Full wwPDB EM Validation Report (i)

Feb 25, 2024 – 07:37 PM EST

PDB ID	:	6W2E
EMDB ID	:	EMD-21526
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	:	4.40 Å(reported)

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

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

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

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

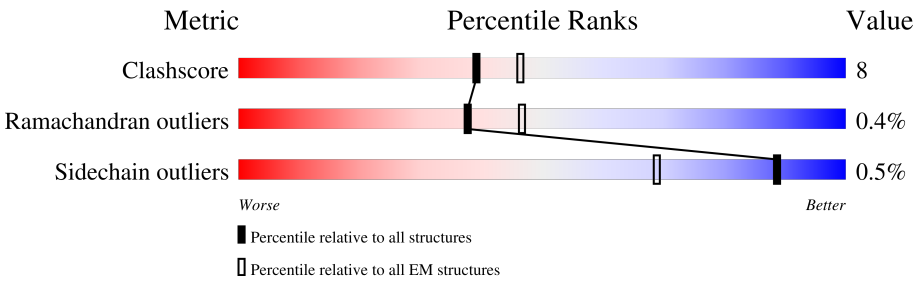
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 4.40 Å.

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



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

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	50% 78% 17% 6%
1	K	1381	54% 84% 15% •
1	N	1381	60% 84% 15% •
1	O	1381	53% 79% 15% 6%
2	v	507	50% 58% 42%
3	w	570	12% 12% 88%
3	x	570	11% 12% 88%
4	y	3149	• • 99%

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Mol	Chain	Length	Quality of chain
4	z	3149	99%
5	Z	176	31% 39% 5% 56%
5	a	176	31% 42% 56%
5	d	176	39% 44% 56%
5	e	176	31% 43% 56%
6	f	364	55% 68% 30%
6	h	364	58% 92% 8%
7	k	301	70% 99%
7	m	301	70% 99%
7	p	301	70% 99%
7	r	301	68% 97%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 62525 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	1305	10252	6507	1779	1908	58	0	0
1	K	1381	10832	6868	1884	2018	62	0	0
1	N	1362	10683	6777	1854	1991	61	0	0
1	O	1299	10194	6468	1771	1895	60	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	293	2288	1472	398	407	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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	f	253	1992	1291	333	361	7	0	0
6	h	336	2604	1667	458	471	8	0	0

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

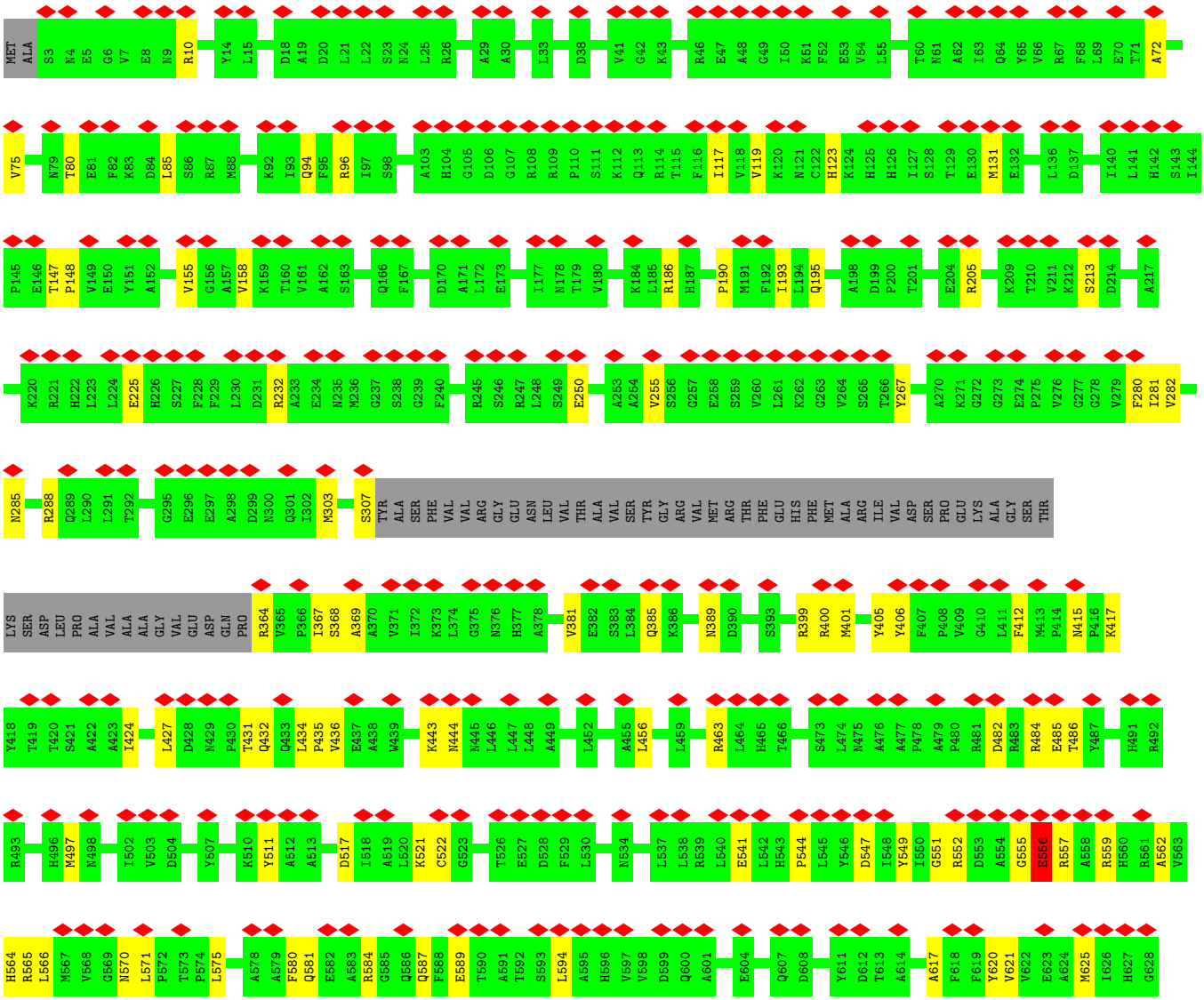
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	k	299	2338	1500	386	434	18	0	0
7	m	299	2338	1500	386	434	18	0	0
7	p	299	2338	1500	386	434	18	0	0
7	r	299	2338	1500	386	434	18	0	0

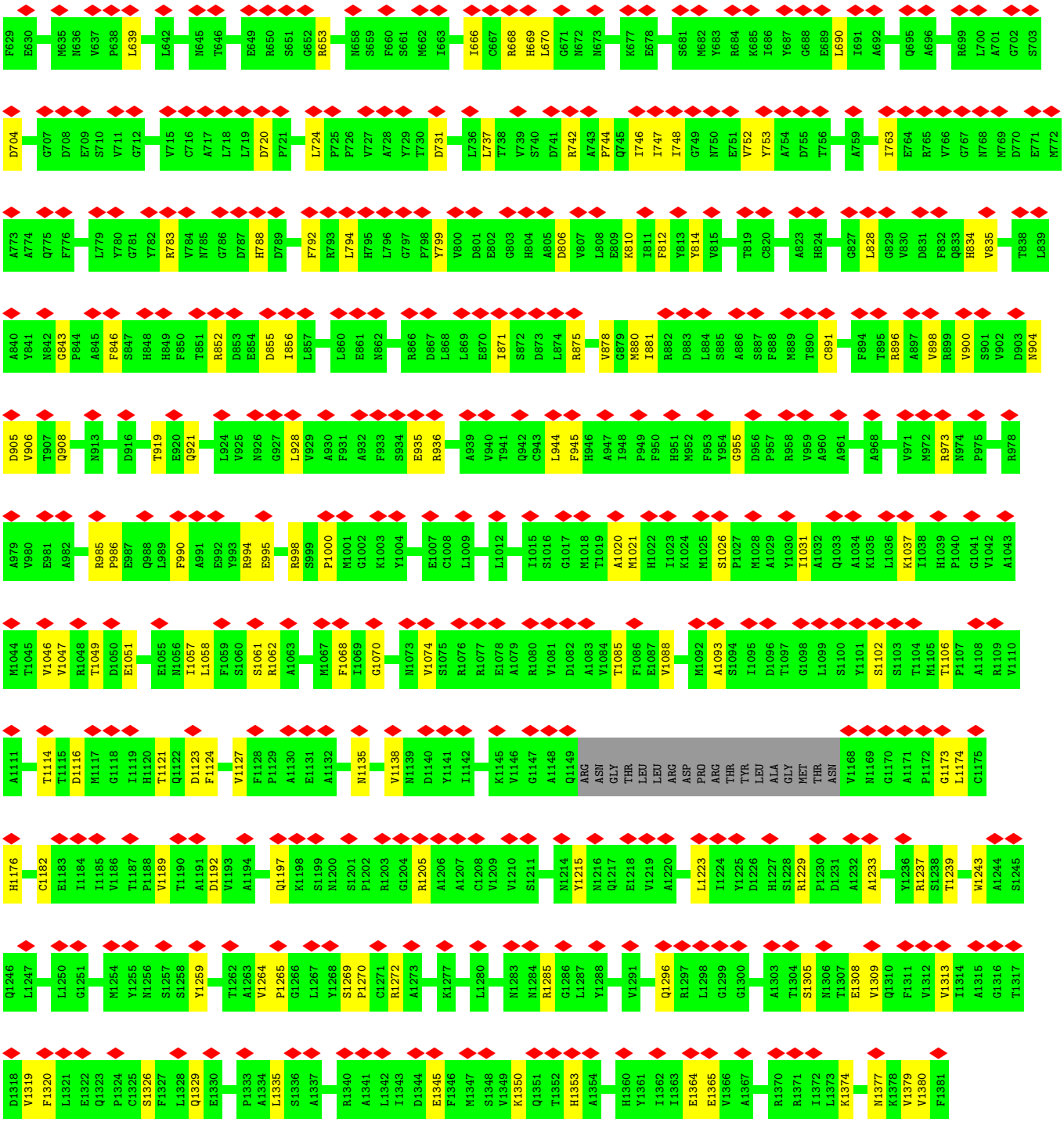
3 Residue-property plots (i)

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

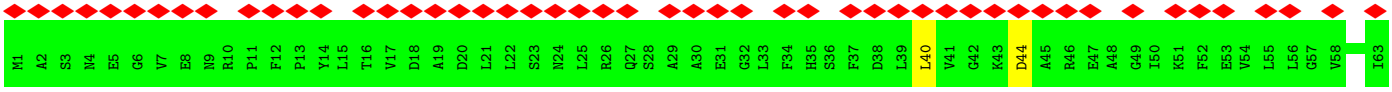
Chain J: 50% 78% 17% 6%

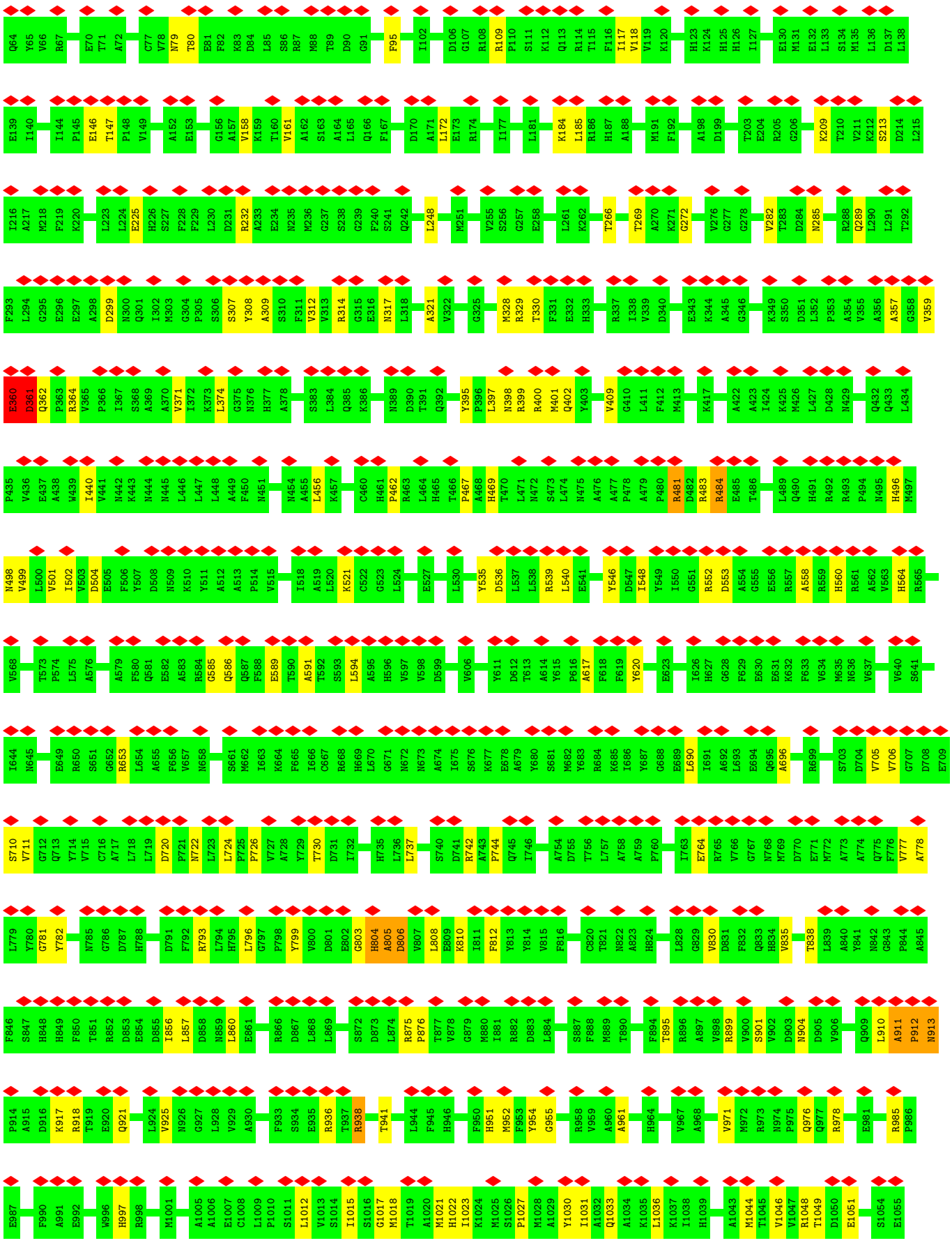


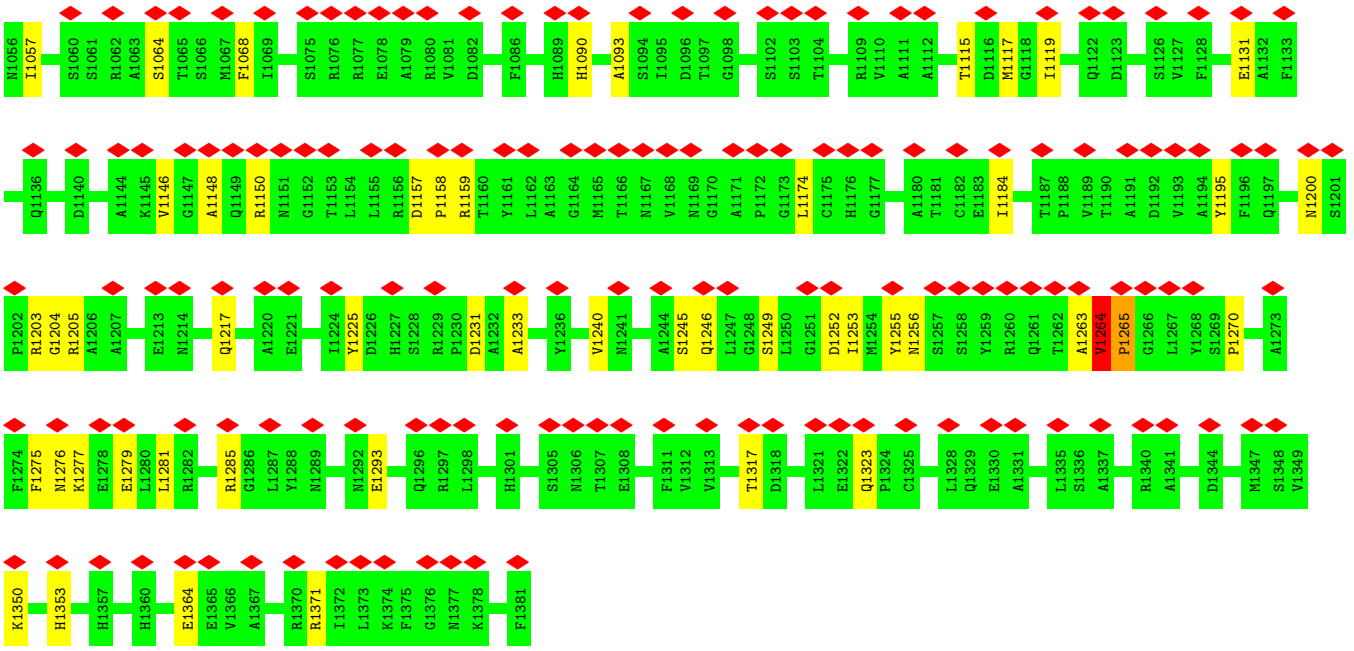


- Molecule 1: Major capsid protein

Chain K:

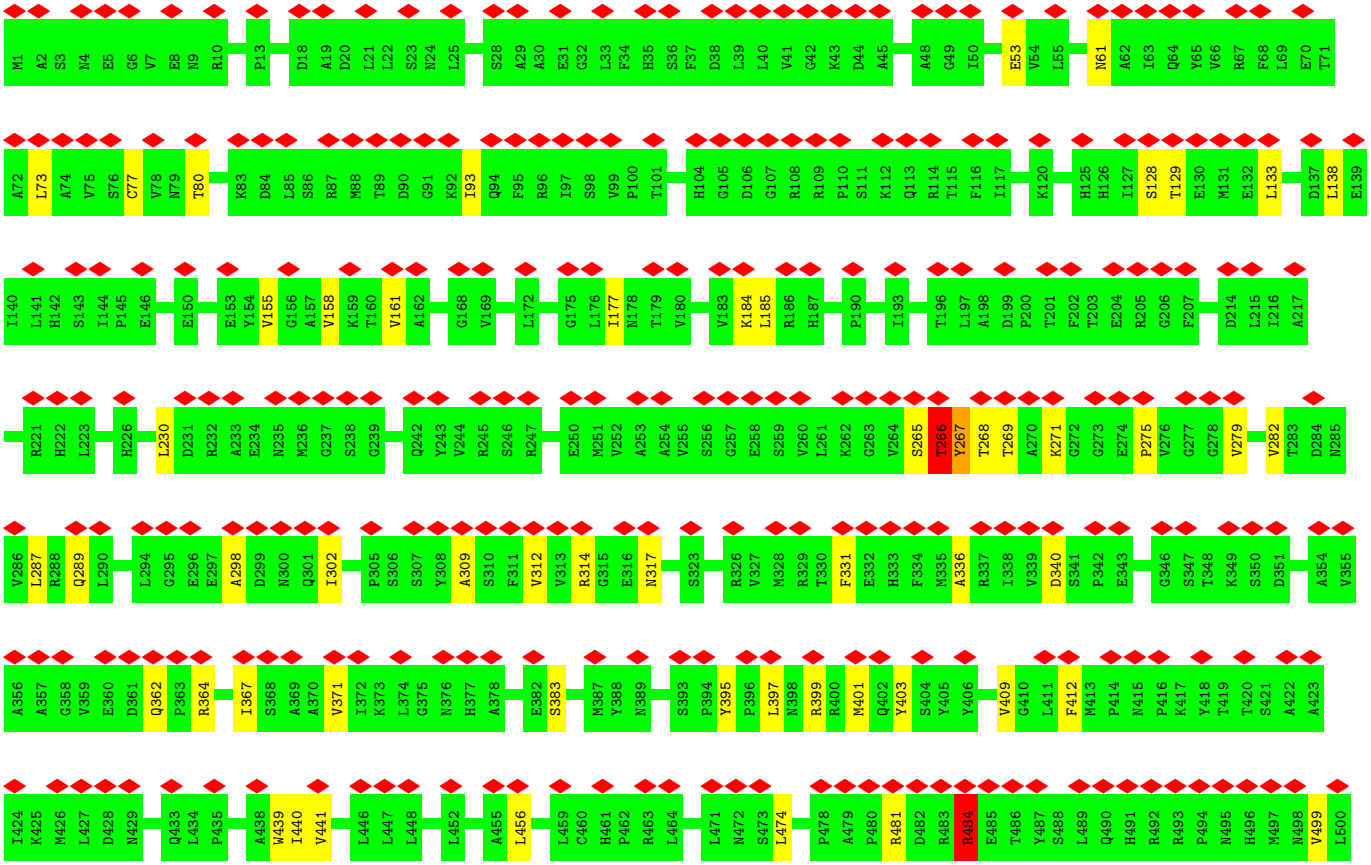


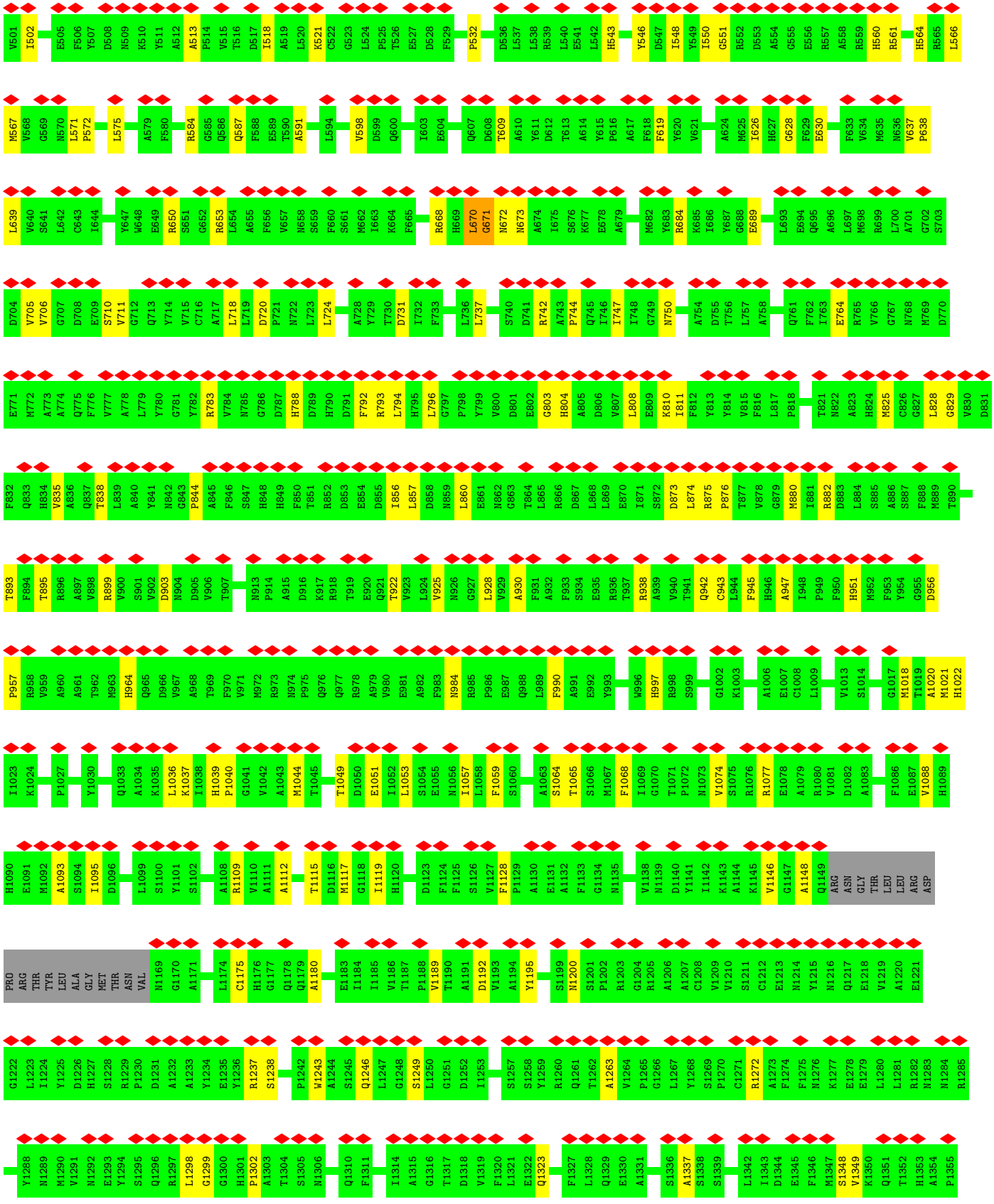

Q64 Y65 V66 R67 E70 T71 A72 C77 V78 N79 T80 E81 F82 K83 D84 L85 S86 R87 M88 T89 D90 G91 F95 I102 D106 G107 R108 R109 P110 S111 K112 Q113 R114 T115 F116 I117 V118 V119 K120 H123 K124 H125 H126 I127 E130 M131 E132 L133 S134 M135 L136 D137 L138
E139 I140 I144 P145 E146 T147 P148 V149 A152 E153 G156 A157 V158 K159 T160 V161 A162 S163 A164 L165 Q166 F167 D170 A171 L172 E173 R174 I177 L181 K184 L185 R186 H187 A188 M191 F192 A198 D199 T203 E204 R205 G206 K209 T210 V211 K212 S213 D214 L215
I216 A217 M218 F219 K220 L223 L224 E225 H226 S227 F228 F229 L230 D231 R232 A233 E234 N235 M236 G237 S238 G239 F240 S241 Q242 L248 M251 V255 S256 G257 E258 L261 K262 T266 T269 A270 K271 G272 V276 G277 G278 V282 T283 D284 N285 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 N317 L318 A321 V322 G325 M328 R329 T330 F331 E332 H333 R337 I338 V339 D340 E343 K344 A345 G346 K349 S350 D351 L352 P353 A354 V355 A356 A357 G358 V359
E360 D361 Q362 P363 R364 V365 P366 I367 S368 A369 A370 V371 I372 K373 L374 G375 N376 H377 A378 S383 L384 Q385 K386 N389 D390 T391 Q392 Y395 P396 L397 N398 R399 R400 M401 Q402 Y403 V409 G410 L411 F412 M413 K417 A422 A423 I424 K425 M426 L427 D428 N429 Q432 Q433 L434
P435 V436 E437 A438 W439 I440 V441 N442 K443 N444 N445 L446 L447 L448 A449 F450 N451 N454 A455 L456 K457 C460 H461 P462 R463 L464 H465 T466 P467 A468 H469 T470 L471 N472 S473 L474 N475 A476 A477 P478 A479 P480 R481 D482 R483 R484 E485 T486 L489 Q490 H491 R492 R493 P494 N495 H496 M497
N498 V499 L500 V501 I502 V503 D504 E505 F506 Y507 D508 N509 K510 Y511 A512 A513 P514 V515 I518 A519 L520 K521 C522 G523 L524 E527 L530 Y535 D536 L537 L538 R539 L540 E541 Y546 D547 I548 Y549 I550 G551 R552 D553 A554 G555 E556 R557 A558 R559 H560 R561 A562 V563 H564 R565
V568 T573 P574 L575 A576 A579 F580 Q581 E582 A583 R584 G585 Q586 Q587 F588 E589 T590 A591 T592 S593 L594 A595 H596 V597 V598 D599 V606 Y611 D612 T613 A614 Y615 P616 A617 F618 F619 Y620 E623 I626 H627 G628 F629 E630 E631 K632 F633 V634 M635 M636 V637 V640 S641
I644 N645 E649 R650 S651 G652 R653 L654 A655 F656 V657 N658 S661 M662 I663 K664 F665 I666 C667 R668 H669 L670 G671 N672 M673 A674 I675 S676 K677 E678 A679 Y680 S681 M682 Y683 R684 K685 I686 Y687 G688 E689 L690 I691 A692 L693 E694 Q695 A696 R699 S703 D704 V705 V706 G707 D708 E709
S710 V711 G712 Q713 Y714 V715 C716 A717 L718 L719 D720 P721 N722 L723 L724 P725 P726 V727 A728 Y729 T730 D731 I732 H735 L736 L737 S740 D741 R742 A743 P744 Q745 I746 A754 D755 T756 L757 A758 A759 P760 I763 E764 R765 V766 G767 N768 M769 D770 E771 M772 A773 A774 Q775 F776 V777 A778
L779 Y780 G781 Y782 N785 G786 D787 H788 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 C820 T821 N822 A823 H824 L828 G829 V830 D831 F832 Q833 H834 V835 T838 L839 A840 Y841 N842 G843 P844 A845
F846 S847 H848 H849 F850 T851 R852 D853 E854 D855 I856 L857 D858 N859 L860 E861 R866 D867 L868 L869 S872 D873 L874 R875 P876 T877 V878 G879 M880 I881 R882 D883 L884 S887 F888 M889 T890 F894 T895 R896 A897 V898 R899 V900 S901 V902 D903 N904 D905 V906 Q909 L910 A911 P912 N913
P914 A915 D916 K917 R918 T919 E920 Q921 L924 V925 N926 G927 L928 V929 A930 F933 S934 E935 R936 T937 R938 T941 L944 F945 H946 F950 H951 M952 F953 Y954 G955 R958 V959 A960 A961 H964 V967 A968 V971 M972 R973 N974 P975 Q976 Q977 R978 E981 R985 P986
E987 F990 A991 E992 W996 H997 R998 M1001 A1005 A1006 E1007 C1008 L1009 P1010 S1011 L1012 V1013 S1014 I1015 S1016 G1017 M1018 T1019 A1020 M1021 H1022 I1023 K1024 M1025 S1026 P1027 M1028 A1029 Y1030 I1031 A1032 Q1033 A1034 K1035 L1036 K1037 I1038 H1039 A1043 M1044 T1045 V1046 V1047 R1048 T1049 D1050 E1051 S1054 E1055



- Molecule 1: Major capsid protein

Chain N:




V501 I502 E505 F506 Y507 D508 N509 K510 Y511 A512 A513 F514 V515 T516 D517 I518 A519 L520 K521 C522 G523 L524 P525 T526 E527 D528 F529 P532 D536 L537 L538 R539 L540 E541 L542 H543 Y546 D547 I548 Y549 I550 G551 R552 D553 A554 G555 E556 R557 A558 R559 H560 R561 H564 R565 L566
M567 V568 G569 N570 L571 P572 L575 A579 F580 R584 G585 Q586 Q587 F588 E589 T590 A591 L594 V598 D599 Q600 I603 E604 Q607 D608 T609 A610 Y611 D612 T613 A614 Y615 P616 A617 F618 F619 Y620 V621 A624 M625 I626 H627 G628 F629 E630 F633 V634 M635 N636 V637 P638
L639 V640 S641 L642 C643 I644 Y647 W648 E649 R650 S651 G652 R653 L654 A655 F656 V657 N658 S659 F660 S661 M662 I663 K664 F665 R668 H669 L670 G671 N672 N673 A674 I675 S676 K677 E678 A679 M682 Y683 R684 K685 I686 Y687 G688 E689 L693 E694 Q695 A696 L697 M698 R699 L700 A701 G702 S703
D704 V705 V706 G707 D708 E709 S710 V711 G712 Q713 Y714 V715 C716 A717 L718 L719 D720 P721 N722 L723 L724 A728 Y729 T730 D731 I732 F733 L736 L737 S740 D741 R742 A743 P744 Q745 I746 I747 I748 G749 N750 A754 D755 T756 L757 A758 Q761 F762 I763 E764 R765 V766 G767 N768 M769 D770
E771 M772 A773 A774 Q775 F776 V777 A778 L779 Y780 G781 Y782 R783 V784 N785 G786 D787 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 T821 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
T893 F894 T895 R896 A897 V898 R899 V900 S901 V902 D903 N904 D905 V906 T907 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 D956
P957 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 W996 H997 R998 S999 G1002 K1003 A1006 E1007 C1008 L1009 V1013 S1014 G1017 M1018 T1019 A1020 M1021 H1022
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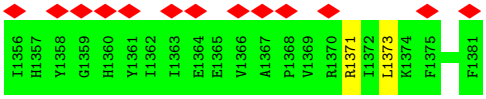
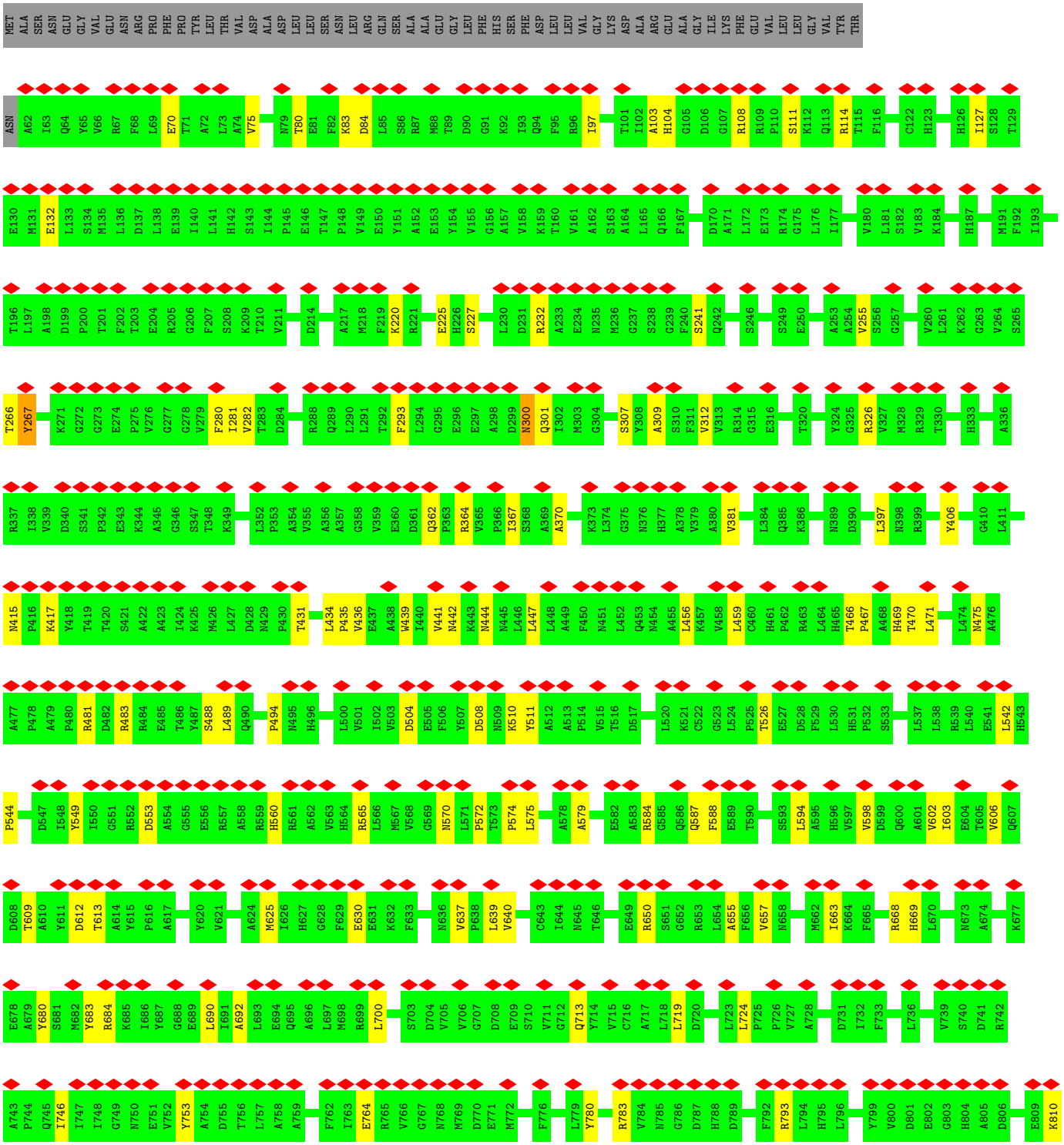
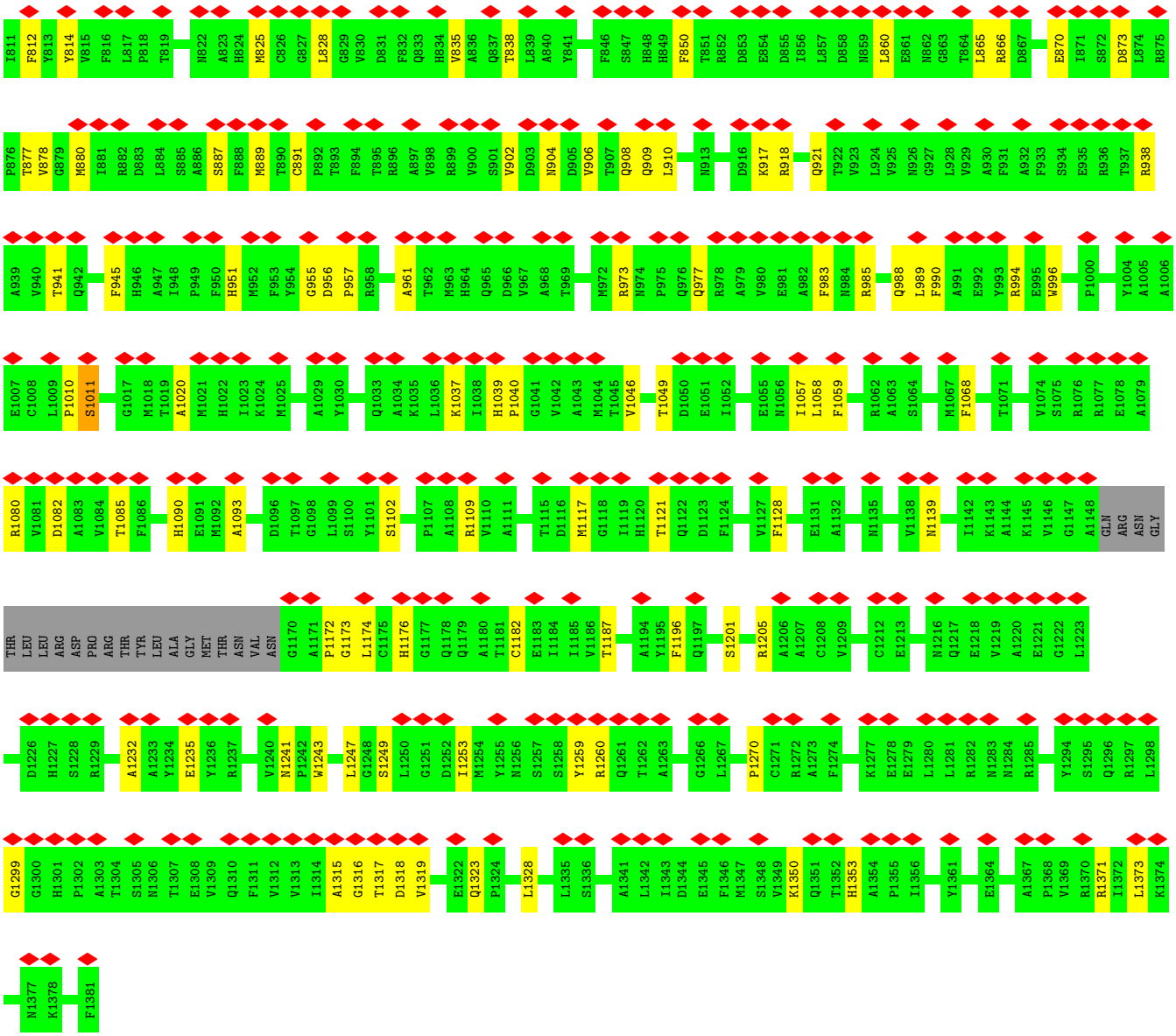
H1090 E1091 M1092 A1093 S1094 I1095 D1096 L1099 S1100 Y1101 S1102 A1108 R1109 V1110 A1111 A1112 T1115 D1116 M1117 G1118 I1119 H1120 D1123 F1124 F1125 S1126 V1127 F1128 P1129 A1130 E1131 A1132 F1133 G1134 N1135 V1138 N1139 D1140 Y1141 I1142 K1143 A1144 K1145 V1146 G1147 A1148 Q1149 ARG ASN GLY THR LEU LEU ARG ASP
PRO ARG THR TYR LEU ALA GLY MET THR ASN VAL N1169 G1170 A1171 L1174 C1175 H1176 G1177 Q1178 Q1179 A1180 E1183 I1184 I1185 V1186 T1187 P1188 V1189 T1190 A1191 D1192 V1193 A1194 Y1195 S1199 N1200 S1201 P1202 R1203 G1204 R1205 A1206 A1207 C1208 V1209 V1210 S1211 C1212 E1213 N1214 Y1215 N1216 Q1217 E1218 V1219 A1220 E1221
G1222 L1223 I1224 Y1225 D1226 H1227 S1228 R1229 P1230 D1231 A1232 A1233 Y1234 E1235 Y1236 R1237 S1238 P1242 W1243 A1244 S1245 Q1246 L1247 G1248 S1249 L1250 G1251 D1252 I1253 S1257 S1258 Y1259 R1260 Q1261 T1262 A1263 V1264 P1265 G1266 L1267 Y1268 S1269 P1270 C1271 R1272 A1273 F1274 F1275 N1276 K1277 E1278 E1279 L1280 L1281 R1282 N1283 N1284 R1285
Y1288 N1289 M1290 V1291 N1292 E1293 Y1294 S1295 Q1296 R1297 L1298 G1299 G1300 H1301 P1302 A1303 T1304 S1305 N1306 Q1310 F1311 I1314 A1315 G1316 T1317 D1318 V1319 F1320 L1321 E1322 Q1323 F1327 L1328 Q1329 E1330 A1331 S1336 A1337 S1338 S1339 L1342 I1343 D1344 E1345 F1346 M1347 S1348 V1349 K1350 Q1351 T1352 H1353 A1354 P1355



- Molecule 1: Major capsid protein

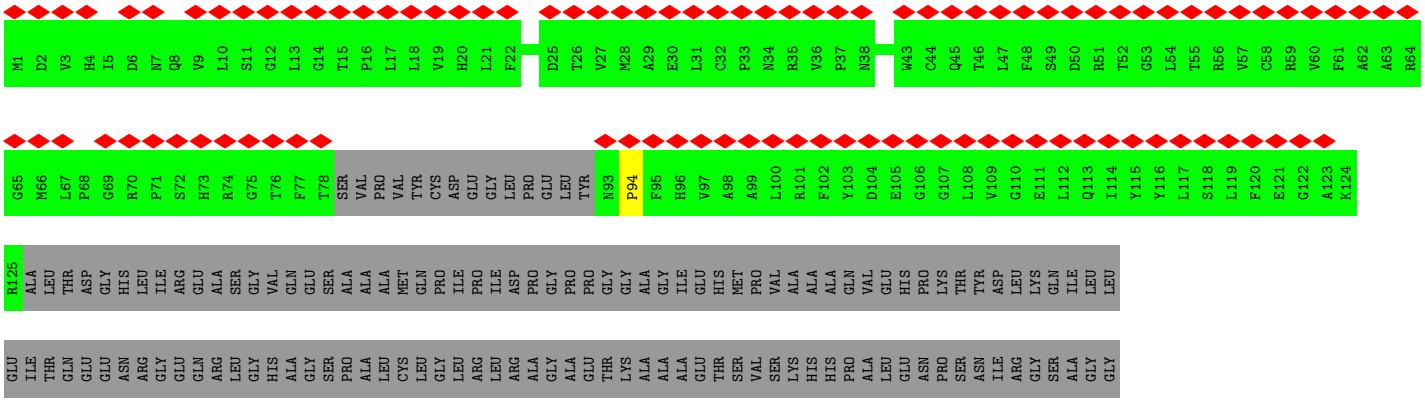
Chain O:





- Molecule 2: Capsid vertex component 1

Chain v:



GLU GLY GLY GLY GLY ARG ALA GLY THR GLY GLY THR VAL GLY VAL GLY SER GLY ALA LEU SER ARG VAL PRO VAL SER PHE SER LYS THR ARG ARG ALA ILE ARG GLU SER ARG A283 L284 V285 R286 G287 I288 A289 H290 I291 F292 S293 P294 H295 A296 L297 V300 T301 Y302 P303 E304 L305

SER ALA GLN GLY ARG LEU HIS ARG MET THR ALA VAL THR HIS ALA SER PRO ALA THR ASP LEU ALA GLU VAL S330 I331 L332 G333 A334 P335 E336 R337 E338 F339 R340 F341 L342 I343 S344 V345 A346 L347 R348 I349 S350 A351 S352 F353 R354 E355 K356 L357 A358 M359 Q360 A361 W362 T363 A364 Q365

Q366 E367 I368 P369 V370 V371 I372 P373 T374 S375 Y376 S377 R378 I379 Y380 K381 N382 S383 D384 L385 I386 R387 E388 A389 F390 F391 T392 V393 Q394 T395 R396 V397 S398 W399 E400 S401 C402 W403 V404 K405 A406 T407 I408 S409 N410 A411 P412 K413 T414 P415 D416 A417 C418 L419 W420 W421 D422 S423 H424 P425

L426 Y427 E428 E429 G430 A431 S432 A433 W434 G435 K436 V437 I438 D439 SER ARG PRO PRO GLY GLY LEU VAL GLY ALA ALA SER GLN LEU V454 A455 L456 G457 T458 D459 G460 H461 C462 V463 H464 L465 A466 T467 T468 S469 D470 G471 Q472 A473 F474 L475 V476 L477 P478 G479 G480 F481 V482 I483 K484 G485

Q486 L487 A488 L489 T490 P491 E492 E493 R494 G495 Y496 I497 L498 A499 R500 H501 G502 ILE ARG ARG GLU GLN

- Molecule 3: Capsid vertex component 2

Chain w: 12% 12% 88%

MET ALA LEU SER GLY HIS VAL LEU ILE ASP PRO ALA ARG LEU PRO ARG ASP SER THR GLY PRO GLU LEU MET TRP ALA PRO SER LEU ARG ASN SER LEU ARG VAL S35 P36 E37 A38 L39 E40 L41 A42 E43 R44 E45 A46 E47 R48 A49 R50 S51 E52 R53 W54 D55 R56 C57 A58 Q59 V60

L61 K62 M63 R64 L65 L66 R67 V68 E69 L70 D71 G72 I73 M74 R75 D76 H77 L78 A79 R80 A81 E82 E83 I84 R85 Q86 D87 L88 D89 A90 V91 V92 A93 F94 S95 D96 G97 L98 E99 S100 M101 Q102 VAL ARG SER PRO SER THR GLY GLY ARG SER ALA PRO ALA PRO PRO SER PRO SER

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

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

LEU LEU LEU GLN GLY GLY SER SER HIS GLN GLN ARG PRO LEU PRO ALA SER ARG GLU GLU LEU LEU LEU GLU 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 LEU PRO

PRO PHE SER SER HIS GLN TRP ASN LEU ARG VAL GLY LEU 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 PRO ASP ALA 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 3: Capsid vertex component 2

Chain x: 11% 12% 88%

MET ALA LEU SER GLY HIS VAL LEU ILE ASP PRO ALA ARG LEU PRO ARG ASP THR GLY PRO GLU LEU MET TRP ALA PRO SER LEU ARG ASN SER LEU ARG VAL S35 P36 E37 A38 L39 E40 L41 A42 E43 R44 E45 A46 E47 R48 A49 R50 S51 E52 R53 W54 D55 R56 C57 A58 Q59 V60

L61 K62 N63 R64 L65 L66 R67 V68 E69 L70 D71 G72 I73 M74 R75 D76 H77 L78 A79 R80 A81 E82 E83 I84 R85 Q86 D87 L88 D89 A90 V91 V92 A93 F94 S95 D96 G97 L98 E99 S100 M101 Q102 VAL ARG SER PRO SER THR GLY GLY ARG SER ALA PRO ALA PRO PRO PRO SER PRO SER

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

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

LEU LEU LEU GLN GLY GLY SER SER HIS GLN GLN ARG PRO LEU PRO ALA SER ARG GLU GLU LEU LEU GLU 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 TRP ASN LEU ARG ARG VAL GLY LEU ALA ALA ALA LEU 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 LEU ALA LEU GLU LEU GLY ALA LYS PRO LEU PHE 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: 99%

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

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

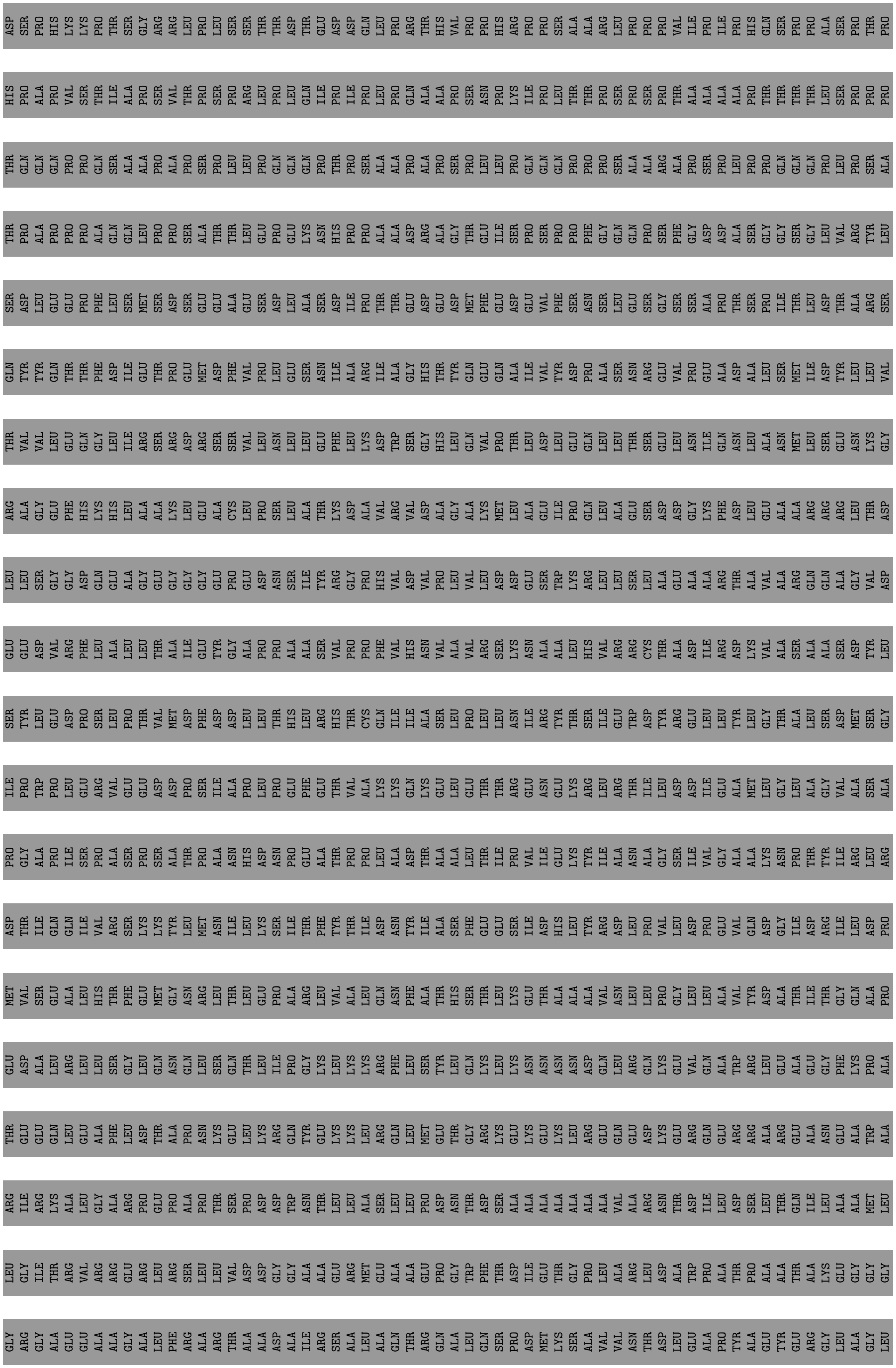
VAL LEU ARG GLY GLY GLY ARG VAL HIS ILE TYR ARG SER ALA GLU ILE PHE GLY LEU VAL LEU PHE PRO ALA GLN ILE ALA ASN SER ALA VAL VAL GLN SER LEU ALA ASN VAL LEU HIS GLY SER TYR ASN GLY VAL ALA GLN PHE ILE LEU TYR ILE CYS ASP ILE TYR ALA GLY GLY

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

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

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

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

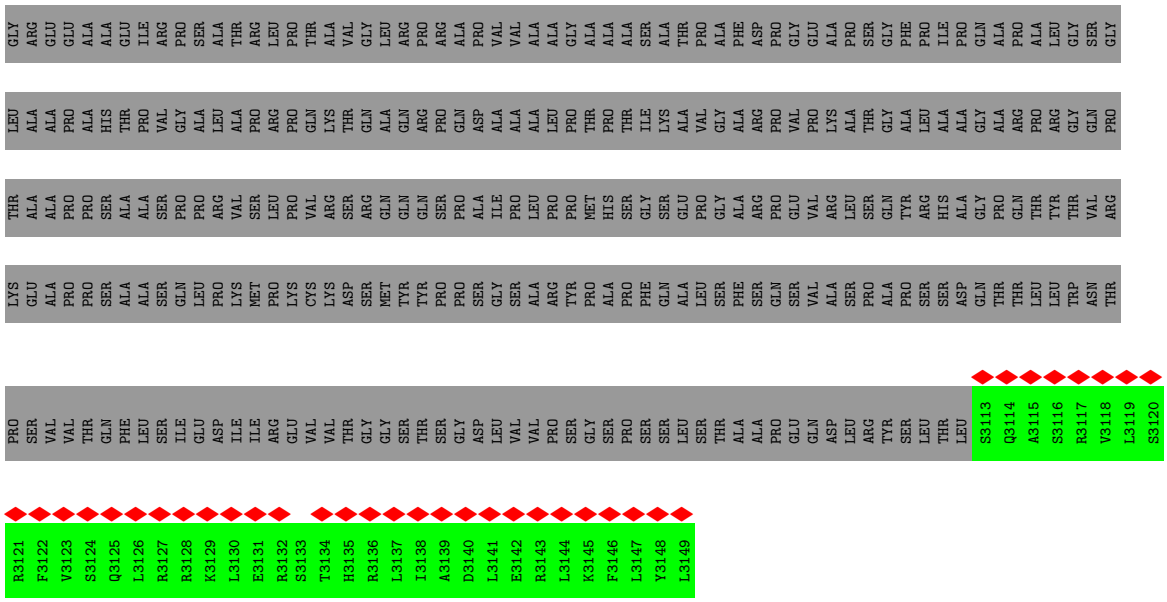
ARG HIS ASN LEU PRO ASP VAL GLN PHE TYR PHE ASN ALA ALA GLY ALA SER ARG TRP PRO THR ASP VAL LEU ASN PRO SER PHE TYR GLU HIS GLU ASP PRO PRO LEU PRO VAL GLY TYR GLN LEU PRO PRO ASN PRO ARG ASN VAL GLN GLU LEU PHE SER GLY PHE PRO PRO ARG VAL

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

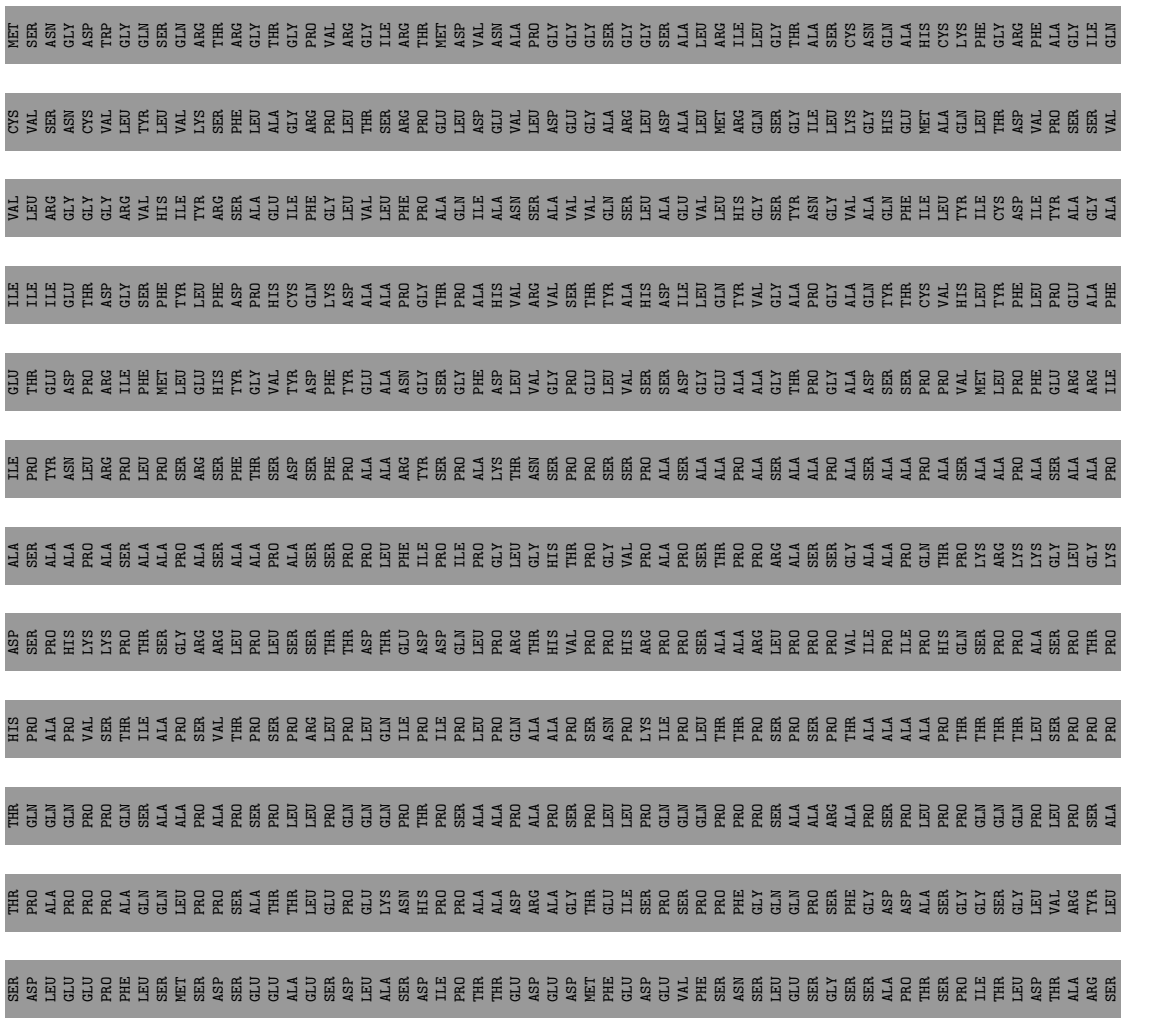
TRP PRO LYS ASP SER LEU GLU LEU LEU PRO GLN PRO ALA PRO GLN GLN PRO PRO SER SER PRO TRP ALA SER GLU GLN GLY PRO ILE VAL TYR THR LEU SER PRO HIS SER THR PRO SER THR ALA SER GLY SER GLN LYS LYS HIS THR ILE GLN ILE PRO GLY LEU VAL PRO SER GLN

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 GLN ASP THR GLN ALA SER SER GLN ASP PRO PRO TYR GLY HIS SER ILE MET GLN ARG GLU LYS LYS GLN GLN GLY



• Molecule 4: Large tegument protein deneddylase

Chain z: 99%



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

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

LEU LEU SER GLY GLY ASP GLN GLU ALA GLY GLU GLY 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

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 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 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 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 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

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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

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 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

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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

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

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

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

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 GLN ASP THR GLN ALA SER SER GLN ASP PRO PRO TYR GLY HIS SER ILE MET GLN ARG GLU LYS LYS GLN GLN GLY

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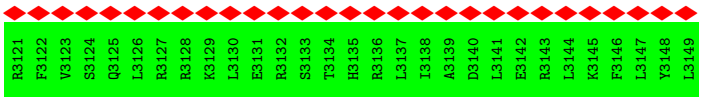
LEU ALA ALA PRO ALA HIS THR PRO VAL GLY ALA LEU ALA PRO ARG PRO GLN LYS THR GLN ALA GLN ARG PRO GLN ASP ALA ALA ALA LEU PRO THR PRO THR ILE LYS ALA VAL GLY ALA ARG PRO VAL PRO LYS ALA THR GLY ALA LEU ALA ALA GLY ALA ARG PRO ARG GLY GLN PRO

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

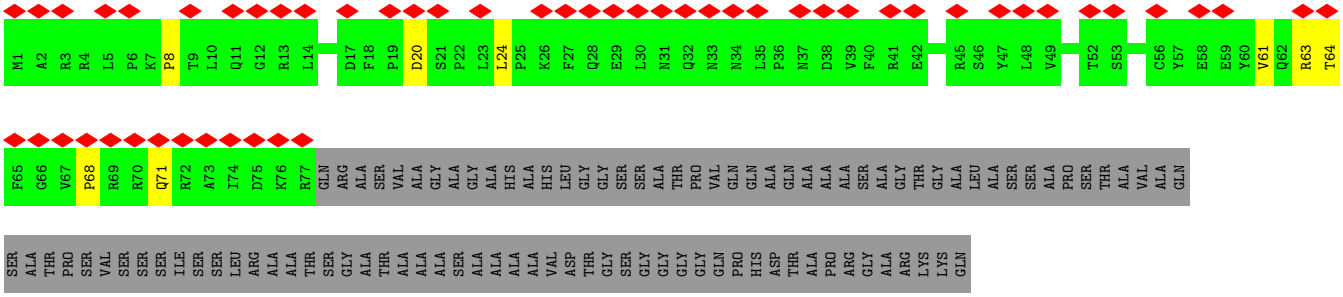
LYS GLU ALA PRO PRO SER ALA ALA ALA SER GLN LEU PRO LYS MET PRO LYS CYS LYS ASP SER MET TYR TYR PRO PRO SER GLY SER ALA ARG TYR PRO ALA PRO PHE GLN ALA LEU SER PHE SER GLN SER VAL ALA SER PRO ALA PRO SER SER ASP GLN THR THR LEU LEU TRP ASN THR

PRO SER VAL VAL THR GLN PHE LEU SER ILE GLU ASP ILE ILE ARG GLU VAL VAL THR GLY GLY SER THR SER GLY ASP LEU VAL VAL PRO SER 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 5: Small capsomere-interacting protein

Chain Z:



• Molecule 5: Small capsomere-interacting protein

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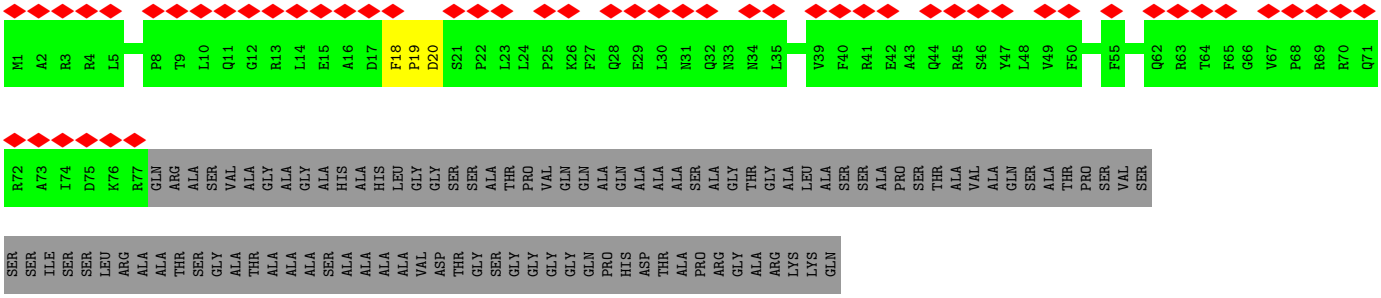

• Molecule 5: Small capsomere-interacting protein

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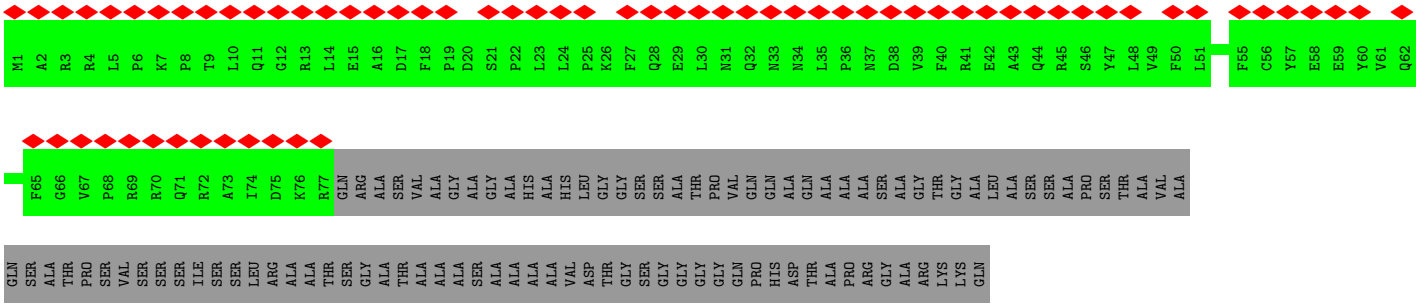

• Molecule 5: Small capsomere-interacting protein

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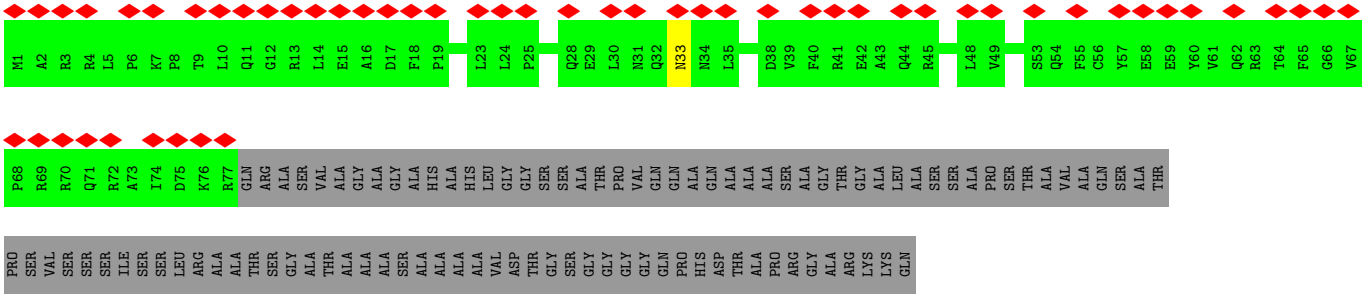
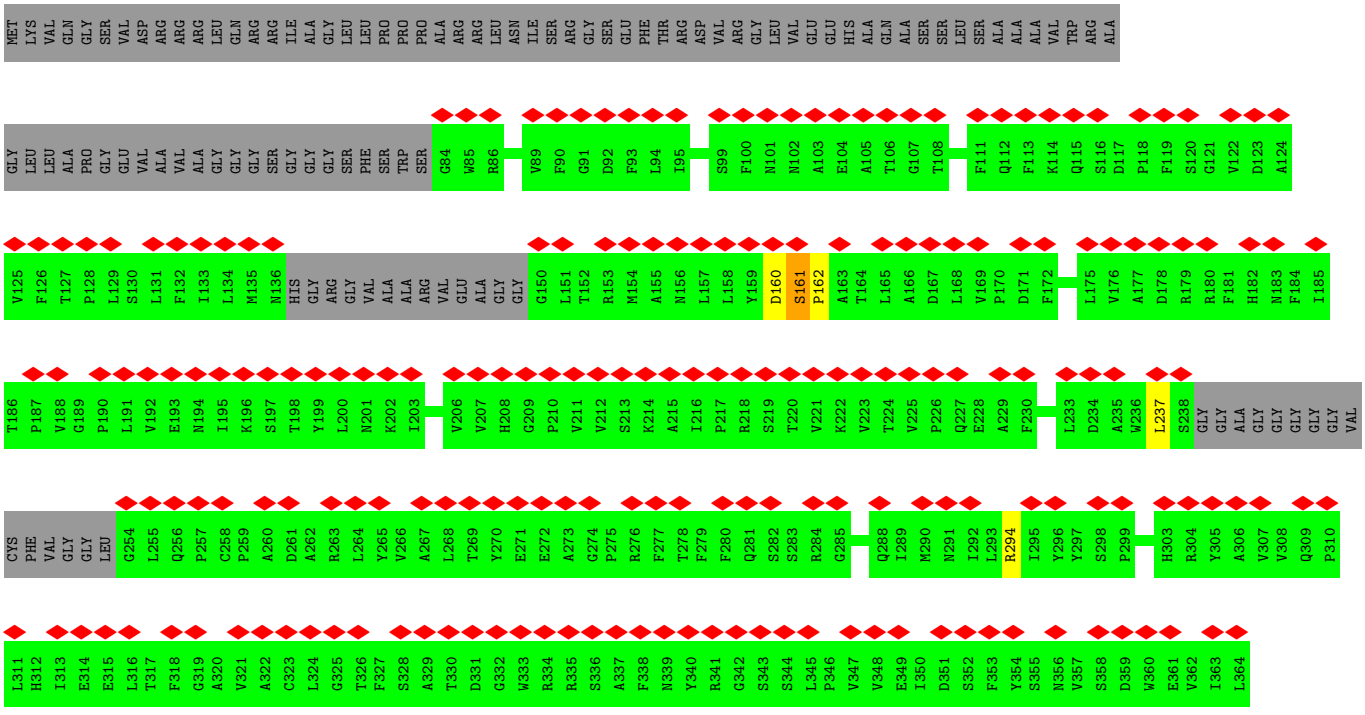


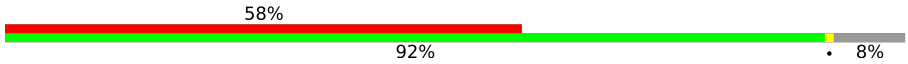
- Molecule 6: Triplex capsid protein 1

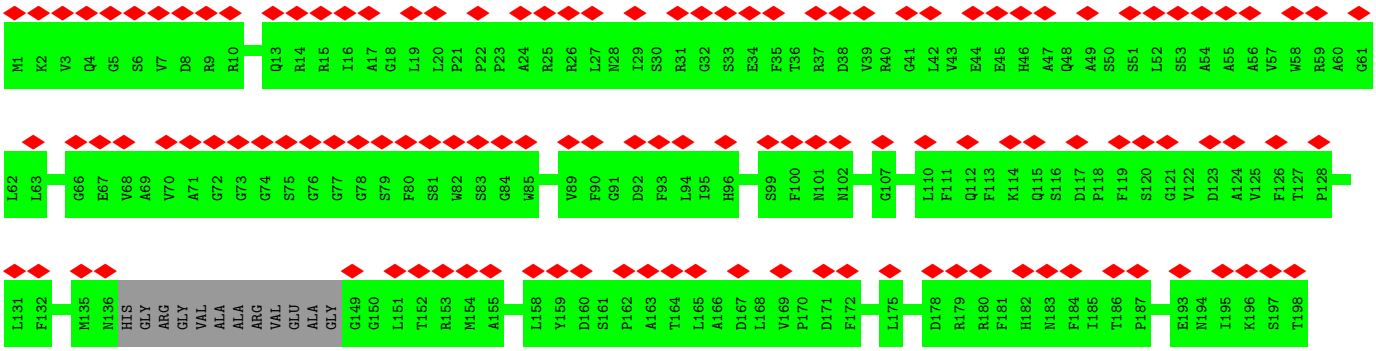
Chain f:

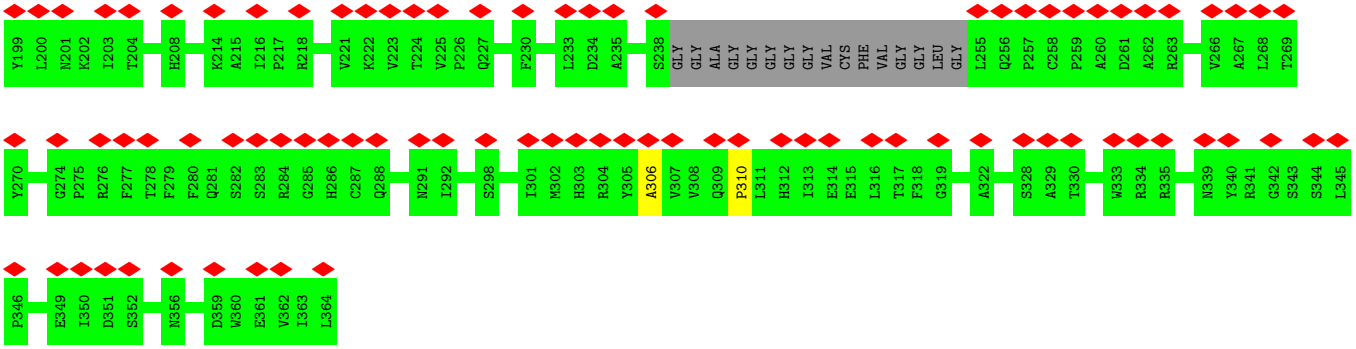


- Molecule 6: Triplex capsid protein 1

Chain h:

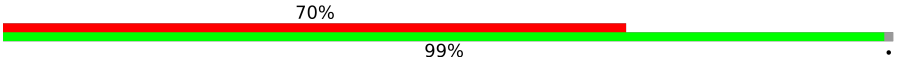


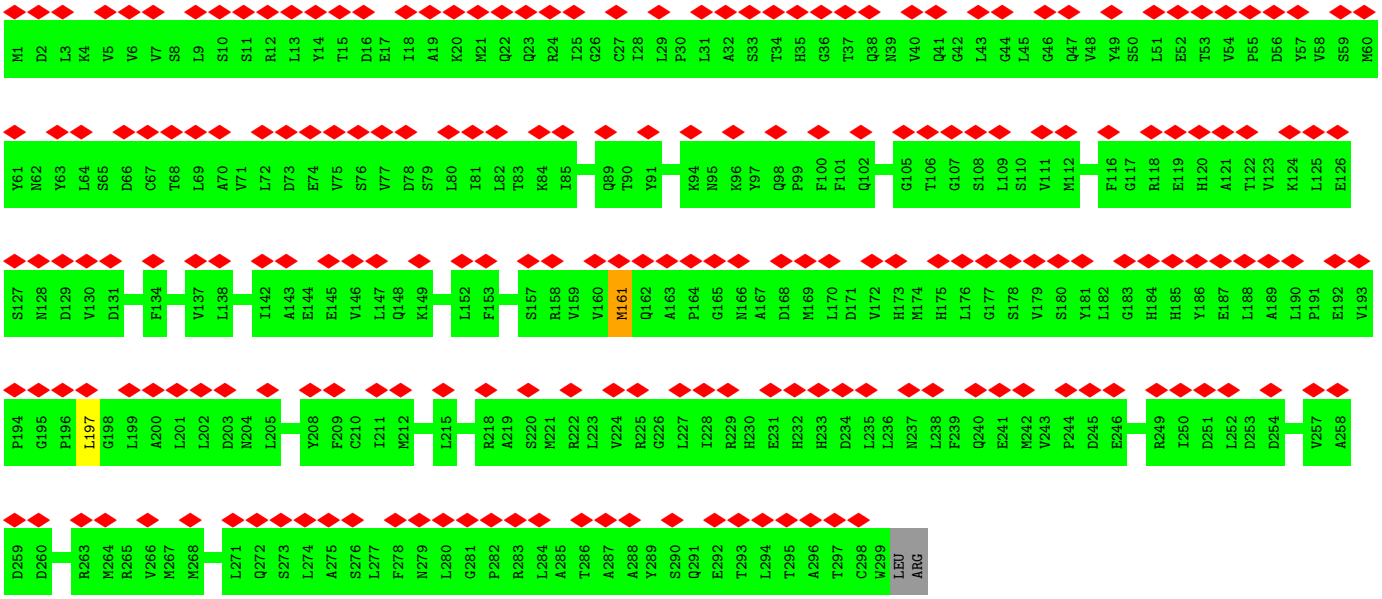




• Molecule 7: Triplex capsid protein 2

Chain k:





• Molecule 7: Triplex capsid protein 2

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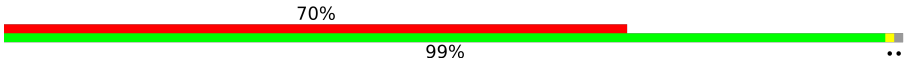

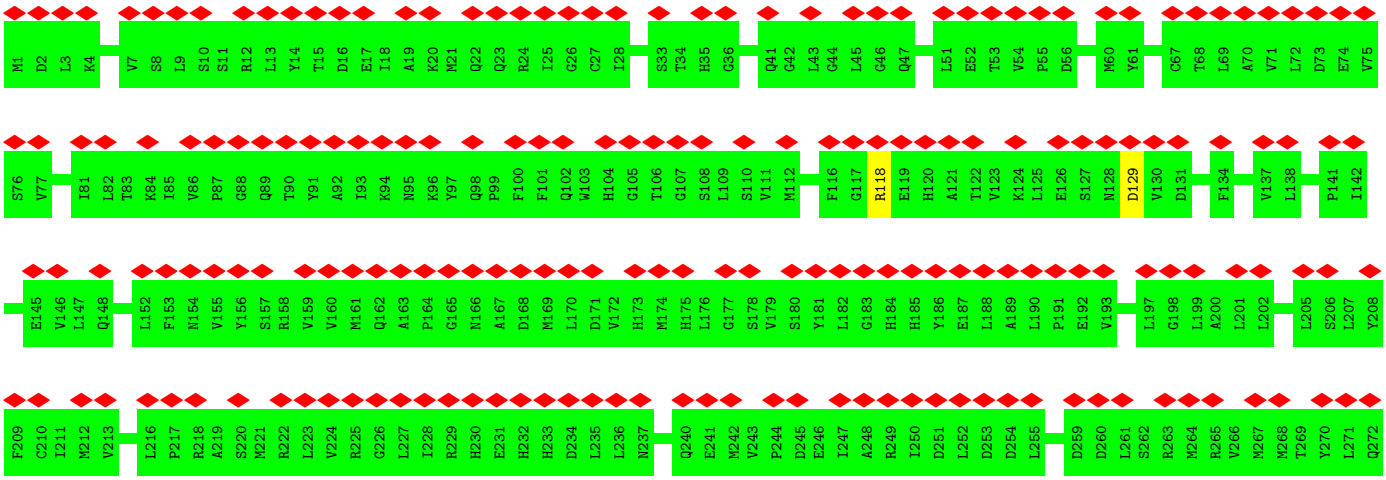

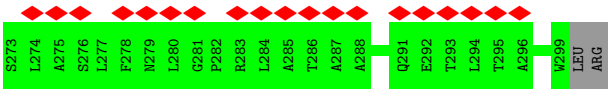

- Molecule 7: Triplex capsid protein 2

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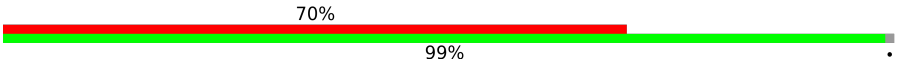

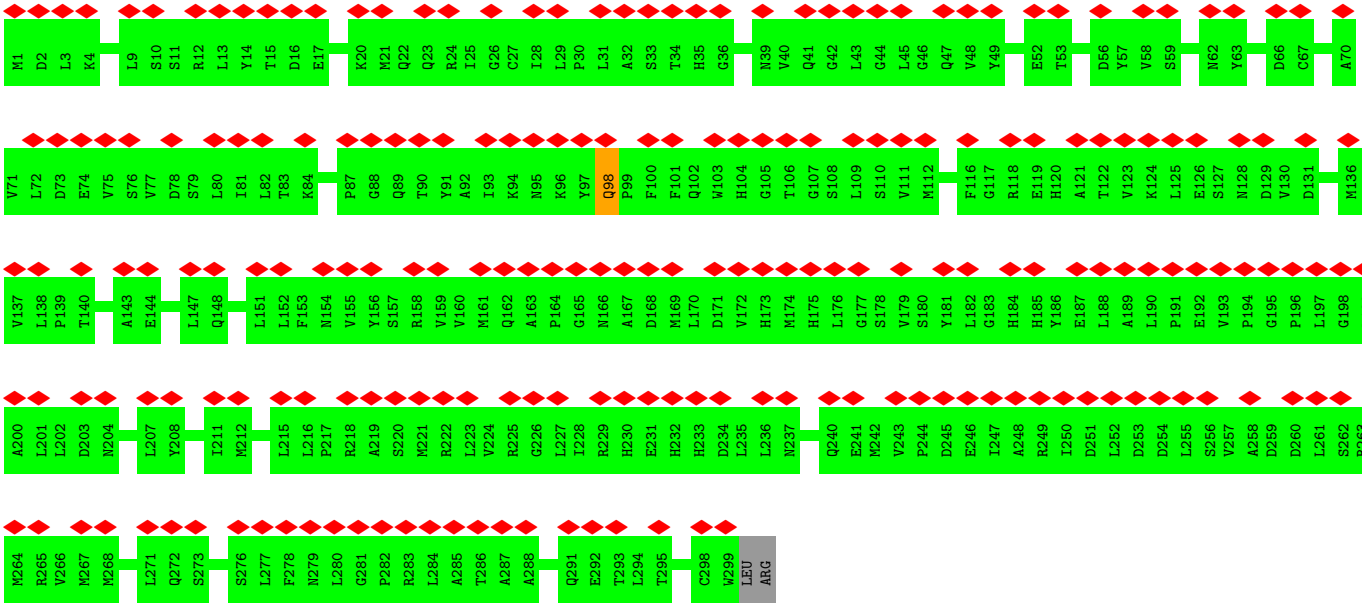

- Molecule 7: Triplex capsid protein 2

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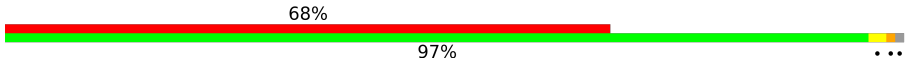

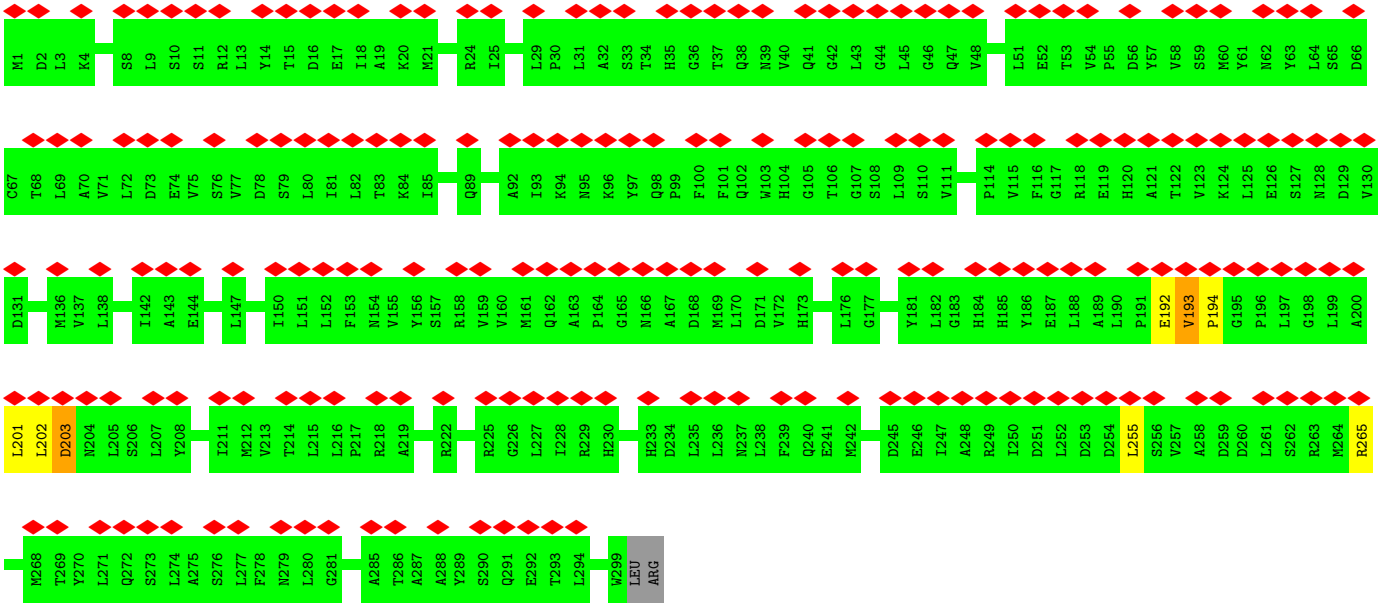

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	2305	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	0.040	Depositor
Minimum map value	-0.027	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.012	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	0.34	0/10492	0.57	0/14259
1	K	0.34	0/11085	0.58	0/15066
1	N	0.34	0/10933	0.57	0/14858
1	O	0.35	0/10435	0.57	0/14183
2	v	0.36	0/2346	0.61	0/3190
3	w	0.32	0/553	0.58	0/741
3	x	0.32	0/553	0.50	0/741
4	y	0.31	0/320	0.58	0/424
4	z	0.30	0/320	0.57	0/424
5	Z	0.35	0/664	0.58	0/896
5	a	0.34	0/664	0.60	1/896 (0.1%)
5	d	0.34	0/664	0.57	0/896
5	e	0.31	0/664	0.51	0/896
6	f	0.34	0/2049	0.63	2/2795 (0.1%)
6	h	0.34	0/2672	0.60	0/3635
7	k	0.34	0/2388	0.61	0/3254
7	m	0.35	0/2388	0.62	0/3254
7	p	0.32	0/2388	0.61	0/3254
7	r	0.33	0/2388	0.65	2/3254 (0.1%)
All	All	0.34	0/63966	0.59	5/86916 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	r	203	ASP	CB-CG-OD1	9.93	127.24	118.30
6	f	161	SER	C-N-CA	-7.42	90.86	122.00
7	r	203	ASP	CB-CG-OD2	-5.82	113.07	118.30
5	a	18	PHE	C-N-CA	-5.42	99.25	122.00
6	f	160	ASP	CB-CG-OD2	5.23	123.00	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	10252	0	10074	154	0
1	K	10832	0	10655	174	0
1	N	10683	0	10500	144	0
1	O	10194	0	10022	135	0
2	v	2288	0	2273	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	5	0
5	a	649	0	649	0	0
5	d	649	0	649	0	0
5	e	649	0	649	0	0
6	f	1992	0	1953	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	62525	0	61868	587	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 8.

All (587) 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:K:857:LEU:HD12	1:K:875:ARG:CD	1.20	1.58
1:J:1264:VAL:CG1	1:J:1265:PRO:HD2	1.34	1.52
1:K:1264:VAL:HB	1:K:1265:PRO:CD	1.09	1.44
1:K:1264:VAL:CB	1:K:1265:PRO:HD2	1.45	1.42
1:K:467:PRO:CG	1:K:912:PRO:HG3	1.59	1.33

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:483:ARG:NH2	1:O:553:ASP:OD2	1.62	1.32
1:K:857:LEU:CD1	1:K:875:ARG:CD	2.08	1.29
1:K:1264:VAL:CB	1:K:1265:PRO:CD	2.02	1.28
1:K:803:GLY:O	1:K:804:HIS:CD2	1.86	1.27
1:K:857:LEU:CD1	1:K:875:ARG:HD3	1.65	1.27
1:K:484:ARG:CD	1:K:552:ARG:HA	1.68	1.23
1:K:803:GLY:C	1:K:804:HIS:CD2	2.16	1.19
1:J:1264:VAL:CG1	1:J:1265:PRO:CD	2.20	1.18
1:J:1264:VAL:HG13	1:J:1265:PRO:CD	1.74	1.18
1:N:670:LEU:CG	1:N:671:GLY:H	1.54	1.18
1:J:871:ILE:HD13	1:J:936:ARG:NH2	1.57	1.17
1:K:1264:VAL:HB	1:K:1265:PRO:HD3	1.16	1.15
1:K:803:GLY:O	1:K:804:HIS:CG	1.98	1.15
1:N:670:LEU:HG	1:N:671:GLY:N	1.30	1.14
1:J:85:LEU:HD11	1:J:1070:GLY:HA2	1.29	1.12
1:K:857:LEU:HD12	1:K:875:ARG:HD2	1.29	1.07
1:J:85:LEU:CD1	1:J:1070:GLY:HA2	1.84	1.07
1:J:1264:VAL:HG12	1:J:1265:PRO:HD2	1.35	1.05
1:K:484:ARG:HD3	1:K:552:ARG:CA	1.88	1.02
1:K:857:LEU:HD11	1:K:875:ARG:HG2	1.37	1.02
1:K:1252:ASP:OD1	1:K:1256:ASN:ND2	1.92	1.02
1:K:467:PRO:HG2	1:K:912:PRO:CG	1.92	1.00
1:K:1264:VAL:CG2	1:K:1265:PRO:HD2	1.90	0.99
1:K:467:PRO:CG	1:K:912:PRO:CG	2.40	0.99
1:J:556:GLU:HG2	1:J:557:ARG:H	1.27	0.97
1:K:467:PRO:HG2	1:K:912:PRO:HG3	0.96	0.95
1:K:484:ARG:HD3	1:K:552:ARG:HA	0.95	0.94
1:N:731:ASP:HA	1:N:796:LEU:HD21	1.45	0.94
1:J:72:ALA:HB2	1:J:369:ALA:HB2	1.50	0.93
1:K:857:LEU:CD1	1:K:875:ARG:CG	2.46	0.92
1:J:556:GLU:HG2	1:J:557:ARG:N	1.87	0.90
1:O:483:ARG:CZ	1:O:553:ASP:OD2	2.20	0.89
1:K:857:LEU:CD1	1:K:875:ARG:HG2	2.03	0.88
1:J:1264:VAL:HG12	1:J:1265:PRO:CD	1.98	0.87
1:O:1010:PRO:O	1:O:1011:SER:O	1.92	0.86
1:J:1264:VAL:HG13	1:J:1265:PRO:HD2	0.87	0.86
1:O:483:ARG:HE	1:O:553:ASP:CG	1.80	0.85
1:N:265:SER:O	1:N:266:THR:O	1.93	0.85
1:J:871:ILE:HD13	1:J:936:ARG:HH21	1.37	0.84
1:J:556:GLU:CG	1:J:557:ARG:N	2.41	0.84
1:K:857:LEU:HD11	1:K:875:ARG:CG	2.07	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:484:ARG:HH11	1:N:484:ARG:HG2	1.41	0.83
1:N:619:PHE:HE1	1:N:874:LEU:HD23	1.41	0.83
1:N:670:LEU:CG	1:N:671:GLY:N	2.20	0.81
1:K:857:LEU:HD12	1:K:875:ARG:HD3	0.82	0.81
1:K:1256:ASN:OD1	1:K:1275:PHE:O	2.00	0.80
1:K:1264:VAL:HB	1:K:1265:PRO:HD2	0.80	0.80
1:J:482:ASP:HB2	1:J:484:ARG:NH1	1.97	0.78
1:N:825:MET:HA	1:N:930:ALA:O	1.84	0.77
1:K:1252:ASP:CG	1:K:1256:ASN:ND2	2.38	0.77
1:N:899:ARG:NH1	1:N:922:THR:HG23	1.99	0.76
1:J:828:LEU:HB3	1:J:928:LEU:O	1.87	0.74
1:K:467:PRO:HG3	1:K:912:PRO:HG3	1.67	0.72
1:K:1252:ASP:CG	1:K:1256:ASN:HD21	1.89	0.72
1:J:936:ARG:HD3	1:O:669:HIS:CD2	2.25	0.72
1:J:85:LEU:HD11	1:J:1070:GLY:CA	2.16	0.72
1:K:617:ALA:O	1:K:620:TYR:HB2	1.90	0.72
1:N:543:HIS:HD2	1:N:546:TYR:H	1.36	0.71
1:N:619:PHE:CE1	1:N:874:LEU:HD23	2.25	0.71
1:K:360:GLU:O	1:K:362:GLN:N	2.23	0.71
1:N:484:ARG:HD3	1:N:550:ILE:HG22	1.72	0.71
1:O:860:LEU:HD22	1:O:866:ARG:HG2	1.72	0.71
1:K:803:GLY:C	1:K:804:HIS:CG	2.52	0.70
1:K:456:LEU:HD11	1:K:1031:ILE:HG13	1.74	0.70
1:K:1252:ASP:CB	1:K:1256:ASN:ND2	2.54	0.70
1:N:899:ARG:HH11	1:N:922:THR:CG2	2.05	0.70
1:J:871:ILE:HD13	1:J:936:ARG:HH22	1.54	0.70
1:O:483:ARG:NE	1:O:553:ASP:CG	2.44	0.70
1:K:804:HIS:HE1	1:K:808:LEU:HD11	1.57	0.69
1:J:96:ARG:HG2	1:J:117:ILE:HG12	1.75	0.68
1:K:805:ALA:O	1:K:806:ASP:OD1	2.11	0.68
1:K:722:ASN:HD22	1:K:742:ARG:HH21	1.40	0.68
1:K:912:PRO:O	1:K:913:ASN:HB3	1.93	0.68
1:K:1252:ASP:CB	1:K:1256:ASN:HD22	2.07	0.67
1:K:1256:ASN:OD1	1:K:1275:PHE:HB3	1.95	0.67
1:O:241:SER:HA	1:O:293:PHE:HZ	1.58	0.67
1:J:856:ILE:HG13	1:J:881:ILE:HD12	1.76	0.67
1:O:639:LEU:HD12	1:O:880:MET:HB3	1.76	0.66
1:N:1068:PHE:HB2	1:N:1093:ALA:HB3	1.78	0.66
1:J:436:VAL:HG11	1:J:587:GLN:HE22	1.59	0.66
1:J:456:LEU:HD21	1:J:1031:ILE:HG13	1.77	0.66
1:K:912:PRO:O	1:K:913:ASN:CB	2.44	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:401:MET:O	1:J:1051:GLU:HA	1.96	0.65
1:O:565:ARG:O	1:O:570:ASN:ND2	2.27	0.65
1:N:650:ARG:NE	1:N:873:ASP:OD2	2.29	0.65
1:O:1117:MET:SD	1:O:1371:ARG:NH1	2.70	0.65
1:O:1068:PHE:HB2	1:O:1093:ALA:HB3	1.77	0.65
1:N:899:ARG:HH11	1:N:922:THR:HG23	1.60	0.65
1:K:467:PRO:HG3	1:K:912:PRO:CG	2.22	0.65
1:K:901:SER:HB3	1:K:918:ARG:HD2	1.80	0.64
1:K:911:ALA:HB3	1:K:912:PRO:CD	2.28	0.64
1:N:129:THR:HG22	1:O:103:ALA:HB2	1.80	0.64
1:O:104:HIS:HE1	1:O:108:ARG:HB2	1.62	0.64
1:J:1192:ASP:OD2	1:J:1237:ARG:NH2	2.31	0.64
1:J:828:LEU:HD11	1:J:945:PHE:HB3	1.80	0.64
1:O:594:LEU:HD11	1:O:692:ALA:HB1	1.79	0.64
1:K:857:LEU:CD1	1:K:875:ARG:HD2	2.06	0.64
1:J:72:ALA:CB	1:J:369:ALA:HB2	2.26	0.64
1:K:803:GLY:C	1:K:804:HIS:HD2	1.96	0.63
1:N:409:VAL:HG13	1:N:1044:MET:HG3	1.80	0.63
1:N:718:LEU:HD13	1:N:811:ILE:HG12	1.81	0.63
1:O:764:GLU:OE1	1:O:793:ARG:NH1	2.32	0.63
1:N:1192:ASP:OD2	1:N:1237:ARG:NH2	2.31	0.63
1:K:764:GLU:HG3	1:K:793:ARG:HH11	1.64	0.62
1:K:1252:ASP:HB3	1:K:1256:ASN:HD22	1.63	0.62
1:J:1264:VAL:HG12	1:J:1265:PRO:N	2.15	0.62
1:K:804:HIS:CE1	1:K:808:LEU:HD11	2.35	0.62
1:K:1195:TYR:O	1:K:1200:ASN:ND2	2.31	0.62
1:N:804:HIS:CD2	1:N:808:LEU:HD11	2.35	0.62
1:O:436:VAL:HG11	1:O:587:GLN:HE22	1.65	0.62
1:J:783:ARG:NH2	1:J:891:CYS:O	2.33	0.61
1:J:72:ALA:HB2	1:J:369:ALA:CB	2.27	0.61
1:J:225:GLU:O	1:J:232:ARG:NH2	2.33	0.61
1:K:400:ARG:NE	1:K:1051:GLU:OE2	2.30	0.61
1:N:747:ILE:HB	1:N:899:ARG:HB2	1.81	0.61
1:N:1246:GLN:HB2	1:N:1249:SER:HB3	1.82	0.61
1:N:362:GLN:O	1:N:364:ARG:NH1	2.34	0.61
1:K:285:ASN:O	1:K:289:GLN:NE2	2.32	0.61
1:K:1252:ASP:HA	1:K:1256:ASN:ND2	2.15	0.61
1:N:53:GLU:OE2	1:O:326:ARG:NH1	2.33	0.61
1:O:225:GLU:O	1:O:232:ARG:NH1	2.34	0.61
1:K:184:LYS:NZ	1:K:1064:SER:OG	2.34	0.61
1:N:93:ILE:HD12	1:N:1095:ILE:HG21	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:439:TRP:HB2	1:N:1337:ALA:HB3	1.83	0.60
1:J:10:ARG:NH1	1:K:321:ALA:O	2.32	0.60
1:N:484:ARG:HG2	1:N:484:ARG:NH1	2.14	0.60
1:N:737:LEU:HD23	1:N:744:PRO:HG2	1.82	0.60
1:N:619:PHE:CE1	1:N:874:LEU:CD2	2.84	0.60
1:K:1068:PHE:HB2	1:K:1093:ALA:HB3	1.83	0.60
1:J:431:THR:HG23	1:J:432:GLN:HG3	1.84	0.59
1:N:783:ARG:HA	1:N:788:HIS:HE1	1.66	0.59
1:K:484:ARG:CD	1:K:552:ARG:CA	2.63	0.59
1:N:184:LYS:NZ	1:N:1064:SER:OG	2.36	0.59
1:O:783:ARG:NH2	1:O:891:CYS:O	2.34	0.59
1:J:1374:LYS:HG2	1:J:1379:VAL:HG22	1.83	0.59
1:K:484:ARG:HD2	1:K:552:ARG:HA	1.76	0.59
1:O:301:GLN:HA	1:O:367:ILE:O	2.01	0.59
1:N:484:ARG:HD2	1:N:551:GLY:O	2.02	0.59
1:K:409:VAL:HG13	1:K:1044:MET:HG3	1.85	0.59
1:K:548:ILE:HD11	1:K:560:HIS:HB3	1.85	0.59
1:N:1074:VAL:HG22	1:N:1088:VAL:HG22	1.84	0.59
1:N:803:GLY:O	1:N:804:HIS:HB2	2.03	0.58
1:O:850:PHE:HE2	1:O:878:VAL:HG21	1.68	0.58
1:J:936:ARG:HD3	1:O:669:HIS:HD2	1.68	0.58
1:N:942:GLN:NE2	1:N:943:CYS:SG	2.76	0.58
1:K:317:ASN:ND2	1:K:328:MET:O	2.36	0.58
1:J:551:GLY:HA3	1:J:559:ARG:HH11	1.67	0.58
1:K:724:LEU:O	1:K:921:GLN:NE2	2.36	0.58
1:N:185:LEU:HD13	1:N:399:ARG:HH21	1.69	0.58
1:J:463:ARG:HH22	1:J:1259:TYR:HB3	1.68	0.58
1:J:720:ASP:OD1	1:J:742:ARG:NH2	2.37	0.58
1:K:496:HIS:HE1	1:K:502:ILE:HG13	1.68	0.58
1:N:1195:TYR:O	1:N:1200:ASN:ND2	2.37	0.58
1:K:185:LEU:HD13	1:K:399:ARG:HH21	1.68	0.58
1:N:997:HIS:HE1	1:N:1022:HIS:HE1	1.52	0.58
1:O:406:TYR:HA	1:O:1046:VAL:O	2.03	0.58
1:O:549:TYR:OH	1:O:994:ARG:NH2	2.36	0.57
1:N:80:THR:HG22	1:N:309:ALA:HB3	1.87	0.57
1:O:904:ASN:ND2	1:O:908:GLN:O	2.37	0.57
1:K:359:VAL:O	1:K:360:GLU:O	2.22	0.57
1:K:496:HIS:ND1	1:K:498:ASN:OD1	2.37	0.57
1:N:401:MET:O	1:N:1051:GLU:HA	2.04	0.57
1:N:441:VAL:HG11	1:N:1373:LEU:HD22	1.85	0.57
1:K:586:GLN:NE2	1:K:589:GLU:OE2	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:439:TRP:HB3	1:O:447:LEU:HD11	1.87	0.57
1:J:406:TYR:HA	1:J:1046:VAL:O	2.05	0.57
1:N:742:ARG:HB3	1:N:903:ASP:HB2	1.85	0.57
1:K:594:LEU:HD13	1:K:696:ALA:HB2	1.87	0.57
1:O:282:VAL:HG12	1:O:1057:ILE:HG12	1.86	0.56
1:J:995:GLU:O	1:J:998:ARG:NH2	2.38	0.56
1:J:85:LEU:CD1	1:J:1070:GLY:CA	2.74	0.56
1:O:584:ARG:NH1	1:O:1020:ALA:O	2.35	0.56
1:O:650:ARG:NH1	1:O:873:ASP:O	2.39	0.56
1:K:585:GLY:HA3	1:K:1017:GLY:HA2	1.88	0.56
1:N:133:LEU:HD13	1:N:138:LEU:HD21	1.87	0.56
1:N:731:ASP:CA	1:N:796:LEU:HD21	2.26	0.56
1:J:443:LYS:HD3	1:J:1116:ASP:HA	1.88	0.56
1:N:673:ASN:HB3	1:O:650:ARG:HH22	1.71	0.56
1:N:567:MET:SD	1:N:1022:HIS:ND1	2.77	0.56
1:O:483:ARG:NE	1:O:553:ASP:OD2	2.39	0.56
1:J:584:ARG:NH1	1:J:1020:ALA:O	2.38	0.56
1:K:1246:GLN:HB2	1:K:1249:SER:HB3	1.88	0.56
1:O:111:SER:OG	1:O:114:ARG:NH2	2.39	0.56
1:J:555:GLY:O	1:J:557:ARG:N	2.39	0.56
1:J:666:ILE:HA	1:J:670:LEU:HD12	1.87	0.56
1:N:230:LEU:HD21	1:N:289:GLN:HG2	1.86	0.56
1:N:670:LEU:HG	1:N:671:GLY:H	0.62	0.56
1:J:400:ARG:NH2	1:J:1051:GLU:OE1	2.38	0.55
1:K:266:THR:O	1:K:364:ARG:NH1	2.34	0.55
1:O:127:ILE:HB	1:O:1090:HIS:O	2.06	0.55
1:O:1080:ARG:HE	1:O:1082:ASP:HB2	1.71	0.55
1:K:307:SER:OG	1:K:362:GLN:NE2	2.39	0.55
1:K:938:ARG:HA	1:K:941:THR:HB	1.88	0.55
1:N:783:ARG:HE	1:N:893:THR:HG22	1.71	0.55
1:K:911:ALA:N	1:K:912:PRO:HD2	2.22	0.55
1:N:269:THR:HG22	1:N:271:LYS:H	1.72	0.55
1:J:746:ILE:HB	1:J:753:TYR:HB3	1.87	0.55
1:J:763:ILE:HG12	1:J:794:LEU:HD11	1.89	0.55
1:K:269:THR:OG1	1:K:272:GLY:O	2.23	0.55
1:N:856:ILE:HD12	1:N:876:PRO:HG2	1.89	0.55
1:N:857:LEU:HD12	1:N:875:ARG:HG2	1.88	0.55
1:J:935:GLU:OE1	1:O:668:ARG:NH1	2.38	0.55
1:J:955:GLY:HA3	1:J:985:ARG:HE	1.72	0.55
1:O:814:TYR:OH	1:O:921:GLN:NE2	2.40	0.55
1:J:1135:ASN:HB3	1:J:1138:VAL:HG12	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:630:GLU:OE2	1:O:669:HIS:NE2	2.36	0.55
1:N:267:TYR:HD1	1:N:267:TYR:N	2.05	0.54
1:J:1174:LEU:O	1:K:213:SER:OG	2.21	0.54
1:J:1308:GLU:HG3	1:J:1309:VAL:HG13	1.88	0.54
1:K:40:LEU:HD22	1:K:44:ASP:HB3	1.88	0.54
1:K:1117:MET:SD	1:K:1371:ARG:NH2	2.80	0.54
1:J:195:GLN:NE2	1:J:250:GLU:OE2	2.40	0.54
1:J:871:ILE:CD1	1:J:936:ARG:HH21	2.14	0.54
1:K:591:ALA:HB1	1:K:1036:LEU:HD12	1.88	0.54
1:K:952:MET:HA	1:K:985:ARG:HH22	1.71	0.54
1:J:303:MET:O	1:J:364:ARG:N	2.41	0.54
1:K:95:PHE:HB2	1:K:118:VAL:HB	1.90	0.54
1:N:287:LEU:HD13	1:N:383:SER:HB3	1.90	0.54
1:N:844:PRO:O	1:N:882:ARG:NH2	2.36	0.54
1:K:720:ASP:O	1:K:810:LYS:NZ	2.40	0.54
1:K:997:HIS:HE1	1:K:1022:HIS:HE1	1.54	0.54
1:N:1119:ILE:HD11	1:O:1235:GLU:HB3	1.90	0.54
1:N:1298:LEU:HD21	1:N:1302:PRO:HG3	1.90	0.54
1:N:572:PRO:HG2	1:N:575:LEU:HD12	1.90	0.54
1:N:1053:LEU:HD12	1:N:1112:ALA:HB3	1.90	0.54
1:O:1299:GLY:O	1:O:1323:GLN:NE2	2.41	0.54
1:J:400:ARG:HH22	1:J:1114:THR:HG21	1.72	0.53
1:K:911:ALA:CB	1:K:912:PRO:CD	2.86	0.53
1:K:910:LEU:C	1:K:912:PRO:HD2	2.29	0.53
1:J:617:ALA:HA	1:J:620:TYR:HD2	1.73	0.53
1:K:329:ARG:HG2	1:K:330:THR:HG23	1.90	0.53
1:J:565:ARG:O	1:J:570:ASN:ND2	2.35	0.53
1:J:589:GLU:HG2	1:J:594:LEU:HD12	1.90	0.53
1:K:312:VAL:HG12	1:K:314:ARG:H	1.73	0.53
1:K:1264:VAL:HG23	1:K:1265:PRO:HD2	1.88	0.53
1:N:282:VAL:HG12	1:N:1057:ILE:HG12	1.90	0.53
1:N:532:PRO:HB3	1:N:1238:SER:HB2	1.90	0.53
1:O:598:VAL:HG13	1:O:602:VAL:HG13	1.89	0.53
1:J:399:ARG:HD3	1:J:1320:PHE:HB3	1.90	0.53
1:J:1326:SER:O	1:J:1329:GLN:NE2	2.42	0.53
1:J:85:LEU:HD13	1:J:1070:GLY:HA2	1.85	0.53
1:K:690:LEU:HD11	1:K:812:PHE:HB2	1.91	0.53
1:K:803:GLY:O	1:K:804:HIS:NE2	2.40	0.53
1:K:804:HIS:HE1	1:K:808:LEU:CD1	2.20	0.53
1:O:307:SER:OG	1:O:362:GLN:OE1	2.27	0.53
1:J:427:LEU:O	1:J:427:LEU:HD23	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:535:TYR:HE2	1:K:539:ARG:HH21	1.57	0.53
1:J:281:ILE:HD12	1:J:1058:LEU:HD23	1.90	0.53
1:K:225:GLU:O	1:K:232:ARG:NH2	2.38	0.53
1:O:417:LYS:NZ	1:O:431:THR:O	2.40	0.53
1:O:625:MET:SD	1:O:887:SER:OG	2.61	0.52
1:O:504:ASP:O	1:O:508:ASP:HB2	2.09	0.52
1:N:484:ARG:HH11	1:N:484:ARG:CG	2.16	0.52
1:O:510:LYS:O	1:O:973:ARG:NH2	2.42	0.52
1:J:904:ASN:ND2	1:J:919:THR:OG1	2.33	0.52
1:O:921:GLN:HB2	1:O:996:TRP:CD1	2.44	0.52
1:J:367:ILE:O	1:J:368:SER:OG	2.21	0.52
1:O:835:VAL:O	1:O:838:THR:OG1	2.26	0.52
1:O:902:VAL:O	1:O:918:ARG:HA	2.09	0.52
1:N:267:TYR:N	1:N:267:TYR:CD1	2.76	0.52
1:N:835:VAL:O	1:N:838:THR:OG1	2.25	0.52
1:O:1128:PHE:HZ	1:O:1260:ARG:HD2	1.75	0.52
1:K:803:GLY:CA	1:K:804:HIS:CD2	2.92	0.52
1:N:513:ALA:HB1	1:N:984:ASN:HD22	1.75	0.52
1:N:1115:THR:HG22	1:N:1180:ALA:HB2	1.92	0.52
1:N:1299:GLY:HA3	1:N:1323:GLN:HE21	1.74	0.52
1:K:553:ASP:HB3	1:K:558:ALA:HB2	1.91	0.51
1:O:266:THR:O	1:O:364:ARG:NH1	2.41	0.51
1:J:731:ASP:HB3	1:J:799:TYR:HB2	1.92	0.51
1:K:401:MET:O	1:K:1051:GLU:HA	2.11	0.51
1:K:1203:ARG:HE	1:K:1245:SER:HA	1.75	0.51
1:J:855:ASP:OD2	1:J:875:ARG:NH2	2.39	0.51
1:K:1205:ARG:HG2	1:K:1231:ASP:HB3	1.93	0.51
1:N:587:GLN:NE2	1:N:1037:LYS:O	2.44	0.51
1:O:603:ILE:HD13	1:O:1011:SER:O	2.11	0.51
1:J:1176:HIS:HE1	1:K:1233:ALA:HA	1.76	0.51
1:O:406:TYR:HE2	1:O:1196:PHE:HD1	1.58	0.51
1:J:1123:ASP:N	1:J:1123:ASP:OD1	2.43	0.51
1:K:1252:ASP:CA	1:K:1256:ASN:ND2	2.74	0.51
1:N:637:VAL:HG23	1:N:638:PRO:HD3	1.92	0.51
1:O:456:LEU:HA	1:O:459:LEU:HB2	1.91	0.51
1:J:587:GLN:NE2	1:J:1037:LYS:O	2.44	0.51
1:K:521:LYS:NZ	1:K:540:LEU:O	2.44	0.51
1:K:1027:PRO:HA	1:K:1030:TYR:HD2	1.74	0.51
1:O:1315:ALA:HB1	1:O:1317:THR:HG23	1.92	0.51
1:K:1159:ARG:NH2	1:K:1317:THR:OG1	2.44	0.51
1:J:581:GLN:HE21	1:J:1021:MET:HG2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:434:LEU:HD12	1:O:435:PRO:HD2	1.93	0.50
1:J:564:HIS:HD2	1:J:566:LEU:HD23	1.76	0.50
1:K:971:VAL:HG13	1:K:978:ARG:HE	1.77	0.50
1:J:482:ASP:HB2	1:J:484:ARG:HH12	1.75	0.50
1:K:777:VAL:O	1:K:781:GLY:N	2.42	0.50
1:N:673:ASN:ND2	1:O:873:ASP:OD2	2.44	0.50
1:O:655:ALA:O	1:O:683:TYR:OH	2.28	0.50
1:J:72:ALA:CB	1:J:369:ALA:CB	2.89	0.50
1:K:440:ILE:HG21	1:K:1048:ARG:HH22	1.77	0.50
1:O:470:THR:HG22	1:O:1253:ILE:HG13	1.94	0.50
1:K:1350:LYS:O	1:K:1353:HIS:ND1	2.45	0.50
1:N:230:LEU:HD22	1:N:1109:ARG:HD2	1.94	0.50
1:N:484:ARG:CD	1:N:551:GLY:O	2.60	0.50
1:O:1350:LYS:O	1:O:1353:HIS:ND1	2.36	0.50
1:J:75:VAL:HG22	1:J:267:TYR:HD2	1.75	0.50
1:J:131:MET:O	1:J:1085:THR:HA	2.12	0.50
1:J:1197:GLN:NE2	1:J:1364:GLU:OE1	2.44	0.50
1:O:70:GLU:HA	1:O:367:ILE:HD12	1.95	0.49
1:J:908:GLN:NE2	1:J:1026:SER:OG	2.45	0.49
1:N:518:ILE:HA	1:N:521:LYS:HB2	1.94	0.49
1:N:548:ILE:HA	1:N:561:ARG:O	2.12	0.49
1:K:361:ASP:O	1:K:362:GLN:C	2.49	0.49
5:Z:61:VAL:O	5:Z:64:THR:OG1	2.27	0.49
1:N:829:GLY:HA2	1:N:895:THR:HG21	1.95	0.49
1:O:780:TYR:O	1:O:783:ARG:HB2	2.12	0.49
1:O:825:MET:N	1:O:956:ASP:OD2	2.43	0.49
1:J:123:HIS:O	1:J:1093:ALA:HA	2.12	0.49
1:J:213:SER:OG	1:O:1174:LEU:O	2.22	0.49
1:N:481:ARG:O	1:N:484:ARG:NH1	2.45	0.49
1:O:657:VAL:HA	1:O:663:ILE:HD11	1.94	0.49
1:J:571:LEU:HB3	1:J:575:LEU:HD23	1.95	0.49
1:J:1350:LYS:O	1:J:1353:HIS:ND1	2.45	0.49
1:N:804:HIS:CG	1:N:808:LEU:HD11	2.48	0.49
1:K:911:ALA:HB3	1:K:912:PRO:HD3	1.95	0.49
1:O:526:THR:HG22	1:O:574:PRO:HA	1.94	0.49
1:K:1264:VAL:CB	1:K:1265:PRO:HD3	2.04	0.48
1:N:951:HIS:HA	1:N:990:PHE:HE1	1.77	0.48
1:N:312:VAL:HG11	1:N:314:ARG:HH11	1.79	0.48
1:O:724:LEU:O	1:O:921:GLN:NE2	2.33	0.48
1:N:73:LEU:HD13	1:N:177:ILE:HD11	1.95	0.48
1:N:403:TYR:O	1:N:1049:THR:HA	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:518:ILE:HG22	1:N:521:LYS:HD2	1.95	0.48
1:J:549:TYR:OH	1:J:994:ARG:NH1	2.35	0.48
1:K:440:ILE:HD12	1:K:1119:ILE:HG22	1.95	0.48
1:O:475:ASN:HB3	1:O:560:HIS:HD2	1.78	0.48
1:O:1121:THR:HA	1:O:1182:CYS:HB2	1.96	0.48
1:J:1049:THR:HG23	1:J:1270:PRO:HB3	1.96	0.48
1:N:1039:HIS:ND1	1:N:1040:PRO:O	2.45	0.48
1:O:80:THR:HG22	1:O:309:ALA:HB3	1.96	0.48
1:O:467:PRO:HB2	1:O:471:LEU:HD23	1.94	0.48
1:O:985:ARG:HH21	1:O:990:PHE:HZ	1.61	0.48
1:J:186:ARG:NH2	1:J:1296:GLN:O	2.46	0.48
1:J:1205:ARG:HG3	1:J:1239:THR:HG23	1.95	0.48
1:N:731:ASP:HA	1:N:796:LEU:CD2	2.32	0.48
1:J:1173:GLY:HA2	1:K:209:LYS:HD3	1.96	0.48
1:J:205:ARG:NH1	1:O:1318:ASP:O	2.46	0.48
1:J:424:ILE:HD11	1:J:1345:GLU:HG2	1.96	0.48
1:J:1121:THR:HA	1:J:1182:CYS:HB2	1.96	0.47
1:K:360:GLU:OE1	1:K:360:GLU:HA	2.11	0.47
1:O:690:LEU:HD21	1:O:812:PHE:HB2	1.96	0.47
1:J:522:CYS:HB3	1:J:1000:PRO:HG3	1.97	0.47
1:J:1068:PHE:HB2	1:J:1093:ALA:HB3	1.95	0.47
1:O:300:ASN:HA	1:O:370:ALA:HA	1.96	0.47
1:J:511:TYR:HD1	1:J:973:ARG:HH12	1.61	0.47
1:K:804:HIS:CE1	1:K:808:LEU:CD1	2.97	0.47
1:N:794:LEU:HD11	1:N:925:VAL:HG21	1.97	0.47
1:N:947:ALA:H	1:N:964:HIS:HE1	1.62	0.47
1:O:588:PHE:HE1	1:O:700:LEU:HG	1.79	0.47
1:J:834:HIS:HD2	5:Z:8:PRO:HD3	1.79	0.47
1:N:484:ARG:NH1	1:N:484:ARG:CG	2.74	0.47
1:N:684:ARG:HH22	1:O:613:THR:H	1.63	0.47
1:O:724:LEU:O	1:O:814:TYR:OH	2.29	0.47
1:J:1233:ALA:HA	1:O:1176:HIS:HE1	1.80	0.47
1:K:730:THR:HB	1:K:799:TYR:HA	1.97	0.47
1:K:835:VAL:O	1:K:838:THR:OG1	2.30	0.47
1:K:857:LEU:CG	1:K:875:ARG:HD2	2.44	0.47
1:N:395:TYR:CE2	1:N:397:LEU:HB2	2.49	0.47
1:N:705:VAL:HG12	1:N:710:SER:HA	1.96	0.47
1:O:1316:GLY:HA2	1:O:1319:VAL:HB	1.97	0.47
5:Z:20:ASP:HA	5:Z:24:LEU:HD11	1.96	0.47
1:J:747:ILE:HG12	1:J:752:VAL:HG12	1.97	0.47
1:N:128:SER:HA	1:N:1088:VAL:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:442:ASN:O	1:O:1371:ARG:NH2	2.45	0.47
1:O:281:ILE:HD12	1:O:1058:LEU:HD23	1.96	0.46
1:K:359:VAL:C	1:K:360:GLU:O	2.53	0.46
1:N:874:LEU:O	1:N:876:PRO:HD3	2.15	0.46
1:N:456:LEU:HD23	1:N:1146:VAL:HG23	1.97	0.46
1:O:957:PRO:O	1:O:961:ALA:HB2	2.15	0.46
1:K:961:ALA:HB2	1:K:971:VAL:HG21	1.98	0.46
1:K:1195:TYR:OH	1:K:1203:ARG:O	2.33	0.46
1:J:282:VAL:HG12	1:J:1057:ILE:HG12	1.96	0.46
1:J:1074:VAL:HG22	1:J:1088:VAL:HG22	1.97	0.46
1:K:1204:GLY:HA3	1:K:1240:VAL:H	1.81	0.46
1:N:440:ILE:HD12	1:N:1119:ILE:HG22	1.97	0.46
1:J:412:PHE:HB2	1:J:1189:VAL:HG12	1.98	0.46
1:J:434:LEU:HD12	1:J:435:PRO:HD2	1.98	0.46
1:J:1215:TYR:HE1	1:J:1285:ARG:HG2	1.80	0.46
1:N:298:ALA:HB3	1:N:371:VAL:HG23	1.97	0.46
1:N:670:LEU:O	1:N:671:GLY:C	2.54	0.46
1:J:806:ASP:HB3	1:J:810:LYS:HE3	1.98	0.46
1:K:706:VAL:HG23	1:K:711:VAL:HG12	1.98	0.46
1:N:499:VAL:HA	1:N:502:ILE:HD12	1.98	0.46
1:N:584:ARG:NH1	1:N:1020:ALA:O	2.44	0.46
1:K:79:ASN:HB3	1:K:308:TYR:CD1	2.51	0.46
1:N:619:PHE:HE1	1:N:874:LEU:CD2	2.15	0.46
1:J:544:PRO:HG3	1:J:1243:TRP:CD2	2.51	0.46
1:K:1263:ALA:O	1:K:1264:VAL:O	2.33	0.46
1:O:544:PRO:HG3	1:O:1243:TRP:CD2	2.51	0.46
1:O:985:ARG:HD2	1:O:990:PHE:CE1	2.51	0.46
1:J:280:PHE:HB2	1:J:381:VAL:HG22	1.97	0.46
1:N:279:VAL:O	1:N:1059:PHE:HA	2.15	0.46
1:K:80:THR:HG22	1:K:309:ALA:HB3	1.98	0.45
1:N:302:ILE:HG13	1:N:367:ILE:HB	1.98	0.45
1:O:281:ILE:HG22	1:O:397:LEU:HD11	1.97	0.45
1:J:486:THR:HG21	1:J:552:ARG:HB2	1.99	0.45
1:K:805:ALA:O	1:K:806:ASP:CG	2.55	0.45
1:O:84:ASP:N	1:O:84:ASP:OD1	2.49	0.45
1:O:860:LEU:HD11	1:O:865:LEU:HB3	1.97	0.45
1:J:190:PRO:HD2	1:J:193:ILE:HD12	1.98	0.45
1:J:255:VAL:HG13	1:J:1102:SER:HA	1.99	0.45
1:J:1350:LYS:HD3	1:J:1380:VAL:HG13	1.98	0.45
1:K:804:HIS:CD2	1:K:804:HIS:N	2.81	0.45
1:N:267:TYR:HD1	1:N:267:TYR:H	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:1146:VAL:HG13	1:N:1148:ALA:H	1.80	0.45
1:O:951:HIS:O	1:O:955:GLY:N	2.49	0.45
1:O:1187:THR:HG23	1:O:1241:ASN:HB3	1.99	0.45
1:J:155:VAL:HA	1:J:158:VAL:HG22	1.98	0.45
1:J:814:TYR:OH	1:J:921:GLN:NE2	2.49	0.45
1:K:402:GLN:HB2	1:K:1323:GLN:HB3	1.99	0.45
1:N:61:ASN:HD22	1:O:97:ILE:HG23	1.82	0.45
1:N:947:ALA:H	1:N:964:HIS:CE1	2.34	0.45
1:O:441:VAL:HG11	1:O:1373:LEU:HD22	1.97	0.45
1:N:630:GLU:OE2	1:N:668:ARG:NH2	2.50	0.45
1:J:1377:ASN:N	1:K:1364:GLU:OE1	2.40	0.45
1:K:955:GLY:O	1:K:985:ARG:NH2	2.49	0.45
1:K:1023:ILE:HG21	1:K:1033:GLN:HE21	1.81	0.45
1:J:497:MET:HE3	1:J:792:PHE:HA	1.98	0.45
1:N:591:ALA:HB1	1:N:1036:LEU:HD12	1.99	0.45
1:N:828:LEU:HD11	1:N:945:PHE:HB3	1.97	0.45
1:J:986:PRO:O	1:J:990:PHE:N	2.48	0.45
1:K:499:VAL:HA	1:K:502:ILE:HD12	1.99	0.45
1:K:1276:ASN:HB3	1:K:1279:GLU:HB2	1.98	0.45
1:K:481:ARG:NH1	1:K:536:ASP:OD2	2.51	0.44
1:K:796:LEU:HD21	1:K:925:VAL:HG13	1.99	0.44
1:K:951:HIS:O	1:K:955:GLY:N	2.50	0.44
1:O:132:GLU:HG2	1:O:1085:THR:HG22	1.98	0.44
1:O:572:PRO:HD2	1:O:575:LEU:HD12	1.99	0.44
1:O:637:VAL:HA	1:O:640:VAL:HG22	1.99	0.44
1:J:94:GLN:HG2	1:J:119:VAL:HG22	1.99	0.44
1:N:619:PHE:CZ	1:N:874:LEU:HD22	2.52	0.44
1:K:1051:GLU:N	1:K:1115:THR:OG1	2.50	0.44
1:O:680:TYR:OH	1:O:684:ARG:NH1	2.50	0.44
1:N:609:THR:HG22	1:N:653:ARG:HB3	1.98	0.44
1:N:1348:SER:OG	1:N:1349:VAL:N	2.51	0.44
1:N:564:HIS:HD2	1:N:566:LEU:HD23	1.82	0.44
1:N:571:LEU:HD12	1:N:572:PRO:HD2	2.00	0.44
1:N:1018:MET:HA	1:N:1021:MET:HE2	1.99	0.44
1:N:598:VAL:HB	1:N:689:GLU:HB2	2.00	0.44
1:K:395:TYR:CE2	1:K:397:LEU:HB2	2.53	0.44
1:K:856:ILE:HD12	1:K:876:PRO:HG2	2.00	0.44
1:N:706:VAL:HG23	1:N:711:VAL:HG12	1.99	0.44
1:O:469:HIS:HB2	1:O:1259:TYR:HE2	1.82	0.44
1:O:1010:PRO:O	1:O:1011:SER:C	2.55	0.44
1:J:1223:LEU:HD11	1:O:1173:GLY:HA3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:483:ARG:O	1:K:483:ARG:HG2	2.16	0.44
1:N:720:ASP:O	1:N:810:LYS:NZ	2.51	0.44
1:J:544:PRO:O	1:J:565:ARG:NH1	2.51	0.44
1:N:639:LEU:HD12	1:N:880:MET:HB3	2.00	0.44
1:O:746:ILE:HB	1:O:753:TYR:HB3	1.98	0.44
1:O:663:ILE:HG23	1:O:683:TYR:HD1	1.83	0.43
1:J:307:SER:OG	1:J:364:ARG:NH1	2.50	0.43
1:J:485:GLU:HB3	1:J:517:ASP:HB2	2.00	0.43
1:N:158:VAL:HA	1:N:161:VAL:HG12	2.00	0.43
1:N:956:ASP:HA	1:N:957:PRO:HD3	1.86	0.43
1:J:668:ARG:HH11	1:J:669:HIS:CE1	2.37	0.43
1:N:857:LEU:HD23	1:N:860:LEU:HD12	1.98	0.43
1:O:227:SER:O	1:O:232:ARG:NH2	2.49	0.43
1:O:866:ARG:O	1:O:870:GLU:HB2	2.18	0.43
1:J:737:LEU:HG	1:J:744:PRO:HG2	2.01	0.43
1:N:412:PHE:HD1	1:N:1189:VAL:HG12	1.83	0.43
1:J:704:ASP:O	1:K:976:GLN:NE2	2.47	0.43
1:K:1255:TYR:HB2	1:K:1275:PHE:HD2	1.83	0.43
1:N:474:LEU:HG	1:N:560:HIS:CE1	2.53	0.43
1:K:282:VAL:HG12	1:K:1057:ILE:HG12	2.00	0.43
1:O:75:VAL:HG23	1:O:267:TYR:CG	2.54	0.43
1:O:83:LYS:HG3	1:O:312:VAL:HG23	1.99	0.43
1:J:1335:LEU:HG	1:J:1365:GLU:HB2	2.00	0.43
1:K:904:ASN:ND2	1:K:917:LYS:O	2.52	0.43
1:N:1117:MET:SD	1:N:1371:ARG:NH1	2.91	0.43
1:O:587:GLN:NE2	1:O:1037:LYS:O	2.52	0.43
1:K:95:PHE:O	1:K:117:ILE:HA	2.19	0.43
1:N:317:ASN:HD21	1:N:331:PHE:HB2	1.82	0.43
1:K:546:TYR:HA	1:K:564:HIS:HA	2.01	0.43
1:K:1049:THR:HG23	1:K:1270:PRO:HB3	2.01	0.43
1:O:280:PHE:HB2	1:O:381:VAL:HG22	2.00	0.43
1:O:444:ASN:HD22	1:O:1176:HIS:CD2	2.36	0.43
1:J:668:ARG:HH11	1:J:669:HIS:HE1	1.67	0.43
1:K:856:ILE:HG22	1:K:860:LEU:HB2	2.01	0.43
1:K:1217:GLN:HE22	1:K:1281:LEU:HD23	1.84	0.43
1:J:639:LEU:HD12	1:J:880:MET:HB3	2.00	0.42
1:J:1313:VAL:HG21	1:J:1319:VAL:HG21	2.01	0.42
1:O:810:LYS:O	1:O:814:TYR:HB2	2.19	0.42
1:J:400:ARG:NE	1:J:1305:SER:OG	2.52	0.42
1:J:547:ASP:O	1:J:562:ALA:HA	2.20	0.42
1:K:172:LEU:HD11	1:K:1090:HIS:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:705:VAL:HA	1:N:711:VAL:HG13	2.00	0.42
1:J:285:ASN:HD22	1:J:288:ARG:HH22	1.68	0.42
1:K:501:VAL:HA	1:K:504:ASP:HB2	2.00	0.42
1:N:77:CYS:SG	1:N:1065:THR:OG1	2.72	0.42
1:N:764:GLU:HB2	1:N:793:ARG:HD3	2.02	0.42
1:N:856:ILE:HG22	1:N:860:LEU:HG	2.01	0.42
1:O:415:ASN:HD21	1:O:579:ALA:HB2	1.85	0.42
1:O:1039:HIS:ND1	1:O:1040:PRO:O	2.53	0.42
1:J:1124:PHE:HA	1:J:1127:VAL:HG12	2.01	0.42
1:O:606:VAL:O	1:O:609:THR:OG1	2.31	0.42
1:K:467:PRO:HG3	1:K:912:PRO:HG2	2.01	0.42
1:K:737:LEU:HD23	1:K:744:PRO:HG2	2.01	0.42
1:J:385:GLN:HG2	1:J:389:ASN:HD21	1.83	0.42
1:J:405:TYR:O	1:J:1047:VAL:HA	2.20	0.42
1:J:690:LEU:HD21	1:J:812:PHE:HB2	2.01	0.42
1:J:724:LEU:HD12	1:J:900:VAL:HG21	2.01	0.42
1:J:905:ASP:OD1	1:J:906:VAL:N	2.51	0.42
1:K:778:ALA:O	1:K:782:TYR:N	2.51	0.42
1:K:1012:LEU:HA	1:K:1015:ILE:HD12	2.01	0.42
1:J:415:ASN:OD1	1:J:417:LYS:NZ	2.39	0.42
1:J:621:VAL:O	1:J:625:MET:HG2	2.20	0.42
1:J:788:HIS:O	1:J:896:ARG:NH1	2.53	0.42
1:N:155:VAL:HA	1:N:158:VAL:HG22	2.02	0.42
1:O:814:TYR:HH	1:O:921:GLN:HE22	1.68	0.42
1:O:1049:THR:HG23	1:O:1270:PRO:HB3	2.02	0.42
1:J:748:ILE:HG13	1:J:898:VAL:HG13	2.02	0.42
1:J:1269:SER:HB2	1:J:1272:ARG:HB2	2.01	0.42
1:K:1146:VAL:HG13	1:K:1148:ALA:H	1.85	0.42
1:K:1225:TYR:CE2	1:K:1277:LYS:HE2	2.55	0.42
1:N:312:VAL:HG12	1:N:314:ARG:H	1.84	0.42
1:O:828:LEU:HD11	1:O:945:PHE:HB3	2.01	0.42
1:J:521:LYS:NZ	1:J:541:GLU:OE2	2.40	0.42
1:K:158:VAL:HA	1:K:161:VAL:HG12	2.01	0.42
1:O:494:PRO:HB3	1:O:988:GLN:HG2	2.01	0.42
1:J:843:GLY:HA2	1:J:846:PHE:HB3	2.02	0.42
1:J:856:ILE:HD11	1:J:878:VAL:HA	2.02	0.42
1:K:726:PRO:HG3	1:K:954:TYR:HE2	1.85	0.42
1:N:638:PRO:HG2	1:N:880:MET:SD	2.59	0.42
1:N:828:LEU:HB3	1:N:928:LEU:O	2.20	0.42
1:N:1175:CYS:H	1:O:1232:ALA:HB1	1.85	0.41
1:O:906:VAL:HA	1:O:909:GLN:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:705:VAL:HG12	1:K:710:SER:HA	2.00	0.41
1:N:626:ILE:HG22	1:N:628:GLY:H	1.85	0.41
1:N:684:ARG:NH2	1:O:612:ASP:HA	2.35	0.41
1:O:909:GLN:HE21	1:O:917:LYS:HD3	1.85	0.41
1:O:977:GLN:HE21	1:O:983:PHE:HA	1.85	0.41
1:K:830:VAL:H	1:K:895:THR:HG21	1.86	0.41
1:O:466:THR:HB	1:O:910:LEU:HD13	2.02	0.41
1:J:80:THR:HG21	1:J:1068:PHE:HE1	1.85	0.41
1:O:713:GLN:NE2	1:O:719:LEU:O	2.44	0.41
1:K:299:ASP:HB2	1:K:371:VAL:HG21	2.03	0.41
1:O:955:GLY:HA3	1:O:985:ARG:NE	2.36	0.41
1:J:444:ASN:HD22	1:J:1176:HIS:HD2	1.69	0.41
1:J:852:ARG:NH2	5:Z:63:ARG:HD3	2.35	0.41
1:N:724:LEU:HD23	1:N:724:LEU:HA	1.85	0.41
1:K:1285:ARG:NH2	1:K:1293:GLU:OE1	2.54	0.41
1:O:220:LYS:HZ3	1:O:1328:LEU:HB3	1.86	0.41
1:O:989:LEU:HD23	1:O:989:LEU:HA	1.75	0.41
1:J:147:THR:HA	1:J:148:PRO:HD3	1.96	0.41
1:J:871:ILE:HD12	1:J:871:ILE:HA	1.89	0.41
1:K:1157:ASP:HA	1:K:1158:PRO:HD3	1.95	0.41
1:K:1046:VAL:HG22	1:K:1184:ILE:HG13	2.02	0.41
1:N:268:THR:HG22	1:N:275:PRO:HB3	2.03	0.41
1:N:336:ALA:HA	1:N:340:ASP:HB2	2.03	0.41
1:O:255:VAL:HG13	1:O:1102:SER:HA	2.02	0.41
1:O:1201:SER:OG	1:O:1205:ARG:O	2.36	0.41
1:N:1128:PHE:CE1	1:N:1263:ALA:HB2	2.56	0.41
1:J:255:VAL:HG11	1:J:1061:SER:HB3	2.03	0.40
1:J:835:VAL:HG22	1:J:944:LEU:HD22	2.02	0.40
1:J:1057:ILE:HB	1:J:1106:THR:HG22	2.03	0.40
1:K:899:ARG:HA	1:K:899:ARG:HD2	1.83	0.40
1:K:1018:MET:HA	1:K:1021:MET:HG3	2.04	0.40
1:N:575:LEU:HD13	1:N:1243:TRP:HH2	1.87	0.40
1:N:750:ASN:H	1:N:792:PHE:HE1	1.68	0.40
1:O:511:TYR:HA	1:O:973:ARG:HH12	1.86	0.40
1:O:542:LEU:HB3	1:O:1249:SER:HA	2.03	0.40
1:J:580:PHE:CE1	1:J:1189:VAL:HG11	2.57	0.40
1:K:469:HIS:HB2	1:K:1253:ILE:HD12	2.03	0.40
1:O:255:VAL:HG21	1:O:1059:PHE:HD2	1.86	0.40
1:K:146:GLU:HG3	1:K:147:THR:HG23	2.02	0.40
1:K:248:LEU:HB3	1:K:374:LEU:HD21	2.02	0.40
1:K:462:PRO:HG2	1:K:1131:GLU:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1229:ARG:HD3	1:O:1172:PRO:HD3	2.04	0.40
1:K:395:TYR:HB3	1:K:398:ASN:ND2	2.36	0.40
1:K:1174:LEU:HD23	1:K:1174:LEU:HA	1.97	0.40
1:N:269:THR:HG22	1:N:271:LYS:N	2.35	0.40
1:O:877:THR:OG1	1:O:880:MET:SD	2.67	0.40
1:O:938:ARG:HA	1:O:941:THR:HG22	2.03	0.40
1:O:1247:LEU:HD23	1:O:1247:LEU:HA	1.91	0.40
5:Z:68:PRO:HG2	5:Z:71:GLN:HB3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	1299/1381 (94%)	1225 (94%)	73 (6%)	1 (0%)	51	85
1	K	1379/1381 (100%)	1313 (95%)	56 (4%)	10 (1%)	22	62
1	N	1358/1381 (98%)	1305 (96%)	49 (4%)	4 (0%)	41	76
1	O	1295/1381 (94%)	1239 (96%)	52 (4%)	4 (0%)	41	76
2	v	283/507 (56%)	260 (92%)	22 (8%)	1 (0%)	34	72
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%)	35 (100%)	0	0	100	100
4	z	35/3149 (1%)	34 (97%)	1 (3%)	0	100	100
5	Z	75/176 (43%)	71 (95%)	4 (5%)	0	100	100
5	a	75/176 (43%)	71 (95%)	3 (4%)	1 (1%)	12	48
5	d	75/176 (43%)	73 (97%)	2 (3%)	0	100	100
5	e	75/176 (43%)	73 (97%)	1 (1%)	1 (1%)	12	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	f	247/364 (68%)	224 (91%)	21 (8%)	2 (1%)	19	60
6	h	330/364 (91%)	308 (93%)	20 (6%)	2 (1%)	25	65
7	k	297/301 (99%)	282 (95%)	14 (5%)	1 (0%)	41	76
7	m	297/301 (99%)	281 (95%)	15 (5%)	1 (0%)	41	76
7	p	297/301 (99%)	285 (96%)	11 (4%)	1 (0%)	41	76
7	r	297/301 (99%)	282 (95%)	10 (3%)	5 (2%)	9	43
All	All	7881/16105 (49%)	7492 (95%)	355 (4%)	34 (0%)	38	72

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	556	GLU
1	K	360	GLU
1	K	911	ALA
1	K	912	PRO
1	K	1264	VAL
1	K	1265	PRO
1	N	266	THR
1	O	488	SER
1	O	1011	SER
5	a	19	PRO
6	h	306	ALA
7	p	98	GLN
7	r	192	GLU
7	r	193	VAL
7	r	203	ASP
1	K	361	ASP
5	e	33	ASN
7	r	255	LEU
1	K	805	ALA
1	O	300	ASN
7	k	161	MET
7	m	129	ASP
1	K	806	ASP
1	K	913	ASN
1	O	489	LEU
6	f	161	SER
6	h	310	PRO
1	N	484	ARG
1	N	671	GLY

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Mol	Chain	Res	Type
1	N	672	ASN
7	r	194	PRO
1	K	357	ALA
6	f	162	PRO
2	v	94	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	1110/1171 (95%)	1107 (100%)	3 (0%)	92	95
1	K	1171/1171 (100%)	1160 (99%)	11 (1%)	78	88
1	N	1155/1171 (99%)	1148 (99%)	7 (1%)	86	92
1	O	1103/1171 (94%)	1098 (100%)	5 (0%)	88	93
2	v	243/400 (61%)	243 (100%)	0	100	100
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%)	35 (100%)	0	100	100
4	z	35/2539 (1%)	35 (100%)	0	100	100
5	Z	71/128 (56%)	71 (100%)	0	100	100
5	a	71/128 (56%)	70 (99%)	1 (1%)	67	81
5	d	71/128 (56%)	71 (100%)	0	100	100
5	e	71/128 (56%)	71 (100%)	0	100	100
6	f	218/289 (75%)	216 (99%)	2 (1%)	78	88
6	h	278/289 (96%)	278 (100%)	0	100	100
7	k	265/267 (99%)	263 (99%)	2 (1%)	81	89
7	m	265/267 (99%)	264 (100%)	1 (0%)	91	94
7	p	265/267 (99%)	264 (100%)	1 (0%)	91	94
7	r	265/267 (99%)	261 (98%)	4 (2%)	65	80
All	All	6806/13250 (51%)	6769 (100%)	37 (0%)	89	93

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	556	GLU
1	J	653	ARG
1	J	1062	ARG
1	K	109	ARG
1	K	360	GLU
1	K	361	ASP
1	K	481	ARG
1	K	484	ARG
1	K	653	ARG
1	K	804	HIS
1	K	936	ARG
1	K	938	ARG
1	K	1150	ARG
1	K	1264	VAL
1	N	266	THR
1	N	267	TYR
1	N	484	ARG
1	N	670	LEU
1	N	938	ARG
1	N	1077	ARG
1	N	1272	ARG
1	O	267	TYR
1	O	481	ARG
1	O	889	MET
1	O	1109	ARG
1	O	1139	ASN
5	a	20	ASP
6	f	237	LEU
6	f	294	ARG
7	k	161	MET
7	k	197	LEU
7	m	118	ARG
7	p	98	GLN
7	r	193	VAL
7	r	201	LEU
7	r	202	LEU
7	r	265	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

Mol	Chain	Res	Type
1	J	126	HIS
1	J	285	ASN
1	J	300	ASN
1	J	389	ASN
1	J	444	ASN
1	J	581	GLN
1	J	587	GLN
1	J	596	HIS
1	J	636	ASN
1	J	669	HIS
1	J	834	HIS
1	J	859	ASN
1	J	904	ASN
1	J	908	GLN
1	J	921	GLN
1	J	1176	HIS
1	J	1241	ASN
1	J	1360	HIS
1	K	123	HIS
1	K	289	GLN
1	K	317	ASN
1	K	362	GLN
1	K	385	GLN
1	K	389	ASN
1	K	543	HIS
1	K	795	HIS
1	K	804	HIS
1	K	822	ASN
1	K	824	HIS
1	K	997	HIS
1	K	1197	GLN
1	K	1217	GLN
1	N	123	HIS
1	N	125	HIS
1	N	317	ASN
1	N	362	GLN
1	N	444	ASN
1	N	496	HIS
1	N	543	HIS
1	N	564	HIS
1	N	587	GLN
1	N	788	HIS
1	N	804	HIS

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Mol	Chain	Res	Type
1	N	942	GLN
1	N	964	HIS
1	N	997	HIS
1	N	1179	GLN
1	N	1284	ASN
1	N	1323	GLN
1	O	121	ASN
1	O	226	HIS
1	O	415	ASN
1	O	432	GLN
1	O	491	HIS
1	O	496	HIS
1	O	531	HIS
1	O	581	GLN
1	O	587	GLN
1	O	824	HIS
1	O	977	GLN
1	O	1090	HIS
1	O	1176	HIS
2	v	7	ASN
2	v	45	GLN
2	v	290	HIS
3	w	77	HIS
6	h	291	ASN
6	h	309	GLN
7	k	120	HIS
7	k	128	ASN
7	k	204	ASN
7	m	128	ASN
7	m	148	GLN
7	m	175	HIS
7	m	204	ASN
7	m	291	GLN
7	p	95	ASN
7	p	102	GLN
7	p	148	GLN
7	r	120	HIS
7	r	154	ASN

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.

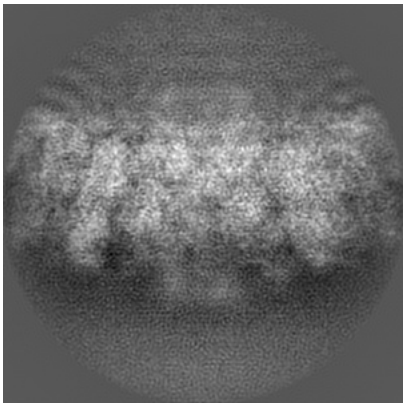
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-21526. These allow visual inspection of the internal detail of the map and identification of artifacts.

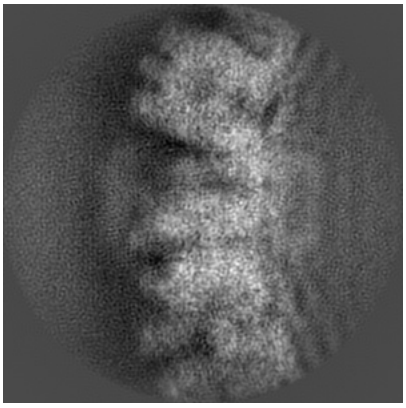
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

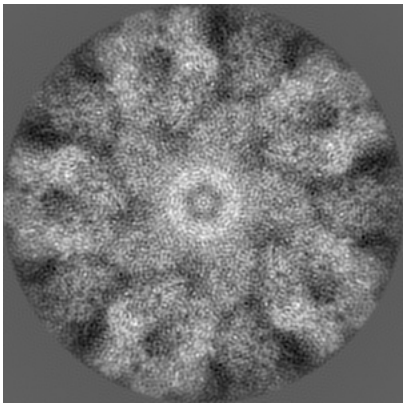
6.1.1 Primary map



X



Y

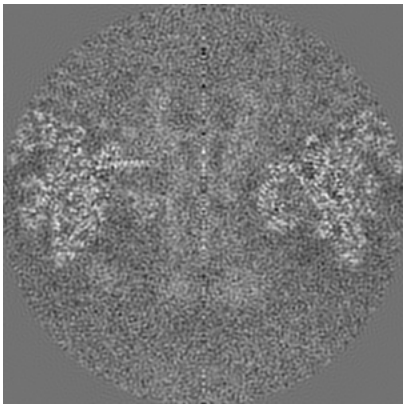


Z

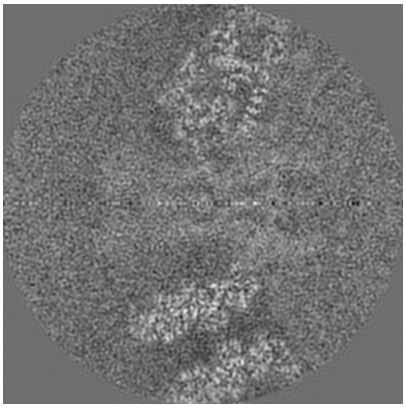
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

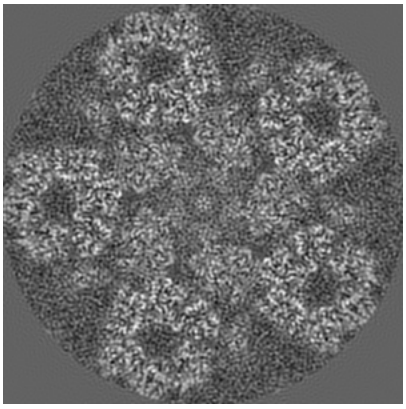
6.2.1 Primary map



X Index: 160



Y Index: 160

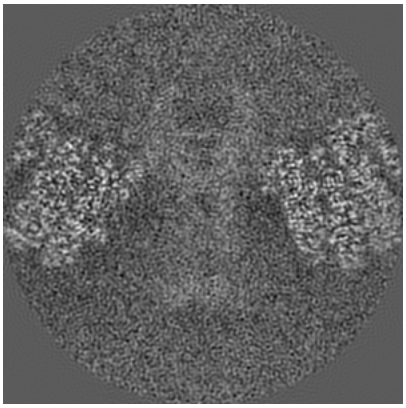


Z Index: 160

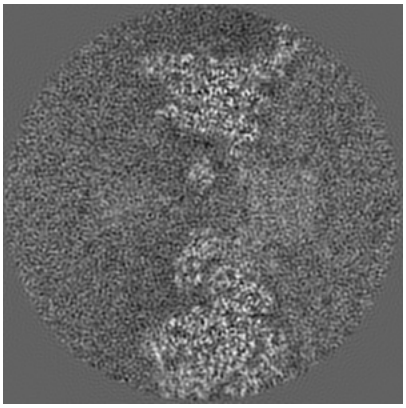
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

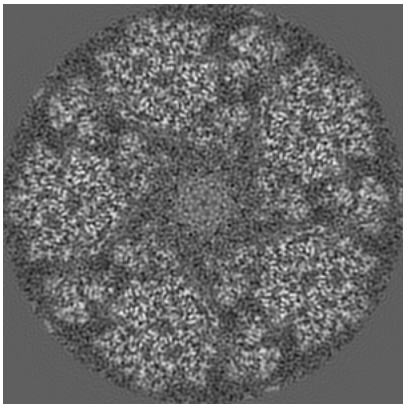
6.3.1 Primary map



X Index: 147



Y Index: 193

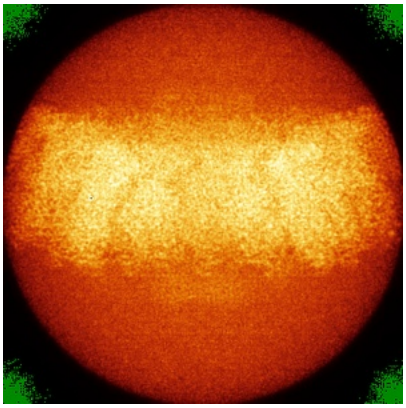


Z Index: 175

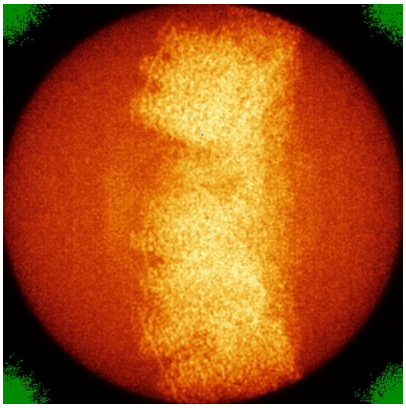
The images above show the largest variance slices of the map in three orthogonal directions.

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

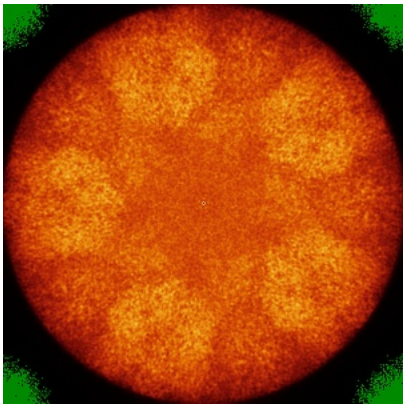
6.4.1 Primary map



X



Y

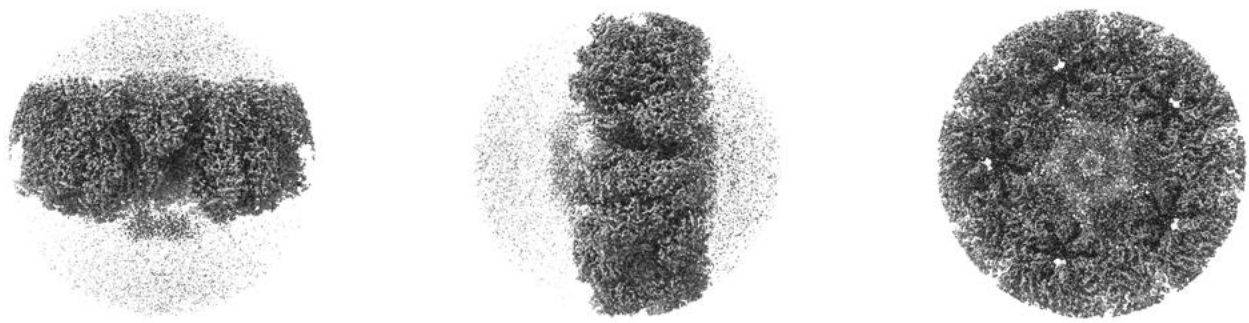


Z

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

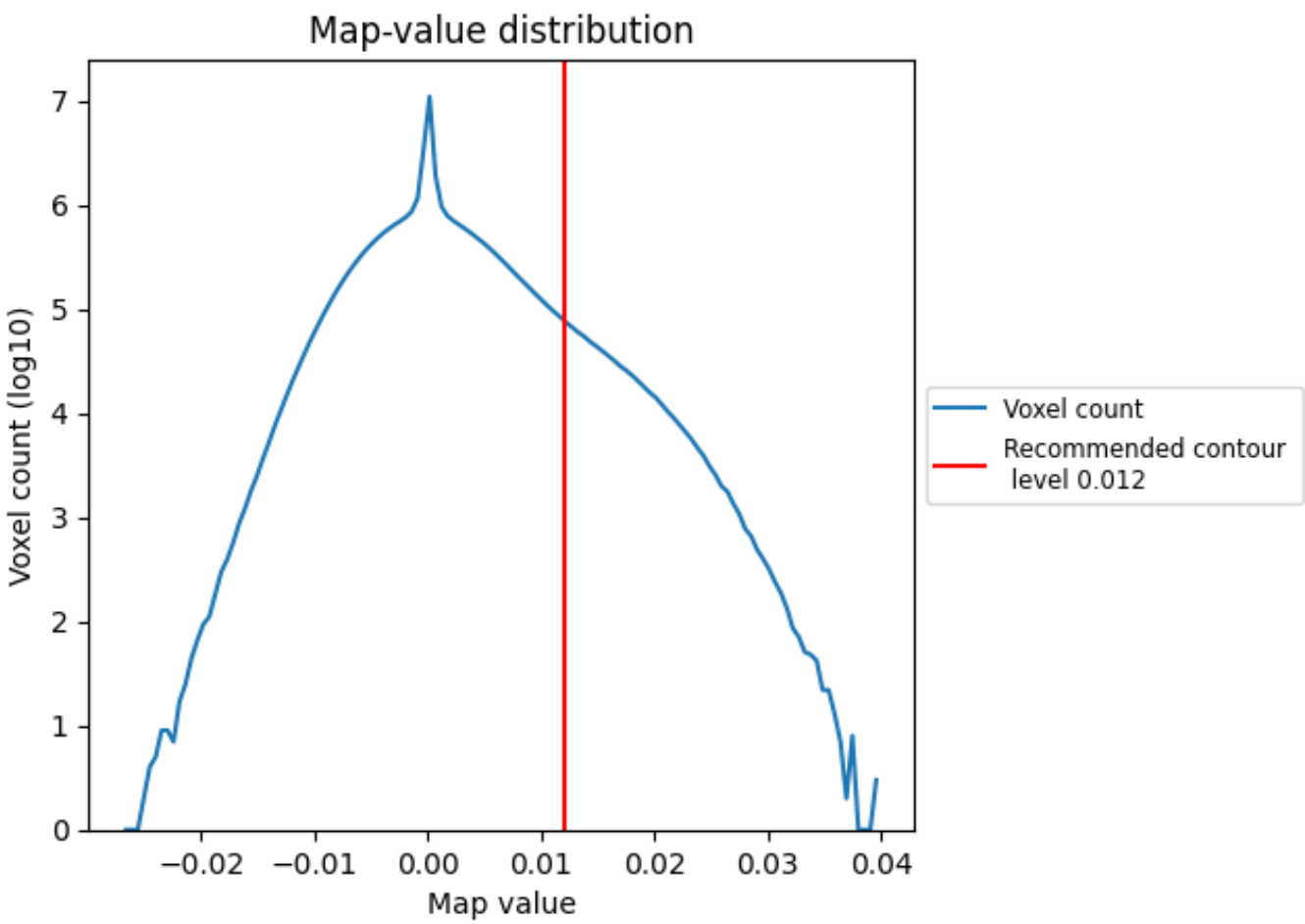
6.6 Mask visualisation (i)

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

7 Map analysis (i)

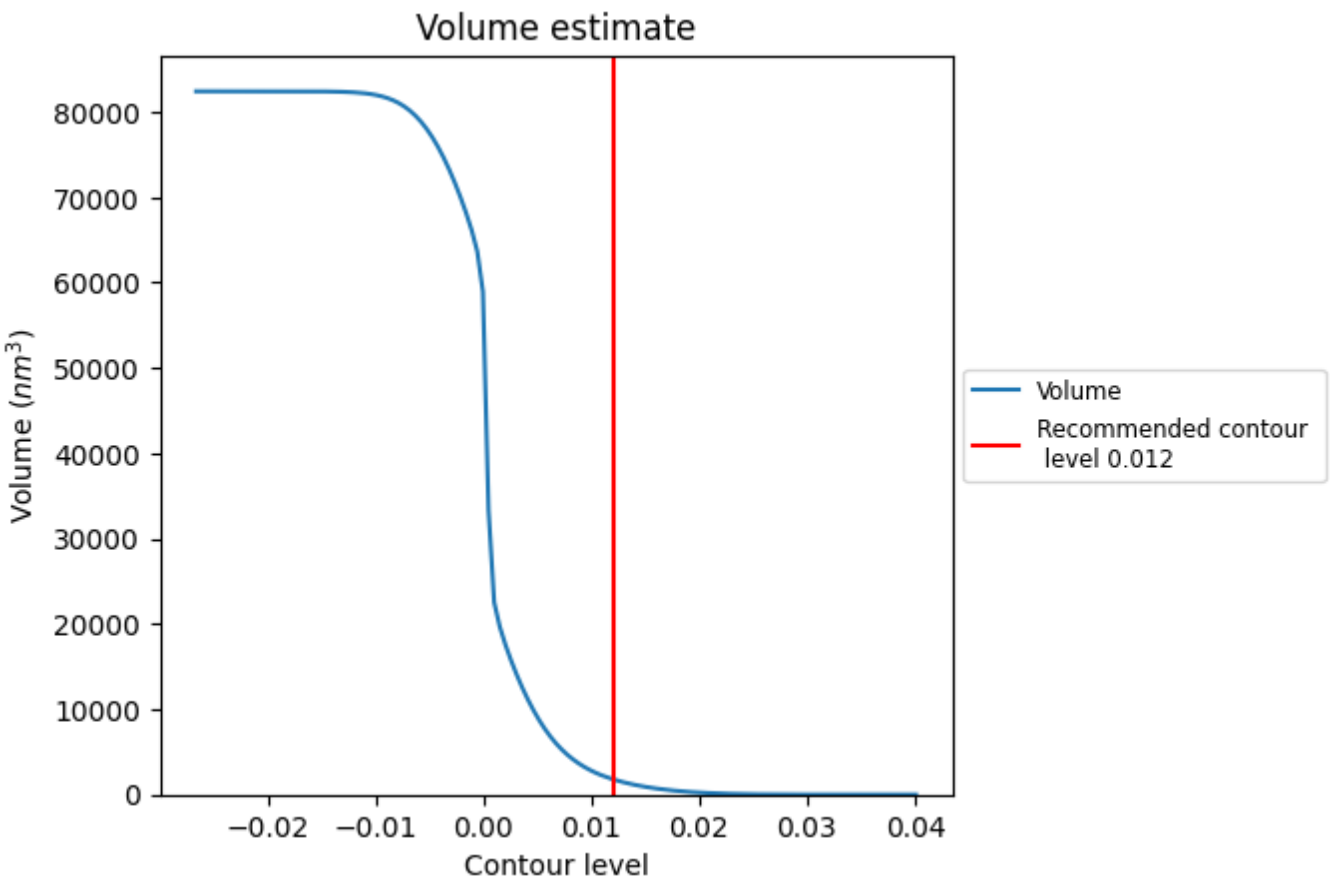
This section contains the results of statistical analysis of the map.

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.

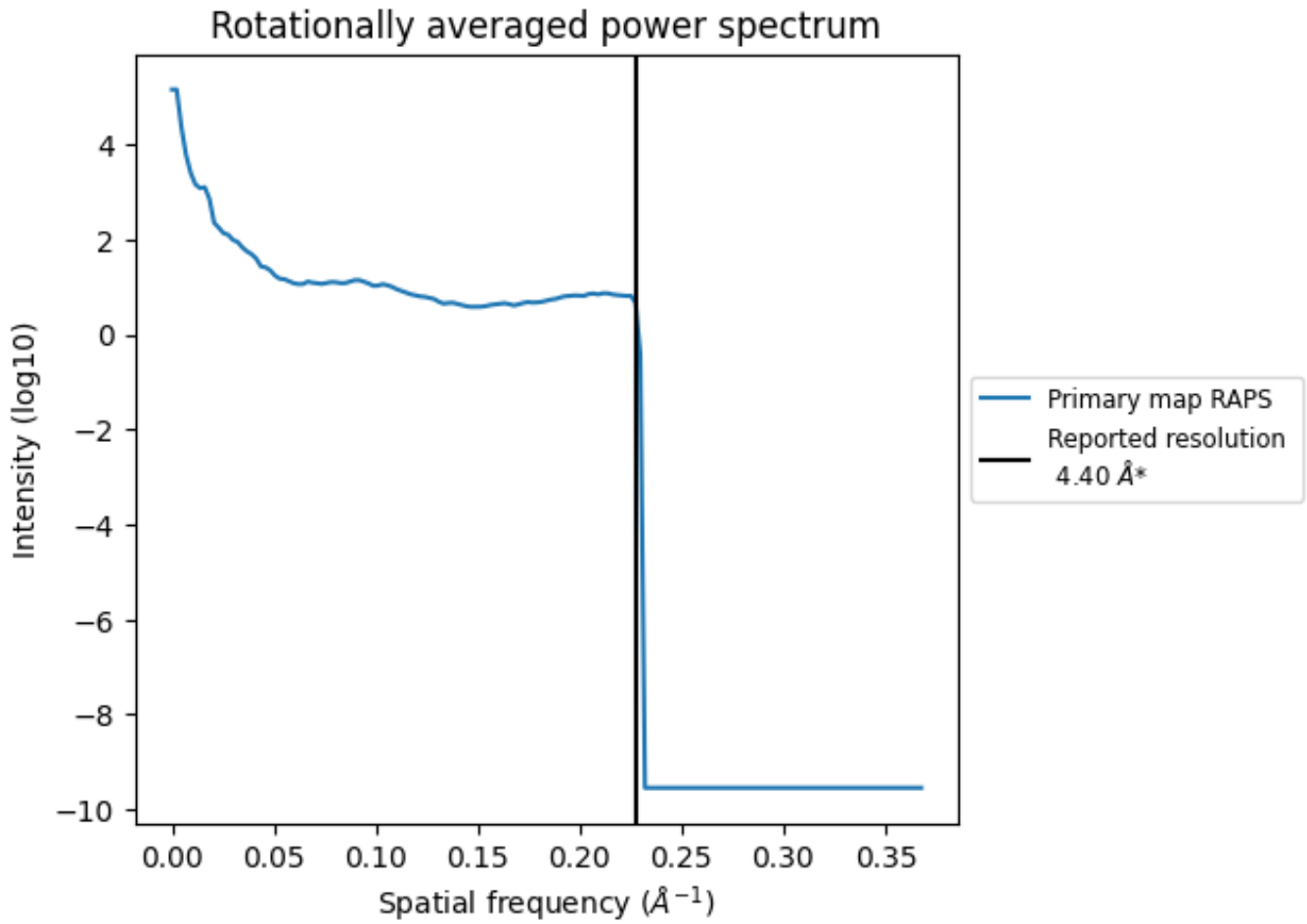
7.2 Volume estimate (i)



The volume at the recommended contour level is 1798 nm^3; this corresponds to an approximate mass of 1624 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 0.227 Å^{-1}

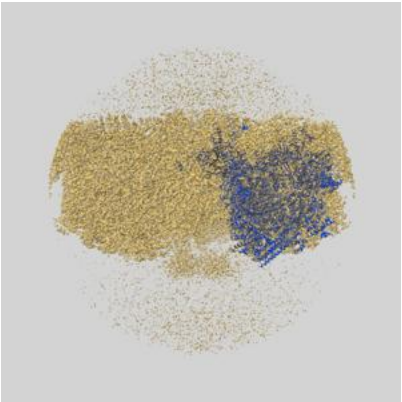
8 Fourier-Shell correlation (i)

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

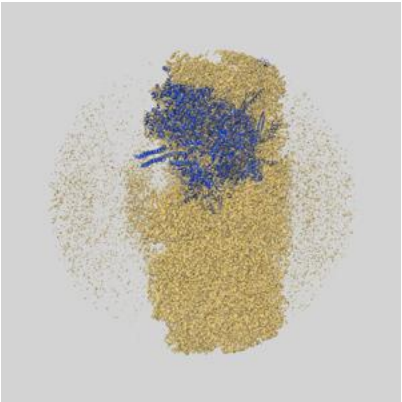
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-21526 and PDB model 6W2E. Per-residue inclusion information can be found in section 3 on page 6.

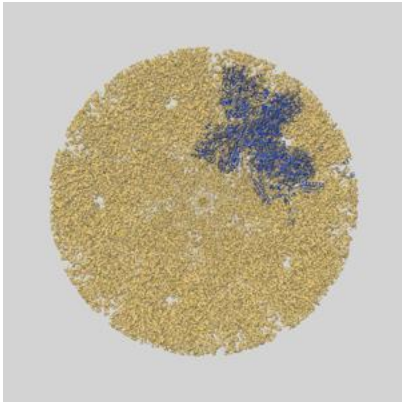
9.1 Map-model overlay (i)



X



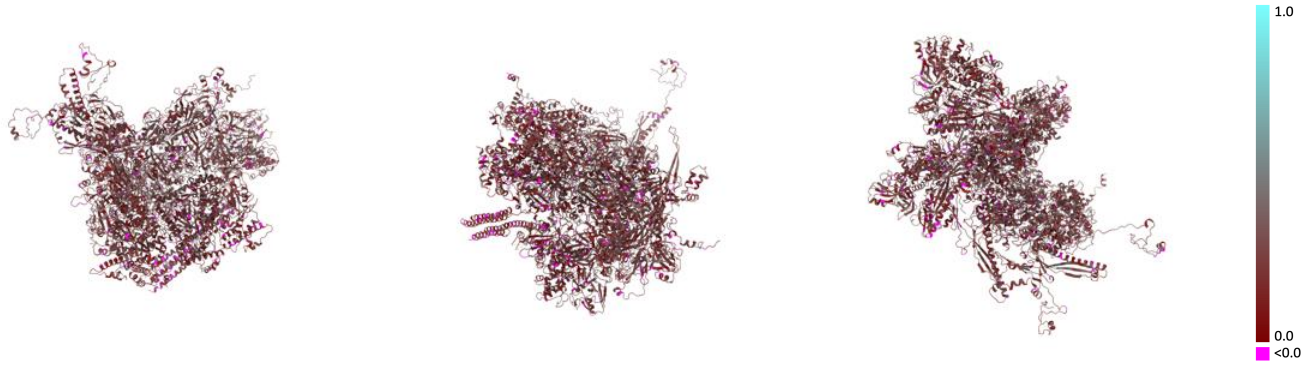
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.012 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.

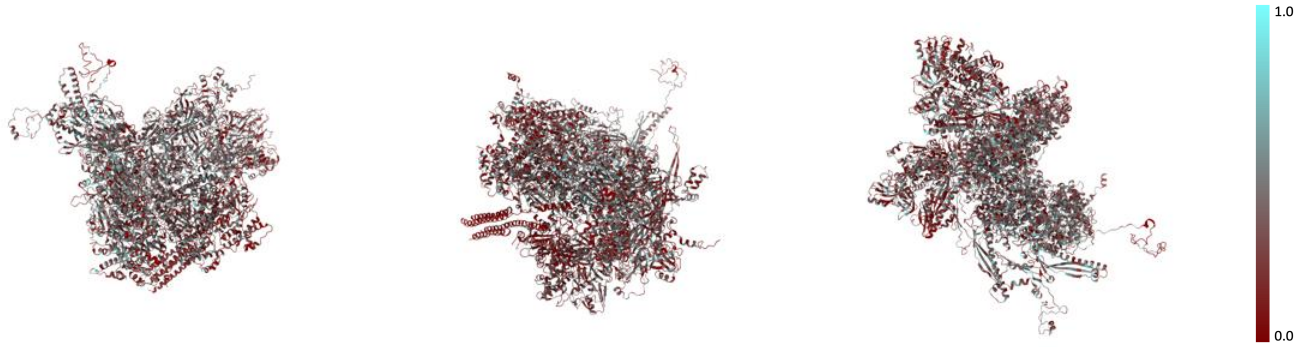
9.2 Q-score mapped to coordinate model (i)



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.

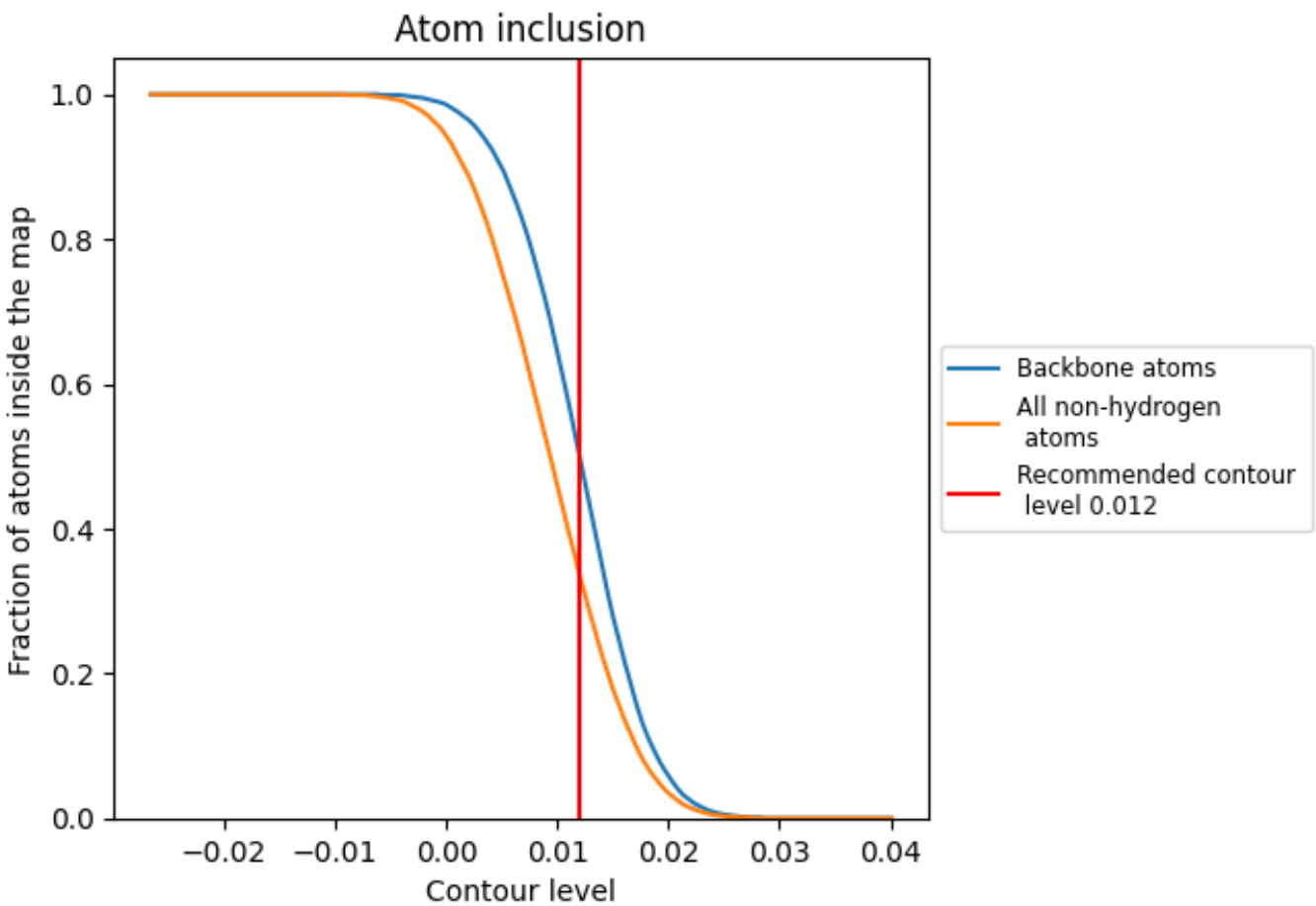
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.012).

9.4 Atom inclusion (i)



At the recommended contour level, 50% of all backbone atoms, 34% 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 (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3360	0.2450
J	0.3910	0.2500
K	0.3870	0.2640
N	0.3500	0.2590
O	0.3700	0.2460
Z	0.3000	0.2300
a	0.3100	0.2180
d	0.1720	0.1880
e	0.2860	0.2230
f	0.2490	0.2260
h	0.3450	0.2610
k	0.2780	0.2310
m	0.2860	0.2490
p	0.2910	0.2330
r	0.2990	0.2550
v	0.1690	0.1870
w	0.0720	0.1710
x	0.1170	0.1700
y	0.0630	0.1150
z	0.0500	0.1040