2:B:1105:ARG:HG2	2:B:1172:GLU:HB3	1.90	0.54
7:G:235:ASN:H	7:G:246:ASP:HB3	1.72	0.54
16:P:229:ARG:HG3	16:P:230:HIS:N	2.21	0.54
17:Q:186:CYS:O	18:R:208:TYR:CZ	2.61	0.54
18:R:357:PRO:HB3	18:R:359:MET:SD	2.48	0.54
2:B:99:VAL:HG12	2:B:100:GLU:H	1.72	0.54
13:M:43:LYS:HB2	14:N:29:PHE:CD1	2.43	0.54
14:N:54:TRP:CD1	14:N:135:LYS:HB2	2.42	0.54
17:Q:6:ARG:HA	17:Q:18:ARG:HD2	1.88	0.54
1:A:111:LYS:HD2	1:A:114:GLU:HG2	1.88	0.54
2:B:683:ASN:HA	14:N:150:TYR:CE1	2.42	0.54
2:B:1074:MET:CE	20:T:18:DT:C4'	2.86	0.54
3:C:105:PRO:HB2	3:C:187:ALA:HB3	1.88	0.54
7:G:235:ASN:HD22	7:G:237:HIS:CE1	2.26	0.54
10:J:31:ASP:OD1	10:J:34:THR:N	2.29	0.54
14:N:125:ALA:C	14:N:127:ASP:H	2.11	0.54
15:O:441:PHE:O	15:O:445:TYR:N	2.28	0.54
16:P:598:LEU:HA	16:P:601:ARG:HG3	1.89	0.54
17:Q:136:ILE:HG12	17:Q:243:PHE:CZ	2.42	0.54
2:B:1114:GLN:OE1	2:B:1129:ARG:NH2	2.38	0.54
16:P:185:GLN:C	18:R:198:LEU:CD2	2.76	0.54
16:P:194:ARG:CZ	16:P:511:ILE:HG12	2.38	0.54
17:Q:366:TYR:HA	17:Q:369:TRP:CE2	2.43	0.54
18:R:427:PRO:HG2	18:R:429:ARG:NH2	2.23	0.54
20:T:7:DT:H3	21:U:43:DA:N6	2.06	0.54
1:A:321:LYS:CE	1:A:325:ASP:OD2	2.56	0.54
2:B:832:TRP:CZ3	2:B:834:LYS:HA	2.43	0.54
2:B:1065:ARG:O	2:B:1066:HIS:CB	2.56	0.54
3:C:134:LEU:HD23	3:C:169:PHE:HA	1.89	0.54
3:C:157:TYR:HB2	3:C:160:ALA:HB2	1.90	0.54
17:Q:314:ILE:O	17:Q:318:LEU:HB2	2.08	0.54
17:Q:323:ASP:N	17:Q:324:ARG:N	2.55	0.54
19:S:5:G:H8	19:S:5:G:O5'	1.90	0.54
1:A:435:ASN:O	1:A:439:ASP:N	2.41	0.54
1:A:578:TYR:N	1:A:578:TYR:CD1	2.75	0.54
1:A:627:ASP:N	1:A:631:ASP:OD2	2.41	0.54
1:A:1018:TYR:HE1	20:T:16:DT:P	2.14	0.54
2:B:101:GLN:HE21	18:R:359:MET:HE1	0.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:396:ALA:HA	2:B:521:LEU:CD1	2.37	0.54
2:B:432:ILE:O	2:B:435:GLY:N	2.31	0.54
2:B:492:ASN:OD1	2:B:495:ARG:N	2.30	0.54
8:H:29:ALA:HA	8:H:37:LYS:HA	1.90	0.54
17:Q:366:TYR:HB2	18:R:215:THR:CG2	2.38	0.54
18:R:252:GLY:O	18:R:256:GLU:CB	2.56	0.54
1:A:462:LYS:O	1:A:464:GLU:N	2.38	0.54
1:A:1443:GLN:HG2	1:A:1446:ARG:NH2	2.23	0.54
2:B:566:TYR:HE1	2:B:572:PRO:HA	1.72	0.54
5:E:185:ALA:O	5:E:189:GLY:N	2.40	0.54
15:O:360:VAL:HA	15:O:363:THR:HG22	1.89	0.54
15:O:532:ALA:O	15:O:536:SER:N	2.41	0.54
16:P:384:ASP:HB3	16:P:389:TRP:HD1	1.71	0.54
17:Q:356:VAL:HG23	18:R:208:TYR:CD2	2.24	0.54
17:Q:374:THR:HG23	18:R:219:LEU:HD13	1.90	0.54
1:A:457:LYS:HG3	1:A:1619:CYS:SG	2.48	0.53
1:A:591:ARG:HB2	1:A:633:MET:HG2	1.90	0.53
1:A:1328:ALA:HA	1:A:1331:LYS:HB3	1.90	0.53
2:B:114:SER:O	18:R:280:SER:O	2.25	0.53
2:B:1051:PRO:HG2	2:B:1059:PRO:HA	1.90	0.53
7:G:45:LEU:HD13	7:G:47:VAL:HG13	1.90	0.53
9:I:11:LEU:N	9:I:37:TYR:OH	2.37	0.53
15:O:361:PHE:HZ	15:O:399:PHE:HB2	1.73	0.53
17:Q:22:ILE:HD12	17:Q:26:ARG:NH1	2.24	0.53
17:Q:330:TRP:O	17:Q:334:LEU:HB2	2.08	0.53
18:R:250:LEU:O	18:R:253:ILE:N	2.40	0.53
2:B:792:SER:O	2:B:796:ARG:HG3	2.08	0.53
3:C:81:GLU:O	12:L:69:ALA:N	2.32	0.53
7:G:170:HIS:HA	7:G:215:GLY:HA3	1.90	0.53
16:P:383:ILE:HG12	16:P:390:GLN:HG2	1.89	0.53
16:P:411:LYS:HB2	16:P:412:ASN:OD1	2.08	0.53
1:A:672:ASP:CG	2:B:783:MET:CE	2.77	0.53
2:B:101:GLN:HE22	18:R:359:MET:HE3	1.71	0.53
5:E:26:ARG:HH21	5:E:187:TYR:C	2.12	0.53
16:P:577:LEU:HD21	17:Q:499:LYS:HB2	1.89	0.53
18:R:231:LEU:O	18:R:235:ILE:HG12	2.08	0.53
18:R:416:LYS:O	18:R:419:LEU:N	2.41	0.53
1:A:1513:GLU:O	1:A:1516:LYS:N	2.37	0.53
2:B:45:HIS:O	2:B:48:SER:OG	2.18	0.53
2:B:994:ASP:HA	2:B:1007:TYR:OH	2.09	0.53
15:O:200:ASN:OD1	17:Q:14:ASN:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:254:ILE:HD11	16:P:365:TRP:CD1	2.43	0.53
16:P:421:ILE:CG2	16:P:423:ILE:HG13	2.38	0.53
16:P:452:THR:HG21	16:P:508:ILE:HG22	1.90	0.53
16:P:778:ASP:OD1	16:P:779:ASP:N	2.42	0.53
1:A:520:ARG:HH21	1:A:559:ASN:ND2	2.06	0.53
1:A:949:GLN:HA	1:A:981:TYR:HA	1.90	0.53
1:A:962:SER:HB3	2:B:670:VAL:HG12	1.90	0.53
1:A:1637:PRO:HB3	1:A:1647:ASN:ND2	2.23	0.53
3:C:43:ASN:O	3:C:55:ASP:N	2.37	0.53
9:I:35:ALA:HB2	13:M:59:ARG:HH22	1.72	0.53
15:O:484:PHE:CZ	15:O:528:PHE:HA	2.43	0.53
16:P:185:GLN:O	18:R:198:LEU:HD21	2.08	0.53
1:A:1136:VAL:HG11	1:A:1140:PHE:HD2	1.74	0.53
1:A:1238:MET:HE1	1:A:1524:VAL:HG13	1.90	0.53
1:A:1239:THR:HG23	1:A:1518:VAL:HG11	1.89	0.53
2:B:650:LEU:HB3	2:B:663:ILE:CG2	2.39	0.53
5:E:83:CYS:HB2	5:E:110:PHE:CZ	2.43	0.53
15:O:487:ARG:NH2	15:O:502:LEU:HD13	2.22	0.53
16:P:436:ILE:HG21	18:R:141:TRP:O	2.09	0.53
1:A:1506:ARG:O	1:A:1522:GLU:OE1	2.26	0.53
2:B:731:VAL:HA	10:J:60:PHE:CE1	2.42	0.53
15:O:434:LEU:HD22	15:O:439:ILE:CD1	2.35	0.53
16:P:186:TYR:CD1	18:R:198:LEU:HD23	2.44	0.53
16:P:715:TYR:CE1	16:P:733:THR:HG23	2.44	0.53
17:Q:350:ARG:CD	17:Q:486:GLN:CG	2.83	0.53
18:R:250:LEU:HD23	18:R:251:TRP:H	1.72	0.53
20:T:17:DT:H6	20:T:17:DT:O5'	1.92	0.53
1:A:646:GLU:OE2	6:F:91:ALA:CB	2.57	0.53
13:M:60:LEU:HA	13:M:102:SER:HA	1.90	0.53
15:O:418:ILE:HG12	15:O:475:ALA:HB2	1.91	0.53
16:P:433:VAL:HG23	16:P:434:ARG:O	2.08	0.53
16:P:470:SER:O	16:P:505:PRO:HD2	2.08	0.53
2:B:75:ASP:OD1	2:B:93:ASN:N	2.42	0.53
2:B:320:LEU:CD2	2:B:326:VAL:N	2.71	0.53
2:B:1106:GLU:O	2:B:1197:ARG:NH2	2.38	0.53
8:H:101:ALA:HB2	8:H:116:TYR:CE2	2.44	0.53
9:I:46:LYS:HE3	9:I:48:VAL:HG23	1.91	0.53
15:O:352:LEU:HD21	15:O:395:LEU:HD11	1.91	0.53
16:P:302:VAL:HG21	16:P:362:ARG:HD2	1.91	0.53
16:P:455:LYS:H	16:P:455:LYS:HD2	1.74	0.53
2:B:954:PHE:CB	2:B:955:PRO:CD	2.87	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1074:MET:HE1	20:T:18:DT:O4'	2.09	0.53
7:G:47:VAL:HB	7:G:65:HIS:CD2	2.44	0.53
15:O:484:PHE:CD1	15:O:528:PHE:HA	2.43	0.53
16:P:215:ASN:N	16:P:220:THR:OG1	2.42	0.53
18:R:209:ARG:H	18:R:209:ARG:HD3	1.74	0.53
1:A:797:LEU:HD23	1:A:809:VAL:HG21	1.91	0.52
1:A:1060:GLU:OE1	1:A:1580:ARG:NH1	2.43	0.52
1:A:1637:PRO:HB3	1:A:1647:ASN:HD21	1.70	0.52
2:B:778:TYR:CE2	2:B:937:PRO:HD3	2.44	0.52
2:B:841:ASP:OD2	12:L:58:LYS:NZ	2.35	0.52
2:B:916:LYS:NZ	19:S:5:G:H4'	2.24	0.52
20:T:14:DG:H2'	20:T:15:DC:C6	2.44	0.52
1:A:1049:MET:HB2	1:A:1052:GLY:HA2	1.92	0.52
2:B:691:PHE:HB2	2:B:695:ASN:HD21	1.73	0.52
2:B:828:GLY:HA3	2:B:862:PHE:CD1	2.43	0.52
2:B:916:LYS:HZ2	19:S:5:G:H4'	1.73	0.52
6:F:137:TYR:CD1	6:F:143:PHE:HB3	2.44	0.52
7:G:219:ASP:OD1	7:G:222:GLY:N	2.42	0.52
15:O:62:ASP:HB3	15:O:67:ASP:HB3	1.91	0.52
15:O:473:PHE:O	15:O:477:PHE:N	2.40	0.52
16:P:261:VAL:HG22	16:P:262:GLY:H	1.74	0.52
1:A:836:THR:N	1:A:915:GLY:O	2.22	0.52
16:P:261:VAL:HG22	16:P:262:GLY:N	2.24	0.52
16:P:681:GLN:HA	16:P:684:GLN:HB2	1.92	0.52
2:B:211:ARG:NH2	2:B:645:GLY:HA3	2.24	0.52
2:B:403:LEU:HD11	2:B:411:MET:HE3	1.91	0.52
2:B:755:ASN:ND2	2:B:980:ASP:OD1	2.43	0.52
4:D:43:PHE:O	4:D:47:LYS:HG2	2.10	0.52
7:G:20:HIS:ND1	7:G:20:HIS:O	2.43	0.52
15:O:78:VAL:HG23	15:O:118:SER:HB3	1.91	0.52
16:P:358:SER:HB3	16:P:377:ARG:CD	2.34	0.52
16:P:544:SER:O	16:P:546:GLU:N	2.40	0.52
17:Q:364:SER:O	17:Q:367:PHE:HB2	2.10	0.52
1:A:50:TYR:OH	1:A:383:ASN:ND2	2.43	0.52
1:A:600:MET:CB	2:B:1082:HIS:CD2	2.91	0.52
1:A:1238:MET:CE	1:A:1525:ASN:C	2.78	0.52
1:A:1297:PHE:HB3	1:A:1301:GLU:OE1	2.10	0.52
1:A:1656:VAL:HG11	6:F:96:THR:HG21	1.89	0.52
2:B:216:ALA:HB1	2:B:384:LEU:HD22	1.90	0.52
2:B:643:PHE:N	2:B:643:PHE:CD1	2.77	0.52
2:B:788:ILE:HB	2:B:948:ILE:HB	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:124:VAL:HB	5:E:125:PRO:HD3	1.91	0.52
6:F:89:GLU:OE2	6:F:136:ARG:NE	2.41	0.52
13:M:81:PHE:HD1	13:M:88:ILE:HB	1.74	0.52
15:O:435:SER:HB3	15:O:438:GLN:HG3	1.91	0.52
16:P:242:ILE:HD13	16:P:273:ARG:HE	1.75	0.52
16:P:314:GLN:OE1	16:P:314:GLN:HA	2.09	0.52
16:P:776:ASP:O	16:P:777:MET:HG2	2.10	0.52
17:Q:159:THR:O	17:Q:163:SER:OG	2.16	0.52
1:A:223:PHE:CE2	1:A:227:LEU:HD11	2.45	0.52
1:A:463:LYS:HZ2	20:T:16:DT:H71	1.73	0.52
1:A:1645:LYS:NZ	1:A:1645:LYS:CB	2.73	0.52
2:B:37:LEU:HD12	2:B:759:ASP:HB3	1.91	0.52
2:B:110:ASN:HA	2:B:118:GLU:HG2	1.92	0.52
8:H:39:THR:HB	8:H:124:ARG:HB3	1.91	0.52
10:J:8:PHE:HB2	10:J:48:ARG:HH22	1.73	0.52
15:O:584:GLN:O	15:O:588:LEU:HG	2.09	0.52
15:O:602:TYR:HA	15:O:605:LEU:HD12	1.92	0.52
16:P:433:VAL:HG23	16:P:434:ARG:N	2.24	0.52
1:A:93:GLN:HB2	1:A:355:PHE:HE2	1.75	0.52
1:A:130:ILE:O	1:A:133:SER:OG	2.22	0.52
1:A:638:PRO:CB	2:B:1087:LEU:HD12	2.39	0.52
1:A:1640:ARG:NH1	1:A:1640:ARG:CG	2.73	0.52
2:B:516:THR:HA	2:B:519:LYS:HE2	1.91	0.52
2:B:773:VAL:HG21	2:B:1033:TYR:HE1	1.73	0.52
2:B:841:ASP:OD1	2:B:842:GLU:N	2.38	0.52
3:C:116:VAL:HG22	3:C:130:ASN:HB3	1.92	0.52
6:F:117:PRO:HA	6:F:120:ILE:HD12	1.91	0.52
9:I:29:GLU:HA	9:I:36:ILE:HA	1.91	0.52
15:O:78:VAL:HG12	15:O:88:ILE:HG21	1.91	0.52
16:P:389:TRP:CH2	18:R:149:LYS:CG	2.93	0.52
18:R:303:THR:HG22	18:R:304:HIS:H	1.75	0.52
1:A:1303:SER:O	1:A:1307:ASP:HA	2.10	0.52
1:A:1654:PHE:HE2	6:F:89:GLU:N	2.07	0.52
2:B:135:GLY:O	2:B:161:LEU:N	2.25	0.52
2:B:368:GLN:O	2:B:372:ARG:NH1	2.43	0.52
10:J:7:CYS:HA	10:J:49:MET:HG3	1.92	0.52
15:O:169:THR:HA	15:O:172:HIS:ND1	2.25	0.52
15:O:477:PHE:HE2	15:O:525:MET:HE1	1.74	0.52
16:P:473:HIS:N	16:P:504:THR:HG21	2.24	0.52
16:P:585:GLU:O	16:P:589:ILE:HG13	2.10	0.52
16:P:622:TYR:O	16:P:626:LEU:CB	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:706:GLU:O	16:P:708:VAL:HG23	2.10	0.52
17:Q:101:LYS:O	17:Q:105:LEU:HG	2.09	0.52
17:Q:414:TYR:CE2	17:Q:419:LEU:HB3	2.45	0.52
18:R:346:ILE:HD11	18:R:374:LEU:HD12	1.91	0.52
18:R:436:LYS:HA	18:R:439:GLU:HB2	1.92	0.52
1:A:464:GLU:HB2	1:A:465:GLY:CA	2.40	0.52
1:A:552:GLU:HG2	1:A:553:GLN:N	2.25	0.52
1:A:1238:MET:HB2	1:A:1521:THR:HB	1.84	0.52
2:B:338:PHE:CE2	2:B:353:VAL:HG22	2.45	0.52
2:B:658:LEU:HD23	2:B:660:LYS:HD3	1.91	0.52
15:O:200:ASN:OD1	17:Q:14:ASN:CG	2.48	0.52
15:O:357:GLY:HA2	15:O:360:VAL:HB	1.91	0.52
16:P:419:ARG:CG	16:P:420:GLU:N	2.73	0.52
17:Q:8:PRO:CB	17:Q:19:LEU:HD23	2.39	0.52
18:R:153:ASN:OD1	18:R:154:LYS:N	2.43	0.52
1:A:462:LYS:C	1:A:464:GLU:H	2.13	0.52
1:A:526:GLY:HA2	1:A:554:ARG:NH1	2.25	0.52
1:A:581:ILE:HD12	1:A:637:PHE:CE1	2.45	0.52
2:B:120:LYS:HE2	18:R:352:TRP:CH2	2.45	0.52
7:G:149:ILE:HG22	7:G:150:HIS:ND1	2.25	0.52
15:O:491:PHE:CB	15:O:498:TRP:HZ3	2.07	0.52
1:A:584:ARG:HD2	6:F:116:ASP:HB2	1.92	0.51
1:A:846:ILE:O	1:A:849:THR:OG1	2.21	0.51
2:B:322:ASN:HB3	2:B:325:GLN:HG3	1.92	0.51
2:B:939:SER:HG	2:B:943:ILE:H	1.55	0.51
2:B:1019:GLY:HA3	3:C:65:ASN:HB2	1.92	0.51
2:B:1063:ARG:CG	20:T:22:DG:P	2.98	0.51
9:I:37:TYR:HB3	9:I:41:GLN:NE2	2.25	0.51
10:J:34:THR:O	10:J:38:ARG:N	2.36	0.51
16:P:532:GLU:HA	16:P:554:ASN:ND2	2.17	0.51
16:P:724:LEU:HD12	17:Q:443:GLN:CA	2.39	0.51
16:P:748:GLU:HG2	16:P:749:LYS:HG3	1.91	0.51
17:Q:355:VAL:HG12	18:R:212:HIS:HA	1.72	0.51
1:A:81:LEU:HD12	1:A:82:PRO:CD	2.37	0.51
1:A:244:ARG:HH22	1:A:312:SER:HA	1.75	0.51
1:A:477:ASN:HB3	2:B:1047:ARG:NH1	2.25	0.51
1:A:480:ALA:HB2	2:B:1046:VAL:HG23	1.92	0.51
1:A:594:THR:HG23	1:A:599:SER:HB2	1.91	0.51
1:A:772:LYS:HE3	8:H:137:GLN:HE21	1.76	0.51
2:B:119:ARG:NH2	2:B:125:GLU:OE2	2.36	0.51
2:B:1104:CYS:HB2	2:B:1128:CYS:SG	2.49	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:243:SER:HA	3:C:246:ARG:HE	1.75	0.51
5:E:64:PRO:HB2	5:E:69:ILE:HG13	1.91	0.51
7:G:40:ARG:HB2	7:G:123:TYR:CE1	2.44	0.51
14:N:113:SER:OG	14:N:115:SER:OG	2.22	0.51
17:Q:8:PRO:CG	17:Q:19:LEU:HD23	2.40	0.51
1:A:1650:GLY:O	1:A:1652:GLY:N	2.44	0.51
2:B:819:ASP:O	2:B:820:PRO:O	2.27	0.51
16:P:712:ASP:OD1	16:P:712:ASP:N	2.44	0.51
16:P:762:ARG:HG3	17:Q:139:LYS:CE	2.40	0.51
1:A:368:ARG:HA	1:A:380:ASN:ND2	2.24	0.51
1:A:1608:SER:O	1:A:1612:LYS:NZ	2.41	0.51
2:B:807:GLU:O	2:B:903:ILE:N	2.38	0.51
7:G:216:HIS:ND1	7:G:224:PRO:HB3	2.25	0.51
13:M:55:GLY:N	13:M:62:TYR:O	2.36	0.51
14:N:85:HIS:CD2	14:N:86:ASP:H	2.28	0.51
16:P:362:ARG:HG3	16:P:363:ILE:N	2.24	0.51
18:R:314:TRP:CD1	18:R:367:ILE:HD11	2.45	0.51
1:A:440:SER:N	1:A:458:GLN:HE22	2.08	0.51
1:A:579:ARG:NH1	1:A:585:ASP:OD2	2.29	0.51
1:A:1651:THR:CG2	2:B:1086:PHE:HB2	2.41	0.51
2:B:757:TYR:CE1	2:B:762:MET:HB2	2.46	0.51
3:C:224:THR:HG21	10:J:43:ARG:NH2	2.25	0.51
16:P:66:CYS:HB2	16:P:547:VAL:HB	1.92	0.51
16:P:389:TRP:CZ2	18:R:147:GLN:CA	2.94	0.51
16:P:389:TRP:CH2	18:R:147:GLN:CA	2.94	0.51
1:A:401:ASP:O	1:A:404:SER:OG	2.24	0.51
1:A:535:GLN:HB2	1:A:578:TYR:CD1	2.46	0.51
2:B:777:SER:OG	2:B:951:PRO:HD2	2.11	0.51
3:C:227:TYR:HB3	3:C:300:PHE:CE1	2.45	0.51
16:P:299:ASP:O	16:P:320:ILE:HB	2.10	0.51
16:P:389:TRP:CZ3	18:R:149:LYS:HB2	2.45	0.51
16:P:417:THR:OG1	16:P:451:ILE:HB	2.10	0.51
1:A:636:HIS:HB3	2:B:1091:ARG:HD2	1.93	0.51
1:A:1516:LYS:HG3	1:A:1518:VAL:HG23	1.92	0.51
2:B:736:ARG:O	2:B:904:LYS:NZ	2.26	0.51
8:H:10:PHE:CD1	8:H:30:SER:HA	2.46	0.51
8:H:112:ILE:HD11	8:H:129:TYR:CD1	2.46	0.51
9:I:31:SER:O	9:I:34:LYS:NZ	2.37	0.51
13:M:57:ASN:ND2	13:M:60:LEU:HB2	2.25	0.51
16:P:704:LEU:HD23	17:Q:258:MET:HE3	1.93	0.51
18:R:173:MET:O	18:R:176:PRO:HD2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:PHE:CE2	1:A:444:GLN:HG2	2.46	0.51
2:B:240:ARG:HG2	2:B:360:VAL:HB	1.93	0.51
3:C:128:ASP:O	3:C:175:GLN:NE2	2.44	0.51
3:C:237:GLN:HE21	3:C:288:LYS:HG2	1.75	0.51
16:P:186:TYR:HD1	18:R:198:LEU:HB3	1.74	0.51
16:P:267:ASN:OD1	16:P:268:SER:N	2.43	0.51
16:P:378:SER:OG	16:P:379:LYS:HD2	2.11	0.51
16:P:474:LYS:H	16:P:474:LYS:CD	2.23	0.51
17:Q:97:GLY:O	17:Q:99:GLU:N	2.39	0.51
17:Q:186:CYS:SG	18:R:208:TYR:HE2	2.31	0.51
17:Q:192:TYR:CD1	17:Q:193:PHE:N	2.76	0.51
17:Q:366:TYR:CG	18:R:215:THR:HG21	2.42	0.51
1:A:409:ASP:OD1	1:A:410:LYS:N	2.42	0.51
1:A:1268:ASP:N	1:A:1295:ARG:O	2.42	0.51
1:A:1272:VAL:O	9:I:49:THR:N	2.38	0.51
8:H:127:GLY:N	8:H:132:LEU:HD11	2.26	0.51
9:I:9:PHE:HA	9:I:15:ASP:O	2.10	0.51
11:K:66:VAL:O	11:K:68:GLU:HG2	2.11	0.51
16:P:233:VAL:HG12	16:P:234:THR:H	1.75	0.51
16:P:405:TYR:HE2	16:P:414:ILE:CG1	2.24	0.51
16:P:438:TRP:HE3	16:P:439:LYS:O	1.93	0.51
18:R:12:LYS:O	18:R:15:GLN:N	2.44	0.51
18:R:406:LYS:O	18:R:410:TYR:HB2	2.11	0.51
1:A:463:LYS:NZ	20:T:16:DT:C7	2.74	0.51
1:A:941:SER:O	1:A:945:CYS:N	2.39	0.51
1:A:991:LYS:N	1:A:994:GLU:OE1	2.43	0.51
1:A:1316:VAL:HG13	1:A:1320:GLN:NE2	2.25	0.51
1:A:1450:ILE:HA	1:A:1453:HIS:CD2	2.46	0.51
2:B:173:ASN:OD1	2:B:174:LYS:N	2.44	0.51
5:E:91:LYS:O	5:E:95:THR:N	2.27	0.51
15:O:52:TYR:CZ	15:O:92:ASN:HB3	2.46	0.51
16:P:330:PRO:HG3	16:P:342:GLN:CG	2.41	0.51
16:P:634:THR:HG22	16:P:686:TYR:CE2	2.46	0.51
17:Q:381:MET:CG	18:R:238:THR:HG21	2.32	0.51
18:R:189:GLN:O	18:R:192:SER:OG	2.29	0.51
1:A:748:ASN:OD1	1:A:773:ASP:N	2.37	0.50
2:B:1078:ALA:O	2:B:1082:HIS:CB	2.59	0.50
5:E:26:ARG:NH2	5:E:187:TYR:O	2.39	0.50
13:M:22:ALA:HA	13:M:94:PRO:HD2	1.93	0.50
16:P:188:GLN:HG2	16:P:360:TRP:CB	2.37	0.50
16:P:380:MET:HB3	16:P:393:VAL:CG2	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:658:LYS:HB3	16:P:659:LEU:HD22	1.93	0.50
17:Q:24:ASP:CG	17:Q:26:ARG:HE	2.14	0.50
17:Q:270:THR:HA	17:Q:273:VAL:HG23	1.92	0.50
17:Q:349:GLY:O	17:Q:352:ILE:N	2.44	0.50
18:R:291:ARG:NH2	20:T:42:DA:OP2	2.43	0.50
1:A:1449:ALA:O	1:A:1452:SER:OG	2.17	0.50
2:B:143:TRP:CD1	2:B:152:LEU:HD12	2.45	0.50
2:B:816:ASN:O	21:U:17:DT:H4'	2.11	0.50
2:B:1079:LEU:CG	2:B:1088:LEU:CB	2.74	0.50
8:H:11:GLN:HA	8:H:54:SER:HA	1.91	0.50
8:H:102:TYR:CZ	8:H:115:TYR:HB3	2.45	0.50
15:O:245:GLN:HG2	15:O:377:TYR:O	2.10	0.50
16:P:272:PHE:HB2	16:P:300:LEU:HD11	1.93	0.50
16:P:658:LYS:C	16:P:660:LYS:N	2.64	0.50
17:Q:378:LEU:HD13	18:R:231:LEU:CD2	2.40	0.50
21:U:40:DT:H6	21:U:40:DT:H5"	1.75	0.50
1:A:1003:ARG:HD3	2:B:520:LEU:HD22	1.92	0.50
1:A:1645:LYS:NZ	1:A:1645:LYS:HB3	2.26	0.50
2:B:731:VAL:HG12	10:J:63:TYR:CE2	2.46	0.50
2:B:1103:VAL:HG12	2:B:1110:ILE:HG22	1.92	0.50
9:I:32:GLN:OE1	13:M:105:SER:HB2	2.11	0.50
15:O:477:PHE:HA	15:O:480:LEU:HG	1.93	0.50
16:P:227:LEU:HD23	16:P:227:LEU:H	1.75	0.50
16:P:408:ILE:HD12	16:P:409:ASP:H	1.76	0.50
16:P:410:ASP:O	16:P:411:LYS:HD3	2.10	0.50
16:P:762:ARG:HG3	17:Q:139:LYS:NZ	2.27	0.50
17:Q:447:ALA:HA	17:Q:450:THR:HB	1.93	0.50
18:R:11:ARG:CZ	21:U:4:DA:O5'	2.45	0.50
1:A:95:TYR:CD1	1:A:245:LYS:HD3	2.47	0.50
1:A:102:CYS:HB3	1:A:107:HIS:H	1.76	0.50
1:A:416:ARG:O	1:A:420:PHE:N	2.45	0.50
1:A:509:GLU:CD	1:A:579:ARG:NE	2.63	0.50
1:A:519:LEU:HA	1:A:522:ALA:HB3	1.92	0.50
1:A:1261:VAL:HG12	1:A:1498:ILE:HB	1.93	0.50
1:A:1648:ASN:OD1	1:A:1648:ASN:N	2.39	0.50
2:B:168:ASN:OD1	2:B:169:ARG:HG2	2.11	0.50
2:B:328:GLN:NE2	13:M:110:GLY:O	2.45	0.50
2:B:428:VAL:O	2:B:432:ILE:N	2.43	0.50
2:B:985:ILE:O	14:N:157:ARG:NH2	2.45	0.50
2:B:1093:LEU:HD11	2:B:1098:TYR:HD1	1.76	0.50
3:C:65:ASN:O	3:C:68:ARG:HB3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:34:CYS:HB3	12:L:51:CYS:SG	2.51	0.50
16:P:446:ASP:N	18:R:200:THR:HG21	2.25	0.50
17:Q:353:VAL:CG1	17:Q:489:VAL:HG12	2.39	0.50
18:R:361:ASP:HB2	18:R:364:VAL:CG1	2.42	0.50
1:A:39:ASP:OD1	1:A:43:HIS:N	2.44	0.50
1:A:56:ALA:HB3	1:A:69:GLU:HA	1.93	0.50
1:A:419:ILE:O	1:A:422:ARG:N	2.43	0.50
1:A:880:GLN:HE21	2:B:633:THR:H	1.59	0.50
1:A:975:ASP:OD1	1:A:976:ALA:N	2.45	0.50
2:B:279:ALA:HB1	2:B:354:LEU:HD11	1.93	0.50
2:B:1093:LEU:HD12	2:B:1098:TYR:CB	2.25	0.50
2:B:1093:LEU:HD11	2:B:1098:TYR:CD1	2.46	0.50
3:C:308:MET:SD	3:C:316:LYS:NZ	2.70	0.50
9:I:6:SER:H	9:I:45:LEU:HD11	1.76	0.50
11:K:104:ARG:NH2	11:K:106:GLN:HE21	1.95	0.50
14:N:124:THR:H	14:N:131:LEU:HB2	1.75	0.50
16:P:50:LEU:HD11	18:R:259:ASP:OD1	2.11	0.50
16:P:444:PRO:HG3	16:P:449:LEU:HD11	1.93	0.50
18:R:257:ILE:HG23	18:R:267:GLY:H	1.75	0.50
18:R:320:CYS:O	18:R:323:SER:HB3	2.11	0.50
1:A:4:SER:HB3	1:A:576:LYS:NZ	2.26	0.50
1:A:618:TYR:OH	2:B:783:MET:HB2	2.11	0.50
2:B:641:TYR:CB	2:B:643:PHE:HE1	2.25	0.50
2:B:790:ASN:HB2	2:B:936:MET:SD	2.51	0.50
9:I:58:SER:HG	9:I:62:ALA:H	1.59	0.50
15:O:198:PHE:CE1	15:O:236:LYS:HG3	2.47	0.50
16:P:190:ALA:O	16:P:248:PRO:HA	2.12	0.50
16:P:262:GLY:C	16:P:263:ILE:HG12	2.31	0.50
16:P:487:ASN:CB	18:R:138:PHE:CE1	2.94	0.50
17:Q:356:VAL:CG1	18:R:208:TYR:CD2	2.90	0.50
17:Q:357:TYR:OH	17:Q:488:LEU:HB3	2.12	0.50
21:U:38:DG:H2"	21:U:39:DT:O4'	2.12	0.50
1:A:804:GLU:H	1:A:804:GLU:CD	2.15	0.50
1:A:1040:ASP:OD1	1:A:1041:ALA:N	2.41	0.50
2:B:532:HIS:CD2	2:B:719:CYS:HB3	2.46	0.50
4:D:80:THR:HG21	15:O:227:PHE:CD2	2.46	0.50
16:P:414:ILE:CD1	16:P:425:GLY:HA3	2.41	0.50
16:P:443:ASP:CB	18:R:2:PHE:HB3	2.30	0.50
16:P:725:VAL:HG23	17:Q:446:TYR:CB	2.26	0.50
17:Q:119:LEU:HD13	17:Q:125:PHE:CG	2.47	0.50
1:A:44:PRO:HG2	1:A:52:LEU:HD21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:ILE:O	1:A:140:THR:OG1	2.29	0.50
1:A:264:ASN:O	1:A:268:GLY:N	2.44	0.50
1:A:543:LEU:HD22	1:A:578:TYR:CZ	2.47	0.50
1:A:1459:LYS:HB2	1:A:1473:LYS:HB3	1.94	0.50
1:A:1646:LEU:HD11	2:B:1086:PHE:CD1	2.47	0.50
2:B:399:HIS:O	2:B:400:GLN:HG3	2.11	0.50
2:B:717:TYR:O	2:B:721:MET:N	2.41	0.50
2:B:790:ASN:CA	2:B:936:MET:SD	3.00	0.50
10:J:53:HIS:NE2	10:J:55:ASP:OD1	2.39	0.50
13:M:44:LYS:NZ	13:M:47:GLU:O	2.40	0.50
15:O:99:ILE:O	15:O:102:SER:OG	2.19	0.50
17:Q:10:CYS:HB2	17:Q:17:SER:N	2.25	0.50
17:Q:10:CYS:SG	17:Q:29:CYS:SG	3.07	0.50
17:Q:326:TYR:HB3	17:Q:330:TRP:CZ3	2.47	0.50
17:Q:374:THR:O	17:Q:377:PHE:HB3	2.12	0.50
18:R:302:ARG:O	18:R:303:THR:OG1	2.21	0.50
1:A:535:GLN:O	1:A:578:TYR:HD1	1.95	0.50
1:A:652:ASN:HB2	1:A:655:SER:CB	2.39	0.50
2:B:396:ALA:HA	2:B:521:LEU:HD12	1.93	0.50
2:B:599:GLU:H	2:B:599:GLU:CD	2.16	0.50
2:B:795:GLU:HB3	3:C:216:HIS:CE1	2.46	0.50
5:E:16:PHE:CZ	5:E:20:LYS:HE3	2.46	0.50
7:G:37:CYS:HB2	7:G:125:TRP:CD1	2.47	0.50
15:O:478:GLN:OE1	15:O:520:CYS:HB3	2.12	0.50
16:P:319:ASP:OD1	16:P:324:TRP:HB3	2.12	0.50
16:P:762:ARG:HG3	17:Q:139:LYS:HE3	1.93	0.50
17:Q:162:ILE:HG22	17:Q:226:LEU:HD21	1.94	0.50
21:U:38:DG:C6	21:U:39:DT:N3	2.80	0.50
1:A:545:SER:CB	17:Q:34:VAL:HG21	2.39	0.49
2:B:216:ALA:HB2	2:B:380:LYS:HE2	1.94	0.49
2:B:954:PHE:HB2	2:B:955:PRO:CD	2.41	0.49
6:F:66:ARG:HH22	7:G:90:LEU:HD13	1.76	0.49
15:O:197:PHE:O	15:O:211:TYR:OH	2.21	0.49
16:P:609:ASN:O	16:P:612:GLU:HB2	2.12	0.49
17:Q:109:GLN:CD	17:Q:137:TRP:HE1	2.16	0.49
1:A:19:LEU:N	2:B:1193:GLY:O	2.35	0.49
1:A:95:TYR:CG	1:A:245:LYS:HD3	2.47	0.49
1:A:621:THR:O	1:A:625:ASN:N	2.45	0.49
1:A:671:GLN:OE1	2:B:783:MET:O	2.29	0.49
1:A:1654:PHE:CB	6:F:134:ILE:HG23	2.33	0.49
2:B:1075:GLU:OE1	2:B:1075:GLU:N	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1116:SER:N	2:B:1125:THR:O	2.44	0.49
3:C:237:GLN:HE21	3:C:288:LYS:HE3	1.78	0.49
6:F:77:ASP:OD1	6:F:78:GLN:N	2.44	0.49
7:G:38:ILE:HG13	7:G:125:TRP:HD1	1.77	0.49
14:N:35:LEU:N	14:N:116:LYS:O	2.35	0.49
16:P:549:TYR:HE1	16:P:551:ALA:HB2	1.76	0.49
16:P:551:ALA:C	16:P:552:LEU:HD23	2.32	0.49
18:R:299:THR:OG1	18:R:300:GLY:N	2.45	0.49
1:A:1242:ILE:HA	1:A:1536:ILE:HA	1.94	0.49
2:B:1154:ASP:HB3	2:B:1157:GLN:HG2	1.94	0.49
5:E:41:ASP:HA	5:E:44:ALA:HB3	1.94	0.49
8:H:100:THR:OG1	8:H:139:ASN:OD1	2.21	0.49
13:M:57:ASN:O	13:M:103:LYS:NZ	2.23	0.49
15:O:429:ALA:HB3	15:O:482:TYR:CE2	2.47	0.49
16:P:405:TYR:OH	16:P:414:ILE:HB	2.12	0.49
18:R:85:ARG:HG2	18:R:85:ARG:HH11	1.77	0.49
18:R:362:ALA:O	18:R:365:TRP:N	2.46	0.49
21:U:38:DG:N2	21:U:39:DT:O2	2.45	0.49
1:A:1246:VAL:HA	1:A:1250:GLN:OE1	2.13	0.49
2:B:1102:SER:HA	2:B:1174:THR:O	2.12	0.49
15:O:351:SER:HA	15:O:355:GLY:HA3	1.93	0.49
15:O:507:GLN:HE22	15:O:543:ILE:HD11	1.78	0.49
16:P:193:LEU:HG	16:P:250:ALA:HA	1.95	0.49
16:P:353:ASP:OD2	16:P:379:LYS:NZ	2.46	0.49
16:P:426:ALA:O	16:P:433:VAL:HG22	2.12	0.49
17:Q:198:ILE:HG21	17:Q:390:THR:H	1.77	0.49
17:Q:232:LEU:HD13	17:Q:287:TRP:HE1	1.77	0.49
17:Q:356:VAL:N	18:R:212:HIS:CE1	2.80	0.49
18:R:23:TYR:CD1	18:R:173:MET:HG3	2.47	0.49
18:R:274:MET:HB3	18:R:308:PHE:HB3	1.94	0.49
18:R:282:SER:O	18:R:282:SER:OG	2.27	0.49
20:T:7:DT:O2	21:U:44:DG:N2	2.46	0.49
1:A:831:ASP:HB3	2:B:1008:HIS:CG	2.47	0.49
1:A:1185:VAL:O	1:A:1189:ALA:N	2.36	0.49
1:A:1191:GLN:HE22	2:B:1078:ALA:HA	1.77	0.49
1:A:1650:GLY:C	1:A:1652:GLY:N	2.66	0.49
15:O:219:ARG:HE	15:O:230:TRP:HE1	1.61	0.49
17:Q:335:THR:HG21	17:Q:478:ARG:HD2	1.95	0.49
17:Q:357:TYR:HE2	17:Q:488:LEU:C	2.16	0.49
18:R:160:HIS:O	18:R:164:LYS:HG3	2.13	0.49
20:T:11:DA:N6	20:T:12:DC:N4	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:990:ILE:HD11	1:A:995:TYR:HD1	1.77	0.49
1:A:1114:TYR:CD1	5:E:146:HIS:HA	2.48	0.49
1:A:1238:MET:HG2	1:A:1524:VAL:HG22	1.94	0.49
1:A:1299:ASN:HA	1:A:1302:TYR:CE2	2.48	0.49
1:A:1657:LEU:O	6:F:133:VAL:N	2.45	0.49
2:B:31:ASP:OD1	2:B:32:LYS:N	2.40	0.49
2:B:1163:GLN:OE1	2:B:1163:GLN:N	2.46	0.49
15:O:116:ILE:HA	15:O:119:ILE:HD12	1.94	0.49
15:O:487:ARG:NH2	15:O:506:PHE:CE2	2.81	0.49
16:P:196:TYR:HB3	16:P:206:ALA:HB1	1.93	0.49
16:P:357:LEU:CD1	18:R:191:ILE:HD12	2.43	0.49
16:P:722:TRP:CZ3	16:P:736:ILE:HD12	2.47	0.49
18:R:206:ARG:C	18:R:207:ASN:CB	2.80	0.49
1:A:1055:ILE:HB	1:A:1580:ARG:HH21	1.77	0.49
1:A:1097:TYR:O	1:A:1101:THR:HG23	2.11	0.49
2:B:42:VAL:HG21	2:B:190:ILE:HD12	1.94	0.49
7:G:90:LEU:HD11	7:G:119:HIS:NE2	2.28	0.49
15:O:474:TYR:O	15:O:478:GLN:N	2.24	0.49
16:P:408:ILE:HB	16:P:453:VAL:HG21	1.95	0.49
17:Q:274:ILE:HG12	17:Q:282:ARG:HH22	1.77	0.49
1:A:129:LEU:HB3	1:A:132:GLU:OE1	2.12	0.49
1:A:1508:VAL:O	1:A:1510:PRO:HD3	2.12	0.49
2:B:368:GLN:HG3	2:B:372:ARG:NH1	2.27	0.49
2:B:398:GLN:NE2	2:B:636:GLN:OE1	2.42	0.49
8:H:38:LEU:HD11	8:H:123:MET:HG3	1.95	0.49
9:I:54:ASP:OD1	9:I:55:ALA:N	2.45	0.49
14:N:114:GLU:HG2	14:N:120:LYS:NZ	2.28	0.49
16:P:274:ILE:CD1	16:P:305:PHE:HE2	2.25	0.49
16:P:305:PHE:HZ	16:P:329:ILE:HG21	1.76	0.49
16:P:357:LEU:HD12	18:R:191:ILE:HD12	1.94	0.49
16:P:458:LYS:HA	16:P:458:LYS:NZ	2.28	0.49
16:P:693:PHE:HA	16:P:746:ARG:NE	2.28	0.49
17:Q:141:LEU:O	17:Q:144:ILE:HG13	2.12	0.49
17:Q:247:ILE:HD12	17:Q:248:SER:H	1.77	0.49
1:A:354:SER:OG	1:A:355:PHE:CE1	2.61	0.49
1:A:552:GLU:OE1	1:A:552:GLU:N	2.38	0.49
1:A:1014:SER:CB	20:T:17:DT:C6	2.91	0.49
1:A:1090:ASP:HB3	1:A:1132:TYR:HD1	1.76	0.49
1:A:1443:GLN:NE2	1:A:1461:ASN:OD1	2.46	0.49
2:B:1079:LEU:H	2:B:1079:LEU:HD12	1.77	0.49
3:C:113:LEU:HD23	3:C:210:LEU:HG	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:315:PHE:HE1	11:K:135:PHE:HD2	1.61	0.49
5:E:107:THR:HG23	5:E:131:THR:HG23	1.95	0.49
8:H:124:ARG:NH1	8:H:126:GLU:OE1	2.27	0.49
15:O:205:ARG:HB2	15:O:331:LYS:HG2	1.95	0.49
16:P:405:TYR:CE2	16:P:414:ILE:HB	2.48	0.49
16:P:458:LYS:HD3	16:P:459:PRO:CD	2.43	0.49
16:P:573:GLU:HB2	17:Q:499:LYS:NZ	2.27	0.49
17:Q:22:ILE:HD12	17:Q:26:ARG:CZ	2.40	0.49
17:Q:356:VAL:HG11	18:R:208:TYR:CD2	2.46	0.49
17:Q:386:LEU:CA	18:R:241:ARG:CZ	2.74	0.49
1:A:257:ASN:O	1:A:261:ILE:HD12	2.13	0.49
1:A:1050:TYR:CE2	1:A:1580:ARG:HD3	2.47	0.49
1:A:1447:GLN:NE2	1:A:1460:TYR:H	2.10	0.49
1:A:1575:ILE:HG22	1:A:1576:SER:H	1.77	0.49
3:C:297:HIS:CD2	3:C:298:PHE:H	2.30	0.49
5:E:28:TYR:HA	5:E:64:PRO:HA	1.95	0.49
15:O:592:PHE:O	15:O:594:TYR:N	2.45	0.49
16:P:274:ILE:HD13	16:P:305:PHE:CE2	2.43	0.49
16:P:319:ASP:HB2	16:P:363:ILE:CG1	2.43	0.49
16:P:319:ASP:HB2	16:P:363:ILE:HG13	1.95	0.49
1:A:1227:MET:O	1:A:1597:ALA:HB1	2.13	0.48
2:B:887:LEU:N	12:L:56:LEU:O	2.42	0.48
2:B:1114:GLN:HE21	2:B:1159:TRP:HZ3	1.61	0.48
7:G:49:LEU:HD11	7:G:53:TYR:HB2	1.95	0.48
15:O:383:TYR:HA	15:O:386:PHE:HB3	1.95	0.48
16:P:300:LEU:N	16:P:300:LEU:HD23	2.27	0.48
16:P:414:ILE:HG12	16:P:425:GLY:N	2.28	0.48
17:Q:352:ILE:HD12	17:Q:380:TRP:CE3	2.48	0.48
17:Q:363:SER:C	17:Q:365:ASP:N	2.65	0.48
17:Q:385:PHE:O	18:R:241:ARG:NE	2.45	0.48
18:R:304:HIS:NE2	18:R:361:ASP:HB3	2.28	0.48
1:A:248:PHE:CD2	1:A:444:GLN:HG2	2.49	0.48
1:A:332:GLN:NE2	1:A:349:LEU:HB3	2.28	0.48
1:A:492:THR:HB	1:A:667:ARG:NH2	2.28	0.48
1:A:646:GLU:OE1	2:B:1086:PHE:CB	2.61	0.48
1:A:651:ALA:H	2:B:1084:THR:CG2	2.27	0.48
1:A:656:GLN:HE22	2:B:1082:HIS:HD1	1.61	0.48
2:B:752:VAL:HB	2:B:920:ARG:HH22	1.78	0.48
8:H:103:LYS:HD2	8:H:115:TYR:CE2	2.47	0.48
15:O:141:LYS:HA	15:O:179:PHE:HZ	1.78	0.48
16:P:61:VAL:HB	16:P:551:ALA:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:347:LEU:HD22	16:P:385:PHE:HD2	1.78	0.48
17:Q:266:PHE:HA	17:Q:269:TYR:HB2	1.94	0.48
1:A:482:SER:OG	1:A:483:VAL:N	2.45	0.48
1:A:1290:TYR:CE1	1:A:1474:LEU:HB2	2.48	0.48
2:B:184:LYS:HZ2	10:J:69:ARG:HH22	1.60	0.48
2:B:402:VAL:O	2:B:647:SER:HB3	2.13	0.48
2:B:747:GLY:HA3	2:B:766:PRO:HB2	1.96	0.48
7:G:24:VAL:O	7:G:128:GLN:NE2	2.36	0.48
11:K:77:ARG:HD2	11:K:91:TYR:HD1	1.77	0.48
13:M:83:PRO:HG2	14:N:49:LYS:HE3	1.94	0.48
16:P:56:ASP:O	16:P:57:LEU:HD23	2.12	0.48
16:P:223:ASN:HD22	16:P:286:VAL:HG11	1.78	0.48
17:Q:10:CYS:HB3	17:Q:16:PRO:HA	1.93	0.48
17:Q:239:PHE:HB2	17:Q:245:SER:OG	2.13	0.48
18:R:15:GLN:OE1	18:R:181:THR:HG23	2.12	0.48
18:R:23:TYR:CE1	18:R:170:LEU:HD23	2.49	0.48
1:A:512:THR:CG2	1:A:513:ALA:H	2.24	0.48
1:A:1025:LYS:HG2	1:A:1615:TYR:CD1	2.48	0.48
1:A:1229:ALA:HB3	1:A:1597:ALA:HB2	1.94	0.48
2:B:129:ARG:HH22	2:B:890:ASP:HA	1.78	0.48
2:B:320:LEU:HD22	2:B:326:VAL:N	2.28	0.48
2:B:736:ARG:HD3	2:B:738:ASP:OD2	2.13	0.48
5:E:67:GLU:H	5:E:67:GLU:CD	2.16	0.48
12:L:48:CYS:HB3	12:L:52:GLY:N	2.22	0.48
13:M:80:LEU:HD21	14:N:38:PHE:CZ	2.49	0.48
15:O:179:PHE:HD2	15:O:183:ILE:HD12	1.78	0.48
15:O:484:PHE:HB2	15:O:528:PHE:CD1	2.48	0.48
1:A:418:VAL:HG13	1:A:419:ILE:HG13	1.94	0.48
1:A:552:GLU:H	1:A:552:GLU:CD	2.16	0.48
1:A:734:THR:O	1:A:738:ASN:ND2	2.46	0.48
2:B:585:CYS:HB2	2:B:595:TRP:CZ3	2.49	0.48
2:B:745:GLN:NE2	10:J:1:MET:SD	2.81	0.48
2:B:1087:LEU:CD2	2:B:1088:LEU:HD23	2.43	0.48
16:P:194:ARG:O	16:P:195:ASN:ND2	2.46	0.48
16:P:238:LEU:HD21	16:P:284:VAL:HG23	1.96	0.48
17:Q:350:ARG:NE	17:Q:486:GLN:CD	2.66	0.48
1:A:463:LYS:NZ	20:T:16:DT:H71	2.27	0.48
1:A:966:LEU:HB3	1:A:969:PHE:CD2	2.49	0.48
5:E:76:GLY:HA3	5:E:106:GLN:HB2	1.96	0.48
15:O:532:ALA:HB1	15:O:537:VAL:HB	1.95	0.48
16:P:294:PHE:CE2	16:P:299:ASP:HA	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:751:SER:O	16:P:753:PHE:N	2.46	0.48
17:Q:22:ILE:HD11	17:Q:26:ARG:CG	2.44	0.48
17:Q:140:ILE:O	17:Q:143:THR:HG22	2.14	0.48
1:A:219:LEU:O	1:A:223:PHE:N	2.32	0.48
1:A:1311:GLU:O	1:A:1314:GLN:HB3	2.13	0.48
2:B:985:ILE:HG13	2:B:986:PHE:CD2	2.48	0.48
2:B:1138:ALA:HB1	2:B:1153:ILE:HG13	1.95	0.48
8:H:103:LYS:HD2	8:H:115:TYR:CD2	2.48	0.48
14:N:56:ILE:HG12	14:N:137:PHE:HB2	1.94	0.48
16:P:348:HIS:CE1	18:R:154:LYS:HE2	2.49	0.48
16:P:475:ARG:HD2	16:P:475:ARG:N	2.28	0.48
1:A:232:LYS:HE2	1:A:239:PHE:CZ	2.48	0.48
1:A:613:THR:OG1	1:A:615:ARG:NH2	2.46	0.48
1:A:647:ALA:HB2	2:B:1087:LEU:HD13	1.94	0.48
1:A:1003:ARG:HD3	2:B:520:LEU:HB2	1.95	0.48
1:A:1013:THR:O	20:T:17:DT:C2	2.67	0.48
1:A:1490:GLU:HB3	1:A:1494:ARG:HH12	1.79	0.48
1:A:1610:PHE:HA	1:A:1613:MET:HB3	1.96	0.48
2:B:18:THR:O	2:B:21:ARG:HB3	2.14	0.48
2:B:52:LEU:HD23	2:B:60:LEU:HD12	1.95	0.48
2:B:211:ARG:HB3	2:B:401:GLU:OE2	2.13	0.48
2:B:1064:LYS:HE2	2:B:1064:LYS:HB3	1.62	0.48
15:O:162:PHE:O	15:O:211:TYR:HA	2.14	0.48
15:O:498:TRP:CZ2	15:O:535:GLU:HB3	2.48	0.48
16:P:60:VAL:HG12	16:P:61:VAL:H	1.78	0.48
16:P:182:LEU:HD12	16:P:185:GLN:HG2	1.95	0.48
16:P:300:LEU:HB3	16:P:320:ILE:HG22	1.96	0.48
16:P:422:ILE:O	16:P:439:LYS:HB3	2.14	0.48
16:P:436:ILE:HG23	18:R:141:TRP:HB2	1.95	0.48
17:Q:234:CYS:SG	17:Q:284:LEU:HB3	2.53	0.48
18:R:368:TYR:CE2	18:R:414:PHE:CZ	3.02	0.48
18:R:402:ASN:O	18:R:406:LYS:HG2	2.14	0.48
2:B:299:ASP:OD1	2:B:300:SER:N	2.47	0.48
2:B:943:ILE:HD11	10:J:43:ARG:HB3	1.96	0.48
2:B:1064:LYS:HD2	2:B:1064:LYS:O	2.13	0.48
2:B:1187:SER:O	2:B:1190:SER:OG	2.27	0.48
3:C:57:ILE:HG22	3:C:58:ASN:ND2	2.29	0.48
7:G:134:GLU:HA	7:G:229:LEU:O	2.14	0.48
15:O:348:THR:HG23	15:O:351:SER:H	1.78	0.48
16:P:463:LEU:HA	16:P:482:SER:HA	1.96	0.48
17:Q:417:PHE:HE1	18:R:265:SER:O	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:158:THR:OG1	18:R:159:TYR:N	2.46	0.48
21:U:39:DT:H2"	21:U:40:DT:H5"	1.96	0.48
1:A:371:SER:N	1:A:378:HIS:O	2.31	0.48
1:A:830:MET:HG3	2:B:967:LEU:HD11	1.95	0.48
2:B:939:SER:OG	2:B:942:GLY:N	2.46	0.48
2:B:1159:TRP:O	2:B:1167:PHE:N	2.40	0.48
12:L:34:CYS:HB3	12:L:51:CYS:HG	1.78	0.48
15:O:61:ASP:O	15:O:65:LYS:N	2.44	0.48
16:P:475:ARG:HH21	17:Q:364:SER:HA	1.78	0.48
16:P:533:LEU:H	16:P:554:ASN:HB2	1.78	0.48
16:P:658:LYS:C	16:P:660:LYS:H	2.17	0.48
16:P:678:LEU:HD22	16:P:679:LEU:HD13	1.96	0.48
17:Q:355:VAL:CA	18:R:212:HIS:CE1	2.60	0.48
18:R:4:VAL:HG13	18:R:6:ILE:H	1.78	0.48
18:R:82:ARG:HD2	18:R:82:ARG:O	2.14	0.48
1:A:15:ASP:OD1	1:A:1631:ARG:HG3	2.13	0.47
1:A:244:ARG:O	1:A:252:PHE:N	2.25	0.47
1:A:367:PHE:CD1	2:B:1184:TYR:HD1	2.31	0.47
1:A:920:PHE:CD1	1:A:921:PRO:HA	2.49	0.47
1:A:1261:VAL:HB	1:A:1499:ARG:H	1.79	0.47
2:B:301:PHE:CE2	2:B:386:ALA:HB2	2.49	0.47
2:B:826:GLY:N	2:B:860:ALA:O	2.46	0.47
2:B:954:PHE:CZ	2:B:963:PHE:CE1	3.03	0.47
2:B:1097:ASP:O	2:B:1179:PRO:HA	2.14	0.47
7:G:74:ASN:HB3	7:G:77:VAL:HG22	1.96	0.47
16:P:389:TRP:HZ2	18:R:147:GLN:N	1.71	0.47
17:Q:15:CYS:CB	17:Q:17:SER:N	2.60	0.47
1:A:511:VAL:CG1	1:A:575:LYS:C	2.74	0.47
1:A:537:GLN:HE21	1:A:541:GLY:HA2	1.78	0.47
1:A:546:LEU:HB3	1:A:554:ARG:CZ	2.44	0.47
1:A:771:PHE:HA	1:A:775:ALA:O	2.15	0.47
1:A:966:LEU:HD11	2:B:525:TRP:CE3	2.49	0.47
1:A:1240:LEU:HB2	1:A:1519:LEU:HB2	1.95	0.47
1:A:1312:GLU:O	1:A:1316:VAL:N	2.26	0.47
9:I:30:CYS:HB3	9:I:35:ALA:N	2.29	0.47
15:O:109:SER:O	15:O:113:THR:OG1	2.29	0.47
16:P:66:CYS:HB2	16:P:547:VAL:CG2	2.44	0.47
16:P:412:ASN:OD1	16:P:412:ASN:N	2.45	0.47
17:Q:123:MET:HE1	17:Q:184:TRP:HE1	1.78	0.47
17:Q:499:LYS:HE3	17:Q:499:LYS:HB3	1.59	0.47
18:R:275:CYS:SG	18:R:309:ALA:HA	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:ARG:NH2	1:A:1615:TYR:O	2.46	0.47
1:A:1013:THR:HB	20:T:17:DT:C2	2.49	0.47
2:B:113:VAL:O	18:R:282:SER:HB2	2.13	0.47
2:B:1128:CYS:N	2:B:1170:GLY:O	2.30	0.47
6:F:83:PRO:HB2	6:F:152:ILE:CD1	2.44	0.47
6:F:137:TYR:HD1	6:F:143:PHE:HB3	1.78	0.47
14:N:53:VAL:O	14:N:134:ASP:HB2	2.14	0.47
15:O:72:GLY:O	15:O:76:ASN:N	2.45	0.47
15:O:192:THR:O	15:O:196:LYS:N	2.27	0.47
15:O:228:GLN:HA	15:O:231:SER:HB2	1.96	0.47
15:O:478:GLN:NE2	15:O:481:CYS:SG	2.87	0.47
18:R:200:THR:H	18:R:203:SER:HB3	1.79	0.47
18:R:250:LEU:HG	18:R:307:LYS:HZ2	1.79	0.47
1:A:248:PHE:O	1:A:249:THR:OG1	2.30	0.47
1:A:597:LYS:CD	2:B:1082:HIS:HA	2.41	0.47
1:A:1460:TYR:OH	1:A:1462:PHE:HB2	2.14	0.47
2:B:207:ILE:HB	2:B:505:ARG:HD2	1.96	0.47
2:B:314:LYS:C	2:B:316:ARG:H	2.18	0.47
2:B:975:HIS:CG	14:N:166:LEU:HD22	2.50	0.47
2:B:1120:ILE:HD12	15:O:117:GLN:HE21	1.79	0.47
3:C:71:MET:HB2	3:C:317:SER:OG	2.15	0.47
9:I:38:PRO:CD	9:I:41:GLN:HE21	2.26	0.47
10:J:68:LYS:HE2	12:L:34:CYS:HB2	1.97	0.47
15:O:63:LEU:HD11	15:O:112:GLY:N	2.28	0.47
15:O:518:LYS:HB2	15:O:547:ASN:ND2	2.29	0.47
17:Q:161:THR:OG1	17:Q:162:ILE:N	2.47	0.47
1:A:440:SER:H	1:A:458:GLN:HE22	1.61	0.47
1:A:597:LYS:HD2	2:B:1082:HIS:CA	2.44	0.47
1:A:672:ASP:CG	2:B:950:ASN:HD21	2.18	0.47
2:B:48:SER:HB3	2:B:404:LEU:HD13	1.96	0.47
2:B:107:PRO:HG2	2:B:133:TYR:CE2	2.49	0.47
2:B:492:ASN:HD21	2:B:723:LYS:HA	1.79	0.47
2:B:1084:THR:CB	2:B:1087:LEU:HD22	2.33	0.47
15:O:390:GLN:OE1	15:O:609:TYR:HB3	2.14	0.47
15:O:602:TYR:O	15:O:606:MET:HG2	2.14	0.47
16:P:271:ILE:HG12	16:P:272:PHE:N	2.29	0.47
16:P:477:TYR:HD2	18:R:2:PHE:CZ	2.30	0.47
16:P:582:ASP:N	16:P:585:GLU:HB2	2.29	0.47
18:R:250:LEU:HD11	18:R:307:LYS:HG3	1.96	0.47
18:R:440:SER:O	18:R:440:SER:OG	2.31	0.47
7:G:48:SER:HB3	7:G:115:PHE:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:302:VAL:O	16:P:363:ILE:HD11	2.13	0.47
16:P:397:LYS:O	16:P:397:LYS:HG2	2.14	0.47
17:Q:319:SER:O	17:Q:319:SER:OG	2.30	0.47
18:R:12:LYS:O	18:R:14:ALA:N	2.47	0.47
1:A:507:TYR:CE1	1:A:639:GLN:O	2.68	0.47
1:A:657:TYR:CZ	1:A:665:PRO:HB3	2.50	0.47
1:A:1114:TYR:CE2	1:A:1115:LYS:HG2	2.49	0.47
1:A:1555:VAL:HG21	5:E:212:ARG:HH12	1.80	0.47
2:B:656:LEU:HD22	14:N:153:VAL:HG21	1.97	0.47
2:B:787:MET:HB2	2:B:927:CYS:HA	1.92	0.47
2:B:963:PHE:O	2:B:1027:TYR:OH	2.31	0.47
2:B:1074:MET:CE	20:T:18:DT:O4'	2.62	0.47
3:C:105:PRO:HG2	10:J:13:VAL:HG21	1.95	0.47
3:C:316:LYS:HA	3:C:319:ARG:HB3	1.97	0.47
5:E:50:MET:HG2	5:E:52:ARG:HB2	1.96	0.47
11:K:50:LEU:O	11:K:54:THR:HG23	2.14	0.47
16:P:465:VAL:HG13	16:P:480:VAL:HG13	1.96	0.47
16:P:498:LEU:CD1	17:Q:368:GLN:HE21	2.26	0.47
16:P:775:TRP:O	17:Q:109:GLN:NE2	2.47	0.47
17:Q:135:ILE:O	17:Q:139:LYS:HD2	2.15	0.47
17:Q:274:ILE:HG23	17:Q:282:ARG:NH2	2.30	0.47
20:T:2:DT:H3	21:U:48:DA:H61	1.61	0.47
20:T:11:DA:C4	20:T:12:DC:C4	3.02	0.47
1:A:407:GLN:H	1:A:410:LYS:HE2	1.80	0.47
2:B:113:VAL:O	18:R:282:SER:CB	2.63	0.47
2:B:938:PHE:CE2	2:B:1014:TYR:HD2	2.32	0.47
3:C:90:SER:HB3	3:C:202:ILE:HD11	1.97	0.47
5:E:110:PHE:O	5:E:134:THR:HA	2.15	0.47
6:F:76:LYS:HA	6:F:79:ARG:NH1	2.29	0.47
7:G:92:ALA:HB3	7:G:104:LEU:HB2	1.97	0.47
14:N:41:ASN:HD22	14:N:51:GLN:CD	2.18	0.47
15:O:548:ASN:OD1	15:O:549:ASN:N	2.48	0.47
1:A:597:LYS:HE3	1:A:660:PRO:HG2	1.97	0.47
1:A:1637:PRO:CG	1:A:1647:ASN:ND2	2.62	0.47
2:B:372:ARG:HH21	2:B:574:SER:HA	1.80	0.47
2:B:541:LEU:O	2:B:543:ASN:ND2	2.47	0.47
2:B:823:GLN:HG2	2:B:863:ASP:HA	1.97	0.47
6:F:140:ASP:OD1	6:F:141:GLY:N	2.47	0.47
7:G:241:ARG:HG2	15:O:189:PHE:CD2	2.49	0.47
1:A:1238:MET:SD	1:A:1526:PHE:CE1	3.08	0.47
1:A:1511:GLU:O	1:A:1513:GLU:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:219:ARG:HG2	2:B:221:SER:H	1.79	0.47
2:B:992:PRO:HA	2:B:995:TYR:HB3	1.97	0.47
9:I:30:CYS:N	9:I:35:ALA:O	2.38	0.47
15:O:201:LYS:HD3	15:O:239:SER:OG	2.15	0.47
16:P:186:TYR:HE1	16:P:447:THR:OG1	1.98	0.47
16:P:263:ILE:CG2	16:P:277:VAL:HG12	2.44	0.47
16:P:363:ILE:HA	16:P:373:LEU:O	2.14	0.47
16:P:428:GLU:HG3	16:P:429:SER:N	2.29	0.47
18:R:320:CYS:SG	18:R:346:ILE:HG13	2.55	0.47
21:U:42:DA:H1'	21:U:43:DA:H5'	1.97	0.47
1:A:239:PHE:HE2	1:A:263:ASN:HD22	1.63	0.46
1:A:440:SER:H	1:A:458:GLN:NE2	2.12	0.46
1:A:970:LYS:HE2	1:A:973:GLU:OE1	2.15	0.46
1:A:1052:GLY:HA2	5:E:208:TYR:CE1	2.51	0.46
2:B:264:TRP:NE1	2:B:265:ARG:HG2	2.30	0.46
2:B:504:HIS:HB3	2:B:542:LEU:HD23	1.97	0.46
3:C:64:ALA:HA	3:C:67:PHE:HB3	1.97	0.46
3:C:87:ASN:OD1	3:C:88:ASN:N	2.48	0.46
11:K:55:SER:OG	11:K:57:ASP:OD1	2.21	0.46
15:O:174:ASP:HA	15:O:177:LYS:HE2	1.97	0.46
15:O:477:PHE:O	15:O:480:LEU:HG	2.15	0.46
16:P:304:ASP:HB2	16:P:363:ILE:O	2.15	0.46
16:P:416:LEU:HD23	16:P:423:ILE:HD12	1.97	0.46
17:Q:129:PHE:HE1	17:Q:169:SER:N	2.12	0.46
1:A:202:THR:HG22	1:A:203:THR:O	2.16	0.46
5:E:91:LYS:HA	5:E:94:LYS:HB3	1.97	0.46
15:O:77:GLN:HE21	15:O:88:ILE:HA	1.80	0.46
15:O:396:MET:HG3	15:O:434:LEU:HD11	1.54	0.46
16:P:363:ILE:HG22	16:P:374:VAL:HG22	1.98	0.46
17:Q:283:ASN:C	17:Q:284:LEU:HD12	2.36	0.46
17:Q:327:PRO:HG2	17:Q:330:TRP:H	1.80	0.46
18:R:356:PRO:CB	18:R:357:PRO:HA	2.45	0.46
20:T:12:DC:C2'	20:T:13:DT:H5'	2.44	0.46
1:A:831:ASP:N	1:A:831:ASP:OD1	2.48	0.46
1:A:1092:GLU:O	1:A:1095:LEU:N	2.48	0.46
2:B:54:GLU:O	2:B:59:GLY:HA2	2.15	0.46
15:O:216:LEU:HB3	15:O:342:HIS:CD2	2.50	0.46
15:O:434:LEU:CD2	15:O:439:ILE:HD11	2.39	0.46
15:O:487:ARG:HG2	15:O:491:PHE:CG	2.50	0.46
16:P:265:THR:HG23	16:P:274:ILE:HG12	1.97	0.46
16:P:322:GLY:N	16:P:361:LYS:HD3	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:436:ILE:CG2	18:R:141:TRP:HB2	2.45	0.46
16:P:442:LEU:N	16:P:442:LEU:HD13	2.31	0.46
16:P:463:LEU:H	16:P:463:LEU:HD22	1.81	0.46
16:P:540:LYS:O	16:P:541:LEU:HD13	2.16	0.46
16:P:573:GLU:HB2	17:Q:499:LYS:HZ1	1.79	0.46
16:P:724:LEU:HD12	17:Q:443:GLN:HG2	1.98	0.46
18:R:200:THR:O	18:R:204:GLU:HG2	2.15	0.46
1:A:590:ASN:HD21	2:B:1075:GLU:HG2	1.81	0.46
2:B:273:VAL:HG21	2:B:378:ILE:HD11	1.98	0.46
2:B:442:ASP:HB3	2:B:445:TYR:HB3	1.97	0.46
2:B:794:ASP:HA	2:B:798:PHE:HB3	1.97	0.46
16:P:361:LYS:HA	16:P:375:PHE:O	2.16	0.46
16:P:751:SER:O	16:P:754:GLU:N	2.44	0.46
18:R:253:ILE:HD13	18:R:257:ILE:HD12	1.97	0.46
1:A:461:GLU:HG2	1:A:1618:THR:HB	1.98	0.46
1:A:535:GLN:NE2	17:Q:26:ARG:HD3	2.31	0.46
1:A:564:PRO:HD2	15:O:371:HIS:HA	1.96	0.46
1:A:812:VAL:HA	1:A:815:ARG:HH21	1.80	0.46
2:B:1104:CYS:SG	2:B:1107:CYS:N	2.70	0.46
15:O:225:LEU:O	15:O:227:PHE:N	2.49	0.46
15:O:241:ASP:OD2	15:O:378:THR:HG22	2.15	0.46
16:P:394:VAL:HG12	16:P:434:ARG:NH1	2.30	0.46
17:Q:128:GLU:O	17:Q:132:VAL:HG23	2.15	0.46
17:Q:384:GLN:HA	17:Q:387:PRO:HD2	1.96	0.46
19:S:3:G:N1	20:T:21:DC:N3	2.51	0.46
1:A:81:LEU:CD2	1:A:85:CYS:SG	3.04	0.46
1:A:1314:GLN:O	1:A:1318:SER:N	2.49	0.46
2:B:212:ASN:CB	2:B:589:ASP:O	2.62	0.46
2:B:517:VAL:HG23	2:B:518:ARG:HG3	1.96	0.46
2:B:679:GLN:OE1	2:B:679:GLN:N	2.38	0.46
2:B:887:LEU:HB2	12:L:56:LEU:HB2	1.97	0.46
4:D:28:PRO:HD2	7:G:24:VAL:HG11	1.97	0.46
15:O:531:ILE:HA	15:O:534:GLN:HB2	1.97	0.46
16:P:659:LEU:HD12	16:P:742:TRP:CD1	2.50	0.46
18:R:171:ARG:C	18:R:174:GLU:H	2.18	0.46
18:R:250:LEU:HD21	18:R:307:LYS:CG	2.41	0.46
18:R:250:LEU:HB2	18:R:270:PHE:CE2	2.45	0.46
21:U:9:DT:H2"	21:U:10:DG:H5'	1.97	0.46
1:A:707:THR:HG22	1:A:709:ARG:N	2.21	0.46
1:A:1038:ILE:N	1:A:1047:GLN:O	2.43	0.46
4:D:86:ILE:HA	4:D:89:LEU:HD12	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:70:HIS:CE1	11:K:93:ILE:HD12	2.50	0.46
11:K:122:LYS:NZ	11:K:126:ASP:OD2	2.49	0.46
15:O:453:TYR:CZ	15:O:473:PHE:HB2	2.51	0.46
16:P:481:PHE:CE1	16:P:491:SER:HB2	2.50	0.46
16:P:604:ILE:HG22	16:P:605:SER:N	2.31	0.46
16:P:724:LEU:HB2	17:Q:446:TYR:HB3	1.96	0.46
17:Q:283:ASN:CG	17:Q:284:LEU:H	2.18	0.46
17:Q:410:ARG:HA	17:Q:413:LEU:CB	2.45	0.46
21:U:5:DT:H2"	21:U:6:DG:H5'	1.98	0.46
1:A:1104:TYR:CZ	1:A:1108:HIS:HD2	2.34	0.46
2:B:71:LYS:HG3	2:B:421:LEU:HB3	1.97	0.46
2:B:215:MET:HE2	2:B:217:ILE:HD11	1.97	0.46
2:B:729:PRO:HG2	2:B:733:LEU:HD21	1.98	0.46
2:B:912:GLN:N	2:B:915:ASP:OD2	2.48	0.46
5:E:43:LYS:O	5:E:47:CYS:HB2	2.15	0.46
15:O:540:CYS:O	15:O:544:ILE:N	2.40	0.46
16:P:288:SER:O	16:P:288:SER:OG	2.31	0.46
16:P:315:PHE:O	16:P:317:ILE:HD12	2.16	0.46
17:Q:139:LYS:HZ3	17:Q:139:LYS:N	2.14	0.46
17:Q:152:LEU:HB2	17:Q:154:LEU:HD13	1.97	0.46
17:Q:282:ARG:HG2	17:Q:302:ALA:HB1	1.98	0.46
17:Q:350:ARG:HD3	17:Q:486:GLN:CG	2.38	0.46
18:R:354:LEU:C	18:R:356:PRO:HD3	2.37	0.46
20:T:11:DA:C5	20:T:12:DC:C5	3.04	0.46
20:T:19:DC:H2'	20:T:20:DG:H8	1.81	0.46
1:A:1018:TYR:N	20:T:17:DT:H4'	2.31	0.46
1:A:1245:ASP:OD1	1:A:1246:VAL:N	2.41	0.46
1:A:1254:PHE:CE1	1:A:1258:ILE:HG21	2.51	0.46
1:A:1270:VAL:HG22	1:A:1294:MET:HG2	1.98	0.46
2:B:204:ARG:HH11	2:B:502:MET:HE1	1.81	0.46
2:B:770:ASN:O	10:J:48:ARG:NH1	2.48	0.46
2:B:815:ARG:HE	2:B:821:ILE:HA	1.80	0.46
2:B:881:TYR:CZ	12:L:67:PHE:HE1	2.34	0.46
2:B:954:PHE:CE1	2:B:963:PHE:CE1	3.04	0.46
3:C:243:SER:O	3:C:247:PHE:N	2.27	0.46
15:O:147:ILE:O	15:O:149:LYS:N	2.47	0.46
16:P:290:GLU:OE2	16:P:291:PRO:HD2	2.16	0.46
1:A:488:PRO:HB3	1:A:618:TYR:HE2	1.80	0.46
1:A:495:ILE:HG22	1:A:604:LYS:O	2.15	0.46
1:A:717:PRO:HG2	1:A:720:PHE:CD1	2.50	0.46
1:A:1238:MET:CE	1:A:1524:VAL:HG13	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:894:LYS:C	2:B:896:GLN:H	2.17	0.46
15:O:147:ILE:C	15:O:149:LYS:H	2.18	0.46
16:P:768:TYR:HB3	16:P:769:GLN:H	1.35	0.46
1:A:643:ALA:CA	2:B:1087:LEU:HB2	2.46	0.45
1:A:1038:ILE:CG1	1:A:1047:GLN:HB2	2.46	0.45
1:A:1297:PHE:HE2	9:I:58:SER:HB2	1.81	0.45
1:A:1556:GLU:O	1:A:1560:ASN:ND2	2.49	0.45
2:B:527:PHE:O	2:B:546:ALA:N	2.32	0.45
2:B:529:CYS:SG	2:B:698:SER:N	2.86	0.45
2:B:966:SER:OG	2:B:1029:GLY:HA3	2.16	0.45
9:I:37:TYR:HB3	9:I:41:GLN:HE22	1.80	0.45
11:K:77:ARG:HD2	11:K:91:TYR:CD1	2.51	0.45
13:M:102:SER:HB3	13:M:105:SER:OG	2.16	0.45
15:O:478:GLN:HA	15:O:481:CYS:SG	2.56	0.45
16:P:182:LEU:HA	16:P:182:LEU:HD22	1.51	0.45
16:P:190:ALA:O	16:P:247:ILE:O	2.34	0.45
16:P:215:ASN:OD1	16:P:218:VAL:HA	2.16	0.45
16:P:475:ARG:C	16:P:476:ILE:HD13	2.36	0.45
1:A:241:PRO:HB2	1:A:254:THR:O	2.16	0.45
1:A:771:PHE:CE1	1:A:776:LEU:HD13	2.43	0.45
1:A:1662:ASN:HB3	7:G:101:SER:HA	1.97	0.45
2:B:99:VAL:HG12	2:B:100:GLU:N	2.31	0.45
2:B:302:LEU:O	2:B:306:LEU:N	2.43	0.45
2:B:679:GLN:HE21	14:N:157:ARG:HA	1.81	0.45
2:B:683:ASN:HA	14:N:150:TYR:CZ	2.50	0.45
2:B:946:ASP:OD2	10:J:48:ARG:NH2	2.48	0.45
3:C:127:THR:OG1	3:C:130:ASN:N	2.47	0.45
3:C:232:GLN:HG2	3:C:232:GLN:O	2.16	0.45
9:I:6:SER:N	9:I:45:LEU:HD11	2.31	0.45
10:J:16:ASP:OD1	10:J:17:LYS:HG3	2.16	0.45
13:M:75:GLN:HB2	14:N:60:SER:HA	1.98	0.45
16:P:301:GLN:N	16:P:319:ASP:O	2.49	0.45
18:R:207:ASN:HD21	18:R:209:ARG:HH21	1.63	0.45
18:R:304:HIS:CD2	18:R:361:ASP:HB3	2.50	0.45
20:T:39:DT:H2"	20:T:40:DG:H5'	1.98	0.45
1:A:262:THR:O	1:A:266:VAL:HG23	2.17	0.45
1:A:643:ALA:HB1	2:B:1087:LEU:HD12	1.98	0.45
1:A:1293:HIS:CD2	1:A:1295:ARG:HH22	2.34	0.45
2:B:554:GLN:HA	2:B:646:HIS:CD2	2.51	0.45
2:B:1062:GLY:HA2	2:B:1067:GLY:H	1.81	0.45
2:B:1104:CYS:HA	2:B:1172:GLU:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1110:ILE:HG13	2:B:1111:LEU:HG	1.98	0.45
2:B:1134:ARG:HH12	2:B:1165:ASN:ND2	2.15	0.45
3:C:121:PRO:O	3:C:125:LYS:N	2.49	0.45
5:E:22:MET:O	5:E:26:ARG:N	2.34	0.45
12:L:68:GLU:OE2	12:L:70:ARG:HD3	2.17	0.45
13:M:58:GLU:O	13:M:103:LYS:NZ	2.49	0.45
15:O:477:PHE:HD2	15:O:520:CYS:SG	2.40	0.45
18:R:240:ILE:O	18:R:240:ILE:HG13	2.15	0.45
1:A:63:SER:O	2:B:1162:GLY:HA3	2.16	0.45
1:A:590:ASN:HD21	2:B:1075:GLU:CG	2.29	0.45
2:B:71:LYS:HB3	2:B:425:ILE:HG13	1.97	0.45
2:B:320:LEU:HD21	2:B:326:VAL:N	2.30	0.45
2:B:335:ARG:NH2	2:B:342:PRO:O	2.49	0.45
2:B:782:ASP:HB3	2:B:788:ILE:HG12	1.98	0.45
3:C:222:VAL:HB	3:C:224:THR:O	2.16	0.45
13:M:56:GLU:OE2	13:M:103:LYS:NZ	2.49	0.45
14:N:38:PHE:CE2	14:N:40:LEU:HB2	2.52	0.45
14:N:54:TRP:NE1	14:N:135:LYS:HD2	2.31	0.45
15:O:189:PHE:HD1	15:O:193:TYR:CE2	2.33	0.45
16:P:194:ARG:CZ	16:P:511:ILE:CG1	2.95	0.45
16:P:198:ASP:CB	16:P:261:VAL:HG23	2.46	0.45
16:P:574:TRP:O	16:P:577:LEU:HB2	2.17	0.45
17:Q:253:LEU:HD11	17:Q:270:THR:CG2	2.46	0.45
17:Q:366:TYR:CG	18:R:215:THR:CB	3.00	0.45
18:R:207:ASN:HD21	18:R:209:ARG:NH2	2.14	0.45
18:R:435:LEU:O	18:R:439:GLU:HG3	2.16	0.45
20:T:31:DT:H2"	20:T:32:DG:H5'	1.99	0.45
1:A:643:ALA:CB	2:B:1087:LEU:HA	2.46	0.45
1:A:1274:GLU:HB2	9:I:47:VAL:HB	1.99	0.45
1:A:1615:TYR:CD2	1:A:1616:GLU:HG3	2.51	0.45
2:B:252:TYR:HB2	2:B:381:LEU:HD21	1.99	0.45
2:B:726:MET:HG3	2:B:742:TYR:HB3	1.98	0.45
2:B:1074:MET:HE2	20:T:18:DT:H4'	1.97	0.45
3:C:273:ASP:CG	3:C:275:VAL:H	2.19	0.45
8:H:90:ALA:HB1	8:H:96:VAL:HG21	1.99	0.45
11:K:116:ALA:O	11:K:120:GLY:N	2.36	0.45
17:Q:360:LYS:HZ1	18:R:211:ARG:HH21	1.58	0.45
1:A:590:ASN:O	1:A:634:ASN:N	2.43	0.45
1:A:1070:LEU:HD13	1:A:1155:PHE:HE1	1.81	0.45
2:B:57:ASP:OD1	2:B:57:ASP:N	2.46	0.45
2:B:134:ARG:HD3	2:B:160:GLY:CA	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:372:ARG:NH2	2:B:574:SER:HA	2.31	0.45
2:B:1058:GLN:HG2	2:B:1096:SER:C	2.33	0.45
2:B:1060:VAL:O	2:B:1068:GLY:N	2.50	0.45
2:B:1079:LEU:CD1	2:B:1079:LEU:H	2.30	0.45
2:B:1093:LEU:HD13	2:B:1093:LEU:C	2.37	0.45
13:M:77:VAL:HG11	13:M:90:LEU:HB3	1.98	0.45
16:P:344:ILE:HG22	16:P:345:ASP:H	1.81	0.45
17:Q:341:ARG:HD3	17:Q:373:GLU:OE1	2.16	0.45
20:T:13:DT:H3	21:U:37:DA:H61	1.65	0.45
21:U:17:DT:H2"	21:U:18:DG:H5'	1.98	0.45
1:A:31:GLN:HB2	1:A:78:HIS:CE1	2.51	0.45
1:A:94:LEU:N	1:A:355:PHE:CE2	2.85	0.45
1:A:782:ASP:H	1:A:785:GLN:HB2	1.81	0.45
1:A:1136:VAL:HA	1:A:1174:TYR:CE2	2.52	0.45
1:A:1299:ASN:HB2	1:A:1466:SER:O	2.17	0.45
2:B:320:LEU:CD1	2:B:326:VAL:HA	2.46	0.45
2:B:600:GLN:HG3	2:B:604:ILE:HD11	1.99	0.45
7:G:62:MET:HA	7:G:66:LEU:HB2	1.99	0.45
11:K:60:SER:OG	11:K:106:GLN:HG2	2.17	0.45
15:O:540:CYS:O	15:O:543:ILE:N	2.50	0.45
16:P:727:PRO:HA	16:P:729:ALA:H	1.82	0.45
17:Q:408:ILE:HG13	17:Q:412:LYS:HD3	1.97	0.45
18:R:25:ASN:HD21	18:R:81:GLU:HG3	0.67	0.45
1:A:628:PHE:CB	2:B:785:ASP:OD1	2.64	0.45
1:A:646:GLU:OE1	2:B:1086:PHE:HB3	2.16	0.45
1:A:1039:ARG:CZ	6:F:139:PRO:HG2	2.47	0.45
1:A:1239:THR:HB	1:A:1542:THR:OG1	2.17	0.45
2:B:575:HIS:HB2	14:N:107:MET:HE2	1.99	0.45
4:D:19:PRO:HG2	4:D:22:ILE:HD11	1.99	0.45
15:O:477:PHE:CE1	15:O:480:LEU:HD11	2.52	0.45
17:Q:361:PRO:C	17:Q:363:SER:H	2.20	0.45
1:A:474:LYS:HD2	2:B:1092:LEU:HD21	1.98	0.45
1:A:557:LEU:O	1:A:561:LEU:N	2.49	0.45
2:B:545:PHE:HB3	2:B:549:CYS:HB3	1.98	0.45
5:E:100:ILE:O	5:E:104:ASN:N	2.50	0.45
11:K:46:LYS:NZ	11:K:67:GLU:HB2	2.32	0.45
15:O:388:VAL:HG22	15:O:395:LEU:HD23	1.99	0.45
15:O:399:PHE:CE2	15:O:403:LEU:HD11	2.51	0.45
18:R:75:GLN:HB2	20:T:43:DT:O3'	2.17	0.45
18:R:239:LEU:HD12	18:R:239:LEU:HA	1.74	0.45
20:T:3:DT:O2	21:U:47:DA:C2	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1048:PHE:CZ	5:E:211:TYR:HB2	2.52	0.45
1:A:1195:GLU:HB3	1:A:1196:PRO:HD3	1.98	0.45
2:B:262:PHE:CZ	2:B:269:TYR:HB2	2.51	0.45
2:B:890:ASP:O	12:L:54:ARG:HD3	2.17	0.45
3:C:123:ASP:OD1	3:C:124:GLU:N	2.48	0.45
3:C:230:LEU:HD22	3:C:231:PRO:HD2	1.97	0.45
3:C:277:ARG:HB3	3:C:280:LEU:HD12	1.98	0.45
3:C:309:THR:O	3:C:312:GLU:HB3	2.16	0.45
8:H:103:LYS:HB3	8:H:115:TYR:CD2	2.50	0.45
14:N:111:VAL:N	14:N:120:LYS:O	2.33	0.45
15:O:396:MET:HE1	15:O:434:LEU:HD12	0.99	0.45
15:O:610:TYR:CE2	15:O:612:GLU:HA	2.52	0.45
16:P:778:ASP:CG	16:P:779:ASP:H	2.19	0.45
18:R:34:ILE:HD12	18:R:34:ILE:HA	1.81	0.45
21:U:37:DA:C2	21:U:38:DG:C5	3.05	0.45
1:A:674:ILE:HA	1:A:786:TYR:OH	2.16	0.44
1:A:1258:ILE:CD1	1:A:1507:CYS:SG	3.00	0.44
2:B:459:SER:O	2:B:463:TYR:N	2.40	0.44
15:O:82:SER:HA	15:O:87:ARG:CZ	2.47	0.44
16:P:221:ARG:NH1	16:P:223:ASN:HD21	2.15	0.44
16:P:577:LEU:HD11	17:Q:503:SER:HB3	1.99	0.44
17:Q:150:GLU:OE1	17:Q:150:GLU:HA	2.17	0.44
18:R:365:TRP:HA	18:R:365:TRP:CE3	2.53	0.44
20:T:3:DT:H2"	20:T:4:DG:C8	2.51	0.44
1:A:537:GLN:HB3	1:A:576:LYS:HB2	2.00	0.44
1:A:547:ILE:HD11	17:Q:26:ARG:NH2	2.23	0.44
1:A:593:PRO:HD3	20:T:18:DT:O2	2.17	0.44
1:A:964:LYS:HE3	1:A:969:PHE:O	2.17	0.44
1:A:1118:VAL:O	1:A:1118:VAL:HG12	2.18	0.44
1:A:1158:SER:OG	1:A:1159:ASP:N	2.50	0.44
2:B:407:PHE:O	2:B:411:MET:HG3	2.18	0.44
2:B:974:LEU:HD23	10:J:44:TYR:HB3	1.99	0.44
2:B:1134:ARG:HH12	2:B:1165:ASN:HD22	1.66	0.44
3:C:74:GLU:HA	3:C:212:ILE:HB	1.99	0.44
10:J:16:ASP:OD1	10:J:17:LYS:N	2.50	0.44
11:K:66:VAL:HG12	11:K:67:GLU:N	2.32	0.44
15:O:124:LYS:HD3	15:O:127:GLU:OE1	2.17	0.44
16:P:399:TRP:CH2	18:R:294:VAL:HG23	2.52	0.44
18:R:157:MET:HG3	18:R:162:PHE:HB2	1.99	0.44
18:R:375:LYS:HA	18:R:375:LYS:HD3	1.57	0.44
1:A:81:LEU:HD23	1:A:85:CYS:SG	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:LYS:HG2	1:A:201:ARG:HH22	1.82	0.44
1:A:1090:ASP:HB3	1:A:1132:TYR:CD1	2.52	0.44
1:A:1303:SER:OG	1:A:1308:VAL:O	2.13	0.44
1:A:1320:GLN:HG3	1:A:1321:PHE:N	2.32	0.44
2:B:184:LYS:HZ3	10:J:69:ARG:HH22	1.65	0.44
2:B:996:PHE:O	2:B:999:GLN:N	2.51	0.44
2:B:1092:LEU:C	2:B:1092:LEU:CD2	2.85	0.44
5:E:13:TRP:HB2	5:E:42:PHE:CD2	2.53	0.44
8:H:116:TYR:HB2	8:H:123:MET:HB3	1.99	0.44
15:O:458:GLU:OE2	15:O:512:SER:HB2	2.18	0.44
15:O:479:ALA:O	15:O:483:ILE:HG13	2.17	0.44
16:P:186:TYR:CE1	16:P:448:THR:HG22	2.52	0.44
16:P:504:THR:HG22	16:P:505:PRO:HD3	2.00	0.44
17:Q:159:THR:HG22	17:Q:229:LYS:CB	2.46	0.44
17:Q:357:TYR:CD2	17:Q:489:VAL:CA	2.92	0.44
17:Q:366:TYR:CZ	18:R:215:THR:CA	2.95	0.44
17:Q:418:PRO:HD3	18:R:233:TYR:OH	2.18	0.44
18:R:15:GLN:HG3	18:R:184:ASN:HD22	1.83	0.44
1:A:564:PRO:HB2	15:O:371:HIS:NE2	2.33	0.44
1:A:697:TYR:CE1	1:A:701:ARG:HA	2.51	0.44
1:A:720:PHE:CE2	8:H:141:TYR:HE2	2.35	0.44
1:A:1136:VAL:HG22	1:A:1174:TYR:CD2	2.52	0.44
1:A:1196:PRO:HB3	1:A:1575:ILE:HG21	1.98	0.44
2:B:173:ASN:OD1	2:B:174:LYS:HG3	2.17	0.44
2:B:449:VAL:O	2:B:453:VAL:HG23	2.17	0.44
2:B:847:TYR:HB2	2:B:850:THR:OG1	2.18	0.44
2:B:908:ARG:HG2	3:C:95:GLU:HG3	1.99	0.44
2:B:949:ILE:CD1	2:B:954:PHE:CE2	3.00	0.44
5:E:76:GLY:H	5:E:106:GLN:HG2	1.82	0.44
5:E:177:ARG:NE	5:E:215:MET:HB2	2.32	0.44
11:K:64:GLN:NE2	11:K:100:LEU:HD13	2.32	0.44
13:M:42:LYS:O	14:N:30:LYS:N	2.46	0.44
15:O:328:LEU:HA	15:O:331:LYS:HD2	1.99	0.44
15:O:428:ILE:HD12	15:O:439:ILE:HD12	1.99	0.44
15:O:492:ARG:C	15:O:493:ASP:O	2.55	0.44
16:P:228:ASN:O	16:P:230:HIS:N	2.50	0.44
16:P:466:ALA:O	16:P:478:MET:HA	2.17	0.44
17:Q:283:ASN:OD1	17:Q:284:LEU:N	2.36	0.44
17:Q:309:TYR:O	17:Q:313:THR:OG1	2.30	0.44
1:A:93:GLN:CB	1:A:355:PHE:HE2	2.30	0.44
1:A:248:PHE:CZ	1:A:444:GLN:HA	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:956:ARG:HH21	1:A:979:GLY:HA3	1.82	0.44
1:A:1216:THR:HG22	1:A:1221:ARG:HB2	1.99	0.44
2:B:228:SER:O	2:B:254:ASN:ND2	2.50	0.44
2:B:649:MET:HE3	2:B:666:PRO:HG2	1.98	0.44
2:B:785:ASP:N	2:B:785:ASP:OD1	2.51	0.44
8:H:107:VAL:HB	8:H:111:LEU:CD1	2.47	0.44
15:O:447:THR:HA	15:O:450:LEU:HD12	2.00	0.44
15:O:477:PHE:CZ	15:O:516:PRO:HB2	2.53	0.44
16:P:214:LEU:HB2	16:P:222:GLN:CD	2.38	0.44
16:P:389:TRP:CH2	18:R:149:LYS:CB	3.00	0.44
16:P:436:ILE:HG23	16:P:436:ILE:O	2.18	0.44
16:P:451:ILE:HA	16:P:467:PHE:O	2.18	0.44
16:P:507:GLY:O	16:P:539:VAL:HA	2.17	0.44
16:P:738:LYS:HA	16:P:741:ILE:HG22	2.00	0.44
17:Q:19:LEU:CD1	17:Q:27:ARG:CB	2.94	0.44
17:Q:365:ASP:N	17:Q:365:ASP:OD1	2.50	0.44
18:R:76:LYS:O	18:R:80:ARG:HG3	2.17	0.44
18:R:350:SER:HB2	18:R:368:TYR:HE1	1.82	0.44
18:R:372:HIS:CD2	18:R:410:TYR:HB3	2.52	0.44
1:A:470:HIS:CD2	2:B:1056:THR:HG21	2.53	0.44
1:A:609:PRO:HB2	1:A:610:ASN:ND2	2.33	0.44
1:A:672:ASP:CB	2:B:783:MET:HE3	2.33	0.44
1:A:680:LEU:HD12	1:A:820:TYR:CG	2.53	0.44
1:A:683:LYS:HB2	8:H:20:TYR:CE1	2.53	0.44
1:A:1229:ALA:HB1	1:A:1595:TYR:CE2	2.53	0.44
1:A:1559:ARG:HG3	1:A:1586:ALA:HB1	2.00	0.44
2:B:65:VAL:CG2	2:B:99:VAL:HB	2.48	0.44
2:B:72:VAL:HG11	2:B:94:LYS:HE3	1.99	0.44
2:B:712:SER:HA	2:B:715:ASN:HD22	1.83	0.44
2:B:840:LEU:HA	2:B:846:PRO:HA	1.99	0.44
2:B:954:PHE:C	2:B:956:SER:N	2.70	0.44
2:B:1079:LEU:HD12	2:B:1079:LEU:N	2.33	0.44
3:C:31:TRP:HA	3:C:35:LYS:HD2	2.00	0.44
5:E:23:VAL:HG13	5:E:28:TYR:HD2	1.83	0.44
9:I:15:ASP:OD2	9:I:31:SER:OG	2.27	0.44
12:L:27:LEU:N	12:L:39:SER:HB2	2.32	0.44
15:O:541:PHE:HA	15:O:544:ILE:HB	2.00	0.44
16:P:343:LEU:N	16:P:343:LEU:HD23	2.32	0.44
16:P:582:ASP:H	16:P:585:GLU:HB2	1.82	0.44
17:Q:104:PHE:CD2	17:Q:105:LEU:HD23	2.53	0.44
17:Q:437:THR:OG1	17:Q:440:GLU:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:305:THR:HB	18:R:308:PHE:CE1	2.52	0.44
1:A:253:GLU:O	1:A:312:SER:N	2.51	0.44
1:A:559:ASN:HD22	15:O:376:TYR:HB2	1.83	0.44
1:A:584:ARG:NH1	1:A:644:ARG:HH12	2.15	0.44
1:A:654:ASP:N	1:A:654:ASP:OD1	2.47	0.44
1:A:672:ASP:CG	2:B:783:MET:HE3	2.38	0.44
1:A:1028:GLU:HG3	1:A:1637:PRO:HD2	1.99	0.44
1:A:1088:HIS:CD2	6:F:152:ILE:HD11	2.52	0.44
1:A:1508:VAL:O	1:A:1509:HIS:C	2.55	0.44
2:B:499:HIS:O	2:B:502:MET:HB3	2.18	0.44
2:B:822:THR:HG22	2:B:823:GLN:HG3	1.99	0.44
2:B:854:GLU:HA	2:B:874:TYR:HD2	1.83	0.44
2:B:916:LYS:HB3	2:B:1036:LEU:HD12	2.00	0.44
2:B:1093:LEU:CD1	2:B:1093:LEU:C	2.86	0.44
3:C:60:ASP:O	3:C:63:ILE:N	2.41	0.44
3:C:227:TYR:HA	3:C:299:ILE:O	2.17	0.44
5:E:205:SER:OG	5:E:206:GLY:N	2.51	0.44
9:I:8:ILE:O	9:I:17:LEU:N	2.50	0.44
13:M:77:VAL:HG21	14:N:64:ILE:HG21	2.00	0.44
15:O:153:ASP:HA	15:O:156:MET:HB3	2.00	0.44
15:O:357:GLY:O	15:O:361:PHE:N	2.27	0.44
16:P:283:ASP:OD1	16:P:284:VAL:N	2.50	0.44
17:Q:108:PHE:O	17:Q:111:ILE:HG22	2.18	0.44
18:R:408:ILE:HA	18:R:411:VAL:HG12	1.99	0.44
1:A:512:THR:CG2	1:A:514:TYR:CE2	2.99	0.44
1:A:584:ARG:HH12	1:A:644:ARG:HH12	1.65	0.44
1:A:793:ILE:O	1:A:796:SER:N	2.48	0.44
1:A:1654:PHE:CG	6:F:89:GLU:HG2	2.51	0.44
3:C:67:PHE:HE2	3:C:314:PHE:CZ	2.35	0.44
3:C:237:GLN:NE2	3:C:288:LYS:HG2	2.32	0.44
3:C:240:LYS:HB2	3:C:263:ASP:OD2	2.18	0.44
7:G:126:GLN:HG3	7:G:126:GLN:O	2.18	0.44
7:G:242:VAL:HG21	15:O:148:PRO:HB2	2.00	0.44
15:O:335:ILE:O	15:O:339:VAL:HG23	2.17	0.44
15:O:450:LEU:HD22	15:O:473:PHE:CE1	2.53	0.44
15:O:487:ARG:NE	15:O:502:LEU:HD13	2.31	0.44
16:P:55:LEU:HB3	18:R:227:HIS:HD1	1.67	0.44
16:P:389:TRP:HE1	18:R:146:SER:CB	2.13	0.44
16:P:632:ILE:O	16:P:636:GLU:HG3	2.18	0.44
17:Q:265:GLU:HB3	17:Q:269:TYR:CE1	2.52	0.44
1:A:530:TRP:CD1	1:A:531:PRO:HA	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:560:GLN:NE2	15:O:239:SER:HA	2.32	0.44
1:A:735:VAL:O	1:A:738:ASN:N	2.51	0.44
1:A:1311:GLU:O	1:A:1315:ASN:N	2.44	0.44
1:A:1492:ILE:O	1:A:1496:SER:N	2.49	0.44
1:A:1646:LEU:HD11	2:B:1086:PHE:HE1	1.79	0.44
2:B:25:PHE:CE1	10:J:59:LYS:HD2	2.53	0.44
2:B:289:PHE:HD1	2:B:306:LEU:HD22	1.83	0.44
2:B:822:THR:HG23	2:B:865:THR:HG23	2.00	0.44
3:C:86:PHE:HB3	12:L:62:LYS:HG3	2.00	0.44
16:P:330:PRO:HG3	16:P:342:GLN:HE21	1.82	0.44
16:P:658:LYS:CB	16:P:660:LYS:H	2.29	0.44
17:Q:22:ILE:HD13	17:Q:26:ARG:CZ	2.46	0.44
17:Q:381:MET:O	17:Q:385:PHE:HB2	2.18	0.44
17:Q:446:TYR:O	17:Q:449:GLN:HG2	2.18	0.44
1:A:263:ASN:HA	1:A:266:VAL:HB	1.99	0.43
1:A:1162:ASN:ND2	1:A:1164:LYS:HB2	2.33	0.43
2:B:174:LYS:NZ	18:R:351:GLU:OE2	2.41	0.43
2:B:292:ILE:O	2:B:579:ALA:HB3	2.18	0.43
2:B:374:LEU:HD12	2:B:374:LEU:HA	1.78	0.43
2:B:840:LEU:HD13	2:B:860:ALA:HB2	1.98	0.43
2:B:891:GLU:O	2:B:892:SER:OG	2.25	0.43
2:B:970:LYS:NZ	2:B:1011:GLU:OE2	2.39	0.43
10:J:14:VAL:CG2	10:J:50:ILE:HG12	2.48	0.43
14:N:87:TYR:HA	14:N:142:THR:HG22	2.00	0.43
15:O:361:PHE:CZ	15:O:399:PHE:HB2	2.53	0.43
16:P:186:TYR:N	18:R:198:LEU:HD23	2.33	0.43
16:P:187:ILE:HG22	16:P:188:GLN:H	1.83	0.43
17:Q:239:PHE:CG	17:Q:240:LYS:N	2.86	0.43
17:Q:334:LEU:HD12	17:Q:334:LEU:HA	1.76	0.43
18:R:161:ASN:O	18:R:164:LYS:HB2	2.18	0.43
20:T:9:DC:H2"	20:T:10:DA:O5'	2.18	0.43
1:A:413:LEU:HG	1:A:417:ARG:HH12	1.82	0.43
1:A:482:SER:HB3	1:A:614:LEU:HG	2.01	0.43
1:A:672:ASP:HA	2:B:952:HIS:NE2	2.33	0.43
1:A:753:ASN:HA	1:A:784:SER:OG	2.18	0.43
1:A:883:LEU:HD23	1:A:884:ARG:HH12	1.82	0.43
1:A:1182:GLY:O	1:A:1650:GLY:HA3	2.18	0.43
1:A:1305:GLU:HG2	9:I:59:SER:HB2	2.00	0.43
2:B:395:ASP:HA	2:B:505:ARG:HH12	1.82	0.43
2:B:881:TYR:HB2	2:B:906:ARG:HB3	1.98	0.43
3:C:67:PHE:HE2	3:C:314:PHE:CE1	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:78:LEU:HD21	5:E:109:ILE:HD12	1.99	0.43
16:P:49:THR:O	16:P:49:THR:OG1	2.35	0.43
16:P:227:LEU:HD21	16:P:234:THR:O	2.17	0.43
16:P:229:ARG:HE	16:P:230:HIS:CB	2.31	0.43
18:R:80:ARG:O	18:R:83:HIS:HB3	2.18	0.43
20:T:47:DT:H2"	20:T:48:DG:H5'	1.99	0.43
1:A:403:LEU:HD22	1:A:419:ILE:HG22	2.00	0.43
1:A:527:PRO:HD3	1:A:554:ARG:CZ	2.49	0.43
1:A:1017:GLY:HA3	20:T:17:DT:O4'	2.18	0.43
2:B:547:HIS:CG	2:B:760:TYR:HH	2.34	0.43
2:B:851:TYR:HD1	2:B:881:TYR:HE1	1.65	0.43
2:B:857:PRO:HG3	2:B:871:ILE:HD11	2.00	0.43
2:B:1063:ARG:CD	20:T:22:DG:P	3.06	0.43
3:C:80:ALA:HA	3:C:208:CYS:HA	2.00	0.43
3:C:165:ARG:HB3	3:C:189:PRO:HB3	2.00	0.43
3:C:334:THR:HG21	11:K:44:ARG:HB3	1.99	0.43
9:I:3:VAL:HA	9:I:7:LEU:O	2.18	0.43
15:O:241:ASP:CG	15:O:380:SER:CB	2.82	0.43
16:P:246:LYS:HD3	16:P:266:GLU:OE2	2.17	0.43
16:P:385:PHE:C	16:P:387:ASN:H	2.21	0.43
16:P:389:TRP:CH2	18:R:147:GLN:C	2.91	0.43
16:P:629:ARG:CZ	16:P:662:LEU:HD11	2.48	0.43
17:Q:356:VAL:CG1	18:R:208:TYR:CZ	2.97	0.43
1:A:481:ARG:NE	1:A:632:GLU:OE1	2.51	0.43
1:A:628:PHE:CB	2:B:785:ASP:CB	2.96	0.43
1:A:1258:ILE:O	1:A:1501:ILE:HD12	2.19	0.43
1:A:1617:THR:CG2	20:T:14:DG:H4'	2.48	0.43
2:B:229:TYR:HE1	2:B:253:LEU:HD11	1.83	0.43
2:B:1116:SER:O	2:B:1124:SER:OG	2.24	0.43
6:F:103:MET:O	6:F:104:ASN:HB2	2.18	0.43
15:O:591:TYR:CE2	15:O:593:PRO:HG3	2.53	0.43
15:O:600:LYS:HG3	15:O:601:ASN:N	2.32	0.43
16:P:389:TRP:CH2	18:R:149:LYS:N	2.79	0.43
16:P:696:PHE:HZ	16:P:745:ALA:HA	1.83	0.43
17:Q:178:THR:HG22	17:Q:303:GLU:OE2	2.18	0.43
17:Q:366:TYR:CG	18:R:215:THR:OG1	2.61	0.43
17:Q:366:TYR:OH	18:R:218:ASP:OD2	2.33	0.43
17:Q:472:ARG:O	17:Q:476:ILE:HG12	2.17	0.43
18:R:76:LYS:HA	18:R:79:ARG:HB2	2.01	0.43
1:A:449:GLY:C	1:A:451:VAL:H	2.21	0.43
1:A:1038:ILE:HG13	1:A:1047:GLN:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1245:ASP:OD1	1:A:1245:ASP:N	2.51	0.43
2:B:37:LEU:HB3	2:B:760:TYR:CE1	2.53	0.43
2:B:790:ASN:CB	2:B:936:MET:SD	3.06	0.43
7:G:45:LEU:HD13	7:G:47:VAL:CG1	2.48	0.43
12:L:33:GLU:HG2	12:L:53:HIS:NE2	2.34	0.43
14:N:149:ASP:O	14:N:153:VAL:HG12	2.19	0.43
15:O:446:LEU:HA	15:O:449:TRP:HB3	1.99	0.43
17:Q:484:ALA:O	17:Q:488:LEU:HG	2.18	0.43
18:R:248:LYS:HA	18:R:298:GLN:CD	2.39	0.43
1:A:109:ARG:HA	1:A:233:CYS:HA	2.01	0.43
2:B:225:ARG:HB2	2:B:229:TYR:CD2	2.53	0.43
2:B:832:TRP:HH2	2:B:837:LEU:HD21	1.83	0.43
7:G:168:PHE:HA	7:G:217:TRP:HA	2.00	0.43
13:M:67:ASP:HB3	13:M:70:SER:OG	2.18	0.43
15:O:600:LYS:O	15:O:603:LYS:HB3	2.19	0.43
16:P:329:ILE:HG13	16:P:330:PRO:O	2.18	0.43
16:P:365:TRP:CE3	16:P:372:ILE:HG22	2.54	0.43
16:P:675:PHE:HZ	16:P:742:TRP:CZ3	2.37	0.43
17:Q:120:ILE:HA	17:Q:125:PHE:HB2	2.00	0.43
17:Q:257:VAL:HG13	17:Q:262:LEU:HB2	2.00	0.43
17:Q:285:THR:OG1	17:Q:287:TRP:HB3	2.19	0.43
17:Q:323:ASP:C	17:Q:325:GLN:H	2.22	0.43
18:R:216:LEU:HD23	18:R:216:LEU:HA	1.91	0.43
18:R:415:LEU:HD21	18:R:428:SER:HB3	2.01	0.43
1:A:474:LYS:HD2	2:B:1092:LEU:CD2	2.48	0.43
1:A:966:LEU:HB3	1:A:969:PHE:HD2	1.84	0.43
1:A:1330:VAL:HA	1:A:1333:ILE:HD12	2.01	0.43
3:C:213:GLY:N	3:C:219:PHE:HB2	2.33	0.43
13:M:80:LEU:C	13:M:88:ILE:HG13	2.39	0.43
16:P:376:ASP:C	16:P:378:SER:N	2.72	0.43
16:P:641:TRP:CE3	16:P:750:PRO:HD3	2.54	0.43
17:Q:177:TYR:O	17:Q:180:ASP:HB2	2.19	0.43
20:T:35:DT:H2"	20:T:36:DG:H5'	1.99	0.43
1:A:194:ALA:O	1:A:198:SER:N	2.49	0.43
1:A:741:PRO:HD2	1:A:801:TYR:CD2	2.54	0.43
1:A:934:LYS:HG3	2:B:956:SER:OG	2.19	0.43
1:A:1074:TYR:OH	1:A:1159:ASP:OD2	2.24	0.43
1:A:1549:VAL:O	1:A:1553:TYR:N	2.51	0.43
1:A:1575:ILE:HG22	1:A:1576:SER:N	2.34	0.43
2:B:186:GLU:OE1	2:B:731:VAL:N	2.43	0.43
2:B:641:TYR:HB3	2:B:643:PHE:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:725:THR:HA	2:B:1036:LEU:HA	1.99	0.43
2:B:808:LYS:HA	2:B:902:SER:HA	1.99	0.43
2:B:916:LYS:O	2:B:917:PHE:HD1	2.02	0.43
3:C:161:HIS:CD2	3:C:195:LYS:HG2	2.53	0.43
6:F:57:ASP:OD1	6:F:58:PHE:N	2.51	0.43
10:J:7:CYS:HB2	10:J:46:CYS:SG	2.52	0.43
15:O:224:GLU:OE1	15:O:224:GLU:N	2.43	0.43
16:P:187:ILE:C	16:P:188:GLN:OE1	2.57	0.43
16:P:446:ASP:H	18:R:200:THR:HG21	1.82	0.43
16:P:745:ALA:O	16:P:747:LEU:N	2.44	0.43
17:Q:488:LEU:HD21	17:Q:498:LEU:HD12	2.01	0.43
18:R:307:LYS:HB3	18:R:308:PHE:H	1.66	0.43
1:A:646:GLU:OE1	2:B:1086:PHE:HB2	2.19	0.43
1:A:729:LYS:HE3	1:A:779:GLY:O	2.19	0.43
1:A:1291:VAL:HA	1:A:1473:LYS:HA	2.01	0.43
2:B:171:HIS:O	2:B:175:MET:HE3	2.19	0.43
2:B:335:ARG:HH21	2:B:342:PRO:HA	1.83	0.43
2:B:949:ILE:HD11	2:B:954:PHE:CE2	2.53	0.43
2:B:1013:MET:SD	2:B:1026:ILE:HD11	2.59	0.43
3:C:222:VAL:C	3:C:224:THR:N	2.69	0.43
3:C:241:GLY:O	3:C:245:ARG:NH1	2.52	0.43
3:C:294:VAL:CG2	3:C:297:HIS:HB3	2.49	0.43
15:O:383:TYR:CE2	15:O:594:TYR:HD1	2.37	0.43
16:P:226:HIS:NE2	16:P:232:ASN:HB3	2.34	0.43
16:P:358:SER:HB2	18:R:196:GLU:CD	2.40	0.43
16:P:650:LEU:HB3	17:Q:242:PHE:CD1	2.54	0.43
17:Q:171:HIS:HA	17:Q:244:ASN:O	2.19	0.43
17:Q:327:PRO:O	17:Q:331:ILE:HD13	2.18	0.43
19:S:6:A:H8	19:S:6:A:O5'	2.02	0.43
21:U:42:DA:H2"	21:U:43:DA:OP2	2.19	0.43
1:A:109:ARG:C	1:A:230:ARG:HG2	2.39	0.43
1:A:1060:GLU:HA	1:A:1063:MET:SD	2.59	0.43
2:B:524:SER:HB3	2:B:528:LEU:HB2	2.00	0.43
2:B:776:ILE:C	2:B:951:PRO:CD	2.77	0.43
3:C:169:PHE:CE2	3:C:171:PRO:HG3	2.54	0.43
3:C:226:SER:OG	3:C:227:TYR:N	2.52	0.43
5:E:114:ASN:OD1	5:E:115:ASN:N	2.48	0.43
5:E:154:ILE:HB	5:E:197:LYS:HB3	2.00	0.43
10:J:49:MET:O	10:J:53:HIS:HB2	2.19	0.43
10:J:53:HIS:CG	10:J:54:VAL:N	2.86	0.43
11:K:49:LEU:HD11	11:K:61:ALA:HB1	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:113:SER:N	14:N:118:SER:O	2.49	0.43
15:O:422:GLN:O	15:O:593:PRO:HD2	2.18	0.43
16:P:381:ILE:HA	16:P:391:THR:O	2.19	0.43
17:Q:177:TYR:OH	17:Q:252:LEU:N	2.52	0.43
17:Q:375:LEU:HA	17:Q:375:LEU:HD23	1.87	0.43
1:A:476:VAL:HG12	2:B:1095:SER:HB3	1.55	0.42
1:A:579:ARG:HH22	1:A:585:ASP:CG	2.22	0.42
1:A:808:LYS:O	1:A:812:VAL:HG23	2.19	0.42
1:A:1261:VAL:N	1:A:1499:ARG:O	2.52	0.42
1:A:1654:PHE:CE2	6:F:89:GLU:HG2	2.50	0.42
2:B:75:ASP:OD1	2:B:76:GLY:N	2.52	0.42
2:B:232:TYR:HD1	2:B:384:LEU:HG	1.83	0.42
2:B:572:PRO:HD2	2:B:575:HIS:CE1	2.54	0.42
2:B:929:ARG:HG2	2:B:930:LYS:O	2.18	0.42
2:B:986:PHE:CD2	2:B:992:PRO:HG3	2.54	0.42
3:C:42:VAL:HB	11:K:138:LYS:HG3	2.00	0.42
3:C:85:PHE:CE1	3:C:204:LEU:HD22	2.47	0.42
5:E:81:GLU:N	5:E:109:ILE:O	2.50	0.42
10:J:45:CYS:SG	10:J:46:CYS:N	2.92	0.42
16:P:192:ASP:OD1	16:P:212:SER:HA	2.19	0.42
16:P:197:ARG:HA	16:P:197:ARG:HD3	1.75	0.42
16:P:263:ILE:CG2	16:P:276:SER:HA	2.43	0.42
16:P:264:ILE:HD13	16:P:265:THR:H	1.84	0.42
16:P:458:LYS:HZ2	16:P:459:PRO:HD3	1.84	0.42
16:P:472:ARG:CZ	16:P:472:ARG:HB3	2.48	0.42
16:P:475:ARG:NH2	17:Q:364:SER:OG	2.52	0.42
18:R:301:SER:C	18:R:302:ARG:HG2	2.39	0.42
18:R:305:THR:O	18:R:306:ALA:C	2.57	0.42
18:R:366:PHE:CE2	18:R:425:ALA:HB2	2.54	0.42
1:A:120:CYS:HB3	1:A:189:VAL:HG21	2.01	0.42
1:A:1121:ASP:OD1	5:E:197:LYS:NZ	2.46	0.42
2:B:812:ALA:HB1	2:B:815:ARG:HD3	2.00	0.42
2:B:1078:ALA:O	2:B:1082:HIS:CA	2.63	0.42
5:E:7:ARG:O	5:E:11:ARG:N	2.36	0.42
10:J:8:PHE:HB2	10:J:48:ARG:NH2	2.34	0.42
14:N:69:SER:OG	14:N:70:LEU:N	2.52	0.42
14:N:82:ILE:HB	14:N:87:TYR:CE1	2.54	0.42
16:P:321:LYS:HB3	16:P:321:LYS:HE2	1.36	0.42
16:P:551:ALA:O	16:P:552:LEU:HD23	2.20	0.42
16:P:691:VAL:HG22	16:P:692:THR:O	2.19	0.42
17:Q:253:LEU:HB3	17:Q:267:TYR:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:269:TYR:HD2	17:Q:317:MET:HG3	1.84	0.42
18:R:242:ILE:HG13	18:R:243:PRO:HD2	2.01	0.42
1:A:651:ALA:H	2:B:1084:THR:HG22	1.84	0.42
1:A:1055:ILE:HD11	1:A:1174:TYR:CZ	2.54	0.42
1:A:1527:GLN:H	1:A:1527:GLN:CD	2.22	0.42
3:C:84:TYR:CE2	3:C:207:HIS:CD2	3.07	0.42
3:C:332:PRO:HG2	11:K:44:ARG:HG2	2.00	0.42
5:E:123:LEU:O	5:E:126:SER:HB3	2.18	0.42
14:N:78:THR:O	14:N:89:ILE:N	2.45	0.42
15:O:97:LEU:O	15:O:101:SER:N	2.42	0.42
15:O:409:ALA:O	15:O:417:LYS:HE2	2.19	0.42
16:P:236:ILE:HD13	16:P:236:ILE:HA	1.91	0.42
16:P:301:GLN:NE2	16:P:359:SER:O	2.52	0.42
18:R:4:VAL:CG1	18:R:6:ILE:HG12	2.49	0.42
18:R:162:PHE:HA	18:R:165:ILE:CD1	2.45	0.42
18:R:374:LEU:HD22	18:R:374:LEU:HA	1.84	0.42
1:A:325:ASP:O	1:A:329:ARG:HG3	2.19	0.42
1:A:1035:ASP:O	1:A:1036:ASN:HB2	2.18	0.42
1:A:1263:LEU:HG	1:A:1267:ILE:HD11	2.02	0.42
2:B:390:SER:HB3	2:B:634:ARG:O	2.20	0.42
2:B:393:ASN:HB3	2:B:396:ALA:HB2	2.01	0.42
2:B:936:MET:HG3	2:B:948:ILE:HD11	2.00	0.42
2:B:1011:GLU:N	2:B:1026:ILE:O	2.45	0.42
8:H:92:ASP:O	8:H:145:ARG:HD3	2.19	0.42
10:J:20:SER:O	10:J:24:LEU:HG	2.20	0.42
15:O:430:ARG:HD2	15:O:610:TYR:CE1	2.54	0.42
16:P:356:GLU:OE2	16:P:378:SER:HB3	2.18	0.42
16:P:715:TYR:HE1	16:P:733:THR:HG23	1.84	0.42
17:Q:167:LEU:HD22	17:Q:167:LEU:HA	1.90	0.42
17:Q:288:GLU:O	17:Q:290:THR:HG22	2.19	0.42
18:R:187:TYR:O	18:R:191:ILE:HG23	2.20	0.42
18:R:358:PHE:O	18:R:360:GLU:N	2.47	0.42
1:A:246:ASP:OD2	1:A:250:LYS:HB2	2.19	0.42
1:A:627:ASP:C	2:B:784:ASP:OD1	2.58	0.42
2:B:417:ILE:O	2:B:420:TYR:HB3	2.20	0.42
2:B:795:GLU:HB3	3:C:216:HIS:NE2	2.34	0.42
3:C:235:ILE:HG22	3:C:237:GLN:H	1.85	0.42
15:O:347:VAL:HG11	15:O:395:LEU:HD21	2.02	0.42
16:P:200:THR:OG1	16:P:280:ARG:NH1	2.53	0.42
16:P:330:PRO:HG3	16:P:342:GLN:HG3	2.00	0.42
16:P:422:ILE:HG12	16:P:442:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:6:ARG:HA	17:Q:18:ARG:CD	2.50	0.42
17:Q:115:GLN:HB3	17:Q:190:MET:HE3	2.00	0.42
17:Q:329:LYS:O	17:Q:332:LEU:HB2	2.19	0.42
17:Q:500:ASP:O	17:Q:503:SER:OG	2.36	0.42
18:R:30:ARG:NE	18:R:168:ILE:HD13	2.34	0.42
1:A:407:GLN:O	1:A:411:VAL:HG23	2.20	0.42
1:A:503:VAL:HG13	1:A:527:PRO:O	2.20	0.42
1:A:511:VAL:HG11	1:A:575:LYS:CA	2.49	0.42
1:A:671:GLN:CB	2:B:783:MET:HE3	2.48	0.42
1:A:690:GLU:OE1	1:A:690:GLU:N	2.46	0.42
1:A:826:PHE:O	2:B:776:ILE:HG13	2.19	0.42
1:A:975:ASP:OD2	1:A:977:MET:HB3	2.20	0.42
2:B:113:VAL:HB	18:R:281:LYS:HE3	2.01	0.42
2:B:314:LYS:O	2:B:316:ARG:N	2.49	0.42
2:B:1103:VAL:O	2:B:1173:THR:HA	2.18	0.42
3:C:100:ARG:NH1	10:J:3:VAL:O	2.47	0.42
5:E:96:PHE:O	5:E:99:HIS:HB3	2.20	0.42
14:N:35:LEU:O	14:N:116:LYS:HD3	2.19	0.42
15:O:82:SER:OG	15:O:87:ARG:NH1	2.53	0.42
16:P:442:LEU:HB3	16:P:477:TYR:OH	2.20	0.42
16:P:475:ARG:NH2	17:Q:364:SER:HA	2.34	0.42
17:Q:7:GLY:HA3	17:Q:8:PRO:HD2	1.45	0.42
17:Q:256:LEU:HG	17:Q:310:PHE:CE2	2.54	0.42
1:A:75:HIS:N	1:A:364:PRO:HB3	2.34	0.42
1:A:91:PHE:CE2	1:A:245:LYS:HD2	2.55	0.42
1:A:246:ASP:HB2	1:A:250:LYS:H	1.85	0.42
1:A:750:ILE:HG12	1:A:770:LEU:HD13	2.01	0.42
2:B:90:TYR:CE2	2:B:92:GLY:HA2	2.54	0.42
2:B:300:SER:O	2:B:303:THR:OG1	2.32	0.42
2:B:343:ASP:OD1	2:B:344:GLN:HG3	2.20	0.42
2:B:439:ASN:HB3	2:B:442:ASP:HB2	2.01	0.42
2:B:654:ARG:NH2	2:B:659:ASP:OD2	2.53	0.42
2:B:702:ASN:HB3	2:B:756:LEU:HD12	2.02	0.42
2:B:1049:THR:O	2:B:1052:VAL:HG13	2.20	0.42
3:C:233:ILE:HG12	3:C:291:LEU:HD22	2.01	0.42
5:E:200:ARG:N	5:E:208:TYR:O	2.36	0.42
8:H:62:SER:OG	8:H:63:LEU:N	2.53	0.42
16:P:426:ALA:HB3	16:P:435:ARG:HD2	2.02	0.42
16:P:473:HIS:CG	16:P:475:ARG:HD3	2.54	0.42
17:Q:356:VAL:CA	18:R:208:TYR:HA	2.49	0.42
17:Q:366:TYR:HE1	18:R:218:ASP:HB2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:GLU:OE2	1:A:1645:LYS:CG	2.63	0.42
1:A:477:ASN:HB3	2:B:1047:ARG:HH11	1.83	0.42
1:A:812:VAL:HG22	1:A:815:ARG:NH2	2.35	0.42
1:A:1238:MET:HE2	1:A:1525:ASN:H	1.83	0.42
2:B:328:GLN:O	2:B:346:ASP:HB3	2.19	0.42
2:B:648:ARG:NH1	2:B:650:LEU:HD21	2.34	0.42
2:B:853:GLU:HG2	2:B:856:ASP:OD2	2.19	0.42
3:C:69:ARG:HH21	11:K:71:THR:N	2.15	0.42
3:C:103:LEU:HD23	3:C:218:LYS:HB3	2.01	0.42
4:D:33:THR:O	4:D:37:LEU:N	2.32	0.42
5:E:68:SER:HB3	5:E:75:MET:SD	2.60	0.42
7:G:73:TYR:CZ	7:G:238:THR:HG21	2.55	0.42
11:K:62:SER:OG	11:K:104:ARG:NH1	2.41	0.42
16:P:324:TRP:CZ2	16:P:383:ILE:HG21	2.55	0.42
16:P:438:TRP:CE3	16:P:439:LYS:O	2.73	0.42
16:P:597:LYS:HD2	17:Q:321:ASP:OD1	2.19	0.42
16:P:740:ILE:O	16:P:744:LEU:HG	2.20	0.42
17:Q:297:ARG:HB2	17:Q:297:ARG:HH11	1.84	0.42
17:Q:302:ALA:O	17:Q:303:GLU:C	2.58	0.42
18:R:253:ILE:HG22	18:R:254:GLY:N	2.34	0.42
20:T:11:DA:N3	20:T:12:DC:C6	2.88	0.42
1:A:132:GLU:O	1:A:136:LEU:N	2.51	0.42
1:A:259:LYS:O	1:A:262:THR:HB	2.18	0.42
1:A:489:ASN:ND2	2:B:781:TYR:CZ	2.85	0.42
1:A:560:GLN:HE22	15:O:238:ILE:HG22	1.85	0.42
1:A:1051:GLY:CA	1:A:1580:ARG:HG2	2.49	0.42
1:A:1482:LYS:HD2	2:B:307:GLU:OE1	2.20	0.42
2:B:95:LEU:HD12	2:B:144:SER:O	2.20	0.42
2:B:561:ILE:HB	2:B:562:PRO:HD3	2.02	0.42
2:B:712:SER:N	2:B:713:PRO:HD2	2.35	0.42
2:B:789:ILE:HD12	2:B:927:CYS:SG	2.59	0.42
3:C:294:VAL:HG21	3:C:297:HIS:HB3	2.02	0.42
4:D:27:LEU:HA	4:D:28:PRO:HD3	1.91	0.42
4:D:89:LEU:HA	4:D:92:ILE:HD12	2.01	0.42
5:E:55:ARG:NE	5:E:113:GLN:HE21	2.18	0.42
7:G:33:GLY:HA3	7:G:230:ARG:HH22	1.85	0.42
7:G:127:PRO:HG2	7:G:236:VAL:HG21	2.01	0.42
9:I:29:GLU:HG3	9:I:36:ILE:HG13	2.01	0.42
9:I:30:CYS:O	9:I:34:LYS:HA	2.20	0.42
13:M:10:ILE:HB	14:N:70:LEU:HB3	2.01	0.42
15:O:474:TYR:HA	15:O:477:PHE:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:393:VAL:HG23	16:P:394:VAL:N	2.31	0.42
17:Q:147:GLN:N	17:Q:148:PRO:HD3	2.34	0.42
17:Q:323:ASP:C	17:Q:325:GLN:N	2.72	0.42
17:Q:439:ILE:H	17:Q:439:ILE:HG13	1.66	0.42
17:Q:512:ARG:HA	17:Q:512:ARG:HD3	1.84	0.42
18:R:426:VAL:HG23	18:R:427:PRO:HD2	2.02	0.42
1:A:821:ILE:O	1:A:825:ALA:N	2.38	0.42
1:A:1645:LYS:CB	1:A:1645:LYS:HZ2	2.33	0.42
2:B:909:ARG:NH2	2:B:1042:ASP:OD1	2.53	0.42
2:B:917:PHE:CE1	2:B:1035:ARG:HG3	2.55	0.42
5:E:50:MET:HB3	5:E:52:ARG:H	1.85	0.42
8:H:33:GLN:HB2	8:H:36:CYS:HB3	2.02	0.42
14:N:83:ASP:C	14:N:85:HIS:H	2.23	0.42
15:O:364:LEU:HB3	15:O:385:MET:HE3	2.02	0.42
16:P:473:HIS:HA	16:P:474:LYS:HE3	2.02	0.42
16:P:582:ASP:HB2	16:P:585:GLU:HG3	2.02	0.42
16:P:607:VAL:O	16:P:611:ILE:HG13	2.20	0.42
16:P:776:ASP:HB3	17:Q:134:LYS:HE3	2.02	0.42
17:Q:112:LEU:CD1	17:Q:164:ILE:HD11	2.50	0.42
17:Q:356:VAL:CB	18:R:208:TYR:CA	2.77	0.42
1:A:103:LEU:CD1	1:A:241:PRO:HD2	2.50	0.41
1:A:476:VAL:HA	2:B:1095:SER:C	2.17	0.41
1:A:525:ASN:ND2	1:A:531:PRO:O	2.36	0.41
1:A:535:GLN:C	1:A:578:TYR:CD1	2.93	0.41
1:A:1246:VAL:CG1	1:A:1250:GLN:HB3	2.41	0.41
1:A:1657:LEU:HD23	7:G:104:LEU:HB3	2.01	0.41
2:B:1087:LEU:HD23	2:B:1088:LEU:CD2	2.50	0.41
6:F:147:SER:O	6:F:150:GLU:HG2	2.19	0.41
11:K:83:ASN:ND2	11:K:119:LYS:HD3	2.35	0.41
13:M:10:ILE:O	14:N:69:SER:HA	2.20	0.41
16:P:473:HIS:ND1	16:P:473:HIS:O	2.53	0.41
16:P:492:LEU:HD22	16:P:492:LEU:N	2.35	0.41
16:P:697:GLU:HB3	16:P:709:PRO:O	2.20	0.41
16:P:768:TYR:O	16:P:771:ILE:N	2.53	0.41
18:R:8:LEU:HB2	18:R:9:THR:HG22	2.01	0.41
18:R:246:GLN:CD	18:R:247:ILE:HD12	2.40	0.41
18:R:372:HIS:CE1	18:R:410:TYR:CD2	3.08	0.41
1:A:1289:SER:CB	1:A:1475:GLU:HG2	2.49	0.41
2:B:527:PHE:HE2	2:B:669:GLN:OE1	2.03	0.41
2:B:565:LEU:HB3	2:B:570:VAL:HG21	2.01	0.41
2:B:612:LYS:CG	2:B:622:ILE:HA	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:146:ALA:HB1	3:C:156:LEU:HD23	2.02	0.41
7:G:65:HIS:O	7:G:68:PRO:HD2	2.20	0.41
8:H:30:SER:HB3	8:H:33:GLN:O	2.20	0.41
14:N:81:THR:HG22	14:N:86:ASP:HB3	2.02	0.41
15:O:502:LEU:HD22	15:O:506:PHE:CE2	2.55	0.41
16:P:300:LEU:HA	16:P:320:ILE:CA	2.48	0.41
16:P:504:THR:O	16:P:542:ARG:HG2	2.20	0.41
17:Q:22:ILE:HD12	17:Q:26:ARG:HE	1.78	0.41
17:Q:26:ARG:HD2	17:Q:34:VAL:HG11	2.02	0.41
18:R:75:GLN:HA	18:R:78:ARG:NE	2.32	0.41
1:A:76:GLN:HB3	1:A:364:PRO:HD3	2.02	0.41
1:A:461:GLU:O	1:A:465:GLY:N	2.54	0.41
1:A:597:LYS:HE3	1:A:660:PRO:CG	2.50	0.41
2:B:311:ARG:NH2	9:I:17:LEU:O	2.53	0.41
2:B:528:LEU:HA	2:B:528:LEU:HD23	1.86	0.41
2:B:775:VAL:HG12	2:B:951:PRO:HB3	2.03	0.41
2:B:929:ARG:HG2	2:B:930:LYS:N	2.34	0.41
2:B:1112:THR:OG1	2:B:1128:CYS:SG	2.64	0.41
3:C:128:ASP:HB2	3:C:175:GLN:HG3	2.02	0.41
4:D:88:GLN:HE21	15:O:184:PRO:HB2	1.84	0.41
7:G:47:VAL:HB	7:G:65:HIS:NE2	2.35	0.41
13:M:42:LYS:HG3	13:M:51:PHE:HE1	1.85	0.41
14:N:31:LYS:HE2	14:N:117:GLU:HG2	2.01	0.41
16:P:64:LEU:CD2	16:P:64:LEU:H	2.33	0.41
16:P:184:SER:C	18:R:198:LEU:HG	2.40	0.41
16:P:348:HIS:HE1	18:R:154:LYS:CE	2.33	0.41
16:P:358:SER:HB2	18:R:196:GLU:OE1	2.16	0.41
17:Q:4:PHE:HE2	17:Q:18:ARG:HH11	1.67	0.41
18:R:297:PHE:N	18:R:297:PHE:CD1	2.89	0.41
18:R:402:ASN:O	18:R:405:ILE:HB	2.20	0.41
1:A:407:GLN:HB2	1:A:410:LYS:HB3	2.01	0.41
1:A:582:LYS:CE	1:A:584:ARG:HE	2.33	0.41
1:A:733:THR:HG23	1:A:775:ALA:HA	2.02	0.41
1:A:1003:ARG:CD	2:B:520:LEU:HD22	2.49	0.41
1:A:1273:THR:HG22	9:I:48:VAL:HG13	2.02	0.41
3:C:128:ASP:OD1	3:C:129:GLU:N	2.53	0.41
5:E:33:GLU:OE1	5:E:33:GLU:N	2.42	0.41
8:H:115:TYR:HE1	8:H:124:ARG:CG	2.32	0.41
10:J:36:LEU:HD11	10:J:51:LEU:HD13	2.03	0.41
14:N:82:ILE:O	14:N:87:TYR:HE1	2.04	0.41
15:O:523:ASN:O	15:O:527:MET:N	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:611:ILE:CD1	16:P:731:LEU:HB2	2.50	0.41
16:P:755:PRO:HB3	17:Q:131:HIS:HB3	2.03	0.41
1:A:54:LEU:HA	1:A:54:LEU:HD23	1.85	0.41
1:A:632:GLU:OE2	2:B:1043:LYS:HB3	2.19	0.41
1:A:1129:PRO:HB2	1:A:1178:LEU:HD11	2.03	0.41
2:B:918:SER:HA	2:B:923:GLN:O	2.21	0.41
2:B:975:HIS:CE1	2:B:1003:ALA:HB2	2.56	0.41
5:E:112:TYR:CD2	5:E:116:ILE:HD11	2.55	0.41
7:G:158:LYS:HG2	15:O:105:ASN:OD1	2.21	0.41
7:G:216:HIS:HD1	7:G:224:PRO:HB3	1.85	0.41
10:J:30:LEU:HD11	10:J:38:ARG:NH1	2.34	0.41
13:M:67:ASP:OD1	13:M:68:SER:N	2.53	0.41
15:O:383:TYR:CE1	15:O:597:LEU:HD21	2.55	0.41
16:P:186:TYR:HD1	18:R:198:LEU:HD23	1.82	0.41
16:P:194:ARG:HA	16:P:209:LYS:O	2.20	0.41
16:P:540:LYS:HE2	16:P:544:SER:O	2.21	0.41
16:P:596:ILE:HB	17:Q:272:GLN:HG2	2.01	0.41
16:P:666:SER:HB3	16:P:742:TRP:CE2	2.54	0.41
16:P:697:GLU:HG2	16:P:698:LYS:N	2.34	0.41
17:Q:353:VAL:HG11	17:Q:489:VAL:HG12	2.01	0.41
18:R:165:ILE:H	18:R:165:ILE:HG13	1.49	0.41
18:R:216:LEU:HD13	18:R:239:LEU:HD13	2.02	0.41
20:T:14:DG:C2	21:U:37:DA:C2	3.09	0.41
1:A:2:ASP:OD2	1:A:4:SER:OG	2.37	0.41
1:A:67:LEU:HD11	2:B:1115:GLN:HG3	2.03	0.41
1:A:91:PHE:O	1:A:94:LEU:HB3	2.21	0.41
1:A:126:GLN:HB3	1:A:343:PRO:HD3	2.01	0.41
1:A:358:ASP:HB2	1:A:359:VAL:H	1.64	0.41
1:A:514:TYR:OH	6:F:102:SER:HA	2.21	0.41
1:A:518:GLU:OE1	1:A:582:LYS:NZ	2.54	0.41
1:A:539:GLU:HB3	1:A:570:THR:HB	2.02	0.41
1:A:581:ILE:CD1	1:A:637:PHE:CE1	3.03	0.41
1:A:772:LYS:HE3	8:H:137:GLN:NE2	2.35	0.41
1:A:934:LYS:HE2	2:B:956:SER:OG	2.21	0.41
1:A:989:GLY:HA3	2:B:709:PHE:HE1	1.85	0.41
1:A:1319:ASN:C	1:A:1323:HIS:HD1	2.16	0.41
2:B:117:VAL:HG23	18:R:276:GLN:HA	1.68	0.41
2:B:178:TYR:O	2:B:182:GLN:HG2	2.20	0.41
2:B:218:ILE:HG23	2:B:231:HIS:ND1	2.36	0.41
2:B:560:ARG:HH22	2:B:618:PRO:HB2	1.85	0.41
2:B:584:CYS:HB3	2:B:596:VAL:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:893:ASN:ND2	20:T:39:DT:H5"	2.36	0.41
2:B:1131:CYS:HB2	2:B:1170:GLY:HA2	2.02	0.41
3:C:44:ILE:HA	3:C:54:PHE:CB	2.51	0.41
9:I:19:ASN:OD1	9:I:21:ASN:N	2.48	0.41
12:L:50:ASP:HA	17:Q:412:LYS:NZ	2.36	0.41
14:N:63:ASP:OD1	14:N:65:SER:OG	2.32	0.41
15:O:457:ARG:HB3	15:O:470:PHE:HE1	1.85	0.41
17:Q:123:MET:HG2	17:Q:184:TRP:CZ2	2.56	0.41
18:R:231:LEU:HD23	18:R:231:LEU:HA	1.78	0.41
1:A:413:LEU:O	1:A:417:ARG:NH1	2.53	0.41
1:A:638:PRO:HB3	1:A:643:ALA:HB1	2.03	0.41
1:A:719:ILE:HG12	8:H:97:MET:HG2	2.02	0.41
1:A:800:VAL:O	1:A:1079:LYS:HD2	2.21	0.41
1:A:1478:ALA:O	9:I:19:ASN:ND2	2.53	0.41
1:A:1481:GLU:OE1	1:A:1481:GLU:N	2.49	0.41
2:B:135:GLY:N	2:B:161:LEU:O	2.52	0.41
2:B:781:TYR:OH	11:K:96:PRO:HD2	2.21	0.41
2:B:806:THR:OG1	2:B:904:LYS:HG2	2.21	0.41
2:B:913:ILE:HD12	2:B:929:ARG:HA	2.02	0.41
2:B:995:TYR:O	2:B:998:GLU:HB3	2.21	0.41
2:B:1061:LYS:HE2	20:T:21:DC:OP2	2.21	0.41
4:D:22:ILE:O	7:G:76:LYS:NZ	2.39	0.41
4:D:88:GLN:O	4:D:92:ILE:HG13	2.21	0.41
5:E:118:PRO:O	5:E:121:MET:HB2	2.20	0.41
7:G:138:PHE:CD1	15:O:182:MET:SD	3.14	0.41
15:O:181:ARG:NH2	15:O:221:TYR:O	2.54	0.41
15:O:200:ASN:OD1	17:Q:14:ASN:CB	2.66	0.41
18:R:219:LEU:O	18:R:223:ASN:ND2	2.51	0.41
1:A:571:HIS:CE1	1:A:572:THR:HG23	2.56	0.41
1:A:597:LYS:HB2	2:B:1082:HIS:CG	2.55	0.41
1:A:793:ILE:HG23	1:A:794:VAL:N	2.32	0.41
1:A:826:PHE:HB3	2:B:777:SER:HB2	2.03	0.41
1:A:886:ASN:OD1	1:A:955:ARG:NH1	2.32	0.41
1:A:1156:LYS:HE2	1:A:1156:LYS:HB2	1.91	0.41
1:A:1233:ILE:HD11	1:A:1236:PRO:HA	2.03	0.41
1:A:1314:GLN:O	1:A:1318:SER:OG	2.36	0.41
1:A:1655:ASP:HB2	6:F:135:ARG:HB3	2.03	0.41
2:B:127:ARG:NH2	2:B:193:TYR:OH	2.50	0.41
3:C:240:LYS:HA	3:C:244:ALA:HB2	2.02	0.41
5:E:39:LEU:O	5:E:42:PHE:HB3	2.21	0.41
5:E:191:LYS:HB2	5:E:194:GLU:OE2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:141:SER:HG	7:G:144:HIS:HD1	1.62	0.41
13:M:42:LYS:HG3	13:M:51:PHE:CE1	2.56	0.41
16:P:645:LYS:O	16:P:647:GLU:N	2.54	0.41
18:R:16:ARG:NH2	18:R:183:GLU:OE2	2.54	0.41
1:A:332:GLN:HG2	1:A:349:LEU:HD22	2.03	0.41
1:A:628:PHE:CG	2:B:784:ASP:HB3	2.54	0.41
1:A:810:LEU:HA	1:A:810:LEU:HD12	1.88	0.41
1:A:1644:GLY:HA3	2:B:1179:PRO:HD3	2.02	0.41
2:B:79:LEU:HB2	2:B:90:TYR:CE2	2.56	0.41
2:B:211:ARG:HH22	2:B:645:GLY:HA3	1.86	0.41
2:B:212:ASN:HD22	2:B:212:ASN:H	1.67	0.41
2:B:460:LYS:O	2:B:463:TYR:HB3	2.21	0.41
2:B:610:TYR:HE1	2:B:658:LEU:HD11	1.86	0.41
2:B:612:LYS:HG2	2:B:622:ILE:HA	2.03	0.41
2:B:1058:GLN:O	2:B:1059:PRO:O	2.39	0.41
2:B:1202:PRO:HG3	7:G:46:TYR:CD2	2.56	0.41
5:E:183:PRO:HA	5:E:186:LEU:HD12	2.03	0.41
11:K:79:VAL:HG21	11:K:124:LEU:HD13	2.02	0.41
14:N:82:ILE:HB	14:N:87:TYR:CD1	2.56	0.41
15:O:484:PHE:CZ	15:O:527:MET:O	2.74	0.41
15:O:487:ARG:HG2	15:O:491:PHE:CD2	2.56	0.41
15:O:606:MET:HA	15:O:609:TYR:CD2	2.56	0.41
15:O:606:MET:HA	15:O:609:TYR:HD2	1.84	0.41
16:P:220:THR:HB	16:P:222:GLN:HE22	1.86	0.41
16:P:329:ILE:HG13	16:P:330:PRO:N	2.33	0.41
16:P:351:ILE:O	16:P:352:PHE:HB2	2.21	0.41
16:P:414:ILE:HD13	16:P:425:GLY:HA3	2.03	0.41
16:P:420:GLU:HB2	16:P:442:LEU:H	1.82	0.41
16:P:484:ARG:HG3	16:P:488:LEU:HD23	2.02	0.41
16:P:510:THR:C	16:P:511:ILE:HG13	2.41	0.41
16:P:596:ILE:O	16:P:596:ILE:HD12	2.21	0.41
16:P:662:LEU:CB	16:P:665:ASN:HD22	2.25	0.41
16:P:732:LEU:O	16:P:733:THR:C	2.58	0.41
16:P:764:LEU:O	16:P:766:GLY:N	2.54	0.41
17:Q:15:CYS:CB	17:Q:17:SER:H	2.30	0.41
17:Q:178:THR:CG2	17:Q:303:GLU:OE1	2.69	0.41
17:Q:229:LYS:HA	17:Q:232:LEU:HB2	2.03	0.41
17:Q:307:LEU:O	17:Q:311:MET:HG2	2.21	0.41
17:Q:356:VAL:CG1	18:R:212:HIS:NE2	2.80	0.41
17:Q:441:ASP:OD2	17:Q:445:ARG:NH1	2.54	0.41
1:A:70:LYS:HZ2	17:Q:27:ARG:CZ	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:ARG:HA	1:A:369:LEU:HG	2.02	0.41
1:A:499:PRO:HG3	1:A:609:PRO:HA	2.03	0.41
1:A:893:ASP:OD2	1:A:955:ARG:HB3	2.21	0.41
1:A:1014:SER:O	20:T:17:DT:C5'	2.60	0.41
1:A:1031:HIS:O	1:A:1039:ARG:N	2.53	0.41
1:A:1104:TYR:OH	1:A:1117:SER:HB3	2.20	0.41
1:A:1152:SER:O	1:A:1156:LYS:NZ	2.53	0.41
1:A:1323:HIS:CE1	1:A:1454:HIS:NE2	2.89	0.41
2:B:461:MET:O	2:B:464:PHE:HB3	2.21	0.41
2:B:1136:GLU:O	2:B:1140:LYS:HG3	2.21	0.41
3:C:40:PHE:O	11:K:134:LYS:NZ	2.54	0.41
5:E:67:GLU:HA	5:E:70:SER:OG	2.20	0.41
7:G:48:SER:OG	7:G:64:GLN:NE2	2.54	0.41
7:G:50:ALA:HB3	7:G:53:TYR:HD2	1.86	0.41
15:O:234:ILE:HA	15:O:237:ILE:HB	2.03	0.41
16:P:450:ARG:O	16:P:468:VAL:HA	2.21	0.41
16:P:698:LYS:HB3	17:Q:124:ARG:HB3	2.03	0.41
17:Q:302:ALA:O	17:Q:305:ARG:N	2.53	0.41
17:Q:435:GLN:H	17:Q:435:GLN:HG3	1.42	0.41
18:R:9:THR:HG21	18:R:13:PHE:HD2	1.83	0.41
18:R:350:SER:HA	18:R:353:VAL:HB	2.03	0.41
1:A:81:LEU:HD11	1:A:430:ILE:HD11	2.01	0.40
1:A:447:THR:O	1:A:447:THR:HG22	2.21	0.40
1:A:511:VAL:HG11	1:A:575:LYS:H	1.85	0.40
1:A:553:GLN:O	1:A:556:ALA:HB3	2.22	0.40
1:A:633:MET:HB3	1:A:633:MET:HE2	1.85	0.40
1:A:701:ARG:NH2	1:A:704:ASP:OD2	2.54	0.40
1:A:718:THR:OG1	1:A:730:GLN:NE2	2.53	0.40
1:A:1061:SER:OG	1:A:1062:HIS:N	2.53	0.40
1:A:1238:MET:HE3	1:A:1525:ASN:C	2.42	0.40
1:A:1300:ASN:OD1	1:A:1301:GLU:HG3	2.20	0.40
1:A:1305:GLU:HG3	1:A:1306:TYR:CD1	2.56	0.40
1:A:1646:LEU:HD22	1:A:1646:LEU:HA	1.76	0.40
2:B:114:SER:O	18:R:281:LYS:HA	2.14	0.40
2:B:212:ASN:N	2:B:212:ASN:ND2	2.68	0.40
2:B:711:GLN:HB2	2:B:958:MET:HB2	2.03	0.40
2:B:792:SER:HA	3:C:217:ALA:HB2	2.03	0.40
2:B:874:TYR:CZ	2:B:876:SER:HB3	2.56	0.40
2:B:1007:TYR:HB3	3:C:281:ARG:HD2	2.03	0.40
5:E:22:MET:HB2	5:E:187:TYR:CE1	2.56	0.40
6:F:93:ILE:HD13	6:F:93:ILE:HA	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:113:SER:OG	14:N:116:LYS:N	2.54	0.40
15:O:236:LYS:HA	15:O:239:SER:HB3	2.03	0.40
15:O:403:LEU:HD13	15:O:424:LEU:HA	2.04	0.40
16:P:302:VAL:C	16:P:363:ILE:HD11	2.40	0.40
16:P:408:ILE:HD11	16:P:455:LYS:HG3	2.03	0.40
16:P:469:TYR:CE2	16:P:508:ILE:HB	2.56	0.40
17:Q:116:ILE:O	17:Q:120:ILE:HG13	2.21	0.40
17:Q:178:THR:HG22	17:Q:178:THR:H	1.63	0.40
17:Q:262:LEU:HA	17:Q:262:LEU:HD23	1.67	0.40
1:A:1124:LEU:HD23	1:A:1135:SER:OG	2.21	0.40
1:A:1559:ARG:NH2	5:E:200:ARG:HD3	2.36	0.40
2:B:26:ILE:HA	10:J:58:GLU:OE2	2.21	0.40
2:B:1093:LEU:CD1	2:B:1098:TYR:CD1	3.04	0.40
2:B:1158:ILE:HA	2:B:1167:PHE:O	2.20	0.40
5:E:9:ILE:HG21	5:E:43:LYS:HD3	2.03	0.40
13:M:55:GLY:HA3	13:M:62:TYR:HB2	2.03	0.40
16:P:198:ASP:HB3	16:P:261:VAL:HG23	2.02	0.40
16:P:272:PHE:HD2	16:P:292:LEU:HD11	1.85	0.40
16:P:656:HIS:CE1	16:P:748:GLU:HG3	2.56	0.40
17:Q:106:LYS:HB3	17:Q:106:LYS:HE3	1.81	0.40
17:Q:187:THR:HG22	17:Q:380:TRP:HE1	1.86	0.40
17:Q:366:TYR:OH	18:R:214:VAL:HG13	2.21	0.40
18:R:357:PRO:HB3	18:R:359:MET:HB3	2.02	0.40
1:A:81:LEU:CD1	1:A:82:PRO:HD2	2.45	0.40
1:A:659:THR:HG1	1:A:664:SER:H	1.64	0.40
1:A:1032:VAL:HG22	1:A:1038:ILE:CD1	2.48	0.40
1:A:1195:GLU:O	1:A:1198:THR:OG1	2.29	0.40
2:B:139:LEU:O	2:B:155:VAL:HA	2.21	0.40
2:B:387:GLY:O	2:B:634:ARG:NH1	2.54	0.40
2:B:883:GLU:HB3	2:B:904:LYS:CB	2.51	0.40
3:C:105:PRO:HG3	10:J:6:ARG:NH2	2.37	0.40
3:C:297:HIS:CD2	3:C:298:PHE:N	2.89	0.40
5:E:154:ILE:O	5:E:197:LYS:N	2.46	0.40
11:K:63:PHE:O	11:K:102:ASN:HA	2.21	0.40
13:M:8:SER:OG	13:M:9:GLU:N	2.53	0.40
14:N:111:VAL:O	14:N:120:LYS:N	2.34	0.40
15:O:151:TRP:HA	15:O:154:VAL:HB	2.04	0.40
15:O:171:CYS:O	15:O:175:MET:N	2.42	0.40
15:O:414:ALA:HA	15:O:417:LYS:HD2	2.02	0.40
15:O:487:ARG:HH21	15:O:502:LEU:CD1	2.29	0.40
15:O:510:VAL:HG13	15:O:517:LEU:HG	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:219:LEU:HB2	16:P:244:SER:O	2.21	0.40
16:P:358:SER:CB	18:R:196:GLU:CD	2.90	0.40
16:P:418:SER:O	16:P:419:ARG:HB3	2.21	0.40
16:P:437:SER:O	16:P:438:TRP:HD1	2.04	0.40
16:P:616:SER:OG	16:P:618:ASP:N	2.48	0.40
18:R:250:LEU:HD22	18:R:298:GLN:NE2	2.36	0.40
18:R:253:ILE:O	18:R:255:VAL:N	2.54	0.40
1:A:463:LYS:HD3	20:T:16:DT:C7	2.52	0.40
1:A:628:PHE:CE2	2:B:784:ASP:HB2	2.41	0.40
1:A:752:LYS:O	1:A:785:GLN:NE2	2.55	0.40
1:A:771:PHE:CD1	1:A:776:LEU:HA	2.56	0.40
2:B:119:ARG:HH22	2:B:125:GLU:CD	2.23	0.40
2:B:286:ARG:HD3	9:I:9:PHE:CD2	2.57	0.40
2:B:572:PRO:HG3	13:M:74:ASN:ND2	2.37	0.40
2:B:698:SER:HB3	24:B:1301:SO4:S	2.60	0.40
2:B:1114:GLN:HG3	2:B:1115:GLN:O	2.21	0.40
5:E:29:PHE:N	5:E:63:ASN:O	2.46	0.40
8:H:108:SER:OG	8:H:111:LEU:HG	2.21	0.40
9:I:12:ASP:HB2	9:I:33:CYS:SG	2.61	0.40
9:I:19:ASN:HB3	9:I:22:ALA:CB	2.51	0.40
10:J:69:ARG:NH2	12:L:33:GLU:OE2	2.54	0.40
16:P:68:THR:HG23	16:P:214:LEU:O	2.21	0.40
18:R:205:VAL:O	18:R:205:VAL:HG12	2.20	0.40
18:R:297:PHE:N	18:R:297:PHE:HD1	2.20	0.40
1:A:184:LYS:HA	1:A:187:GLU:OE2	2.22	0.40
1:A:510:PRO:HG2	6:F:102:SER:HB2	2.03	0.40
1:A:590:ASN:OD1	1:A:591:ARG:N	2.54	0.40
1:A:665:PRO:O	1:A:788:ALA:HB1	2.21	0.40
1:A:980:GLY:HA2	1:A:997:PHE:CD2	2.56	0.40
2:B:75:ASP:OD1	2:B:75:ASP:N	2.54	0.40
2:B:228:SER:O	2:B:254:ASN:N	2.35	0.40
2:B:338:PHE:HE2	2:B:353:VAL:HA	1.87	0.40
7:G:91:ASP:OD1	7:G:104:LEU:N	2.44	0.40
7:G:219:ASP:OD1	7:G:223:GLU:N	2.55	0.40
16:P:217:ALA:O	16:P:219:LEU:N	2.51	0.40
16:P:389:TRP:CZ3	18:R:149:LYS:N	2.89	0.40
16:P:773:SER:O	16:P:775:TRP:N	2.54	0.40
17:Q:6:ARG:HA	17:Q:18:ARG:HG3	2.02	0.40
17:Q:348:ILE:HG12	17:Q:376:GLU:HB3	2.04	0.40
18:R:219:LEU:HD23	18:R:219:LEU:HA	1.66	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1447/1664 (87%)	1307 (90%)	131 (9%)	9 (1%)	25	57
2	B	1171/1203 (97%)	1094 (93%)	61 (5%)	16 (1%)	11	37
3	C	303/335 (90%)	276 (91%)	26 (9%)	1 (0%)	41	72
4	D	50/137 (36%)	48 (96%)	2 (4%)	0	100	100
5	E	210/215 (98%)	199 (95%)	11 (5%)	0	100	100
6	F	98/155 (63%)	92 (94%)	6 (6%)	0	100	100
7	G	189/326 (58%)	180 (95%)	9 (5%)	0	100	100
8	H	127/146 (87%)	123 (97%)	4 (3%)	0	100	100
9	I	61/125 (49%)	52 (85%)	8 (13%)	1 (2%)	9	34
10	J	67/70 (96%)	61 (91%)	6 (9%)	0	100	100
11	K	99/142 (70%)	94 (95%)	5 (5%)	0	100	100
12	L	42/70 (60%)	38 (90%)	4 (10%)	0	100	100
13	M	106/415 (26%)	101 (95%)	5 (5%)	0	100	100
14	N	121/233 (52%)	112 (93%)	9 (7%)	0	100	100
15	O	457/627 (73%)	418 (92%)	36 (8%)	3 (1%)	22	55
16	P	573/894 (64%)	414 (72%)	113 (20%)	46 (8%)	1	6
17	Q	377/514 (73%)	311 (82%)	49 (13%)	17 (4%)	2	16
18	R	289/507 (57%)	219 (76%)	41 (14%)	29 (10%)	0	4
All	All	5787/7778 (74%)	5139 (89%)	526 (9%)	122 (2%)	10	30

All (122) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	819	ASP
2	B	820	PRO
2	B	954	PHE
2	B	1097	ASP

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Mol	Chain	Res	Type
15	O	493	ASP
16	P	218	VAL
16	P	229	ARG
16	P	248	PRO
16	P	271	ILE
16	P	321	LYS
16	P	332	ASN
16	P	393	VAL
16	P	432	PRO
16	P	444	PRO
16	P	743	SER
16	P	752	LEU
17	Q	8	PRO
17	Q	9	ILE
17	Q	15	CYS
17	Q	289	ARG
18	R	11	ARG
18	R	155	GLN
18	R	247	ILE
18	R	294	VAL
18	R	295	PRO
18	R	296	PRO
18	R	302	ARG
18	R	306	ALA
18	R	307	LYS
18	R	359	MET
18	R	427	PRO
1	A	90	PHE
1	A	91	PHE
1	A	358	ASP
1	A	1651	THR
2	B	955	PRO
2	B	1059	PRO
2	B	1066	HIS
15	O	492	ARG
16	P	61	VAL
16	P	67	ASP
16	P	216	ILE
16	P	259	ASN
16	P	377	ARG
16	P	396	ALA
16	P	657	SER

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Mol	Chain	Res	Type
16	P	659	LEU
16	P	726	SER
16	P	774	SER
17	Q	7	GLY
17	Q	196	SER
17	Q	280	ASP
17	Q	316	TRP
17	Q	317	MET
17	Q	362	THR
18	R	254	GLY
18	R	420	ASP
1	A	1259	SER
1	A	1505	ASP
2	B	322	ASN
2	B	784	ASP
2	B	1100	GLN
16	P	191	SER
16	P	201	GLU
16	P	269	PHE
16	P	301	GLN
16	P	365	TRP
16	P	437	SER
16	P	591	ALA
16	P	746	ARG
17	Q	364	SER
18	R	5	PRO
18	R	141	TRP
18	R	151	PRO
18	R	239	LEU
18	R	301	SER
18	R	323	SER
1	A	1650	GLY
2	B	815	ARG
16	P	263	ILE
16	P	290	GLU
16	P	394	VAL
16	P	446	ASP
16	P	545	SER
16	P	745	ALA
17	Q	13	ASP
17	Q	492	ALA
18	R	149	LYS

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Mol	Chain	Res	Type
18	R	421	LYS
1	A	1050	TYR
1	A	1061	SER
2	B	786	ALA
2	B	1063	ARG
3	C	232	GLN
15	O	225	LEU
16	P	58	HIS
16	P	445	ASP
16	P	458	LYS
16	P	487	ASN
16	P	666	SER
17	Q	16	PRO
18	R	18	LYS
18	R	232	ALA
18	R	425	ALA
2	B	1052	VAL
16	P	187	ILE
16	P	297	ILE
16	P	500	ILE
18	R	262	SER
18	R	423	GLY
2	B	491	ILE
16	P	709	PRO
17	Q	451	PRO
17	Q	470	PRO
18	R	267	GLY
2	B	699	ILE
17	Q	327	PRO
9	I	47	VAL
16	P	233	VAL
18	R	293	ILE
16	P	568	ILE
18	R	357	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1289/1465 (88%)	1271 (99%)	18 (1%)	67	83
2	B	1030/1053 (98%)	1017 (99%)	13 (1%)	69	84
3	C	269/296 (91%)	269 (100%)	0	100	100
4	D	52/116 (45%)	52 (100%)	0	100	100
5	E	194/197 (98%)	194 (100%)	0	100	100
6	F	90/137 (66%)	90 (100%)	0	100	100
7	G	171/291 (59%)	171 (100%)	0	100	100
8	H	115/128 (90%)	115 (100%)	0	100	100
9	I	55/110 (50%)	55 (100%)	0	100	100
10	J	64/65 (98%)	63 (98%)	1 (2%)	62	81
11	K	91/130 (70%)	91 (100%)	0	100	100
12	L	39/57 (68%)	39 (100%)	0	100	100
13	M	98/371 (26%)	98 (100%)	0	100	100
14	N	119/220 (54%)	119 (100%)	0	100	100
15	O	427/576 (74%)	420 (98%)	7 (2%)	62	81
16	P	543/828 (66%)	374 (69%)	169 (31%)	0	1
17	Q	364/476 (76%)	293 (80%)	71 (20%)	1	4
18	R	286/474 (60%)	209 (73%)	77 (27%)	0	1
All	All	5296/6990 (76%)	4940 (93%)	356 (7%)	20	46

All (356) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	CYS
1	A	321	LYS
1	A	355	PHE
1	A	357	MET
1	A	358	ASP
1	A	578	TYR
1	A	646	GLU
1	A	1248	ASP
1	A	1249	GLU
1	A	1255	CYS
1	A	1506	ARG
1	A	1507	CYS
1	A	1640	ARG
1	A	1641	ILE

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Mol	Chain	Res	Type
1	A	1645	LYS
1	A	1646	LEU
1	A	1647	ASN
1	A	1648	ASN
2	B	784	ASP
2	B	787	MET
2	B	817	ARG
2	B	936	MET
2	B	949	ILE
2	B	1060	VAL
2	B	1064	LYS
2	B	1065	ARG
2	B	1086	PHE
2	B	1087	LEU
2	B	1091	ARG
2	B	1093	LEU
2	B	1096	SER
10	J	45	CYS
15	O	380	SER
15	O	434	LEU
15	O	435	SER
15	O	484	PHE
15	O	486	PHE
15	O	490	ILE
15	O	491	PHE
16	P	26	TYR
16	P	49	THR
16	P	50	LEU
16	P	56	ASP
16	P	64	LEU
16	P	66	CYS
16	P	181	ARG
16	P	182	LEU
16	P	183	ASP
16	P	185	GLN
16	P	187	ILE
16	P	192	ASP
16	P	193	LEU
16	P	194	ARG
16	P	195	ASN
16	P	198	ASP
16	P	201	GLU

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Mol	Chain	Res	Type
16	P	205	TYR
16	P	207	SER
16	P	212	SER
16	P	213	VAL
16	P	214	LEU
16	P	219	LEU
16	P	220	THR
16	P	221	ARG
16	P	226	HIS
16	P	227	LEU
16	P	229	ARG
16	P	238	LEU
16	P	247	ILE
16	P	248	PRO
16	P	259	ASN
16	P	260	LEU
16	P	263	ILE
16	P	264	ILE
16	P	267	ASN
16	P	268	SER
16	P	269	PHE
16	P	273	ARG
16	P	276	SER
16	P	278	HIS
16	P	282	CYS
16	P	288	SER
16	P	292	LEU
16	P	295	VAL
16	P	296	GLU
16	P	300	LEU
16	P	314	GLN
16	P	320	ILE
16	P	321	LYS
16	P	329	ILE
16	P	342	GLN
16	P	343	LEU
16	P	345	ASP
16	P	347	LEU
16	P	348	HIS
16	P	355	GLU
16	P	360	TRP
16	P	362	ARG

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Mol	Chain	Res	Type
16	P	364	GLU
16	P	365	TRP
16	P	367	SER
16	P	377	ARG
16	P	379	LYS
16	P	380	MET
16	P	381	ILE
16	P	384	ASP
16	P	386	MET
16	P	390	GLN
16	P	392	GLU
16	P	394	VAL
16	P	403	ARG
16	P	407	ARG
16	P	410	ASP
16	P	412	ASN
16	P	414	ILE
16	P	415	LEU
16	P	424	VAL
16	P	427	SER
16	P	428	GLU
16	P	433	VAL
16	P	438	TRP
16	P	439	LYS
16	P	442	LEU
16	P	443	ASP
16	P	453	VAL
16	P	455	LYS
16	P	456	VAL
16	P	458	LYS
16	P	461	HIS
16	P	463	LEU
16	P	465	VAL
16	P	468	VAL
16	P	469	TYR
16	P	474	LYS
16	P	480	VAL
16	P	491	SER
16	P	492	LEU
16	P	495	SER
16	P	496	THR
16	P	498	LEU

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Mol	Chain	Res	Type
16	P	500	ILE
16	P	504	THR
16	P	508	ILE
16	P	511	ILE
16	P	531	PHE
16	P	534	VAL
16	P	535	VAL
16	P	538	LEU
16	P	539	VAL
16	P	555	THR
16	P	567	ILE
16	P	573	GLU
16	P	574	TRP
16	P	577	LEU
16	P	583	GLU
16	P	592	LEU
16	P	600	GLU
16	P	604	ILE
16	P	606	ARG
16	P	608	GLN
16	P	609	ASN
16	P	614	GLU
16	P	617	HIS
16	P	625	ASP
16	P	626	LEU
16	P	632	ILE
16	P	635	ASN
16	P	637	LEU
16	P	638	LEU
16	P	643	LYS
16	P	645	LYS
16	P	646	ASP
16	P	647	GLU
16	P	653	SER
16	P	656	HIS
16	P	657	SER
16	P	659	LEU
16	P	660	LYS
16	P	662	LEU
16	P	663	LEU
16	P	664	GLU
16	P	666	SER

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Mol	Chain	Res	Type
16	P	667	ASP
16	P	671	SER
16	P	676	SER
16	P	679	LEU
16	P	692	THR
16	P	693	PHE
16	P	694	ILE
16	P	700	LEU
16	P	703	PHE
16	P	711	LEU
16	P	712	ASP
16	P	713	ILE
16	P	728	GLN
16	P	731	LEU
16	P	736	ILE
16	P	742	TRP
16	P	746	ARG
16	P	749	LYS
16	P	751	SER
16	P	753	PHE
16	P	754	GLU
16	P	762	ARG
16	P	770	ASP
16	P	771	ILE
16	P	772	ILE
16	P	777	MET
17	Q	17	SER
17	Q	21	ARG
17	Q	26	ARG
17	Q	27	ARG
17	Q	94	LYS
17	Q	95	LEU
17	Q	98	HIS
17	Q	101	LYS
17	Q	103	LEU
17	Q	119	LEU
17	Q	138	LEU
17	Q	139	LYS
17	Q	149	GLN
17	Q	150	GLU
17	Q	151	GLU
17	Q	152	LEU

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Mol	Chain	Res	Type
17	Q	154	LEU
17	Q	164	ILE
17	Q	167	LEU
17	Q	169	SER
17	Q	176	VAL
17	Q	178	THR
17	Q	187	THR
17	Q	192	TYR
17	Q	226	LEU
17	Q	229	LYS
17	Q	232	LEU
17	Q	234	CYS
17	Q	241	GLU
17	Q	248	SER
17	Q	252	LEU
17	Q	254	LEU
17	Q	255	LYS
17	Q	256	LEU
17	Q	272	GLN
17	Q	273	VAL
17	Q	280	ASP
17	Q	285	THR
17	Q	286	LEU
17	Q	295	THR
17	Q	297	ARG
17	Q	299	SER
17	Q	301	HIS
17	Q	312	LEU
17	Q	318	LEU
17	Q	321	ASP
17	Q	324	ARG
17	Q	328	LEU
17	Q	337	SER
17	Q	348	ILE
17	Q	363	SER
17	Q	364	SER
17	Q	378	LEU
17	Q	384	GLN
17	Q	412	LYS
17	Q	419	LEU
17	Q	435	GLN
17	Q	436	LEU

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Mol	Chain	Res	Type
17	Q	437	THR
17	Q	444	GLU
17	Q	445	ARG
17	Q	453	PHE
17	Q	478	ARG
17	Q	486	GLN
17	Q	494	SER
17	Q	495	LYS
17	Q	498	LEU
17	Q	502	ILE
17	Q	512	ARG
17	Q	513	MET
17	Q	514	ASN
18	R	1	MET
18	R	4	VAL
18	R	8	LEU
18	R	28	SER
18	R	74	GLN
18	R	80	ARG
18	R	84	TRP
18	R	85	ARG
18	R	87	VAL
18	R	143	THR
18	R	146	SER
18	R	149	LYS
18	R	156	LYS
18	R	158	THR
18	R	160	HIS
18	R	165	ILE
18	R	167	LYS
18	R	168	ILE
18	R	175	ILE
18	R	177	LEU
18	R	178	LEU
18	R	181	THR
18	R	182	LYS
18	R	189	GLN
18	R	202	THR
18	R	206	ARG
18	R	209	ARG
18	R	211	ARG
18	R	212	HIS

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Mol	Chain	Res	Type
18	R	214	VAL
18	R	216	LEU
18	R	230	SER
18	R	231	LEU
18	R	238	THR
18	R	240	ILE
18	R	242	ILE
18	R	245	VAL
18	R	246	GLN
18	R	247	ILE
18	R	249	SER
18	R	250	LEU
18	R	253	ILE
18	R	255	VAL
18	R	257	ILE
18	R	258	LEU
18	R	261	LEU
18	R	264	SER
18	R	272	GLN
18	R	275	CYS
18	R	276	GLN
18	R	282	SER
18	R	294	VAL
18	R	296	PRO
18	R	299	THR
18	R	307	LYS
18	R	308	PHE
18	R	324	MET
18	R	345	LEU
18	R	347	ASP
18	R	348	LYS
18	R	354	LEU
18	R	355	THR
18	R	361	ASP
18	R	365	TRP
18	R	373	LEU
18	R	374	LEU
18	R	375	LYS
18	R	403	GLN
18	R	409	HIS
18	R	410	TYR
18	R	411	VAL

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Mol	Chain	Res	Type
18	R	426	VAL
18	R	427	PRO
18	R	429	ARG
18	R	430	LEU
18	R	437	SER
18	R	440	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	107	HIS
1	A	383	ASN
1	A	458	GLN
1	A	470	HIS
1	A	489	ASN
1	A	537	GLN
1	A	559	ASN
1	A	560	GLN
1	A	610	ASN
1	A	639	GLN
1	A	730	GLN
1	A	880	GLN
1	A	949	GLN
1	A	1108	HIS
1	A	1314	GLN
1	A	1320	GLN
1	A	1443	GLN
1	A	1447	GLN
1	A	1453	HIS
1	A	1647	ASN
2	B	27	ASN
2	B	101	GLN
2	B	212	ASN
2	B	213	HIS
2	B	254	ASN
2	B	267	ASN
2	B	399	HIS
2	B	422	GLN
2	B	504	HIS
2	B	543	ASN
2	B	555	GLN
2	B	646	HIS

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Mol	Chain	Res	Type
2	B	695	ASN
2	B	816	ASN
2	B	952	HIS
2	B	1066	HIS
2	B	1157	GLN
2	B	1165	ASN
2	B	1171	ASN
3	C	161	HIS
3	C	237	GLN
3	C	297	HIS
4	D	88	GLN
7	G	26	ASN
7	G	32	ASN
7	G	237	HIS
8	H	11	GLN
8	H	52	GLN
9	I	44	ASN
11	K	64	GLN
11	K	106	GLN
12	L	53	HIS
14	N	41	ASN
14	N	51	GLN
14	N	85	HIS
14	N	128	ASN
15	O	77	GLN
15	O	117	GLN
15	O	173	HIS
15	O	362	ASN
15	O	391	GLN
15	O	438	GLN
15	O	472	HIS
15	O	507	GLN
16	P	222	GLN
16	P	223	ASN
16	P	348	HIS
16	P	554	ASN
16	P	665	ASN
17	Q	145	ASN
17	Q	157	HIS
17	Q	368	GLN
17	Q	507	ASN
18	R	25	ASN

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Mol	Chain	Res	Type
18	R	184	ASN
18	R	207	ASN
18	R	298	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
19	S	4/5 (80%)	1 (25%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
19	S	3	G

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 8 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
24	SO4	B	1301	-	4,4,4	0.17	0	6,6,6	0.07	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	B	1301	SO4	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
17	Q	2
18	R	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	R	206:ARG	C	207:ASN	N	2.76
1	Q	323:ASP	C	324:ARG	N	1.79
1	Q	356:VAL	C	357:TYR	N	1.17

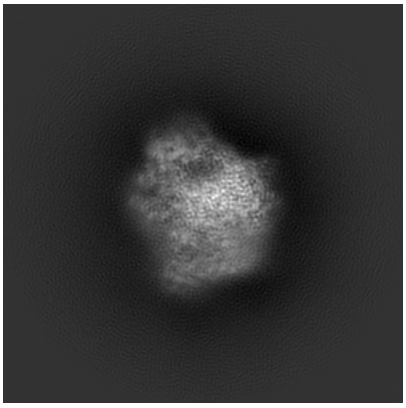
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-3593. These allow visual inspection of the internal detail of the map and identification of artifacts.

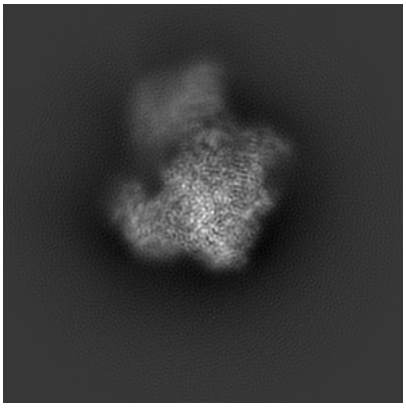
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

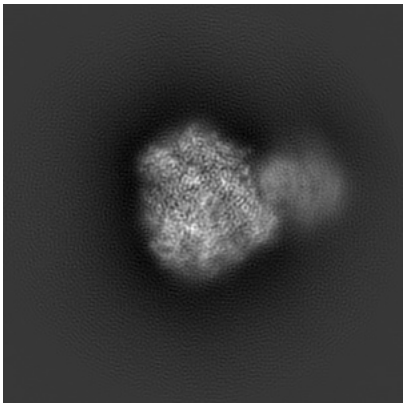
6.1.1 Primary map



X



Y

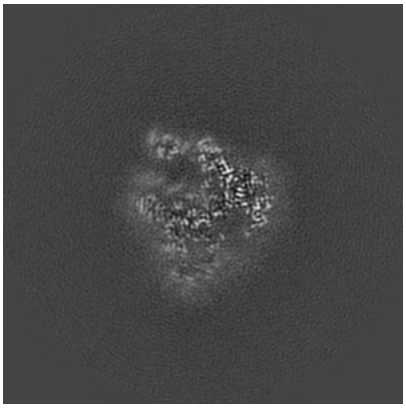


Z

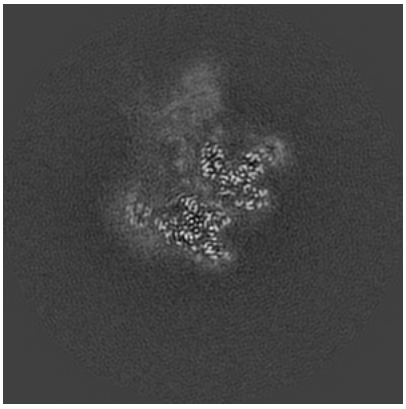
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

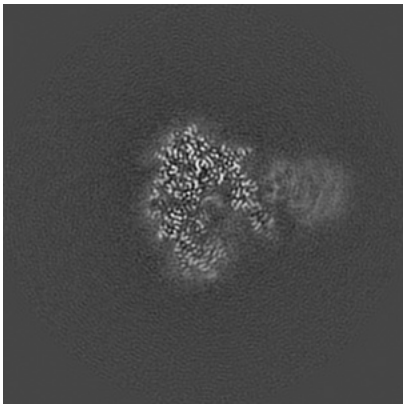
6.2.1 Primary map



X Index: 165



Y Index: 165

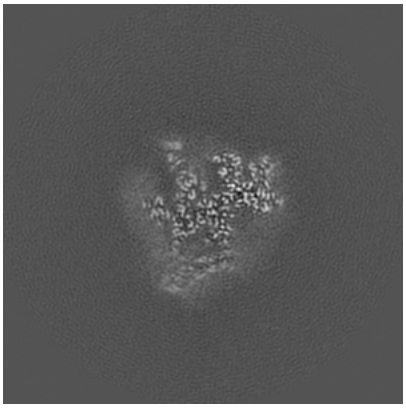


Z Index: 165

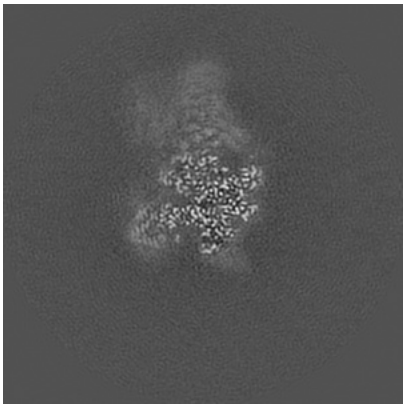
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

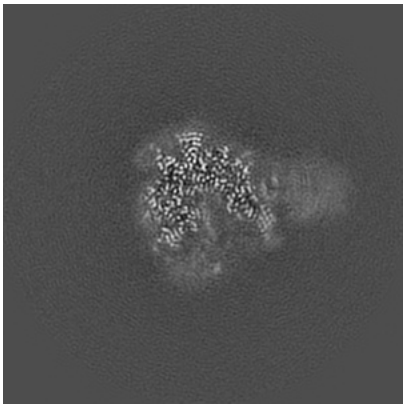
6.3.1 Primary map



X Index: 157



Y Index: 182

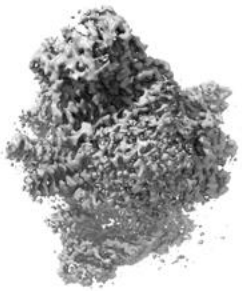


Z Index: 172

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

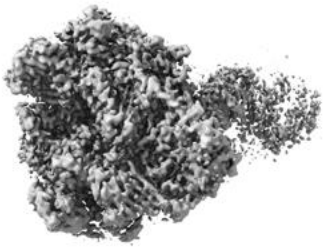
6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.065. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

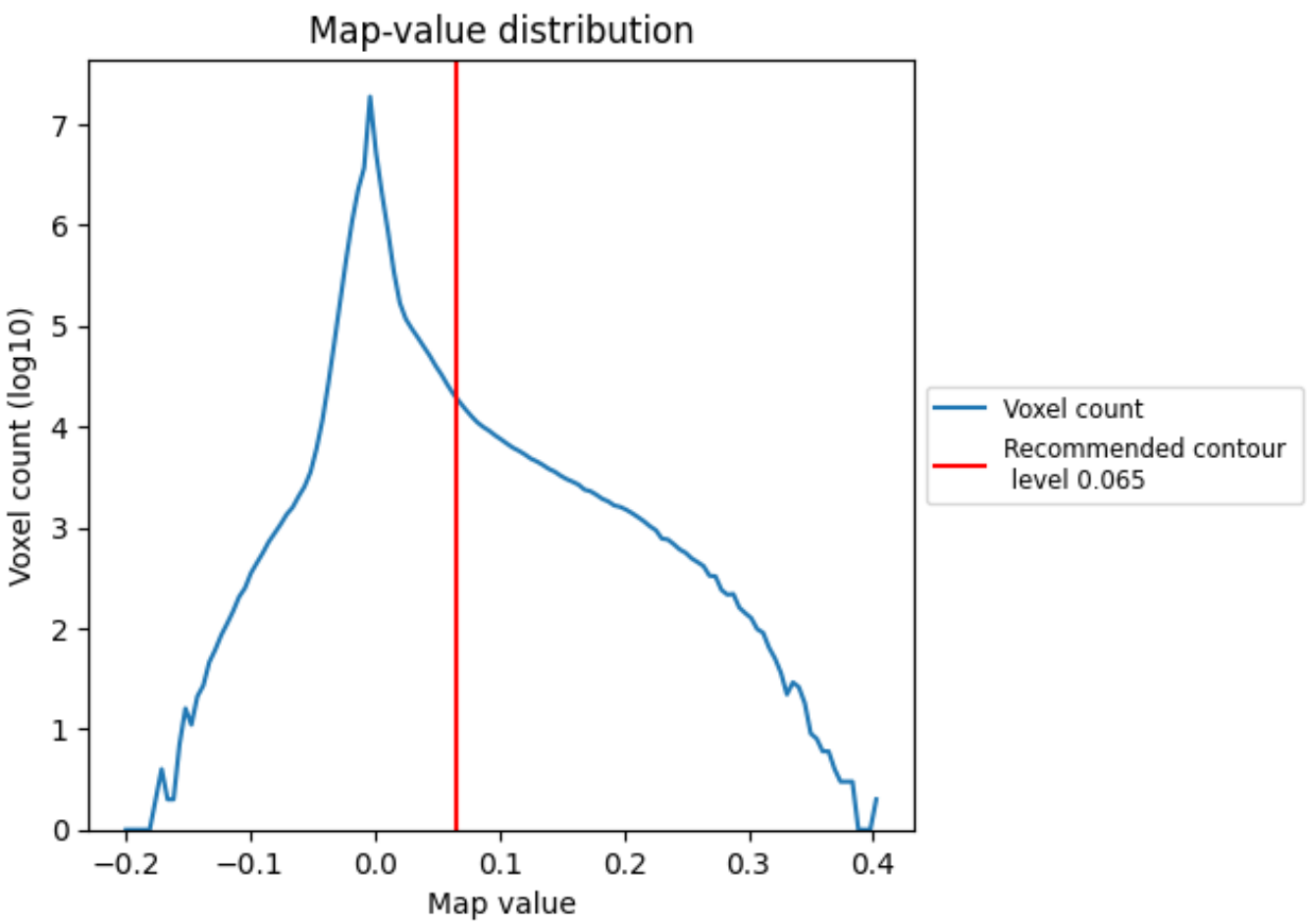
6.5 Mask visualisation (i)

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

7 Map analysis (i)

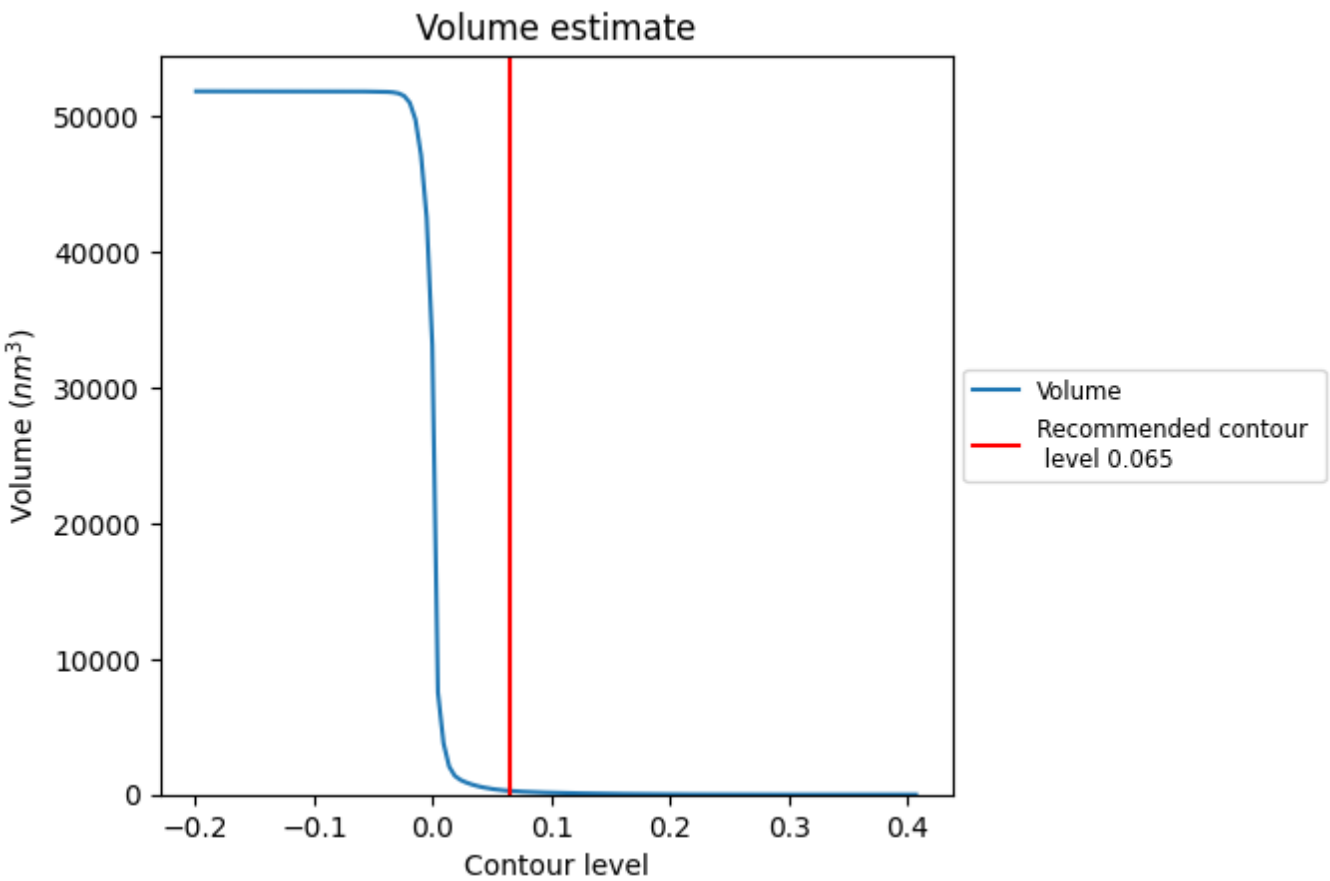
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

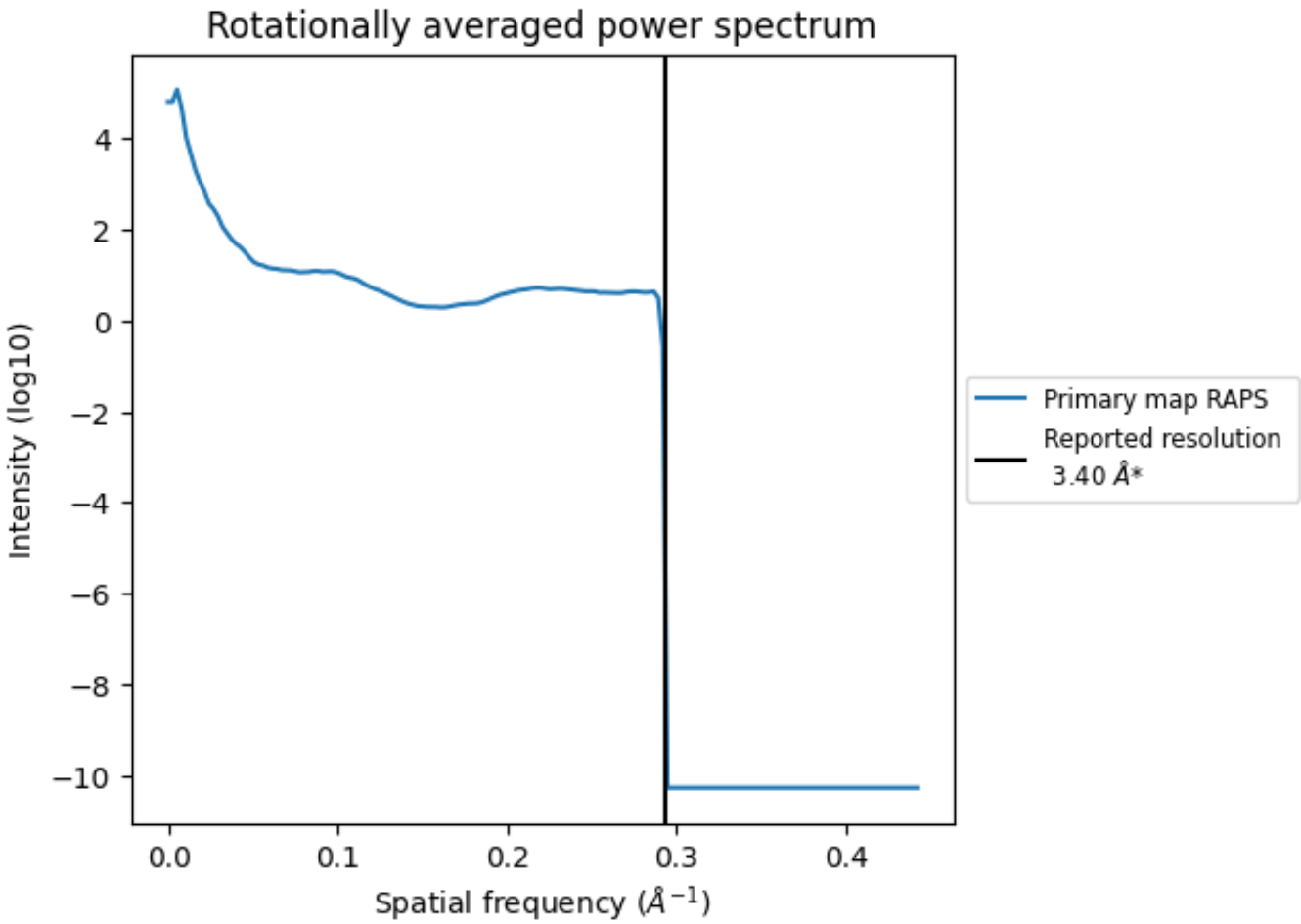
7.2 Volume estimate (i)



The volume at the recommended contour level is 273 nm^3; this corresponds to an approximate mass of 246 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 0.294 Å^{-1}

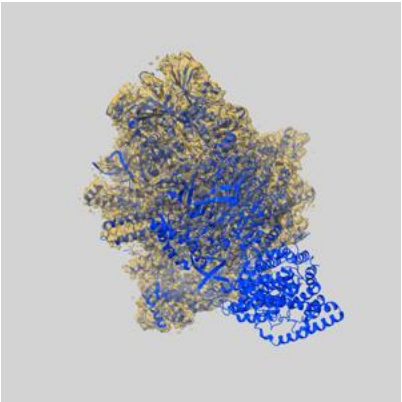
8 Fourier-Shell correlation (i)

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

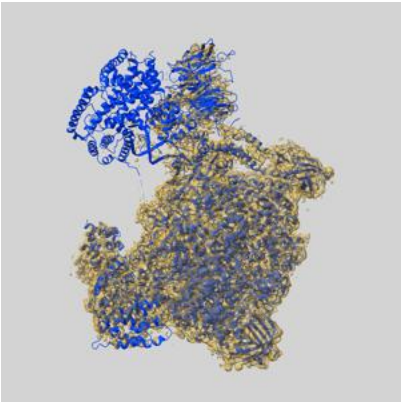
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-3593 and PDB model 5N61. Per-residue inclusion information can be found in section 3 on page 9.

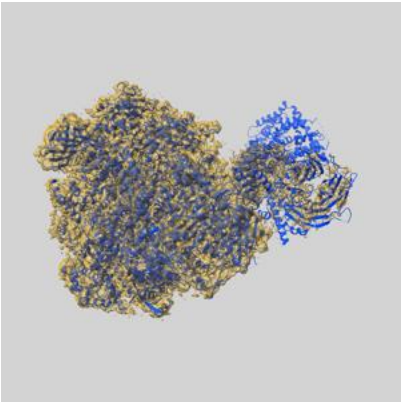
9.1 Map-model overlay (i)



X



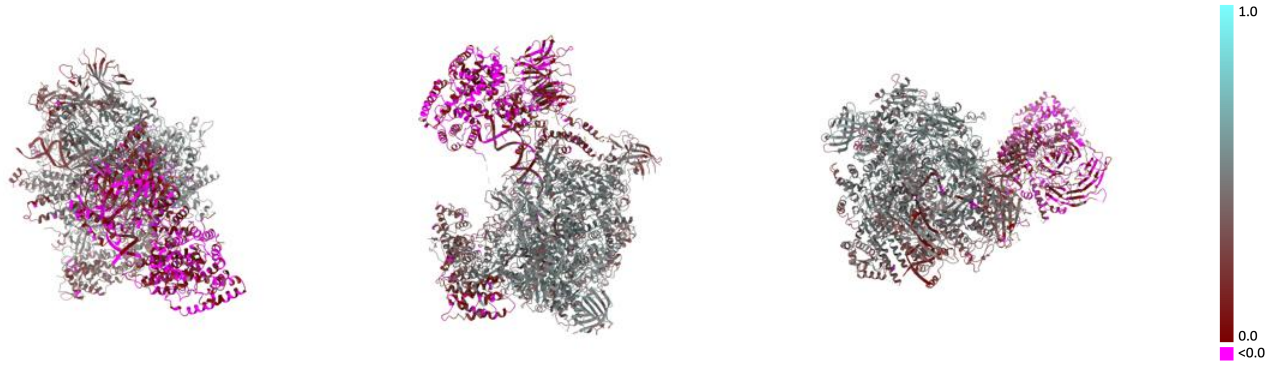
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.065 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

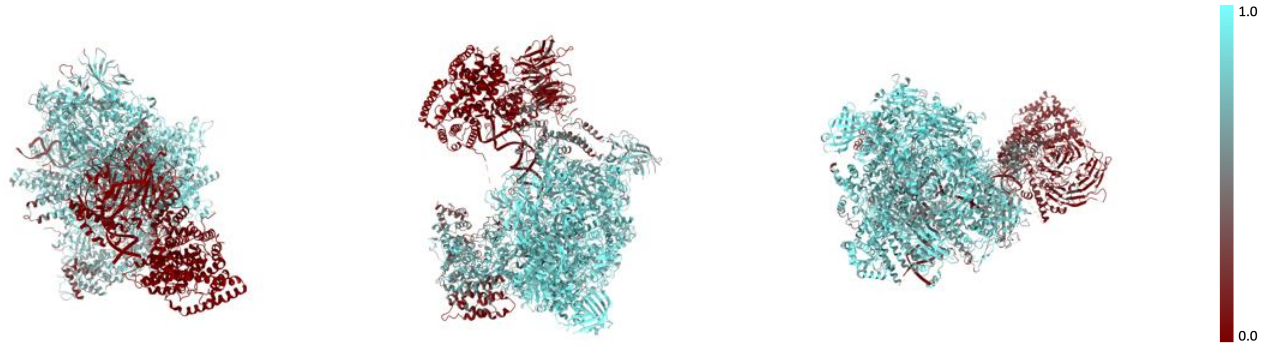
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

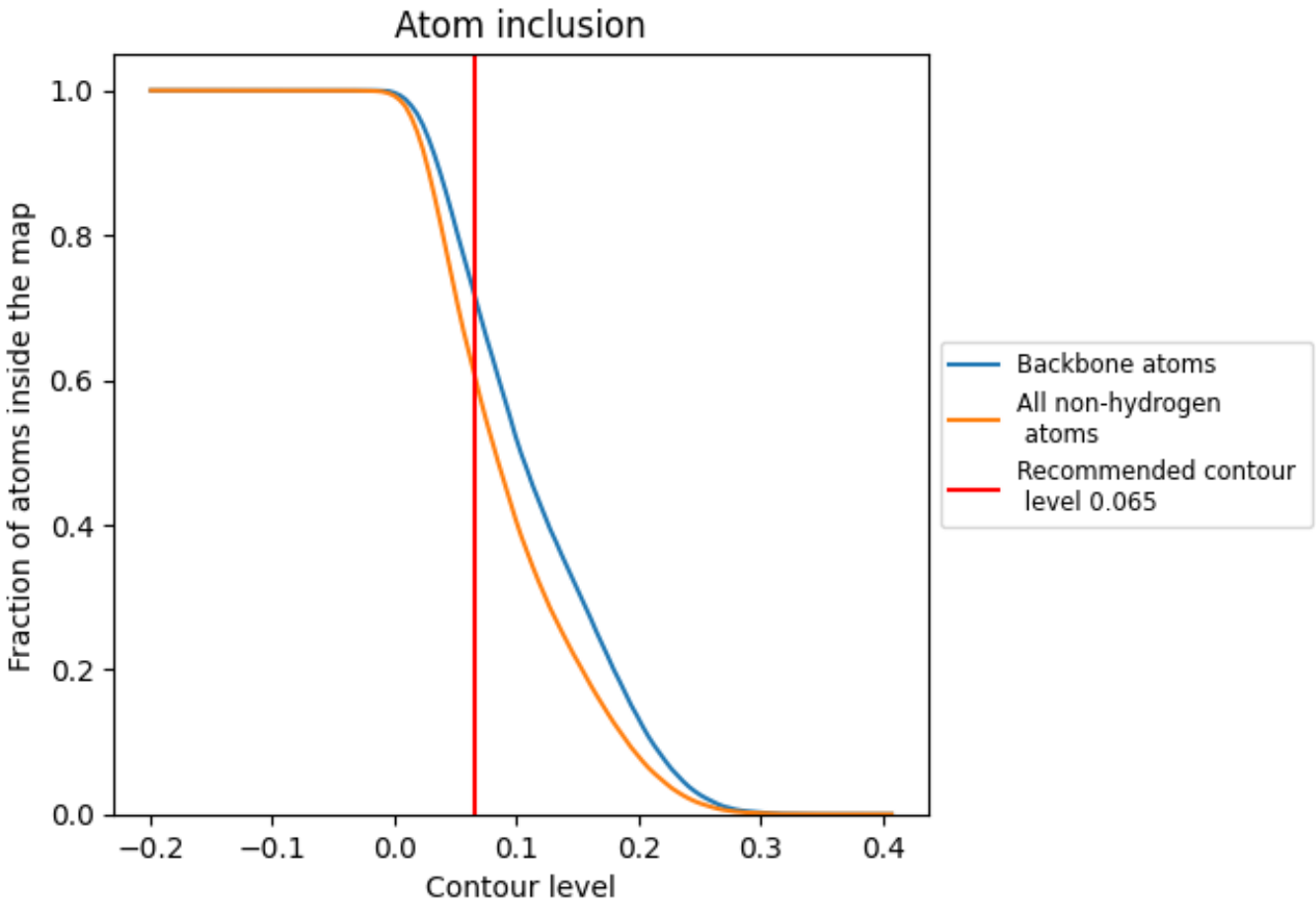
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.065).

9.4 Atom inclusion (i)



At the recommended contour level, 72% of all backbone atoms, 61% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.065) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6108	0.3430
A	0.8017	0.4510
B	0.8256	0.4740
C	0.8764	0.4830
D	0.7377	0.4080
E	0.8304	0.4280
F	0.7965	0.4770
G	0.7098	0.3960
H	0.8801	0.4860
I	0.6875	0.3020
J	0.8967	0.5110
K	0.8431	0.4840
L	0.8382	0.4670
M	0.6355	0.3390
N	0.6268	0.3470
O	0.4817	0.2610
P	0.0552	0.0410
Q	0.0487	0.0480
R	0.2271	0.1240
S	0.4722	0.2280
T	0.2683	0.1150
U	0.2163	0.1170