Full wwPDB EM Validation Report (i)

Feb 26, 2024 – 12:16 AM EST

PDB ID	:	6W2D
EMDB ID	:	EMD-21525
Title	:	Structures of Capsid and Capsid-Associated Tegument Complex inside the Epstein-Barr Virus
Authors	:	Liu, W.; Cui, Y.X.; Wang, C.Y.; Li, Z.H.; Gong, D.Y.; Dai, X.H.; Bi, G.Q.; Sun, R.; Zhou, Z.H.
Deposited on	:	2020-03-05
Resolution	:	4.00 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:

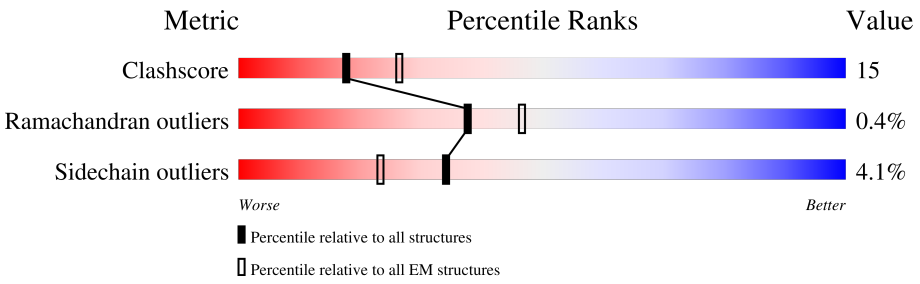
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.00 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	J	1381	40% 65% 31% • •
1	K	1381	42% 70% 29% •
1	N	1381	51% 68% 28% • •
1	O	1381	43% 67% 27% • •
1	P	1381	59% 65% 27% • 7%
2	v	507	46% 54% • 42%
3	w	570	12% 12% 88%
3	x	570	11% 12% 88%

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Mol	Chain	Length	Quality of chain
4	y	3149	99%
4	z	3149	99%
5	Z	176	26% 34% 9% 56%
5	a	176	30% 43% 56%
5	d	176	33% 41% 56%
5	e	176	32% 43% 56%
5	u	176	33% 36% 64%
6	f	364	72% 85% 13%
6	h	364	52% 88% 5% 8%
7	k	301	80% 97%
7	m	301	61% 93% 6%
7	p	301	77% 94% 5%
7	r	301	59% 96%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 74272 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 Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	J	1352	10628	6744	1849	1974	61	0	0
1	K	1381	10832	6868	1884	2018	62	0	0
1	N	1362	10683	6777	1854	1991	61	0	0
1	O	1332	10447	6633	1812	1942	60	0	0
1	P	1283	10113	6429	1754	1871	59	0	0

- Molecule 2 is a protein called Capsid vertex component 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	v	292	2283	1469	397	406	11	0	0

- Molecule 3 is a protein called Capsid vertex component 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	w	68	549	332	106	108	3	0	0
3	x	68	549	332	106	108	3	0	0

- Molecule 4 is a protein called Large tegument protein deneddylase.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	y	37	317	200	64	53	0	0
4	z	37	317	200	64	53	0	0

- Molecule 5 is a protein called Small capsomere-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	Z	77	649	411	121	115	2	0	0
5	a	77	649	411	121	115	2	0	0
5	d	77	649	411	121	115	2	0	0
5	e	77	649	411	121	115	2	0	0
5	u	63	528	339	90	98	1	0	0

- Molecule 6 is a protein called Triplex capsid protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	f	315	2474	1586	436	444	8	0	0
6	h	336	2604	1667	458	471	8	0	0

- Molecule 7 is a protein called Triplex capsid protein 2.

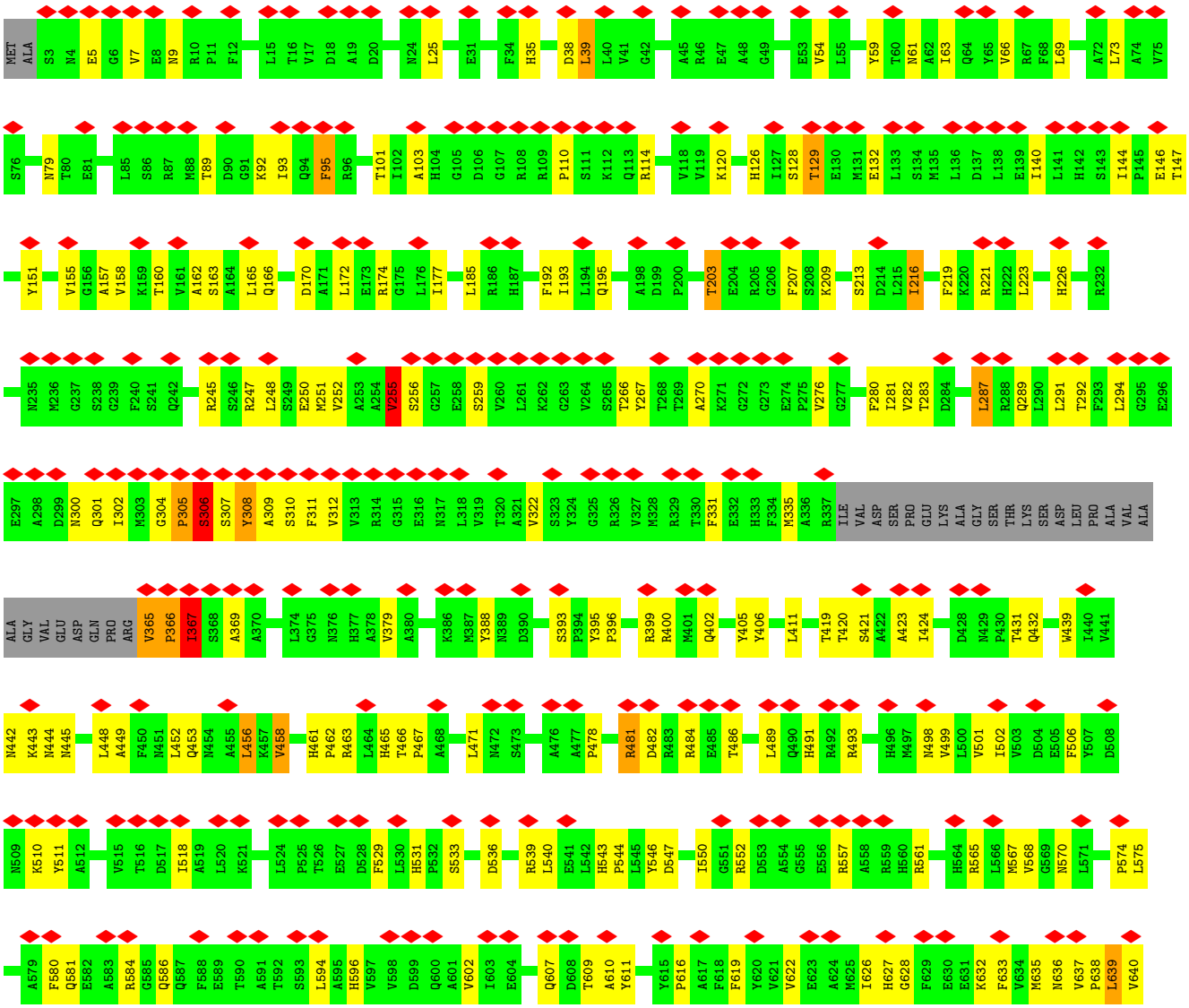
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	k	299	2338	1500	386	434	18	0	0
7	m	299	2338	1500	386	434	18	0	0
7	p	299	2338	1500	386	434	18	0	0
7	r	299	2338	1500	386	434	18	0	0

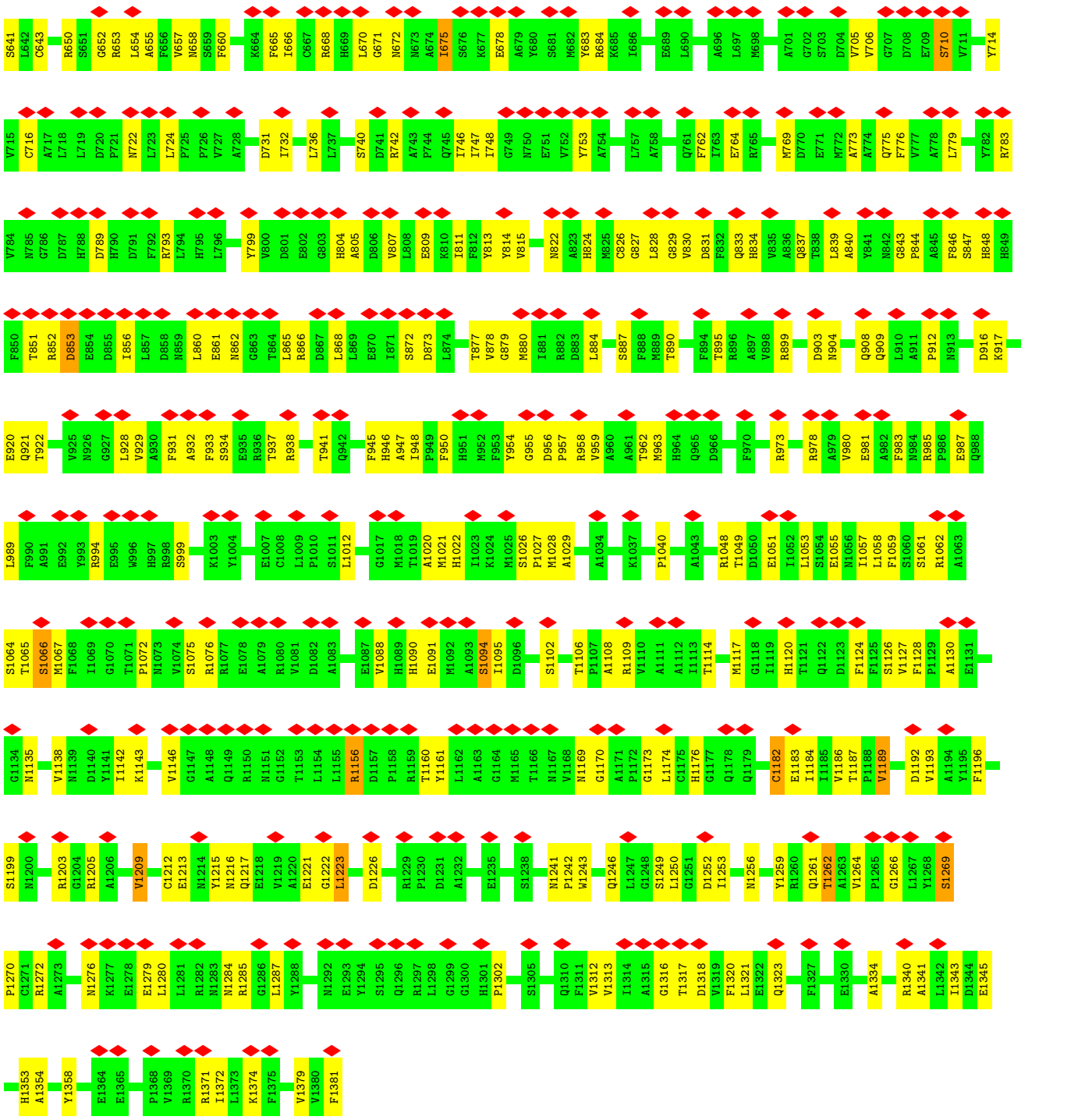
3 Residue-property plots (i)

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

- Molecule 1: Major capsid protein

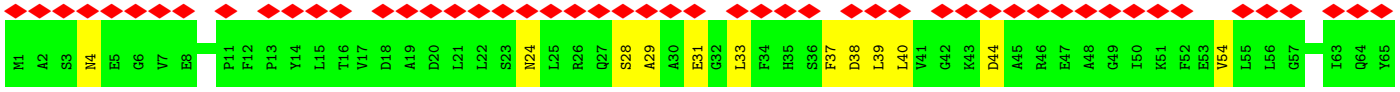
Chain J:

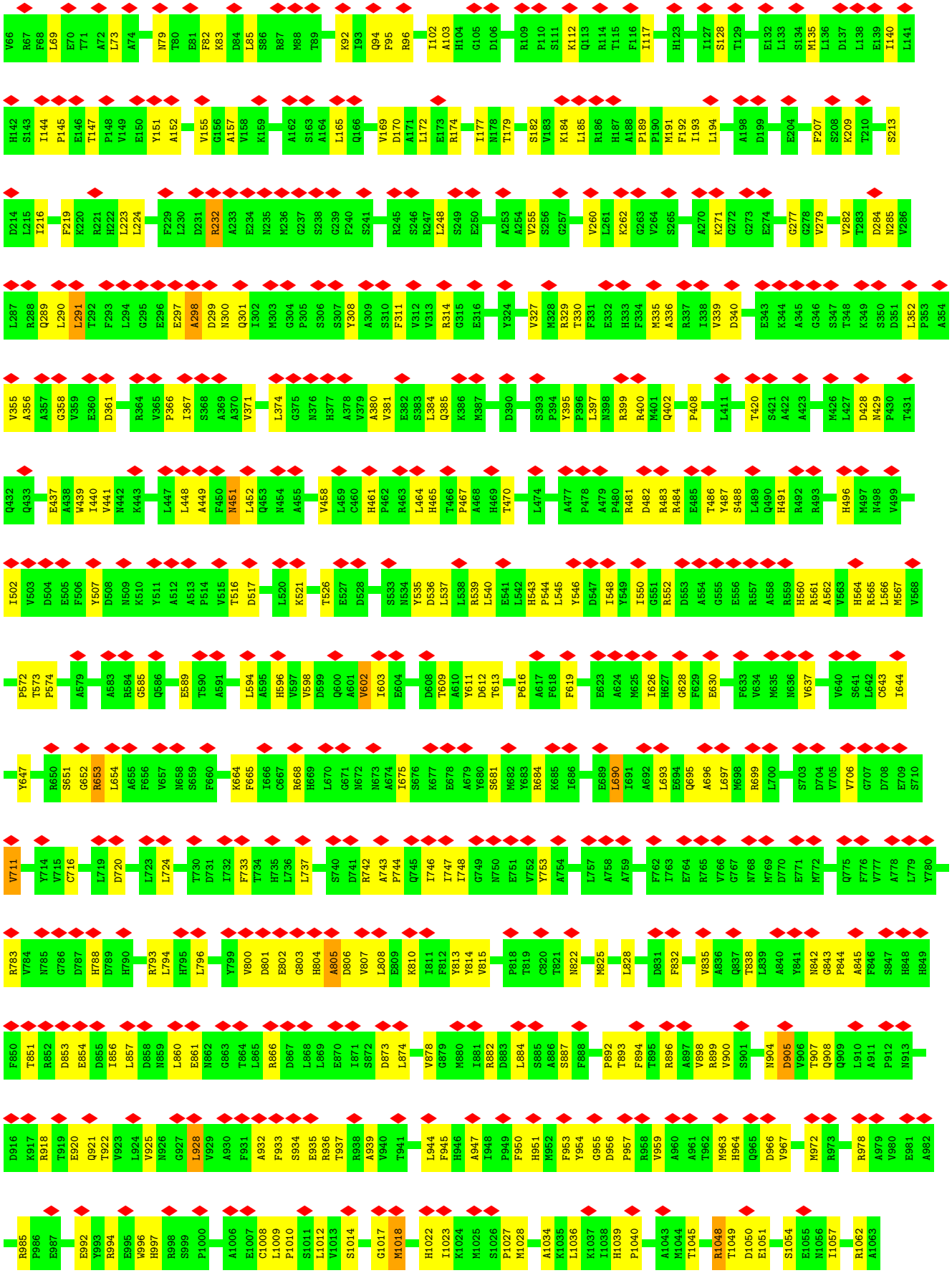


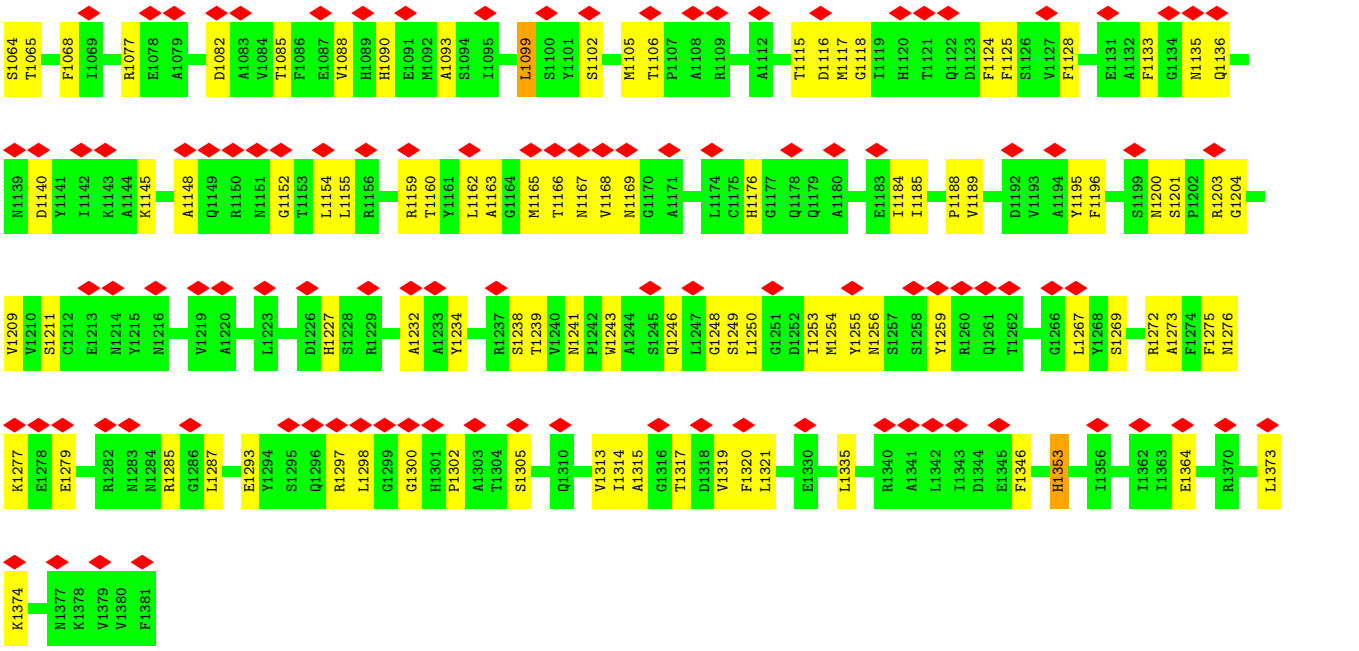


- Molecule 1: Major capsid protein

Chain K:

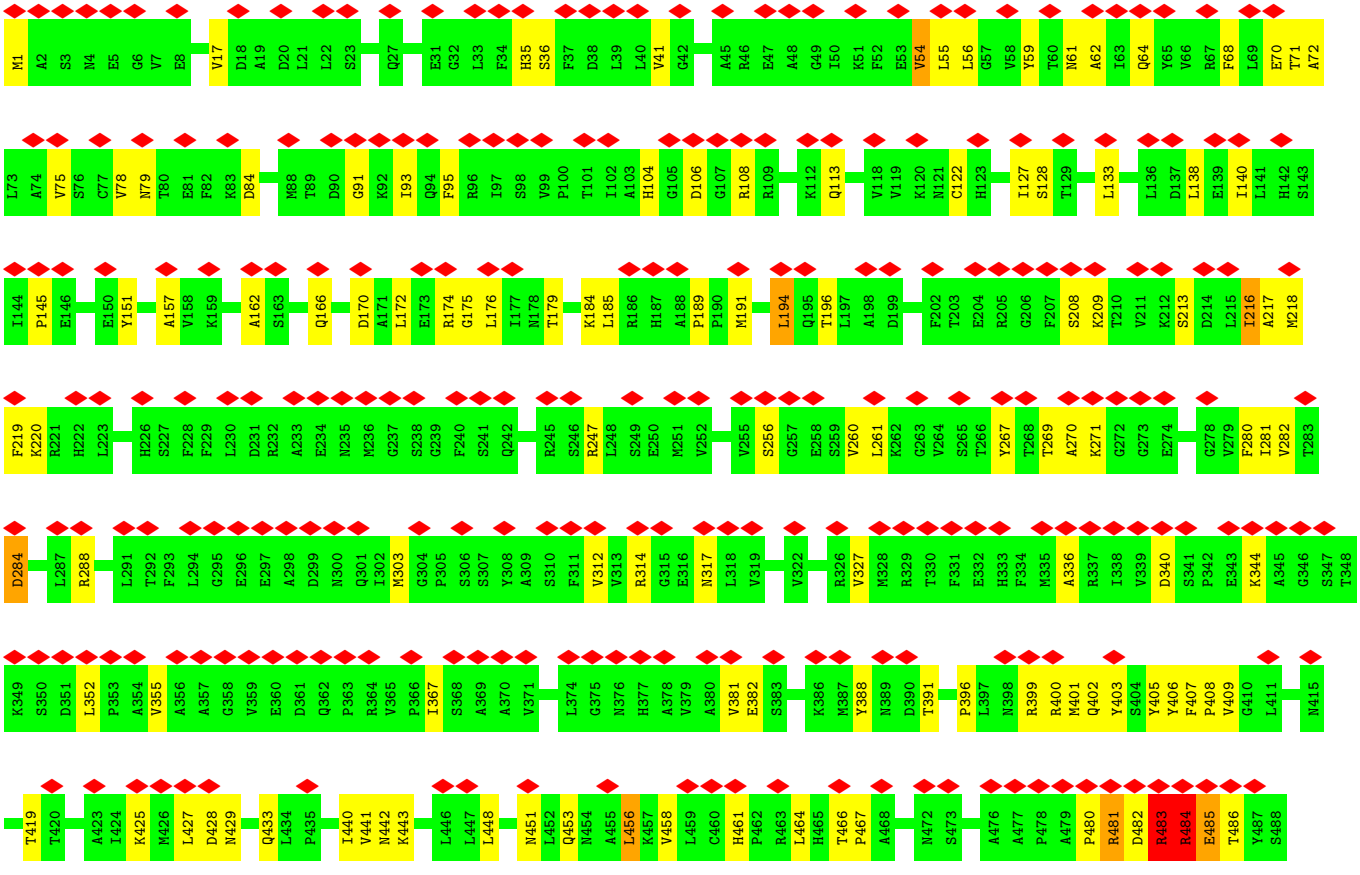


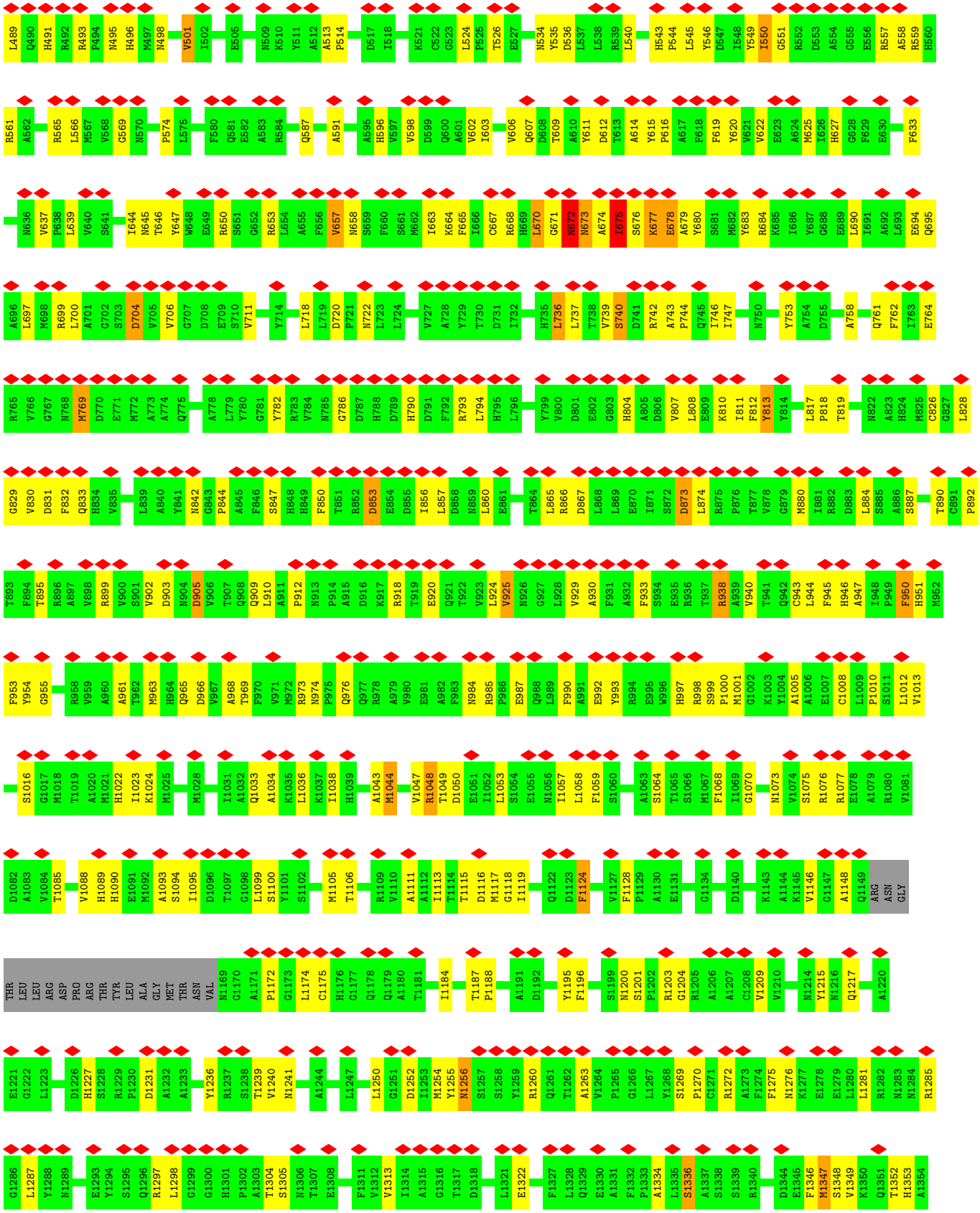

V66 R67 F68 L69 E70 T71 A72 L73 A74 N79 T80 E81 F82 K83 D84 L85 S86 R87 M88 T89 K92 I93 Q94 F95 R96 I102 A103 H104 G105 D106 R109 P110 S111 K112 Q113 R114 T115 F116 I117 H123 I127 S128 T129 E132 L133 S134 M135 L136 D137 L138 E139 I140 L141
H142 S143 I144 P145 E146 T147 P148 V149 E150 Y151 A152 V155 G156 A157 V158 K159 A162 S163 A164 L165 Q166 V169 D170 A171 L172 E173 R174 I177 N178 T179 S182 V183 K184 L185 R186 H187 A188 P189 P190 M191 F192 I193 L194 A198 D199 E204 F207 S208 K209 T210 S213
D214 L215 I216 F219 K220 R221 H222 L223 L224 F229 L230 D231 R232 A233 E234 N235 M236 G237 S238 G239 F240 S241 R245 S246 R247 L248 S249 E250 A253 A254 V255 S256 G257 V260 L261 K262 G263 V264 S265 A270 K271 G272 G273 E274 G277 G278 V279 V282 T283 D284 N285 V286
L287 R288 Q289 L290 L291 T292 F293 L294 G295 E296 E297 A298 D299 N300 Q301 I302 M303 G304 P305 S306 S307 Y308 A309 S310 F311 V312 V313 R314 G315 E316 Y324 V327 M328 R329 T330 F331 E332 H333 F334 M335 A336 R337 I338 V339 D340 E343 K344 A345 G346 S347 T348 K349 S350 D351 L352 P353 A354
V355 A356 A357 G358 V359 E360 D361 R364 V365 P366 I367 S368 A369 A370 V371 L374 G375 N376 H377 A378 V379 A380 V381 E382 S383 L384 Q385 K386 M387 D390 S393 P394 Y395 P396 L397 N398 R399 R400 M401 Q402 P408 L411 T420 S421 A422 A423 M426 L427 D428 N429 P430 T431
Q432 Q433 E437 A438 W439 I440 V441 N442 K443 L447 L448 A449 F450 N451 L452 Q453 N454 A455 V458 L459 C460 H461 P462 R463 L464 H465 T466 P467 A468 H469 T470 L474 A477 P478 A479 P480 R481 D482 R483 R484 E485 T486 Y487 S488 L489 Q490 H491 R492 R493 H496 M497 N498 V499
I502 V503 D504 E505 F506 Y507 D508 N509 K510 Y511 A512 A513 P514 V515 T516 D517 L520 K521 T526 E527 D528 S533 N534 Y535 D536 L537 L538 R539 L540 E541 L542 H543 P544 L545 Y546 D547 I548 Y549 I550 G551 R552 D553 A554 G555 E556 R557 A558 R559 H560 R561 A562 V563 H564 R565 L566 M567 V568
P572 T573 P574 A579 A583 R584 G585 Q586 E589 T590 A591 L594 A595 H596 V597 V598 D599 Q600 A601 V602 I603 E604 D608 T609 A610 Y611 D612 T613 P616 A617 F618 F619 E623 A624 M625 I626 H627 G628 F629 E630 F633 V634 M635 N636 V637 V640 S641 L642 C643 I644
Y647 R650 S651 G652 R653 L654 A655 F656 V657 N658 S659 F660 K664 F665 I666 C667 R668 H669 L670 G671 N672 N673 A674 I675 S676 K677 E678 A679 Y680 S681 M682 Y683 R684 K685 I686 E689 L690 I691 A692 L693 E694 Q695 A696 L697 M698 R699 L700 S703 D704 V705 V706 G707 D708 E709 S710
V711 Y714 V715 C716 L719 D720 L723 L724 T730 D731 I732 F733 T734 H735 L736 L737 S740 D741 R742 A743 P744 Q745 I746 I747 I748 G749 N750 E751 V752 Y753 A754 L757 A758 A759 F762 I763 E764 R765 V766 G767 N768 M769 D770 E771 M772 Q775 F776 V777 A778 L779 Y780
R783 V784 N785 G786 D787 H788 D789 H790 R793 L794 H795 L796 Y799 V800 D801 E802 G803 H804 A805 D806 V807 L808 E809 K810 I811 F812 Y813 Y814 V815 P818 T819 C820 T821 N822 M825 L828 D831 F832 V835 A836 Q837 T838 L839 A840 Y841 N842 G843 P844 A845 F846 S847 H848 H849
F850 T851 R852 D853 E854 D855 I856 L857 D858 N859 L860 E861 N862 G863 T864 L865 R866 D867 L868 L869 E870 I871 S872 D873 L874 V878 G879 M880 I881 R882 D883 L884 S885 A886 S887 F888 P892 T893 F894 T895 R896 A897 V898 R899 V900 S901 N904 D905 V906 T907 Q908 Q909 L910 A911 P912 N913
D916 K917 R918 T919 E920 Q921 T922 V923 L924 V925 N926 G927 L928 V929 A930 F931 A932 F933 S934 E935 R936 T937 R938 A939 V940 T941 L944 F945 H946 A947 I948 P949 F950 H951 M952 F953 Y954 G955 D956 P957 R958 V959 A960 A961 T962 M963 H964 Q965 D966 V967 M972 R973 R978 A979 V980 E981 A982
R985 P986 E987 E992 Y993 R994 E995 W996 H997 R998 S999 P1000 A1006 E1007 C1008 L1009 P1010 S1011 L1012 V1013 S1014 G1017 M1018 H1022 I1023 K1024 M1025 S1026 P1027 M1028 A1034 K1035 L1036 K1037 I1038 H1039 P1040 A1043 M1044 T1045 R1048 T1049 D1050 E1051 S1054 E1055 N1056 I1057 R1062 A1063



- Molecule 1: Major capsid protein

Chain N: 51% 68% 28%

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R561 A562 R565 L566 H567 V568 G569 N570 P574 L575 F580 Q581 E582 A583 R584 Q587 A591 A595 H596 V597 V598 D599 Q600 A601 V602 I603 V606 Q607 D608 T609 A610 Y611 D612 T613 A614 Y615 P616 A617 F618 F619 Y620 V621 V622 E623 A624 M625 I626 H627 G628 F629 E630 F633
M636 V637 F638 L639 V640 S641 I644 N645 T646 Y647 W648 E649 R650 S651 E652 R653 L654 A655 F656 V657 N658 S659 F660 S661 M662 I663 K664 F665 I666 C667 R668 H669 L670 G671 M672 N673 A674 I675 S676 K677 E678 A679 Y680 S681 M682 Y683 R684 K685 I686 Y687 G688 E689 L690 I691 A692 L693 E694 Q695
A696 L697 M698 R699 L700 A701 G702 S703 D704 V705 V706 G707 D708 E709 S710 V711 Y714 L718 L719 D720 P721 N722 L723 L724 V727 A728 Y729 T730 D731 I732 H735 L736 L737 T738 V739 S740 D741 R742 A743 P744 Q745 I746 I747 N750 Y753 A754 D755 A758 Q761 F762 I763 E764
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G829 V830 D831 F832 Q833 H834 V835 L839 A840 Y841 N842 G843 P844 A845 F846 S847 H848 H849 F850 T851 R852 D853 E854 D855 I856 L857 D858 N859 L860 E861 T864 L865 R866 D867 L868 L869 E870 I871 S872 D873 L874 R875 P876 T877 V878 G879 M880 I881 R882 D883 L884 S885 A886 S887 T890 C891 P892
T893 F894 T895 R896 A897 V898 R899 V900 S901 V902 D903 N904 D905 V906 T907 Q908 Q909 L910 A911 P912 N913 P914 A915 D916 K917 R918 T919 E920 Q921 T922 V923 L924 V925 N926 G927 L928 V929 A930 F931 A932 F933 S934 E935 R936 T937 R938 A939 V940 T941 Q942 C943 L944 F945 H946 A947 I948 P949 F950 H951 M952
F953 Y954 G955 R958 V959 A960 A961 T962 M963 H964 Q965 D966 V967 A968 T969 F970 V971 M972 R973 N974 P975 Q976 Q977 R978 A979 V980 E981 A982 F983 N984 R985 P986 E987 Q988 L989 F990 A991 E992 Y993 R994 E995 W996 H997 R998 S999 P1000 M1001 G1002 K1003 Y1004 A1005 A1006 E1007 C1008 L1009 P1010 S1011 L1012 V1013
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D1082 A1083 V1084 T1085 V1088 H1089 H1090 E1091 M1092 A1093 S1094 I1095 D1096 T1097 G1098 L1099 S1100 Y1101 S1102 M1105 T1106 R1109 V1110 A1111 A1112 I1113 T1114 T1115 D1116 M1117 G1118 I1119 Q1122 D1123 F1124 V1127 F1128 P1129 A1130 E1131 G1134 D1140 K1143 A1144 K1145 V1146 G1147 A1148 Q1149 ARG ASN GLY
THR LEU LEU ARG ASP PRO ARG THR TYR LEU ALA GLY MET THR ASN VAL N1169 G1170 A1171 P1172 G1173 L1174 C1175 H1176 G1177 Q1178 Q1179 A1180 T1181 I1184 T1187 P1188 A1191 D1192 Y1195 F1196 S1199 N1200 S1201 P1202 R1203 G1204 R1205 A1206 A1207 C1208 V1209 V1210 N1214 Y1215 N1216 Q1217 A1220
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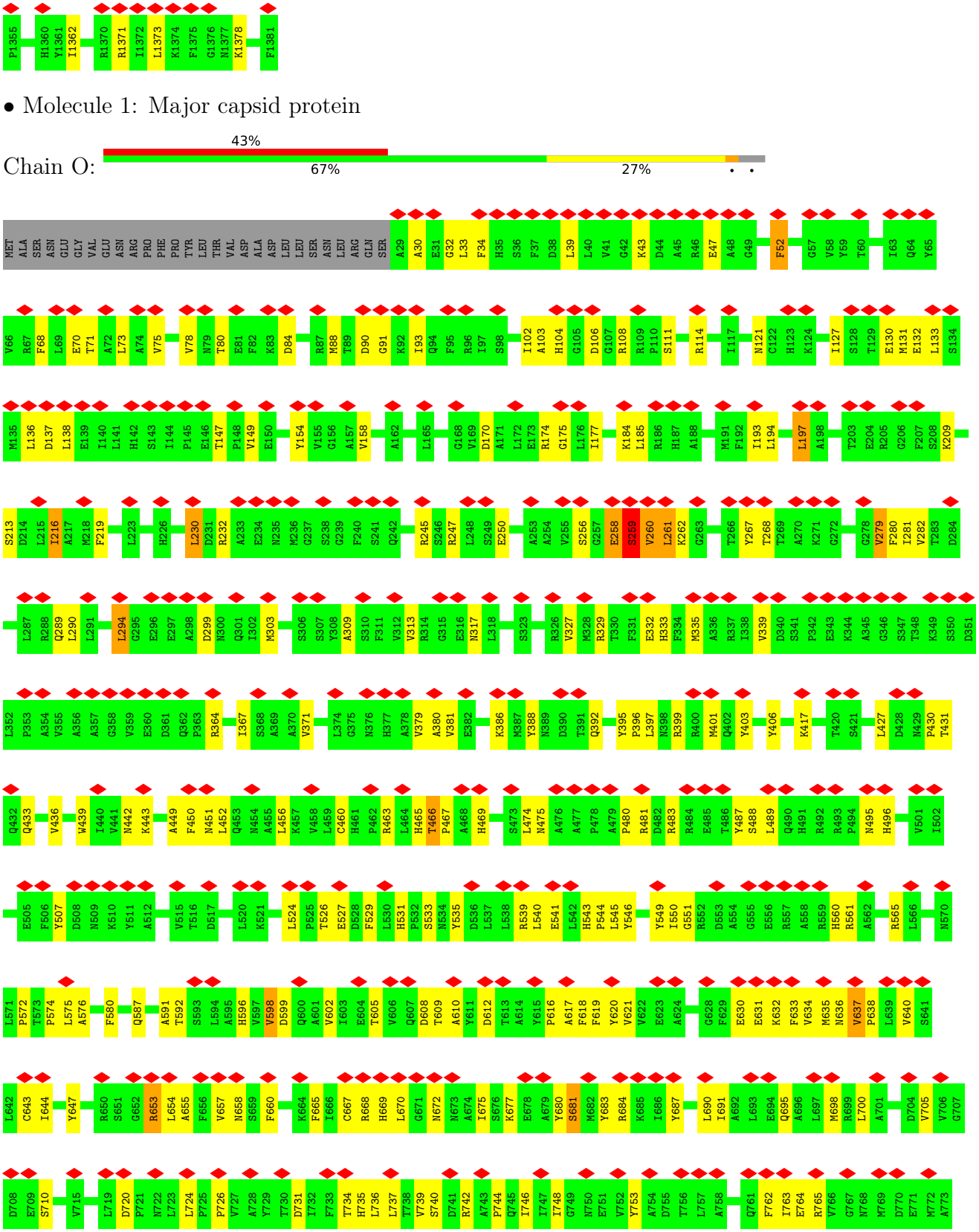
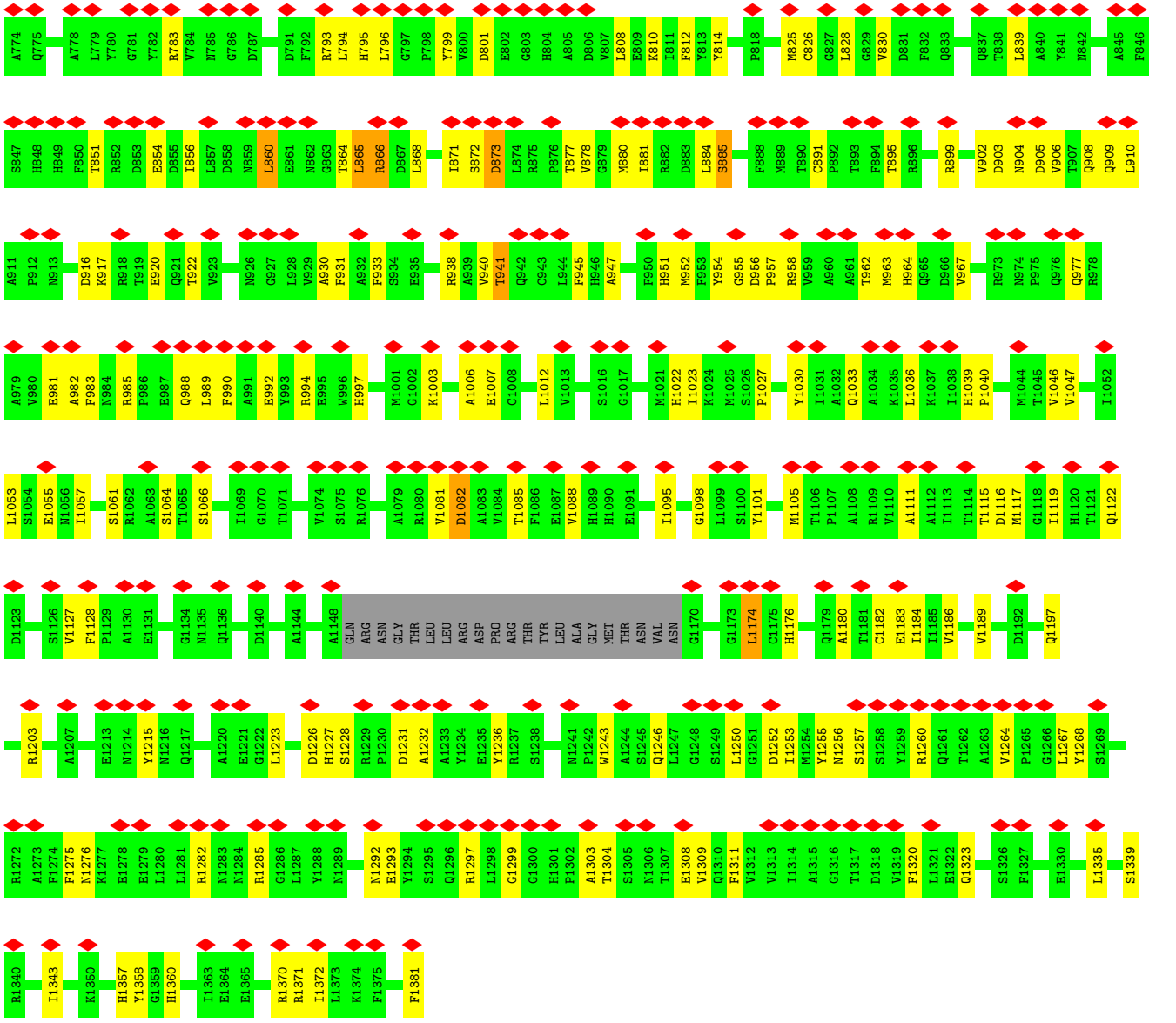
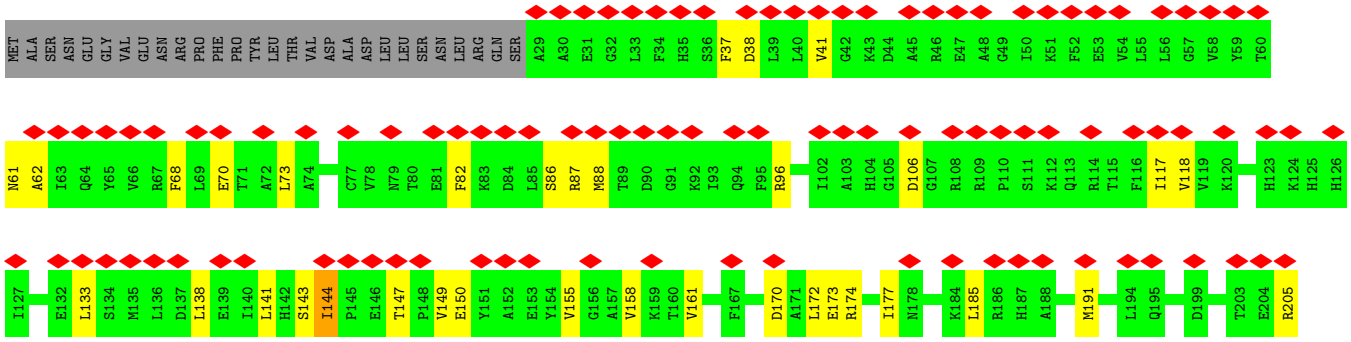
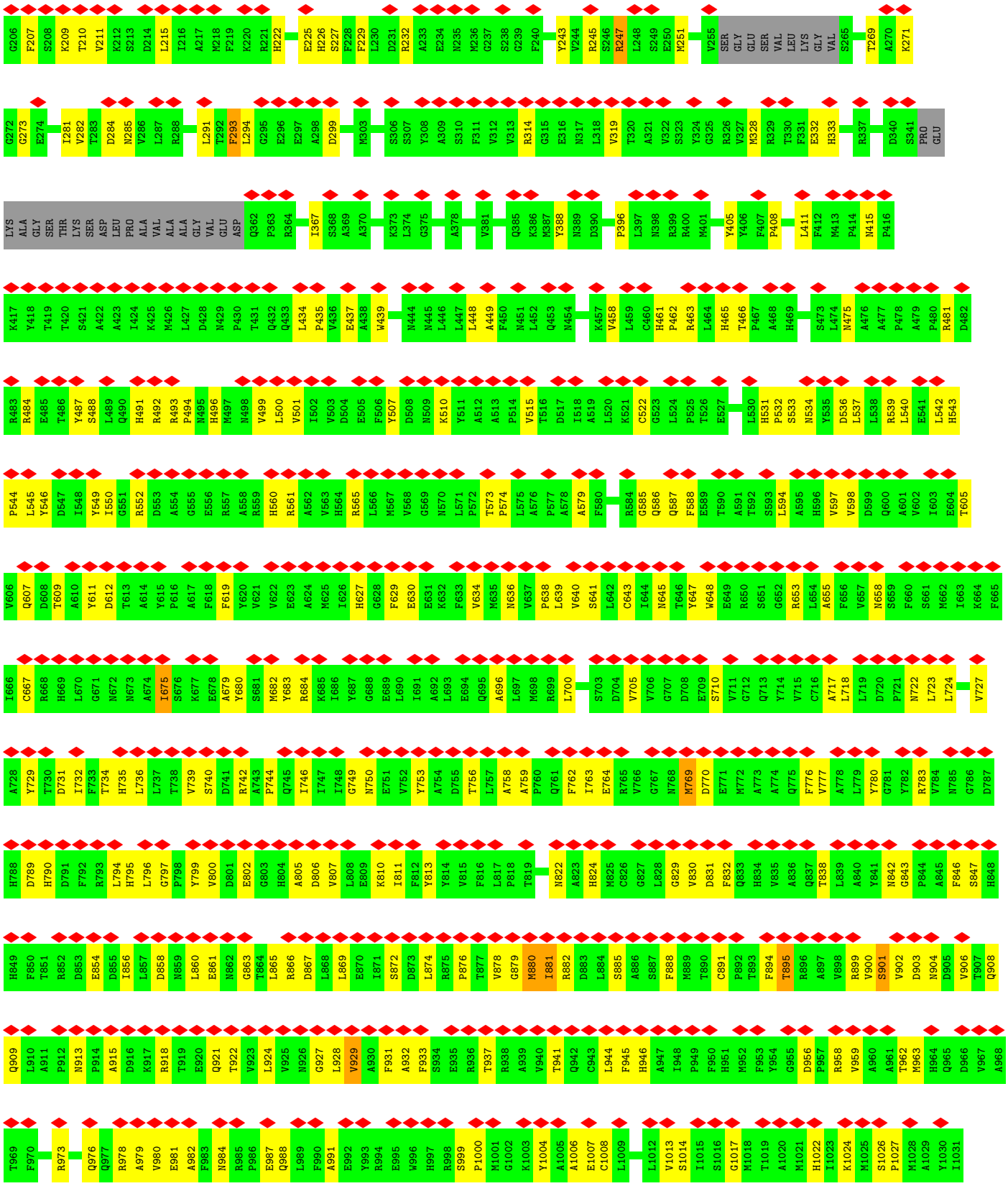

P1355 H1360 Y1361 I1362 R1370 R1371 I1372 L1373 K1374 F1375 G1376 N1377 K1378 F1381
• Molecule 1: Major capsid protein
Chain O:
43%
67%
27%
MET ALA SER ASN GLU GLY VAL GLU ASN ARG PRO PHE PRO TYR LEU THR VAL ASP ALA ASP LEU LEU SER ASN LEU ARG GLN SER A29 A30 E31 G32 L33 F34 H35 S36 F37 D38 L39 L40 V41 G42 K43 D44 A45 R46 E47 A48 G49 F52 G57 V58 Y59 T60 I63 Q64 Y65
V66 R67 F68 L69 E70 T71 A72 L73 A74 V75 V78 N79 T80 E81 F82 K83 D84 R87 M88 T89 D90 G91 K92 I93 Q94 F95 R96 I97 S98 I102 A103 H104 G105 D106 G107 R108 R109 P110 S111 R114 I117 N121 C122 H123 K124 I127 S128 T129 E130 M131 E132 L133 S134
M135 L136 D137 L138 E139 I140 L141 H142 S143 I144 P145 E146 T147 P148 V149 E150 Y154 V155 G156 A157 V158 A162 L165 G168 V169 D170 A171 L172 E173 R174 G175 L176 I177 K184 L185 R186 H187 A188 M191 F192 I193 L194 L197 A198 T203 E204 R205 G206 F207 S208 K209
S213 D214 L215 I216 A217 M218 F219 L223 H226 L230 D231 R232 A233 E234 N235 M236 G237 S238 G239 F240 S241 Q242 R245 S246 R247 L248 S249 E250 A253 A254 V255 S256 G257 E258 S259 V260 L261 K262 G263 T266 Y267 T268 T269 A270 K271 G272 G278 V279 F280 I281 V282 T283 D284
L287 R288 Q289 L290 L291 L294 G295 E296 E297 A298 D299 N300 Q301 I302 M303 S306 S307 Y308 A309 S310 F311 V312 V313 R314 G315 E316 N317 L318 S323 R326 V327 M328 R329 T330 F331 E332 H333 F334 M335 A336 R337 I338 V339 D340 S341 P342 E343 K344 A345 G346 S347 T348 K349 S350 D351
L352 P353 A354 V355 A356 A357 G358 V359 E360 D361 Q362 P363 R364 I367 S368 A369 A370 V371 L374 G375 N376 H377 A378 V379 A380 V381 E382 K386 M387 Y388 N389 D390 T391 Q392 Y395 P396 L397 N398 R399 R400 M401 Q402 Y403 Y406 K417 T420 S421 L427 D428 N429 P430 T431
Q432 Q433 V436 W439 I440 V441 N442 K443 A449 F450 N451 L452 Q453 N454 A455 L456 K457 V458 L459 C460 H461 P462 R463 L464 H465 T466 P467 A468 H469 S473 L474 N475 A476 A477 P478 A479 P480 R481 D482 R483 R484 E485 T486 Y487 S488 L489 Q490 H491 R492 R493 P494 N495 H496 V501 I502
E505 F506 Y507 D508 N509 K510 Y511 A512 V515 T516 D517 L520 K521 L524 P525 T526 E527 D528 F529 L530 H531 P532 S533 N534 Y535 D536 L537 L538 R539 L540 E541 L542 H543 P544 L545 Y546 Y549 I550 G551 R552 D553 A554 G555 E556 R557 A558 R559 H560 R561 A562 R565 L566 N570
L571 P572 T573 P574 L575 A576 F580 Q587 A591 T592 S593 L594 A595 H596 V597 V598 D599 Q600 A601 V602 I603 E604 T605 V606 Q607 D608 T609 A610 Y611 D612 T613 A614 Y615 P616 A617 F618 F619 Y620 V621 V622 E623 A624 G628 F629 E630 E631 K632 F633 V634 M635 M636 V637 P638 L639 V640 S641
L642 C643 I644 Y647 R650 S651 G652 R653 L654 A655 F656 V657 N658 S659 F660 K664 F665 I666 C667 R668 H669 L670 G671 N672 N673 A674 I675 S676 K677 E678 A679 Y680 S681 M682 Y683 R684 K685 I686 Y687 L690 I691 A692 L693 E694 Q695 A696 L697 M698 R699 L700 A701 D704 V705 V706 G707
D708 E709 S710 V715 L719 D720 P721 N722 L723 L724 P725 P726 V727 A728 Y729 T730 D731 I732 F733 T734 H735 L736 L737 T738 V739 S740 D741 R742 A743 P744 Q745 I746 I747 I748 G749 N750 E751 V752 Y753 A754 D755 T756 L757 A758 Q761 F762 I763 E764 R765 V766 G767 N768 M769 D770 E771 M772 A773



- Molecule 1: Major capsid protein

Chain P:

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G272 G273 E274 I281 V282 T283 D284 N285 V286 L287 R288 L291 T292 F293 L294 G295 E296 E297 A298 D299 M303 S306 S307 Y308 A309 S310 F311 V312 V313 R314 G315 E316 N317 L318 V319 T320 A321 V322 S323 Y324 G325 R326 V327 M328 R329 T330 F331 E332 H333 R337 D340 S341 PRO GLU
LYS ALA GLY SER THR LYS SER ASP LEU PRO ALA VAL ALA ALA GLY VAL GLU ASP Q362 P363 R364 I367 S368 A369 A370 K373 L374 G375 A378 V381 Q385 K386 M387 Y388 N389 D390 P396 L397 N398 R399 R400 M401 Y405 Y406 F407 P408 L411 F412 M413 P414 N415 P416
K417 Y418 T419 T420 S421 A422 A423 I424 K425 M426 L427 D428 N429 P430 T431 Q432 Q433 L434 P435 V436 E437 A438 W439 N444 N445 L446 L447 L448 A449 F450 N451 L452 Q453 N454 K457 V458 L459 C460 H461 P462 R463 L464 H465 T466 P467 A468 H469 S473 L474 N475 A476 A477 P478 A479 P480 R481 D482
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P544 L545 Y546 D547 T548 Y549 I550 G551 R552 D553 A554 G555 E556 R557 A558 R559 H560 R561 A562 V563 H564 R565 L566 M567 V568 G569 N570 L571 P572 T573 P574 L575 A576 P577 A578 A579 F580 R584 G585 Q586 Q587 F588 E589 T590 A591 T592 S593 L594 A595 H596 V597 V598 D599 Q600 A601 V602 I603 E604 T605
V606 Q607 D608 T609 A610 Y611 D612 T613 A614 Y615 P616 A617 F618 F619 Y620 V621 V622 E623 A624 M625 I626 H627 G628 F629 E630 E631 K632 F633 V634 M635 N636 V637 P638 L639 V640 S641 L642 C643 I644 N645 T646 Y647 W648 E649 R650 S651 G652 R653 L654 A655 F656 V657 N658 S659 F660 S661 M662 I663 K664 F665
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H788 D789 H790 D791 F792 R793 L794 H795 L796 G797 P798 Y799 V800 D801 E802 G803 H804 A805 D806 V807 L808 E809 K810 I811 F812 Y813 Y814 V815 F816 L817 P818 T819 N822 A823 H824 M825 C826 G827 L828 G829 V830 D831 F832 Q833 H834 V835 A836 Q837 T838 L839 A840 Y841 N842 G843 P844 A845 F846 S847 H848
H849 F850 T851 R852 D853 E854 D855 I856 L857 D858 N859 L860 E861 N862 G863 T864 L865 R866 D867 L868 L869 E870 I871 S872 D873 L874 R875 P876 T877 V878 G879 M880 I881 R882 D883 L884 S885 A886 S887 F888 M889 T890 C891 P892 T893 F894 T895 R896 A897 V898 R899 V900 S901 V902 D903 N904 D905 V906 T907 Q908
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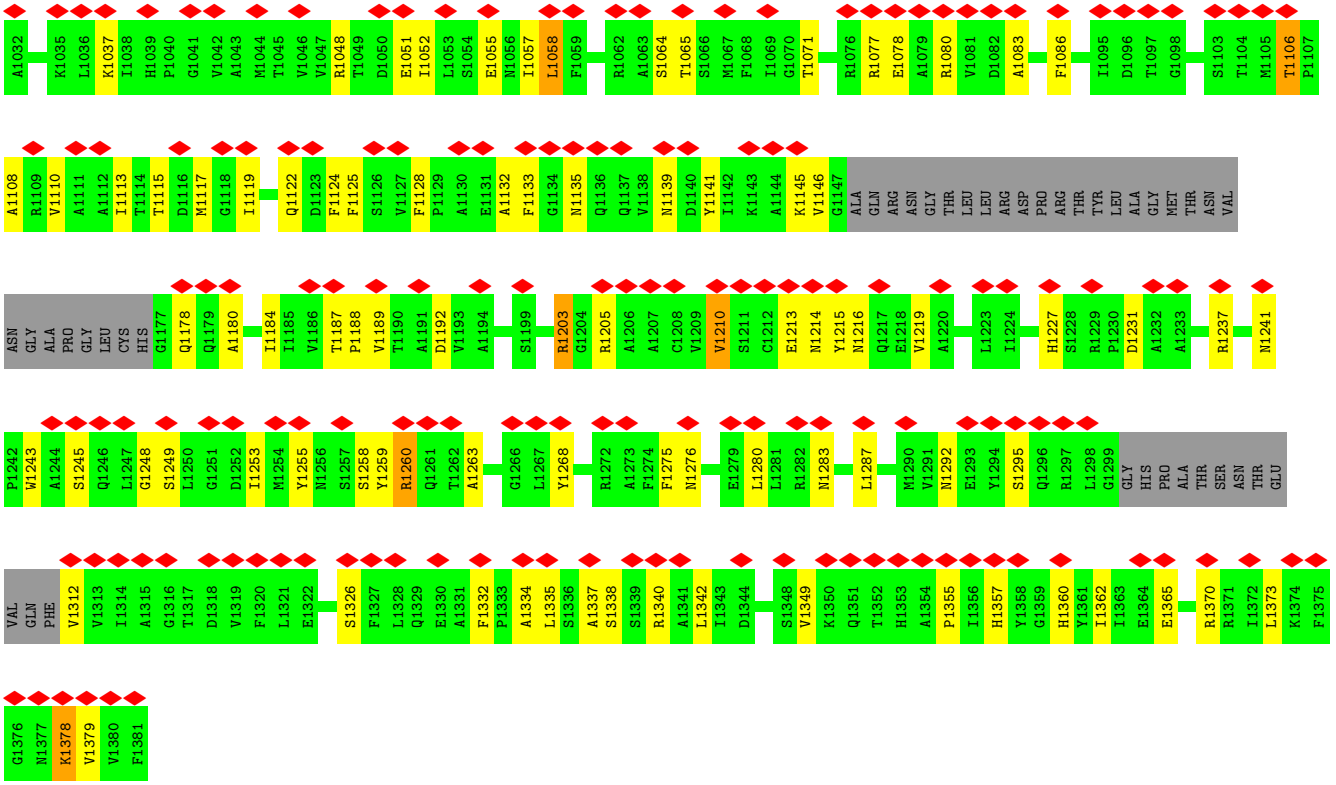
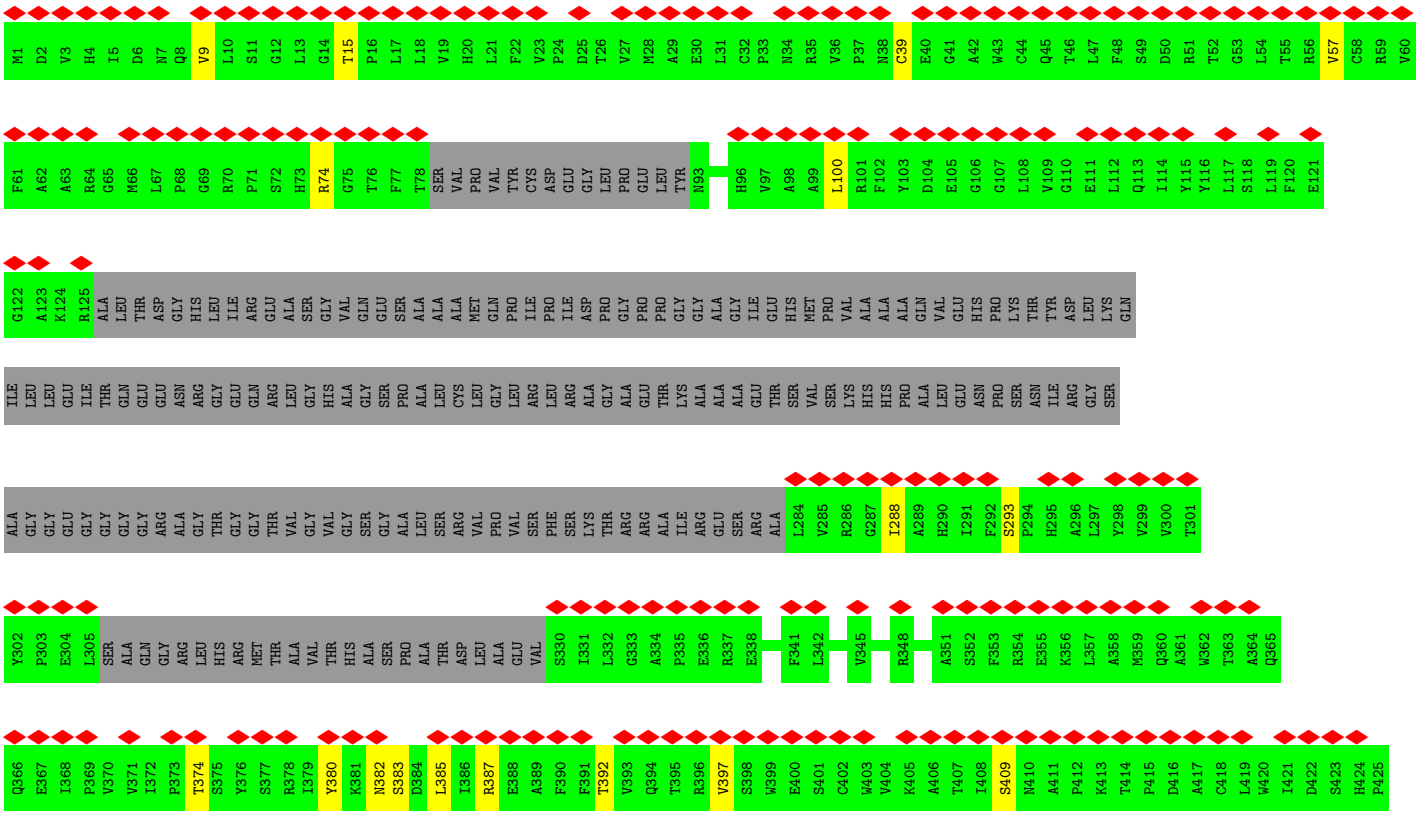
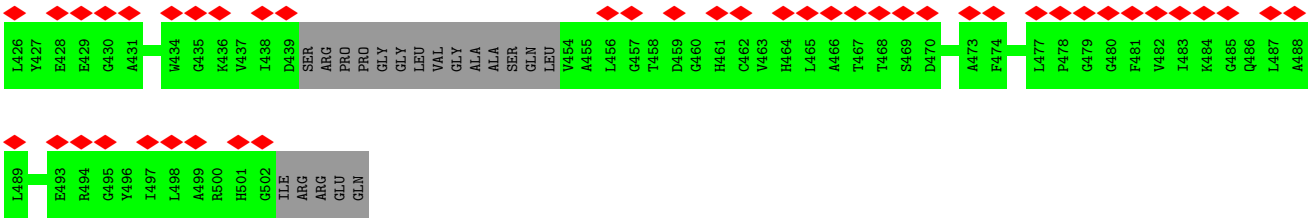
T969 F970 R973 Q976 Q977 R978 A979 V980 E981 A982 F983 N984 R985 P986 E987 Q988 L989 F990 A991 E992 Y993 R994 E995 W996 H997 R998 S999 P1000 M1001 G1002 K1003 Y1004 A1005 A1006 E1007 C1008 L1009 L1012 V1013 S1014 I1015 S1016 G1017 M1018 T1019 A1020 M1021 H1022 I1023 K1024 M1025 S1026 P1027 M1028 A1029 Y1030 I1031



- Molecule 2: Capsid vertex component 1

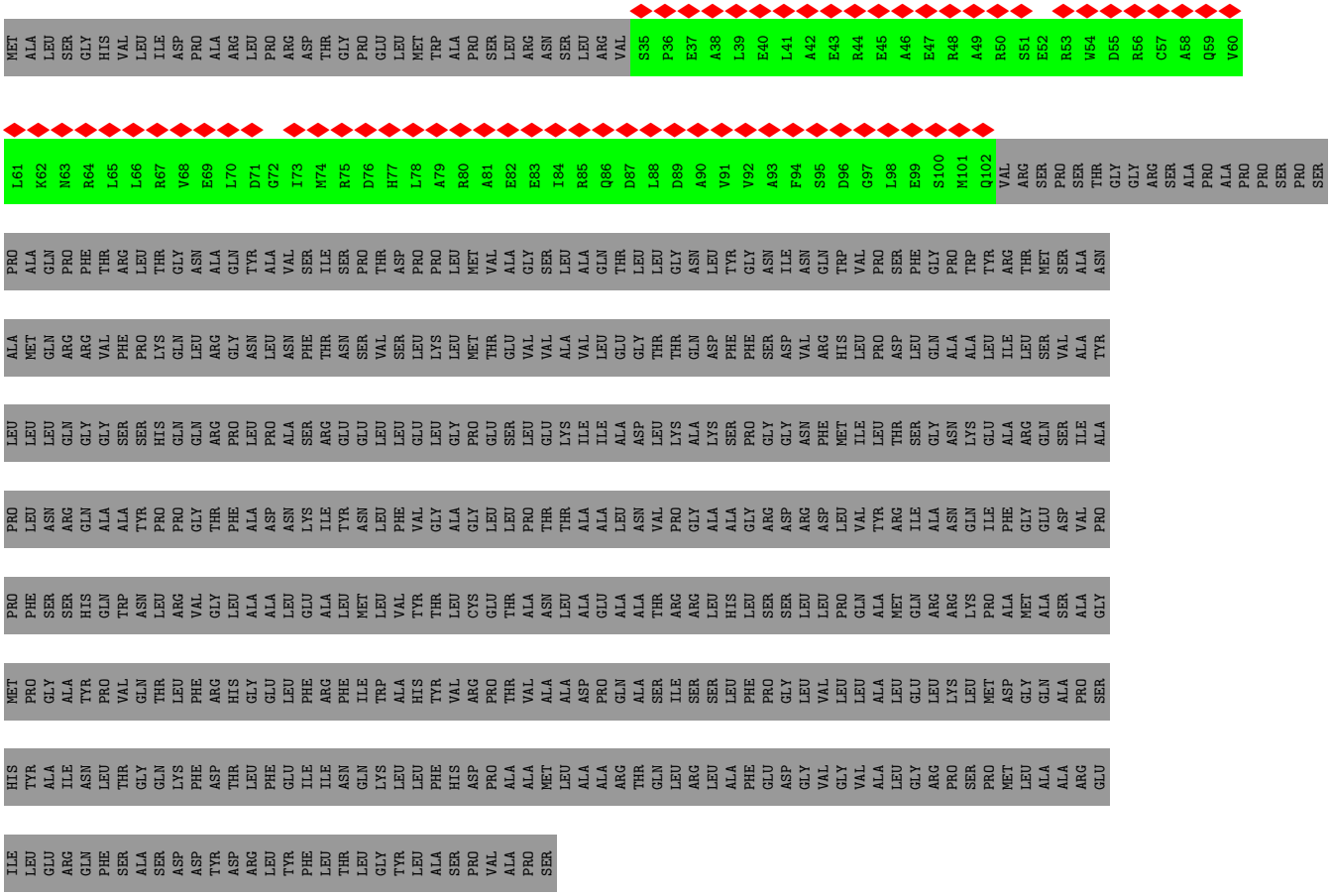
Chain v:





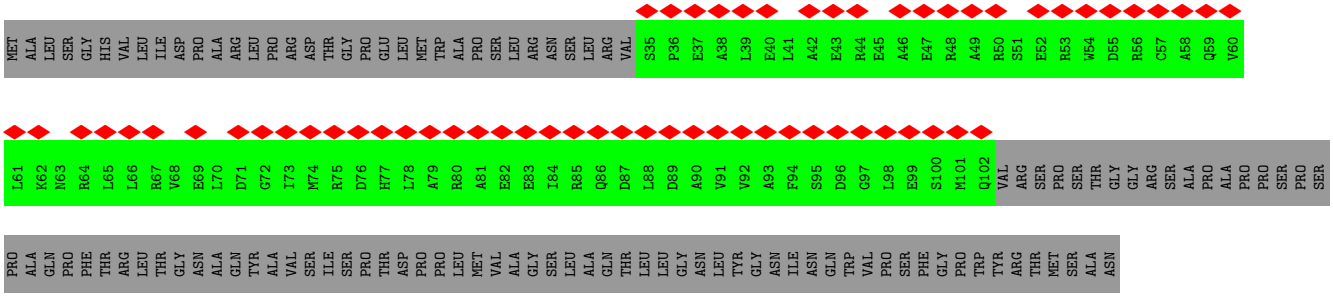
- Molecule 3: Capsid vertex component 2

Chain w:



- Molecule 3: Capsid vertex component 2

Chain x:



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

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

PRO PHE SER SER HIS GLN TRP ASN LEU ARG VAL GLY LEU ALA ALA LEU GLU ALA LEU MET LEU VAL TYR THR LEU CYS GLU THR ALA ASN LEU ALA GLU ALA ALA THR ARG ARG LEU HIS LEU SER SER LEU LEU PRO GLN ALA MET GLN ARG ARG LYS PRO ALA MET ALA SER ALA GLY

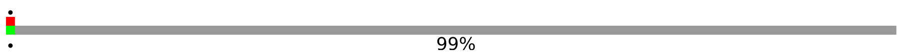
MET PRO GLY ALA TYR PRO VAL GLN THR LEU PHE ARG HIS GLY GLU LEU PHE ARG PHE ILE TRP ALA HIS TYR VAL ARG PRO THR VAL ALA ALA ASP PRO GLN ALA SER ILE SER SER LEU PHE PRO GLY LEU VAL LEU LEU ALA LEU GLU LEU LYS LEU MET ASP GLY GLN ALA PRO SER

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

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

- Molecule 4: Large tegument protein deneddylase

Chain y:



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

VAL LEU ARG GLY GLY GLY ARG VAL HIS ILE TYR ARG SER ALA GLU ILE PHE GLY LEU VAL LEU PHE PRO ALA GLN ILE ALA ASN SER ALA VAL VAL GLN SER LEU ALA GLU VAL LEU HIS GLY SER TYR ASN GLY VAL ALA GLN PHE ILE LEU TYR ILE CYS ASP ILE TYR ALA GLY ALA

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

GLU THR GLU ASP PRO ARG ILE PHE MET LEU GLU HIS TYR GLY VAL TYR ASP PHE TYR GLU ALA ASN GLY SER GLY PHE ASP LEU VAL GLY PRO GLU LEU VAL SER SER ASP GLY GLU ALA ALA GLY THR PRO GLY ALA ASP SER SER PRO PRO VAL MET LEU PRO PHE GLU ARG ARG ILE

ILE PRO TYR ASN LEU ARG PRO LEU PRO SER ARG SER PHE THR SER ASP SER PHE PRO ALA ALA ARG TYR SER PRO ALA LYS THR ASN SER PRO PRO SER SER PRO ALA SER ALA ALA PRO ALA SER ALA ALA PRO ALA SER ALA ALA PRO ALA SER ALA ALA PRO ALA SER ALA ALA PRO

ALA SER ALA ALA PRO ALA SER ALA ALA PRO ALA SER ALA ALA PRO ALA SER SER PRO PRO LEU PHE ILE PRO ILE PRO GLY LEU GLY HIS THR PRO GLY VAL PRO ALA PRO SER THR PRO PRO ARG ALA SER SER GLY ALA ALA PRO GLN THR PRO LYS ARG LYS LYS GLY LEU GLY LYS

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

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

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

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

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

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

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

SER TYR LEU GLU ASP PRO SER LEU PRO THR VAL MET ASP PHE ASP ASP LEU LEU THR HIS LEU ARG HIS THR CYS GLN ILE ILE ALA SER LEU PRO LEU LEU ASN ILE ARG TYR THR SER ILE GLU TRP ASP TYR ARG GLU LEU LEU TYR LEU GLY THR ALA LEU SER ASP MET SER GLY

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

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

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THR GLU GLU GLN LEU GLU ALA PHE LEU ASP THR ALA PRO ASN LYS GLU LEU LYS ARG GLN TYR GLU LYS LYS LEU ARG GLN LEU MET GLU THR GLY ARG LYS GLU LYS GLU LYS LEU ARG GLU GLN GLU ASP LYS GLU ARG GLN GLU ARG ARG ALA ARG GLU ALA ASN GLU ALA TRP ALA

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TRP ILE ARG GLY ILE CYS GLU ALA VAL ARG GLY LEU SER GLU GLY ALA LEU ALA LEU ALA GLY GLY ALA GLY ALA TRP LEU ASN LEU ALA ALA ALA ALA ASP GLY GLU ILE HIS GLU LEU THR ARG LEU LEU GLU VAL GLU GLY MET ALA GLN ASN SER MET ASP GLY MET GLU GLU LEU

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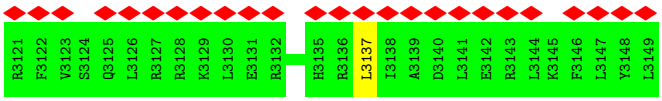
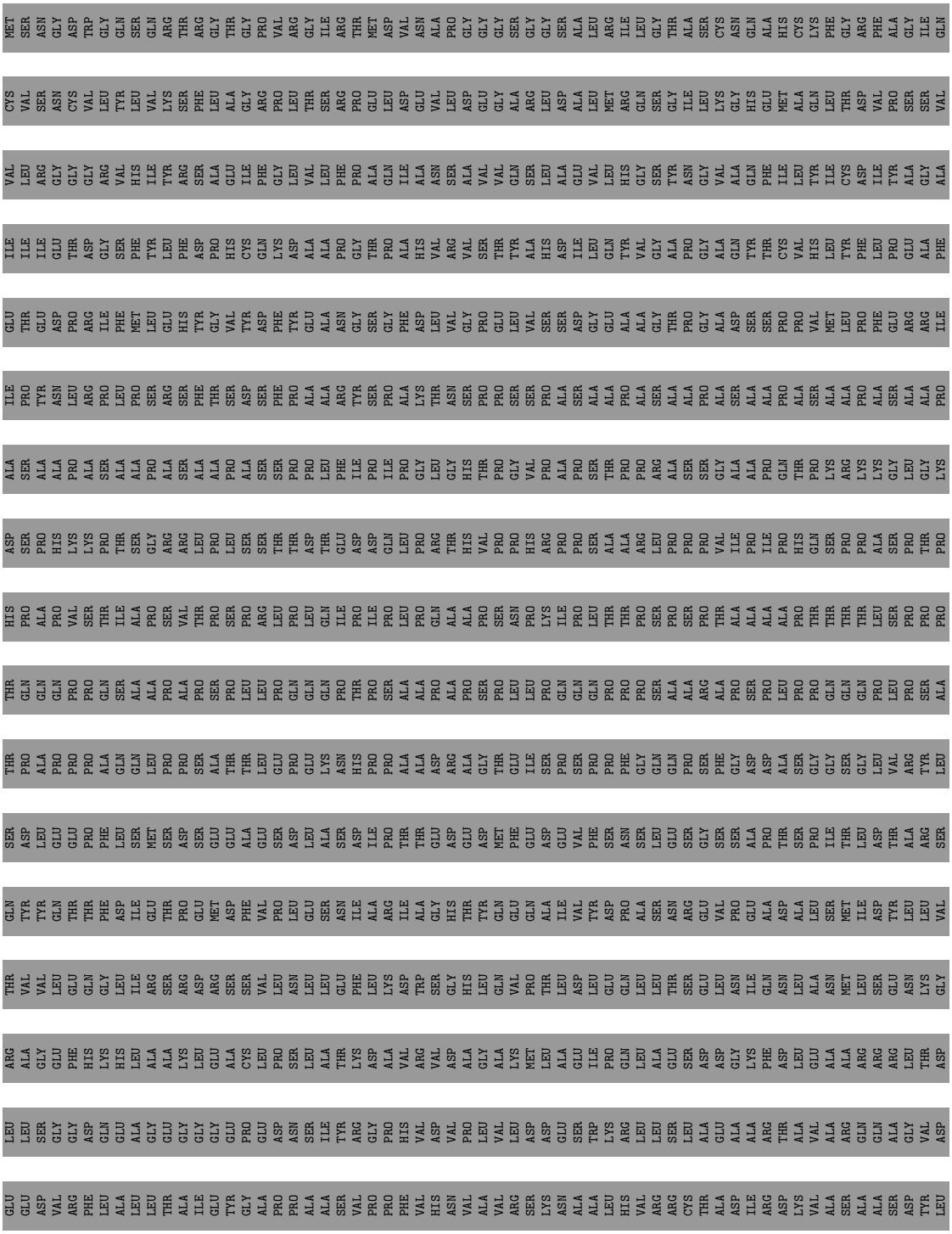
ALA LEU TRP PRO HIS PRO GLU PHE LEU GLY LEU VAL HIS ASN GLN SER THR ALA ARG ALA ARG ALA ALA CYS MET LEU LEU LEU ALA ARG ARG CYS PHE ALA PRO GLU ALA ALA LEU VAL ARG PRO LEU LEU ALA ASP ALA GLY PRO PRO TRP LEU ALA ASP PHE
VAL LYS GLN ALA TYR THR ARG GLY GLU GLU LEU PRO ARG ALA GLU GLY LEU GLU VAL PRO ARG GLU THR PRO SER SER TYR GLY THR VAL THR GLY ARG ALA ASN LEU MET PRO TYR GLY THR PRO ILE THR GLY PRO LYS ARG GLY SER GLY ASP THR VAL SER VAL
PHE GLU ALA ALA VAL ALA ALA ALA PHE PHE LEU GLY ARG PRO LEU THR LEU PHE VAL SER SER GLN TYR LEU PHE ASN LEU LYS THR LEU GLY GLN VAL ARG VAL ALA PRO LEU LEU TYR CYS ASP GLY HIS SER GLU PRO PHE ARG SER LEU VAL GLU THR ILE SER LEU ASN PHE LEU
GLN ASP LEU ASP GLY TYR SER GLU SER PHE GLU PRO MET SER ILE PHE ALA ARG GLN ALA VAL TRP LEU ARG GLU LEU THR GLU ALA ARG ALA ALA LYS PRO LYS GLU ALA ARG PRO PRO THR VAL ALA ILE ILE LEU ALA ASN ARG LYS ASN ILE ILE TRP LYS CYS PHE THR TYR
ARG HIS ASN LEU PRO ASP VAL GLN PHE TYR PHE ASN ALA ALA GLY ALA SER ARG TRP PRO THR ASP VAL LEU ASN PRO SER PHE PHE TYR GLU HIS GLU ASP PRO PRO VAL GLY TYR GLN LEU PRO PRO PRO ASN PRO ARG ASN VAL GLN GLU LEU PHE SER PRO ARG VAL
GLY HIS GLY LEU VAL SER GLY ASP GLY PHE GLN SER ALA ASP ASN THR THR PRO ALA SER SER ASP ARG LEU GLN GLN LEU GLY GLY GLY GLU THR ASP GLN GLY GLU LYS GLY SER THR THR ALA GLU SER GLU ALA SER GLY PRO PRO GLN SER SER PRO GLN LYS VAL ALA
PRO GLY ARG PRO ARG ASP TRP LEU SER PRO THR SER SER PRO ARG ASP VAL THR VAL THR PRO GLY LEU LEU ALA ALA ALA SER PRO ILE THR LEU PRO GLY PRO ARG LEU MET ALA ARG PRO TYR PHE GLY ALA GLU THR ARG ALA SER GLU PRO PRO ASP ARG SER PRO ARG PRO
TRP PRO LYS ASP SER LEU GLU LEU LEU PRO GLN PRO ALA PRO GLN GLN PRO PRO SER SER PRO TRP ALA SER GLU GLN GLY PRO ILE VAL TYR THR THR LEU SER PRO HIS SER THR PRO SER THR ALA SER GLY SER GLN LYS LYS HIS THR ILE GLN ILE PRO LEU VAL PRO GLY LEU GLY
LYS PRO SER TYR PRO PRO SER ALA PRO TYR LYS PRO GLY GLN SER THR GLY GLY ILE ALA PRO THR PRO SER ALA ALA SER LEU THR THR PHE GLY LEU GLN PRO HIS GLN ASP THR GLN ALA SER SER GLN ASP PRO PRO TYR GLY HIS SER ILE MET GLN ARG GLN GLN GLN GLY
GLY ARG GLU GLU ALA ALA GLU ILE ARG PRO SER ALA THR ARG PRO GLY GLY ALA LEU ARG PRO PRO ARG ALA ALA ALA GLY ALA ALA ALA SER ALA THR PRO ALA PHE ASP PRO GLY GLU ALA PRO ILE ALA PRO PRO SER GLY PHE GLY ALA PRO GLN ILE ILE ALA GLN GLY ALA ALA
LEU ALA ALA PRO ALA HIS THR PRO VAL GLY PRO ARG ALA ALA LEU ALA ALA ALA LEU PRO THR ALA ALA ALA ARG PRO GLN ASP ALA ALA ALA LEU PRO THR ALA ALA VAL GLY LEU GLN ALA ARG PRO VAL PRO LYS ALA THR GLY LYS GLY HIS ALA SER ILE MET GLN ARG ALA ALA
THR ALA ALA PRO PRO SER ALA ALA SER PRO PRO ARG VAL SER LEU PRO VAL ARG SER ARG GLN GLN SER PRO ALA ILE PRO LEU PRO PRO MET HIS SER GLY SER GLU PRO GLY ALA ARG PRO PRO GLN TYR ARG HIS ALA ALA GLY PRO GLN THR TYR THR VAL ARG
LYS GLU ALA PRO PRO SER ALA ALA LEU PRO LYS MET PRO LYS CYS LYS ASP SER MET TYR TYR PRO PRO SER GLY SER ALA ARG TYR PRO ALA PHE GLN ALA LEU SER PHE SER GLN GLN SER VAL ALA SER PRO ALA GLN THR THR LEU LEU TRP ASN THR
PRO SER VAL VAL THR GLY GLY SER THR THR SER GLY ASP LEU VAL VAL THR GLY SER PRO SER SER LEU SER THR ALA ALA PRO GLU GLN ASP LEU ARG TYR SER LEU THR LEU
S3113 Q3114 A3115 S3116 R3117 V3118 L3119 S3120



• Molecule 4: Large tegument protein deneddylase

Chain z: 99%



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

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

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

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

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

THR GLU GLU GLN LEU GLU ALA PHE LEU ASP THR ALA PRO ASN LYS GLU LEU LYS ARG GLN TYR GLU LYS LYS LEU ARG GLN LEU MET GLU THR GLY ARG LYS GLU LYS GLU LYS LEU ARG GLU GLN GLU ASP LYS GLU ARG GLN GLU ARG ARG ALA ARG GLU ALA ASN GLU ALA TRP ALA

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

LEU GLY ILE THR ARG VAL ARG ARG GLU ARG LEU ARG SER LEU LEU VAL ASP ASP GLY GLY ALA ALA GLU ARG MET GLU ALA ALA GLU PRO GLY TRP PHE THR ASP ILE GLU THR GLY PRO LEU ALA ARG LEU ASP ALA TRP PRO ALA THR PRO ALA ALA THR ALA LYS GLU GLY GLY GLY

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

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

PRO GLN LEU LEU THR ARG ARG GLU ARG ASP ASP LEU LEU GLN ALA THR GLY ASP PHE PHE SER GLU LEU LEU THR GLU ALA GLU ALA ALA GLU VAL ARG ALA LEU GLU GLU GLN VAL ARG GLU SER GLN THR LEU MET ALA LYS ALA HIS GLU MET ALA ALA SER THR ARG ARG GLY PHE

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

TRP ILE ARG GLY ILE CYS GLU ALA VAL ARG GLY LEU SER GLU GLY ALA LEU ALA LEU ALA GLY GLY ALA GLY ALA TRP LEU ASN LEU ALA ALA ALA ALA ASP GLY GLU ILE HIS GLU LEU THR ARG LEU LEU GLU VAL GLU GLY MET ALA GLN ASN SER MET ASP GLY MET GLU GLU LEU

ARG LEU ALA LEU ALA THR LEU ASP PRO LYS ARG VAL ALA GLY GLY LYS GLU THR VAL ALA ASP TRP LYS ARG ARG LEU SER ARG LEU GLU GLU ALA ILE ILE GLN GLU ALA GLN GLU GLU SER GLN LEU GLN GLY THR LEU GLN ASP LEU VAL THR GLN ALA ARG GLY HIS THR ASP PRO ARG

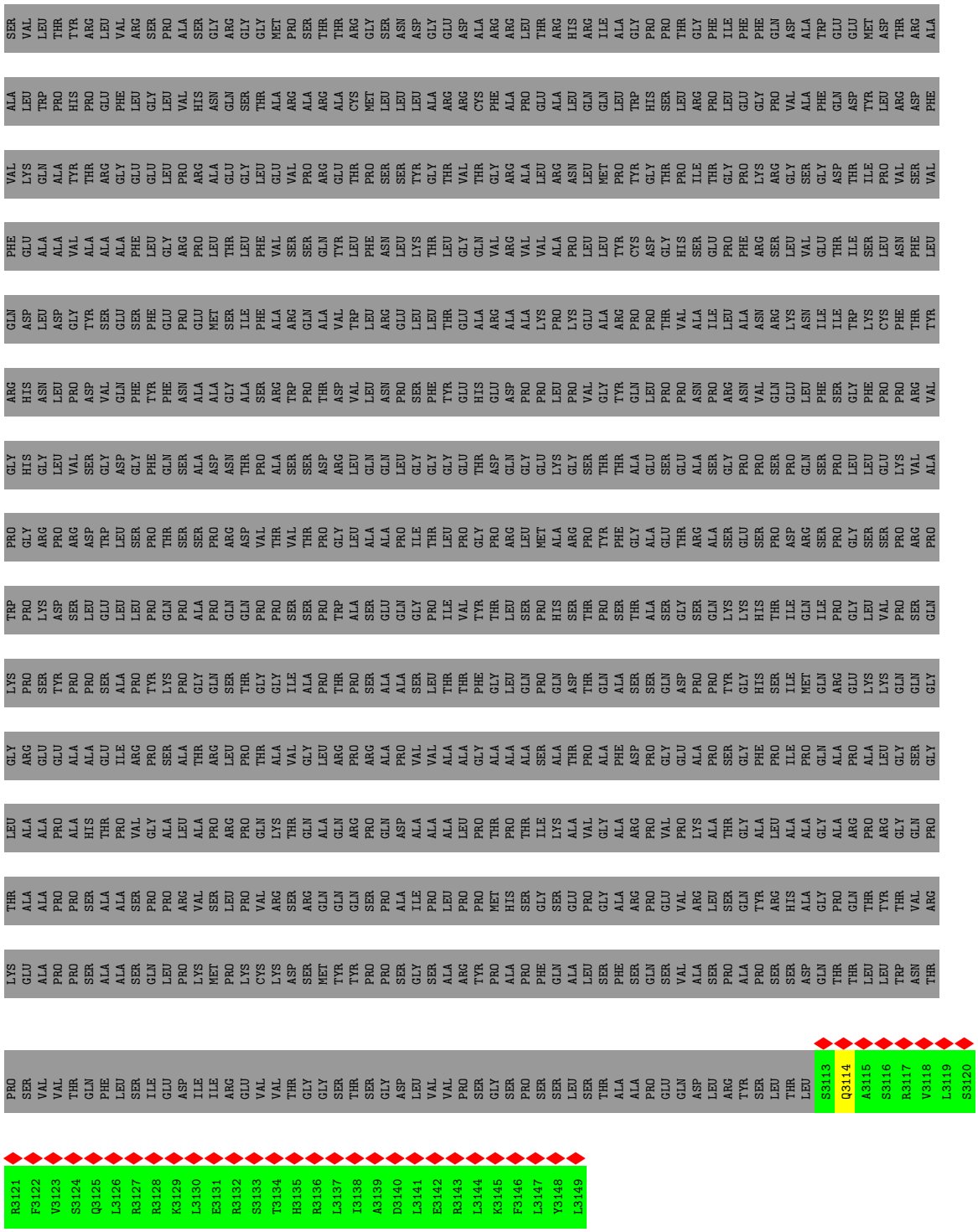
GLN LEU LYS ILE VAL VAL GLU ALA ALA ARG GLY LEU ALA LEU GLY ALA SER ALA GLY SER GLN TYR ALA LEU LEU LYS ASP LYS LEU LEU ARG TYR ALA SER ALA LYS GLN SER PHE LEU ALA PHE TYR GLU THR ALA GLN PRO THR VAL PHE VAL LYS HIS PRO LEU THR ASN ASN LEU

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

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

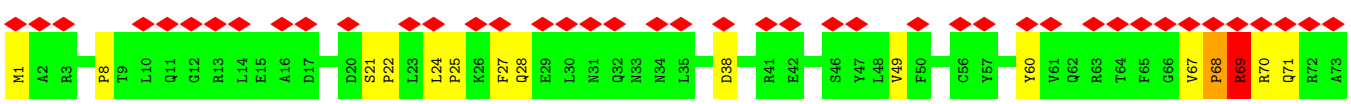
ALA ALA ALA ASP SER TYR TRP ASP THR TRP PRO ASP VAL GLU SER ASN ALA GLY GLU LEU LEU ARG GLU TYR VAL SER ALA PRO LYS ALA LEU MET GLU ASP LEU ALA ASP ASN PRO ILE VAL ALA MET THR LEU LEU ALA HIS ALA SER LEU ILE ALA SER ARG ASN HIS PRO PRO TYR

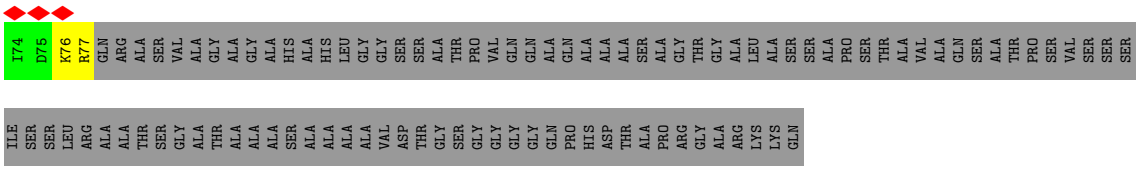
PRO ALA PRO ALA THR ASP ARG GLU VAL ILE LEU LEU GLU GLN ARG GLU MET MET ALA LEU LEU VAL GLY THR HIS PRO ALA TYR ALA ALA ALA PHE LEU GLY ALA PRO SER PHE TYR ALA GLY LEU GLY LEU VAL SER ALA LEU ALA ARG ASP GLY GLY LEU GLY ASP LEU LEU SER ASP



- Molecule 5: Small capsomere-interacting protein

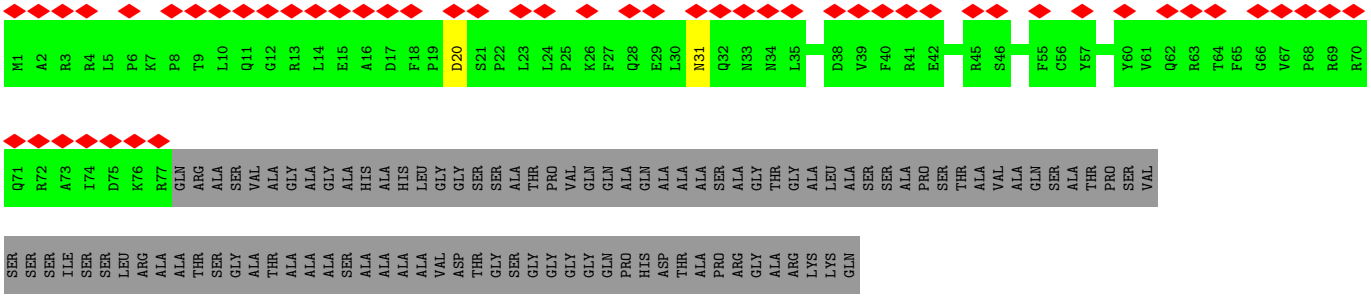
Chain Z:





• Molecule 5: Small capsomere-interacting protein

Chain a:



• Molecule 5: Small capsomere-interacting protein

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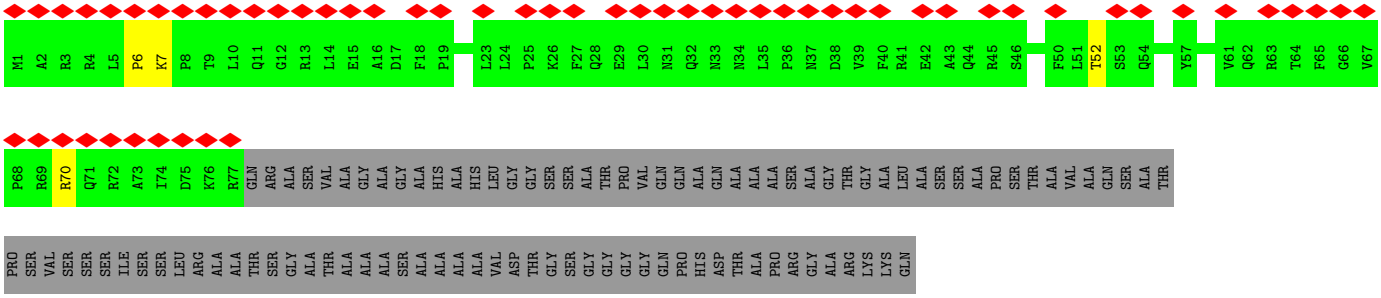

• Molecule 5: Small capsomere-interacting protein

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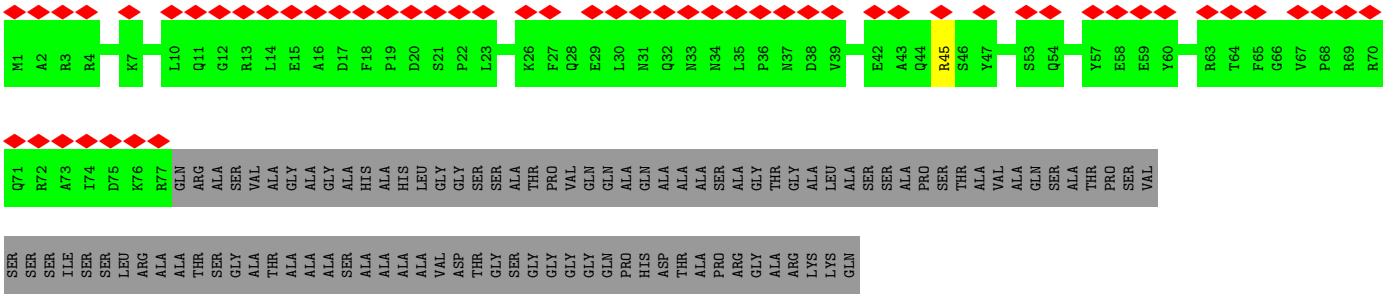
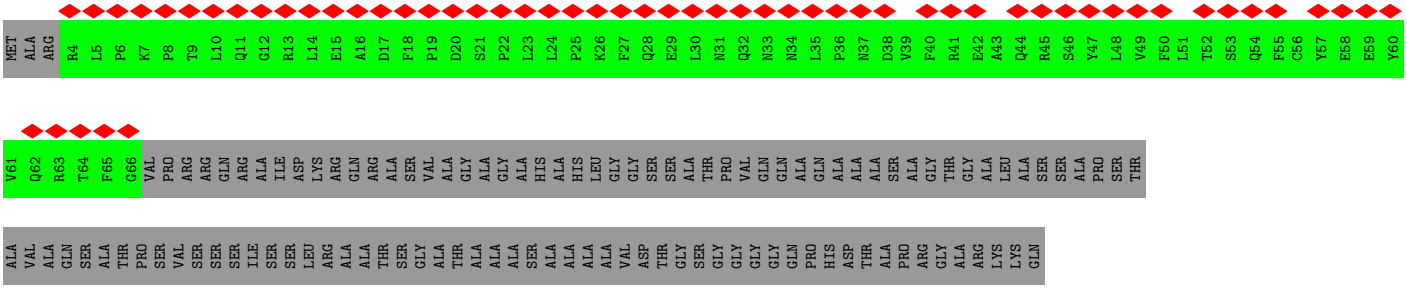


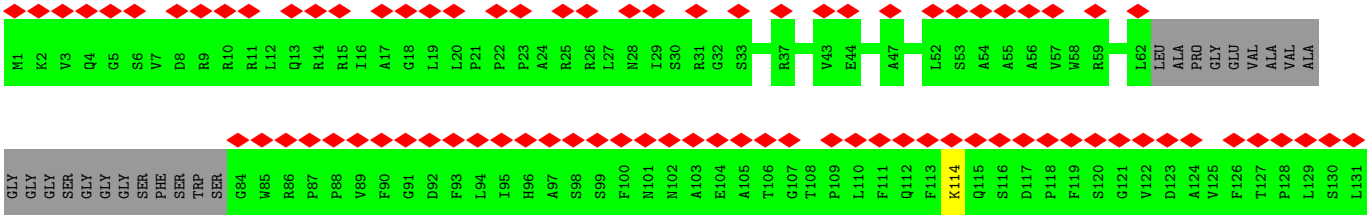
• Molecule 5: Small capsomere-interacting protein

Chain u:



- Molecule 6: Triplex capsid protein 1

Chain f:



- Molecule 6: Triplex capsid protein 1

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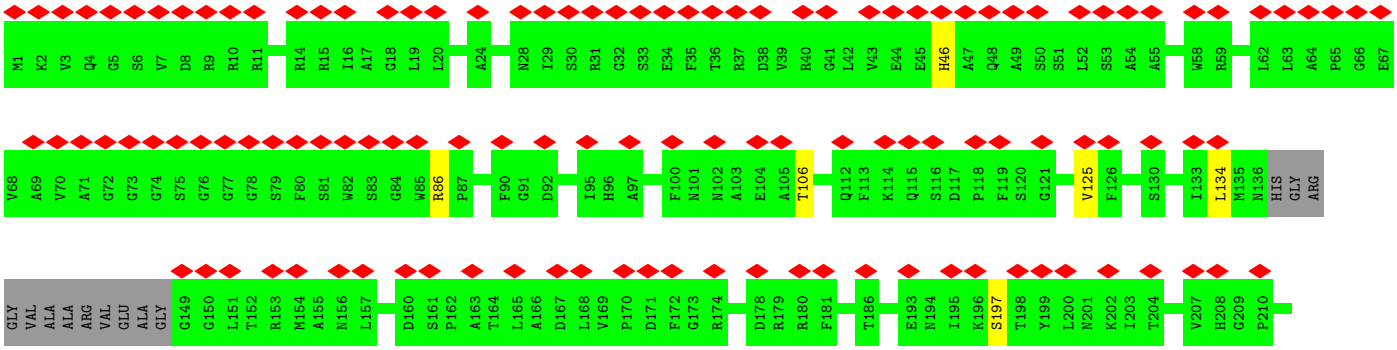
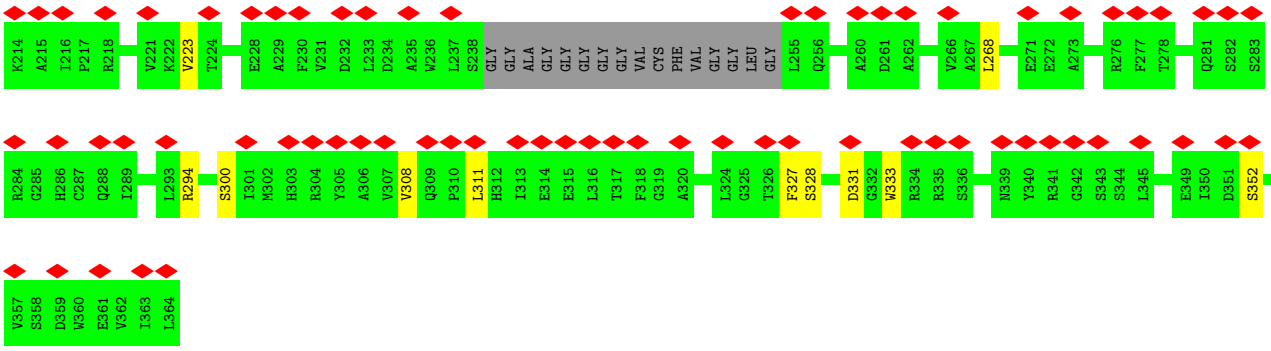
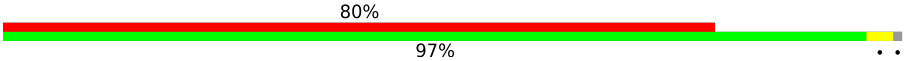
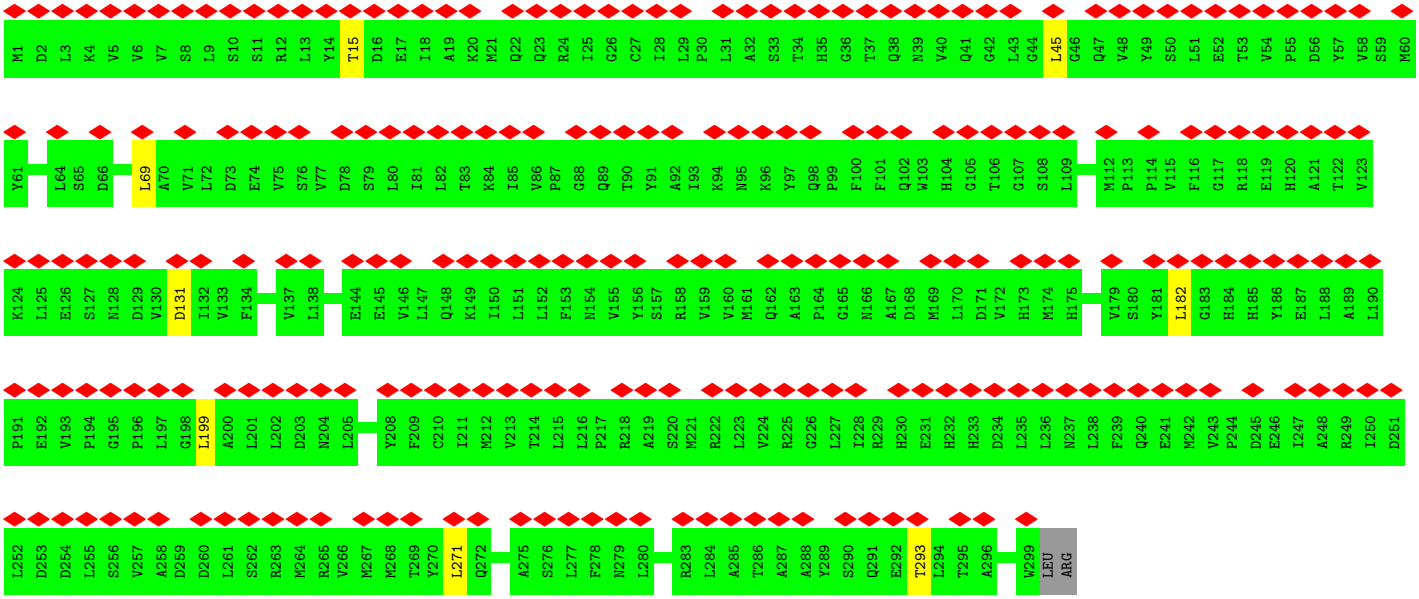




- Molecule 7: Triplex capsid protein 2

Chain k:





- Molecule 7: Triplex capsid protein 2

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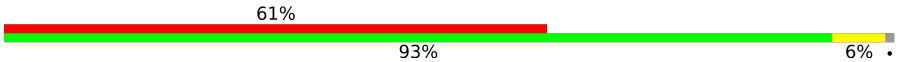

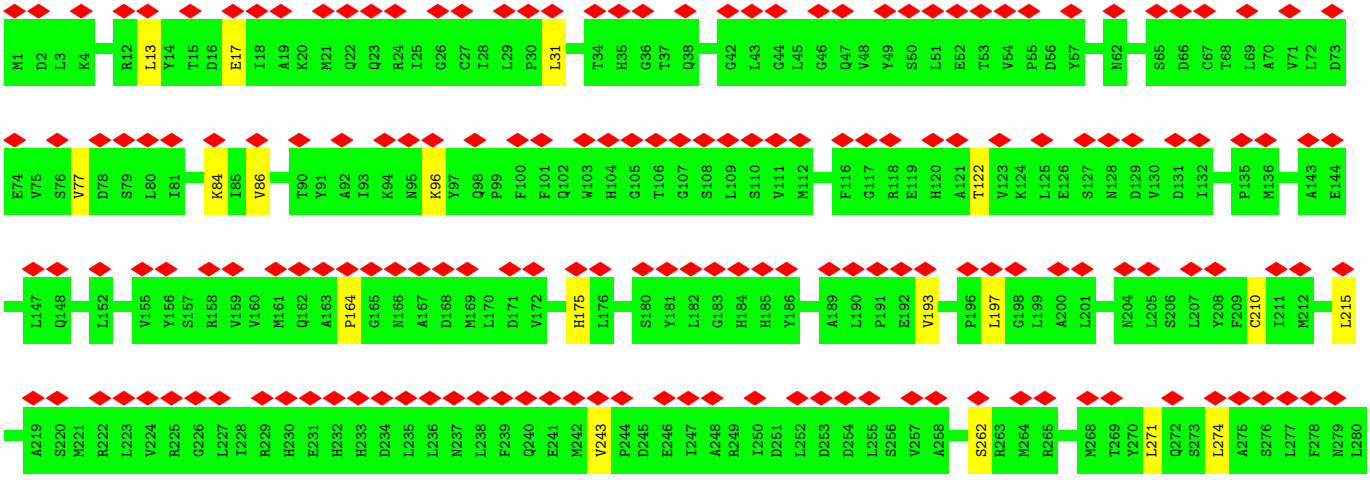

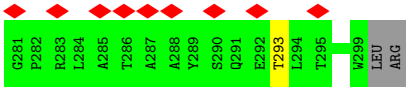

• Molecule 7: Triplex capsid protein 2

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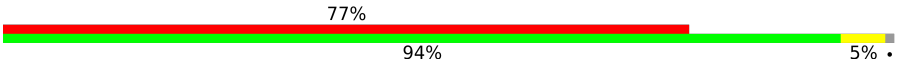
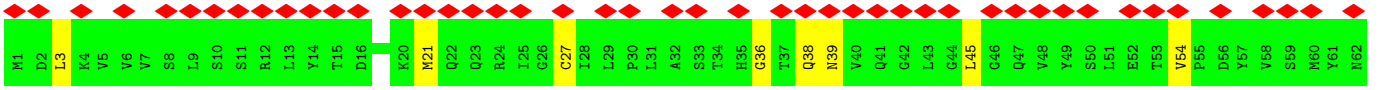
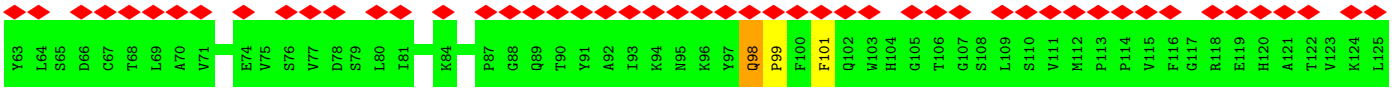
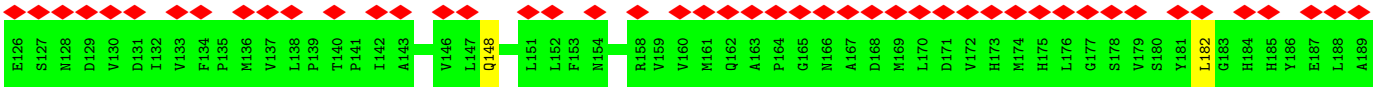
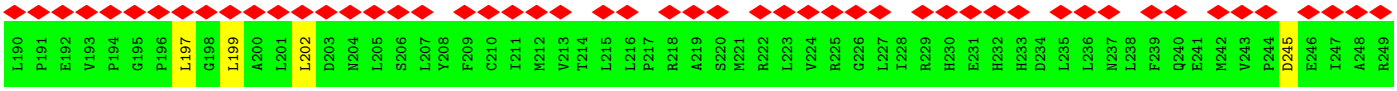
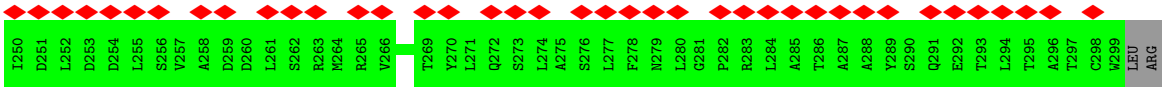






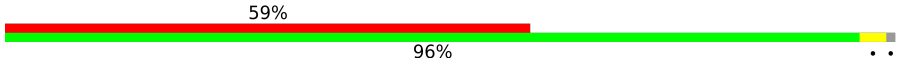


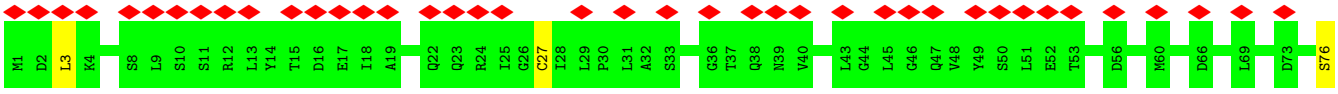


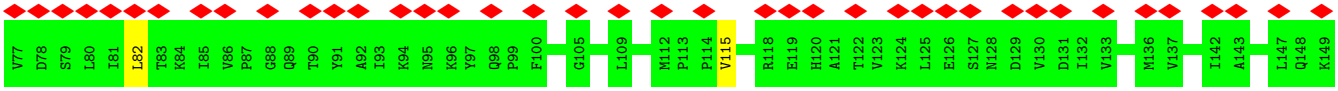


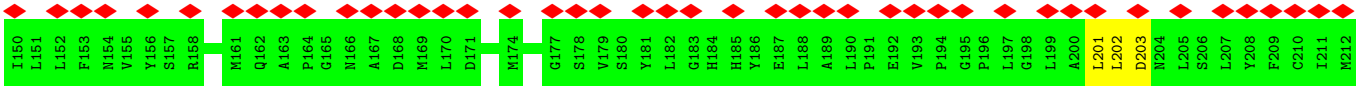
• Molecule 7: Triplex capsid protein 2

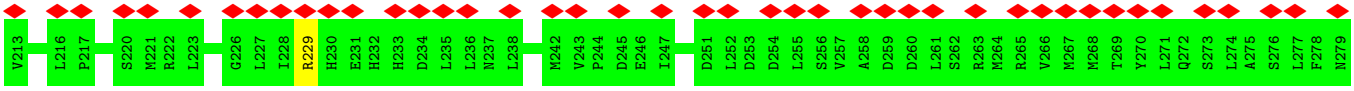
Chain r:

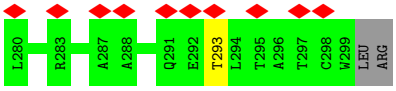












4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	21085	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 ($e^-/Å^2$)	28	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.058	Depositor
Minimum map value	-0.035	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	435.2, 435.2, 435.2	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.36, 1.36, 1.36	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	J	0.36	0/10877	0.49	0/14781
1	K	0.36	0/11085	0.47	0/15066
1	N	0.34	0/10933	0.47	0/14858
1	O	0.35	0/10693	0.47	0/14531
1	P	0.32	0/10349	0.47	0/14057
2	v	0.32	0/2341	0.48	0/3183
3	w	0.26	0/553	0.41	0/741
3	x	0.30	0/553	0.44	0/741
4	y	0.30	0/320	0.45	0/424
4	z	0.29	0/320	0.45	0/424
5	Z	0.30	0/664	0.42	0/896
5	a	0.31	0/664	0.44	0/896
5	d	0.30	0/664	0.48	0/896
5	e	0.29	0/664	0.45	0/896
5	u	0.30	0/542	0.47	0/735
6	f	0.30	0/2537	0.48	0/3450
6	h	0.34	0/2672	0.48	0/3635
7	k	0.30	0/2388	0.50	0/3254
7	m	0.32	0/2388	0.50	0/3254
7	p	0.29	0/2388	0.50	0/3254
7	r	0.33	0/2388	0.50	0/3254
All	All	0.34	0/75983	0.48	0/103226

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	10628	0	10448	344	0
1	K	10832	0	10655	309	0
1	N	10683	0	10500	345	0
1	O	10447	0	10273	306	0
1	P	10113	0	9949	260	0
2	v	2283	0	2268	0	0
3	w	549	0	540	0	0
3	x	549	0	540	0	0
4	y	317	0	341	0	0
4	z	317	0	341	0	0
5	Z	649	0	649	45	0
5	a	649	0	649	0	0
5	d	649	0	649	0	0
5	e	649	0	649	0	0
5	u	528	0	510	0	0
6	f	2474	0	2459	0	0
6	h	2604	0	2577	0	0
7	k	2338	0	2364	0	0
7	m	2338	0	2364	0	0
7	p	2338	0	2364	0	0
7	r	2338	0	2364	0	0
All	All	74272	0	73453	1530	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 15.

All (1530) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:258:GLU:CG	1:O:262:LYS:CD	1.74	1.55
1:O:258:GLU:HG2	1:O:262:LYS:CD	1.28	1.53
1:N:483:ARG:NH1	1:N:485:GLU:HG2	1.25	1.40
1:O:258:GLU:CG	1:O:262:LYS:HD2	0.91	1.39
5:Z:68:PRO:HB3	5:Z:71:GLN:NE2	1.29	1.38
1:O:258:GLU:CB	1:O:262:LYS:HD2	1.63	1.29
1:N:672:ASN:ND2	1:O:871:ILE:O	1.67	1.28
1:N:484:ARG:HB3	1:N:551:GLY:O	1.36	1.22
5:Z:68:PRO:CB	5:Z:71:GLN:NE2	2.03	1.21
1:N:484:ARG:NH2	1:N:558:ALA:HA	1.58	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:483:ARG:HH11	1:N:485:GLU:CG	1.59	1.15
1:J:69:LEU:HD13	1:J:308:TYR:CD2	1.84	1.11
1:N:483:ARG:NH1	1:N:485:GLU:CG	2.13	1.10
1:O:258:GLU:HG2	1:O:262:LYS:HD3	1.31	1.09
1:N:480:PRO:O	1:N:481:ARG:HG2	1.50	1.08
1:N:484:ARG:HH21	1:N:558:ALA:HA	0.94	1.06
1:N:484:ARG:CB	1:N:551:GLY:O	2.06	1.04
1:N:484:ARG:HD2	1:N:550:ILE:CG2	1.86	1.03
1:N:484:ARG:HH21	1:N:558:ALA:CA	1.71	1.03
1:J:365:VAL:O	1:J:366:PRO:O	1.77	1.02
1:N:484:ARG:NH2	1:N:558:ALA:CA	2.23	1.01
1:O:258:GLU:HG3	1:O:262:LYS:HD2	1.10	1.00
1:O:258:GLU:HG3	1:O:262:LYS:CD	1.62	0.98
1:K:464:LEU:HD11	1:K:1254:MET:CG	1.94	0.98
1:N:670:LEU:O	1:N:674:ALA:HB3	1.64	0.97
5:Z:68:PRO:HB3	5:Z:71:GLN:HE22	1.17	0.96
1:N:480:PRO:O	1:N:481:ARG:NE	1.99	0.95
1:O:258:GLU:O	1:O:259:SER:O	1.85	0.94
1:N:483:ARG:HH12	1:N:485:GLU:HG2	1.23	0.94
1:J:69:LEU:HD13	1:J:308:TYR:CE2	2.02	0.92
1:N:484:ARG:NH2	1:N:558:ALA:CB	2.33	0.92
1:N:677:LYS:O	1:N:679:ALA:N	2.03	0.90
1:J:308:TYR:HB3	1:J:312:VAL:HG23	1.52	0.90
1:O:258:GLU:HG3	1:O:262:LYS:HZ2	1.34	0.89
1:N:480:PRO:O	1:N:481:ARG:CG	2.20	0.89
1:J:308:TYR:O	1:J:312:VAL:N	2.06	0.88
1:J:1205:ARG:NH2	1:J:1223:LEU:O	2.07	0.88
1:N:677:LYS:O	1:N:680:TYR:N	2.07	0.88
1:K:271:LYS:HD3	1:K:299:ASP:HB2	1.54	0.87
1:O:258:GLU:O	1:O:262:LYS:HB3	1.73	0.87
1:K:465:HIS:CE1	1:K:1027:PRO:HD3	2.10	0.86
1:N:565:ARG:HA	1:N:998:ARG:HH12	1.40	0.86
1:K:464:LEU:HD11	1:K:1254:MET:SD	2.16	0.86
1:K:861:GLU:OE2	5:Z:67:VAL:HG11	1.74	0.86
1:N:644:ILE:HG22	1:N:675:ILE:HG21	1.57	0.85
1:O:488:SER:HB2	1:O:992:GLU:H	1.43	0.84
1:N:59:TYR:CD1	1:O:260:VAL:HG21	2.11	0.84
1:O:258:GLU:HG3	1:O:262:LYS:NZ	1.94	0.82
1:O:258:GLU:HG3	1:O:262:LYS:CE	2.08	0.82
1:N:677:LYS:HG2	1:N:678:GLU:N	1.95	0.82
1:K:804:HIS:O	1:K:805:ALA:HB2	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:861:GLU:CB	5:Z:69:ARG:HD2	2.09	0.82
1:J:463:ARG:NH2	1:J:1253:ILE:O	2.13	0.81
1:N:484:ARG:HD2	1:N:550:ILE:HG22	1.61	0.81
1:J:301:GLN:HB3	1:J:366:PRO:HB2	1.61	0.81
1:O:303:MET:SD	1:O:364:ARG:NH2	2.53	0.81
1:O:258:GLU:O	1:O:262:LYS:CB	2.29	0.81
1:K:185:LEU:HD13	1:K:399:ARG:HH21	1.47	0.80
1:K:399:ARG:NH1	1:K:1320:PHE:O	2.14	0.80
1:N:974:ASN:HD21	1:N:976:GLN:HE21	1.27	0.80
1:N:670:LEU:O	1:N:674:ALA:CB	2.30	0.80
1:O:245:ARG:NH2	1:O:294:LEU:O	2.13	0.80
1:J:848:HIS:HE2	5:Z:21:SER:HG	1.24	0.80
1:P:776:PHE:O	1:P:780:TYR:CB	2.29	0.80
1:O:591:ALA:HB1	1:O:1036:LEU:HD12	1.62	0.79
1:N:740:SER:HB2	1:N:744:PRO:HG3	1.64	0.79
1:O:1372:ILE:HG23	1:O:1381:PHE:HB3	1.62	0.79
1:N:483:ARG:HH11	1:N:485:GLU:HG2	0.99	0.79
1:N:672:ASN:OD1	1:O:873:ASP:HB2	1.82	0.79
1:P:205:ARG:HH21	1:P:209:LYS:HG2	1.47	0.79
1:K:544:PRO:O	1:K:565:ARG:NH1	2.15	0.79
1:O:258:GLU:CG	1:O:262:LYS:HD3	1.93	0.79
1:K:861:GLU:HB2	5:Z:69:ARG:HD2	1.63	0.79
1:K:861:GLU:HG3	5:Z:69:ARG:HD2	1.65	0.79
1:N:484:ARG:HD2	1:N:550:ILE:HG21	1.65	0.79
1:K:184:LYS:NZ	1:K:1064:SER:OG	2.14	0.78
1:K:804:HIS:O	1:K:805:ALA:CB	2.29	0.78
1:P:776:PHE:O	1:P:780:TYR:HB3	1.83	0.78
1:K:997:HIS:HE1	1:K:1022:HIS:HE1	1.32	0.78
1:N:56:LEU:HA	1:O:329:ARG:HB2	1.64	0.78
1:O:690:LEU:HD21	1:O:812:PHE:HB2	1.65	0.78
1:J:69:LEU:HD13	1:J:308:TYR:CG	2.18	0.78
1:N:442:ASN:OD1	1:N:443:LYS:N	2.16	0.78
1:J:955:GLY:HA3	1:J:985:ARG:HE	1.47	0.78
1:K:861:GLU:CG	5:Z:69:ARG:HD2	2.14	0.78
1:N:737:LEU:HD23	1:N:744:PRO:HG2	1.64	0.78
5:Z:68:PRO:O	5:Z:70:ARG:N	2.17	0.78
1:N:844:PRO:HG2	1:N:856:ILE:HG23	1.67	0.77
1:J:195:GLN:NE2	1:J:250:GLU:OE2	2.17	0.77
1:O:185:LEU:HD13	1:O:399:ARG:HH21	1.50	0.77
1:N:484:ARG:CD	1:N:550:ILE:CG2	2.62	0.77
1:O:258:GLU:HG2	1:O:262:LYS:CG	2.14	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:769:MET:HG2	1:J:890:THR:HG21	1.67	0.77
1:N:391:THR:HG21	1:O:102:ILE:HG13	1.65	0.77
1:N:722:ASN:HB3	1:N:902:VAL:HG11	1.67	0.77
1:N:842:ASN:HD21	1:N:860:LEU:HD21	1.50	0.77
1:N:856:ILE:HG22	1:N:860:LEU:HG	1.67	0.76
1:P:491:HIS:O	1:P:899:ARG:NH2	2.17	0.76
1:N:674:ALA:O	1:N:675:ILE:HG12	1.86	0.76
1:O:436:VAL:HG11	1:O:587:GLN:HE22	1.50	0.76
1:O:1117:MET:SD	1:O:1371:ARG:NH1	2.59	0.76
1:N:924:LEU:HB2	1:N:950:PHE:HZ	1.51	0.76
1:J:166:GLN:HG2	1:J:322:VAL:HG13	1.66	0.76
1:O:1252:ASP:OD1	1:O:1256:ASN:ND2	2.19	0.76
1:P:1283:ASN:ND2	1:P:1326:SER:OG	2.19	0.75
1:J:481:ARG:HD2	1:J:539:ARG:HD2	1.68	0.75
1:J:670:LEU:HD11	1:J:675:ILE:HG13	1.67	0.75
1:N:860:LEU:O	1:N:866:ARG:NH1	2.20	0.75
1:O:764:GLU:HB2	1:O:795:HIS:HA	1.66	0.74
1:N:480:PRO:C	1:N:481:ARG:HG2	2.08	0.74
1:O:78:VAL:HG21	1:O:261:LEU:HD13	1.70	0.74
1:J:565:ARG:O	1:J:570:ASN:ND2	2.20	0.73
1:N:674:ALA:C	1:N:675:ILE:HG12	2.08	0.73
1:N:484:ARG:CD	1:N:550:ILE:HG21	2.18	0.73
1:J:498:ASN:ND2	5:Z:1:MET:O	2.20	0.73
1:N:493:ARG:HH12	1:N:747:ILE:HG12	1.54	0.73
1:P:594:LEU:HD13	1:P:696:ALA:HB2	1.70	0.73
1:P:655:ALA:O	1:P:683:TYR:OH	2.08	0.72
1:P:1378:LYS:HG2	1:P:1379:VAL:HG23	1.70	0.72
1:J:626:ILE:HG22	1:J:628:GLY:H	1.54	0.72
1:K:329:ARG:HG2	1:K:330:THR:HG23	1.72	0.72
1:K:737:LEU:HD23	1:K:744:PRO:HG2	1.70	0.72
1:K:483:ARG:NH2	1:K:536:ASP:OD2	2.23	0.72
1:J:452:LEU:HD11	1:J:1040:PRO:HD3	1.70	0.72
1:J:140:ILE:HD11	1:J:157:ALA:HB2	1.71	0.72
1:K:1068:PHE:HB2	1:K:1093:ALA:HB3	1.72	0.72
1:O:258:GLU:HG2	1:O:262:LYS:HD2	0.92	0.72
1:K:609:THR:HG22	1:K:653:ARG:HB3	1.72	0.71
5:Z:68:PRO:CB	5:Z:71:GLN:HE21	1.98	0.71
1:P:727:VAL:HG22	1:P:924:LEU:HB2	1.72	0.71
1:N:743:ALA:O	1:N:918:ARG:NH2	2.23	0.71
1:O:612:ASP:OD2	1:O:647:TYR:OH	2.08	0.71
1:O:1299:GLY:O	1:O:1323:GLN:NE2	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:941:THR:HA	1:P:944:LEU:O	1.89	0.71
1:N:484:ARG:NH2	1:N:558:ALA:HB2	2.06	0.71
1:N:658:ASN:ND2	1:N:929:VAL:O	2.23	0.71
1:O:947:ALA:HB2	1:O:963:MET:HB2	1.71	0.70
1:J:478:PRO:O	1:J:557:ARG:NH2	2.24	0.70
1:O:401:MET:SD	1:O:403:TYR:OH	2.48	0.70
1:J:1187:THR:OG1	1:J:1241:ASN:ND2	2.24	0.70
1:P:499:VAL:H	1:P:894:PHE:HE2	1.39	0.70
1:K:535:TYR:HE2	1:K:539:ARG:HH21	1.37	0.70
1:J:213:SER:OG	1:O:1174:LEU:O	2.08	0.70
1:J:611:TYR:OH	1:J:822:ASN:ND2	2.25	0.70
1:J:722:ASN:ND2	1:J:740:SER:OG	2.23	0.70
1:K:464:LEU:HD21	1:K:1254:MET:SD	2.32	0.70
1:J:146:GLU:OE1	1:J:146:GLU:N	2.25	0.70
1:P:609:THR:HG22	1:P:653:ARG:HB2	1.72	0.70
1:N:495:ASN:OD1	1:N:496:HIS:N	2.25	0.69
1:N:832:PHE:HE2	1:N:892:PRO:HG2	1.56	0.69
1:N:625:MET:SD	1:N:887:SER:OG	2.51	0.69
1:O:133:LEU:HB3	1:O:138:LEU:HD21	1.74	0.69
1:J:226:HIS:HB3	1:J:247:ARG:HH22	1.57	0.69
1:K:464:LEU:HD11	1:K:1254:MET:HG3	1.75	0.69
1:O:731:ASP:OD2	1:O:765:ARG:NH1	2.25	0.69
1:P:492:ARG:HD3	1:P:987:GLU:HB3	1.72	0.69
1:K:172:LEU:HD11	1:K:1090:HIS:HB2	1.73	0.69
1:N:544:PRO:O	1:N:565:ARG:NH1	2.25	0.69
1:O:80:THR:HG22	1:O:309:ALA:HB3	1.75	0.69
1:N:905:ASP:OD1	1:N:905:ASP:N	2.25	0.69
1:J:1061:SER:HG	1:J:1064:SER:HG	1.41	0.69
1:N:938:ARG:HH22	1:N:965:GLN:HE21	1.39	0.69
1:P:465:HIS:O	1:P:546:TYR:OH	2.07	0.69
5:Z:68:PRO:O	5:Z:71:GLN:N	2.25	0.69
1:K:1255:TYR:HB2	1:K:1275:PHE:HD2	1.57	0.69
1:O:877:THR:OG1	1:O:880:MET:SD	2.50	0.69
1:J:302:ILE:HB	1:J:367:ILE:HG21	1.76	0.68
1:N:622:VAL:HG21	1:N:639:LEU:HD21	1.75	0.68
1:O:1128:PHE:HZ	1:O:1260:ARG:HD2	1.57	0.68
1:O:1285:ARG:NH2	1:O:1293:GLU:OE1	2.27	0.68
1:K:828:LEU:HD11	1:K:945:PHE:HB3	1.74	0.68
1:O:399:ARG:HD3	1:O:1320:PHE:HB3	1.75	0.68
1:K:585:GLY:HA3	1:K:1017:GLY:HA2	1.74	0.68
1:P:534:ASN:HD21	1:P:537:LEU:HD22	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:1187:THR:OG1	1:P:1241:ASN:ND2	2.26	0.68
1:K:860:LEU:O	1:K:866:ARG:NH1	2.27	0.68
1:N:312:VAL:HG12	1:N:314:ARG:H	1.59	0.68
1:P:729:TYR:OH	1:P:927:GLY:O	2.09	0.68
1:J:834:HIS:HD2	5:Z:8:PRO:HD3	1.60	0.67
1:N:281:ILE:HD12	1:N:1058:LEU:HD23	1.77	0.67
1:N:1204:GLY:HA3	1:N:1239:THR:HG23	1.76	0.67
1:O:450:PHE:HD2	1:O:1119:ILE:HD12	1.59	0.67
1:K:1297:ARG:NH2	1:K:1298:LEU:O	2.27	0.67
1:N:172:LEU:HD11	1:N:1090:HIS:HB2	1.75	0.67
1:O:317:ASN:HB3	1:O:327:VAL:HG13	1.75	0.67
5:Z:67:VAL:O	5:Z:69:ARG:N	2.26	0.67
1:P:903:ASP:OD2	1:P:909:GLN:NE2	2.27	0.67
1:J:402:GLN:HG2	1:J:1051:GLU:HG2	1.77	0.67
1:O:475:ASN:HB3	1:O:560:HIS:HD2	1.58	0.67
1:K:1246:GLN:HB2	1:K:1249:SER:HB3	1.76	0.67
1:O:1293:GLU:OE2	1:O:1297:ARG:NH1	2.27	0.67
1:P:764:GLU:HG2	1:P:795:HIS:HA	1.77	0.66
1:N:650:ARG:CZ	1:N:873:ASP:OD2	2.43	0.66
1:N:336:ALA:HA	1:N:340:ASP:HB2	1.76	0.66
1:O:1226:ASP:OD1	1:O:1228:SER:N	2.21	0.66
1:P:484:ARG:HG3	1:P:552:ARG:HG2	1.75	0.66
1:P:944:LEU:HD22	1:P:945:PHE:H	1.58	0.66
1:J:1124:PHE:HA	1:J:1127:VAL:HG12	1.77	0.66
1:K:484:ARG:HG2	1:K:552:ARG:HA	1.76	0.66
1:N:924:LEU:HB2	1:N:950:PHE:CZ	2.30	0.66
1:N:899:ARG:NE	1:N:920:GLU:OE2	2.28	0.66
1:O:644:ILE:HG21	1:O:675:ILE:HD11	1.78	0.66
1:P:742:ARG:NH1	1:P:903:ASP:O	2.22	0.66
1:N:543:HIS:HD2	1:N:546:TYR:H	1.43	0.66
1:O:630:GLU:OE2	1:O:669:HIS:NE2	2.28	0.66
1:J:899:ARG:NH2	1:J:920:GLU:OE1	2.26	0.66
1:P:536:ASP:OD1	1:P:539:ARG:NH2	2.28	0.66
1:P:899:ARG:NH2	1:P:988:GLN:O	2.29	0.66
1:J:1374:LYS:HG2	1:J:1379:VAL:HG22	1.78	0.66
1:N:407:PHE:CZ	1:N:440:ILE:HD11	2.31	0.66
1:N:706:VAL:HG23	1:N:711:VAL:HG12	1.78	0.66
1:O:442:ASN:OD1	1:O:443:LYS:N	2.29	0.66
1:O:899:ARG:HH12	1:O:990:PHE:HA	1.61	0.65
1:N:483:ARG:O	1:N:485:GLU:N	2.29	0.65
1:J:7:VAL:HG11	1:J:38:ASP:HB2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:184:LYS:NZ	1:N:1064:SER:OG	2.28	0.65
1:O:258:GLU:HA	1:O:262:LYS:CE	2.26	0.65
1:K:743:ALA:HB3	1:K:918:ARG:HH12	1.61	0.65
1:J:853:ASP:OD1	1:J:853:ASP:N	2.27	0.65
1:O:1215:TYR:HE1	1:O:1285:ARG:HG2	1.61	0.65
1:J:266:THR:HG21	1:J:1062:ARG:HE	1.61	0.65
1:J:1272:ARG:NH2	1:J:1279:GLU:OE2	2.29	0.65
1:K:297:GLU:O	1:K:298:ALA:HB2	1.96	0.65
1:O:388:TYR:CE2	1:O:396:PRO:HD3	2.32	0.65
1:O:1203:ARG:HG2	1:O:1275:PHE:HE1	1.61	0.65
1:K:825:MET:N	1:K:956:ASP:OD2	2.29	0.65
1:N:456:LEU:HD23	1:N:1146:VAL:HG23	1.78	0.65
1:N:675:ILE:HD13	1:N:675:ILE:N	2.12	0.65
1:J:267:TYR:HA	1:J:305:PRO:HD3	1.79	0.65
1:K:452:LEU:HD23	1:K:1034:ALA:HB2	1.78	0.65
1:P:639:LEU:HD13	1:P:880:MET:HB2	1.77	0.65
1:J:658:ASN:ND2	1:J:929:VAL:O	2.26	0.65
1:J:1242:PRO:O	1:J:1246:GLN:NE2	2.30	0.65
1:K:861:GLU:HB2	5:Z:69:ARG:CD	2.26	0.65
1:P:1192:ASP:OD2	1:P:1237:ARG:NH2	2.30	0.65
1:J:129:THR:HG23	1:K:103:ALA:HB2	1.79	0.64
1:P:1357:HIS:ND1	1:P:1357:HIS:O	2.30	0.64
1:J:302:ILE:O	1:J:367:ILE:HB	1.98	0.64
1:J:958:ARG:HH11	1:O:695:GLN:HG3	1.62	0.64
1:O:951:HIS:O	1:O:955:GLY:N	2.30	0.64
1:P:587:GLN:NE2	1:P:1037:LYS:O	2.29	0.64
1:P:776:PHE:O	1:P:780:TYR:HB2	1.96	0.64
1:K:1188:PRO:HD2	1:K:1241:ASN:HB2	1.79	0.64
1:J:1264:VAL:HG12	1:J:1266:GLY:H	1.62	0.64
1:N:677:LYS:O	1:N:678:GLU:C	2.36	0.64
1:P:1203:ARG:NH1	1:P:1205:ARG:O	2.31	0.64
1:K:664:LYS:NZ	1:K:802:GLU:OE1	2.30	0.64
1:O:68:PHE:HD1	1:O:177:ILE:HG12	1.61	0.64
1:K:400:ARG:NH2	1:K:1051:GLU:OE2	2.30	0.64
1:N:1068:PHE:HB2	1:N:1093:ALA:HB3	1.79	0.64
1:O:938:ARG:NH2	1:O:962:THR:O	2.30	0.64
1:K:1353:HIS:NE2	1:K:1364:GLU:OE2	2.31	0.64
1:N:451:ASN:ND2	1:O:527:GLU:OE2	2.31	0.64
1:P:150:GLU:OE1	1:P:150:GLU:N	2.31	0.64
1:K:298:ALA:HB2	1:K:371:VAL:O	1.98	0.64
1:N:1195:TYR:O	1:N:1200:ASN:ND2	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:804:HIS:O	1:K:978:ARG:NH1	2.28	0.64
1:K:1203:ARG:HG2	1:K:1275:PHE:HE1	1.63	0.64
1:J:908:GLN:NE2	1:J:1026:SER:OG	2.30	0.63
1:K:1008:CYS:SG	1:K:1014:SER:HB3	2.37	0.63
1:P:585:GLY:HA3	1:P:1017:GLY:HA2	1.80	0.63
1:K:1051:GLU:N	1:K:1115:THR:OG1	2.31	0.63
1:K:128:SER:HA	1:K:1088:VAL:O	1.97	0.63
1:K:951:HIS:HD2	1:K:953:PHE:H	1.47	0.63
1:N:70:GLU:HA	1:N:367:ILE:HD12	1.79	0.63
1:P:958:ARG:NH1	1:P:978:ARG:O	2.31	0.63
1:J:402:GLN:HG3	1:J:1321:LEU:HD11	1.79	0.63
1:J:561:ARG:NH2	1:J:916:ASP:OD1	2.31	0.63
1:O:705:VAL:HG12	1:O:710:SER:HA	1.80	0.63
1:J:365:VAL:C	1:J:366:PRO:O	2.37	0.63
1:K:482:ASP:N	1:K:482:ASP:OD1	2.31	0.63
1:N:481:ARG:HB2	1:N:484:ARG:HD3	1.80	0.63
1:P:147:THR:OG1	1:P:150:GLU:OE1	2.16	0.63
1:O:539:ARG:HG2	1:O:540:LEU:HD22	1.79	0.62
1:P:1283:ASN:HD21	1:P:1326:SER:HG	1.46	0.62
1:K:491:HIS:CD2	1:K:899:ARG:HD2	2.34	0.62
1:O:1101:TYR:OH	1:O:1292:ASN:OD1	2.12	0.62
1:K:1204:GLY:HA3	1:K:1239:THR:HG23	1.81	0.62
1:J:938:ARG:HA	1:J:941:THR:HG22	1.80	0.62
1:P:1122:GLN:NE2	1:P:1268:TYR:O	2.32	0.62
1:O:531:HIS:HD2	1:O:533:SER:H	1.47	0.62
1:O:535:TYR:HE1	1:O:1227:HIS:HB2	1.64	0.62
1:K:465:HIS:NE2	1:K:1027:PRO:HD3	2.14	0.62
1:N:609:THR:HG22	1:N:653:ARG:HB3	1.82	0.62
1:K:950:PHE:CD1	1:K:951:HIS:HB2	2.34	0.62
1:O:258:GLU:HA	1:O:262:LYS:HE3	1.82	0.62
1:J:170:ASP:OD1	1:J:174:ARG:NE	2.33	0.62
1:O:495:ASN:OD1	1:O:496:HIS:N	2.33	0.62
1:K:428:ASP:OD1	1:K:429:ASN:N	2.32	0.61
1:O:565:ARG:NH1	1:O:572:PRO:HD3	2.15	0.61
1:N:1255:TYR:HB2	1:N:1275:PHE:HD2	1.64	0.61
1:P:546:TYR:O	1:P:565:ARG:NH2	2.33	0.61
1:N:704:ASP:OD1	1:N:704:ASP:N	2.33	0.61
1:N:1043:ALA:HB3	1:N:1187:THR:O	2.00	0.61
1:O:39:LEU:HD11	1:O:149:VAL:HG21	1.80	0.61
1:O:388:TYR:HE2	1:O:396:PRO:HD3	1.65	0.61
1:P:1335:LEU:HD12	1:P:1373:LEU:HD13	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:92:LYS:HB2	1:J:1095:ILE:HD11	1.83	0.61
1:J:547:ASP:HB2	1:J:565:ARG:HE	1.66	0.61
1:K:451:ASN:OD1	1:K:451:ASN:N	2.29	0.61
1:K:1057:ILE:O	1:K:1105:MET:HA	2.00	0.61
1:N:1231:ASP:N	1:N:1231:ASP:OD1	2.33	0.61
1:J:1142:ILE:O	1:J:1146:VAL:HG12	1.99	0.61
1:K:73:LEU:HD13	1:K:177:ILE:HD11	1.82	0.61
1:K:311:PHE:HE2	1:K:329:ARG:HG3	1.64	0.61
1:J:132:GLU:HG3	1:K:112:LYS:HD3	1.82	0.61
1:J:308:TYR:HB3	1:J:312:VAL:CG2	2.29	0.61
1:O:1122:GLN:HE21	1:O:1127:VAL:HG21	1.65	0.61
1:N:480:PRO:O	1:N:481:ARG:CD	2.48	0.61
1:O:68:PHE:O	1:O:71:THR:OG1	2.19	0.61
1:J:308:TYR:O	1:J:312:VAL:HG23	2.01	0.60
1:J:501:VAL:HG21	5:Z:1:MET:HB3	1.82	0.60
1:N:684:ARG:HH22	1:O:612:ASP:HA	1.66	0.60
1:N:947:ALA:HB2	1:N:963:MET:HB2	1.83	0.60
1:N:484:ARG:HB2	1:N:551:GLY:O	2.01	0.60
1:P:611:TYR:OH	1:P:822:ASN:ND2	2.29	0.60
1:P:1213:GLU:N	1:P:1213:GLU:OE1	2.34	0.60
1:J:92:LYS:HG2	1:J:93:ILE:N	2.16	0.60
1:J:481:ARG:CD	1:J:481:ARG:H	2.12	0.60
1:K:566:LEU:HD21	1:K:904:ASN:ND2	2.16	0.60
1:O:39:LEU:HB2	1:O:52:PHE:HB2	1.82	0.60
1:O:443:LYS:NZ	1:O:1176:HIS:O	2.23	0.60
1:P:1283:ASN:ND2	1:P:1326:SER:O	2.34	0.60
1:P:1334:ALA:HA	1:P:1365:GLU:HG3	1.82	0.60
1:J:1259:TYR:HE2	1:J:1262:THR:HB	1.65	0.60
1:J:1323:GLN:OE1	1:J:1323:GLN:N	2.34	0.60
1:O:480:PRO:O	1:O:539:ARG:NH1	2.34	0.60
1:N:405:TYR:HD2	1:N:1334:ALA:HB2	1.66	0.60
1:O:268:THR:OG1	1:O:364:ARG:NH1	2.35	0.60
1:J:814:TYR:OH	1:J:921:GLN:NE2	2.34	0.59
1:J:830:VAL:H	1:J:895:THR:HG21	1.67	0.59
1:N:828:LEU:HD21	1:N:945:PHE:CG	2.37	0.59
1:N:1023:ILE:HG21	1:N:1033:GLN:HE21	1.67	0.59
1:P:680:TYR:OH	1:P:684:ARG:NH2	2.33	0.59
1:N:513:ALA:HB1	1:N:984:ASN:HD22	1.67	0.59
1:N:746:ILE:HB	1:N:753:TYR:HB3	1.83	0.59
1:K:248:LEU:HB3	1:K:374:LEU:HD21	1.84	0.59
1:K:746:ILE:HB	1:K:753:TYR:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:288:ARG:NH2	1:O:250:GLU:OE2	2.31	0.59
1:J:310:SER:O	1:J:311:PHE:HD1	1.85	0.59
1:J:1216:ASN:O	1:J:1284:ASN:ND2	2.35	0.59
1:K:596:HIS:NE2	1:K:1012:LEU:HB3	2.18	0.59
1:O:70:GLU:HA	1:O:367:ILE:HD12	1.83	0.59
1:J:544:PRO:HG3	1:J:1243:TRP:CD2	2.37	0.59
1:K:845:ALA:O	1:K:882:ARG:NE	2.34	0.59
1:K:1285:ARG:NH2	1:K:1293:GLU:OE1	2.35	0.59
1:J:824:HIS:ND1	1:J:956:ASP:OD1	2.31	0.59
1:K:861:GLU:HG3	5:Z:69:ARG:CD	2.32	0.59
1:K:1195:TYR:O	1:K:1200:ASN:ND2	2.30	0.59
1:P:807:VAL:O	1:P:810:LYS:N	2.36	0.59
1:K:546:TYR:HA	1:K:564:HIS:HA	1.85	0.59
1:N:847:SER:HB2	1:N:850:PHE:HD2	1.68	0.59
1:O:184:LYS:HZ3	1:O:1064:SER:HB2	1.68	0.59
1:K:630:GLU:OE2	1:K:668:ARG:NH2	2.36	0.59
1:N:804:HIS:CD2	1:N:808:LEU:HG	2.38	0.59
1:O:720:ASP:O	1:O:810:LYS:NZ	2.36	0.59
1:P:1080:ARG:HD2	1:P:1083:ALA:HB3	1.84	0.59
1:J:489:LEU:O	1:J:994:ARG:NH2	2.36	0.59
1:P:491:HIS:HB2	1:P:899:ARG:NH1	2.18	0.58
1:J:266:THR:O	1:J:305:PRO:HG3	2.03	0.58
1:J:301:GLN:HB3	1:J:366:PRO:CB	2.33	0.58
1:O:864:THR:O	1:O:868:LEU:HB2	2.03	0.58
1:P:718:LEU:HD13	1:P:811:ILE:HG12	1.83	0.58
1:J:1302:PRO:HB2	1:J:1321:LEU:HD23	1.84	0.58
1:K:1050:ASP:HA	1:K:1115:THR:HG21	1.85	0.58
1:N:1128:PHE:HZ	1:N:1260:ARG:HG3	1.68	0.58
1:J:748:ILE:HD12	1:J:762:PHE:HD2	1.69	0.58
1:N:484:ARG:CD	1:N:550:ILE:HG22	2.29	0.58
1:N:720:ASP:O	1:N:810:LYS:NZ	2.36	0.58
1:J:909:GLN:NE2	1:J:917:LYS:HD3	2.17	0.58
1:K:611:TYR:OH	1:K:822:ASN:ND2	2.36	0.58
1:K:644:ILE:HG21	1:K:675:ILE:HD11	1.85	0.58
1:K:793:ARG:O	1:K:896:ARG:NH2	2.36	0.58
1:O:1039:HIS:ND1	1:O:1040:PRO:O	2.30	0.58
1:J:904:ASN:HB2	1:J:917:LYS:O	2.04	0.58
1:K:1077:ARG:O	1:K:1085:THR:OG1	2.15	0.58
1:N:674:ALA:C	1:N:675:ILE:CG1	2.72	0.58
1:K:619:PHE:CE1	1:K:643:CYS:HB3	2.38	0.58
1:K:950:PHE:HD1	1:K:951:HIS:HB2	1.66	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:402:GLN:HA	1:N:1050:ASP:O	2.04	0.58
1:O:417:LYS:NZ	1:O:431:THR:O	2.37	0.58
1:O:736:LEU:O	1:O:740:SER:OG	2.14	0.58
1:J:209:LYS:HB3	1:O:1174:LEU:HD11	1.85	0.57
1:P:170:ASP:O	1:P:174:ARG:HG2	2.04	0.57
1:K:4:ASN:ND2	1:K:38:ASP:HB2	2.18	0.57
1:K:40:LEU:HB3	1:K:44:ASP:HB3	1.85	0.57
1:K:282:VAL:HG12	1:K:1057:ILE:HG12	1.86	0.57
1:K:905:ASP:N	1:K:905:ASP:OD1	2.37	0.57
1:N:591:ALA:HB1	1:N:1036:LEU:HD12	1.86	0.57
1:O:258:GLU:O	1:O:259:SER:C	2.42	0.57
1:J:1169:ASN:OD1	1:J:1170:GLY:N	2.37	0.57
1:K:828:LEU:HB3	1:K:928:LEU:O	2.04	0.57
1:O:828:LEU:HD11	1:O:945:PHE:HB3	1.85	0.57
1:J:170:ASP:O	1:J:174:ARG:HG2	2.03	0.57
1:N:1117:MET:SD	1:N:1371:ARG:NH2	2.77	0.57
1:O:258:GLU:CA	1:O:262:LYS:HD2	2.32	0.57
1:O:561:ARG:NH2	1:O:916:ASP:OD1	2.36	0.57
1:J:501:VAL:HB	5:Z:1:MET:HE3	1.87	0.57
1:O:977:GLN:NE2	1:O:982:ALA:O	2.38	0.57
1:P:475:ASN:OD1	1:P:560:HIS:N	2.35	0.57
1:J:310:SER:O	1:J:311:PHE:CD1	2.57	0.57
1:J:1183:GLU:OE2	1:J:1269:SER:OG	2.17	0.57
1:K:947:ALA:HB2	1:K:963:MET:HB2	1.87	0.57
1:O:170:ASP:O	1:O:174:ARG:HG2	2.04	0.57
1:O:565:ARG:HH12	1:O:572:PRO:HD3	1.68	0.57
1:J:731:ASP:HB3	1:J:799:TYR:HB2	1.87	0.57
1:J:1372:ILE:HG12	1:J:1381:PHE:HD2	1.69	0.57
1:J:742:ARG:HB3	1:J:903:ASP:HB2	1.86	0.57
1:K:140:ILE:HD11	1:K:157:ALA:HB2	1.86	0.57
1:N:832:PHE:CE2	1:N:892:PRO:HG2	2.38	0.57
1:O:43:LYS:HA	1:P:314:ARG:HH22	1.70	0.57
1:N:282:VAL:HG12	1:N:1057:ILE:HG12	1.86	0.57
1:O:881:ILE:O	1:O:885:SER:OG	2.23	0.57
1:O:952:MET:HE1	1:O:981:GLU:HA	1.85	0.57
1:N:758:ALA:HB1	1:N:761:GLN:HG2	1.86	0.56
1:N:1174:LEU:O	1:O:213:SER:OG	2.15	0.56
1:J:844:PRO:HG2	1:J:860:LEU:HD23	1.87	0.56
1:J:1135:ASN:HB3	1:J:1138:VAL:HG12	1.87	0.56
1:K:285:ASN:O	1:K:289:GLN:NE2	2.38	0.56
1:N:736:LEU:O	1:N:740:SER:OG	2.17	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:68:PHE:N	1:P:173:GLU:OE1	2.37	0.56
1:J:185:LEU:HD13	1:J:399:ARG:HH21	1.70	0.56
1:J:310:SER:C	1:J:311:PHE:CD1	2.79	0.56
1:J:655:ALA:O	1:J:683:TYR:OH	2.16	0.56
1:J:1072:PRO:HB3	1:J:1090:HIS:HD2	1.69	0.56
1:N:969:THR:O	1:N:973:ARG:HG2	2.06	0.56
1:O:856:ILE:HD11	1:O:878:VAL:HA	1.87	0.56
1:P:861:GLU:OE1	1:P:861:GLU:N	2.38	0.56
1:P:899:ARG:HG2	1:P:922:THR:HG22	1.86	0.56
1:P:913:ASN:HD21	1:P:915:ALA:HB3	1.70	0.56
1:J:302:ILE:HB	1:J:367:ILE:CG2	2.36	0.56
1:K:626:ILE:HG22	1:K:628:GLY:H	1.69	0.56
1:N:485:GLU:OE2	1:N:993:TYR:OH	2.23	0.56
1:N:997:HIS:HE1	1:N:1022:HIS:NE2	2.04	0.56
1:O:1231:ASP:OD1	1:O:1231:ASP:N	2.39	0.56
1:N:145:PRO:HG3	1:N:151:TYR:HD1	1.70	0.56
1:N:535:TYR:CE1	1:N:1227:HIS:HB2	2.41	0.56
1:N:596:HIS:CD2	1:N:1012:LEU:HB2	2.40	0.56
1:O:73:LEU:HD12	1:O:281:ILE:HD11	1.88	0.56
1:P:434:LEU:HD12	1:P:435:PRO:HD2	1.87	0.56
1:J:922:THR:HG21	1:J:989:LEU:O	2.06	0.56
1:N:461:HIS:CD2	1:N:1124:PHE:HB3	2.40	0.56
1:O:947:ALA:HB3	1:O:964:HIS:CE1	2.41	0.56
1:O:1252:ASP:O	1:O:1256:ASN:HB2	2.06	0.56
1:P:869:LEU:HD13	1:P:876:PRO:HG2	1.88	0.56
1:P:1027:PRO:HG2	1:P:1133:PHE:HZ	1.69	0.56
1:N:620:TYR:HE1	1:N:828:LEU:HD22	1.71	0.56
1:P:856:ILE:HD11	1:P:878:VAL:HA	1.88	0.56
1:J:226:HIS:HB3	1:J:247:ARG:NH2	2.21	0.56
1:J:652:GLY:H	1:O:677:LYS:NZ	2.04	0.56
1:K:612:ASP:OD2	1:K:647:TYR:OH	2.22	0.56
1:N:483:ARG:NH1	1:N:485:GLU:CB	2.68	0.56
1:N:543:HIS:CD2	1:N:545:LEU:H	2.23	0.56
1:N:607:GLN:HE21	1:N:611:TYR:HE2	1.53	0.56
1:O:280:PHE:HB2	1:O:381:VAL:HG22	1.87	0.56
1:K:1255:TYR:HB2	1:K:1275:PHE:CD2	2.41	0.56
1:O:1226:ASP:OD1	1:O:1227:HIS:N	2.38	0.56
1:P:612:ASP:OD2	1:P:653:ARG:NH1	2.39	0.56
1:P:667:CYS:O	1:P:684:ARG:NH2	2.28	0.56
1:J:61:ASN:HD21	1:J:63:ILE:HG12	1.71	0.56
1:J:724:LEU:HD21	1:J:736:LEU:HD12	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:515:VAL:HG11	1:P:976:GLN:HE22	1.70	0.56
1:P:932:ALA:HA	1:P:959:VAL:HG13	1.88	0.56
1:O:1197:GLN:NE2	1:O:1197:GLN:O	2.39	0.55
1:P:222:HIS:HE1	1:P:247:ARG:HH12	1.51	0.55
1:N:650:ARG:NH1	1:N:873:ASP:OD2	2.39	0.55
1:N:718:LEU:HD13	1:N:811:ILE:HG12	1.88	0.55
1:P:1057:ILE:HG13	1:P:1108:ALA:HB2	1.86	0.55
1:J:444:ASN:HD22	1:J:1176:HIS:CD2	2.24	0.55
1:J:746:ILE:HB	1:J:753:TYR:HB3	1.88	0.55
1:O:1061:SER:O	1:O:1064:SER:OG	2.23	0.55
1:P:605:THR:O	1:P:609:THR:HG23	2.06	0.55
1:P:705:VAL:HA	1:P:710:SER:HA	1.86	0.55
1:N:990:PHE:CE2	1:N:992:GLU:HG2	2.41	0.55
1:O:1203:ARG:HG2	1:O:1275:PHE:CE1	2.42	0.55
1:P:1342:LEU:HB3	1:P:1362:ILE:HD12	1.89	0.55
1:K:566:LEU:HD21	1:K:904:ASN:HD21	1.71	0.55
1:N:175:GLY:HA3	1:O:103:ALA:HB3	1.88	0.55
1:N:764:GLU:HB2	1:N:793:ARG:HD3	1.89	0.55
1:N:400:ARG:HH11	1:N:1305:SER:HB3	1.72	0.55
1:N:483:ARG:HH11	1:N:485:GLU:CB	2.20	0.55
1:N:998:ARG:HB3	1:N:1000:PRO:HD2	1.89	0.55
1:J:69:LEU:CD1	1:J:308:TYR:CG	2.90	0.55
1:O:576:ALA:HB1	1:O:580:PHE:HD2	1.72	0.55
1:O:667:CYS:O	1:O:680:TYR:OH	2.20	0.55
1:P:494:PRO:O	1:P:750:ASN:ND2	2.39	0.55
1:J:110:PRO:HB2	1:O:130:GLU:HG3	1.87	0.55
1:N:208:SER:OG	1:N:209:LYS:N	2.39	0.55
1:N:535:TYR:HE1	1:N:1227:HIS:HB2	1.71	0.55
1:N:842:ASN:ND2	1:N:860:LEU:HD21	2.21	0.55
1:J:670:LEU:HG	1:J:671:GLY:H	1.72	0.54
1:J:92:LYS:HD2	1:J:120:LYS:H	1.72	0.54
1:O:111:SER:OG	1:O:114:ARG:NH2	2.39	0.54
1:O:938:ARG:HA	1:O:941:THR:HG22	1.89	0.54
1:P:607:GLN:HE21	1:P:611:TYR:HE2	1.55	0.54
1:K:298:ALA:CB	1:K:371:VAL:O	2.55	0.54
1:O:762:PHE:O	1:O:793:ARG:HG3	2.07	0.54
1:J:114:ARG:NH2	1:O:392:GLN:OE1	2.36	0.54
1:J:856:ILE:HD11	1:J:878:VAL:HA	1.88	0.54
1:N:1128:PHE:CE1	1:N:1263:ALA:HB2	2.43	0.54
1:J:465:HIS:CE1	1:J:1027:PRO:HD3	2.43	0.54
1:J:607:GLN:HE21	1:J:611:TYR:HE2	1.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:684:ARG:HH22	1:K:653:ARG:HH22	1.56	0.54
1:N:453:GLN:HB2	1:N:1034:ALA:HB1	1.89	0.54
1:P:70:GLU:HA	1:P:367:ILE:HD12	1.89	0.54
1:P:491:HIS:HD2	1:P:493:ARG:HG3	1.72	0.54
1:N:481:ARG:CG	1:N:550:ILE:HD13	2.37	0.54
1:K:546:TYR:HB3	1:K:562:ALA:HB1	1.90	0.54
1:K:1165:MET:SD	1:K:1166:THR:N	2.81	0.54
1:O:905:ASP:O	1:O:909:GLN:HG2	2.08	0.54
1:O:1003:LYS:NZ	1:O:1007:GLU:OE2	2.38	0.54
1:P:744:PRO:HB3	1:P:902:VAL:HG22	1.88	0.54
1:N:690:LEU:HD21	1:N:812:PHE:HB2	1.89	0.54
1:N:857:LEU:HD23	1:N:860:LEU:HD12	1.89	0.54
1:O:90:ASP:OD1	1:O:91:GLY:N	2.41	0.54
1:J:1186:VAL:HG22	1:J:1250:LEU:HD22	1.89	0.54
1:K:262:LYS:HD2	1:K:1062:ARG:HH21	1.73	0.54
1:K:481:ARG:HG2	1:K:550:ILE:HD12	1.89	0.54
1:P:462:PRO:HG2	1:P:1132:ALA:HA	1.90	0.54
1:P:732:ILE:HG22	1:P:799:TYR:CE2	2.43	0.54
1:N:72:ALA:HB3	1:N:382:GLU:HB2	1.90	0.53
1:J:827:GLY:HA3	1:J:950:PHE:HE1	1.73	0.53
1:N:78:VAL:HG21	1:N:261:LEU:HD12	1.90	0.53
1:P:829:GLY:HA3	1:P:946:HIS:CE1	2.44	0.53
1:K:461:HIS:NE2	1:K:1128:PHE:HB2	2.23	0.53
1:K:1250:LEU:O	1:K:1253:ILE:HG22	2.08	0.53
1:N:543:HIS:CE1	1:N:1250:LEU:HD12	2.43	0.53
1:N:1195:TYR:OH	1:N:1203:ARG:O	2.25	0.53
1:J:575:LEU:HD21	1:J:1243:TRP:CZ2	2.44	0.53
1:J:668:ARG:HD2	1:K:935:GLU:HB3	1.91	0.53
1:K:1195:TYR:OH	1:K:1201:SER:O	2.26	0.53
1:O:258:GLU:CB	1:O:262:LYS:CD	2.55	0.53
1:P:789:ASP:OD1	1:P:790:HIS:N	2.41	0.53
1:P:881:ILE:O	1:P:885:SER:OG	2.25	0.53
1:J:59:TYR:HB2	1:K:95:PHE:HD1	1.72	0.53
1:K:861:GLU:CG	5:Z:69:ARG:CD	2.86	0.53
1:N:853:ASP:OD1	1:N:853:ASP:N	2.37	0.53
1:P:251:MET:SD	1:P:1106:THR:OG1	2.66	0.53
1:J:388:TYR:CE2	1:J:396:PRO:HD3	2.43	0.53
1:J:805:ALA:HA	1:K:972:MET:HE1	1.89	0.53
1:K:951:HIS:O	1:K:955:GLY:N	2.42	0.53
1:O:825:MET:N	1:O:956:ASP:OD2	2.30	0.53
1:P:207:PHE:C	1:P:209:LYS:H	2.12	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:1214:ASN:OD1	1:P:1215:TYR:N	2.36	0.53
5:Z:38:ASP:OD1	5:Z:38:ASP:N	2.40	0.53
1:N:441:VAL:HG11	1:N:1373:LEU:HD22	1.91	0.53
1:J:399:ARG:HD3	1:J:1320:PHE:HB3	1.91	0.53
1:J:568:VAL:HG21	1:J:584:ARG:NH2	2.24	0.53
1:N:399:ARG:HG3	1:N:1105:MET:HE1	1.90	0.53
1:N:646:THR:HG21	1:N:874:LEU:HD13	1.90	0.53
1:P:510:LYS:O	1:P:973:ARG:NH2	2.42	0.53
1:K:543:HIS:CE1	1:K:1250:LEU:HD12	2.44	0.53
1:P:906:VAL:HG11	1:P:1135:ASN:H	1.73	0.53
5:Z:24:LEU:HA	5:Z:27:PHE:HB3	1.90	0.53
1:J:852:ARG:HD2	1:J:879:GLY:HA3	1.90	0.52
1:N:672:ASN:HD21	1:O:871:ILE:C	2.07	0.52
1:P:68:PHE:HA	1:P:177:ILE:HD11	1.90	0.52
1:N:91:GLY:HA3	1:N:122:CYS:SG	2.49	0.52
1:N:677:LYS:CG	1:N:678:GLU:N	2.69	0.52
1:P:1210:VAL:HG21	1:P:1287:LEU:HD22	1.91	0.52
1:J:309:ALA:HA	1:J:312:VAL:HB	1.91	0.52
1:J:1217:GLN:O	1:J:1221:GLU:HG2	2.09	0.52
1:J:1340:ARG:HA	1:J:1343:ILE:HG22	1.89	0.52
1:K:934:SER:HB3	1:K:937:THR:OG1	2.10	0.52
1:N:644:ILE:HG22	1:N:675:ILE:CG2	2.32	0.52
1:O:1227:HIS:CE1	1:O:1246:GLN:HG2	2.45	0.52
1:P:732:ILE:HG22	1:P:799:TYR:HE2	1.75	0.52
1:J:478:PRO:HA	1:J:557:ARG:HH22	1.74	0.52
1:K:170:ASP:O	1:K:174:ARG:HG2	2.10	0.52
1:K:408:PRO:HB3	1:K:1196:PHE:CD2	2.44	0.52
1:K:957:PRO:HG2	1:K:978:ARG:O	2.10	0.52
1:N:481:ARG:HG3	1:N:550:ILE:HD13	1.90	0.52
1:N:543:HIS:CD2	1:N:546:TYR:HD1	2.27	0.52
1:K:297:GLU:O	1:K:298:ALA:CB	2.57	0.52
1:K:918:ARG:O	1:K:994:ARG:NH1	2.39	0.52
1:K:857:LEU:HD22	1:K:866:ARG:NH2	2.25	0.52
1:N:269:THR:HG22	1:N:271:LYS:H	1.75	0.52
1:O:232:ARG:HH12	1:O:1370:ARG:NH2	2.07	0.52
1:P:1355:PRO:HG2	1:P:1357:HIS:HD2	1.75	0.52
5:Z:68:PRO:C	5:Z:70:ARG:N	2.60	0.52
1:J:481:ARG:N	1:J:481:ARG:HD3	2.25	0.52
1:K:835:VAL:HG22	1:K:944:LEU:HD13	1.91	0.52
1:P:980:VAL:HG11	1:P:1006:ALA:HB2	1.91	0.52
1:J:255:VAL:HG11	1:J:1102:SER:C	2.30	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:1013:VAL:O	1:N:1016:SER:OG	2.25	0.52
1:J:103:ALA:HB1	1:O:127:ILE:HG23	1.92	0.52
1:J:424:ILE:HD11	1:J:1345:GLU:HB2	1.90	0.52
1:K:402:GLN:HG3	1:K:1321:LEU:HD13	1.92	0.52
1:N:1304:THR:HG22	1:N:1313:VAL:HB	1.91	0.52
1:O:290:LEU:O	1:O:294:LEU:HB2	2.09	0.52
1:K:284:ASP:H	1:K:385:GLN:NE2	2.08	0.52
1:N:742:ARG:HB3	1:N:903:ASP:HB2	1.91	0.52
1:O:216:ILE:HA	1:O:219:PHE:CD2	2.45	0.52
1:O:997:HIS:HE1	1:O:1022:HIS:NE2	2.07	0.52
1:P:500:LEU:HD13	1:P:946:HIS:CG	2.45	0.52
1:J:252:VAL:HG23	1:J:1059:PHE:CZ	2.44	0.51
1:N:133:LEU:HD13	1:N:138:LEU:HD21	1.92	0.51
1:P:937:THR:O	1:P:941:THR:HG23	2.10	0.51
1:J:419:THR:OG1	1:J:420:THR:N	2.44	0.51
1:K:461:HIS:CD2	1:K:1124:PHE:HB3	2.46	0.51
1:K:955:GLY:O	1:K:985:ARG:NH2	2.32	0.51
1:K:1159:ARG:NH2	1:K:1317:THR:OG1	2.43	0.51
1:P:724:LEU:HD11	1:P:736:LEU:HD22	1.92	0.51
1:P:1004:TYR:O	1:P:1008:CYS:HB2	2.11	0.51
1:J:848:HIS:CD2	5:Z:22:PRO:HD2	2.45	0.51
1:K:311:PHE:CE2	1:K:329:ARG:HG3	2.44	0.51
1:K:487:TYR:HH	1:K:985:ARG:H	1.59	0.51
1:N:216:ILE:HD12	1:N:219:PHE:HD2	1.76	0.51
1:O:258:GLU:O	1:O:262:LYS:HB2	2.10	0.51
1:O:1055:GLU:HG3	1:O:1111:ALA:HB2	1.93	0.51
1:P:858:ASP:OD1	1:P:858:ASP:N	2.37	0.51
1:P:908:GLN:NE2	1:P:1026:SER:OG	2.44	0.51
1:K:543:HIS:CD2	1:K:545:LEU:H	2.29	0.51
1:N:443:LYS:HD2	1:N:1113:ILE:HB	1.92	0.51
1:N:1353:HIS:HE1	1:N:1362:ILE:HD13	1.73	0.51
1:P:1253:ILE:HD12	1:P:1259:TYR:HD2	1.75	0.51
1:J:481:ARG:CD	1:J:481:ARG:N	2.73	0.51
1:J:1126:SER:HB2	1:J:1156:ARG:HB2	1.93	0.51
1:K:189:PRO:HG2	1:K:194:LEU:HD12	1.93	0.51
1:P:225:GLU:O	1:P:1370:ARG:NH1	2.43	0.51
1:J:622:VAL:HG21	1:J:639:LEU:HD21	1.92	0.51
1:P:415:ASN:HD21	1:P:579:ALA:HB3	1.76	0.51
1:J:486:THR:OG1	1:J:552:ARG:NH1	2.42	0.51
1:O:230:LEU:HD21	1:O:289:GLN:HG2	1.92	0.51
1:O:988:GLN:OE1	1:O:988:GLN:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:133:LEU:HD12	1:P:1086:PHE:HE2	1.76	0.51
1:P:531:HIS:CD2	1:P:533:SER:H	2.29	0.51
1:J:1049:THR:HG23	1:J:1270:PRO:HB3	1.92	0.51
1:K:284:ASP:OD1	1:K:385:GLN:HB2	2.10	0.51
1:K:484:ARG:HG2	1:K:552:ARG:CA	2.40	0.51
1:K:716:CYS:SG	1:K:1023:ILE:HG12	2.50	0.51
1:N:498:ASN:HB3	1:N:501:VAL:HG12	1.93	0.51
1:N:753:TYR:HE1	1:N:762:PHE:HB2	1.75	0.51
1:J:367:ILE:HG22	1:J:367:ILE:O	2.11	0.51
1:N:317:ASN:HB3	1:N:327:VAL:HG13	1.92	0.51
1:K:191:MET:HB2	1:K:1106:THR:HB	1.93	0.50
1:O:783:ARG:NH2	1:O:891:CYS:O	2.43	0.50
1:J:632:LYS:NZ	1:J:887:SER:HB2	2.26	0.50
1:J:1067:MET:SD	1:J:1094:SER:HB3	2.52	0.50
1:K:271:LYS:HB3	1:K:299:ASP:CG	2.31	0.50
1:K:594:LEU:HD13	1:K:696:ALA:HB2	1.93	0.50
1:K:955:GLY:HA3	1:K:985:ARG:HE	1.75	0.50
1:N:620:TYR:OH	1:N:930:ALA:HB2	2.10	0.50
1:J:331:PHE:O	1:J:335:MET:HG2	2.12	0.50
1:J:1213:GLU:OE1	1:J:1213:GLU:N	2.36	0.50
1:N:782:TYR:CE1	1:N:786:GLY:HA3	2.46	0.50
1:P:832:PHE:CE2	1:P:891:CYS:HB3	2.46	0.50
1:J:283:THR:HG22	1:J:395:TYR:CE2	2.47	0.50
1:J:411:LEU:HD23	1:J:1193:VAL:HG22	1.94	0.50
1:K:706:VAL:HG23	1:K:711:VAL:HG12	1.94	0.50
1:N:127:ILE:HG23	1:O:103:ALA:HB1	1.94	0.50
1:N:481:ARG:CB	1:N:550:ILE:HD13	2.42	0.50
1:N:813:TYR:O	1:N:954:TYR:OH	2.12	0.50
1:N:1348:SER:OG	1:N:1349:VAL:N	2.45	0.50
1:O:258:GLU:C	1:O:259:SER:O	2.49	0.50
5:Z:24:LEU:O	5:Z:28:GLN:HG2	2.12	0.50
1:J:567:MET:HB2	1:J:570:ASN:ND2	2.26	0.50
1:K:800:VAL:HB	1:K:802:GLU:HG3	1.92	0.50
1:K:815:VAL:HG13	1:K:1018:MET:HG2	1.93	0.50
1:N:140:ILE:HD11	1:N:157:ALA:HB2	1.93	0.50
1:N:481:ARG:HG3	1:N:550:ILE:HG21	1.92	0.50
1:N:990:PHE:HE2	1:N:992:GLU:HG2	1.75	0.50
1:P:155:VAL:HA	1:P:158:VAL:HG22	1.93	0.50
1:P:282:VAL:HG12	1:P:1057:ILE:HG12	1.92	0.50
1:P:913:ASN:ND2	1:P:915:ALA:HB3	2.26	0.50
1:P:959:VAL:O	1:P:962:THR:OG1	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:482:ASP:O	1:K:484:ARG:NH1	2.44	0.50
1:K:507:TYR:CD1	1:K:967:VAL:HG22	2.47	0.50
1:O:529:PHE:HZ	1:O:541:GLU:HG3	1.77	0.50
1:O:572:PRO:HB2	1:O:574:PRO:HD2	1.93	0.50
1:P:522:CYS:SG	1:P:1000:PRO:HG3	2.51	0.50
1:P:876:PRO:HB3	1:P:880:MET:SD	2.51	0.50
1:P:981:GLU:OE1	1:P:999:SER:HA	2.12	0.50
1:J:856:ILE:HG23	1:J:860:LEU:HD21	1.94	0.50
1:K:461:HIS:HE2	1:K:1128:PHE:HB2	1.76	0.50
1:N:170:ASP:O	1:N:174:ARG:HG2	2.12	0.50
1:O:658:ASN:HD21	1:O:930:ALA:HA	1.77	0.50
1:K:550:ILE:HG12	1:K:560:HIS:CD2	2.46	0.50
1:K:616:PRO:HG2	1:K:619:PHE:CE2	2.47	0.50
1:O:1128:PHE:CZ	1:O:1260:ARG:HD2	2.42	0.50
1:P:769:MET:SD	1:P:769:MET:N	2.76	0.50
1:J:458:VAL:HG11	1:J:1184:ILE:HB	1.93	0.49
1:J:957:PRO:HG3	1:J:983:PHE:CG	2.47	0.49
1:N:35:HIS:O	1:N:36:SER:OG	2.29	0.49
1:P:879:GLY:O	1:P:882:ARG:NE	2.44	0.49
1:J:1130:ALA:HB3	1:J:1261:GLN:HE21	1.76	0.49
1:K:79:ASN:HB3	1:K:308:TYR:HD1	1.77	0.49
1:K:437:GLU:OE2	1:K:439:TRP:NE1	2.42	0.49
1:K:1256:ASN:HD21	1:K:1277:LYS:H	1.61	0.49
1:N:1353:HIS:HE1	1:N:1362:ILE:HG21	1.77	0.49
1:O:465:HIS:CE1	1:O:1027:PRO:HD3	2.47	0.49
1:O:677:LYS:O	1:O:681:SER:OG	2.28	0.49
1:P:484:ARG:NH1	1:P:550:ILE:HD12	2.26	0.49
1:P:487:TYR:OH	1:P:984:ASN:HB3	2.12	0.49
1:K:548:ILE:HD11	1:K:560:HIS:HB3	1.95	0.49
1:N:657:VAL:HA	1:N:663:ILE:HD11	1.94	0.49
1:N:75:VAL:HA	1:N:267:TYR:CE1	2.48	0.49
1:N:196:THR:HG21	1:N:218:MET:HB3	1.94	0.49
1:N:559:ARG:HH22	1:N:561:ARG:HE	1.58	0.49
1:O:480:PRO:HG2	1:O:483:ARG:NH2	2.26	0.49
1:P:229:PHE:HB2	1:P:243:TYR:HE2	1.77	0.49
1:P:824:HIS:ND1	1:P:956:ASP:OD2	2.44	0.49
1:P:901:SER:OG	1:P:918:ARG:NH2	2.45	0.49
5:Z:68:PRO:CG	5:Z:71:GLN:HE21	2.25	0.49
1:K:467:PRO:HD3	1:K:546:TYR:CZ	2.48	0.49
1:N:1252:ASP:O	1:N:1256:ASN:HB2	2.11	0.49
1:N:1260:ARG:NH1	1:N:1269:SER:OG	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:399:ARG:CD	1:O:1320:PHE:HB3	2.42	0.49
1:N:526:THR:HG22	1:N:574:PRO:HA	1.94	0.49
1:N:1272:ARG:HH21	1:N:1276:ASN:ND2	2.11	0.49
1:O:731:ASP:HA	1:O:796:LEU:HD13	1.95	0.49
1:O:860:LEU:HD11	1:O:865:LEU:HB3	1.94	0.49
1:J:764:GLU:HB2	1:J:793:ARG:HH11	1.78	0.49
1:J:840:ALA:HB3	5:Z:49:VAL:HG22	1.95	0.49
1:O:933:PHE:HD2	1:O:963:MET:HG2	1.78	0.49
1:P:439:TRP:N	1:P:1337:ALA:O	2.45	0.49
1:P:675:ILE:HD13	1:P:680:TYR:HB2	1.95	0.49
1:J:203:THR:O	1:J:203:THR:OG1	2.24	0.49
1:J:932:ALA:HB2	1:J:959:VAL:HG22	1.95	0.49
1:K:932:ALA:HA	1:K:959:VAL:HG13	1.95	0.49
1:N:93:ILE:HD12	1:N:1095:ILE:HG21	1.94	0.49
1:N:667:CYS:SG	1:N:683:TYR:HB3	2.52	0.49
1:O:655:ALA:O	1:O:683:TYR:OH	2.28	0.49
5:Z:68:PRO:O	5:Z:69:ARG:C	2.50	0.49
1:J:406:TYR:HE2	1:J:1196:PHE:HD1	1.61	0.49
1:N:847:SER:HB2	1:N:850:PHE:CD2	2.46	0.49
1:O:690:LEU:HB3	1:O:808:LEU:HD22	1.94	0.49
1:O:947:ALA:HB3	1:O:964:HIS:ND1	2.28	0.49
1:P:800:VAL:HG23	1:P:802:GLU:HG2	1.94	0.49
1:J:103:ALA:HB3	1:O:175:GLY:HA3	1.94	0.49
1:J:155:VAL:HA	1:J:158:VAL:HG22	1.94	0.49
1:J:421:SER:HB3	1:J:1354:ALA:HB2	1.94	0.49
1:J:714:TYR:HD2	1:J:1028:MET:HG3	1.77	0.49
1:J:934:SER:HB3	1:J:937:THR:HG23	1.95	0.49
1:N:467:PRO:HG2	1:N:912:PRO:HD3	1.94	0.49
1:N:1353:HIS:CE1	1:N:1362:ILE:HD13	2.48	0.49
1:P:531:HIS:CG	1:P:532:PRO:HD2	2.48	0.49
1:J:93:ILE:HA	1:O:32:GLY:O	2.13	0.48
1:K:1313:VAL:HG21	1:K:1319:VAL:HG21	1.93	0.48
1:N:466:THR:HG22	1:N:910:LEU:HB3	1.94	0.48
1:N:606:VAL:O	1:N:609:THR:OG1	2.22	0.48
1:N:620:TYR:CE1	1:N:828:LEU:HD22	2.47	0.48
1:O:906:VAL:HA	1:O:909:GLN:CG	2.43	0.48
1:O:906:VAL:HA	1:O:909:GLN:HG2	1.94	0.48
1:K:1152:GLY:O	1:K:1167:ASN:ND2	2.46	0.48
1:N:64:GLN:OE1	1:N:64:GLN:N	2.28	0.48
1:N:645:ASN:HA	1:N:675:ILE:CG2	2.43	0.48
1:N:1353:HIS:CE1	1:N:1362:ILE:HG21	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:406:TYR:HA	1:O:1046:VAL:O	2.13	0.48
1:O:596:HIS:CG	1:O:1012:LEU:HD11	2.47	0.48
1:O:1255:TYR:HA	1:O:1260:ARG:NH1	2.28	0.48
1:P:724:LEU:HD22	1:P:732:ILE:HD12	1.95	0.48
1:J:266:THR:HG21	1:J:1062:ARG:NE	2.26	0.48
1:J:1252:ASP:O	1:J:1256:ASN:HB2	2.13	0.48
1:K:1195:TYR:OH	1:K:1203:ARG:O	2.32	0.48
1:N:217:ALA:HA	1:N:220:LYS:HE3	1.95	0.48
1:N:832:PHE:HD2	1:N:892:PRO:O	1.97	0.48
1:O:30:ALA:HB1	1:O:33:LEU:HD13	1.95	0.48
1:O:670:LEU:O	1:O:672:ASN:N	2.46	0.48
1:P:586:GLN:HE21	1:P:1013:VAL:HG13	1.79	0.48
1:P:734:THR:HG22	1:P:753:TYR:OH	2.13	0.48
1:P:863:GLY:HA2	1:P:866:ARG:HB3	1.95	0.48
1:J:192:PHE:CE2	1:J:193:ILE:HG13	2.48	0.48
1:K:352:LEU:O	1:K:355:VAL:HG12	2.13	0.48
1:N:191:MET:HB2	1:N:1106:THR:HB	1.96	0.48
1:N:388:TYR:CE2	1:N:396:PRO:HD3	2.48	0.48
1:N:1023:ILE:HG21	1:N:1033:GLN:NE2	2.28	0.48
1:N:1128:PHE:CZ	1:N:1260:ARG:HG3	2.47	0.48
1:O:726:PRO:HD3	1:O:814:TYR:CE1	2.49	0.48
1:P:37:PHE:O	1:P:41:VAL:HG13	2.14	0.48
1:J:442:ASN:OD1	1:J:443:LYS:N	2.43	0.48
1:K:135:MET:N	1:K:1082:ASP:O	2.37	0.48
1:N:677:LYS:C	1:N:679:ALA:N	2.63	0.48
1:O:826:CYS:HA	1:O:954:TYR:O	2.13	0.48
1:P:226:HIS:HD2	1:P:243:TYR:OH	1.96	0.48
1:P:842:ASN:HD22	1:P:865:LEU:HD12	1.79	0.48
1:P:1205:ARG:HG3	1:P:1231:ASP:HB3	1.95	0.48
1:J:824:HIS:HD1	1:J:956:ASP:CG	2.15	0.48
1:K:548:ILE:HD12	1:K:561:ARG:O	2.13	0.48
1:K:861:GLU:CD	5:Z:67:VAL:HG11	2.34	0.48
1:O:904:ASN:ND2	1:O:908:GLN:O	2.47	0.48
1:P:933:PHE:CD2	1:P:963:MET:HG2	2.49	0.48
1:J:267:TYR:O	1:J:276:VAL:HG23	2.14	0.48
1:J:461:HIS:CG	1:J:462:PRO:HD2	2.49	0.48
1:K:921:GLN:HB2	1:K:996:TRP:HD1	1.77	0.48
1:K:1188:PRO:HD2	1:K:1241:ASN:CB	2.43	0.48
1:P:61:ASN:OD1	1:P:62:ALA:N	2.46	0.48
1:N:104:HIS:CD2	1:N:108:ARG:HH11	2.31	0.48
1:N:162:ALA:O	1:N:166:GLN:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:1053:LEU:HD22	1:N:1111:ALA:HB3	1.96	0.48
1:N:1297:ARG:NH2	1:N:1298:LEU:O	2.47	0.48
1:O:489:LEU:H	1:O:489:LEU:HD12	1.79	0.48
1:O:764:GLU:OE2	1:O:793:ARG:NE	2.28	0.48
1:P:481:ARG:NH2	1:P:540:LEU:HD11	2.28	0.48
1:J:830:VAL:HG22	1:J:945:PHE:HD1	1.78	0.48
1:N:559:ARG:NH2	1:N:561:ARG:HE	2.12	0.48
1:N:619:PHE:HE2	1:N:647:TYR:HB2	1.79	0.48
1:N:794:LEU:HD21	1:N:925:VAL:HG11	1.96	0.48
1:O:524:LEU:O	1:O:574:PRO:HG3	2.14	0.48
1:O:633:PHE:CE2	1:O:665:PHE:HB3	2.49	0.48
1:P:544:PRO:HG3	1:P:1243:TRP:CD2	2.49	0.48
1:P:861:GLU:HB3	1:P:866:ARG:NH1	2.28	0.48
1:J:59:TYR:HB2	1:K:95:PHE:CD1	2.48	0.48
1:J:543:HIS:CE1	1:J:1250:LEU:HD12	2.48	0.48
1:J:831:ASP:OD2	1:J:834:HIS:ND1	2.47	0.48
1:K:384:LEU:O	1:K:395:TYR:HE2	1.96	0.48
1:K:560:HIS:HD1	1:K:560:HIS:H	1.60	0.48
1:K:842:ASN:OD1	1:K:843:GLY:N	2.47	0.48
1:K:1136:GLN:NE2	1:K:1140:ASP:OD2	2.46	0.48
1:K:1346:PHE:HD1	1:K:1353:HIS:CD2	2.32	0.48
1:N:467:PRO:HD3	1:N:546:TYR:CZ	2.49	0.48
1:N:484:ARG:HG3	1:N:484:ARG:NH1	2.28	0.48
1:P:437:GLU:OE1	1:P:437:GLU:N	2.47	0.48
1:P:843:GLY:O	1:P:847:SER:N	2.29	0.48
1:J:69:LEU:HD13	1:J:308:TYR:CZ	2.47	0.47
1:O:483:ARG:HE	1:O:550:ILE:HG21	1.78	0.47
1:J:203:THR:HB	1:J:207:PHE:HE1	1.79	0.47
1:K:184:LYS:HZ3	1:K:1064:SER:HG	1.55	0.47
1:K:813:TYR:O	1:K:954:TYR:OH	2.22	0.47
1:N:639:LEU:HD12	1:N:880:MET:HB3	1.96	0.47
1:O:388:TYR:HD2	1:O:395:TYR:HA	1.80	0.47
5:Z:68:PRO:CG	5:Z:71:GLN:NE2	2.73	0.47
1:J:783:ARG:HG2	1:J:833:GLN:HE21	1.79	0.47
1:K:452:LEU:HD13	1:K:1040:PRO:HG2	1.96	0.47
1:K:543:HIS:CD2	1:K:546:TYR:HD1	2.31	0.47
1:N:269:THR:HG22	1:N:271:LYS:N	2.29	0.47
1:O:154:TYR:O	1:O:158:VAL:HG13	2.14	0.47
1:P:658:ASN:HB2	1:P:931:PHE:CE2	2.50	0.47
1:J:848:HIS:NE2	5:Z:21:SER:OG	2.29	0.47
1:J:1075:SER:OG	1:J:1076:ARG:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:884:LEU:O	1:K:887:SER:OG	2.20	0.47
1:O:854:GLU:O	1:O:878:VAL:HG23	2.15	0.47
1:P:723:LEU:HB3	1:P:810:LYS:HZ2	1.79	0.47
1:K:1045:THR:OG1	1:K:1185:ILE:HB	2.14	0.47
1:O:436:VAL:CG1	1:O:587:GLN:HE22	2.24	0.47
1:P:641:SER:O	1:P:645:ASN:ND2	2.47	0.47
1:P:863:GLY:O	1:P:867:ASP:N	2.35	0.47
1:N:644:ILE:HG21	1:N:675:ILE:HG13	1.95	0.47
1:N:790:HIS:ND1	1:N:790:HIS:O	2.45	0.47
1:O:543:HIS:CE1	1:O:545:LEU:HB2	2.49	0.47
1:O:724:LEU:O	1:O:814:TYR:OH	2.29	0.47
1:P:549:TYR:CZ	1:P:561:ARG:HB3	2.49	0.47
1:P:1255:TYR:HB2	1:P:1275:PHE:HD2	1.79	0.47
1:J:128:SER:HA	1:J:1088:VAL:O	2.15	0.47
1:J:493:ARG:HE	1:J:747:ILE:HD13	1.80	0.47
1:J:584:ARG:NH1	1:J:1020:ALA:O	2.33	0.47
1:J:1117:MET:SD	1:J:1371:ARG:NH1	2.88	0.47
1:K:546:TYR:CD2	1:K:564:HIS:HB3	2.50	0.47
1:K:1159:ARG:HD3	1:K:1315:ALA:HB3	1.97	0.47
1:N:344:LYS:HB3	1:N:344:LYS:HE2	1.73	0.47
1:N:699:ARG:HH22	1:O:1006:ALA:HB1	1.79	0.47
1:N:950:PHE:HD1	1:N:950:PHE:HA	1.61	0.47
1:N:1215:TYR:CE1	1:N:1285:ARG:HG2	2.50	0.47
1:O:951:HIS:HE2	1:O:997:HIS:HD2	1.61	0.47
1:P:481:ARG:HH22	1:P:540:LEU:HD11	1.80	0.47
1:J:1287:LEU:HD12	1:J:1287:LEU:HA	1.80	0.47
1:K:1048:ARG:NH2	1:K:1117:MET:O	2.48	0.47
1:N:176:LEU:O	1:N:179:THR:OG1	2.30	0.47
1:O:93:ILE:HD11	1:O:1095:ILE:HG21	1.96	0.47
1:O:388:TYR:CD2	1:O:395:TYR:HA	2.50	0.47
1:P:133:LEU:HD22	1:P:161:VAL:HG12	1.96	0.47
1:P:630:GLU:O	1:P:634:VAL:HG23	2.14	0.47
1:P:830:VAL:HG13	1:P:944:LEU:HD11	1.97	0.47
1:P:1342:LEU:HD13	1:P:1362:ILE:HB	1.96	0.47
5:Z:68:PRO:C	5:Z:70:ARG:H	2.18	0.47
1:J:283:THR:HG22	1:J:395:TYR:HE2	1.79	0.47
1:K:1154:LEU:HD23	1:K:1167:ASN:HB2	1.97	0.47
1:N:483:ARG:NH1	1:N:485:GLU:HB3	2.29	0.47
1:N:557:ARG:HG2	1:N:558:ALA:N	2.29	0.47
1:N:1347:MET:HE2	1:N:1378:LYS:HG3	1.97	0.47
1:O:977:GLN:HE21	1:O:983:PHE:HA	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:1081:VAL:HG23	1:O:1082:ASP:OD1	2.15	0.47
1:P:405:TYR:HA	1:P:1332:PHE:O	2.15	0.47
1:J:162:ALA:O	1:J:166:GLN:HG3	2.15	0.47
1:J:431:THR:HG23	1:J:432:GLN:HG3	1.97	0.47
1:J:635:MET:HG2	5:Z:60:TYR:CE2	2.50	0.47
1:J:637:VAL:HA	1:J:640:VAL:HG22	1.97	0.47
1:J:1174:LEU:O	1:K:213:SER:OG	2.31	0.47
1:K:1160:THR:HG21	1:K:1314:ILE:HD11	1.97	0.47
1:N:826:CYS:HA	1:N:954:TYR:O	2.15	0.47
1:J:420:THR:O	1:J:420:THR:OG1	2.33	0.46
1:J:423:ALA:HB1	1:K:420:THR:O	2.15	0.46
1:J:609:THR:HG22	1:J:653:ARG:HB3	1.97	0.46
1:K:832:PHE:CE2	1:K:892:PRO:HG2	2.49	0.46
1:K:861:GLU:CG	5:Z:69:ARG:HE	2.28	0.46
1:K:933:PHE:CD2	1:K:963:MET:HG2	2.50	0.46
1:O:526:THR:OG1	1:O:527:GLU:N	2.47	0.46
1:O:860:LEU:HB3	1:O:866:ARG:HD3	1.98	0.46
1:P:736:LEU:O	1:P:740:SER:OG	2.30	0.46
1:J:126:HIS:CD2	1:J:1091:GLU:HG2	2.49	0.46
1:J:482:ASP:N	1:J:482:ASP:OD1	2.42	0.46
1:J:1259:TYR:CE2	1:J:1262:THR:HB	2.47	0.46
1:K:441:VAL:HG11	1:K:1373:LEU:HD22	1.98	0.46
1:K:1152:GLY:HA2	1:K:1169:ASN:O	2.16	0.46
1:N:955:GLY:HA3	1:N:985:ARG:HH21	1.81	0.46
1:O:397:LEU:O	1:O:399:ARG:N	2.49	0.46
1:O:605:THR:O	1:O:609:THR:HG23	2.15	0.46
1:O:922:THR:HG21	1:O:989:LEU:O	2.15	0.46
1:P:269:THR:OG1	1:P:273:GLY:HA2	2.14	0.46
1:P:542:LEU:HB3	1:P:1249:SER:HA	1.95	0.46
1:P:1227:HIS:NE2	1:P:1245:SER:O	2.49	0.46
5:Z:22:PRO:O	5:Z:25:PRO:HD2	2.15	0.46
1:J:400:ARG:HH22	1:J:1114:THR:HG21	1.79	0.46
1:J:633:PHE:CE2	1:J:665:PHE:HB3	2.50	0.46
1:K:997:HIS:HE1	1:K:1022:HIS:CE1	2.22	0.46
1:N:84:ASP:OD1	1:N:84:ASP:N	2.37	0.46
1:N:536:ASP:OD1	1:N:536:ASP:N	2.47	0.46
1:O:964:HIS:HB3	1:O:967:VAL:H	1.80	0.46
1:J:306:SER:HB2	1:J:307:SER:H	1.54	0.46
1:J:666:ILE:O	1:J:670:LEU:HB3	2.16	0.46
1:K:1269:SER:HB2	1:K:1272:ARG:HB2	1.97	0.46
1:N:428:ASP:OD1	1:N:429:ASN:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:513:ALA:HB1	1:N:984:ASN:ND2	2.30	0.46
1:O:193:ILE:HG22	1:O:197:LEU:HD22	1.97	0.46
1:O:734:THR:HG23	1:O:763:ILE:HD12	1.98	0.46
1:O:933:PHE:CD2	1:O:963:MET:HG2	2.51	0.46
1:O:1268:TYR:CG	1:O:1303:ALA:HB2	2.50	0.46
1:P:872:SER:O	1:P:874:LEU:HG	2.16	0.46
1:J:172:LEU:HD23	1:J:172:LEU:HA	1.71	0.46
1:J:267:TYR:CD2	1:J:304:GLY:HA2	2.51	0.46
1:K:336:ALA:HA	1:K:340:ASP:HB3	1.98	0.46
1:K:861:GLU:HG2	5:Z:69:ARG:HE	1.81	0.46
1:N:484:ARG:HH11	1:N:484:ARG:CG	2.29	0.46
1:P:461:HIS:CD2	1:P:1124:PHE:HB3	2.50	0.46
1:P:831:ASP:H	1:P:944:LEU:HD21	1.80	0.46
1:J:877:THR:H	1:J:880:MET:HE2	1.80	0.46
1:K:172:LEU:HD21	1:K:1090:HIS:ND1	2.31	0.46
1:K:835:VAL:O	1:K:838:THR:OG1	2.25	0.46
1:K:1039:HIS:ND1	1:K:1040:PRO:O	2.49	0.46
1:N:217:ALA:O	1:N:220:LYS:HG2	2.15	0.46
1:N:658:ASN:HD21	1:N:930:ALA:HA	1.80	0.46
1:N:818:PRO:HB3	1:N:953:PHE:HB3	1.98	0.46
1:O:184:LYS:NZ	1:O:1064:SER:HB2	2.30	0.46
1:O:487:TYR:OH	1:O:985:ARG:O	2.23	0.46
1:O:609:THR:HG22	1:O:653:ARG:HB3	1.98	0.46
1:O:660:PHE:HB2	1:O:812:PHE:CD2	2.51	0.46
1:O:668:ARG:HD2	1:O:669:HIS:CE1	2.50	0.46
1:P:731:ASP:HB2	1:P:797:GLY:HA3	1.98	0.46
1:P:1008:CYS:SG	1:P:1014:SER:HB2	2.55	0.46
1:K:4:ASN:HD22	1:K:38:ASP:HB2	1.81	0.46
1:K:216:ILE:HD12	1:K:219:PHE:HD2	1.80	0.46
1:K:899:ARG:HH21	1:K:920:GLU:HG3	1.81	0.46
1:N:1070:GLY:O	1:N:1090:HIS:NE2	2.49	0.46
1:O:386:LYS:HD2	1:O:386:LYS:HA	1.73	0.46
1:P:488:SER:O	1:P:991:ALA:HB1	2.15	0.46
1:P:491:HIS:CD2	1:P:493:ARG:HG3	2.50	0.46
1:J:1120:HIS:N	1:J:1182:CYS:SG	2.80	0.46
1:K:783:ARG:O	1:K:788:HIS:NE2	2.47	0.46
1:N:680:TYR:O	1:N:684:ARG:HG3	2.16	0.46
5:Z:76:LYS:HD2	5:Z:77:ARG:H	1.80	0.46
1:N:1174:LEU:HD13	1:O:209:LYS:HD2	1.97	0.46
1:N:1322:GLU:OE1	1:N:1322:GLU:N	2.49	0.46
1:O:610:ALA:HA	1:O:931:PHE:CD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:636:ASN:O	1:O:640:VAL:HG13	2.16	0.46
1:J:287:LEU:O	1:J:291:LEU:HG	2.16	0.46
1:J:402:GLN:NE2	1:J:1051:GLU:OE2	2.44	0.46
1:J:724:LEU:HD22	1:J:732:ILE:HD11	1.98	0.46
1:P:627:HIS:CE1	1:P:629:PHE:HB2	2.51	0.46
1:P:1077:ARG:HD3	1:P:1078:GLU:O	2.16	0.46
1:J:289:GLN:O	1:J:292:THR:OG1	2.27	0.45
1:J:789:ASP:OD2	5:Z:1:MET:N	2.43	0.45
1:J:933:PHE:CE2	1:J:963:MET:HG2	2.51	0.45
1:J:1215:TYR:HE1	1:J:1285:ARG:HG2	1.80	0.45
1:K:184:LYS:HZ3	1:K:1065:THR:HG23	1.81	0.45
1:N:189:PRO:HG2	1:N:194:LEU:HD21	1.97	0.45
1:O:1023:ILE:HG21	1:O:1033:GLN:NE2	2.31	0.45
1:P:73:LEU:HD13	1:P:281:ILE:HD11	1.99	0.45
1:P:96:ARG:HA	1:P:117:ILE:HG13	1.97	0.45
1:J:531:HIS:HD2	1:J:533:SER:H	1.65	0.45
1:J:619:PHE:CE1	1:J:643:CYS:HB3	2.51	0.45
1:K:496:HIS:HE1	1:K:502:ILE:HG12	1.81	0.45
1:K:690:LEU:HD23	1:K:808:LEU:HB3	1.98	0.45
1:N:128:SER:HA	1:N:1088:VAL:O	2.15	0.45
1:N:172:LEU:HD21	1:N:1090:HIS:ND1	2.31	0.45
1:N:830:VAL:HB	1:N:832:PHE:CE1	2.51	0.45
1:O:529:PHE:HE2	1:O:575:LEU:HD21	1.80	0.45
1:P:735:HIS:CE1	1:P:739:VAL:HG21	2.52	0.45
1:K:301:GLN:HE21	1:K:366:PRO:HB2	1.81	0.45
1:K:856:ILE:HG13	1:K:878:VAL:HG22	1.98	0.45
1:O:460:CYS:HB3	1:O:1027:PRO:HB3	1.98	0.45
1:P:1027:PRO:HG2	1:P:1133:PHE:CZ	2.50	0.45
1:J:270:ALA:HB3	1:J:301:GLN:HB2	1.98	0.45
1:J:1243:TRP:O	1:J:1249:SER:HB2	2.16	0.45
1:K:165:LEU:O	1:K:169:VAL:HG23	2.15	0.45
1:O:488:SER:HB2	1:O:992:GLU:N	2.21	0.45
1:P:172:LEU:HD23	1:P:172:LEU:HA	1.74	0.45
1:P:463:ARG:HD2	1:P:463:ARG:HA	1.80	0.45
1:P:843:GLY:O	1:P:846:PHE:N	2.49	0.45
1:J:978:ARG:HB3	1:O:698:MET:SD	2.56	0.45
1:J:978:ARG:H	1:O:698:MET:HE3	1.80	0.45
1:K:395:TYR:HD1	1:K:397:LEU:H	1.62	0.45
1:N:428:ASP:HB3	1:N:433:GLN:HE21	1.81	0.45
1:O:258:GLU:HB3	1:O:262:LYS:HB3	1.98	0.45
1:P:718:LEU:HD21	1:P:1022:HIS:CD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:69:LEU:HD22	1:J:308:TYR:CE2	2.52	0.45
1:J:424:ILE:HD13	1:J:1341:ALA:HB1	1.98	0.45
1:J:828:LEU:HD13	1:J:963:MET:HE2	1.98	0.45
1:K:82:PHE:CE2	1:K:85:LEU:HA	2.52	0.45
1:K:936:ARG:HH11	1:K:939:ALA:HB3	1.81	0.45
1:N:1336:SER:O	1:N:1362:ILE:HA	2.17	0.45
1:O:451:ASN:OD1	1:O:452:LEU:N	2.49	0.45
1:O:550:ILE:HG12	1:O:560:HIS:ND1	2.31	0.45
1:O:608:ASP:HB3	1:O:653:ARG:HD2	1.99	0.45
1:O:1339:SER:HB3	1:O:1360:HIS:ND1	2.31	0.45
1:J:174:ARG:HB2	1:K:102:ILE:HG23	1.98	0.45
1:J:773:ALA:HA	1:J:776:PHE:CE2	2.51	0.45
1:J:789:ASP:OD1	1:J:789:ASP:N	2.49	0.45
1:J:837:GLN:HG3	5:Z:49:VAL:HG21	1.99	0.45
1:K:543:HIS:CG	1:K:544:PRO:HD2	2.51	0.45
1:N:145:PRO:HG3	1:N:151:TYR:CD1	2.50	0.45
1:N:524:LEU:HD13	1:N:534:ASN:HD22	1.80	0.45
1:N:819:THR:HG23	1:N:1008:CYS:SG	2.57	0.45
1:O:637:VAL:HG13	1:O:638:PRO:HD3	1.97	0.45
1:J:93:ILE:HG21	1:O:34:PHE:CE1	2.52	0.45
1:J:151:TYR:O	1:J:155:VAL:HG13	2.16	0.45
1:J:192:PHE:CE2	1:J:223:LEU:HD12	2.52	0.45
1:K:29:ALA:HB1	1:K:37:PHE:CE2	2.52	0.45
1:K:335:MET:HG2	1:K:339:VAL:HG12	1.98	0.45
1:K:452:LEU:HD22	1:K:1040:PRO:HG3	1.98	0.45
5:Z:68:PRO:HB2	5:Z:71:GLN:HB2	1.99	0.45
1:N:514:PRO:O	1:N:984:ASN:ND2	2.47	0.45
1:N:736:LEU:HA	1:N:739:VAL:HG22	1.98	0.45
1:N:938:ARG:HH12	1:N:965:GLN:NE2	2.15	0.45
1:O:439:TRP:CZ3	1:O:449:ALA:HB2	2.51	0.45
1:P:291:LEU:HA	1:P:291:LEU:HD23	1.73	0.45
1:P:507:TYR:OH	1:P:984:ASN:O	2.31	0.45
1:P:979:ALA:HB3	1:P:982:ALA:HB3	1.99	0.45
1:J:491:HIS:ND1	1:J:987:GLU:O	2.50	0.45
1:J:575:LEU:HD21	1:J:1243:TRP:CH2	2.52	0.45
1:J:1066:SER:OG	1:J:1095:ILE:HG22	2.17	0.45
1:K:546:TYR:CE2	1:K:564:HIS:HB3	2.52	0.45
1:K:748:ILE:HG13	1:K:898:VAL:HG13	1.99	0.45
1:N:427:LEU:HG	1:O:417:LYS:O	2.17	0.45
1:N:867:ASP:HB2	1:N:940:VAL:HG11	1.97	0.45
1:P:1258:SER:OG	1:P:1259:TYR:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:862:ASN:HA	1:J:866:ARG:HD3	1.98	0.44
1:J:1345:GLU:OE2	1:J:1353:HIS:HA	2.16	0.44
1:K:255:VAL:HG13	1:K:1102:SER:HA	1.99	0.44
1:K:402:GLN:HA	1:K:1050:ASP:O	2.17	0.44
1:N:860:LEU:HA	1:N:860:LEU:HD23	1.71	0.44
1:O:535:TYR:CE1	1:O:1227:HIS:HB2	2.47	0.44
1:O:737:LEU:HD23	1:O:744:PRO:HG2	1.99	0.44
1:P:222:HIS:CE1	1:P:247:ARG:HH12	2.32	0.44
1:P:759:ALA:O	1:P:763:ILE:HG12	2.17	0.44
1:P:805:ALA:C	1:P:807:VAL:H	2.20	0.44
1:P:1048:ARG:NH2	1:P:1117:MET:O	2.50	0.44
1:P:1178:GLN:HE21	1:P:1180:ALA:HB3	1.81	0.44
1:J:529:PHE:CD2	1:J:574:PRO:HB2	2.52	0.44
1:K:31:GLU:O	1:K:33:LEU:HG	2.18	0.44
1:N:401:MET:HE3	1:N:403:TYR:HE1	1.82	0.44
1:N:481:ARG:HB3	1:N:550:ILE:HD13	1.98	0.44
1:N:627:HIS:O	1:N:627:HIS:ND1	2.47	0.44
1:N:699:ARG:NH1	1:O:1007:GLU:OE2	2.50	0.44
1:P:619:PHE:CE1	1:P:643:CYS:HB3	2.53	0.44
1:P:830:VAL:O	1:P:894:PHE:HA	2.17	0.44
1:J:255:VAL:HG12	1:J:1102:SER:HA	1.98	0.44
1:J:811:ILE:O	1:J:815:VAL:HB	2.17	0.44
1:K:806:ASP:O	1:K:807:VAL:C	2.55	0.44
1:N:55:LEU:HD23	1:N:55:LEU:HA	1.87	0.44
1:N:1260:ARG:HH22	1:N:1269:SER:HB2	1.81	0.44
1:O:106:ASP:HB2	1:O:108:ARG:HG2	1.99	0.44
1:P:82:PHE:CE2	1:P:88:MET:HG3	2.52	0.44
1:P:1338:SER:O	1:P:1360:HIS:ND1	2.47	0.44
1:K:470:THR:HG23	1:K:1248:GLY:O	2.18	0.44
1:K:743:ALA:CB	1:K:918:ARG:HH12	2.29	0.44
1:K:1135:ASN:OD1	1:K:1136:GLN:N	2.50	0.44
1:K:1188:PRO:HD3	1:K:1243:TRP:CE3	2.52	0.44
1:N:1236:TYR:HD1	1:N:1236:TYR:H	1.65	0.44
1:O:748:ILE:HD13	1:O:794:LEU:HD22	1.99	0.44
1:O:830:VAL:H	1:O:895:THR:CG2	2.29	0.44
1:P:118:VAL:HG12	1:P:1312:VAL:HB	1.99	0.44
1:P:170:ASP:OD1	1:P:174:ARG:NE	2.50	0.44
1:J:567:MET:SD	1:J:1022:HIS:HA	2.58	0.44
1:J:705:VAL:HG12	1:J:710:SER:HA	1.99	0.44
1:J:805:ALA:HB3	1:J:807:VAL:H	1.83	0.44
1:K:291:LEU:HD13	1:K:291:LEU:HA	1.78	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:400:ARG:NH1	1:N:1305:SER:HB3	2.32	0.44
1:N:903:ASP:OD1	1:N:918:ARG:HD3	2.18	0.44
1:O:279:VAL:HA	1:O:380:ALA:O	2.18	0.44
1:P:586:GLN:HG2	1:P:1013:VAL:HG13	1.99	0.44
1:J:95:PHE:HD1	1:J:95:PHE:HA	1.59	0.44
1:J:266:THR:C	1:J:305:PRO:HG3	2.38	0.44
1:J:581:GLN:CB	1:J:1021:MET:HE2	2.48	0.44
1:J:627:HIS:NE2	1:J:632:LYS:HE2	2.33	0.44
1:J:868:LEU:HD23	1:J:868:LEU:HA	1.69	0.44
1:J:1055:GLU:OE2	1:J:1109:ARG:NH2	2.51	0.44
1:K:279:VAL:HA	1:K:380:ALA:O	2.18	0.44
1:K:297:GLU:OE2	1:K:300:ASN:ND2	2.50	0.44
1:K:461:HIS:CD2	1:K:1125:PHE:CD1	3.06	0.44
1:K:464:LEU:HD11	1:K:1254:MET:HG2	1.93	0.44
1:K:921:GLN:HB2	1:K:996:TRP:CD1	2.52	0.44
1:N:409:VAL:HG11	1:N:1044:MET:HE2	1.99	0.44
1:N:867:ASP:CB	1:N:940:VAL:HG11	2.48	0.44
1:N:1050:ASP:OD2	1:N:1117:MET:HG2	2.17	0.44
1:O:282:VAL:HG12	1:O:1057:ILE:HG12	1.98	0.44
1:O:742:ARG:HD3	1:O:903:ASP:O	2.17	0.44
1:P:448:LEU:HB3	1:P:1119:ILE:HD12	1.98	0.44
1:P:488:SER:C	1:P:991:ALA:HB1	2.38	0.44
1:P:515:VAL:HG11	1:P:976:GLN:NE2	2.33	0.44
1:J:300:ASN:HB3	1:J:369:ALA:O	2.17	0.44
1:J:828:LEU:HD12	1:J:946:HIS:O	2.18	0.44
1:J:829:GLY:O	1:J:946:HIS:ND1	2.50	0.44
1:J:1048:ARG:HD3	1:J:1182:CYS:SG	2.58	0.44
1:K:193:ILE:HA	1:K:219:PHE:CE1	2.52	0.44
1:K:400:ARG:HD3	1:K:1051:GLU:OE2	2.18	0.44
1:N:68:PHE:HE2	1:N:79:ASN:HD21	1.65	0.44
1:N:491:HIS:HB2	1:N:899:ARG:NH2	2.33	0.44
1:N:831:ASP:OD1	1:N:833:GLN:HG2	2.18	0.44
1:P:531:HIS:ND1	1:P:532:PRO:HD2	2.33	0.44
1:P:830:VAL:H	1:P:895:THR:HG23	1.83	0.44
1:J:388:TYR:HD2	1:J:395:TYR:CD1	2.36	0.44
1:J:616:PRO:HB3	1:J:872:SER:HB2	2.00	0.44
1:J:934:SER:O	1:J:937:THR:OG1	2.34	0.44
1:K:458:VAL:HG21	1:K:1184:ILE:HD13	2.00	0.44
1:K:507:TYR:O	1:K:966:ASP:HB3	2.17	0.44
1:K:1374:LYS:HB2	1:K:1374:LYS:HE3	1.77	0.44
1:O:131:MET:HE3	1:O:1088:VAL:HG21	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:216:ILE:HA	1:J:219:PHE:CD2	2.53	0.44
1:N:448:LEU:HD22	1:O:1236:TYR:HE1	1.83	0.44
1:N:951:HIS:NE2	1:N:997:HIS:CD2	2.86	0.44
1:O:185:LEU:HD11	1:O:397:LEU:HD23	1.99	0.44
1:P:461:HIS:CE1	1:P:1128:PHE:HB2	2.53	0.44
1:P:1125:PHE:HE2	1:P:1146:VAL:HG11	1.82	0.44
5:Z:68:PRO:HB2	5:Z:71:GLN:NE2	2.19	0.44
1:J:209:LYS:NZ	1:O:1308:GLU:OE2	2.47	0.43
1:J:511:TYR:O	1:J:973:ARG:NH2	2.51	0.43
1:J:1321:LEU:HD12	1:J:1321:LEU:HA	1.78	0.43
1:K:564:HIS:CE1	1:K:908:GLN:HB3	2.52	0.43
1:N:1050:ASP:OD1	1:N:1115:THR:OG1	2.34	0.43
1:O:121:ASN:OD1	1:O:121:ASN:N	2.49	0.43
1:P:1132:ALA:HB1	1:P:1139:ASN:CG	2.39	0.43
1:K:733:PHE:N	1:K:733:PHE:CD1	2.85	0.43
1:N:569:GLY:HA3	1:N:1001:MET:SD	2.59	0.43
1:N:612:ASP:C	1:N:614:ALA:H	2.22	0.43
1:N:1255:TYR:HB2	1:N:1275:PHE:CD2	2.50	0.43
1:P:588:PHE:HE1	1:P:700:LEU:HD22	1.83	0.43
1:P:1052:ILE:HD12	1:P:1113:ILE:HG12	2.00	0.43
1:P:1216:ASN:HB2	1:P:1219:VAL:HG22	1.99	0.43
1:J:467:PRO:HD3	1:J:546:TYR:CZ	2.53	0.43
1:J:594:LEU:HD23	1:J:594:LEU:HA	1.86	0.43
1:J:826:CYS:HA	1:J:954:TYR:O	2.18	0.43
1:J:830:VAL:H	1:J:895:THR:CG2	2.31	0.43
1:K:448:LEU:HD23	1:K:448:LEU:HA	1.84	0.43
1:K:1125:PHE:HD2	1:K:1148:ALA:HB3	1.83	0.43
1:N:1:MET:HG2	1:N:35:HIS:ND1	2.33	0.43
1:N:106:ASP:N	1:N:106:ASP:OD1	2.50	0.43
1:N:903:ASP:HB3	1:N:909:GLN:NE2	2.33	0.43
1:J:1026:SER:O	1:J:1029:ALA:N	2.50	0.43
1:K:465:HIS:CD2	1:K:1133:PHE:HZ	2.36	0.43
1:K:796:LEU:HD21	1:K:925:VAL:HG13	2.01	0.43
1:K:1273:ALA:HA	1:K:1279:GLU:OE1	2.17	0.43
1:N:540:LEU:HD11	1:N:550:ILE:HD11	2.01	0.43
1:N:830:VAL:H	1:N:895:THR:CG2	2.31	0.43
1:N:943:CYS:O	1:N:944:LEU:HD23	2.17	0.43
1:O:956:ASP:HA	1:O:957:PRO:HD3	1.89	0.43
1:O:1127:VAL:O	1:O:1264:VAL:HG23	2.18	0.43
1:P:38:ASP:O	1:P:41:VAL:HG22	2.18	0.43
1:P:648:TRP:CZ3	1:P:682:MET:HE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:1378:LYS:H	1:P:1378:LYS:HD3	1.83	0.43
1:J:59:TYR:CD2	1:K:260:VAL:HG11	2.54	0.43
1:J:281:ILE:HD12	1:J:1058:LEU:HD23	2.01	0.43
1:J:282:VAL:HG12	1:J:1057:ILE:HG12	1.99	0.43
1:K:1048:ARG:NH2	1:K:1118:GLY:O	2.46	0.43
1:N:406:TYR:HD1	1:N:1047:VAL:HG22	1.84	0.43
1:N:722:ASN:CB	1:N:902:VAL:HG11	2.43	0.43
1:O:463:ARG:NH2	1:O:1253:ILE:O	2.51	0.43
1:O:634:VAL:O	1:O:637:VAL:HG12	2.18	0.43
1:O:1186:VAL:HG22	1:O:1250:LEU:HD22	2.01	0.43
1:J:92:LYS:HB3	1:J:120:LYS:O	2.19	0.43
1:J:399:ARG:CD	1:J:1320:PHE:HB3	2.48	0.43
1:J:439:TRP:CZ3	1:J:449:ALA:HB2	2.53	0.43
1:J:843:GLY:HA2	1:J:846:PHE:HB3	2.01	0.43
1:J:848:HIS:NE2	5:Z:22:PRO:HD2	2.34	0.43
1:J:1317:THR:OG1	1:J:1318:ASP:N	2.51	0.43
1:K:922:THR:HG23	1:K:950:PHE:CZ	2.53	0.43
1:N:664:LYS:HE2	1:N:668:ARG:HH21	1.83	0.43
1:N:1024:LYS:HE2	1:N:1024:LYS:HB3	1.84	0.43
1:N:1195:TYR:CG	1:N:1240:VAL:HG21	2.54	0.43
1:O:299:ASP:HB3	1:O:371:VAL:CG2	2.49	0.43
1:O:507:TYR:OH	1:O:985:ARG:HA	2.18	0.43
1:O:1357:HIS:CG	1:O:1358:TYR:H	2.36	0.43
1:P:496:HIS:CE1	1:P:501:VAL:HB	2.54	0.43
1:P:874:LEU:O	1:P:876:PRO:HD3	2.18	0.43
1:J:632:LYS:HZ1	1:J:887:SER:HB2	1.84	0.43
1:J:1246:GLN:H	1:J:1246:GLN:HG3	1.57	0.43
1:K:144:ILE:HA	1:K:145:PRO:HD3	1.91	0.43
1:K:801:ASP:OD1	1:K:801:ASP:N	2.42	0.43
1:K:853:ASP:O	1:K:854:GLU:HG3	2.18	0.43
1:N:903:ASP:HB3	1:N:909:GLN:HE21	1.83	0.43
1:N:1172:PRO:HB2	1:O:1223:LEU:HB2	2.00	0.43
1:N:1346:PHE:HB2	1:N:1353:HIS:CE1	2.53	0.43
1:O:531:HIS:CD2	1:O:533:SER:H	2.33	0.43
1:O:619:PHE:CE1	1:O:643:CYS:HB3	2.54	0.43
1:P:143:SER:OG	1:P:144:ILE:N	2.52	0.43
1:P:439:TRP:NE1	1:P:1340:ARG:HB2	2.34	0.43
1:P:544:PRO:HG3	1:P:1243:TRP:CE3	2.53	0.43
1:P:1260:ARG:HG2	1:P:1263:ALA:HB2	2.00	0.43
1:K:301:GLN:HE21	1:K:366:PRO:CB	2.32	0.43
1:K:481:ARG:HB3	1:K:539:ARG:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:572:PRO:HB2	1:K:574:PRO:HD2	2.01	0.43
1:K:810:LYS:O	1:K:814:TYR:HB2	2.19	0.43
1:K:1256:ASN:HD22	1:K:1276:ASN:HA	1.83	0.43
1:N:68:PHE:O	1:N:71:THR:OG1	2.35	0.43
1:O:75:VAL:HG23	1:O:267:TYR:CG	2.53	0.43
1:O:247:ARG:HD2	1:O:247:ARG:HA	1.74	0.43
1:O:335:MET:O	1:O:339:VAL:HG12	2.19	0.43
1:O:933:PHE:O	1:O:962:THR:HG21	2.19	0.43
1:O:1066:SER:HB3	1:O:1095:ILE:HG13	2.00	0.43
1:P:141:LEU:HA	1:P:141:LEU:HD23	1.85	0.43
1:J:805:ALA:CB	1:J:807:VAL:H	2.32	0.43
1:K:695:GLN:O	1:K:699:ARG:HG3	2.19	0.43
1:K:1099:LEU:H	1:K:1099:LEU:HG	1.44	0.43
1:N:280:PHE:CE1	1:N:1059:PHE:HB2	2.54	0.43
1:N:1073:ASN:HB2	1:N:1089:HIS:HB2	2.01	0.43
1:N:1124:PHE:HD1	1:N:1124:PHE:HA	1.68	0.43
1:O:132:GLU:HG2	1:O:1085:THR:HG22	2.01	0.43
1:P:133:LEU:HD13	1:P:138:LEU:HD21	2.00	0.43
1:P:491:HIS:HB2	1:P:899:ARG:CZ	2.48	0.43
1:P:543:HIS:HE1	1:P:545:LEU:HD12	1.84	0.43
1:P:638:PRO:HG2	1:P:882:ARG:HH22	1.84	0.43
1:J:839:LEU:HD23	1:J:865:LEU:HD11	2.01	0.43
1:J:933:PHE:N	1:J:962:THR:HG21	2.34	0.43
1:J:1276:ASN:O	1:J:1280:LEU:HB2	2.19	0.43
1:K:24:ASN:HB3	1:K:28:SER:HB3	2.00	0.43
1:K:711:VAL:HB	1:K:1028:MET:HE1	2.01	0.43
1:N:694:GLU:HG3	1:N:807:VAL:HG11	2.01	0.43
1:N:924:LEU:HD22	1:N:950:PHE:CE2	2.54	0.43
1:N:961:ALA:HB1	1:N:968:ALA:HA	2.00	0.43
1:O:549:TYR:CE1	1:O:561:ARG:HB2	2.53	0.43
1:O:742:ARG:O	1:O:744:PRO:HD3	2.19	0.43
1:P:439:TRP:CE2	1:P:449:ALA:HB2	2.54	0.43
1:P:1188:PRO:HD3	1:P:1243:TRP:CE3	2.54	0.43
1:K:83:LYS:HE3	1:K:83:LYS:HB3	1.85	0.42
1:K:152:ALA:O	1:K:155:VAL:HG22	2.19	0.42
1:K:192:PHE:CZ	1:K:223:LEU:HD12	2.54	0.42
1:K:458:VAL:HG21	1:K:1184:ILE:HB	2.01	0.42
1:K:598:VAL:HG13	1:K:602:VAL:HG22	2.00	0.42
1:K:613:THR:O	1:K:934:SER:HB2	2.18	0.42
1:K:783:ARG:HA	1:K:788:HIS:CE1	2.54	0.42
1:K:1353:HIS:CE1	1:K:1364:GLU:OE2	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:484:ARG:HH22	1:N:558:ALA:CA	2.26	0.42
1:O:456:LEU:HD22	1:O:1030:TYR:HB3	2.01	0.42
1:O:487:TYR:CD2	1:O:488:SER:HB3	2.54	0.42
1:P:763:ILE:HA	1:P:794:LEU:HB3	2.01	0.42
1:P:980:VAL:HG22	1:P:981:GLU:OE2	2.19	0.42
1:P:1064:SER:OG	1:P:1065:THR:N	2.52	0.42
1:J:69:LEU:HD21	1:J:79:ASN:ND2	2.34	0.42
1:J:1222:GLY:O	1:J:1226:ASP:HB3	2.19	0.42
1:K:1259:TYR:O	1:K:1259:TYR:CG	2.72	0.42
1:N:61:ASN:OD1	1:N:62:ALA:N	2.52	0.42
1:N:122:CYS:HA	1:N:1094:SER:O	2.19	0.42
1:P:215:LEU:HD23	1:P:215:LEU:HA	1.98	0.42
1:P:723:LEU:O	1:P:810:LYS:NZ	2.40	0.42
1:J:280:PHE:CE2	1:J:379:VAL:HG11	2.55	0.42
1:J:388:TYR:CD2	1:J:396:PRO:HD3	2.53	0.42
1:J:660:PHE:CD2	1:J:809:GLU:HG2	2.53	0.42
1:J:678:GLU:OE1	1:J:678:GLU:N	2.38	0.42
1:K:567:MET:SD	1:K:1022:HIS:ND1	2.91	0.42
1:N:484:ARG:HH22	1:N:558:ALA:HB2	1.81	0.42
1:N:769:MET:HB2	1:N:890:THR:HG21	2.00	0.42
1:P:458:VAL:HG21	1:P:1184:ILE:HD13	2.00	0.42
1:J:255:VAL:HB	1:J:256:SER:H	1.52	0.42
1:J:388:TYR:HD2	1:J:395:TYR:HD1	1.68	0.42
1:J:626:ILE:HD11	1:J:636:ASN:HD22	1.84	0.42
1:K:507:TYR:CG	1:K:967:VAL:HG22	2.54	0.42
1:K:681:SER:HA	1:K:684:ARG:NH1	2.33	0.42
1:K:842:ASN:ND2	1:K:844:PRO:HD2	2.35	0.42
1:N:587:GLN:NE2	1:N:1038:ILE:HA	2.35	0.42
1:N:615:TYR:CD1	1:N:616:PRO:HD2	2.54	0.42
1:N:829:GLY:HA3	1:N:946:HIS:NE2	2.34	0.42
1:N:1048:ARG:NH2	1:N:1118:GLY:O	2.53	0.42
1:N:1049:THR:HG23	1:N:1270:PRO:HB3	2.02	0.42
1:O:466:THR:HB	1:O:910:LEU:HB3	2.02	0.42
1:O:507:TYR:CD2	1:O:967:VAL:HG22	2.54	0.42
1:O:1184:ILE:O	1:O:1255:TYR:OH	2.26	0.42
1:J:221:ARG:HE	1:J:221:ARG:HB3	1.72	0.42
1:J:531:HIS:HD2	1:J:533:SER:HB3	1.83	0.42
1:J:580:PHE:CE1	1:J:1189:VAL:HG11	2.54	0.42
1:J:610:ALA:HA	1:J:931:PHE:CE1	2.55	0.42
1:J:1127:VAL:HG13	1:J:1128:PHE:CD2	2.55	0.42
1:J:1203:ARG:H	1:J:1203:ARG:HG3	1.71	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1209:VAL:HG12	1:J:1212:CYS:SG	2.59	0.42
1:K:209:LYS:HG3	1:K:1211:SER:O	2.19	0.42
1:O:259:SER:OG	1:O:1098:GLY:HA2	2.19	0.42
1:P:1141:TYR:CZ	1:P:1145:LYS:HG3	2.54	0.42
1:J:160:THR:O	1:J:163:SER:OG	2.32	0.42
1:J:448:LEU:HD23	1:J:448:LEU:HA	1.90	0.42
1:J:653:ARG:HH22	1:O:684:ARG:CZ	2.33	0.42
1:J:947:ALA:HB2	1:J:963:MET:HB2	2.02	0.42
1:K:277:GLY:O	1:K:1062:ARG:HB2	2.19	0.42
1:K:439:TRP:CZ3	1:K:449:ALA:HB2	2.54	0.42
1:N:247:ARG:HD2	1:N:247:ARG:HA	1.77	0.42
1:O:507:TYR:CG	1:O:967:VAL:HG22	2.54	0.42
1:O:617:ALA:O	1:O:620:TYR:HD1	2.03	0.42
1:P:185:LEU:HD23	1:P:1058:LEU:HD13	2.00	0.42
1:P:293:PHE:HD1	1:P:293:PHE:HA	1.66	0.42
1:P:636:ASN:O	1:P:640:VAL:HG13	2.19	0.42
1:P:724:LEU:O	1:P:921:GLN:NE2	2.41	0.42
1:P:1051:GLU:N	1:P:1115:THR:OG1	2.38	0.42
5:Z:67:VAL:O	5:Z:67:VAL:HG12	2.19	0.42
1:J:660:PHE:N	1:J:813:TYR:OH	2.40	0.42
1:J:824:HIS:HA	1:J:956:ASP:CG	2.39	0.42
1:K:603:ILE:HG21	1:K:1010:PRO:O	2.20	0.42
1:N:566:LEU:HD23	1:N:566:LEU:HA	1.93	0.42
1:P:1203:ARG:H	1:P:1203:ARG:HG3	1.52	0.42
1:J:35:HIS:CD2	1:J:35:HIS:H	2.36	0.42
1:J:499:VAL:HA	1:J:502:ILE:HD12	2.02	0.42
1:J:637:VAL:HG13	1:J:638:PRO:HD3	2.02	0.42
1:J:980:VAL:HG23	1:J:981:GLU:OE2	2.19	0.42
1:K:207:PHE:CE2	1:K:1287:LEU:HD21	2.55	0.42
1:K:1300:GLY:O	1:K:1302:PRO:HD3	2.20	0.42
1:K:1353:HIS:ND1	1:K:1353:HIS:O	2.52	0.42
1:N:1075:SER:OG	1:N:1076:ARG:N	2.52	0.42
1:O:687:TYR:CE2	1:O:691:ILE:HD11	2.54	0.42
1:O:884:LEU:HD23	1:O:884:LEU:HA	1.94	0.42
1:P:232:ARG:HB3	1:P:1370:ARG:HD2	2.02	0.42
1:J:650:ARG:NH2	1:J:873:ASP:HB3	2.35	0.42
1:J:1057:ILE:HG13	1:J:1108:ALA:HB2	2.02	0.42
1:J:1173:GLY:O	1:K:1232:ALA:HB2	2.20	0.42
1:K:92:LYS:HB2	1:K:92:LYS:HE3	1.80	0.42
1:K:539:ARG:O	1:K:540:LEU:HD23	2.20	0.42
1:J:471:LEU:HD12	1:J:912:PRO:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:506:PHE:CE2	1:J:510:LYS:HE3	2.55	0.42
1:K:491:HIS:CG	1:K:899:ARG:HD2	2.55	0.42
1:K:521:LYS:HG2	1:K:537:LEU:HD13	2.01	0.42
1:K:573:THR:N	1:K:574:PRO:HD2	2.34	0.42
1:K:630:GLU:CD	1:K:665:PHE:HE1	2.24	0.42
1:N:54:VAL:HA	1:O:327:VAL:O	2.20	0.42
1:N:602:VAL:O	1:N:606:VAL:HG23	2.20	0.42
1:O:917:LYS:HB2	1:O:917:LYS:HE3	1.63	0.42
1:P:245:ARG:NH2	1:P:294:LEU:HB3	2.35	0.42
1:P:904:ASN:HB3	1:P:908:GLN:HB2	2.01	0.42
5:Z:69:ARG:HG3	5:Z:69:ARG:O	2.20	0.42
1:J:294:LEU:HD23	1:J:294:LEU:HA	1.84	0.41
1:J:852:ARG:O	1:J:879:GLY:N	2.53	0.41
1:K:720:ASP:O	1:K:810:LYS:NZ	2.53	0.41
1:N:408:PRO:HG3	1:N:1196:PHE:CD2	2.54	0.41
1:N:543:HIS:HD2	1:N:546:TYR:N	2.14	0.41
1:N:842:ASN:ND2	1:N:865:LEU:HD23	2.34	0.41
1:N:961:ALA:O	1:N:968:ALA:HB2	2.20	0.41
1:N:1298:LEU:HA	1:N:1298:LEU:HD13	1.74	0.41
1:O:78:VAL:HG21	1:O:261:LEU:CD1	2.46	0.41
1:P:573:THR:N	1:P:574:PRO:HD2	2.35	0.41
1:P:658:ASN:OD1	1:P:929:VAL:HG23	2.20	0.41
1:J:174:ARG:CB	1:K:102:ILE:HG12	2.50	0.41
1:K:290:LEU:HD23	1:K:290:LEU:HA	1.88	0.41
1:K:652:GLY:C	1:K:653:ARG:HD3	2.41	0.41
1:K:1036:LEU:HD13	1:K:1036:LEU:HA	1.90	0.41
1:N:672:ASN:HB3	1:N:673:ASN:H	1.61	0.41
1:N:1146:VAL:HG13	1:N:1148:ALA:H	1.84	0.41
1:O:735:HIS:O	1:O:739:VAL:HG22	2.21	0.41
1:O:765:ARG:HA	1:O:765:ARG:HD3	1.91	0.41
1:O:799:TYR:CE2	1:O:801:ASP:HB3	2.55	0.41
1:P:758:ALA:HB1	1:P:762:PHE:CD1	2.54	0.41
1:K:69:LEU:HA	1:K:69:LEU:HD12	1.80	0.41
1:K:151:TYR:O	1:K:155:VAL:HG13	2.19	0.41
1:K:279:VAL:HG22	1:K:380:ALA:HB3	2.02	0.41
1:K:724:LEU:HD12	1:K:900:VAL:HG21	2.01	0.41
1:K:803:GLY:O	1:K:805:ALA:N	2.53	0.41
1:O:258:GLU:HA	1:O:262:LYS:CD	2.50	0.41
1:O:632:LYS:HA	1:O:635:MET:SD	2.60	0.41
1:J:255:VAL:CG1	1:J:1102:SER:HA	2.50	0.41
1:J:304:GLY:HA2	1:J:305:PRO:HD3	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:482:ASP:CG	1:J:484:ARG:HE	2.23	0.41
1:J:539:ARG:O	1:J:540:LEU:HD23	2.20	0.41
1:J:654:LEU:HB2	1:J:683:TYR:CE2	2.55	0.41
1:J:684:ARG:NH2	1:K:653:ARG:HH22	2.18	0.41
1:K:232:ARG:HE	1:K:232:ARG:HB2	1.32	0.41
1:K:1115:THR:O	1:K:1116:ASP:HB3	2.20	0.41
1:N:484:ARG:NE	1:N:550:ILE:HG22	2.36	0.41
1:N:1175:CYS:H	1:O:1232:ALA:HB1	1.86	0.41
1:O:332:GLU:OE1	1:O:333:HIS:HD2	2.04	0.41
1:O:467:PRO:HG3	1:O:546:TYR:CD1	2.55	0.41
1:P:542:LEU:HD23	1:P:1248:GLY:C	2.41	0.41
1:P:746:ILE:HG23	1:P:900:VAL:HG22	2.02	0.41
1:J:722:ASN:OD1	1:J:742:ARG:NH2	2.54	0.41
1:J:775:GLN:O	1:J:779:LEU:HG	2.20	0.41
1:J:884:LEU:HD23	1:J:884:LEU:HA	1.84	0.41
1:J:981:GLU:OE1	1:J:999:SER:HB3	2.21	0.41
1:J:1160:THR:O	1:J:1160:THR:OG1	2.36	0.41
1:K:395:TYR:CE1	1:K:397:LEU:HB2	2.55	0.41
1:K:488:SER:O	1:K:488:SER:OG	2.38	0.41
1:N:884:LEU:HD23	1:N:884:LEU:HA	1.80	0.41
1:O:618:PHE:O	1:O:621:VAL:HB	2.21	0.41
1:O:631:GLU:O	1:O:635:MET:HG3	2.21	0.41
1:O:920:GLU:HG2	1:O:994:ARG:HB3	2.03	0.41
1:O:1047:VAL:O	1:O:1182:CYS:HA	2.20	0.41
1:P:647:TYR:CE2	1:P:653:ARG:HG3	2.55	0.41
1:P:770:ASP:HA	1:P:776:PHE:CE1	2.55	0.41
1:P:831:ASP:H	1:P:944:LEU:CD2	2.33	0.41
1:P:981:GLU:HB3	1:P:999:SER:HB3	2.02	0.41
1:J:672:ASN:OD1	1:K:873:ASP:HB2	2.21	0.41
1:K:488:SER:OG	1:K:992:GLU:HB3	2.21	0.41
1:K:1145:LYS:HD2	1:K:1145:LYS:HA	1.84	0.41
1:O:280:PHE:CE2	1:O:379:VAL:HG11	2.55	0.41
1:O:399:ARG:HG3	1:O:1105:MET:HE1	2.03	0.41
1:O:475:ASN:HB3	1:O:560:HIS:CD2	2.47	0.41
1:O:985:ARG:HD3	1:O:990:PHE:HE2	1.84	0.41
1:P:462:PRO:O	1:P:466:THR:HG23	2.20	0.41
1:P:658:ASN:HB2	1:P:931:PHE:HE2	1.85	0.41
1:P:682:MET:HE3	1:P:682:MET:HB2	1.87	0.41
1:P:832:PHE:CD2	1:P:891:CYS:HB3	2.55	0.41
1:J:544:PRO:HG3	1:J:1243:TRP:CE3	2.56	0.41
1:J:568:VAL:HG12	1:J:581:GLN:HE22	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1053:LEU:HA	1:J:1053:LEU:HD23	1.77	0.41
1:N:95:PHE:HE1	1:N:260:VAL:HG21	1.85	0.41
1:N:284:ASP:N	1:N:284:ASP:OD1	2.50	0.41
1:N:429:ASN:O	1:N:433:GLN:HG3	2.20	0.41
1:N:697:LEU:HD23	1:N:697:LEU:HA	1.91	0.41
1:N:1119:ILE:H	1:N:1119:ILE:HG13	1.67	0.41
1:O:469:HIS:HB3	1:O:1253:ILE:HD12	2.02	0.41
1:O:902:VAL:HG23	1:O:903:ASP:O	2.20	0.41
1:P:722:ASN:OD1	1:P:742:ARG:NH2	2.54	0.41
1:P:807:VAL:HG12	1:P:811:ILE:HG13	2.03	0.41
1:J:596:HIS:HD2	1:J:1012:LEU:HD22	1.86	0.41
1:J:616:PRO:HB3	1:J:872:SER:CB	2.50	0.41
1:N:987:GLU:H	1:N:987:GLU:HG3	1.72	0.41
1:O:616:PRO:HB3	1:O:872:SER:HB3	2.02	0.41
1:O:1267:LEU:HD23	1:O:1267:LEU:HA	1.81	0.41
1:J:38:ASP:OD1	1:J:39:LEU:N	2.54	0.41
1:J:400:ARG:O	1:J:1321:LEU:HD12	2.21	0.41
1:J:544:PRO:HG3	1:J:1243:TRP:CE2	2.56	0.41
1:J:596:HIS:CD2	1:J:1012:LEU:HD22	2.56	0.41
1:J:637:VAL:N	1:J:638:PRO:HD2	2.35	0.41
1:J:670:LEU:HD21	1:J:675:ILE:CG1	2.51	0.41
1:J:1261:GLN:O	1:J:1261:GLN:HG2	2.21	0.41
1:K:94:GLN:HE21	1:K:117:ILE:HG21	1.85	0.41
1:K:747:ILE:HB	1:K:899:ARG:HB2	2.02	0.41
1:K:814:TYR:OH	1:K:921:GLN:NE2	2.53	0.41
1:K:947:ALA:HB2	1:K:963:MET:CB	2.51	0.41
1:K:1154:LEU:O	1:K:1155:LEU:HD13	2.20	0.41
1:K:1335:LEU:HD23	1:K:1335:LEU:HA	1.88	0.41
1:N:216:ILE:HD12	1:N:216:ILE:HA	1.82	0.41
1:N:256:SER:OG	1:N:1100:SER:HB2	2.21	0.41
1:N:458:VAL:HG21	1:N:1184:ILE:HB	2.03	0.41
1:N:633:PHE:CE2	1:N:665:PHE:HB3	2.56	0.41
1:N:736:LEU:HG	1:N:740:SER:OG	2.21	0.41
1:N:753:TYR:CE1	1:N:762:PHE:HB2	2.55	0.41
1:N:1077:ARG:O	1:N:1085:THR:OG1	2.26	0.41
1:N:1188:PRO:HD2	1:N:1241:ASN:HB3	2.01	0.41
1:O:1304:THR:HG22	1:O:1311:PHE:O	2.21	0.41
1:P:328:MET:O	1:P:332:GLU:HG2	2.21	0.41
1:P:408:PRO:HB2	1:P:411:LEU:HD13	2.02	0.41
1:P:863:GLY:CA	1:P:866:ARG:HB3	2.50	0.41
1:P:1276:ASN:O	1:P:1280:LEU:HG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:1292:ASN:HA	1:P:1295:SER:OG	2.20	0.41
1:J:453:GLN:HA	1:J:456:LEU:HD22	2.01	0.41
1:K:1116:ASP:OD1	1:K:1176:HIS:HB3	2.21	0.41
1:K:1162:LEU:HD12	1:K:1163:ALA:N	2.36	0.41
1:N:464:LEU:HD11	1:N:1254:MET:SD	2.61	0.41
1:N:484:ARG:HD2	1:N:550:ILE:CB	2.45	0.41
1:N:549:TYR:CZ	1:N:561:ARG:HB2	2.55	0.41
1:N:817:LEU:HA	1:N:817:LEU:HD23	1.84	0.41
1:O:68:PHE:HA	1:O:177:ILE:HD11	2.02	0.41
1:O:598:VAL:HG13	1:O:599:ASP:O	2.21	0.41
1:O:985:ARG:HD3	1:O:990:PHE:CE2	2.56	0.41
1:P:285:ASN:ND2	1:P:1055:GLU:OE2	2.51	0.41
1:P:717:ALA:HA	1:P:1024:LYS:HE3	2.03	0.41
1:P:854:GLU:O	1:P:878:VAL:HG23	2.21	0.41
1:J:73:LEU:HD13	1:J:177:ILE:HD11	2.03	0.40
1:J:282:VAL:HG23	1:J:283:THR:O	2.21	0.40
1:J:540:LEU:HD11	1:J:550:ILE:HD11	2.03	0.40
1:K:535:TYR:CE1	1:K:1227:HIS:HB2	2.56	0.40
1:N:59:TYR:CE1	1:O:260:VAL:HG21	2.51	0.40
1:N:270:ALA:HA	1:N:303:MET:HG2	2.03	0.40
1:N:1215:TYR:HE1	1:N:1285:ARG:HG2	1.86	0.40
1:O:483:ARG:HD3	1:O:551:GLY:O	2.20	0.40
1:O:544:PRO:HG3	1:O:1243:TRP:CD2	2.57	0.40
1:P:70:GLU:O	1:P:367:ILE:HG23	2.21	0.40
1:P:783:ARG:NH1	1:P:888:PHE:O	2.46	0.40
1:J:245:ARG:HA	1:J:245:ARG:HD2	1.94	0.40
1:K:356:ALA:C	1:K:358:GLY:H	2.24	0.40
1:K:367:ILE:HD13	1:K:367:ILE:HA	1.87	0.40
1:K:487:TYR:HD1	1:K:516:THR:HG23	1.86	0.40
1:K:487:TYR:OH	1:K:985:ARG:N	2.44	0.40
1:K:1250:LEU:HA	1:K:1253:ILE:HG22	2.03	0.40
1:N:899:ARG:HH21	1:N:920:GLU:CD	2.24	0.40
1:N:999:SER:N	1:N:1000:PRO:HD2	2.35	0.40
1:N:1217:GLN:OE1	1:N:1281:LEU:HD13	2.21	0.40
1:O:43:LYS:C	1:P:314:ARG:HH12	2.25	0.40
1:O:481:ARG:NH2	1:O:540:LEU:HD23	2.36	0.40
1:O:839:LEU:HD23	1:O:839:LEU:HA	1.88	0.40
1:P:271:LYS:H	1:P:299:ASP:HB3	1.85	0.40
1:P:534:ASN:OD1	1:P:537:LEU:HB2	2.21	0.40
1:P:777:VAL:HA	1:P:780:TYR:HB3	2.03	0.40
1:J:251:MET:HE3	1:J:251:MET:HB2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:432:GLN:CD	1:J:586:GLN:HG3	2.42	0.40
1:J:456:LEU:HA	1:J:456:LEU:HD12	1.82	0.40
1:J:714:TYR:N	1:J:714:TYR:CD1	2.89	0.40
1:J:1143:LYS:HE3	1:J:1143:LYS:HB2	1.94	0.40
1:N:185:LEU:HD13	1:N:399:ARG:HH21	1.87	0.40
1:N:830:VAL:H	1:N:895:THR:HG23	1.86	0.40
1:O:474:LEU:HG	1:O:560:HIS:NE2	2.37	0.40
1:O:545:LEU:HD23	1:O:545:LEU:HA	1.91	0.40
1:O:576:ALA:HB1	1:O:580:PHE:CD2	2.55	0.40
1:O:746:ILE:HB	1:O:753:TYR:HB3	2.03	0.40
1:O:951:HIS:NE2	1:O:997:HIS:HD2	2.18	0.40
1:O:1257:SER:HB3	1:O:1276:ASN:CG	2.42	0.40
1:P:86:SER:OG	1:P:87:ARG:NH2	2.54	0.40
1:P:191:MET:HE2	1:P:251:MET:HA	2.04	0.40
1:P:388:TYR:HE2	1:P:396:PRO:HD3	1.86	0.40
1:P:679:ALA:O	1:P:683:TYR:HD1	2.03	0.40
1:P:759:ALA:HB1	1:P:763:ILE:HD13	2.03	0.40
1:P:1007:GLU:H	1:P:1007:GLU:HG2	1.73	0.40
5:Z:68:PRO:HB3	5:Z:71:GLN:CD	2.20	0.40
1:J:405:TYR:CD1	1:J:1334:ALA:HB2	2.56	0.40
1:J:948:ILE:HG22	1:J:950:PHE:HD1	1.86	0.40
1:J:1358:TYR:CZ	1:O:427:LEU:HD11	2.57	0.40
1:K:224:LEU:HD23	1:K:224:LEU:HA	1.90	0.40
1:K:893:THR:OG1	1:K:894:PHE:N	2.54	0.40
1:N:352:LEU:HD23	1:N:352:LEU:HA	1.83	0.40
1:O:989:LEU:HD23	1:O:989:LEU:HA	1.95	0.40
1:O:1115:THR:CG2	1:O:1180:ALA:HB2	2.52	0.40
1:O:1122:GLN:NE2	1:O:1127:VAL:HG21	2.32	0.40
1:J:25:LEU:HA	1:J:25:LEU:HD23	1.89	0.40
1:J:54:VAL:HG12	1:K:327:VAL:HB	2.04	0.40
1:J:955:GLY:HA3	1:J:985:ARG:NE	2.25	0.40
1:K:399:ARG:HD2	1:K:1320:PHE:HB3	2.04	0.40
1:K:651:SER:HB2	1:K:653:ARG:HE	1.86	0.40
1:K:1009:LEU:HA	1:K:1010:PRO:HD3	1.92	0.40
1:K:1195:TYR:HD1	1:K:1234:TYR:HE2	1.69	0.40
1:N:603:ILE:HG21	1:N:1010:PRO:O	2.21	0.40
1:N:671:GLY:O	1:N:672:ASN:O	2.40	0.40
1:N:695:GLN:HG2	1:O:958:ARG:CZ	2.51	0.40
1:N:966:ASP:O	1:N:969:THR:OG1	2.31	0.40
1:N:1005:ALA:HA	1:N:1008:CYS:HB2	2.04	0.40
1:O:430:PRO:O	1:O:433:GLN:HG2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:670:LEU:HD22	1:O:680:TYR:CD1	2.57	0.40
1:O:947:ALA:HB2	1:O:963:MET:CB	2.45	0.40
1:P:494:PRO:HG2	1:P:749:GLY:HA2	2.04	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	J	1348/1381 (98%)	1269 (94%)	72 (5%)	7 (0%)	29	67
1	K	1379/1381 (100%)	1310 (95%)	67 (5%)	2 (0%)	51	84
1	N	1358/1381 (98%)	1288 (95%)	62 (5%)	8 (1%)	25	63
1	O	1328/1381 (96%)	1259 (95%)	68 (5%)	1 (0%)	51	84
1	P	1273/1381 (92%)	1202 (94%)	69 (5%)	2 (0%)	47	79
2	v	282/507 (56%)	262 (93%)	19 (7%)	1 (0%)	34	71
3	w	66/570 (12%)	65 (98%)	1 (2%)	0	100	100
3	x	66/570 (12%)	66 (100%)	0	0	100	100
4	y	35/3149 (1%)	34 (97%)	1 (3%)	0	100	100
4	z	35/3149 (1%)	34 (97%)	1 (3%)	0	100	100
5	Z	75/176 (43%)	67 (89%)	6 (8%)	2 (3%)	5	34
5	a	75/176 (43%)	70 (93%)	5 (7%)	0	100	100
5	d	75/176 (43%)	69 (92%)	4 (5%)	2 (3%)	5	34
5	e	75/176 (43%)	72 (96%)	3 (4%)	0	100	100
5	u	61/176 (35%)	56 (92%)	5 (8%)	0	100	100
6	f	307/364 (84%)	289 (94%)	18 (6%)	0	100	100
6	h	330/364 (91%)	305 (92%)	25 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	k	297/301 (99%)	282 (95%)	14 (5%)	1 (0%)	41	75
7	m	297/301 (99%)	282 (95%)	13 (4%)	2 (1%)	22	61
7	p	297/301 (99%)	282 (95%)	10 (3%)	5 (2%)	9	43
7	r	297/301 (99%)	288 (97%)	8 (3%)	1 (0%)	41	75
All	All	9356/17662 (53%)	8851 (95%)	471 (5%)	34 (0%)	38	71

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	305	PRO
1	J	366	PRO
1	K	298	ALA
1	K	805	ALA
1	N	483	ARG
1	N	484	ARG
1	N	672	ASN
1	N	675	ILE
1	N	678	GLU
1	O	259	SER
5	Z	69	ARG
5	d	7	LYS
7	p	39	ASN
7	p	98	GLN
1	J	255	VAL
1	N	481	ARG
1	N	677	LYS
7	k	15	THR
1	J	9	ASN
1	N	873	ASP
1	P	806	ASP
7	p	36	GLY
1	J	306	SER
1	J	1316	GLY
2	v	382	ASN
5	Z	68	PRO
7	r	202	LEU
1	P	106	ASP
7	m	197	LEU
7	p	38	GLN
5	d	6	PRO
1	J	367	ILE

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Mol	Chain	Res	Type
7	m	164	PRO
7	p	99	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	J	1149/1171 (98%)	1092 (95%)	57 (5%)	24	52
1	K	1171/1171 (100%)	1126 (96%)	45 (4%)	33	59
1	N	1155/1171 (99%)	1102 (95%)	53 (5%)	27	54
1	O	1128/1171 (96%)	1080 (96%)	48 (4%)	29	56
1	P	1093/1171 (93%)	1058 (97%)	35 (3%)	39	62
2	v	243/400 (61%)	227 (93%)	16 (7%)	16	45
3	w	57/465 (12%)	57 (100%)	0	100	100
3	x	57/465 (12%)	57 (100%)	0	100	100
4	y	35/2539 (1%)	34 (97%)	1 (3%)	42	65
4	z	35/2539 (1%)	34 (97%)	1 (3%)	42	65
5	Z	71/128 (56%)	70 (99%)	1 (1%)	67	81
5	a	71/128 (56%)	69 (97%)	2 (3%)	43	65
5	d	71/128 (56%)	69 (97%)	2 (3%)	43	65
5	e	71/128 (56%)	70 (99%)	1 (1%)	67	81
5	u	59/128 (46%)	59 (100%)	0	100	100
6	f	267/289 (92%)	261 (98%)	6 (2%)	52	71
6	h	278/289 (96%)	261 (94%)	17 (6%)	18	47
7	k	265/267 (99%)	258 (97%)	7 (3%)	46	67
7	m	265/267 (99%)	248 (94%)	17 (6%)	17	45
7	p	265/267 (99%)	252 (95%)	13 (5%)	25	52
7	r	265/267 (99%)	256 (97%)	9 (3%)	37	61
All	All	8071/14549 (56%)	7740 (96%)	331 (4%)	34	57

All (331) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	5	GLU
1	J	39	LEU
1	J	66	VAL
1	J	89	THR
1	J	95	PHE
1	J	101	THR
1	J	129	THR
1	J	144	ILE
1	J	147	THR
1	J	165	LEU
1	J	203	THR
1	J	216	ILE
1	J	248	LEU
1	J	255	VAL
1	J	259	SER
1	J	287	LEU
1	J	306	SER
1	J	308	TYR
1	J	365	VAL
1	J	367	ILE
1	J	393	SER
1	J	445	ASN
1	J	456	LEU
1	J	458	VAL
1	J	466	THR
1	J	481	ARG
1	J	518	ILE
1	J	536	ASP
1	J	602	VAL
1	J	639	LEU
1	J	641	SER
1	J	657	VAL
1	J	675	ILE
1	J	706	VAL
1	J	710	SER
1	J	716	CYS
1	J	847	SER
1	J	851	THR
1	J	853	ASP
1	J	861	GLU
1	J	928	LEU
1	J	1065	THR

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Mol	Chain	Res	Type
1	J	1066	SER
1	J	1094	SER
1	J	1106	THR
1	J	1156	ARG
1	J	1161	TYR
1	J	1182	CYS
1	J	1189	VAL
1	J	1192	ASP
1	J	1199	SER
1	J	1209	VAL
1	J	1223	LEU
1	J	1262	THR
1	J	1269	SER
1	J	1312	VAL
1	J	1313	VAL
1	K	39	LEU
1	K	54	VAL
1	K	96	ARG
1	K	147	THR
1	K	179	THR
1	K	182	SER
1	K	232	ARG
1	K	291	LEU
1	K	314	ARG
1	K	361	ASP
1	K	381	VAL
1	K	440	ILE
1	K	451	ASN
1	K	486	THR
1	K	517	ASP
1	K	526	THR
1	K	589	GLU
1	K	602	VAL
1	K	637	VAL
1	K	653	ARG
1	K	654	LEU
1	K	690	LEU
1	K	693	LEU
1	K	697	LEU
1	K	711	VAL
1	K	742	ARG
1	K	794	LEU

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Mol	Chain	Res	Type
1	K	851	THR
1	K	874	LEU
1	K	905	ASP
1	K	907	THR
1	K	928	LEU
1	K	964	HIS
1	K	1018	MET
1	K	1048	ARG
1	K	1049	THR
1	K	1054	SER
1	K	1099	LEU
1	K	1168	VAL
1	K	1189	VAL
1	K	1209	VAL
1	K	1238	SER
1	K	1267	LEU
1	K	1305	SER
1	K	1353	HIS
1	N	17	VAL
1	N	41	VAL
1	N	54	VAL
1	N	113	GLN
1	N	194	LEU
1	N	213	SER
1	N	216	ILE
1	N	284	ASP
1	N	355	VAL
1	N	381	VAL
1	N	419	THR
1	N	425	LYS
1	N	456	LEU
1	N	482	ASP
1	N	483	ARG
1	N	484	ARG
1	N	485	GLU
1	N	486	THR
1	N	489	LEU
1	N	501	VAL
1	N	550	ILE
1	N	598	VAL
1	N	637	VAL
1	N	657	VAL

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Mol	Chain	Res	Type
1	N	670	LEU
1	N	672	ASN
1	N	673	ASN
1	N	675	ILE
1	N	676	SER
1	N	700	LEU
1	N	704	ASP
1	N	736	LEU
1	N	740	SER
1	N	769	MET
1	N	813	TYR
1	N	853	ASP
1	N	905	ASP
1	N	925	VAL
1	N	933	PHE
1	N	938	ARG
1	N	950	PHE
1	N	1044	MET
1	N	1048	ARG
1	N	1099	LEU
1	N	1116	ASP
1	N	1124	PHE
1	N	1201	SER
1	N	1209	VAL
1	N	1256	ASN
1	N	1287	LEU
1	N	1336	SER
1	N	1347	MET
1	N	1352	THR
1	O	47	GLU
1	O	52	PHE
1	O	84	ASP
1	O	88	MET
1	O	104	HIS
1	O	136	LEU
1	O	137	ASP
1	O	147	THR
1	O	194	LEU
1	O	197	LEU
1	O	216	ILE
1	O	230	LEU
1	O	256	SER

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Mol	Chain	Res	Type
1	O	258	GLU
1	O	259	SER
1	O	260	VAL
1	O	261	LEU
1	O	279	VAL
1	O	294	LEU
1	O	313	VAL
1	O	466	THR
1	O	592	THR
1	O	598	VAL
1	O	602	VAL
1	O	637	VAL
1	O	653	ARG
1	O	654	LEU
1	O	657	VAL
1	O	681	SER
1	O	700	LEU
1	O	851	THR
1	O	860	LEU
1	O	865	LEU
1	O	866	ARG
1	O	873	ASP
1	O	885	SER
1	O	940	VAL
1	O	941	THR
1	O	1053	LEU
1	O	1082	ASP
1	O	1116	ASP
1	O	1174	LEU
1	O	1183	GLU
1	O	1189	VAL
1	O	1282	ARG
1	O	1309	VAL
1	O	1335	LEU
1	O	1343	ILE
1	P	144	ILE
1	P	149	VAL
1	P	210	THR
1	P	211	VAL
1	P	227	SER
1	P	247	ARG
1	P	284	ASP

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Mol	Chain	Res	Type
1	P	293	PHE
1	P	319	VAL
1	P	333	HIS
1	P	597	VAL
1	P	598	VAL
1	P	675	ILE
1	P	756	THR
1	P	769	MET
1	P	796	LEU
1	P	813	TYR
1	P	838	THR
1	P	860	LEU
1	P	880	MET
1	P	881	ILE
1	P	895	THR
1	P	901	SER
1	P	928	LEU
1	P	929	VAL
1	P	1058	LEU
1	P	1071	THR
1	P	1106	THR
1	P	1110	VAL
1	P	1189	VAL
1	P	1203	ARG
1	P	1210	VAL
1	P	1260	ARG
1	P	1349	VAL
1	P	1378	LYS
2	v	9	VAL
2	v	15	THR
2	v	39	CYS
2	v	57	VAL
2	v	74	ARG
2	v	100	LEU
2	v	288	ILE
2	v	293	SER
2	v	374	THR
2	v	380	TYR
2	v	383	SER
2	v	385	LEU
2	v	387	ARG
2	v	392	THR

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Mol	Chain	Res	Type
2	v	397	VAL
2	v	409	SER
4	y	3137	LEU
4	z	3114	GLN
5	Z	69	ARG
5	a	20	ASP
5	a	31	ASN
5	d	52	THR
5	d	70	ARG
5	e	45	ARG
6	f	114	LYS
6	f	179	ARG
6	f	212	VAL
6	f	237	LEU
6	f	256	GLN
6	f	338	PHE
6	h	46	HIS
6	h	86	ARG
6	h	106	THR
6	h	125	VAL
6	h	134	LEU
6	h	197	SER
6	h	223	VAL
6	h	268	LEU
6	h	294	ARG
6	h	300	SER
6	h	308	VAL
6	h	311	LEU
6	h	327	PHE
6	h	328	SER
6	h	331	ASP
6	h	333	TRP
6	h	352	SER
7	k	45	LEU
7	k	69	LEU
7	k	131	ASP
7	k	182	LEU
7	k	199	LEU
7	k	271	LEU
7	k	293	THR
7	m	13	LEU
7	m	17	GLU

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Mol	Chain	Res	Type
7	m	31	LEU
7	m	77	VAL
7	m	84	LYS
7	m	86	VAL
7	m	96	LYS
7	m	122	THR
7	m	175	HIS
7	m	193	VAL
7	m	210	CYS
7	m	215	LEU
7	m	243	VAL
7	m	262	SER
7	m	271	LEU
7	m	274	LEU
7	m	293	THR
7	p	3	LEU
7	p	21	MET
7	p	27	CYS
7	p	45	LEU
7	p	54	VAL
7	p	98	GLN
7	p	101	PHE
7	p	148	GLN
7	p	182	LEU
7	p	197	LEU
7	p	199	LEU
7	p	202	LEU
7	p	245	ASP
7	r	3	LEU
7	r	27	CYS
7	r	76	SER
7	r	82	LEU
7	r	115	VAL
7	r	201	LEU
7	r	203	ASP
7	r	229	ARG
7	r	293	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (161) such sidechains are listed below:

Mol	Chain	Res	Type
1	J	35	HIS

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Mol	Chain	Res	Type
1	J	79	ASN
1	J	121	ASN
1	J	126	HIS
1	J	195	GLN
1	J	285	ASN
1	J	389	ASN
1	J	531	HIS
1	J	564	HIS
1	J	581	GLN
1	J	596	HIS
1	J	600	GLN
1	J	636	ASN
1	J	695	GLN
1	J	722	ASN
1	J	822	ASN
1	J	859	ASN
1	J	862	ASN
1	J	921	GLN
1	J	984	ASN
1	J	997	HIS
1	J	1022	HIS
1	J	1090	HIS
1	J	1176	HIS
1	J	1241	ASN
1	J	1292	ASN
1	J	1301	HIS
1	K	79	ASN
1	K	94	GLN
1	K	104	HIS
1	K	126	HIS
1	K	142	HIS
1	K	289	GLN
1	K	301	GLN
1	K	317	ASN
1	K	385	GLN
1	K	398	ASN
1	K	444	ASN
1	K	496	HIS
1	K	531	HIS
1	K	543	HIS
1	K	564	HIS
1	K	570	ASN

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Mol	Chain	Res	Type
1	K	722	ASN
1	K	822	ASN
1	K	904	ASN
1	K	951	HIS
1	K	984	ASN
1	K	997	HIS
1	K	1137	GLN
1	K	1167	ASN
1	K	1256	ASN
1	K	1284	ASN
1	K	1289	ASN
1	N	79	ASN
1	N	104	HIS
1	N	126	HIS
1	N	317	ASN
1	N	402	GLN
1	N	444	ASN
1	N	491	HIS
1	N	496	HIS
1	N	531	HIS
1	N	534	ASN
1	N	543	HIS
1	N	587	GLN
1	N	596	HIS
1	N	824	HIS
1	N	834	HIS
1	N	908	GLN
1	N	926	ASN
1	N	965	GLN
1	N	974	ASN
1	N	997	HIS
1	N	1033	GLN
1	N	1169	ASN
1	N	1276	ASN
1	N	1310	GLN
1	N	1353	HIS
1	O	79	ASN
1	O	125	HIS
1	O	317	ASN
1	O	333	HIS
1	O	432	GLN
1	O	465	HIS

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Mol	Chain	Res	Type
1	O	496	HIS
1	O	531	HIS
1	O	581	GLN
1	O	587	GLN
1	O	695	GLN
1	O	824	HIS
1	O	909	GLN
1	O	977	GLN
1	O	997	HIS
1	O	1033	GLN
1	O	1176	HIS
1	O	1351	GLN
1	P	222	HIS
1	P	226	HIS
1	P	415	ASN
1	P	472	ASN
1	P	509	ASN
1	P	531	HIS
1	P	586	GLN
1	P	596	HIS
1	P	627	HIS
1	P	735	HIS
1	P	750	ASN
1	P	837	GLN
1	P	842	ASN
1	P	908	GLN
1	P	942	GLN
1	P	964	HIS
1	P	977	GLN
1	P	984	ASN
1	P	1120	HIS
1	P	1178	GLN
1	P	1241	ASN
1	P	1283	ASN
2	v	7	ASN
2	v	34	ASN
2	v	45	GLN
2	v	290	HIS
2	v	295	HIS
2	v	382	ASN
2	v	394	GLN
4	y	3114	GLN

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Mol	Chain	Res	Type
4	z	3114	GLN
5	Z	11	GLN
5	Z	54	GLN
5	Z	71	GLN
5	a	44	GLN
5	e	31	ASN
5	e	54	GLN
5	u	11	GLN
6	f	102	ASN
6	f	303	HIS
6	h	13	GLN
6	h	28	ASN
6	h	46	HIS
6	h	182	HIS
6	h	288	GLN
6	h	291	ASN
7	k	148	GLN
7	k	184	HIS
7	m	38	GLN
7	m	62	ASN
7	m	98	GLN
7	m	128	ASN
7	m	148	GLN
7	m	230	HIS
7	m	233	HIS
7	p	22	GLN
7	p	23	GLN
7	p	89	GLN
7	p	184	HIS
7	p	185	HIS
7	p	204	ASN
7	r	128	ASN
7	r	162	GLN
7	r	184	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

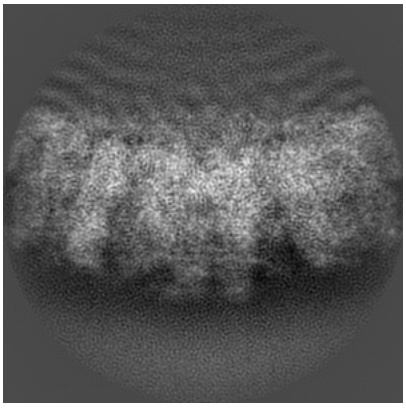
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-21525. These allow visual inspection of the internal detail of the map and identification of artifacts.

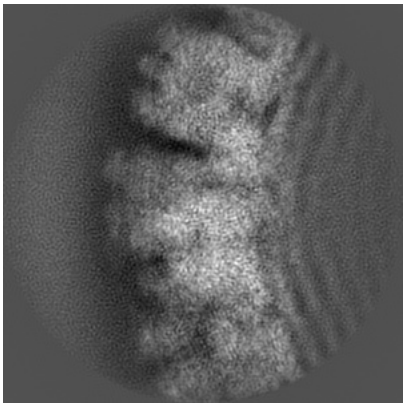
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

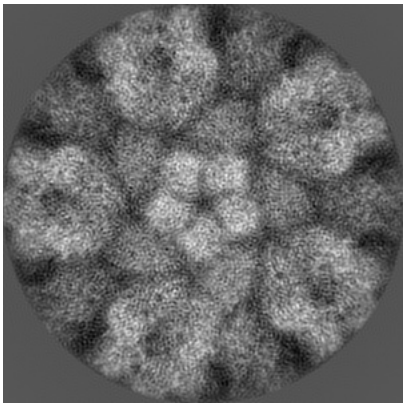
6.1.1 Primary map



X



Y

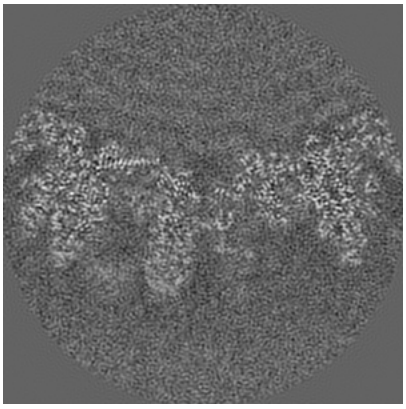


Z

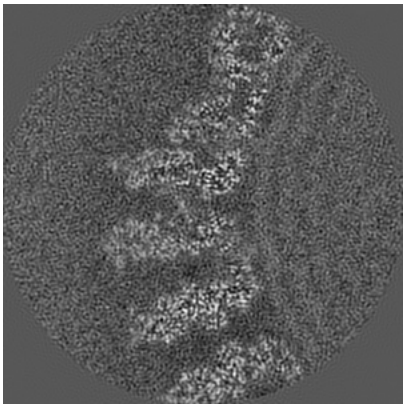
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

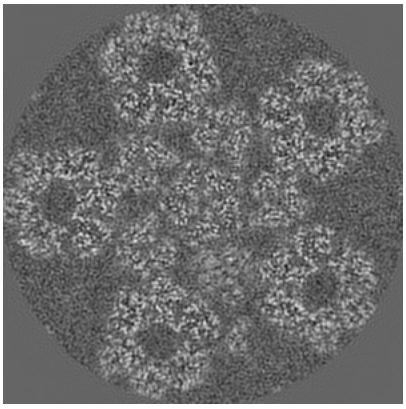
6.2.1 Primary map



X Index: 160



Y Index: 160

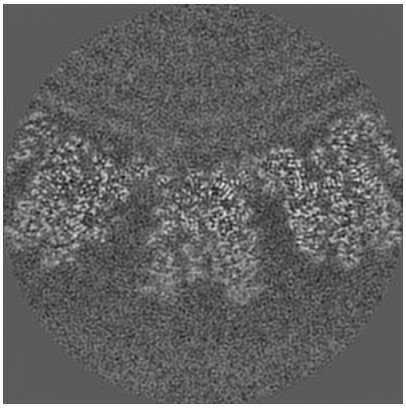


Z Index: 160

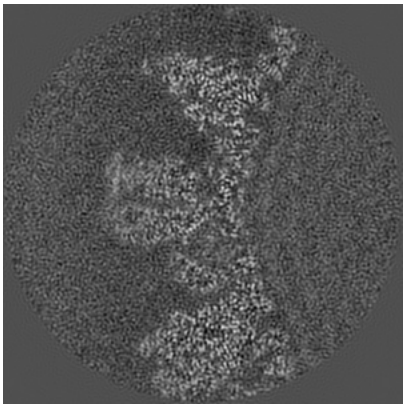
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

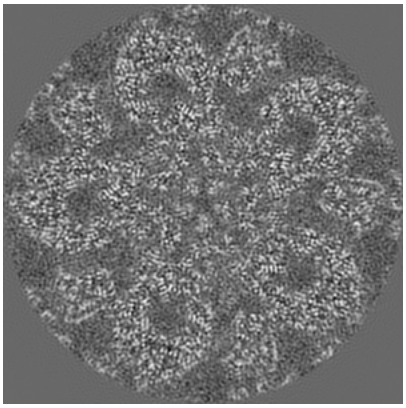
6.3.1 Primary map



X Index: 147



Y Index: 189

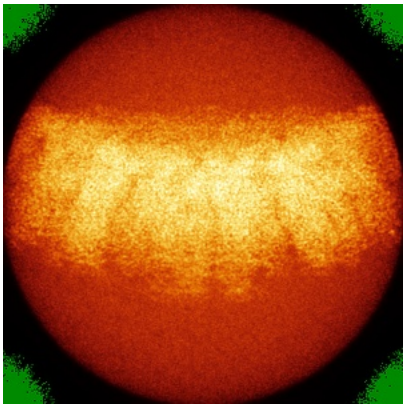


Z Index: 185

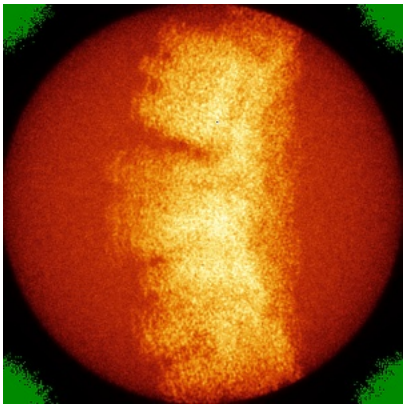
The images above show the largest variance slices of the map in three orthogonal directions.

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

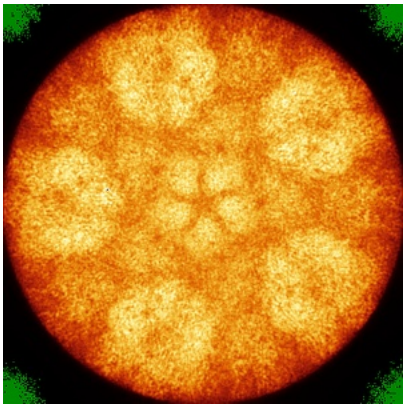
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

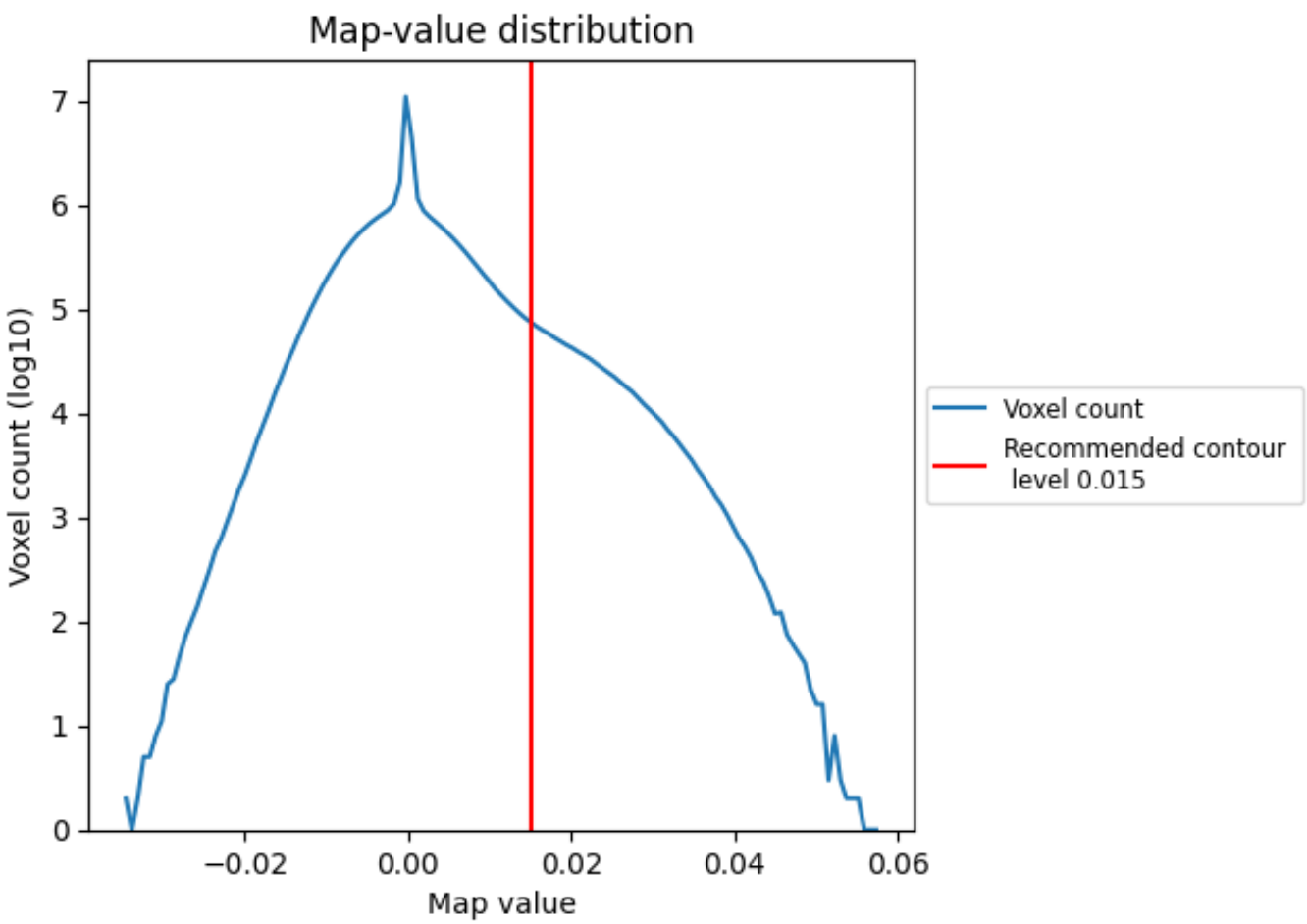
6.6 Mask visualisation (i)

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

7 Map analysis (i)

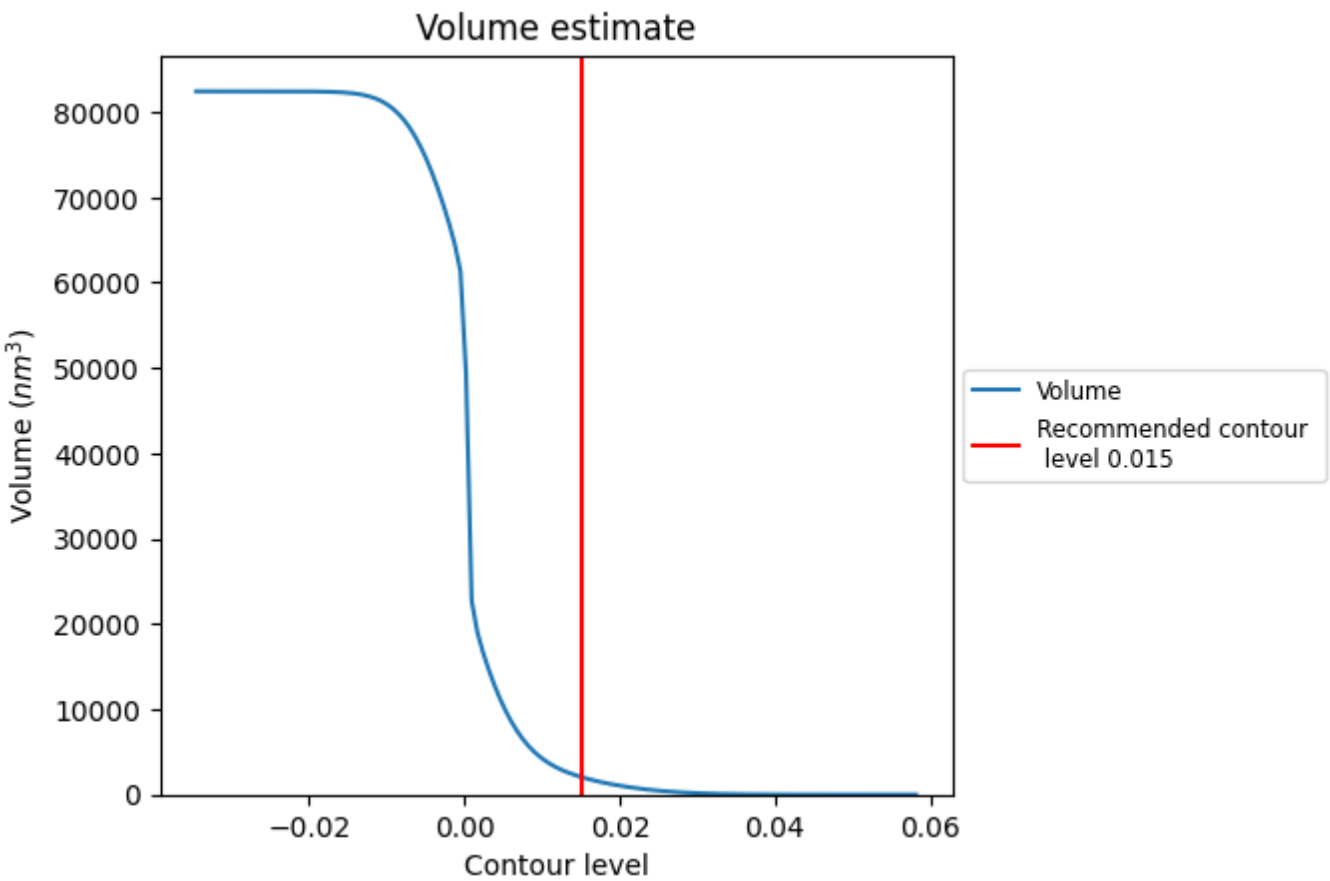
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

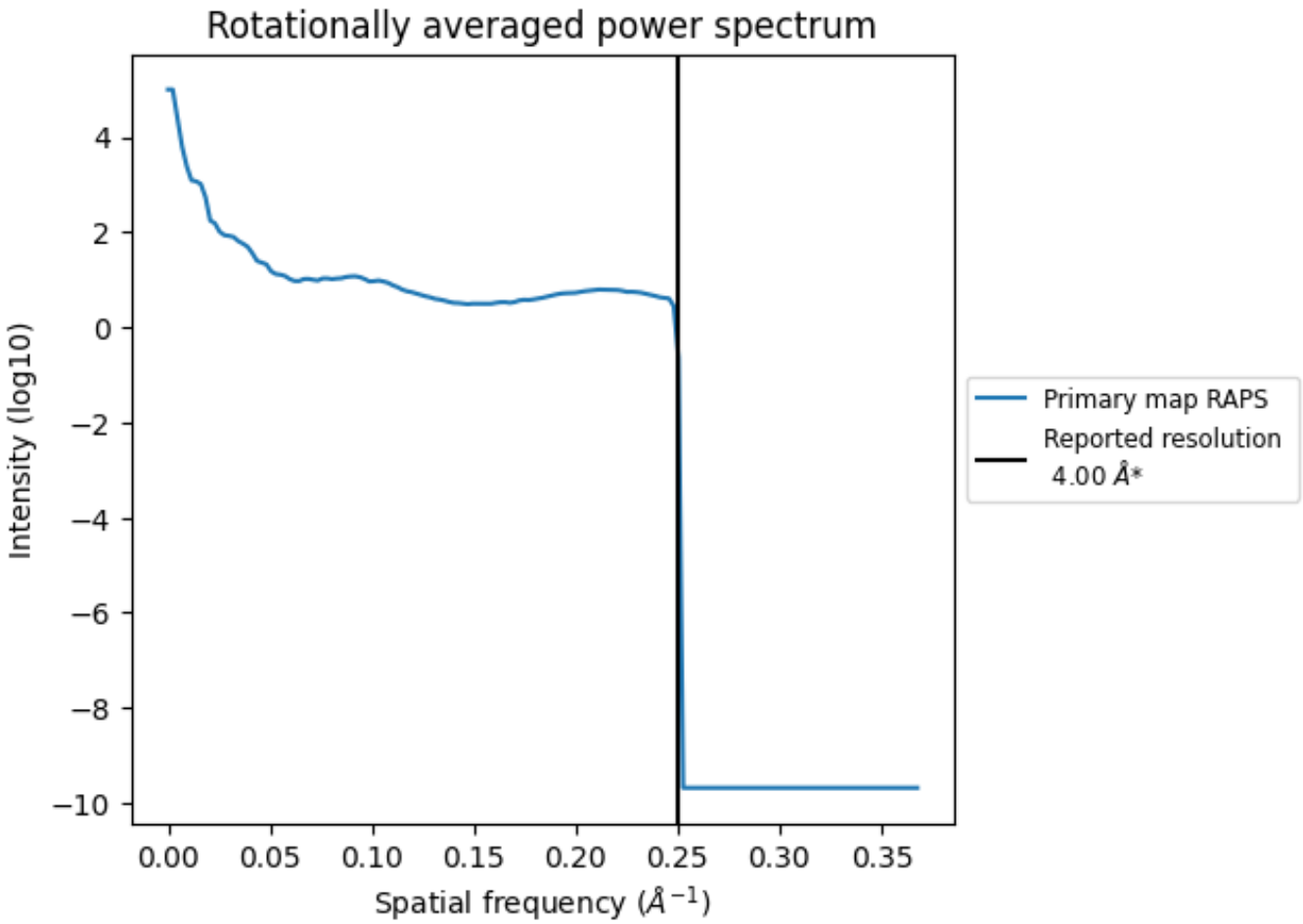
7.2 Volume estimate (i)



The volume at the recommended contour level is 2067 nm^3; this corresponds to an approximate mass of 1867 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 0.250 Å^{-1}

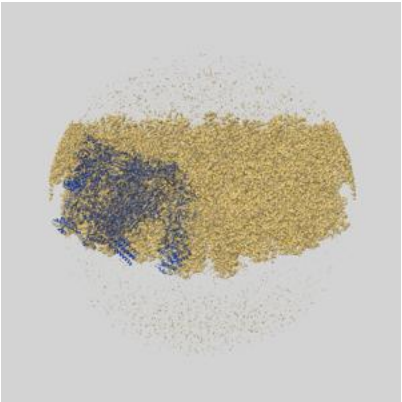
8 Fourier-Shell correlation (i)

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

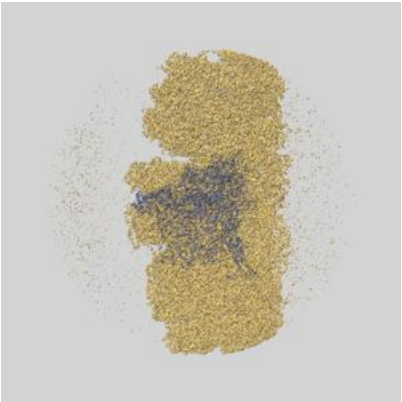
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-21525 and PDB model 6W2D. Per-residue inclusion information can be found in section 3 on page 6.

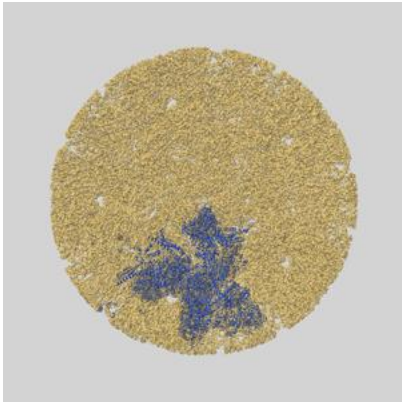
9.1 Map-model overlay (i)



X



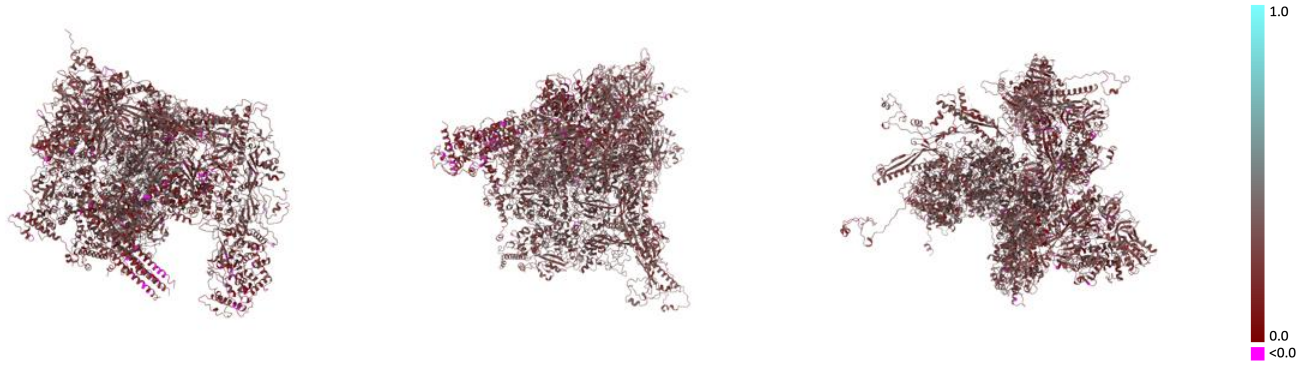
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015 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.

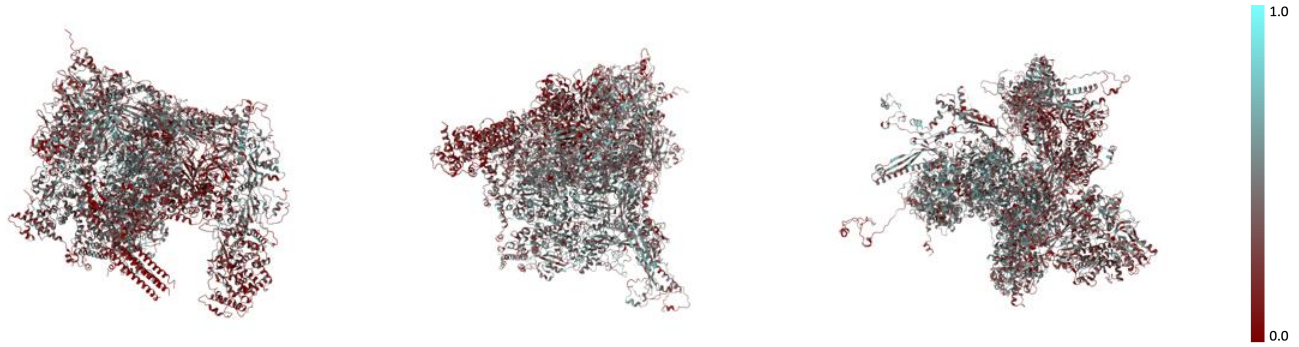
9.2 Q-score mapped to coordinate model (i)



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.

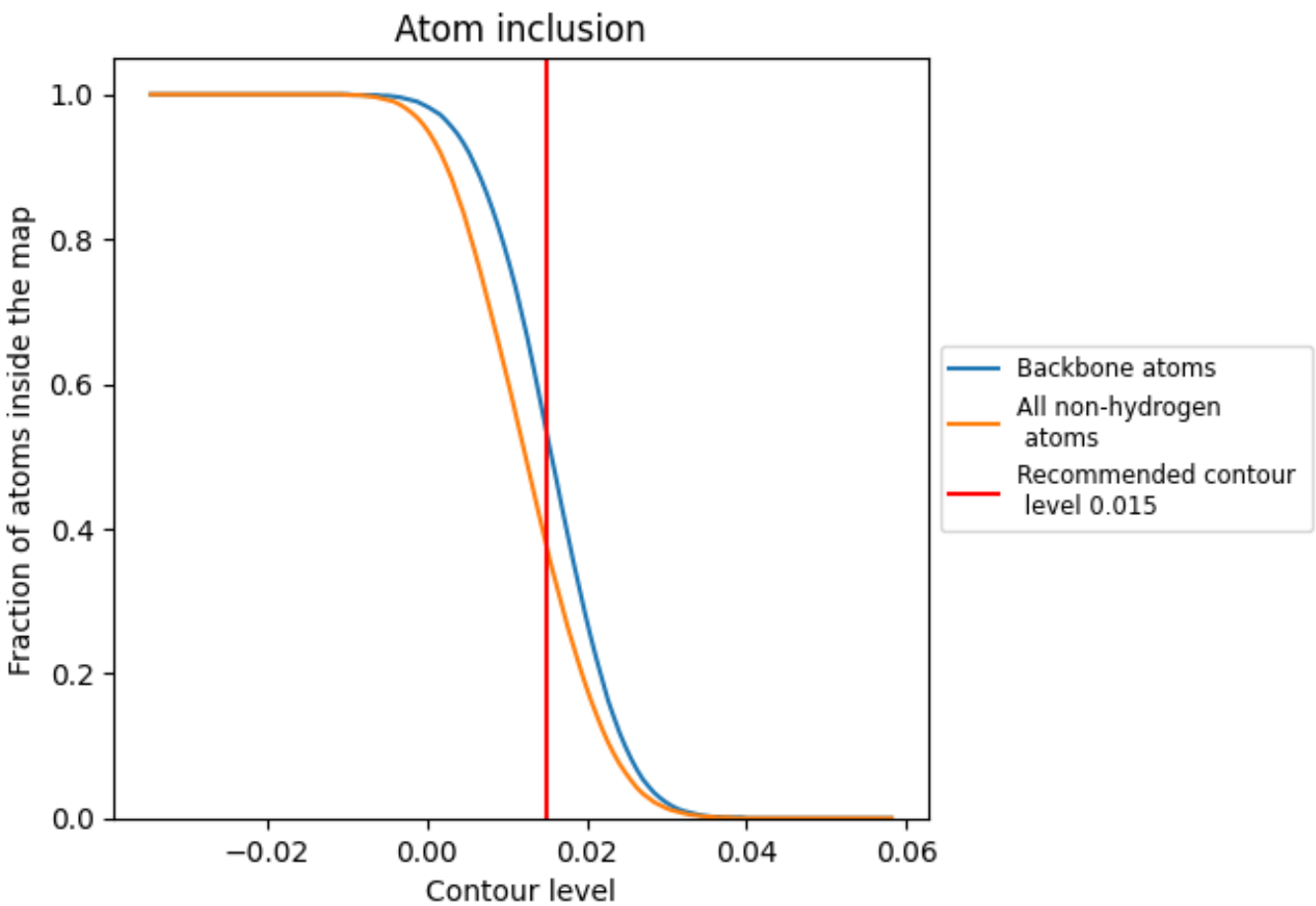
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.015).

9.4 Atom inclusion (i)



At the recommended contour level, 53% of all backbone atoms, 37% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3740	0.2800
J	0.4580	0.3060
K	0.4470	0.3030
N	0.4050	0.2910
O	0.4400	0.3030
P	0.3240	0.2580
Z	0.3450	0.2420
a	0.3080	0.2810
d	0.2430	0.2360
e	0.2950	0.2580
f	0.2000	0.2340
h	0.3770	0.2720
k	0.2460	0.2530
m	0.3430	0.2700
p	0.2390	0.2550
r	0.3660	0.2810
u	0.1380	0.1670
v	0.2220	0.2410
w	0.1000	0.1630
x	0.1880	0.1900
y	0.1090	0.1880
z	0.0960	0.1620