# wwPDB EM Validation Summary Report

May 18, 2024 – 11:39 PM EDT

| | | |
|---|---|---|
| PDB ID | : | 7LFH |
| EMDB ID | : | EMD-23302 |
| Title | : | Cryo-EM structure of NLRP3 double-ring cage, 6-fold (12-mer) |
| Authors | : | Andreeva, L.; Rawson, S.; Wu, H. |
| Deposited on | : | 2021-01-17 |
| Resolution | : | 4.20 Å(reported) |
| Based on initial model | : | 6NPY |

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

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

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

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

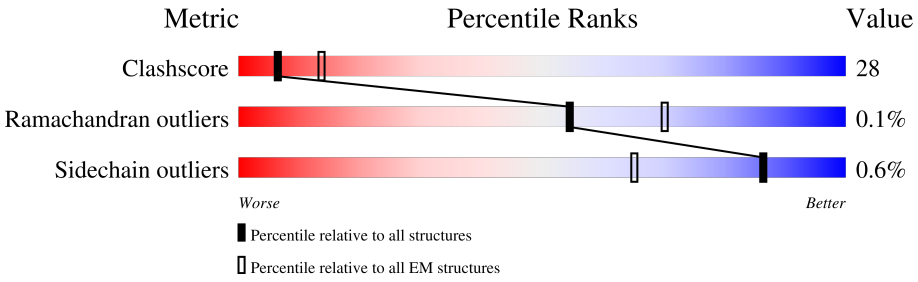
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev92 |
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | 1.9.13 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.36.2 |

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.20 Å.

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




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

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

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 1037 | 24% 38% 39% 22% |
| 1 | B | 1037 | 23% 39% 38% 22% |
| 1 | C | 1037 | 27% 38% 39% 22% |
| 1 | D | 1037 | 22% 39% 38% 22% |
| 1 | E | 1037 | 25% 38% 39% 22% |
| 1 | F | 1037 | 21% 38% 39% 22% |
| 1 | G | 1037 | 25% 39% 39% 22% |
| 1 | H | 1037 | 24% 38% 39% 22% |

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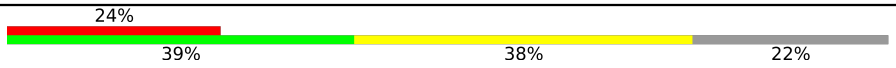
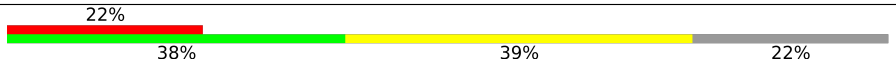
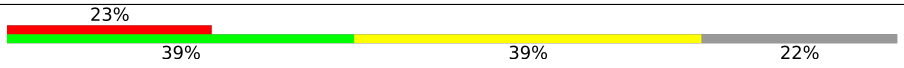
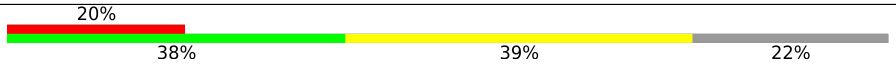
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | I | 1037 |   |
| 1 | J | 1037 |   |
| 1 | K | 1037 |   |
| 1 | L | 1037 |   |

## 2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 76884 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 NACHT, LRR and PYD domains-containing protein 3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 806 | Total | C | N | O | S | 0 | 0 |
| | | | 6407 | 4099 | 1089 | 1166 | 53 | | |
| 1 | B | 806 | Total | C | N | O | S | 0 | 0 |
| | | | 6407 | 4099 | 1089 | 1166 | 53 | | |
| 1 | C | 806 | Total | C | N | O | S | 0 | 0 |
| | | | 6407 | 4099 | 1089 | 1166 | 53 | | |
| 1 | D | 806 | Total | C | N | O | S | 0 | 0 |
| | | | 6407 | 4099 | 1089 | 1166 | 53 | | |
| 1 | E | 806 | Total | C | N | O | S | 0 | 0 |
| | | | 6407 | 4099 | 1089 | 1166 | 53 | | |
| 1 | F | 806 | Total | C | N | O | S | 0 | 0 |
| | | | 6407 | 4099 | 1089 | 1166 | 53 | | |
| 1 | G | 806 | Total | C | N | O | S | 0 | 0 |
| | | | 6407 | 4099 | 1089 | 1166 | 53 | | |
| 1 | H | 806 | Total | C | N | O | S | 0 | 0 |
| | | | 6407 | 4099 | 1089 | 1166 | 53 | | |
| 1 | I | 806 | Total | C | N | O | S | 0 | 0 |
| | | | 6407 | 4099 | 1089 | 1166 | 53 | | |
| 1 | J | 806 | Total | C | N | O | S | 0 | 0 |
| | | | 6407 | 4099 | 1089 | 1166 | 53 | | |
| 1 | K | 806 | Total | C | N | O | S | 0 | 0 |
| | | | 6407 | 4099 | 1089 | 1166 | 53 | | |
| 1 | L | 806 | Total | C | N | O | S | 0 | 0 |
| | | | 6407 | 4099 | 1089 | 1166 | 53 | | |

There are 48 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | -3 | GLY | - | expression tag | UNP Q8R4B8 |
| A | -2 | ARG | - | expression tag | UNP Q8R4B8 |
| A | -1 | SER | - | expression tag | UNP Q8R4B8 |
| A | 0 | ALA | - | expression tag | UNP Q8R4B8 |
| B | -3 | GLY | - | expression tag | UNP Q8R4B8 |
| B | -2 | ARG | - | expression tag | UNP Q8R4B8 |

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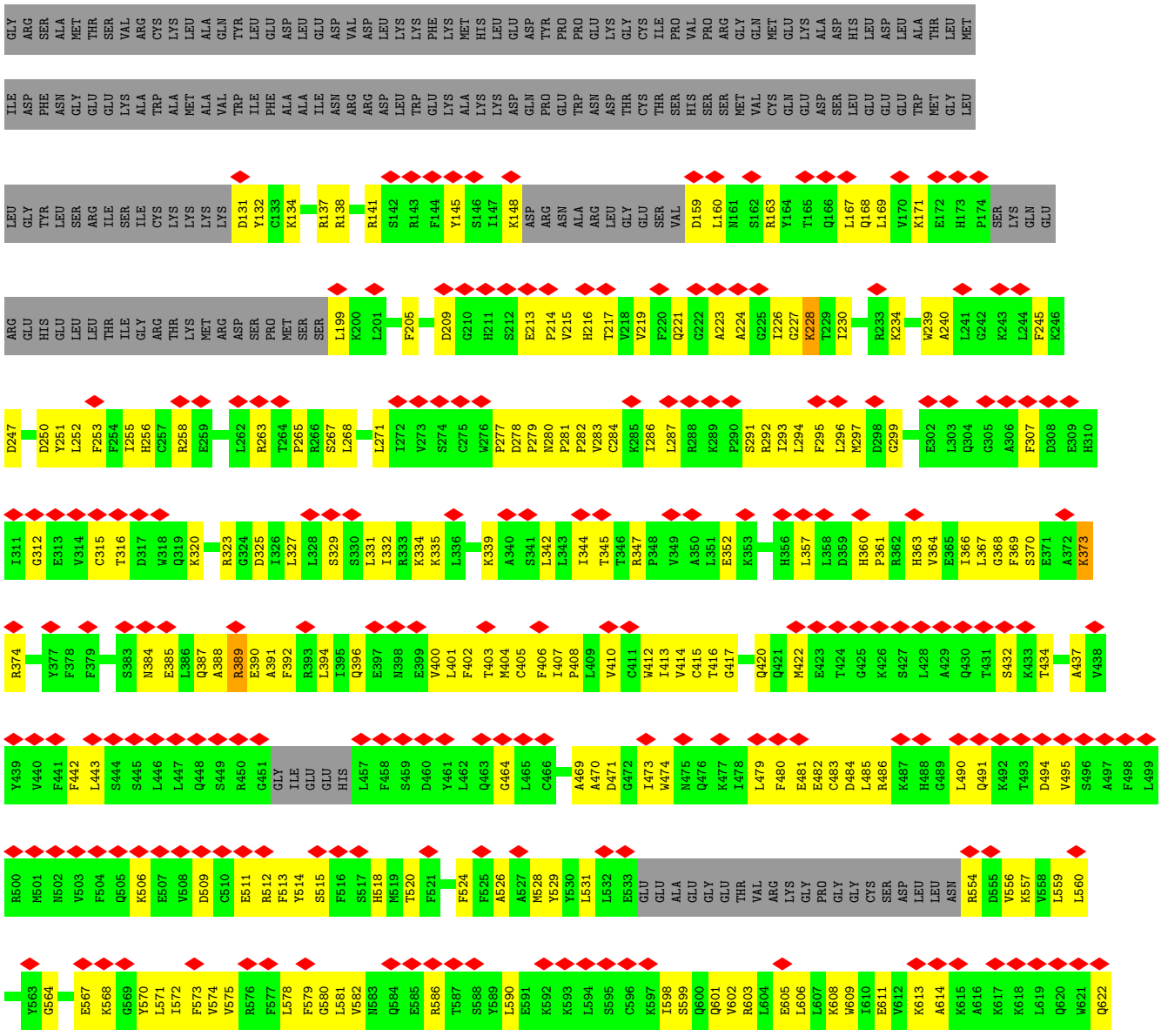
| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| B | -1 | SER | - | expression tag | UNP Q8R4B8 |
| B | 0 | ALA | - | expression tag | UNP Q8R4B8 |
| C | -3 | GLY | - | expression tag | UNP Q8R4B8 |
| C | -2 | ARG | - | expression tag | UNP Q8R4B8 |
| C | -1 | SER | - | expression tag | UNP Q8R4B8 |
| C | 0 | ALA | - | expression tag | UNP Q8R4B8 |
| D | -3 | GLY | - | expression tag | UNP Q8R4B8 |
| D | -2 | ARG | - | expression tag | UNP Q8R4B8 |
| D | -1 | SER | - | expression tag | UNP Q8R4B8 |
| D | 0 | ALA | - | expression tag | UNP Q8R4B8 |
| E | -3 | GLY | - | expression tag | UNP Q8R4B8 |
| E | -2 | ARG | - | expression tag | UNP Q8R4B8 |
| E | -1 | SER | - | expression tag | UNP Q8R4B8 |
| E | 0 | ALA | - | expression tag | UNP Q8R4B8 |
| F | -3 | GLY | - | expression tag | UNP Q8R4B8 |
| F | -2 | ARG | - | expression tag | UNP Q8R4B8 |
| F | -1 | SER | - | expression tag | UNP Q8R4B8 |
| F | 0 | ALA | - | expression tag | UNP Q8R4B8 |
| G | -3 | GLY | - | expression tag | UNP Q8R4B8 |
| G | -2 | ARG | - | expression tag | UNP Q8R4B8 |
| G | -1 | SER | - | expression tag | UNP Q8R4B8 |
| G | 0 | ALA | - | expression tag | UNP Q8R4B8 |
| H | -3 | GLY | - | expression tag | UNP Q8R4B8 |
| H | -2 | ARG | - | expression tag | UNP Q8R4B8 |
| H | -1 | SER | - | expression tag | UNP Q8R4B8 |
| H | 0 | ALA | - | expression tag | UNP Q8R4B8 |
| I | -3 | GLY | - | expression tag | UNP Q8R4B8 |
| I | -2 | ARG | - | expression tag | UNP Q8R4B8 |
| I | -1 | SER | - | expression tag | UNP Q8R4B8 |
| I | 0 | ALA | - | expression tag | UNP Q8R4B8 |
| J | -3 | GLY | - | expression tag | UNP Q8R4B8 |
| J | -2 | ARG | - | expression tag | UNP Q8R4B8 |
| J | -1 | SER | - | expression tag | UNP Q8R4B8 |
| J | 0 | ALA | - | expression tag | UNP Q8R4B8 |
| K | -3 | GLY | - | expression tag | UNP Q8R4B8 |
| K | -2 | ARG | - | expression tag | UNP Q8R4B8 |
| K | -1 | SER | - | expression tag | UNP Q8R4B8 |
| K | 0 | ALA | - | expression tag | UNP Q8R4B8 |
| L | -3 | GLY | - | expression tag | UNP Q8R4B8 |
| L | -2 | ARG | - | expression tag | UNP Q8R4B8 |
| L | -1 | SER | - | expression tag | UNP Q8R4B8 |
| L | 0 | ALA | - | expression tag | UNP Q8R4B8 |

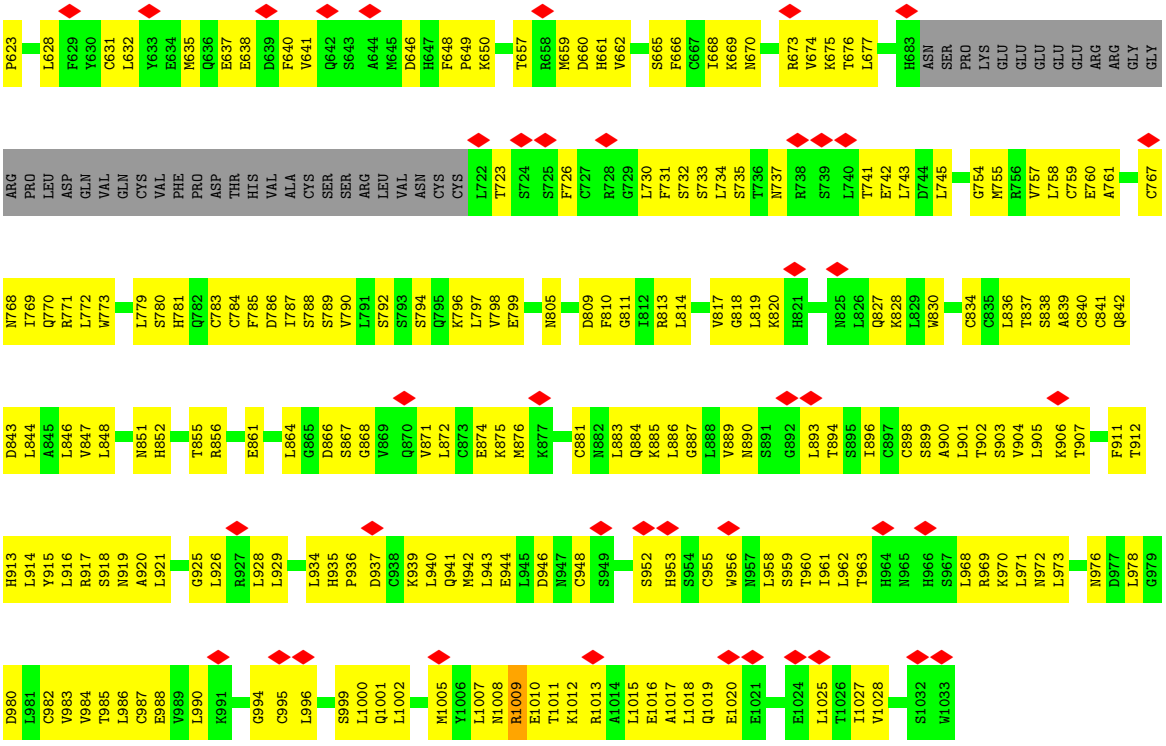
# 3 Residue-property plots (i)

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: NACHT, LRR and PYD domains-containing protein 3

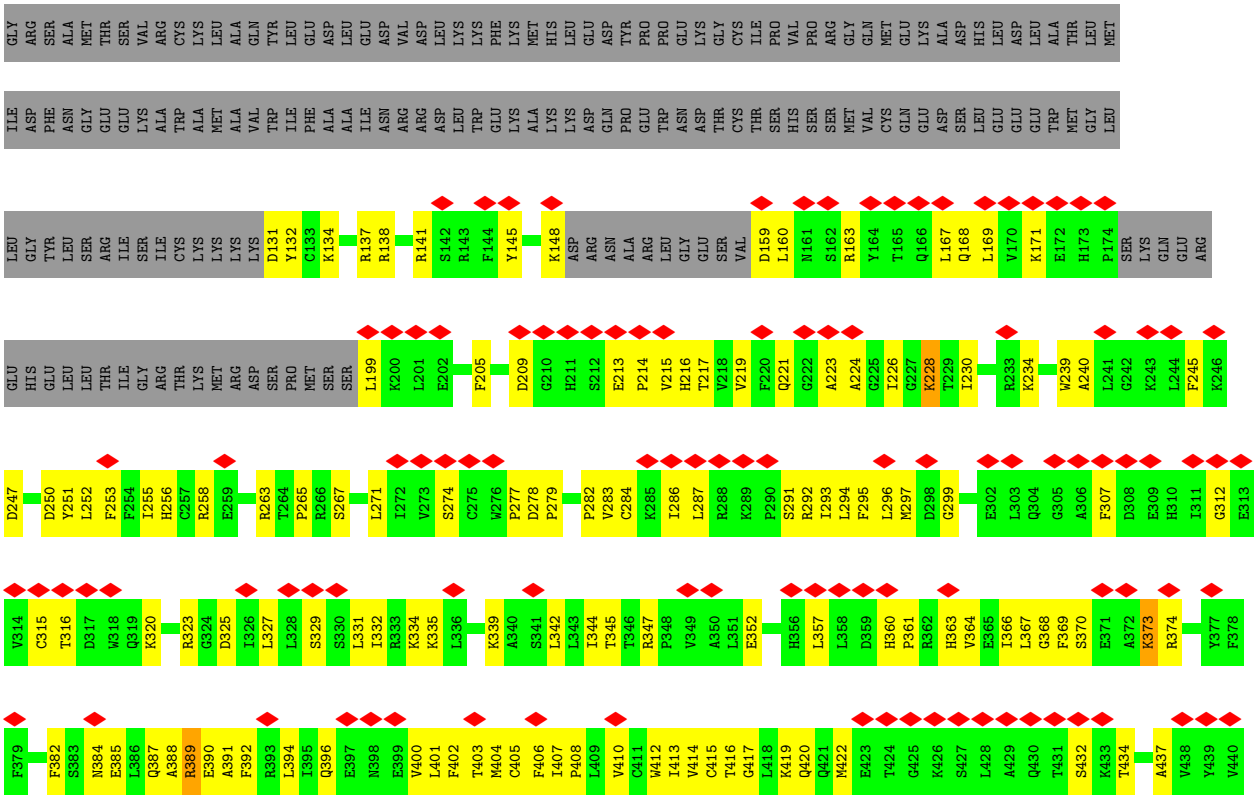
Chain A:

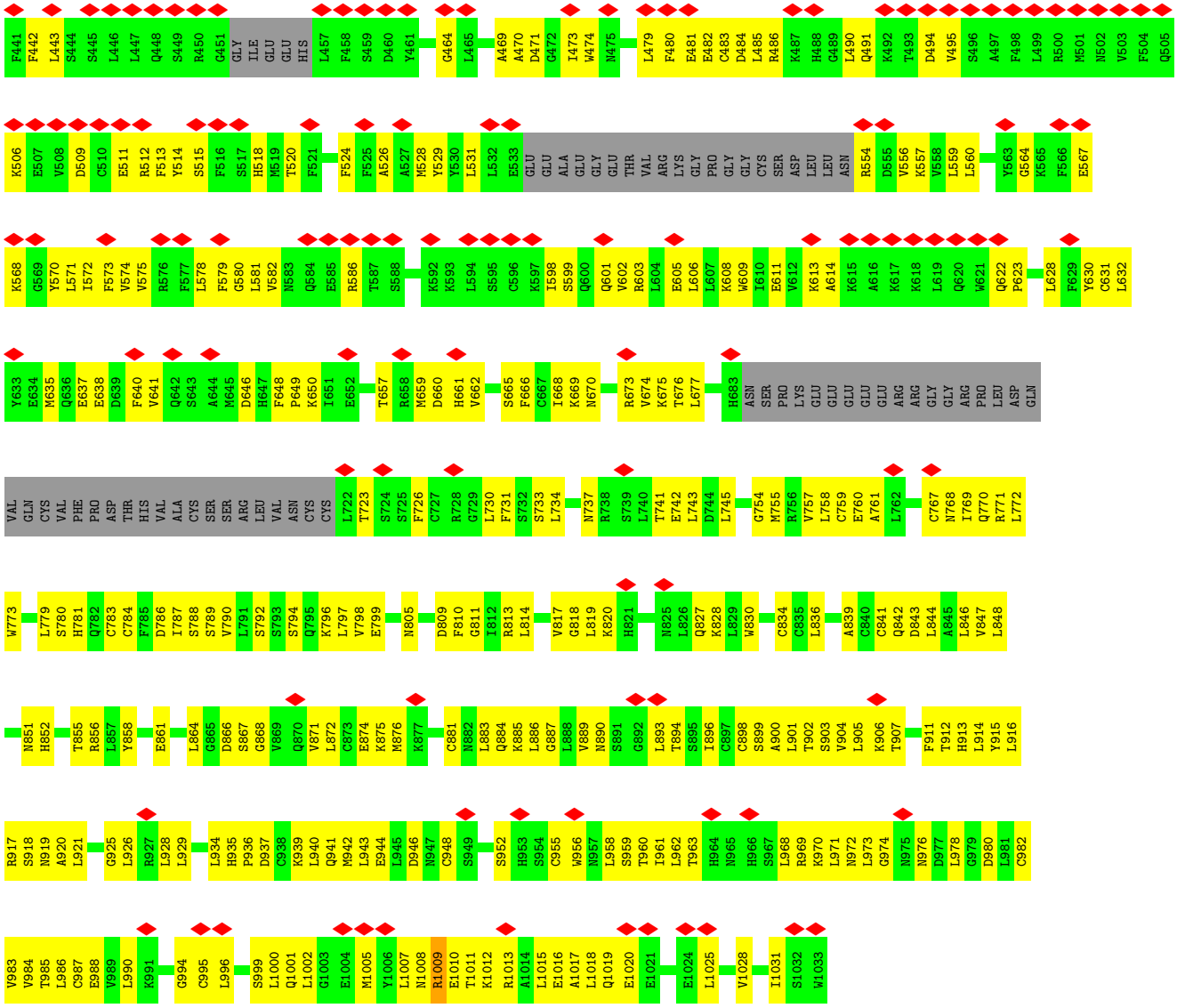





• Molecule 1: NACHT, LRR and PYD domains-containing protein 3

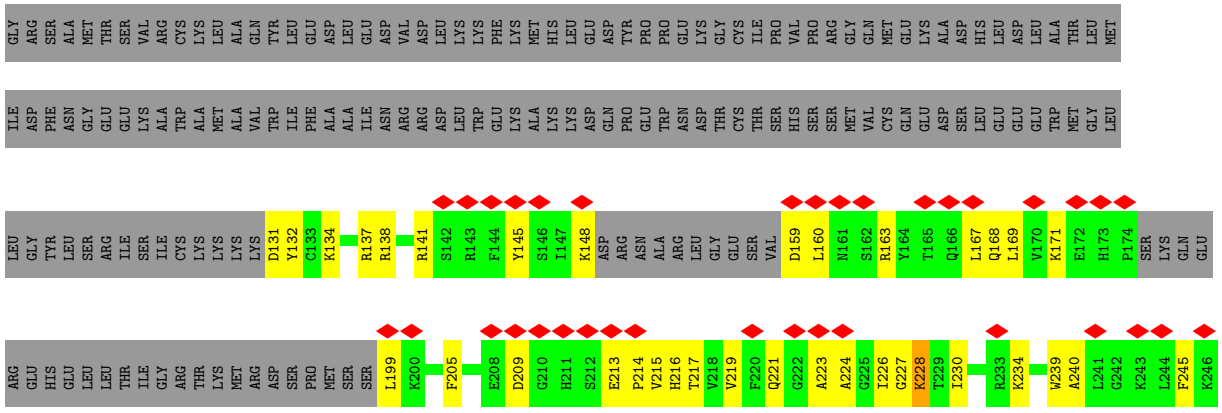
Chain B:

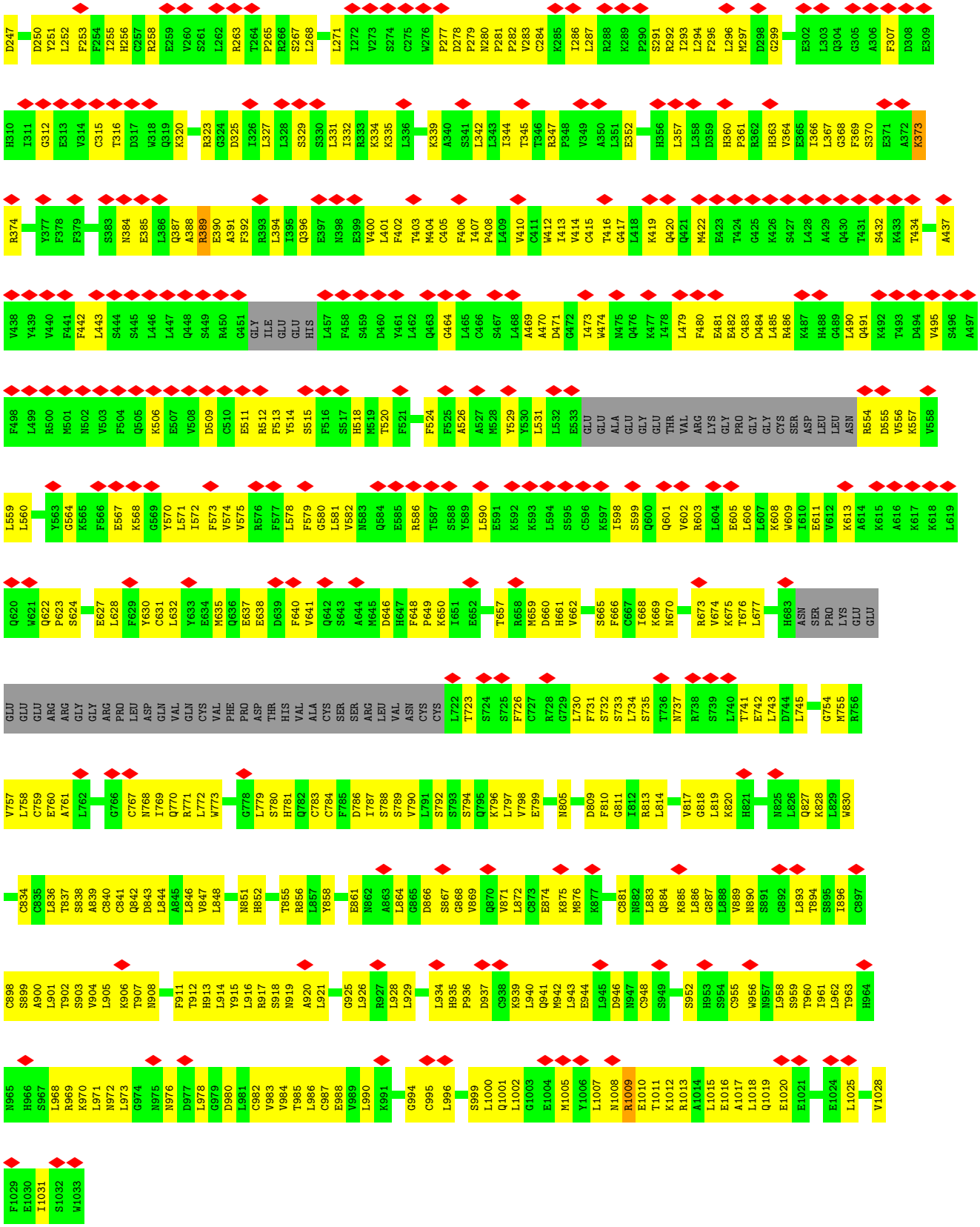





• Molecule 1: NACHT, LRR and PYD domains-containing protein 3

Chain C:

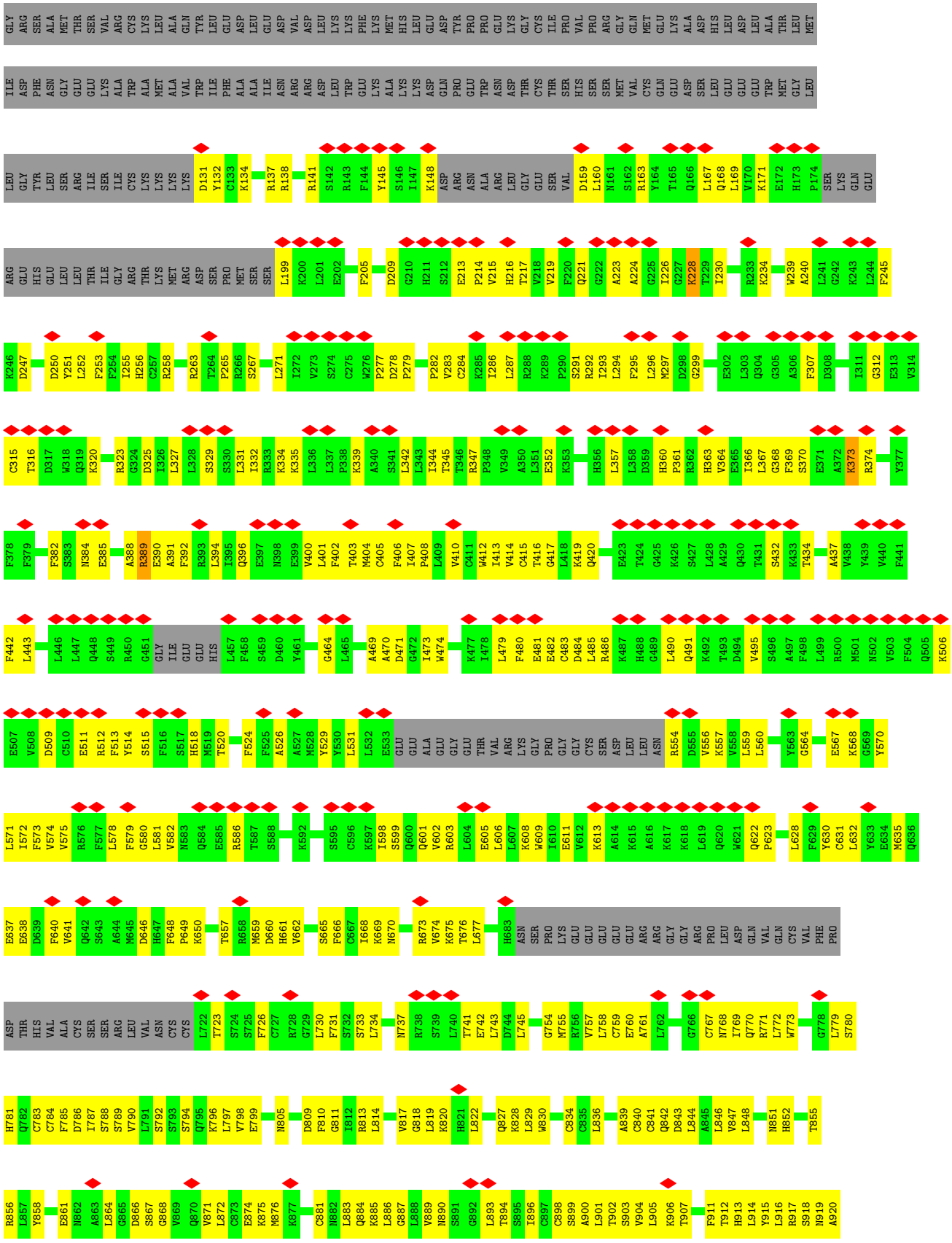



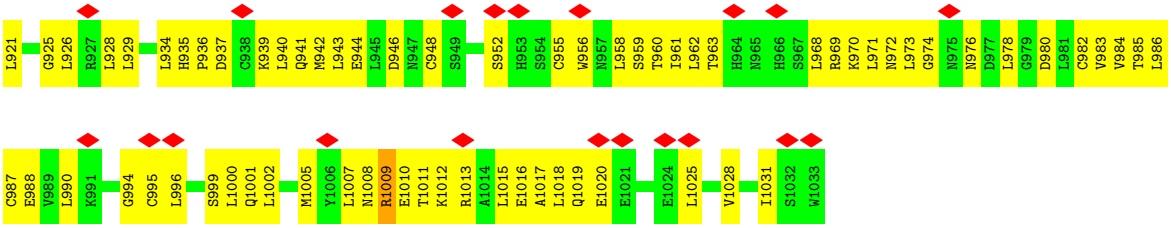


• Molecule 1: NACHT, LRR and PYD domains-containing protein 3

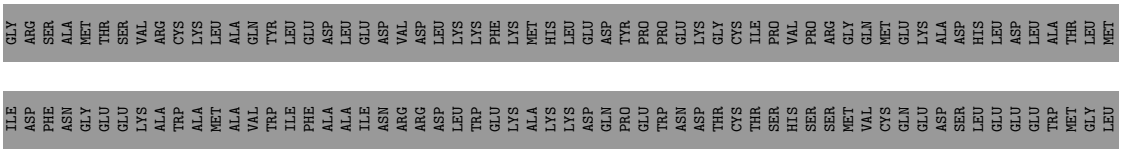
Chain D:

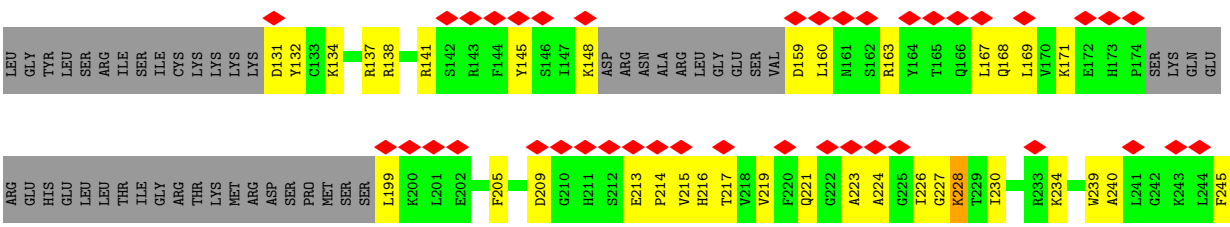

22%
39%
38%
22%

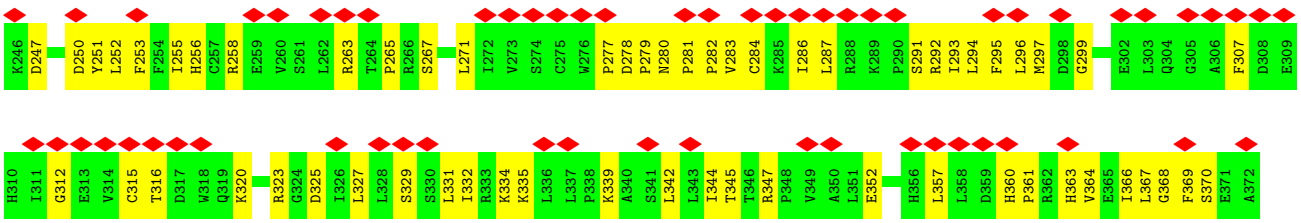

GLY ARG SER ALA MET THR SER VAL ARG CYS LYS LEU ALA GLN TYR LEU GLU ASP LEU GLU ASP VAL ASP LEU LYS LYS PHE LYS MET HIS LEU GLU ASP TYR PRO PRO GLU LYS GLY CYS ILE PRO VAL PRO ARG GLY GLN MET GLU LYS ALA ASP HIS LEU ASP LEU ALA THR LEU MET
ILE ASP PHE ASN GLY GLU GLU LYS ALA TRP ALA MET ALA VAL TRP ILE PHE ALA ALA ILE ASN ARG ARG ASP LEU TRP GLU LYS ALA LYS LYS ASP GLN PRO GLU TRP ASN ASP THR CYS THR SER HIS SER SER MET VAL CYS GLN GLU ASP SER LEU GLU GLU GLU TRP MET GLY LEU
LEU GLY TYR LEU SER ARG ILE SER ILE CYS LYS LYS LYS LYS D131 Y132 C133 K134 R137 R138 R141 S142 R143 F144 Y145 S146 I147 K148 ASP ARG ASN ALA ARG LEU GLY GLU SER VAL D159 L160 N161 S162 R163 Y164 T165 Q166 L167 Q168 L169 V170 K171 E172 H173 P174 SER LYS GLN GLU
ARG GLU HIS GLU LEU LEU THR ILE GLY ARG THR LYS MET ARG ASP SER PRO MET SER SER L199 K200 L201 E202 F205 D209 G210 H211 S212 E213 P214 V215 H216 T217 V218 V219 F220 Q221 G222 A223 A224 G225 I226 G227 K228 T229 I230 R233 K234 W239 A240 L241 G242 K243 L244 F245
K246 D247 D250 Y251 L252 F253 F254 I255 H256 C257 R258 R263 T264 P265 R266 S267 L271 I272 V273 S274 C275 W276 P277 D278 P279 P282 V283 C284 K285 I286 L287 R288 K289 P290 S291 R292 I293 L294 F295 L296 M297 D298 G299 E302 L303 Q304 G305 A306 F307 D308 I311 G312 E313 V314
C315 T316 D317 W318 Q319 K320 R323 G324 D325 I326 L327 L328 S329 S330 L331 I332 R333 K334 K335 L336 L337 P338 K339 A340 S341 L342 L343 I344 T345 T346 R347 P348 V349 A350 L351 E352 K353 H356 L357 L358 D359 H360 P361 R362 H363 V364 E365 I366 L367 G368 F369 S370 E371 A372 K373 R374 Y377
F378 F379 F382 S383 N384 E385 A388 R389 E390 A391 F392 R393 L394 I395 Q396 E397 N398 E399 V400 L401 F402 T403 M404 C405 F406 I407 P408 L409 V410 C411 W412 I413 V414 C415 T416 G417 L418 K419 Q420 E423 T424 G425 K426 S427 L428 A429 Q430 T431 S432 K433 T434 A437 V438 Y439 V440 F441
F442 L443 L446 L447 Q448 S449 R450 G451 GLY ILE GLU GLU HIS L457 F458 S459 D460 Y461 G464 L465 A469 A470 D471 G472 I473 W474 K477 I478 L479 F480 E481 E482 C483 D484 L485 R486 K487 H488 G489 L490 Q491 K492 T493 D494 V495 S496 A497 F498 L499 R500 M501 N502 V503 F504 Q505 K506
E507 V508 D509 C510 E511 R512 F513 Y514 S515 F516 S517 H518 M519 T520 F524 F525 A526 A527 M528 Y529 Y530 L531 L532 E533 GLU GLU ALA GLU GLY GLU THR VAL ARG LYS GLY PRO GLY GLY CYS SER ASP LEU LEU ASN R554 D555 V556 K557 V558 L559 L560 Y563 G564 E567 K568 G569 Y570
L571 I572 F573 V574 V575 R576 F577 L578 F579 G580 L581 V582 N583 Q584 E585 R586 T587 S588 K592 S595 C596 K597 I598 S599 Q600 Q601 V602 R603 L604 E605 L606 L607 K608 W609 I610 E611 V612 K613 A614 K615 A616 K617 K618 L619 Q620 W621 Q622 P623 L628 F629 Y630 C631 L632 Y633 E634 M635 Q636
E637 E638 D639 F640 V641 Q642 S643 A644 M645 D646 H647 F648 P649 K650 T657 R658 M659 D660 H661 V662 S665 F666 C667 I668 K669 N670 R673 V674 K675 T676 L677 H683 ASN SER PRO LYS GLU GLU GLU GLU GLU ARG GLY GLY ARG PRO LEU ASP GLN VAL GLN CYS VAL PHE PRO
ASP THR HIS VAL ALA CYS SER SER ARG LEU VAL ASN CYS CYS L722 T723 S724 S725 F726 C727 R728 G729 L730 F731 S732 S733 L734 N737 R738 S739 L740 T741 E742 L743 D744 L745 G754 M755 R756 V757 L758 C759 E760 A761 L762 G766 C767 N768 I769 Q770 R771 L772 W773 G778 L779 S780
H781 Q782 C783 C784 F785 D786 I787 S788 S789 V790 L791 S792 S793 S794 Q795 K796 L797 V798 E799 N805 D809 F810 G811 I812 R813 L814 V817 G818 L819 K820 H821 L822 Q827 K828 L829 W830 C834 C835 L836 A839 C840 C841 Q842 D843 L844 A845 L846 V847 L848 N851 H852 T855
R856 L857 Y858 E861 N862 A863 L864 G865 D866 S867 G868 V869 Q870 V871 L872 C873 E874 K875 M876 K877 C881 N882 L883 Q884 K885 L886 G887 L888 V889 N890 S891 G892 L893 T894 S895 I896 C897 C898 S899 A900 L901 T902 S903 V904 L905 K906 T907 F911 T912 H913 L914 Y915 L916 R917 S918 N919 A920

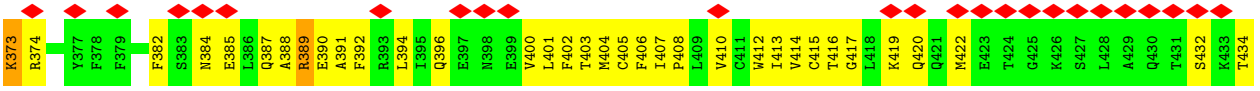


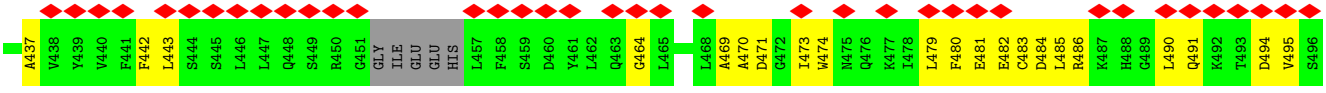

• Molecule 1: NACHT, LRR and PYD domains-containing protein 3

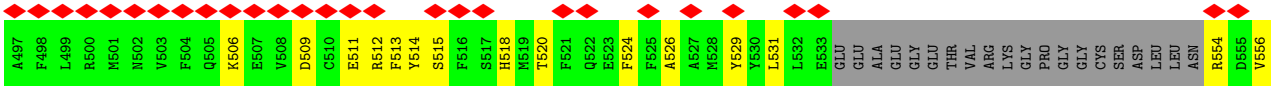



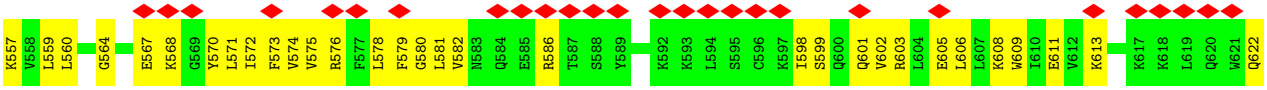



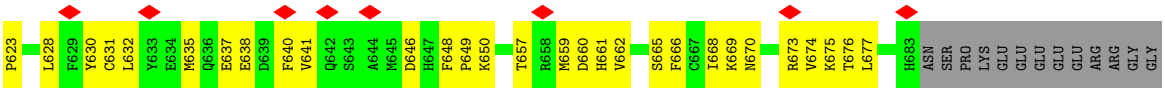



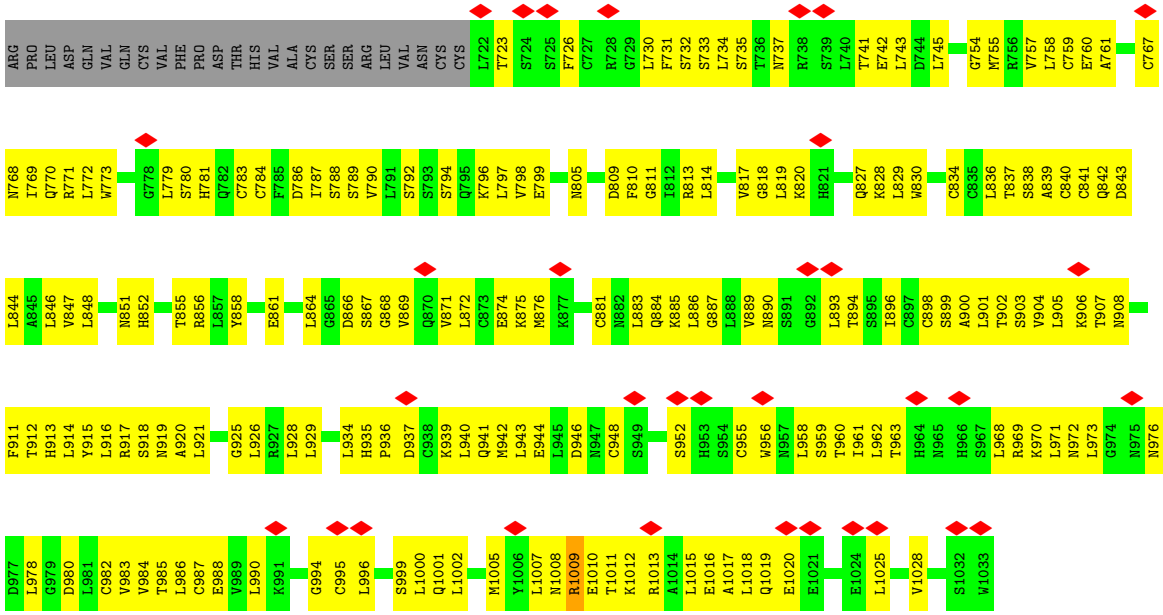



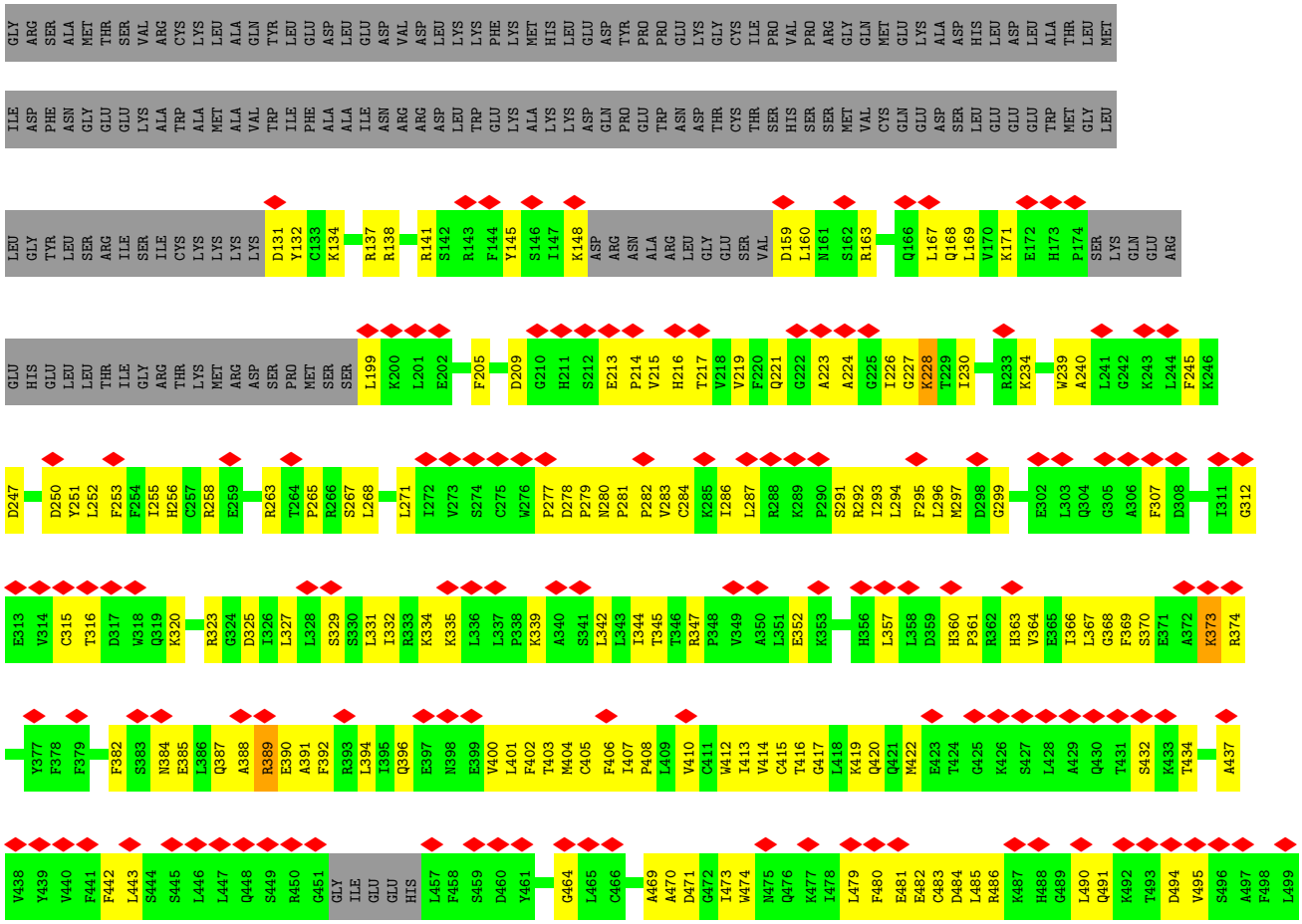



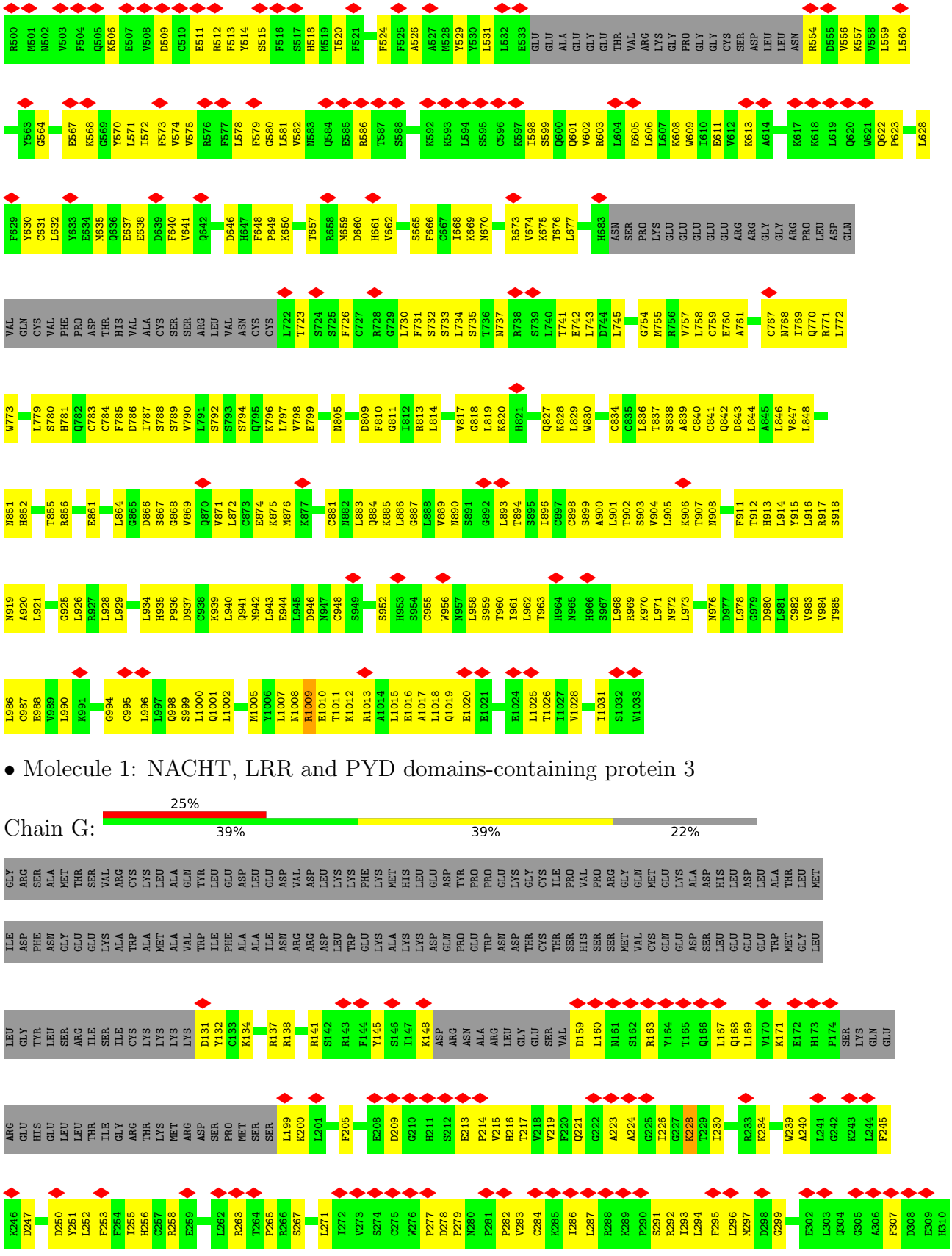





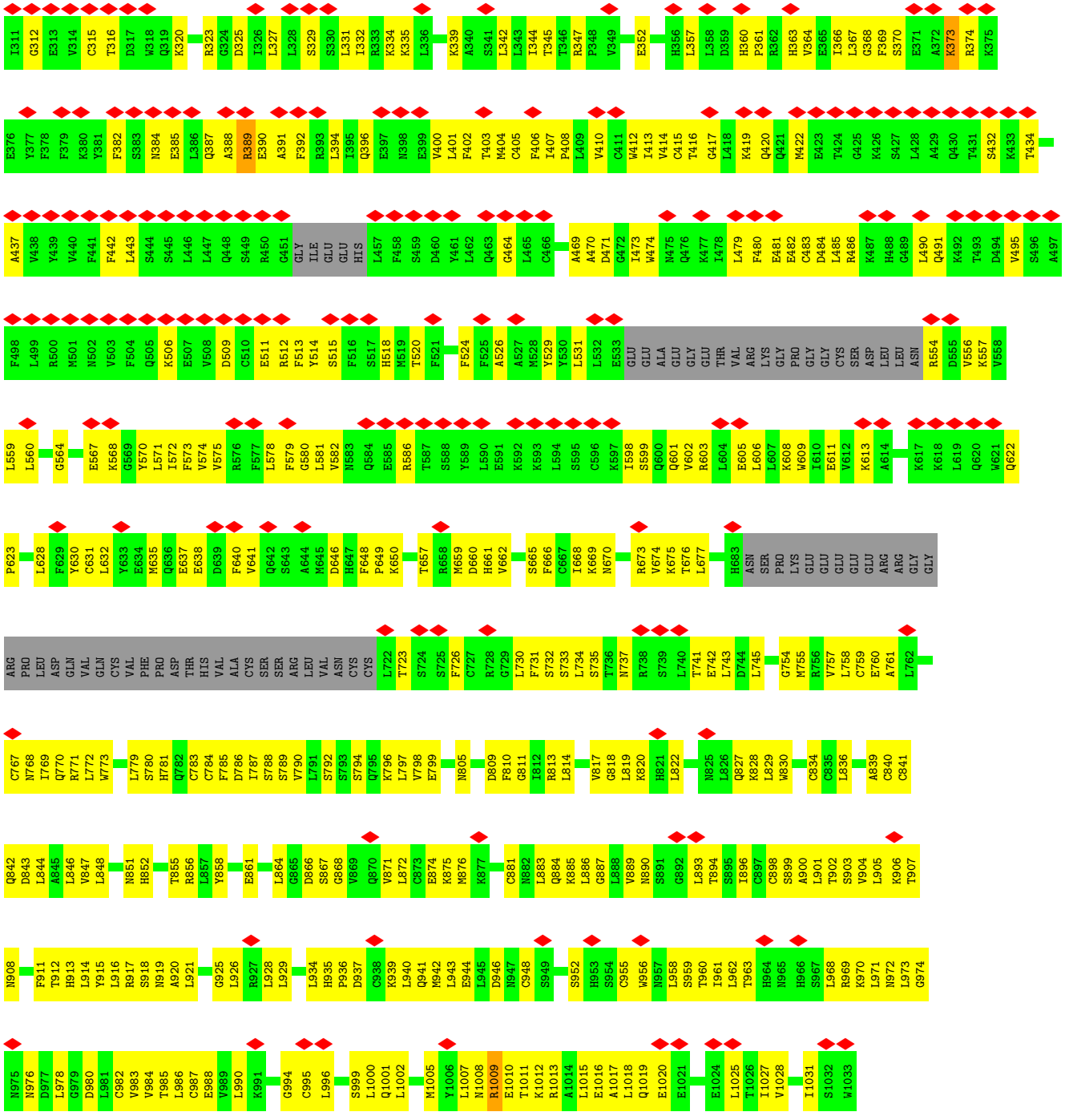
• Molecule 1: NACHT, LRR and PYD domains-containing protein 3

Chain F:

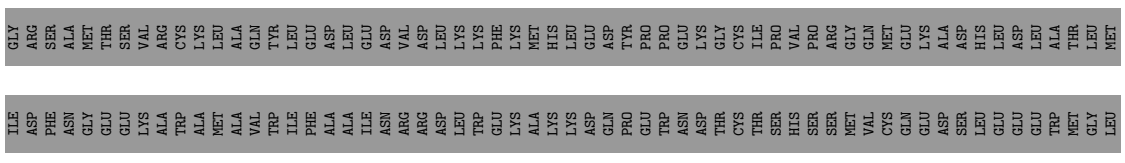


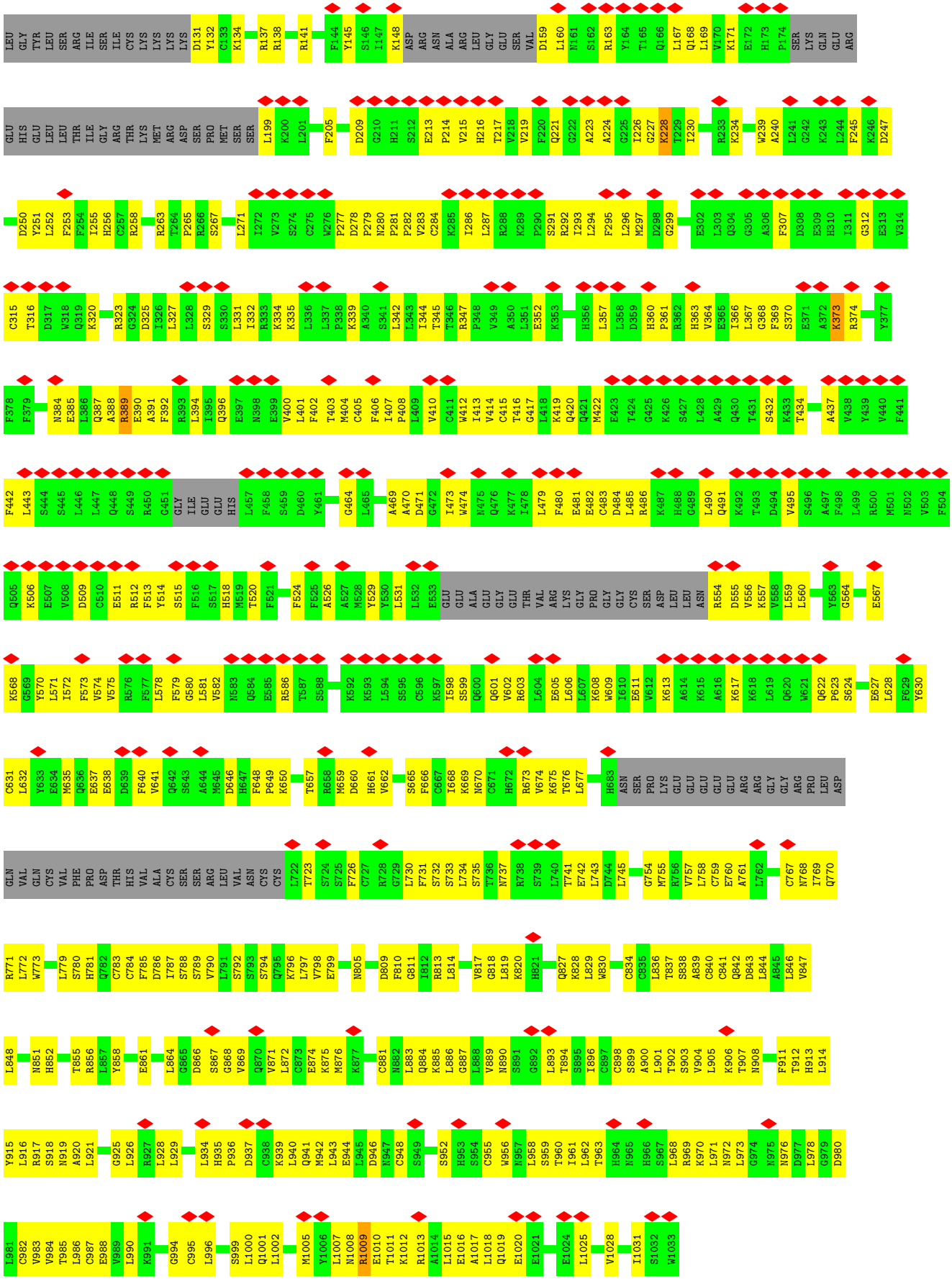
• Molecule 1: NACHT, LRR and PYD domains-containing protein 3



• Molecule 1: NACHT, LRR and PYD domains-containing protein 3

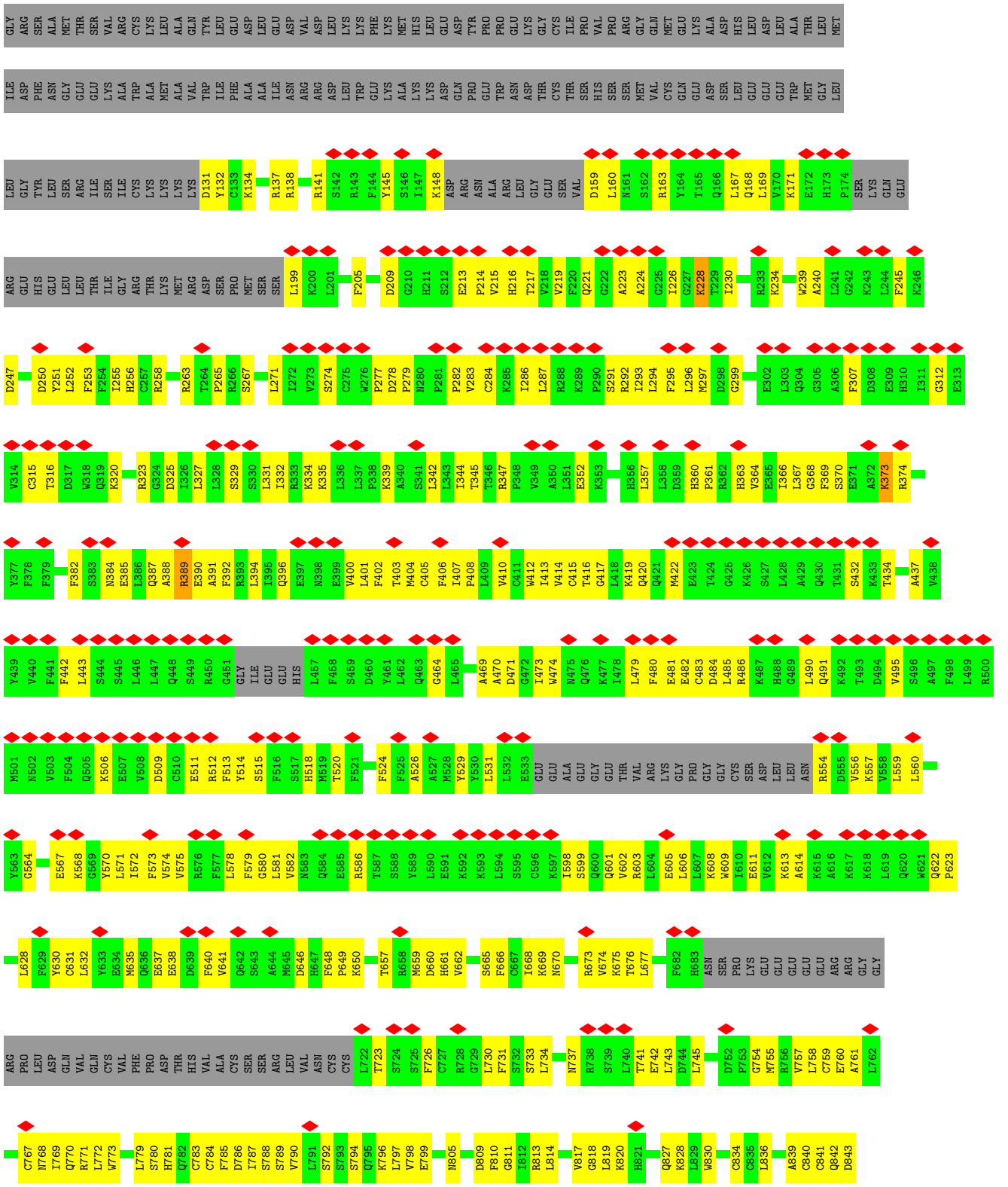
Chain H:

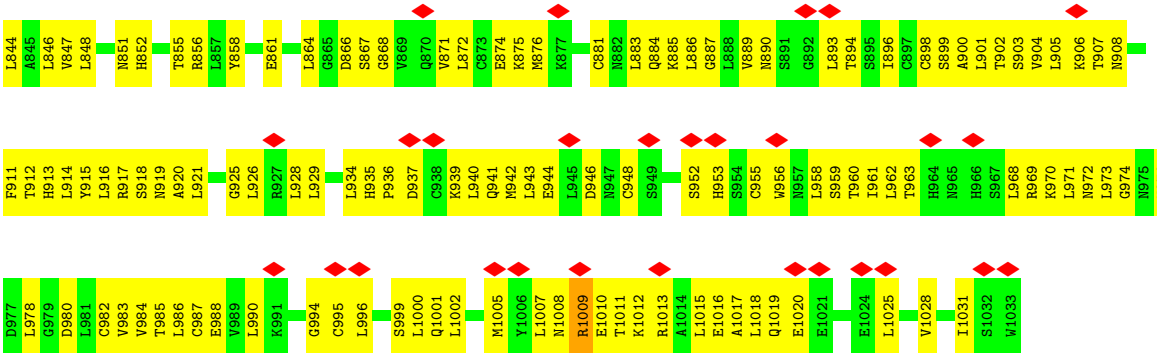



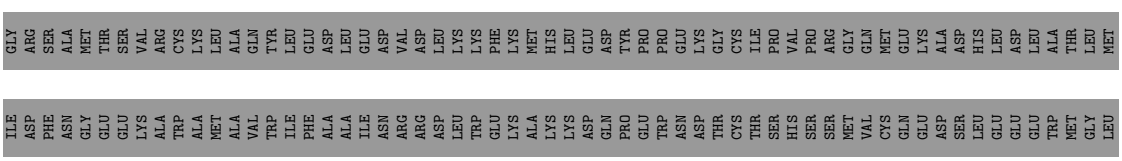


• Molecule 1: NACHT, LRR and PYD domains-containing protein 3

Chain I:

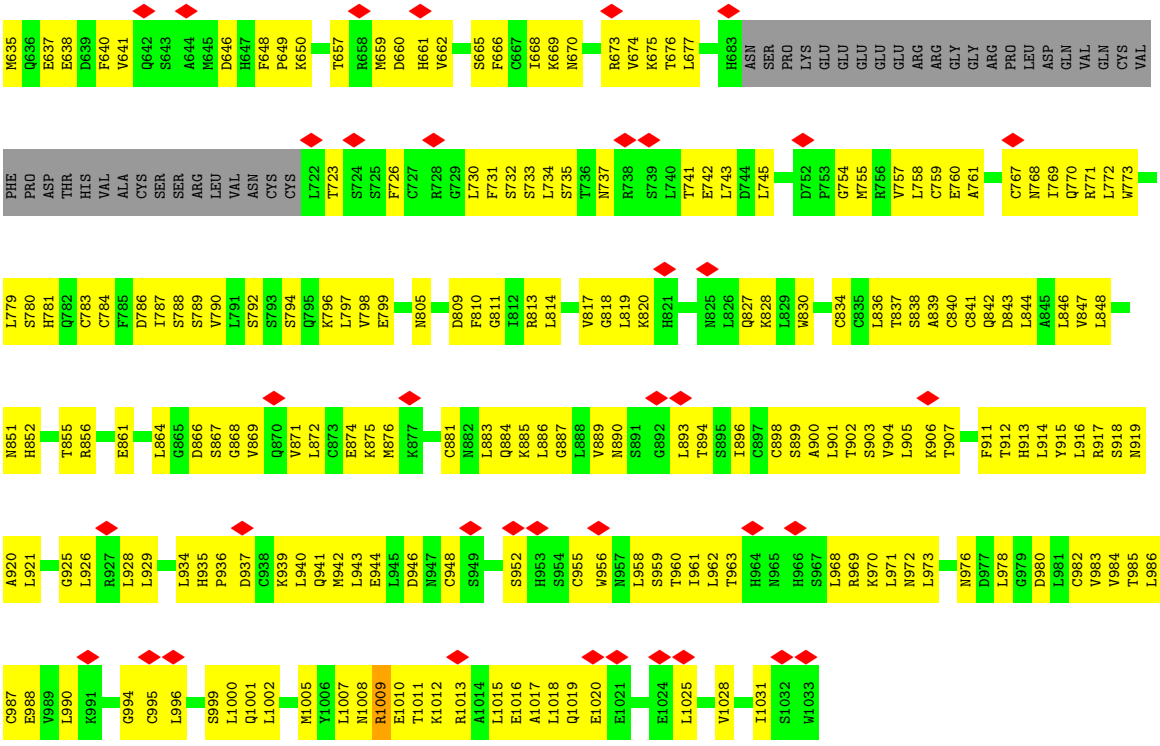







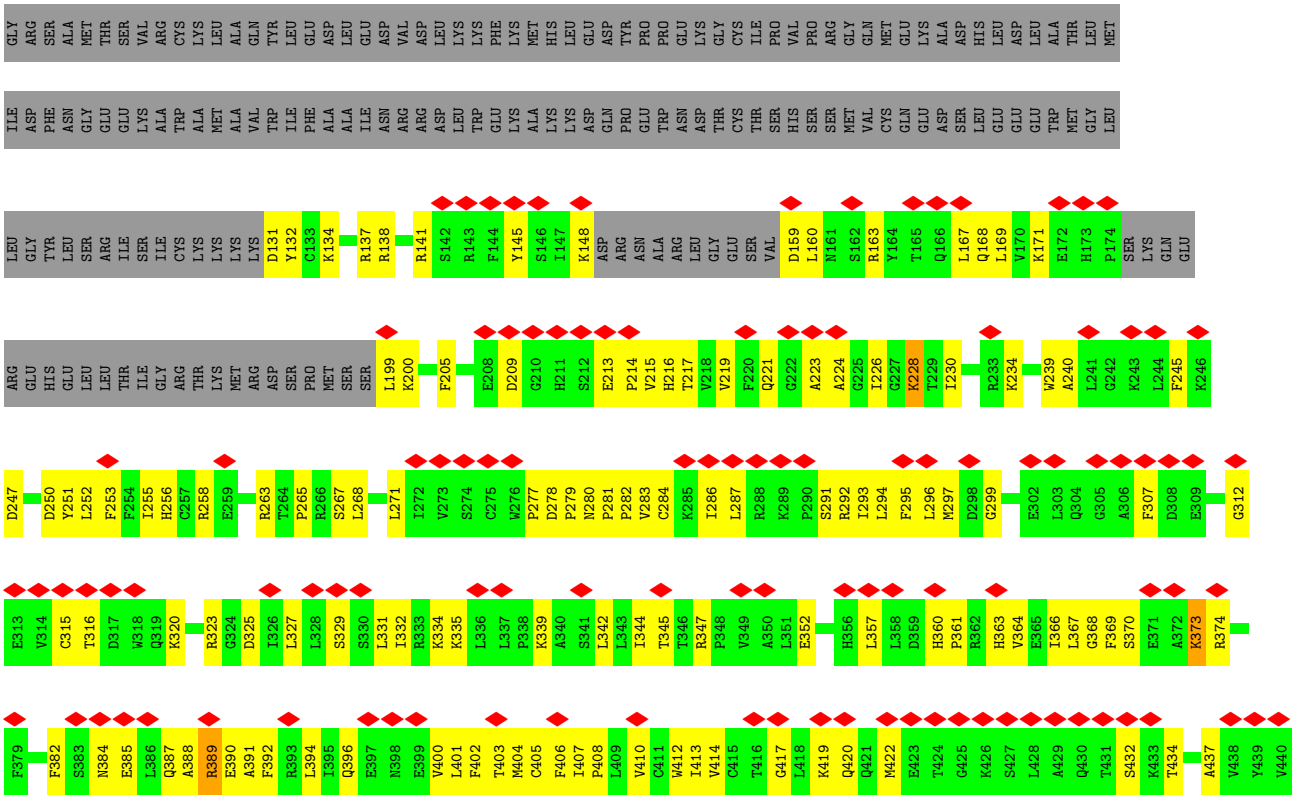
• Molecule 1: NACHT, LRR and PYD domains-containing protein 3

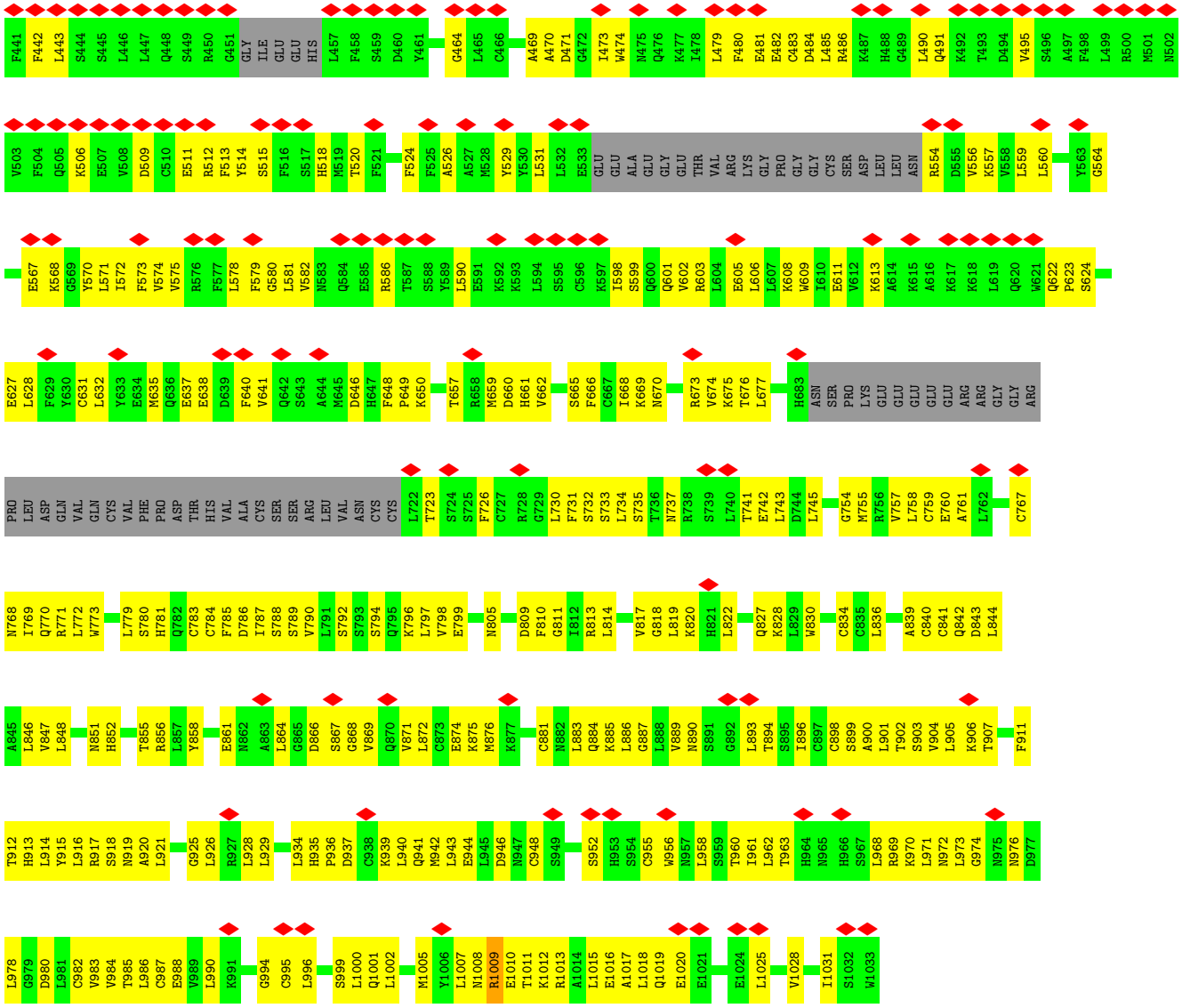
Chain J:



• Molecule 1: NACHT, LRR and PYD domains-containing protein 3

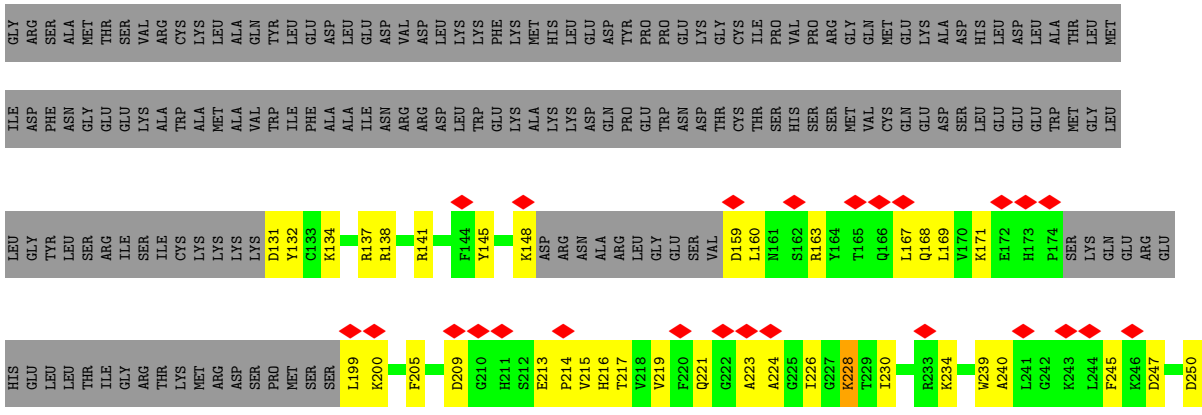
Chain K:

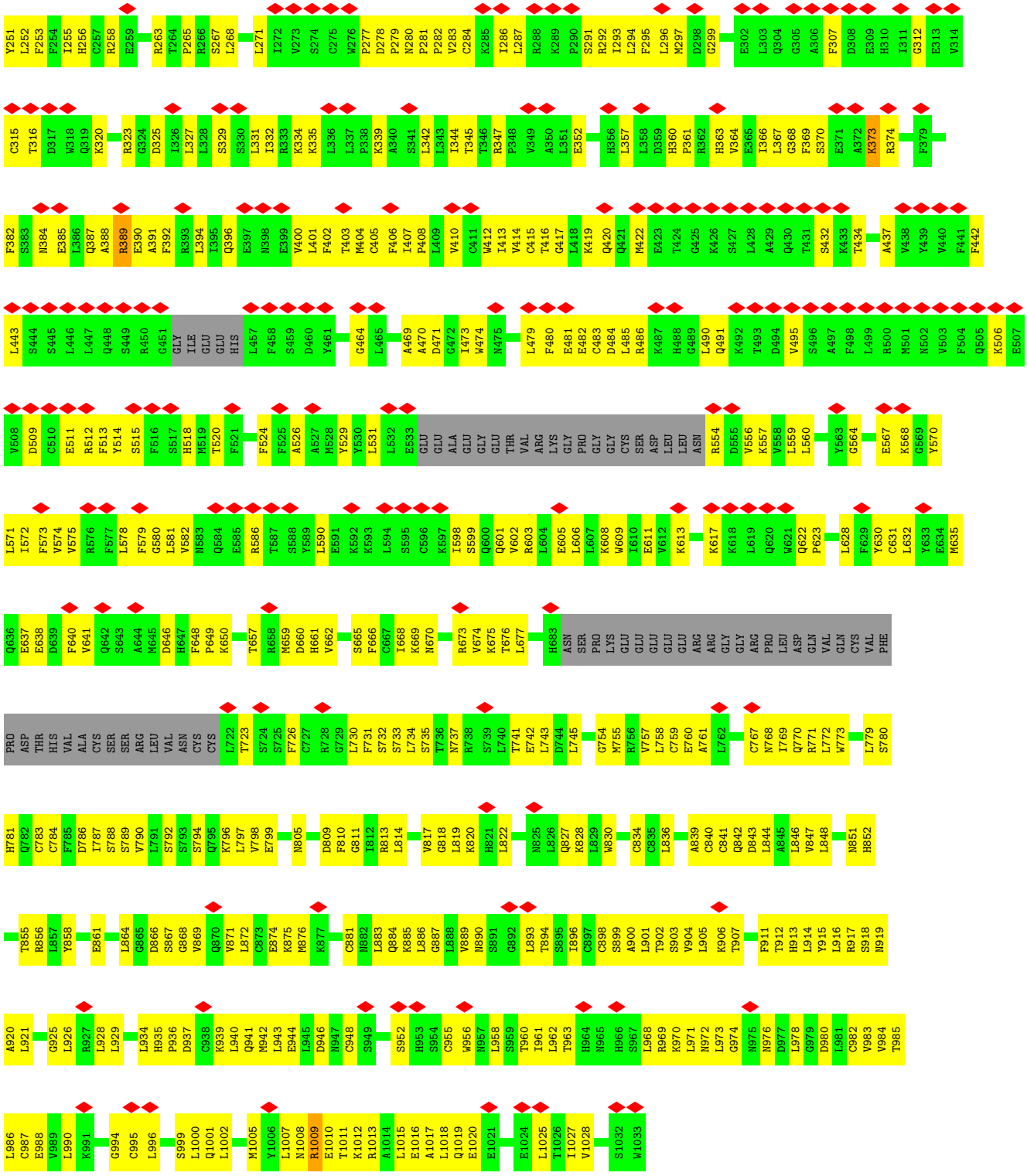





• Molecule 1: NACHT, LRR and PYD domains-containing protein 3

Chain L:


Y251 L252 F253 F254 I255 H256 C257 R258 E259 R263 T264 P265 R266 S267 L268 L271 I272 V273 S274 C275 W276 P277 D278 P279 N280 P281 P282 V283 C284 K285 I286 L287 R288 K289 P290 S291 R292 I293 L294 F295 L296 M297 D298 G299 E302 L303 Q304 G305 A306 F307 D308 E309 H310 I311 G312 E313 V314
C315 T316 D317 H318 Q319 K320 R323 G324 D325 I326 L327 L328 S329 S330 L331 I332 R333 K334 K335 L336 L337 P338 K339 A340 S341 L342 L343 I344 T345 T346 R347 P348 V349 A350 L351 E352 H356 L357 L358 D359 H360 P361 R362 H363 V364 E365 I366 I367 G368 F369 S370 E371 A372 K373 R374 F379
F382 S383 N384 E385 L386 Q387 A388 R389 E390 A391 F392 R393 L394 I395 Q396 E397 N398 E399 V400 L401 F402 T403 M404 C405 F406 I407 P408 I409 V410 C411 W412 I413 V414 C415 T416 G417 L418 K419 Q420 Q421 M422 E423 T424 G425 K426 S427 L428 A429 Q430 T431 S432 K433 T434 A437 W438 Y439 V440 F441 F442
L443 S444 S445 L446 L447 Q448 S449 R450 G451 GLY ILE GLU GLU HIS L457 F458 S459 D460 Y461 G464 L465 A469 A470 D471 G472 I473 W474 N475 L479 F480 E481 E482 C483 D484 L485 R486 K487 H488 G489 L490 Q491 K492 T493 D494 V495 S496 A497 F498 L499 R500 M501 N502 V503 F504 Q505 K506 E507
V508 D509 C510 E511 R512 F513 Y514 S515 F516 S517 H518 M519 T520 F521 F524 F525 A526 A527 M528 Y529 Y530 L531 L532 E533 GLU GLU ALA GLU GLY GLU THR VAL ARG LYS GLY PRO GLY GLY CYS SER ASP LEU LEU ASN R554 D555 V556 K557 V558 L559 L560 Y563 G564 E567 K568 G569 Y570
L571 I572 F573 V574 V575 R576 F577 L578 F579 G580 L581 V582 N583 Q584 E585 R586 T587 S588 Y589 L590 E591 K592 K593 L594 S595 C596 K597 I598 S599 Q600 Q601 V602 R603 L604 E605 L606 L607 K608 W609 I610 E611 V612 K613 K617 K618 L619 Q620 W621 Q622 P623 L628 F629 Y630 C631 L632 Y633 E634 M635
Q636 E637 E638 D639 F640 V641 Q642 S643 A644 M645 D646 H647 F648 P649 K650 T657 R658 M659 D660 H661 V662 S665 F666 C667 I668 K669 N670 R673 V674 K675 T676 L677 H683 ASN SER PRO LYS GLU GLU GLU GLU GLU ARG ARG GLY GLY GLY ARG PRO LEU ASP GLN VAL GLN CYS VAL PHE
PRO ASP THR HIS VAL ALA CYS SER SER ARG LEU VAL ASN CYS CYS L722 T723 S724 S725 F726 C727 R728 G729 L730 F731 S732 S733 L734 S735 T736 N737 R738 S739 L740 T741 E742 L743 D744 L745 G754 M755 R756 V757 L758 C759 E760 A761 L762 C767 N768 I769 Q770 R771 L772 W773 L779 S780
H781 Q782 C783 C784 F785 D786 I787 S788 S789 V790 L791 S792 S793 S794 Q795 K796 L797 V798 E799 N805 D809 F810 G811 I812 R813 L814 V817 G818 L819 K820 H821 L822 N825 L826 Q827 K828 L829 W830 C834 C835 L836 A839 C840 C841 Q842 D843 L844 A845 L846 V847 L848 N851 H852
T855 R856 L857 Y858 E861 L864 G865 D866 S867 G868 V869 Q870 V871 L872 C873 E874 K875 M876 K877 C881 N882 L883 Q884 K885 L886 G887 L888 V889 N890 S891 G892 L893 T894 S895 I896 C897 C898 S899 A900 L901 T902 S903 V904 L905 K906 T907 F911 T912 H913 L914 Y915 L916 R917 N919
A920 L921 G925 L926 R927 L928 L929 L934 H935 P936 D937 C938 K939 L940 Q941 M942 L943 E944 L945 D946 N947 C948 S949 S952 H953 S954 C955 W956 N957 L958 S959 T960 I961 L962 T963 H964 N965 H966 S967 L968 R969 K970 L971 N972 L973 G974 N975 N976 D977 L978 G979 D980 L981 C982 V983 Y984 T985
L986 C987 E988 V989 L990 K991 G994 C995 L996 S999 L1000 Q1001 L1002 M1005 Y1006 L1007 N1008 R1009 E1010 T1011 K1012 R1013 A1014 L1015 E1016 A1017 L1018 Q1019 E1020 E1021 E1024 L1025 T1026 I1027 V1028 S1032 W1033

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, D6 | Depositor |
| Number of particles used | 122941 | 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 ($e^-/Å^2$) | 53.225 | Depositor |
| Minimum defocus (nm) | -800 | Depositor |
| Maximum defocus (nm) | -2400 | Depositor |
| Magnification | 105000 | Depositor |
| Image detector | GATAN K3 (6k x 4k) | Depositor |
| Maximum map value | 1.730 | Depositor |
| Minimum map value | -0.002 | Depositor |
| Average map value | 0.002 | Depositor |
| Map value standard deviation | 0.031 | Depositor |
| Recommended contour level | 0.09 | Depositor |
| Map size (Å) | 422.4, 422.4, 422.4 | wwPDB |
| Map dimensions | 512, 512, 512 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 0.825, 0.825, 0.825 | Depositor |

# 5 Model quality

## 5.1 Standard geometry

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

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | $\#\|Z\| > 5$ | RMSZ | $\#\|Z\| > 5$ |
| 1 | A | 0.28 | 0/6527 | 0.56 | 0/8804 |
| 1 | B | 0.28 | 0/6527 | 0.56 | 0/8804 |
| 1 | C | 0.28 | 0/6527 | 0.56 | 0/8804 |
| 1 | D | 0.28 | 0/6527 | 0.56 | 0/8804 |
| 1 | E | 0.28 | 0/6527 | 0.56 | 0/8804 |
| 1 | F | 0.28 | 0/6527 | 0.56 | 0/8804 |
| 1 | G | 0.28 | 0/6527 | 0.56 | 0/8804 |
| 1 | H | 0.28 | 0/6527 | 0.56 | 0/8804 |
| 1 | I | 0.28 | 0/6527 | 0.56 | 0/8804 |
| 1 | J | 0.28 | 0/6527 | 0.56 | 0/8804 |
| 1 | K | 0.28 | 0/6527 | 0.56 | 0/8804 |
| 1 | L | 0.28 | 0/6527 | 0.56 | 0/8804 |
| All | All | 0.28 | 0/78324 | 0.56 | 0/105648 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | A | 6407 | 0 | 6446 | 367 | 0 |
| 1 | B | 6407 | 0 | 6446 | 365 | 0 |
| 1 | C | 6407 | 0 | 6446 | 370 | 0 |
| 1 | D | 6407 | 0 | 6446 | 365 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | E | 6407 | 0 | 6446 | 368 | 0 |
| 1 | F | 6407 | 0 | 6446 | 374 | 0 |
| 1 | G | 6407 | 0 | 6446 | 371 | 0 |
| 1 | H | 6407 | 0 | 6446 | 370 | 0 |
| 1 | I | 6407 | 0 | 6446 | 366 | 0 |
| 1 | J | 6407 | 0 | 6446 | 367 | 0 |
| 1 | K | 6407 | 0 | 6446 | 361 | 0 |
| 1 | L | 6407 | 0 | 6446 | 367 | 0 |
| All | All | 76884 | 0 | 77352 | 4371 | 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 28.

The worst 5 of 4371 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:785:PHE:HB3 | 1:L:810:PHE:HZ | 1.35 | 0.92 |
| 1:C:810:PHE:HZ | 1:D:785:PHE:HB3 | 1.31 | 0.91 |
| 1:A:773:TRP:HH2 | 1:L:1013:ARG:HG2 | 1.39 | 0.88 |
| 1:A:385:GLU:HA | 1:A:389:ARG:HH12 | 1.44 | 0.83 |
| 1:J:385:GLU:HA | 1:J:389:ARG:HH12 | 1.44 | 0.83 |

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 1 | A | 794/1037 (77%) | 688 (87%) | 105 (13%) | 1 (0%) | 51 85 |
| 1 | B | 794/1037 (77%) | 689 (87%) | 104 (13%) | 1 (0%) | 51 85 |
| 1 | C | 794/1037 (77%) | 689 (87%) | 104 (13%) | 1 (0%) | 51 85 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 1 | D | 794/1037 (77%) | 689 (87%) | 104 (13%) | 1 (0%) | 51 85 |
| 1 | E | 794/1037 (77%) | 689 (87%) | 104 (13%) | 1 (0%) | 51 85 |
| 1 | F | 794/1037 (77%) | 688 (87%) | 105 (13%) | 1 (0%) | 51 85 |
| 1 | G | 794/1037 (77%) | 688 (87%) | 105 (13%) | 1 (0%) | 51 85 |
| 1 | H | 794/1037 (77%) | 690 (87%) | 103 (13%) | 1 (0%) | 51 85 |
| 1 | I | 794/1037 (77%) | 690 (87%) | 103 (13%) | 1 (0%) | 51 85 |
| 1 | J | 794/1037 (77%) | 689 (87%) | 104 (13%) | 1 (0%) | 51 85 |
| 1 | K | 794/1037 (77%) | 689 (87%) | 104 (13%) | 1 (0%) | 51 85 |
| 1 | L | 794/1037 (77%) | 689 (87%) | 104 (13%) | 1 (0%) | 51 85 |
| All | All | 9528/12444 (77%) | 8267 (87%) | 1249 (13%) | 12 (0%) | 54 85 |

5 of 12 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 571 | LEU |
| 1 | B | 571 | LEU |
| 1 | C | 571 | LEU |
| 1 | D | 571 | LEU |
| 1 | E | 571 | LEU |

### 5.3.2 Protein sidechains (i)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 1 | A | 720/937 (77%) | 716 (99%) | 4 (1%) | 86 92 |
| 1 | B | 720/937 (77%) | 716 (99%) | 4 (1%) | 86 92 |
| 1 | C | 720/937 (77%) | 716 (99%) | 4 (1%) | 86 92 |
| 1 | D | 720/937 (77%) | 716 (99%) | 4 (1%) | 86 92 |
| 1 | E | 720/937 (77%) | 716 (99%) | 4 (1%) | 86 92 |
| 1 | F | 720/937 (77%) | 716 (99%) | 4 (1%) | 86 92 |
| 1 | G | 720/937 (77%) | 716 (99%) | 4 (1%) | 86 92 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 1 | H | 720/937 (77%) | 716 (99%) | 4 (1%) | 86 92 |
| 1 | I | 720/937 (77%) | 716 (99%) | 4 (1%) | 86 92 |
| 1 | J | 720/937 (77%) | 716 (99%) | 4 (1%) | 86 92 |
| 1 | K | 720/937 (77%) | 716 (99%) | 4 (1%) | 86 92 |
| 1 | L | 720/937 (77%) | 716 (99%) | 4 (1%) | 86 92 |
| All | All | 8640/11244 (77%) | 8592 (99%) | 48 (1%) | 86 92 |

5 of 48 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | H | 228 | LYS |
| 1 | I | 1009 | ARG |
| 1 | H | 373 | LYS |
| 1 | I | 228 | LYS |
| 1 | J | 373 | LYS |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | H | 670 | ASN |
| 1 | I | 976 | ASN |
| 1 | H | 737 | ASN |
| 1 | I | 670 | ASN |
| 1 | J | 737 | 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

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

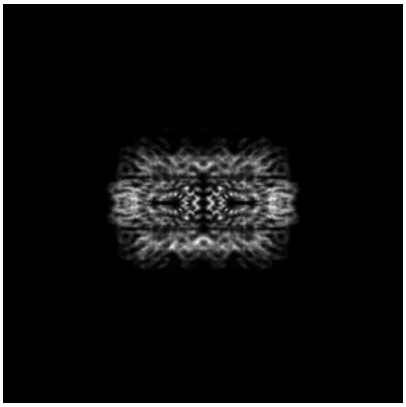
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-23302. These allow visual inspection of the internal detail of the map and identification of artifacts.

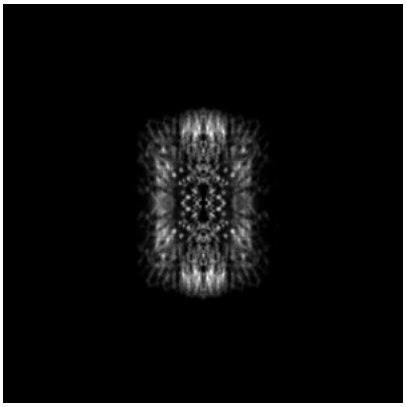
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

## 6.1 Orthogonal projections

### 6.1.1 Primary map



X



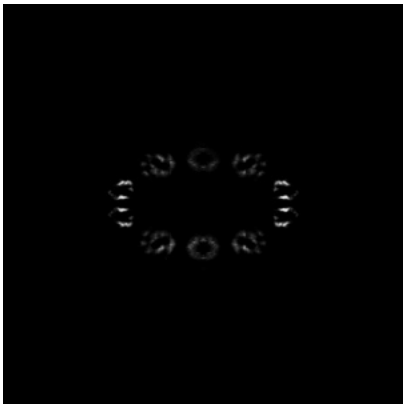
Y

Z

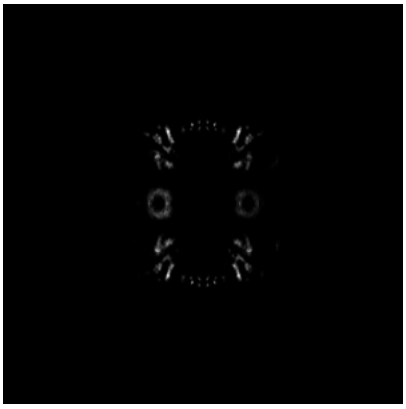
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices

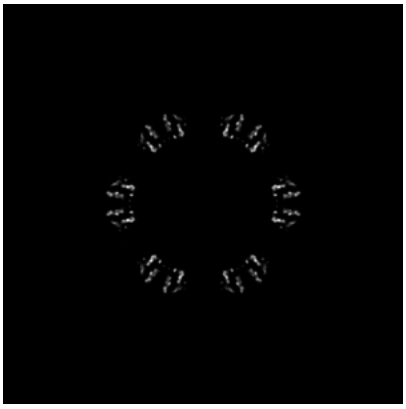
### 6.2.1 Primary map



X Index: 256



Y Index: 256

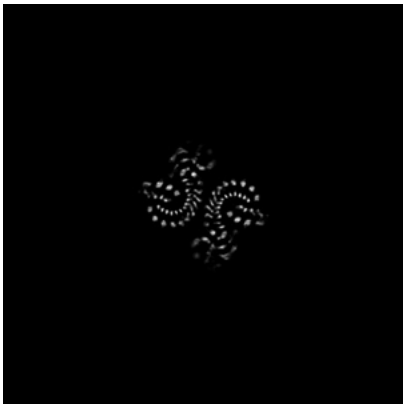


Z Index: 256

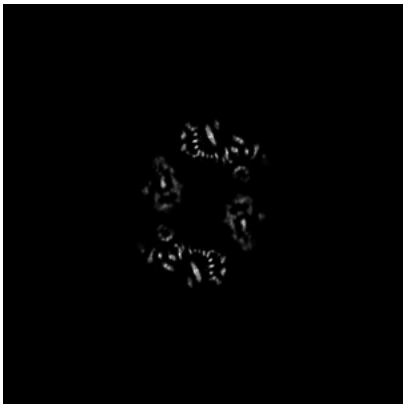
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

### 6.3.1 Primary map



X Index: 348



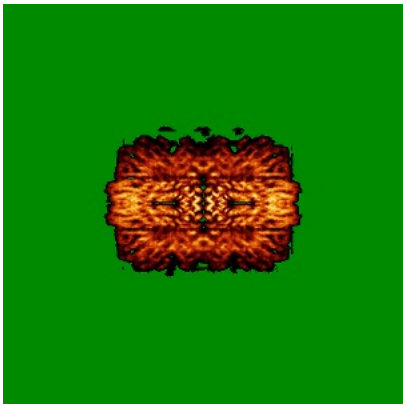
Y Index: 323

Z Index: 266

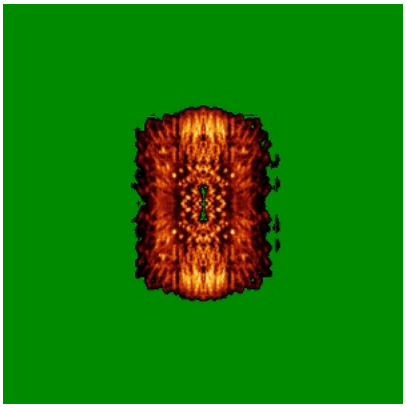
The images above show the largest variance slices of the map in three orthogonal directions.

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

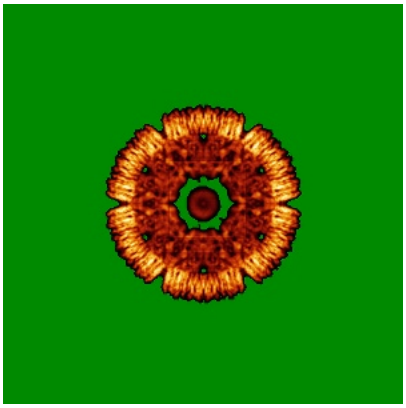
### 6.4.1 Primary map



X



Y

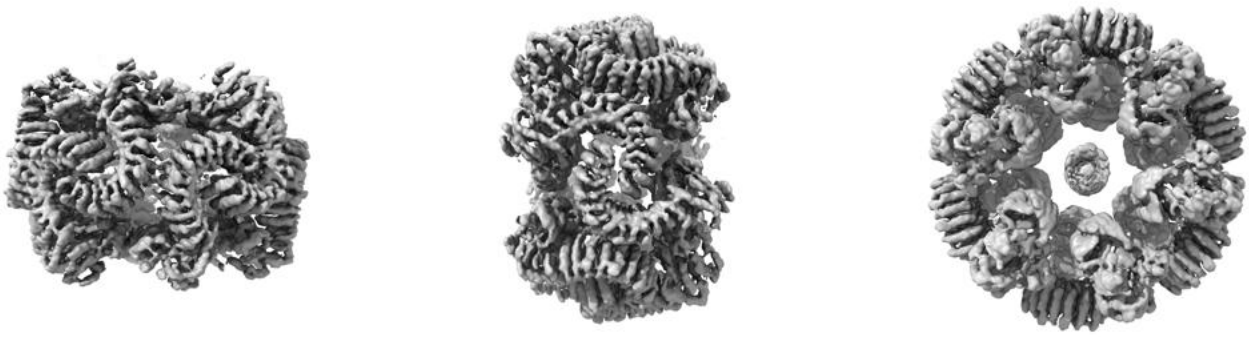


Z

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

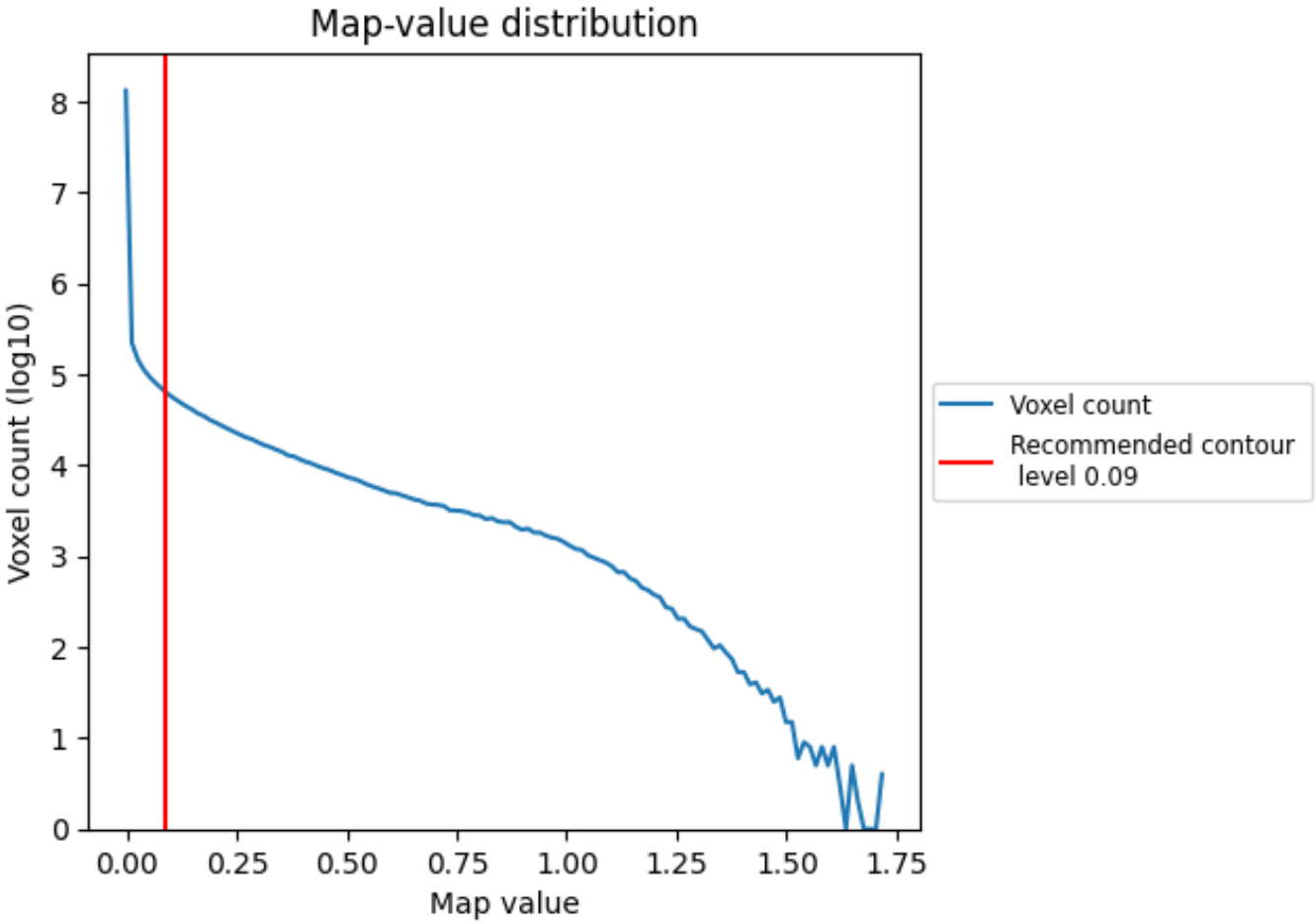
## 6.6 Mask visualisation (i)

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

# 7 Map analysis

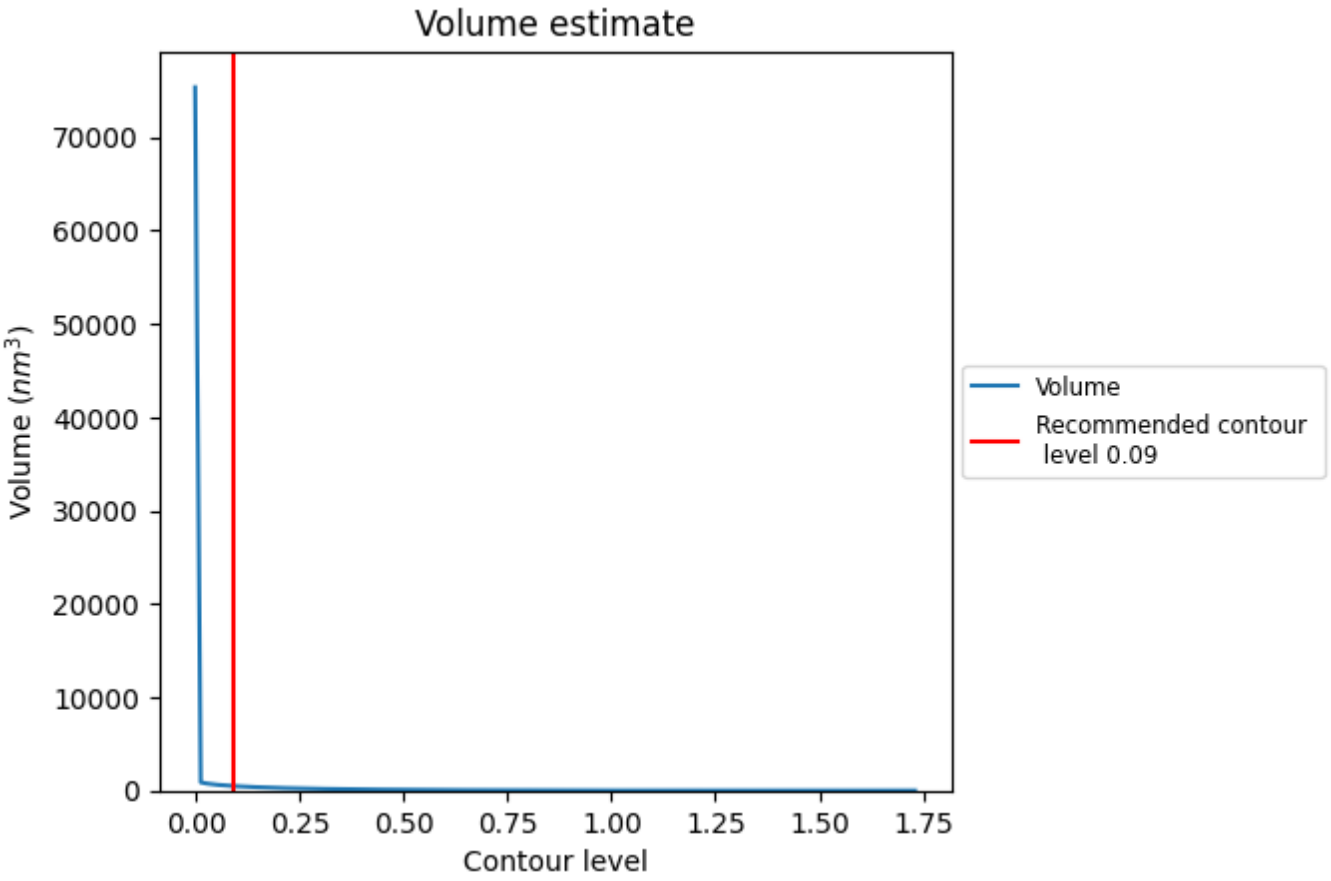
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution




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

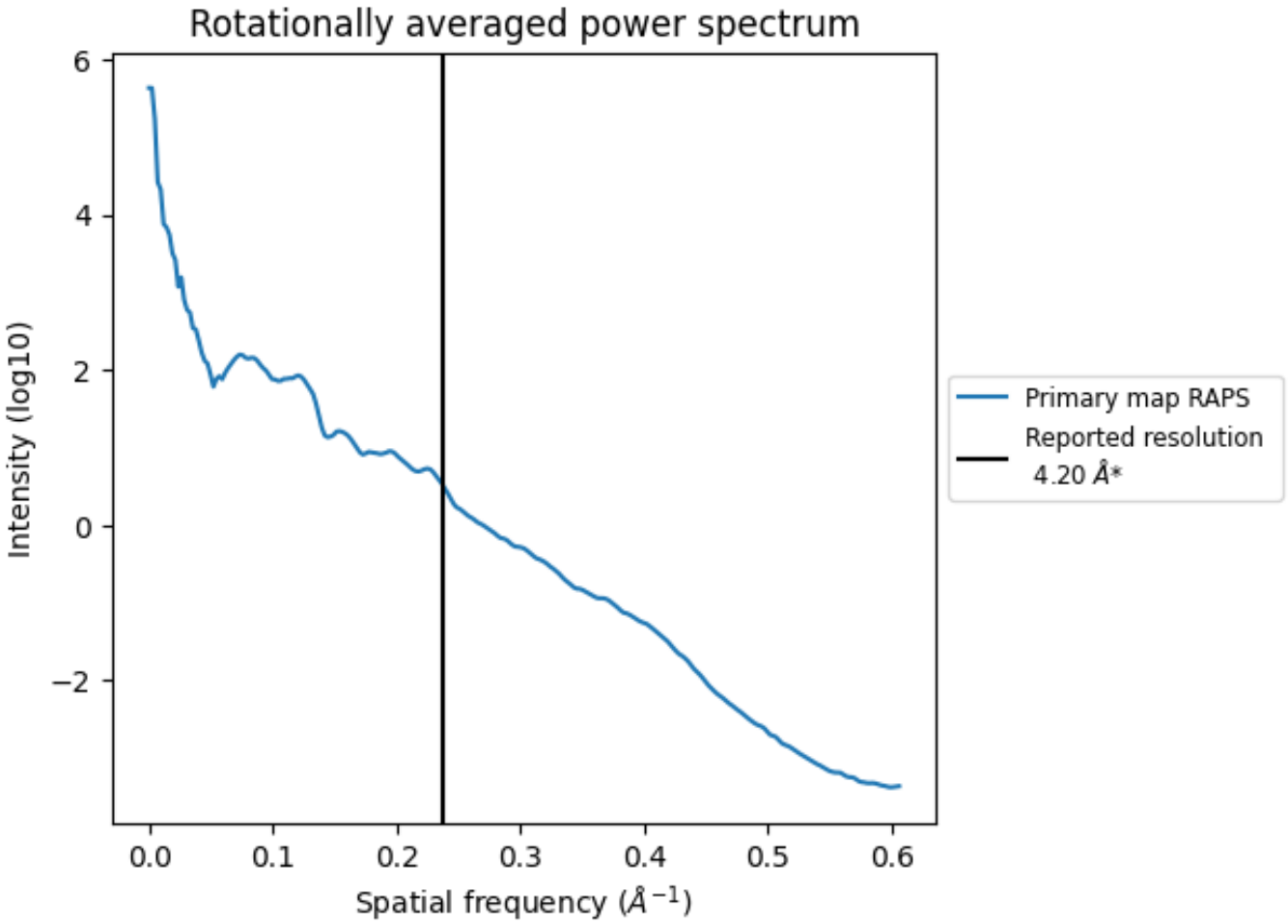
## 7.2 Volume estimate (i)




The volume at the recommended contour level is 489 $nm^3$; this corresponds to an approximate mass of 442 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)

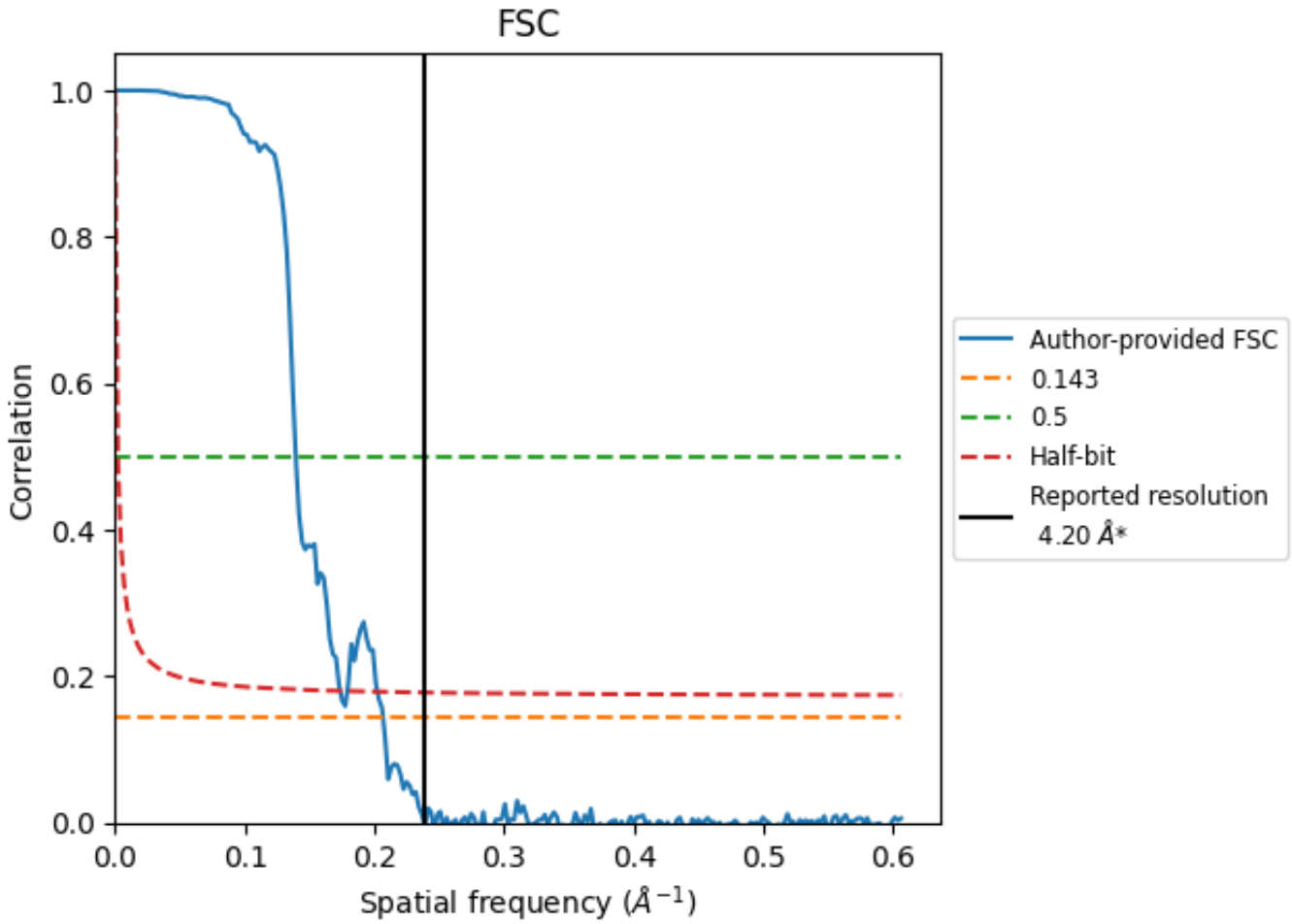



*Reported resolution corresponds to spatial frequency of 0.238 Å$^{-1}$

# 8 Fourier-Shell correlation

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

## 8.1 FSC




*Reported resolution corresponds to spatial frequency of 0.238 Å$^{-1}$

## 8.2 Resolution estimates (i)

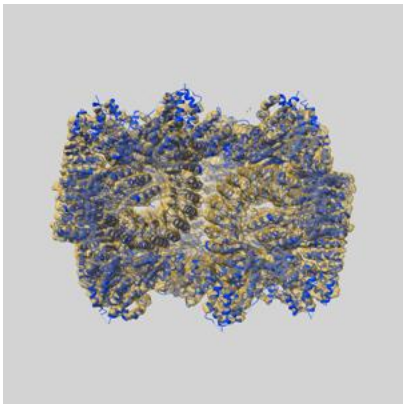
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 4.20 | - | - |
| Author-provided FSC curve | 4.84 | 7.17 | 5.76 |
| Unmasked-calculated* | - | - | - |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 4.84 differs from the reported value 4.2 by more than 10 %

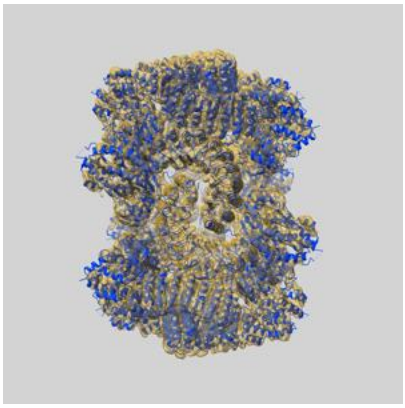
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-23302 and PDB model 7LFH. Per-residue inclusion information can be found in section 3 on page 6.

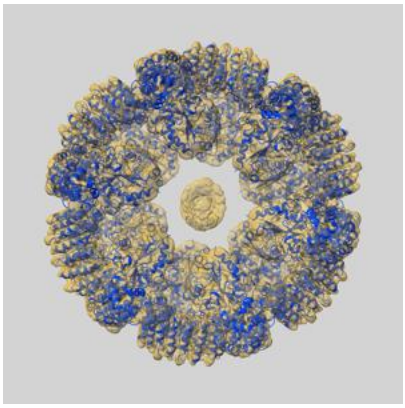
## 9.1 Map-model overlay



X



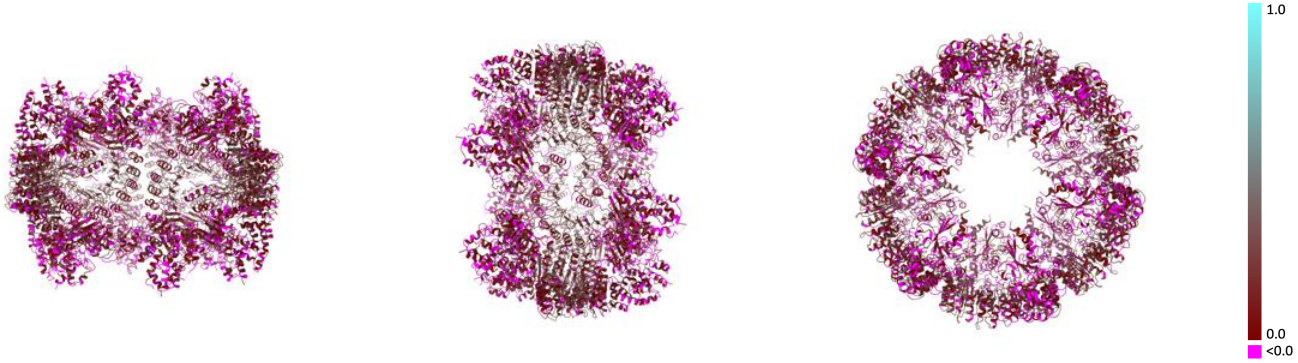
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.09 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.

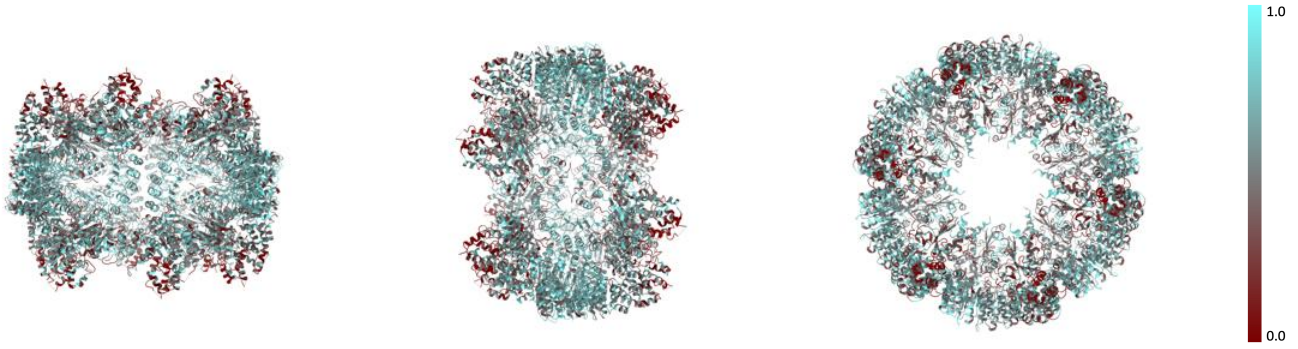
## 9.2 Q-score mapped to coordinate model (i)




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.

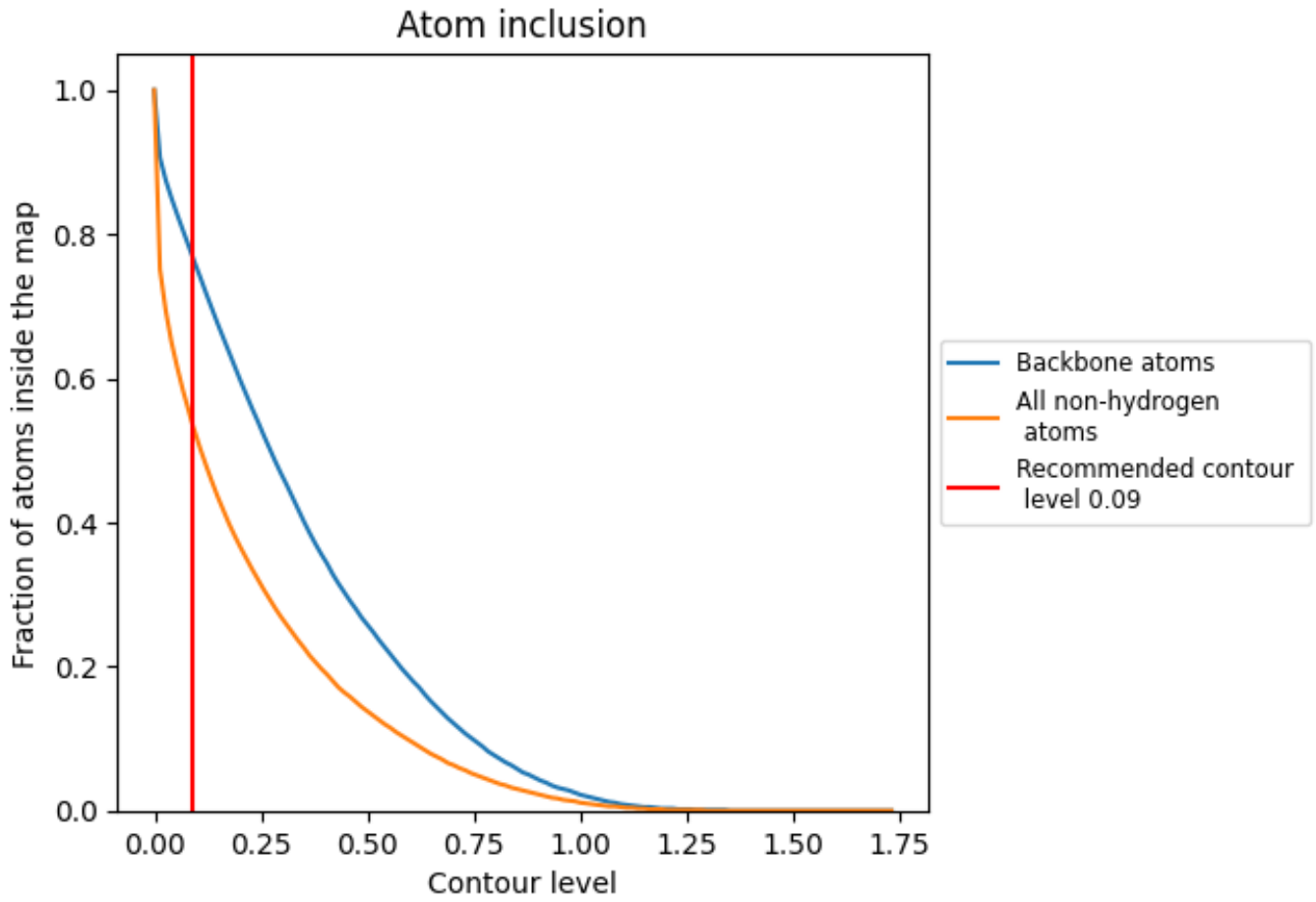
## 9.3 Atom inclusion mapped to coordinate model (i)




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 (0.09).

## 9.4 Atom inclusion (i)




At the recommended contour level, 77% of all backbone atoms, 53% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.09) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.5320 | 0.1150 |
| A | 0.5310 | 0.1180 |
| B | 0.5360 | 0.1150 |
| C | 0.5020 | 0.1070 |
| D | 0.5540 | 0.1190 |
| E | 0.5160 | 0.1140 |
| F | 0.5430 | 0.1160 |
| G | 0.5200 | 0.1120 |
| H | 0.5280 | 0.1140 |
| I | 0.5180 | 0.1140 |
| J | 0.5430 | 0.1160 |
| K | 0.5370 | 0.1180 |
| L | 0.5600 | 0.1170 |