wwPDB EM Validation Summary Report (i)

May 27, 2024 – 03:14 PM JST

PDB ID	:	7DZY
EMDB ID	:	EMD-30921
Title	:	Spike protein from SARS-CoV2 with Fab fragment of enhancing antibody 2490
Authors	:	Liu, Y.; Soh, W.T.; Li, S.; Kishikawa, J.; Hirose, M.; Kato, T.; Standley, D.; Okada, M.; Arase, H.
Deposited on	:	2021-01-26
Resolution	:	3.60 Å(reported)
Based on initial models	:	5K8M, 7KEW

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 (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:

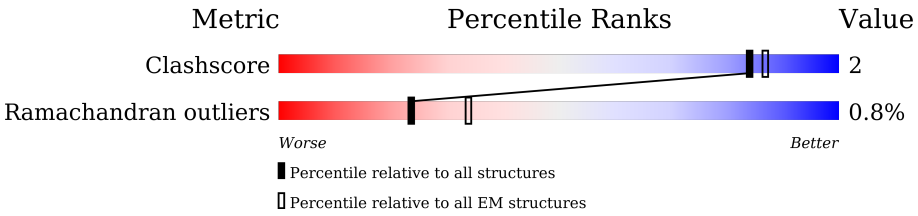
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.60 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

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	1249	68% 88% · 10%
1	B	1249	73% 88% · 10%
1	C	1249	71% 88% · 10%
2	H	225	100% 99% ·
2	M	225	100% 99% ·
2	O	225	100% 99% ·
3	L	266	80% 80% 20%
3	N	266	80% 80% 20%
3	P	266	80% 80% 20%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 18708 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	1121	Total 4484	C 2242	N 1121	O 1121	0	0
1	B	1121	Total 4484	C 2242	N 1121	O 1121	0	0
1	C	1121	Total 4484	C 2242	N 1121	O 1121	0	0

There are 210 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	GLN	-	expression tag	UNP P0DTC2
A	15	CYS	-	expression tag	UNP P0DTC2
A	16	VAL	-	expression tag	UNP P0DTC2
A	17	ASN	-	expression tag	UNP P0DTC2
A	18	LEU	-	expression tag	UNP P0DTC2
A	19	THR	-	expression tag	UNP P0DTC2
A	20	THR	-	expression tag	UNP P0DTC2
A	21	ARG	-	expression tag	UNP P0DTC2
A	22	THR	-	expression tag	UNP P0DTC2
A	23	GLN	-	expression tag	UNP P0DTC2
A	24	LEU	-	expression tag	UNP P0DTC2
A	25	PRO	-	expression tag	UNP P0DTC2
A	26	PRO	-	expression tag	UNP P0DTC2
A	614	GLY	ASP	engineered mutation	UNP P0DTC2
A	682	GLY	ARG	engineered mutation	UNP P0DTC2
A	683	SER	ARG	engineered mutation	UNP P0DTC2
A	685	GLY	ARG	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1212	GLY	-	expression tag	UNP P0DTC2
A	1213	SER	-	expression tag	UNP P0DTC2
A	1214	GLY	-	expression tag	UNP P0DTC2
A	1215	ARG	-	expression tag	UNP P0DTC2
A	1216	GLU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1217	ASN	-	expression tag	UNP P0DTC2
A	1218	LEU	-	expression tag	UNP P0DTC2
A	1219	TYR	-	expression tag	UNP P0DTC2
A	1220	PHE	-	expression tag	UNP P0DTC2
A	1221	GLN	-	expression tag	UNP P0DTC2
A	1222	GLY	-	expression tag	UNP P0DTC2
A	1223	GLY	-	expression tag	UNP P0DTC2
A	1224	GLY	-	expression tag	UNP P0DTC2
A	1225	GLY	-	expression tag	UNP P0DTC2
A	1226	SER	-	expression tag	UNP P0DTC2
A	1227	GLY	-	expression tag	UNP P0DTC2
A	1228	TYR	-	expression tag	UNP P0DTC2
A	1229	ILE	-	expression tag	UNP P0DTC2
A	1230	PRO	-	expression tag	UNP P0DTC2
A	1231	GLU	-	expression tag	UNP P0DTC2
A	1232	ALA	-	expression tag	UNP P0DTC2
A	1233	PRO	-	expression tag	UNP P0DTC2
A	1234	ARG	-	expression tag	UNP P0DTC2
A	1235	ASP	-	expression tag	UNP P0DTC2
A	1236	GLY	-	expression tag	UNP P0DTC2
A	1237	GLN	-	expression tag	UNP P0DTC2
A	1238	ALA	-	expression tag	UNP P0DTC2
A	1239	TYR	-	expression tag	UNP P0DTC2
A	1240	VAL	-	expression tag	UNP P0DTC2
A	1241	ARG	-	expression tag	UNP P0DTC2
A	1242	LYS	-	expression tag	UNP P0DTC2
A	1243	ASP	-	expression tag	UNP P0DTC2
A	1244	GLY	-	expression tag	UNP P0DTC2
A	1245	GLU	-	expression tag	UNP P0DTC2
A	1246	TRP	-	expression tag	UNP P0DTC2
A	1247	VAL	-	expression tag	UNP P0DTC2
A	1248	LEU	-	expression tag	UNP P0DTC2
A	1249	LEU	-	expression tag	UNP P0DTC2
A	1250	SER	-	expression tag	UNP P0DTC2
A	1251	THR	-	expression tag	UNP P0DTC2
A	1252	PHE	-	expression tag	UNP P0DTC2
A	1253	LEU	-	expression tag	UNP P0DTC2
A	1254	GLY	-	expression tag	UNP P0DTC2
A	1255	HIS	-	expression tag	UNP P0DTC2
A	1256	HIS	-	expression tag	UNP P0DTC2
A	1257	HIS	-	expression tag	UNP P0DTC2
A	1258	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1259	HIS	-	expression tag	UNP P0DTC2
A	1260	HIS	-	expression tag	UNP P0DTC2
A	1261	HIS	-	expression tag	UNP P0DTC2
A	1262	HIS	-	expression tag	UNP P0DTC2
B	14	GLN	-	expression tag	UNP P0DTC2
B	15	CYS	-	expression tag	UNP P0DTC2
B	16	VAL	-	expression tag	UNP P0DTC2
B	17	ASN	-	expression tag	UNP P0DTC2
B	18	LEU	-	expression tag	UNP P0DTC2
B	19	THR	-	expression tag	UNP P0DTC2
B	20	THR	-	expression tag	UNP P0DTC2
B	21	ARG	-	expression tag	UNP P0DTC2
B	22	THR	-	expression tag	UNP P0DTC2
B	23	GLN	-	expression tag	UNP P0DTC2
B	24	LEU	-	expression tag	UNP P0DTC2
B	25	PRO	-	expression tag	UNP P0DTC2
B	26	PRO	-	expression tag	UNP P0DTC2
B	614	GLY	ASP	engineered mutation	UNP P0DTC2
B	682	GLY	ARG	engineered mutation	UNP P0DTC2
B	683	SER	ARG	engineered mutation	UNP P0DTC2
B	685	GLY	ARG	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1212	GLY	-	expression tag	UNP P0DTC2
B	1213	SER	-	expression tag	UNP P0DTC2
B	1214	GLY	-	expression tag	UNP P0DTC2
B	1215	ARG	-	expression tag	UNP P0DTC2
B	1216	GLU	-	expression tag	UNP P0DTC2
B	1217	ASN	-	expression tag	UNP P0DTC2
B	1218	LEU	-	expression tag	UNP P0DTC2
B	1219	TYR	-	expression tag	UNP P0DTC2
B	1220	PHE	-	expression tag	UNP P0DTC2
B	1221	GLN	-	expression tag	UNP P0DTC2
B	1222	GLY	-	expression tag	UNP P0DTC2
B	1223	GLY	-	expression tag	UNP P0DTC2
B	1224	GLY	-	expression tag	UNP P0DTC2
B	1225	GLY	-	expression tag	UNP P0DTC2
B	1226	SER	-	expression tag	UNP P0DTC2
B	1227	GLY	-	expression tag	UNP P0DTC2
B	1228	TYR	-	expression tag	UNP P0DTC2
B	1229	ILE	-	expression tag	UNP P0DTC2
B	1230	PRO	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1231	GLU	-	expression tag	UNP P0DTC2
B	1232	ALA	-	expression tag	UNP P0DTC2
B	1233	PRO	-	expression tag	UNP P0DTC2
B	1234	ARG	-	expression tag	UNP P0DTC2
B	1235	ASP	-	expression tag	UNP P0DTC2
B	1236	GLY	-	expression tag	UNP P0DTC2
B	1237	GLN	-	expression tag	UNP P0DTC2
B	1238	ALA	-	expression tag	UNP P0DTC2
B	1239	TYR	-	expression tag	UNP P0DTC2
B	1240	VAL	-	expression tag	UNP P0DTC2
B	1241	ARG	-	expression tag	UNP P0DTC2
B	1242	LYS	-	expression tag	UNP P0DTC2
B	1243	ASP	-	expression tag	UNP P0DTC2
B	1244	GLY	-	expression tag	UNP P0DTC2
B	1245	GLU	-	expression tag	UNP P0DTC2
B	1246	TRP	-	expression tag	UNP P0DTC2
B	1247	VAL	-	expression tag	UNP P0DTC2
B	1248	LEU	-	expression tag	UNP P0DTC2
B	1249	LEU	-	expression tag	UNP P0DTC2
B	1250	SER	-	expression tag	UNP P0DTC2
B	1251	THR	-	expression tag	UNP P0DTC2
B	1252	PHE	-	expression tag	UNP P0DTC2
B	1253	LEU	-	expression tag	UNP P0DTC2
B	1254	GLY	-	expression tag	UNP P0DTC2
B	1255	HIS	-	expression tag	UNP P0DTC2
B	1256	HIS	-	expression tag	UNP P0DTC2
B	1257	HIS	-	expression tag	UNP P0DTC2
B	1258	HIS	-	expression tag	UNP P0DTC2
B	1259	HIS	-	expression tag	UNP P0DTC2
B	1260	HIS	-	expression tag	UNP P0DTC2
B	1261	HIS	-	expression tag	UNP P0DTC2
B	1262	HIS	-	expression tag	UNP P0DTC2
C	14	GLN	-	expression tag	UNP P0DTC2
C	15	CYS	-	expression tag	UNP P0DTC2
C	16	VAL	-	expression tag	UNP P0DTC2
C	17	ASN	-	expression tag	UNP P0DTC2
C	18	LEU	-	expression tag	UNP P0DTC2
C	19	THR	-	expression tag	UNP P0DTC2
C	20	THR	-	expression tag	UNP P0DTC2
C	21	ARG	-	expression tag	UNP P0DTC2
C	22	THR	-	expression tag	UNP P0DTC2
C	23	GLN	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	24	LEU	-	expression tag	UNP P0DTC2
C	25	PRO	-	expression tag	UNP P0DTC2
C	26	PRO	-	expression tag	UNP P0DTC2
C	614	GLY	ASP	engineered mutation	UNP P0DTC2
C	682	GLY	ARG	engineered mutation	UNP P0DTC2
C	683	SER	ARG	engineered mutation	UNP P0DTC2
C	685	GLY	ARG	engineered mutation	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	1212	GLY	-	expression tag	UNP P0DTC2
C	1213	SER	-	expression tag	UNP P0DTC2
C	1214	GLY	-	expression tag	UNP P0DTC2
C	1215	ARG	-	expression tag	UNP P0DTC2
C	1216	GLU	-	expression tag	UNP P0DTC2
C	1217	ASN	-	expression tag	UNP P0DTC2
C	1218	LEU	-	expression tag	UNP P0DTC2
C	1219	TYR	-	expression tag	UNP P0DTC2
C	1220	PHE	-	expression tag	UNP P0DTC2
C	1221	GLN	-	expression tag	UNP P0DTC2
C	1222	GLY	-	expression tag	UNP P0DTC2
C	1223	GLY	-	expression tag	UNP P0DTC2
C	1224	GLY	-	expression tag	UNP P0DTC2
C	1225	GLY	-	expression tag	UNP P0DTC2
C	1226	SER	-	expression tag	UNP P0DTC2
C	1227	GLY	-	expression tag	UNP P0DTC2
C	1228	TYR	-	expression tag	UNP P0DTC2
C	1229	ILE	-	expression tag	UNP P0DTC2
C	1230	PRO	-	expression tag	UNP P0DTC2
C	1231	GLU	-	expression tag	UNP P0DTC2
C	1232	ALA	-	expression tag	UNP P0DTC2
C	1233	PRO	-	expression tag	UNP P0DTC2
C	1234	ARG	-	expression tag	UNP P0DTC2
C	1235	ASP	-	expression tag	UNP P0DTC2
C	1236	GLY	-	expression tag	UNP P0DTC2
C	1237	GLN	-	expression tag	UNP P0DTC2
C	1238	ALA	-	expression tag	UNP P0DTC2
C	1239	TYR	-	expression tag	UNP P0DTC2
C	1240	VAL	-	expression tag	UNP P0DTC2
C	1241	ARG	-	expression tag	UNP P0DTC2
C	1242	LYS	-	expression tag	UNP P0DTC2
C	1243	ASP	-	expression tag	UNP P0DTC2
C	1244	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1245	GLU	-	expression tag	UNP P0DTC2
C	1246	TRP	-	expression tag	UNP P0DTC2
C	1247	VAL	-	expression tag	UNP P0DTC2
C	1248	LEU	-	expression tag	UNP P0DTC2
C	1249	LEU	-	expression tag	UNP P0DTC2
C	1250	SER	-	expression tag	UNP P0DTC2
C	1251	THR	-	expression tag	UNP P0DTC2
C	1252	PHE	-	expression tag	UNP P0DTC2
C	1253	LEU	-	expression tag	UNP P0DTC2
C	1254	GLY	-	expression tag	UNP P0DTC2
C	1255	HIS	-	expression tag	UNP P0DTC2
C	1256	HIS	-	expression tag	UNP P0DTC2
C	1257	HIS	-	expression tag	UNP P0DTC2
C	1258	HIS	-	expression tag	UNP P0DTC2
C	1259	HIS	-	expression tag	UNP P0DTC2
C	1260	HIS	-	expression tag	UNP P0DTC2
C	1261	HIS	-	expression tag	UNP P0DTC2
C	1262	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Fab Heavy chain of enhancing antibody 2490.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	H	225	Total	C	N	O	0	0
			900	450	225	225		
2	M	225	Total	C	N	O	0	0
			900	450	225	225		
2	O	225	Total	C	N	O	0	0
			900	450	225	225		

- Molecule 3 is a protein called Fab light chain of enhancing antibody 2490.

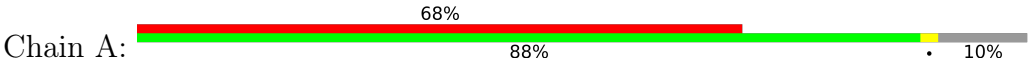
Mol	Chain	Residues	Atoms				AltConf	Trace
3	L	213	Total	C	N	O	0	0
			852	426	213	213		
3	N	213	Total	C	N	O	0	0
			852	426	213	213		
3	P	213	Total	C	N	O	0	0
			852	426	213	213		

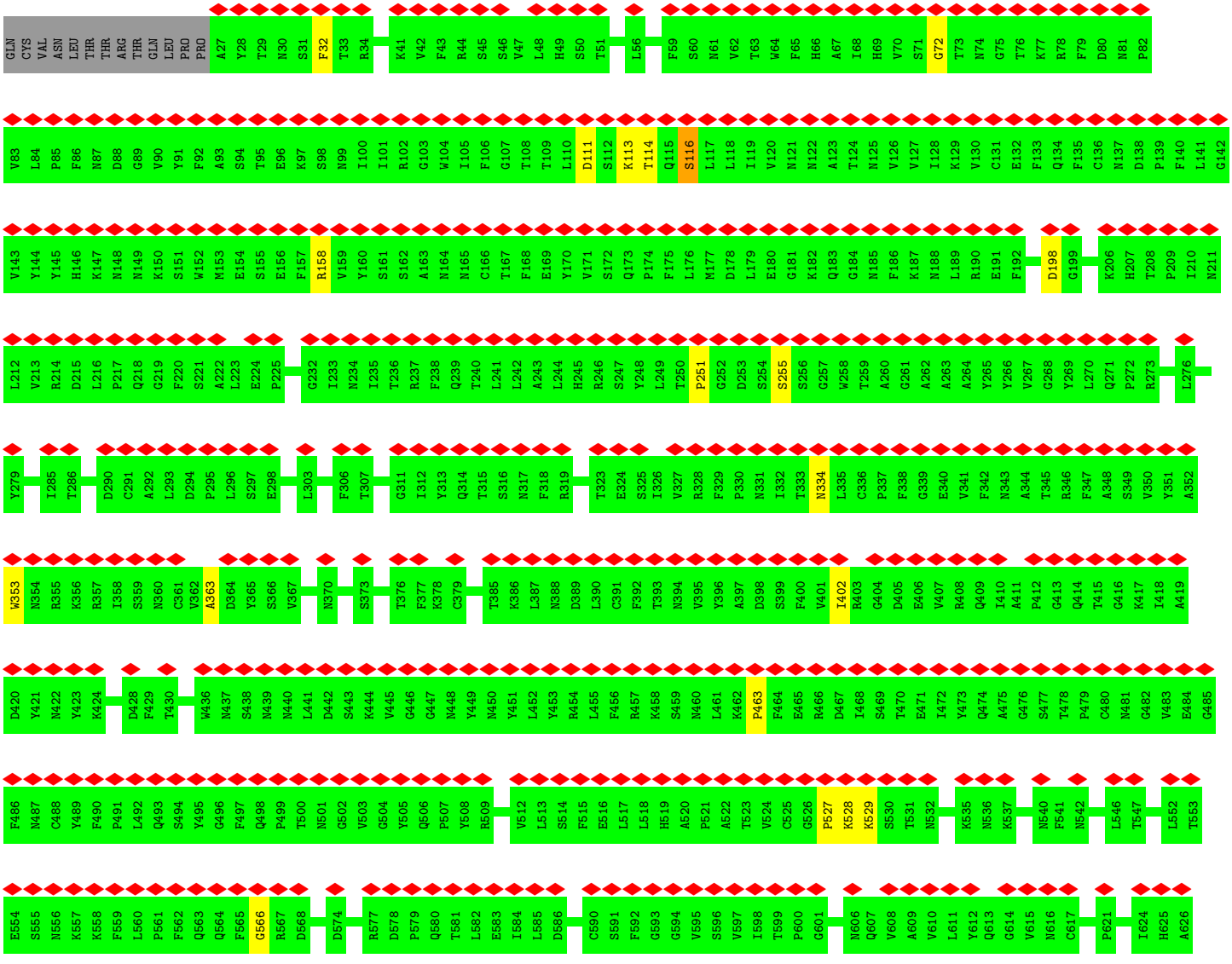
3 Residue-property plots (i)

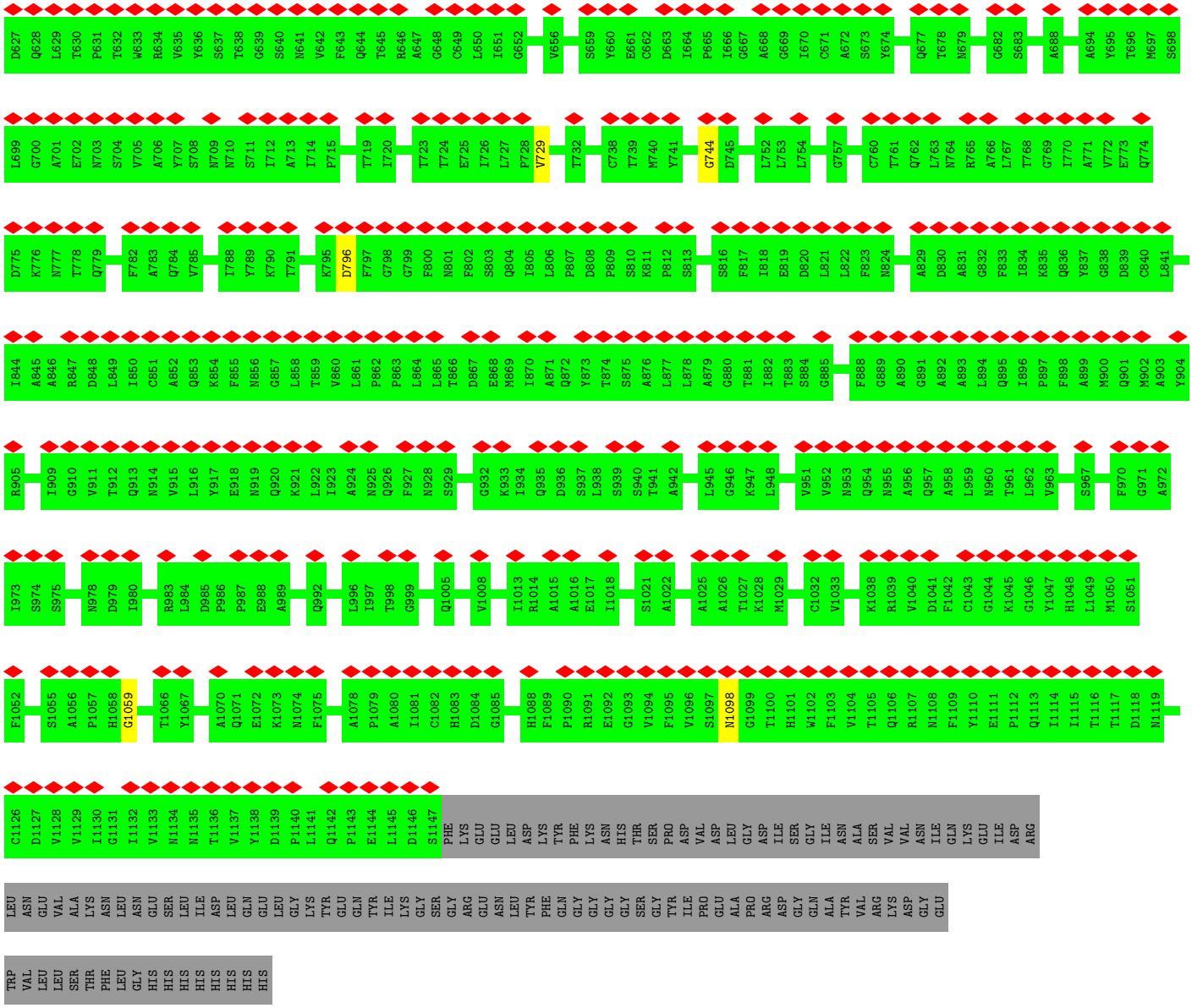
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Spike glycoprotein

Chain A:

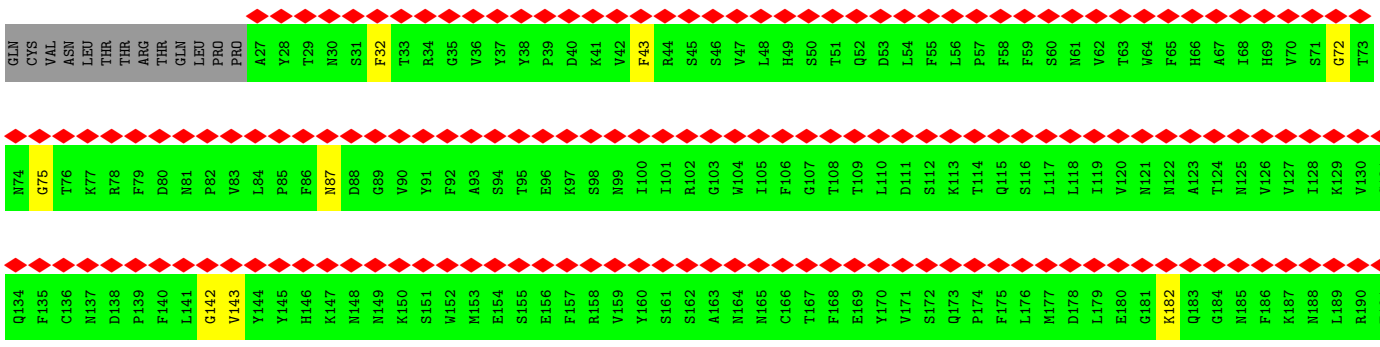


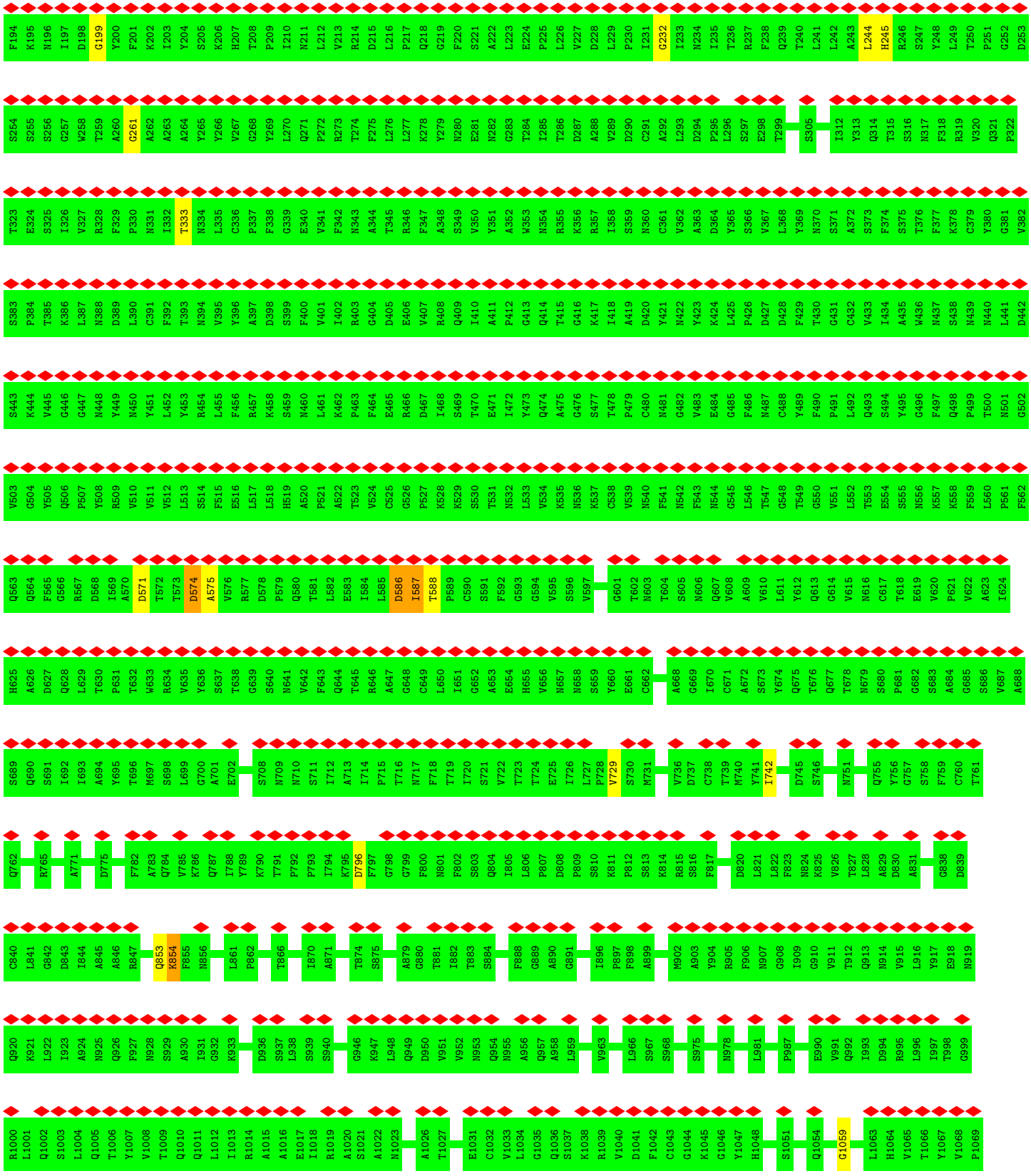


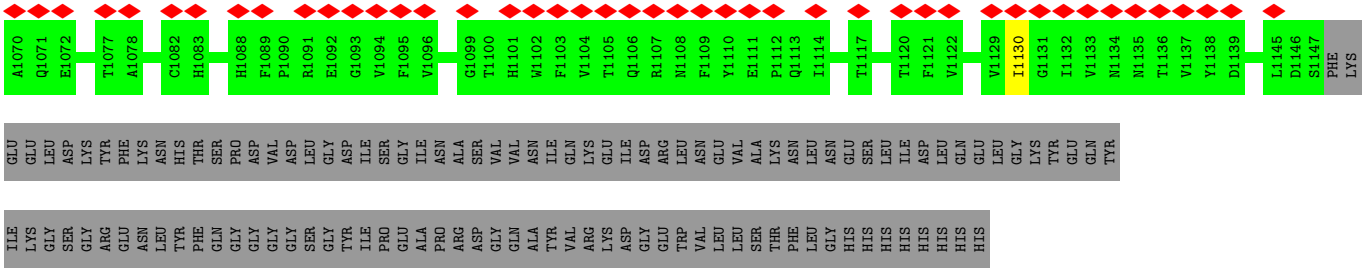


- Molecule 1: Spike glycoprotein

Chain B:

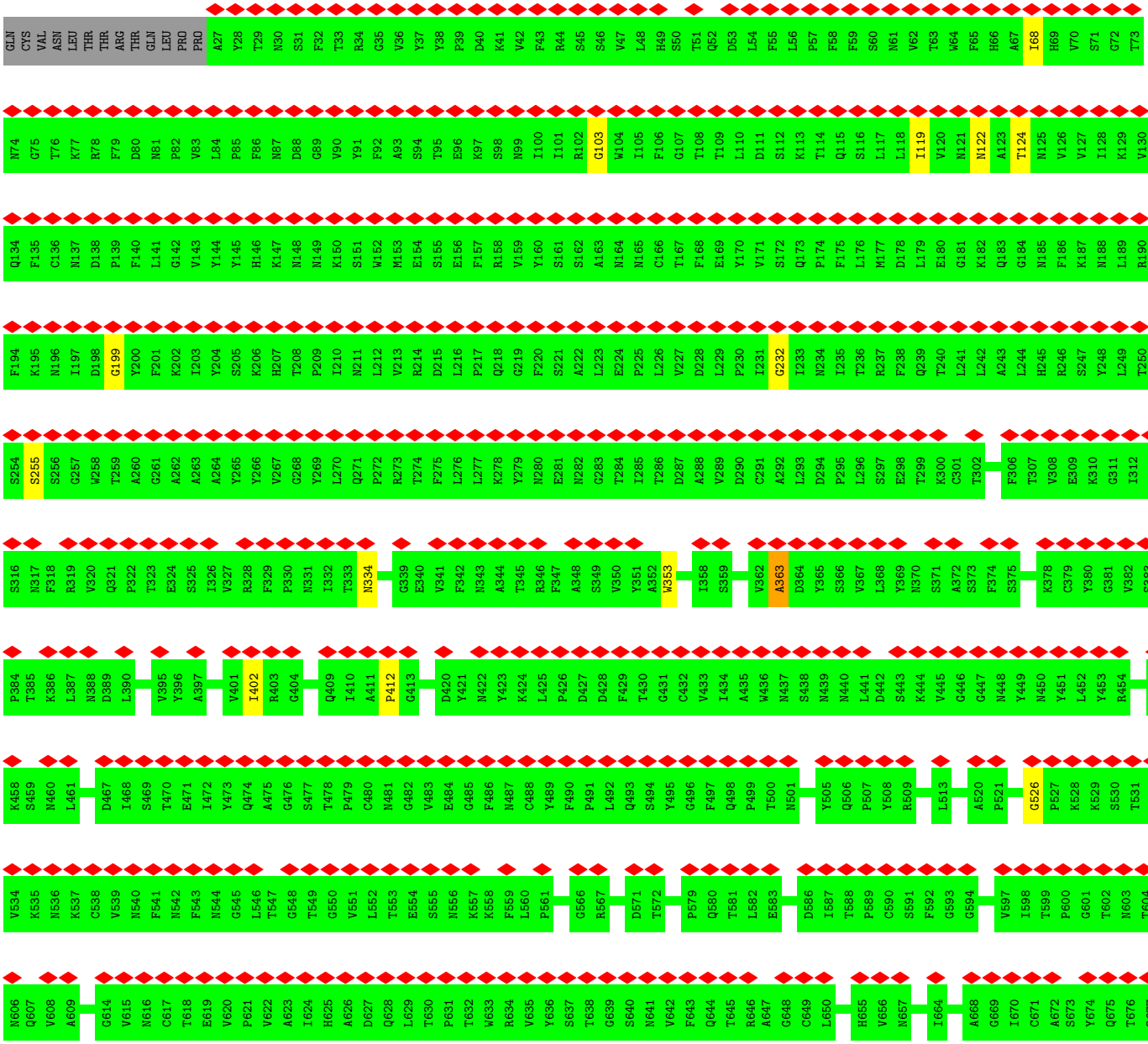


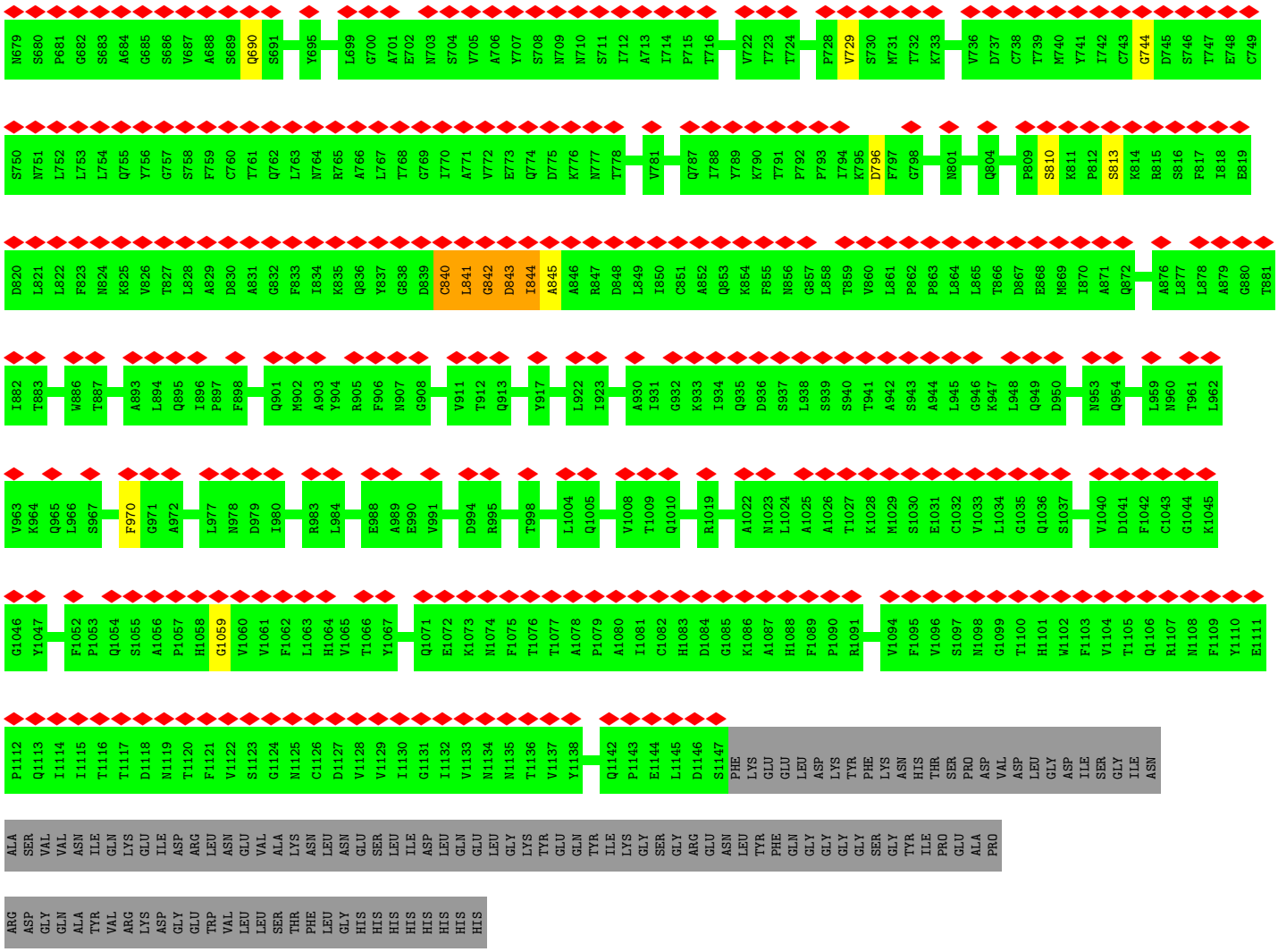

F194 K195 N196 I197 D198 G199 Y200 F201 K202 I203 Y204 S205 K206 H207 T208 P209 I210 N211 L212 V213 R214 D215 L216 P217 Q218 G219 F220 S221 A222 L223 E224 P225 L226 V227 D228 L229 P230 I231 G232 I233 N234 I235 T236 R237 F238 Q239 T240 L241 L242 A243 L244 H245 R246 S247 Y248 L249 T250 P251 G252 D253
S254 S255 S256 C257 W258 T259 A260 G261 A262 A263 A264 Y265 Y266 V267 G268 Y269 L270 Q271 P272 R273 T274 F275 L276 L277 K278 Y279 N280 E281 N282 G283 T284 I285 T286 D287 A288 V289 D290 C291 A292 L293 D294 P295 L296 S297 E298 T299 S305 I312 Y313 Q314 T315 S316 N317 F318 R319 V320 Q321 P322
T323 E324 S325 I326 V327 R328 F329 P330 N331 I332 T333 N334 L335 C336 P337 F338 G339 E340 V341 P342 N343 A344 T345 R346 F347 A348 S349 V350 Y351 A352 W353 N354 R355 K356 R357 I358 S359 N360 C361 V362 A363 D364 Y365 S366 V367 L368 Y369 N370 S371 A372 S373 F374 S375 T376 F377 K378 C379 Y380 G381 V382
S383 P384 T385 K386 L387 N388 D389 L390 C391 F392 T393 N394 V395 Y396 A397 D398 S399 F400 V401 I402 R403 G404 D405 E406 V407 R408 Q409 I410 A411 P412 G413 Q414 T415 G416 K417 I418 A419 D420 Y421 N422 Y423 K424 L425 P426 D427 D428 F429 T430 G431 C432 V433 I434 A435 W436 N437 S438 N439 N440 L441 D442
S443 K444 V445 G446 G447 N448 Y449 N450 Y451 L452 Y453 R454 L455 F456 R457 K458 S459 N460 L461 K462 P463 F464 E465 R466 D467 I468 S469 T470 E471 I472 Y473 Q474 A475 G476 S477 T478 P479 C480 N481 G482 V483 E484 G485 F486 N487 C488 Y489 F490 P491 L492 Q493 S494 Y495 G496 F497 Q498 P499 T500 N501 G502
V503 G504 Y505 Q506 P507 Y508 R509 V510 V511 V512 L513 S514 F515 E516 L517 L518 H519 A520 P521 A522 T523 V524 C525 G526 P527 K528 K529 S530 T531 N532 L533 V534 K535 N536 K537 C538 V539 N540 F541 N542 F543 N544 G545 L546 T547 G548 T549 G550 V551 L552 T553 E554 S555 N556 K557 K558 F559 L560 P561 F562
Q563 Q564 F565 G566 R567 D568 I569 A570 D571 T572 T573 D574 A575 V576 R577 D578 P579 Q580 T581 L582 E583 I584 L585 D586 I587 T588 P589 C590 S591 F592 G593 G594 V595 S596 V597 G601 T602 N603 T604 S605 N606 Q607 V608 A609 V610 L611 Y612 Q613 G614 V615 N616 C617 T618 E619 V620 P621 V622 A623 I624
H625 A626 D627 Q628 L629 T630 P631 T632 W633 R634 V635 Y636 S637 T638 G639 S640 N641 V642 F643 Q644 T645 R646 A647 G648 C649 L650 I651 G652 A653 E654 H655 V656 N657 N658 S659 Y660 E661 C662 A668 G669 I670 C671 A672 S673 Y674 Q675 T676 Q677 T678 N679 S680 P681 G682 S683 A684 G685 S686 V687 A688
S689 Q690 S691 I692 I693 A694 Y695 T696 M697 S698 L699 G700 A701 E702 S708 N709 N710 S711 I712 A713 I714 P715 T716 N717 F718 T719 I720 S721 V722 T723 T724 E725 I726 L727 P728 V729 S730 M731 V736 D737 C738 T739 M740 Y741 I742 D745 S746 N751 Q755 Y756 G757 S758 F759 C760 T761
Q762 R765 A771 D775 F782 A783 Q784 V785 K786 Q787 I788 Y789 K790 T791 P792 P793 I794 K795 D796 F797 G798 G799 F800 N801 F802 S803 Q804 I805 L806 P807 D808 P809 S810 K811 P812 S813 K814 R815 S816 F817 D820 L821 L822 F823 N824 K825 V826 T827 L828 A829 D830 A831 G838 D839
C840 L841 G842 D843 I844 A845 A846 R847 Q853 K854 F855 N856 L861 P862 T866 I870 A871 T874 S875 A879 G880 T881 I882 T883 S884 F888 G889 A890 G891 I896 P897 F898 A899 N902 A903 Y904 R905 F906 N907 G908 I909 G910 V911 T912 Q913 N914 Y915 L916 Y917 E918 N919
Q920 K921 L922 I923 A924 N925 Q926 F927 N928 S929 A930 I931 G932 K933 D936 S937 L938 S939 S940 G946 K947 L948 Q949 D950 V951 V952 N953 Q954 N955 A956 Q957 A958 L959 V963 L966 S967 S968 S975 N978 L981 P987 E990 V991 Q992 I993 D994 R995 L996 I997 T998 G999
R1000 L1001 Q1002 S1003 L1004 Q1005 T1006 Y1007 V1008 T1009 Q1010 Q1011 L1012 I1013 R1014 A1015 A1016 E1017 I1018 R1019 A1020 S1021 A1022 N1023 A1026 T1027 E1031 C1032 V1033 L1034 G1035 Q1036 S1037 K1038 R1039 V1040 D1041 F1042 C1043 G1044 K1045 G1046 Y1047 H1048 S1051 Q1054 G1059 L1063 H1064 V1065 T1066 Y1067 V1068 P1069



- Molecule 1: Spike glycoprotein

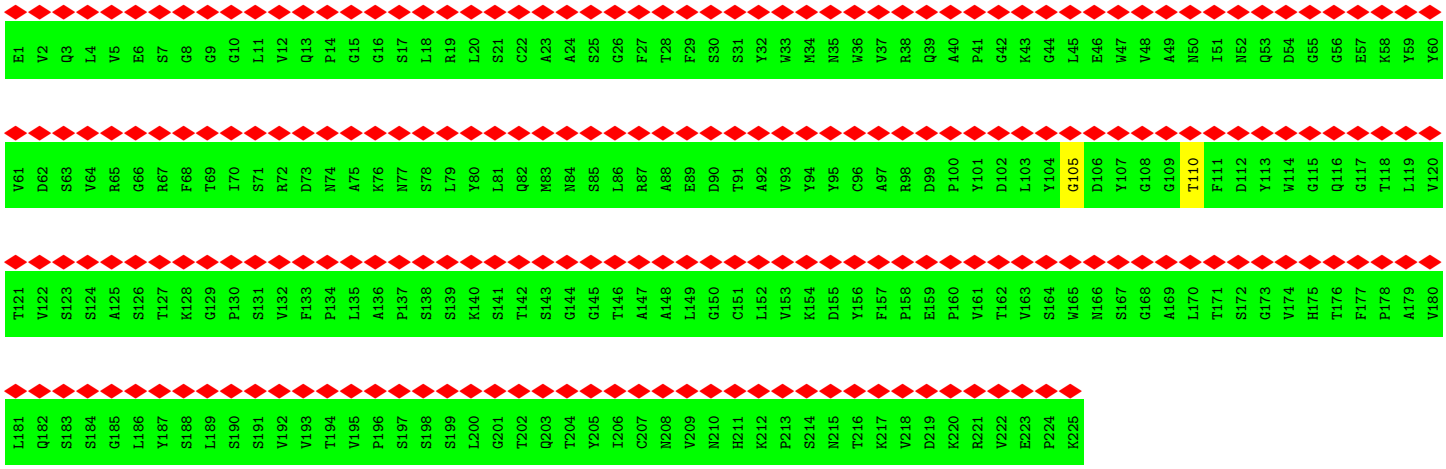
Chain C:





• Molecule 2: Fab Heavy chain of enhancing antibody 2490

Chain H:



• Molecule 2: Fab Heavy chain of enhancing antibody 2490

Chain M:

E1 V2 Q3 L4 V5 E6 S7 G8 G9 G10 L11 V12 Q13 P14 G15 G16 S17 L18 R19 L20 S21 C22 A23 A24 S25 G26 F27 T28 F29 S30 S31 Y32 W33 M34 N35 W36 V37 R38 Q39 A40 P41 G42 K43 G44 L45 E46 W47 V48 A49 N50 I51 N52 Q53 D54 G55 G56 E57 K58 Y59 Y60

V61 D62 S63 V64 R65 G66 R67 F68 T69 I70 S71 R72 D73 N74 A75 K76 N77 S78 L79 Y80 L81 Q82 M83 N84 S85 L86 R87 A88 E89 D90 T91 A92 V93 Y94 Y95 C96 A97 R98 D99 P100 Y101 D102 L103 Y104 G105 D106 Y107 G108 G109 T110 F111 D112 Y113 W114 G115 Q116 G117 T118 L119 V120

T121 V122 S123 S124 A125 S126 T127 K128 G129 P130 S131 V132 F133 P134 L135 A136 P137 S138 S139 K140 S141 T142 S143 G144 G145 T146 A147 A148 L149 G150 C151 L152 V153 K154 D155 Y156 F157 P158 E159 P160 V161 T162 V163 S164 W165 N166 S167 G168 A169 L170 T171 S172 G173 V174 H175 T176 F177 P178 A179 V180

L181 Q182 S183 S184 G185 L186 Y187 S188 L189 S190 S191 V192 V193 T194 V195 P196 S197 S198 S199 L200 G201 T202 Q203 T204 Y205 I206 C207 N208 V209 N210 H211 K212 P213 S214 N215 T216 K217 V218 D219 K220 R221 V222 E223 P224 K225

• Molecule 2: Fab Heavy chain of enhancing antibody 2490

Chain O:

E1 V2 Q3 L4 V5 E6 S7 G8 G9 G10 L11 V12 Q13 P14 G15 G16 S17 L18 R19 L20 S21 C22 A23 A24 S25 G26 F27 T28 F29 S30 S31 Y32 W33 M34 N35 W36 V37 R38 Q39 A40 P41 G42 K43 G44 L45 E46 W47 V48 A49 N50 I51 N52 Q53 D54 G55 G56 E57 K58 Y59 Y60

V61 D62 S63 V64 R65 G66 R67 F68 T69 I70 S71 R72 D73 N74 A75 K76 N77 S78 L79 Y80 L81 Q82 M83 N84 S85 L86 R87 A88 E89 D90 T91 A92 V93 Y94 Y95 C96 A97 R98 D99 P100 Y101 D102 L103 Y104 G105 D106 Y107 G108 G109 T110 F111 D112 Y113 W114 G115 Q116 G117 T118 L119 V120

T121 V122 S123 S124 A125 S126 T127 K128 G129 P130 S131 V132 F133 P134 L135 A136 P137 S138 S139 K140 S141 T142 S143 G144 G145 T146 A147 A148 L149 G150 C151 L152 V153 K154 D155 Y156 F157 P158 E159 P160 V161 T162 V163 S164 W165 N166 S167 G168 A169 L170 T171 S172 G173 V174 H175 T176 F177 P178 A179 V180

L181 Q182 S183 S184 G185 L186 Y187 S188 L189 S190 S191 V192 V193 T194 V195 P196 S197 S198 S199 L200 G201 T202 Q203 T204 Y205 I206 C207 N208 V209 N210 H211 K212 P213 S214 N215 T216 K217 V218 D219 K220 R221 V222 E223 P224 K225

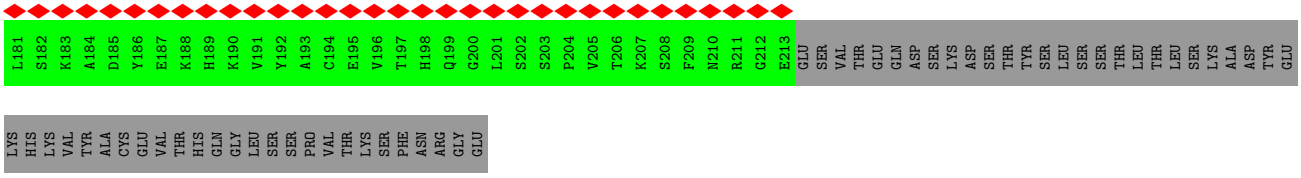
• Molecule 3: Fab light chain of enhancing antibody 2490

Chain L:

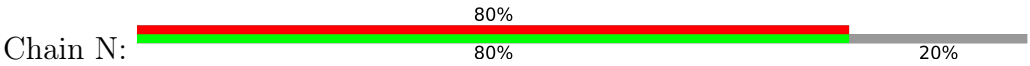
D1 I2 Q3 M4 T5 Q6 S7 P8 S9 T10 L11 S12 A13 S14 V15 G16 D17 R18 V19 T20 I21 T22 C23 R24 A25 S26 Q27 S28 I29 S30 S31 W32 L33 A34 W35 Y36 Q37 Q38 K39 P40 R41 K42 A43 P44 K45 L46 L47 I48 Y49 K50 A51 S52 T53 L54 E55 S56 G57 V58 P59 S60

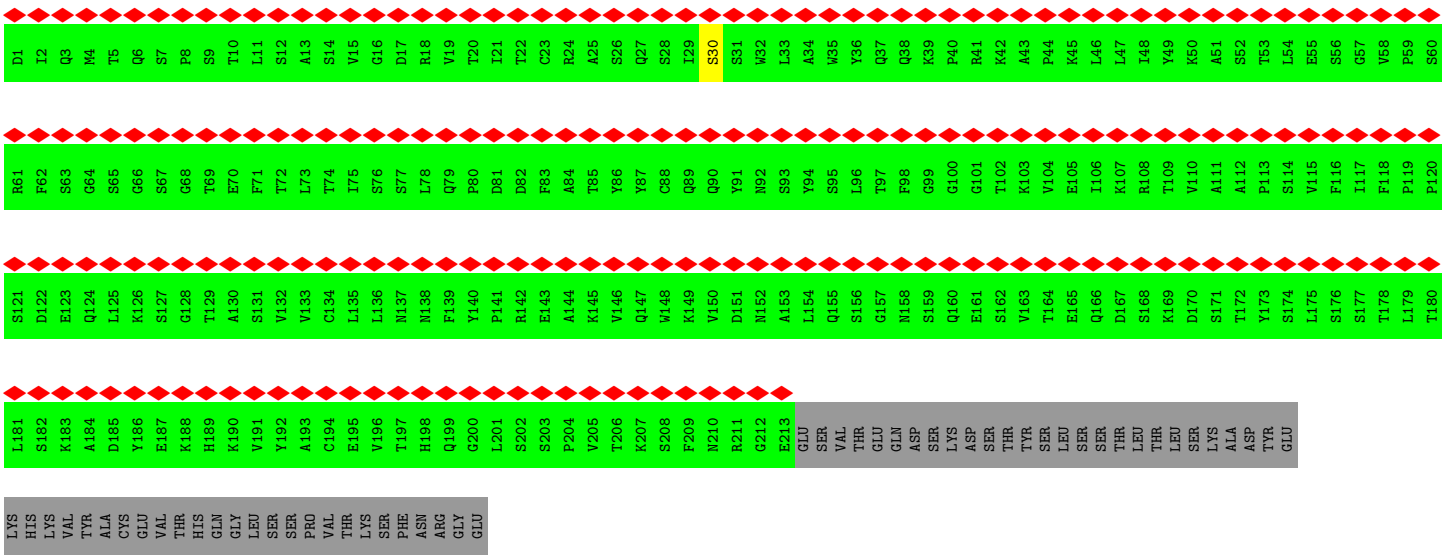
R61 F62 S63 G64 S65 G66 S67 G68 T69 E70 F71 T72 L73 T74 I75 S76 S77 L78 Q79 P80 D81 D82 F83 A84 T85 Y86 Y87 C88 Q89 Q90 Y91 N92 S93 Y94 S95 L96 T97 F98 G99 G100 G101 T102 K103 V104 E105 I106 K107 R108 T109 V110 A111 A112 P113 S114 V115 F116 I117 F118 P119 P120

S121 D122 E123 Q124 L125 K126 S127 G128 T129 A130 S131 V132 V133 C134 L135 L136 N137 N138 F139 Y140 P141 R142 E143 A144 K145 V146 Q147 W148 K149 V150 D151 N152 A153 L154 Q155 S156 G157 N158 S159 Q160 E161 S162 V163 T164 E165 Q166 D167 S168 K169 D170 S171 T172 Y173 S174 L175 S176 S177 T178 L179 T180

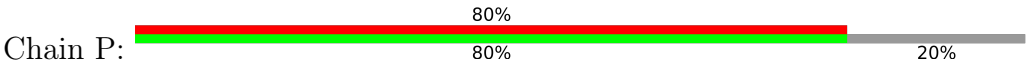


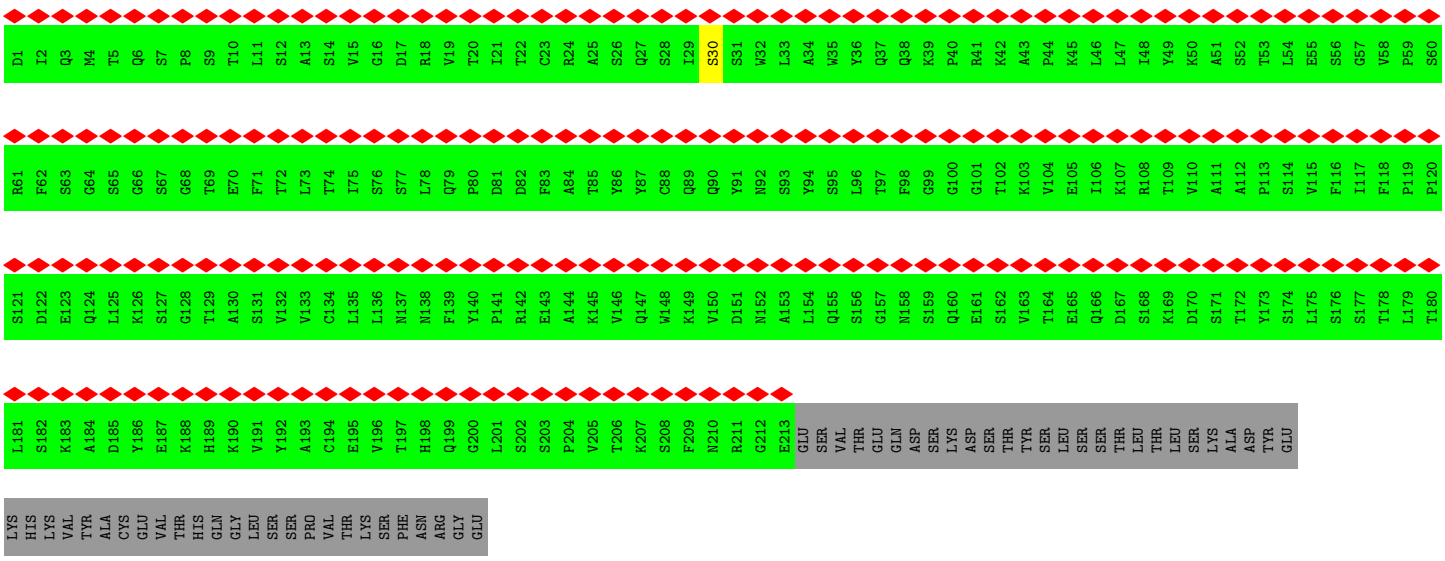
• Molecule 3: Fab light chain of enhancing antibody 2490





• Molecule 3: Fab light chain of enhancing antibody 2490





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	131312	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.491	Depositor
Minimum map value	-0.623	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.042	Depositor
Recommended contour level	0.18	Depositor
Map size (Å)	334.4, 334.4, 334.4	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.88, 0.88, 0.88	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	0.92	0/4483	0.90	5/5602 (0.1%)
1	B	0.94	3/4483 (0.1%)	0.92	7/5602 (0.1%)
1	C	0.97	8/4483 (0.2%)	0.95	16/5602 (0.3%)
2	H	0.95	1/899 (0.1%)	0.88	0/1122
2	M	0.95	1/899 (0.1%)	0.88	0/1122
2	O	0.95	1/899 (0.1%)	0.88	0/1122
3	L	0.88	0/851	0.77	0/1062
3	N	0.88	0/851	0.77	0/1062
3	P	0.88	0/851	0.77	0/1062
All	All	0.94	14/18699 (0.1%)	0.90	28/23358 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	841	LEU	N-CA	9.30	1.65	1.46
1	C	842	GLY	CA-C	8.08	1.64	1.51
1	C	843	ASP	CA-C	7.75	1.73	1.52
1	C	840	CYS	C-N	7.18	1.50	1.34
1	C	841	LEU	C-N	6.91	1.45	1.33

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	574	ASP	C-N-CA	16.36	162.60	121.70
1	C	840	CYS	CA-C-O	-13.98	90.74	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	854	LYS	C-N-CA	-10.90	94.45	121.70
1	B	586	ASP	C-N-CA	9.82	146.26	121.70
1	C	843	ASP	C-N-CA	9.77	146.12	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	853	GLN	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4484	0	1220	7	0
1	B	4484	0	1219	41	0
1	C	4484	0	1220	37	0
2	H	900	0	263	0	0
2	M	900	0	263	0	0
2	O	900	0	263	2	0
3	L	852	0	229	0	0
3	N	852	0	229	0	0
3	P	852	0	229	0	0
All	All	18708	0	5135	54	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 2.

The worst 5 of 54 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:B:587:ILE:CA	1:C:841:LEU:CA	2.55	0.84
1:B:575:ALA:N	1:C:844:ILE:N	2.28	0.81
1:B:182:LYS:O	1:B:261:GLY:HA3	1.82	0.79
1:B:199:GLY:O	1:B:232:GLY:HA2	1.85	0.75
1:C:729:VAL:H	1:C:1059:GLY:HA2	1.57	0.69

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	1119/1249 (90%)	1064 (95%)	43 (4%)	12 (1%)	14	53
1	B	1119/1249 (90%)	1071 (96%)	39 (4%)	9 (1%)	19	59
1	C	1119/1249 (90%)	1050 (94%)	58 (5%)	11 (1%)	15	55
2	H	223/225 (99%)	217 (97%)	5 (2%)	1 (0%)	34	71
2	M	223/225 (99%)	217 (97%)	5 (2%)	1 (0%)	34	71
2	O	223/225 (99%)	217 (97%)	5 (2%)	1 (0%)	34	71
3	L	211/266 (79%)	204 (97%)	6 (3%)	1 (0%)	29	68
3	N	211/266 (79%)	204 (97%)	6 (3%)	1 (0%)	29	68
3	P	211/266 (79%)	204 (97%)	6 (3%)	1 (0%)	29	68
All	All	4659/5220 (89%)	4448 (96%)	173 (4%)	38 (1%)	24	59

5 of 38 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	255	SER
1	A	463	PRO
1	A	528	LYS
1	A	529	LYS
1	A	796	ASP

5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

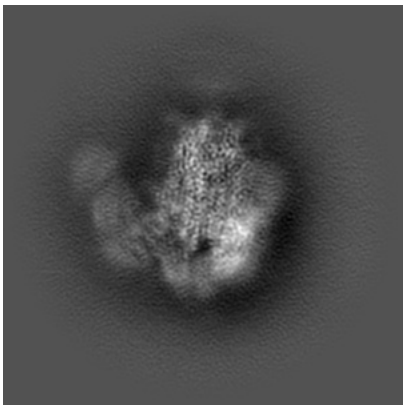
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-30921. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

6.1.1 Primary map



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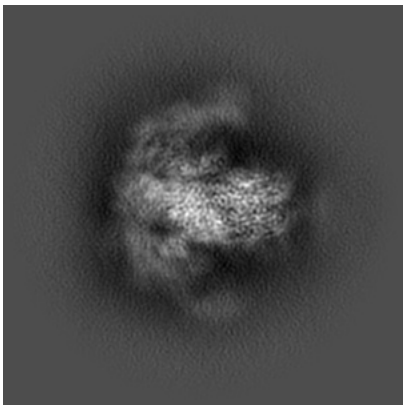

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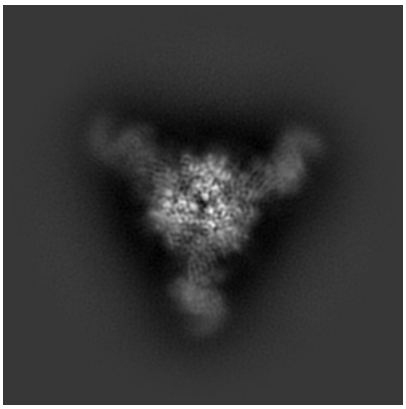
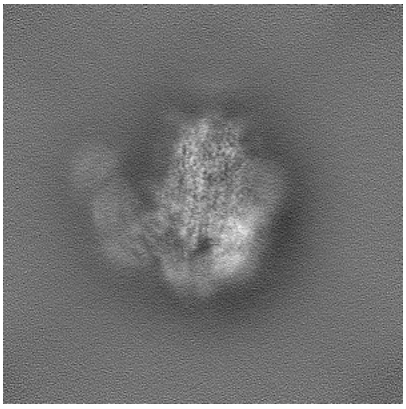


Z

6.1.2 Raw map



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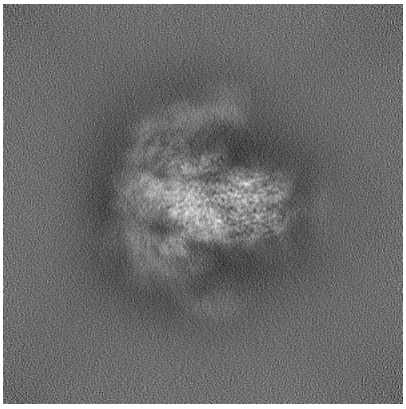

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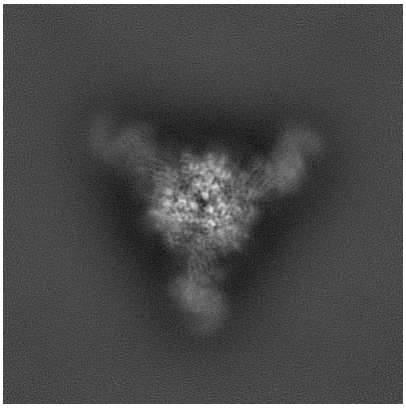
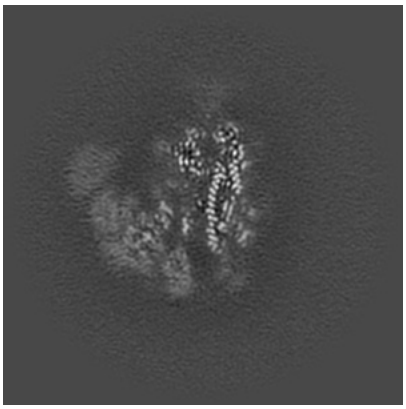


Z

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

6.2 Central slices (i)

6.2.1 Primary map



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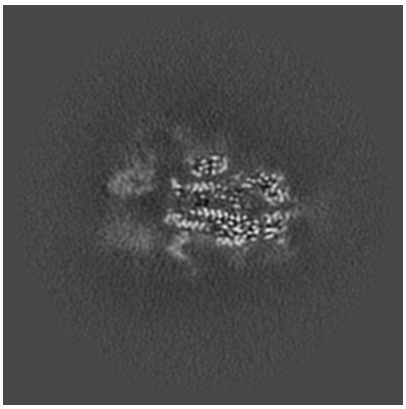

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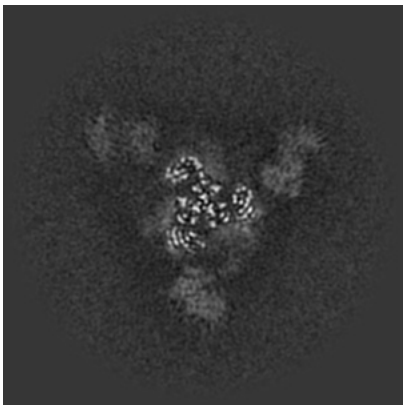

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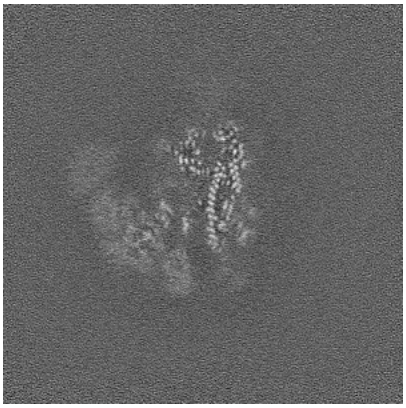
6.2.2 Raw map



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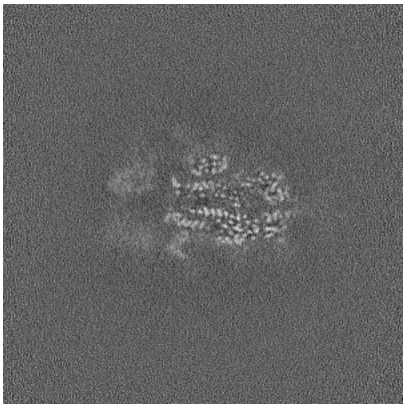

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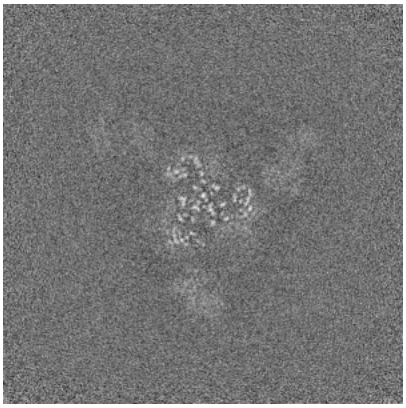
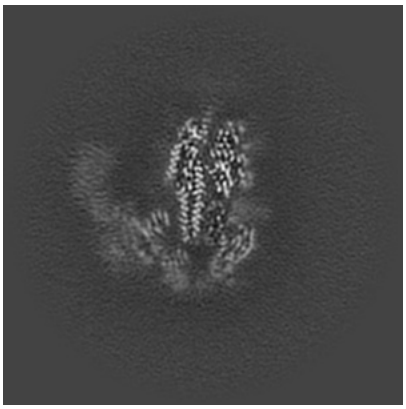


Z Index: 190

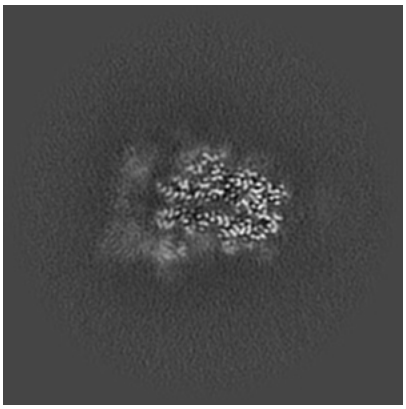
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

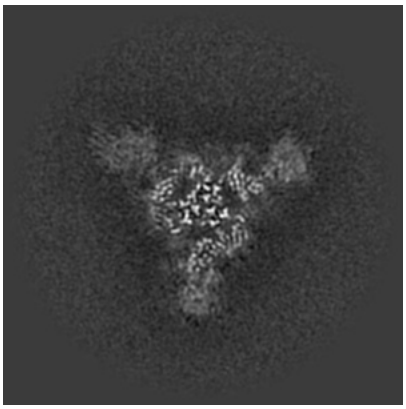
6.3.1 Primary map



X Index: 197

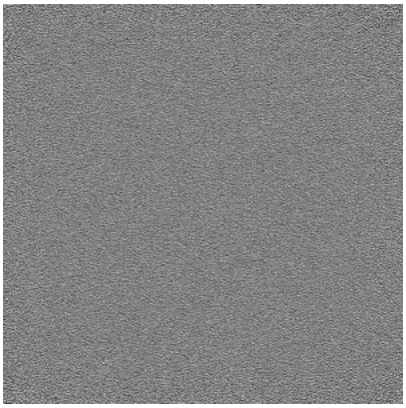


Y Index: 180

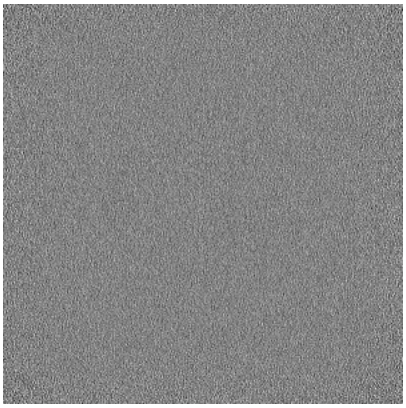


Z Index: 173

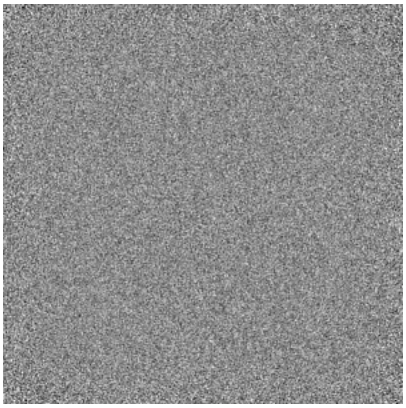
6.3.2 Raw map



X Index: 0



Y Index: 0

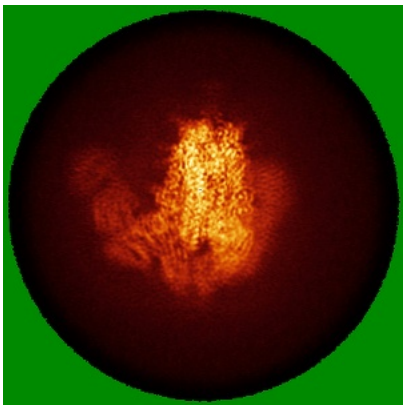


Z Index: 379

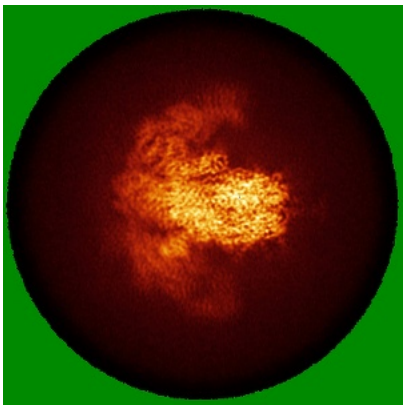
The images above show the largest variance slices of the map in three orthogonal directions.

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

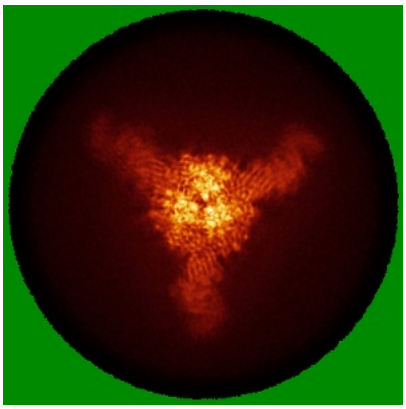
6.4.1 Primary map



X

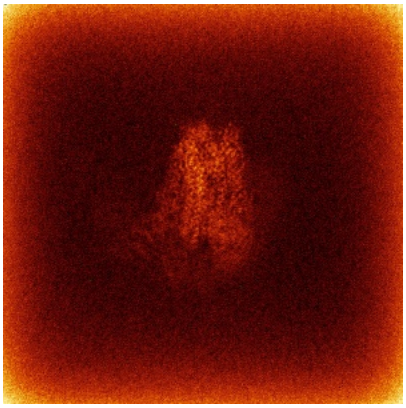


Y

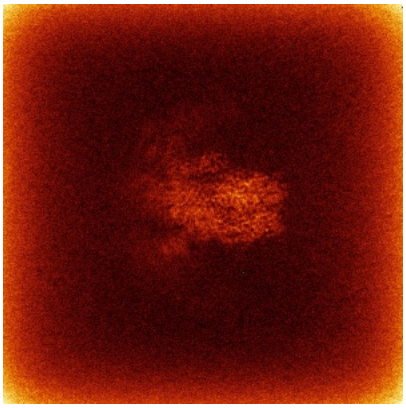


Z

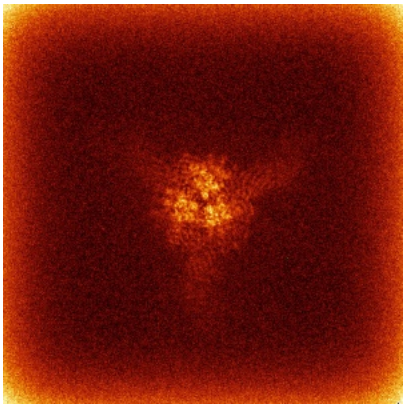
6.4.2 Raw map



X



Y

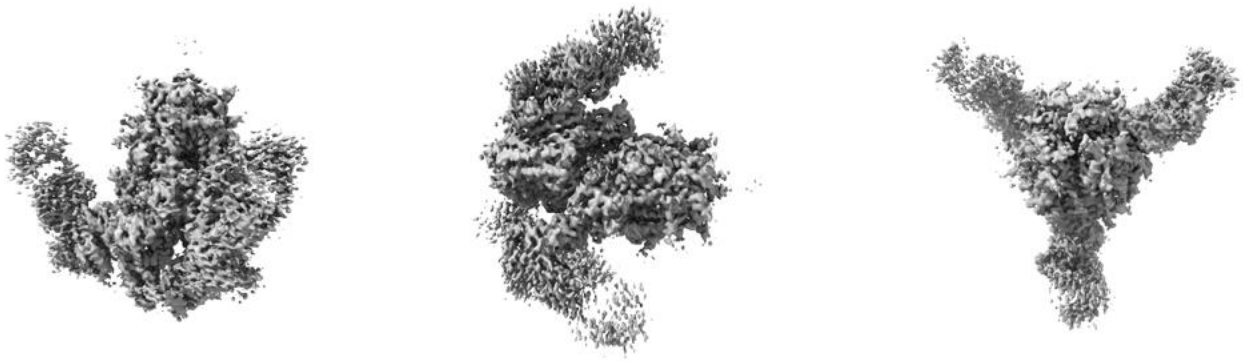


Z

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)

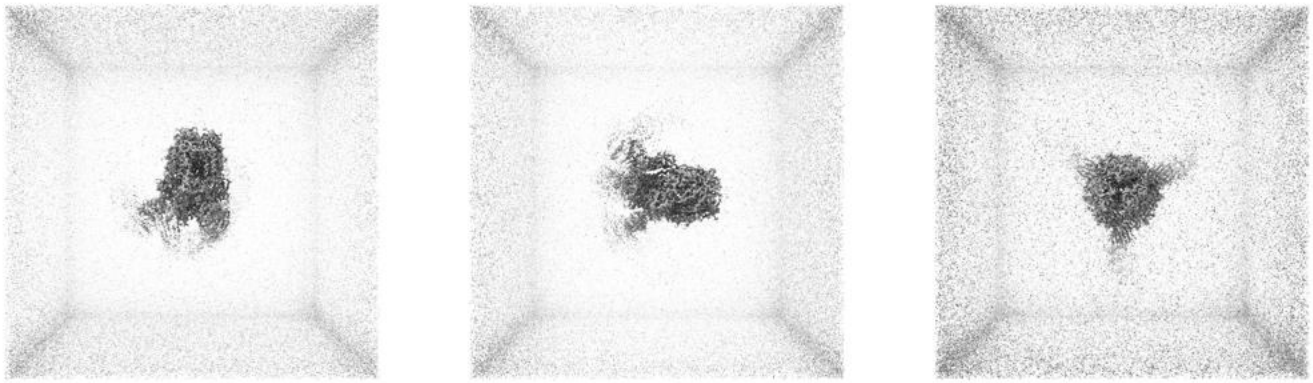
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.18. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

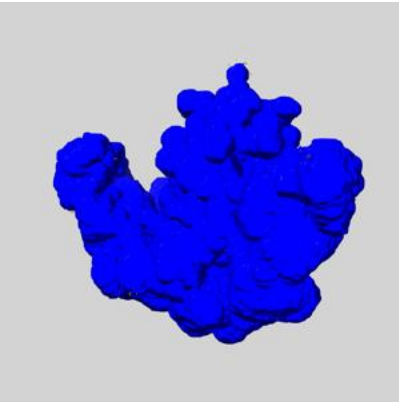
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

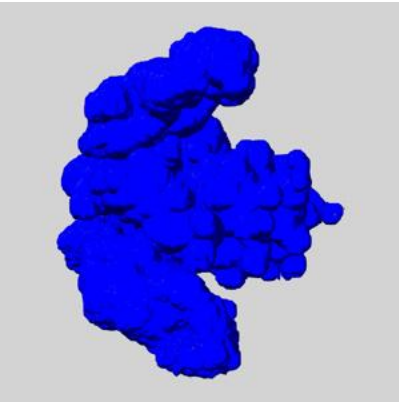
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

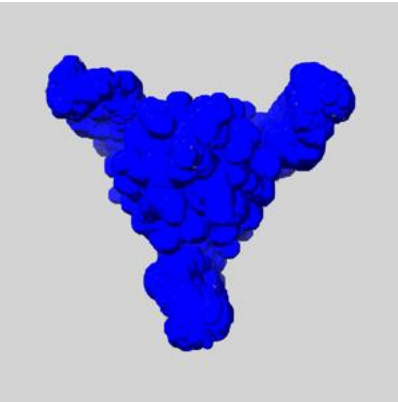
6.6.1 emd_30921_msk_1.map (i)



X



Y

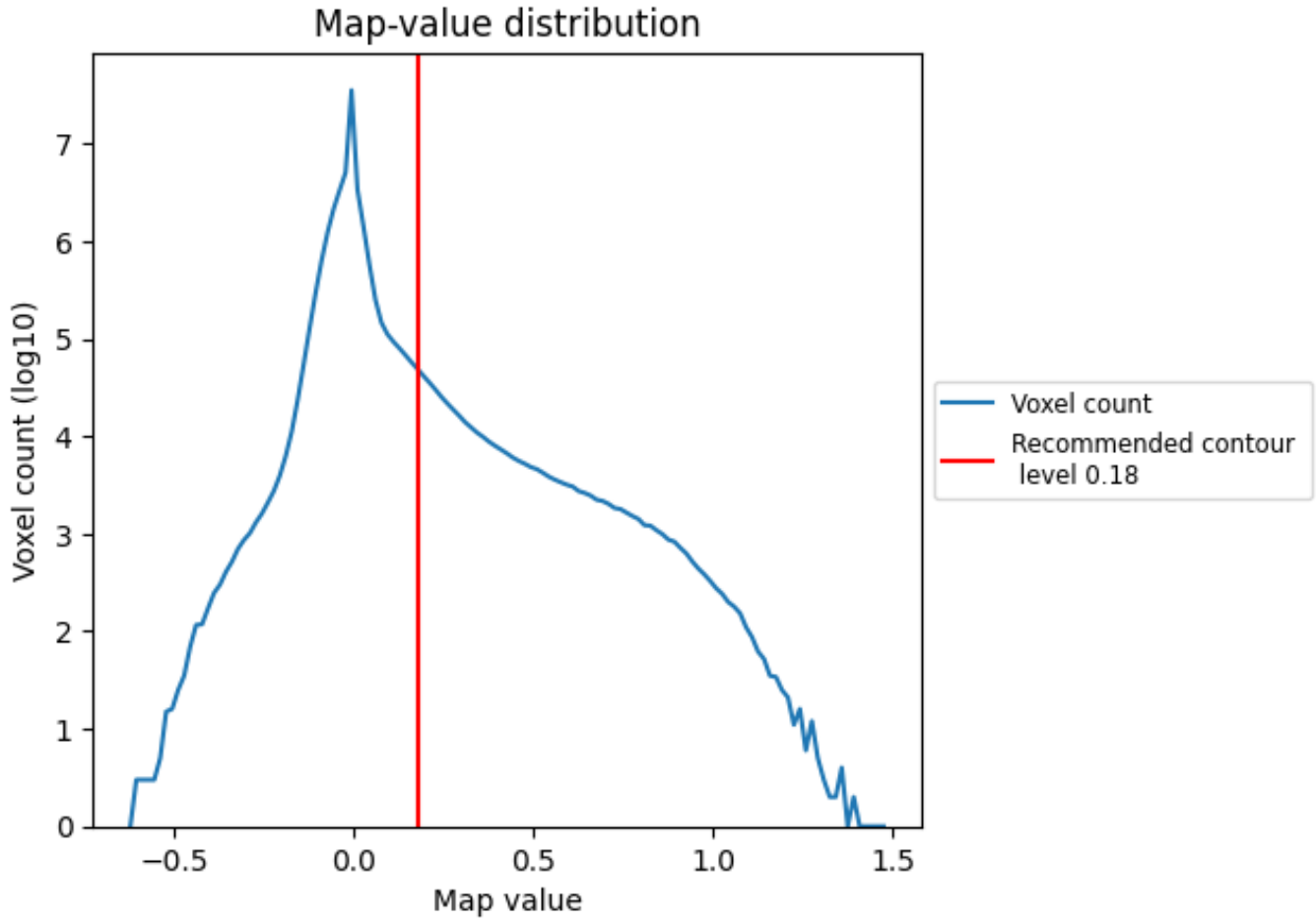


Z

7 Map analysis

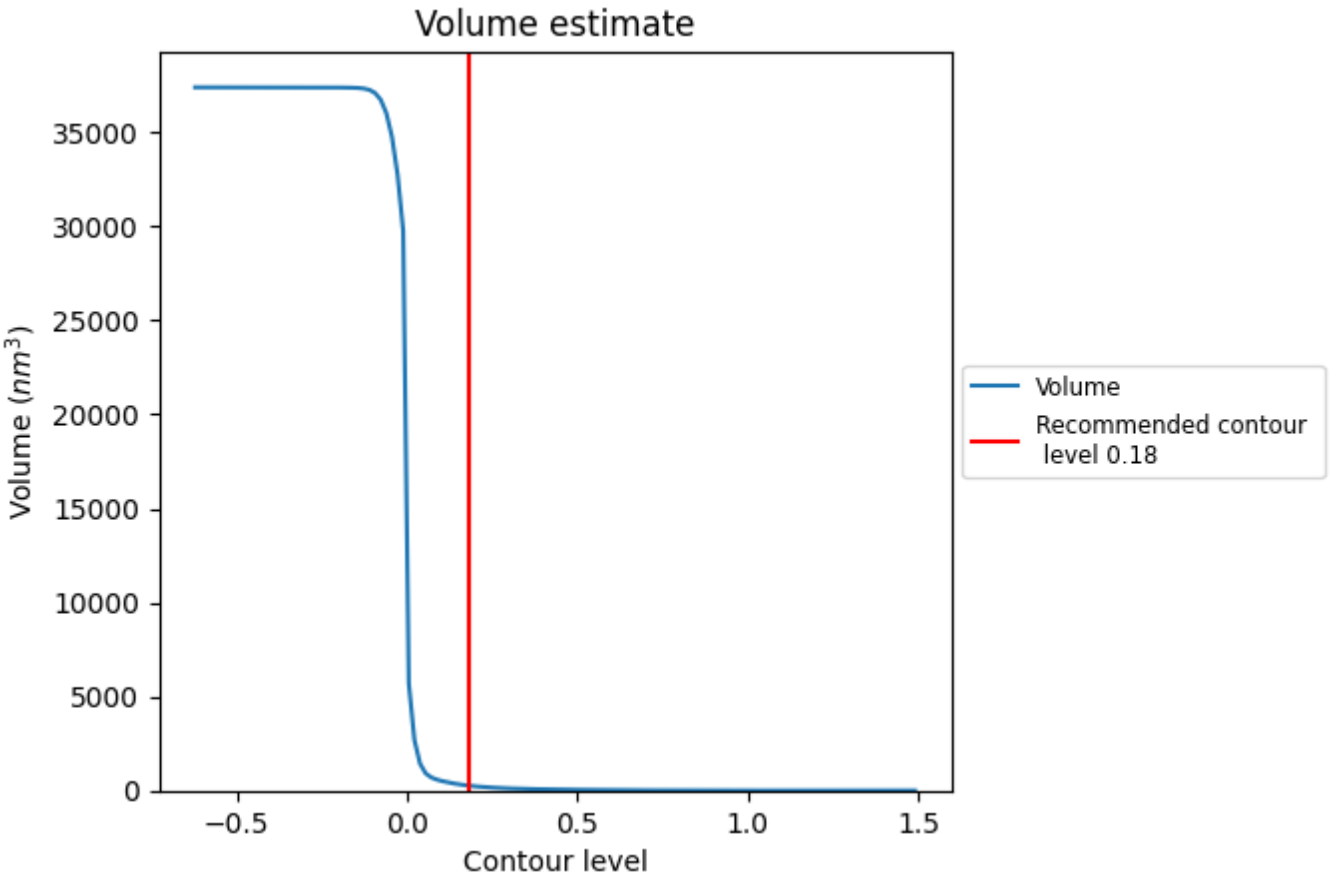
This section contains the results of statistical analysis of the map.

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.

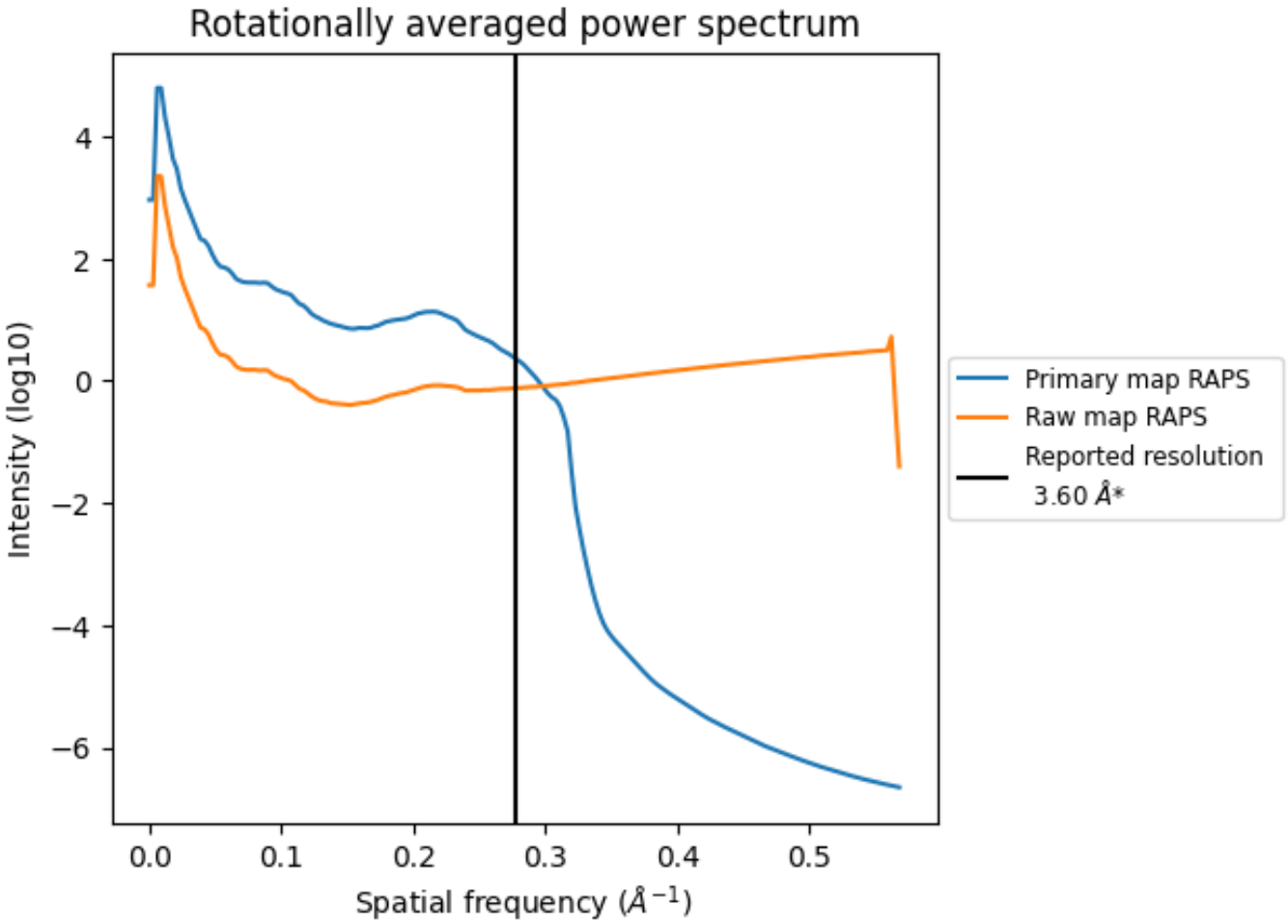
7.2 Volume estimate (i)



The volume at the recommended contour level is 263 nm^3; this corresponds to an approximate mass of 238 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)

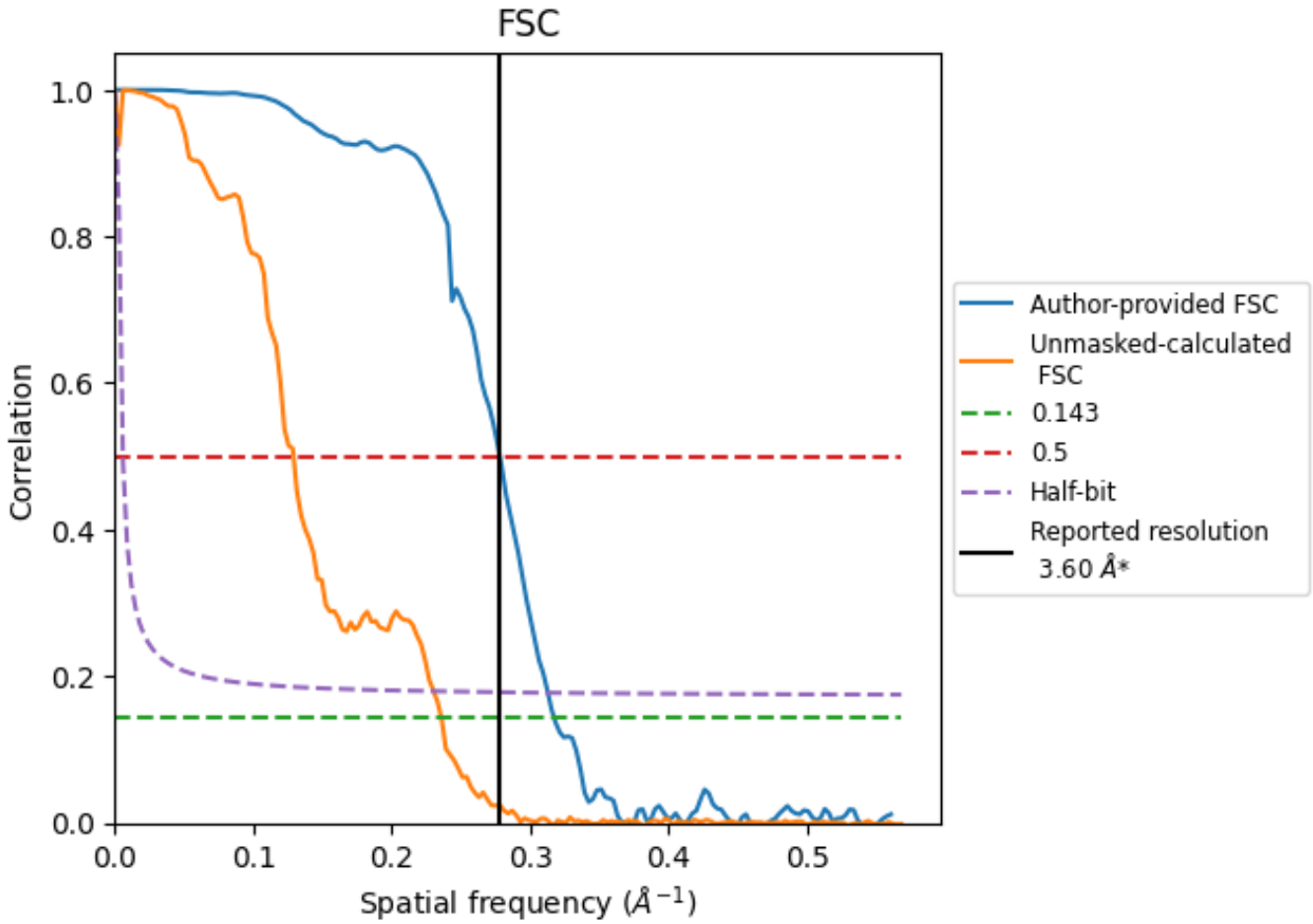


*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

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 0.278 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.15	3.59	3.20
Unmasked-calculated*	4.24	7.75	4.34

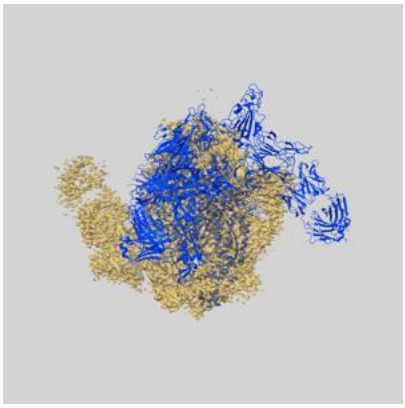
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.15 differs from the reported value 3.6 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.24 differs from the reported value 3.6 by more than 10 %

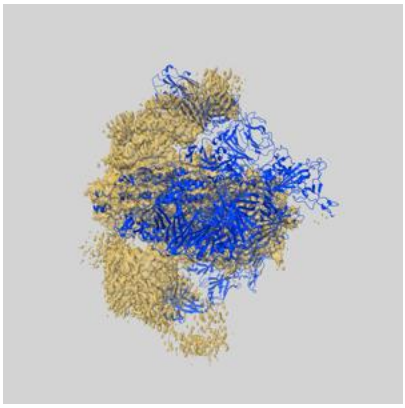
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-30921 and PDB model 7DZY. Per-residue inclusion information can be found in section 3 on page 9.

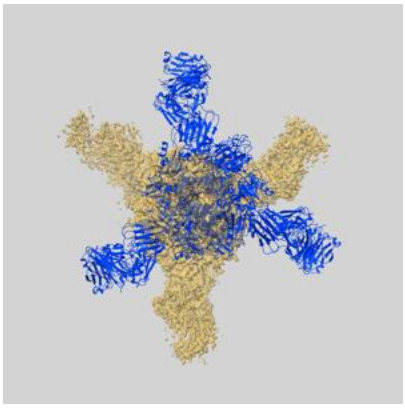
9.1 Map-model overlay



X



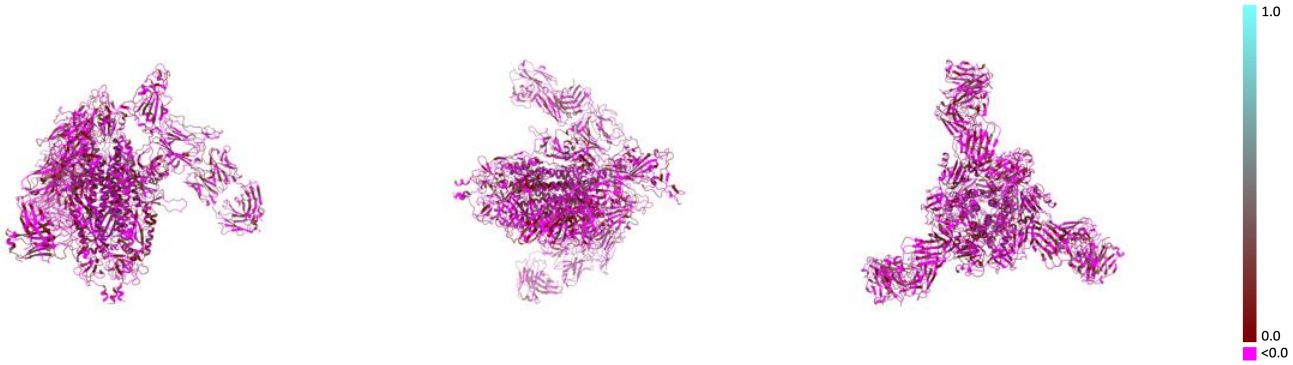
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.18 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.

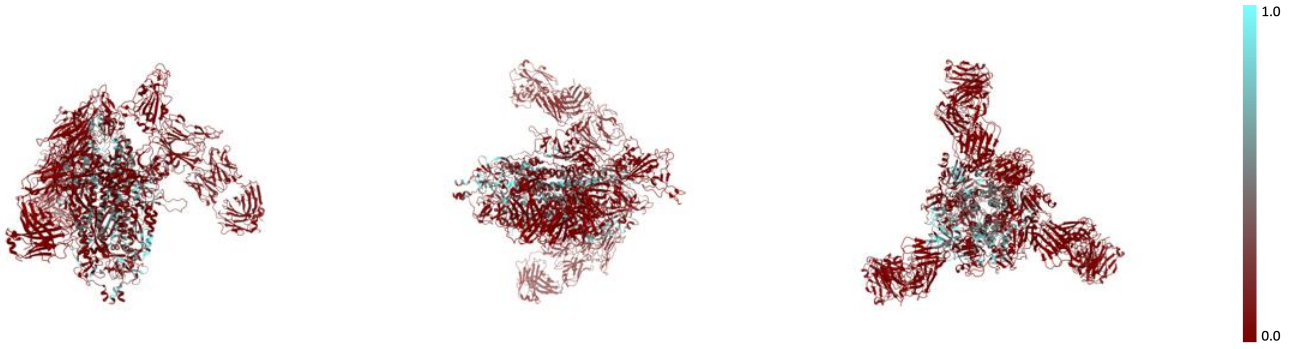
9.2 Q-score mapped to coordinate model



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.

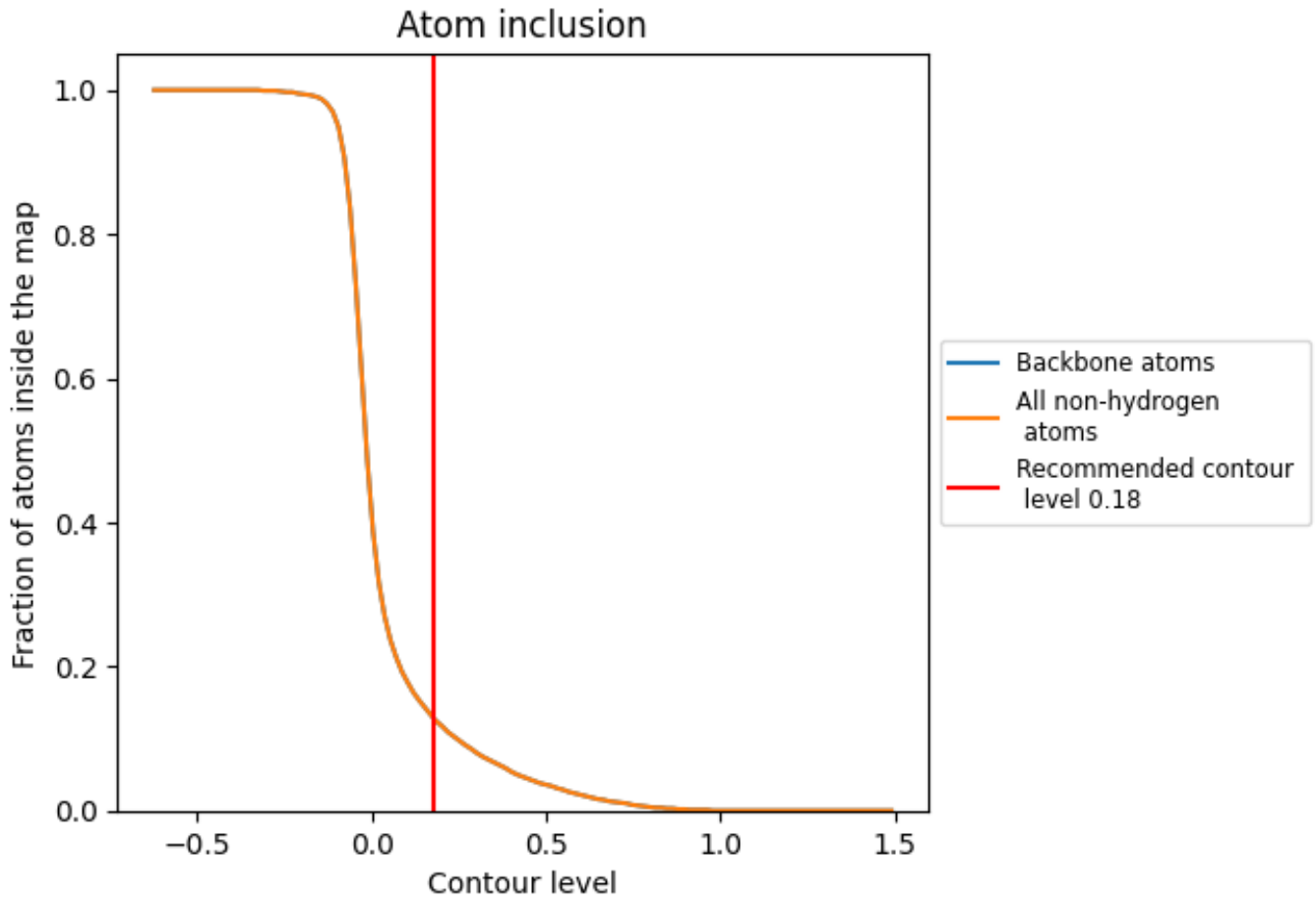
9.3 Atom inclusion mapped to coordinate model



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 (0.18).

9.4 Atom inclusion (i)



At the recommended contour level, 13% of all backbone atoms, 13% 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 (0.18) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.1270	-0.0100
A	0.2020	-0.0270
B	0.1500	-0.0140
C	0.1780	0.0000
H	0.0000	0.0010
L	0.0000	0.0260
M	0.0000	-0.0080
N	0.0000	0.0050
O	0.0000	-0.0250
P	0.0000	-0.0040