wwPDB EM Validation Summary Report ⓘ

Nov 9, 2022 – 01:35 AM JST

PDB ID	:	6ACG
EMDB ID	:	EMD-9591
Title	:	Trypsin-cleaved and low pH-treated SARS-CoV spike glycoprotein and ACE2 complex, ACE2-bound conformation 1
Authors	:	Gui, M.; Song, W.
Deposited on	:	2018-07-26
Resolution	:	5.40 Å(reported)

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:

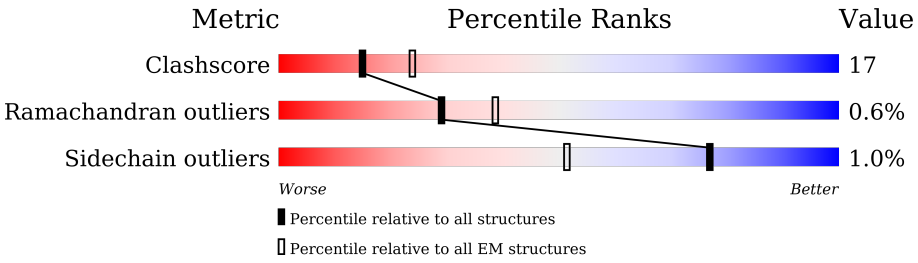
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 5.40 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	A	1203	43% 51% 36% · 11%
1	B	1203	37% 52% 35% · 11%
1	C	1203	45% 53% 33% •• 12%
2	D	603	99% 75% 24% ·

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 29715 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	1065	Total	C	N	O	S	0	0
			8302	5304	1374	1579	45		
1	B	1065	Total	C	N	O	S	0	0
			8302	5304	1374	1579	45		
1	C	1057	Total	C	N	O	S	0	0
			8241	5264	1364	1568	45		

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1197	SER	-	expression tag	UNP P59594
A	1198	HIS	-	expression tag	UNP P59594
A	1199	PRO	-	expression tag	UNP P59594
A	1200	GLN	-	expression tag	UNP P59594
A	1201	PHE	-	expression tag	UNP P59594
A	1202	GLU	-	expression tag	UNP P59594
A	1203	LYS	-	expression tag	UNP P59594
B	1197	SER	-	expression tag	UNP P59594
B	1198	HIS	-	expression tag	UNP P59594
B	1199	PRO	-	expression tag	UNP P59594
B	1200	GLN	-	expression tag	UNP P59594
B	1201	PHE	-	expression tag	UNP P59594
B	1202	GLU	-	expression tag	UNP P59594
B	1203	LYS	-	expression tag	UNP P59594
C	1197	SER	-	expression tag	UNP P59594
C	1198	HIS	-	expression tag	UNP P59594
C	1199	PRO	-	expression tag	UNP P59594
C	1200	GLN	-	expression tag	UNP P59594
C	1201	PHE	-	expression tag	UNP P59594
C	1202	GLU	-	expression tag	UNP P59594
C	1203	LYS	-	expression tag	UNP P59594

- Molecule 2 is a protein called Angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	597	Total	C	N	O	S	0	0
			4870	3115	806	920	29		

There are 6 discrepancies between the modelled and reference sequences:

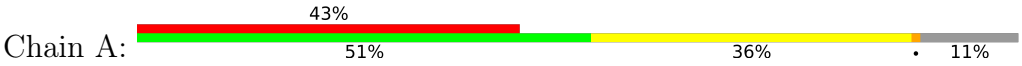
Chain	Residue	Modelled	Actual	Comment	Reference
D	616	HIS	-	expression tag	UNP Q9BYF1
D	617	HIS	-	expression tag	UNP Q9BYF1
D	618	HIS	-	expression tag	UNP Q9BYF1
D	619	HIS	-	expression tag	UNP Q9BYF1
D	620	HIS	-	expression tag	UNP Q9BYF1
D	621	HIS	-	expression tag	UNP Q9BYF1

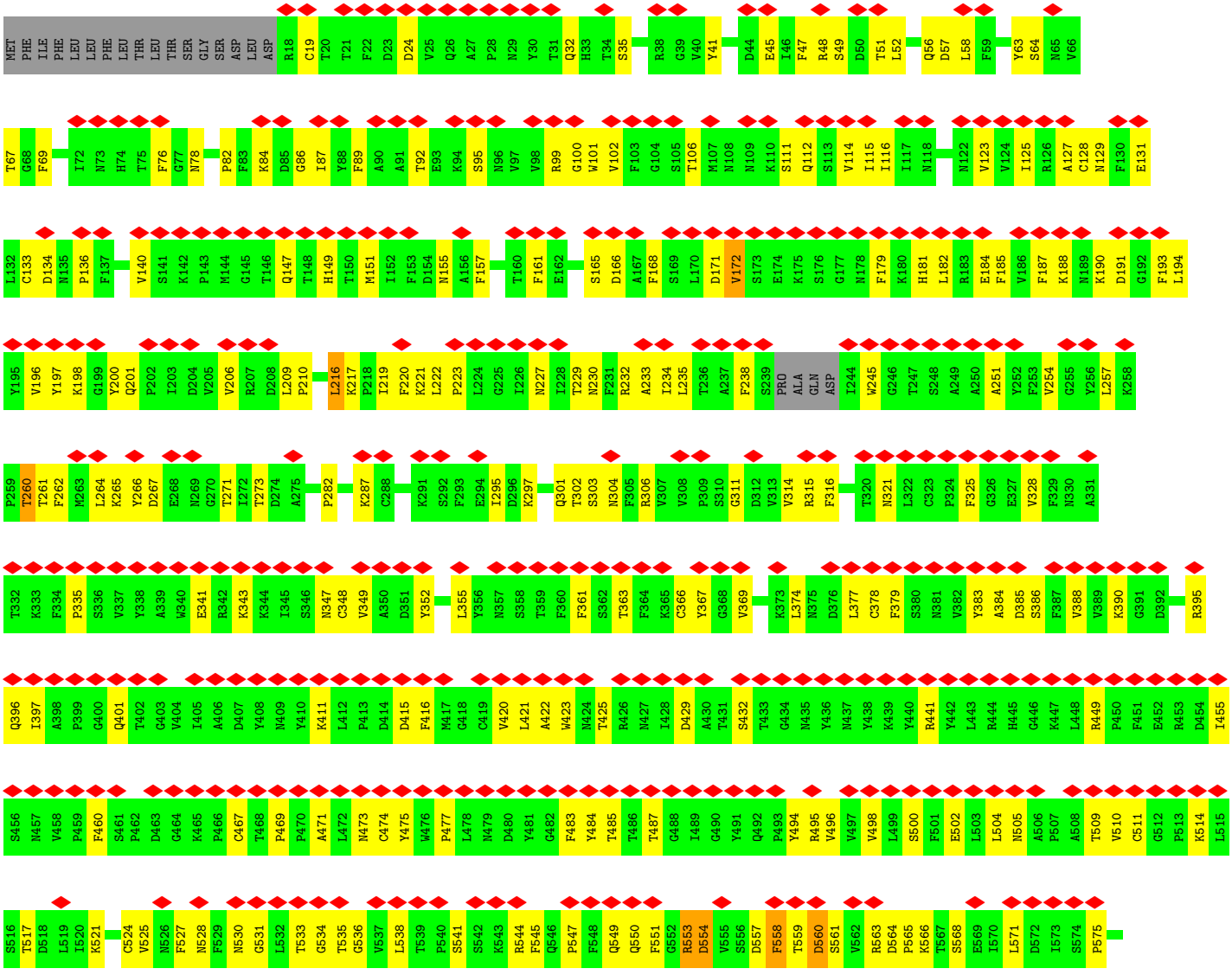
3 Residue-property plots (i)

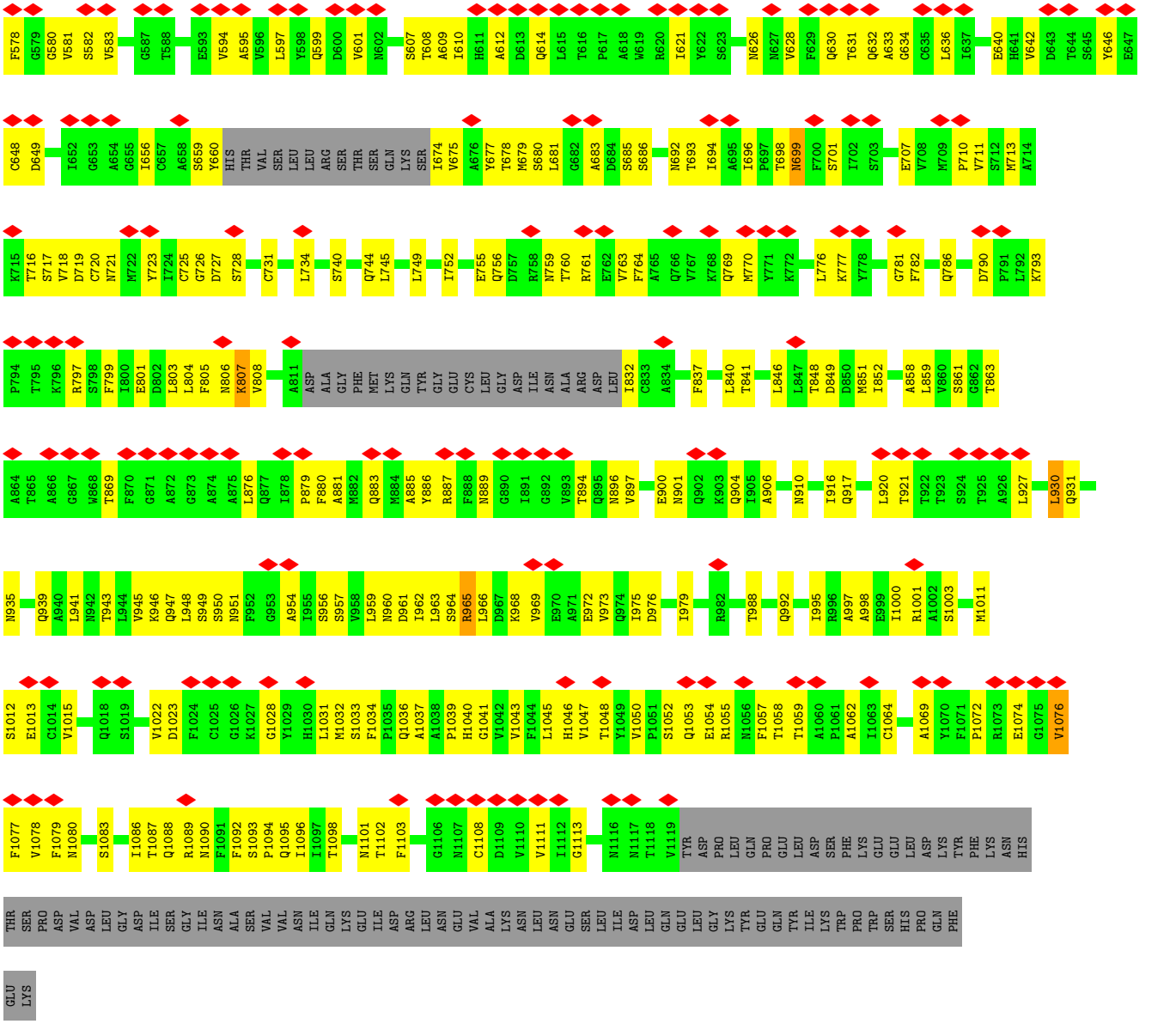
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

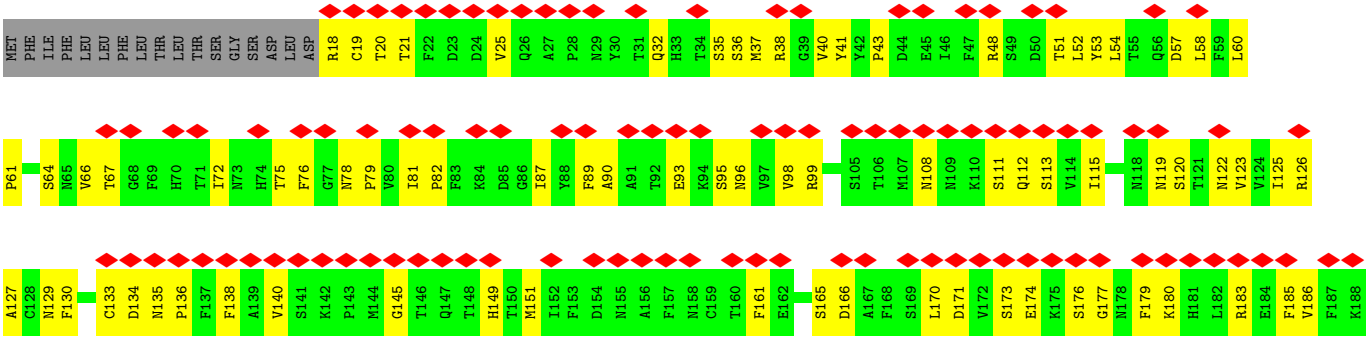


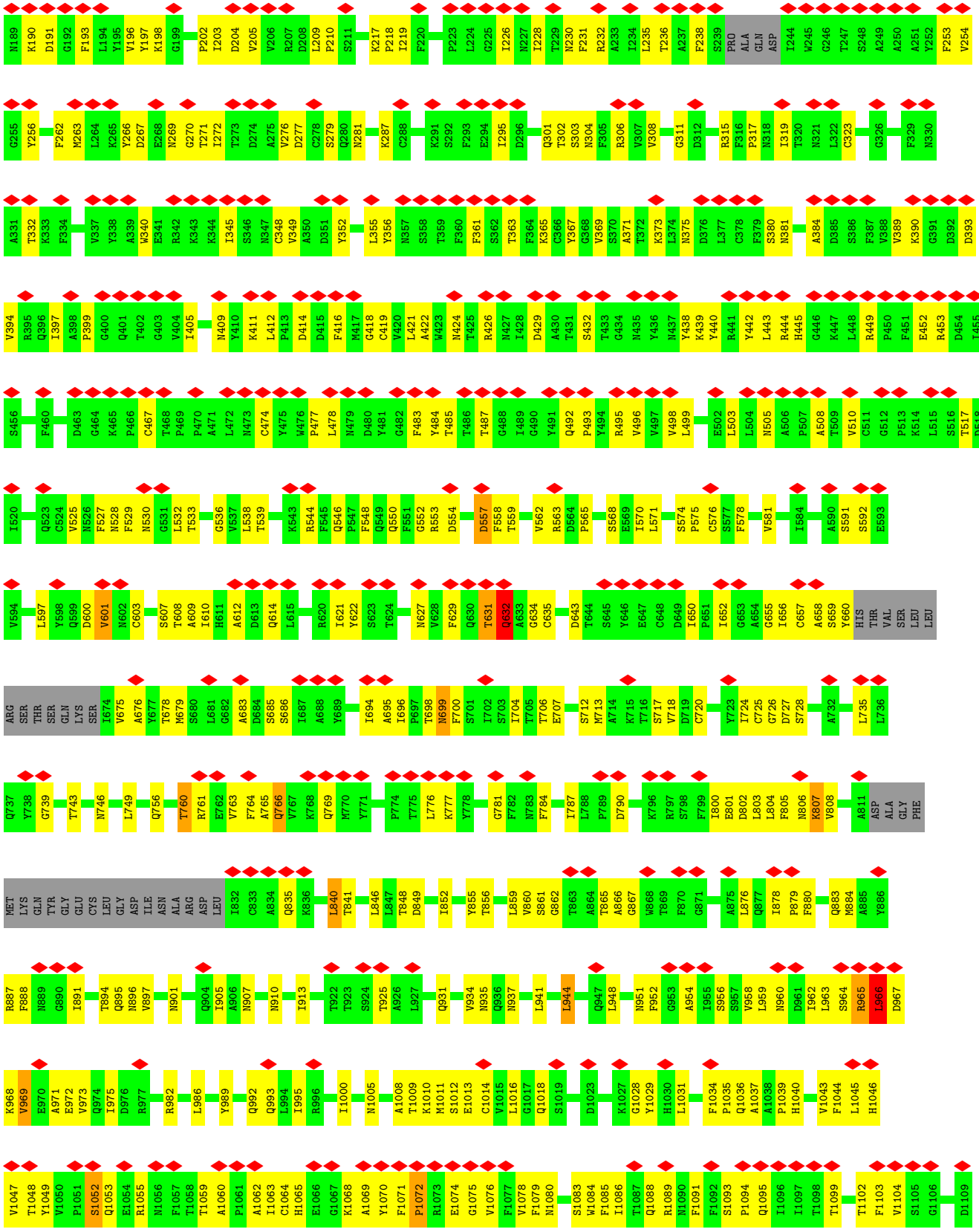


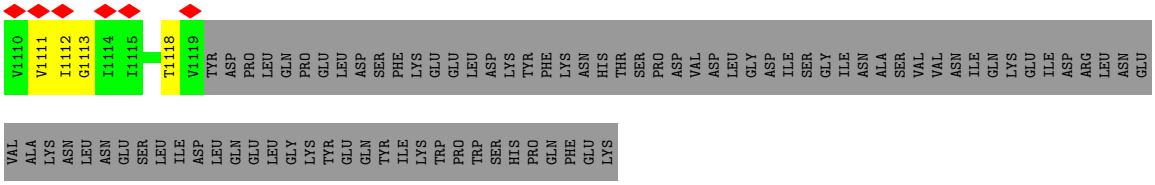


• Molecule 1: Spike glycoprotein

Chain B:

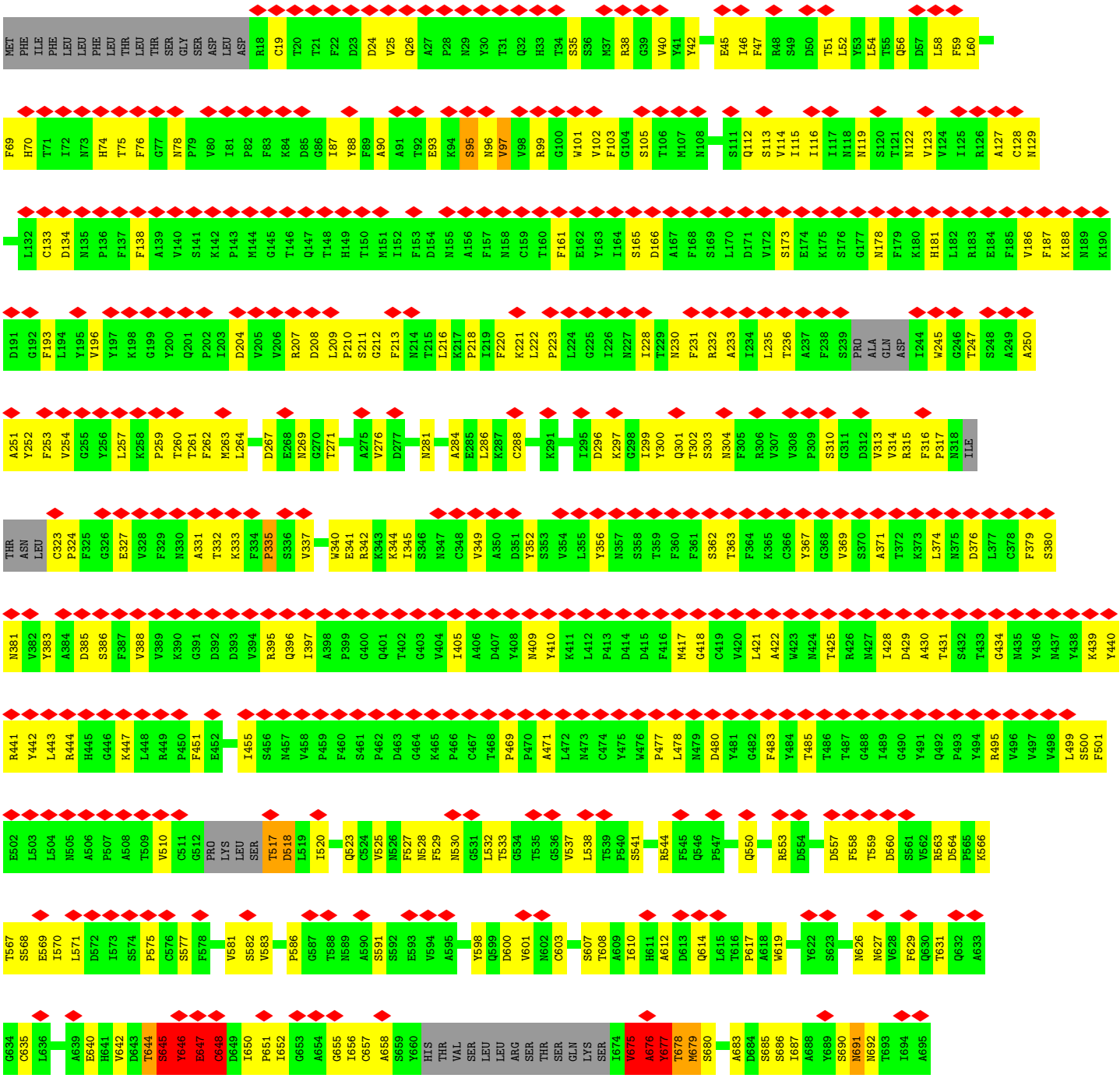


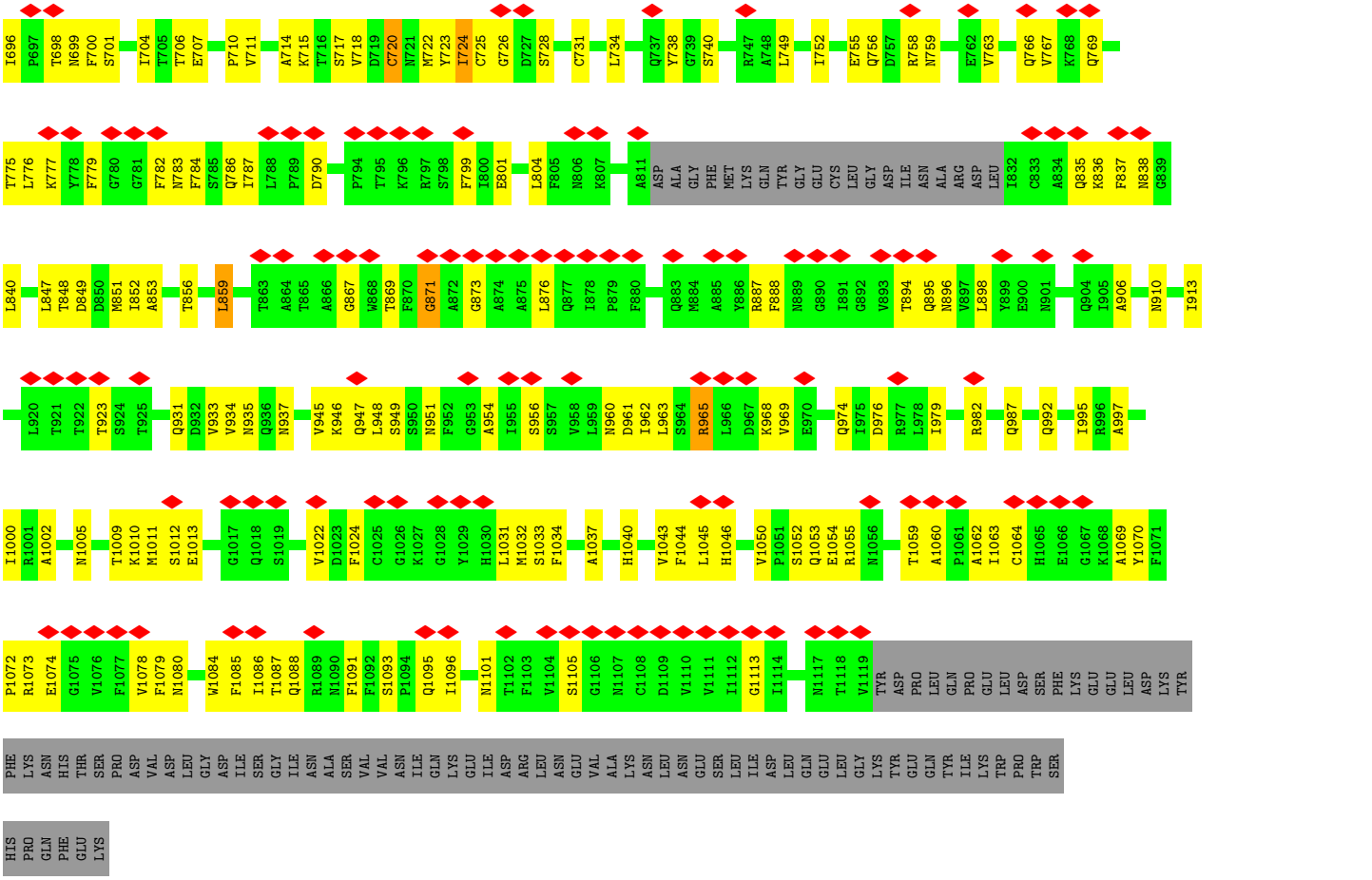

N189 K190 D191 G192 F193 L194 Y195 V196 Y197 K198 G199 P202 I203 D204 V205 V206 R207 D208 L209 P210 S211 K217 P218 I219 F220 P223 L224 G225 I226 N227 I228 T229 N230 F231 R232 A233 I234 L235 T236 A237 F238 S239 PRO ALA GLN ASP I244 W245 G246 T247 S248 A249 A250 A251 Y252 F253 V254
G255 Y256 F262 M263 L264 K265 Y266 D267 E268 N269 G270 T271 I272 T273 D274 A275 V276 D277 C278 S279 Q280 N281 K287 C288 K291 S292 F293 E294 I295 D296 Q301 T302 S303 N304 F305 R306 V307 V308 G311 D312 R315 F316 P317 N318 I319 T320 N321 L322 G323 G326 F329 N330
A331 T332 K333 F334 V337 Y338 A339 W340 E341 R342 K343 K344 I345 S346 N347 C348 V349 A350 D351 Y352 L355 Y356 N357 S358 T359 F360 F361 S362 T363 F364 K365 C366 Y367 G368 V369 S370 A371 T372 K373 L374 N375 D376 L377 C378 F379 S380 N381 A384 D385 S386 F387 V388 V389 K390 G391 D392 D393
V394 R395 Q396 I397 A398 P399 G400 Q401 T402 G403 V404 I405 N409 Y410 K411 L412 P413 D414 D415 F416 M417 G418 C419 V420 L421 A422 W423 N424 T425 R426 N427 I428 D429 A430 T431 S432 T433 G434 N435 Y436 N437 Y438 K439 Y440 R441 Y442 L443 R444 H445 G446 K447 L448 R449 P450 F451 E452 R453 D454 I455
S456 F460 D463 G464 K465 P466 C467 T468 P469 P470 A471 L472 N473 C474 Y475 W476 P477 L478 N479 D480 Y481 G482 F483 Y484 T485 T486 T487 G488 I489 G490 Y491 Q492 P493 Y494 R495 V496 V497 V498 L499 E502 L503 L504 N505 A506 P507 A508 T509 V510 C511 G512 P513 K514 L515 S516 T517 D518 L519
I520 Q523 C524 V525 N526 F527 N528 F529 N530 G531 L532 T533 G536 V537 L538 T539 K543 R544 F545 Q546 F547 F548 Q549 Q550 F551 G552 R553 D554 D557 F558 T559 V562 R563 D564 P565 S568 E569 I570 L571 S574 P575 C576 S577 F578 V581 I584 A590 S591 S592 E593
V594 L597 Y598 Q599 D600 V601 N602 C603 S607 T608 A609 I610 H611 A612 D613 Q614 L615 R620 I621 Y622 S623 T624 N627 V628 F629 Q630 T631 G632 A633 G634 C635 D643 T644 S645 Y646 E647 C648 D649 I650 P651 I652 G653 A654 G655 I656 C657 A658 S659 Y660 HIS THR VAL SER LEU LEU
ARG SER THR SER GLN LYS SER I674 V675 A676 Y677 T678 M679 S680 L681 G682 A683 D684 S685 S686 I687 A688 Y689 I694 A695 I696 P697 T698 N699 F700 S701 I702 S703 I704 T705 T706 E707 S712 M713 A714 K715 T716 S717 V718 D719 C720 Y723 I724 C725 G726 D727 S728 A732 L735 L736
Q737 Y738 G739 T743 N746 L749 Q756 T760 R761 E762 V763 F764 A765 Q766 V767 K768 Q769 M770 Y771 P774 T775 L776 K777 Y778 G781 F782 N783 F784 I787 L788 P789 D790 K796 R797 S798 F799 I800 E801 D802 L803 L804 F805 N806 K807 V808 A811 ASP ALA GLY PHE
MET LYS GLN TYR GLY GLU CYS LEU GLY ASP ILE ASN ALA ARG ASP LEU I832 C833 A834 Q835 K836 L840 T841 L846 L847 T848 D849 I852 Y855 T856 L859 V860 S861 G862 T863 A864 T865 A866 G867 W868 T869 F870 G871 A875 L876 Q877 I878 F880 Q883 M884 A885 Y886
R887 F888 N889 G890 I891 T894 Q895 N896 V897 N901 Q904 I905 A906 N907 N910 I913 T922 T923 S924 T925 A926 L927 Q931 V934 N935 Q936 N937 L941 L944 Q947 L948 N951 F952 G953 A954 I955 S956 S957 V958 L959 N960 D961 I962 L963 S964 R965 L966 D967
K968 V969 E970 A971 E972 V973 Q974 I975 D976 R977 R982 L986 Y989 Q992 Q993 L994 I995 R996 I1000 N1005 A1008 T1009 K1010 M1011 S1012 E1013 C1014 V1015 L1016 G1017 Q1018 S1019 D1023 K1027 G1028 Y1029 H1030 L1031 F1034 P1035 Q1036 A1037 A1038 P1039 H1040 V1043 F1044 L1045 H1046
V1047 T1048 Y1049 V1050 P1051 S1052 Q1053 E1054 R1055 N1056 F1057 T1058 T1059 A1060 P1061 A1062 I1063 C1064 H1065 E1066 G1067 K1068 A1069 Y1070 F1071 P1072 R1073 E1074 G1075 V1076 F1077 V1078 F1079 N1080 S1083 W1084 F1085 I1086 T1087 Q1088 R1089 N1090 F1091 F1092 S1093 P1094 Q1095 I1096 I1097 T1098 T1099 T1102 F1103 V1104 S1105 G1106 D1109



- Molecule 1: Spike glycoprotein

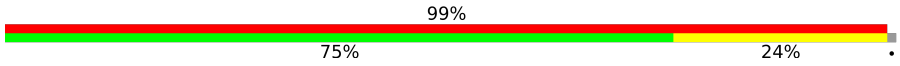
Chain C:

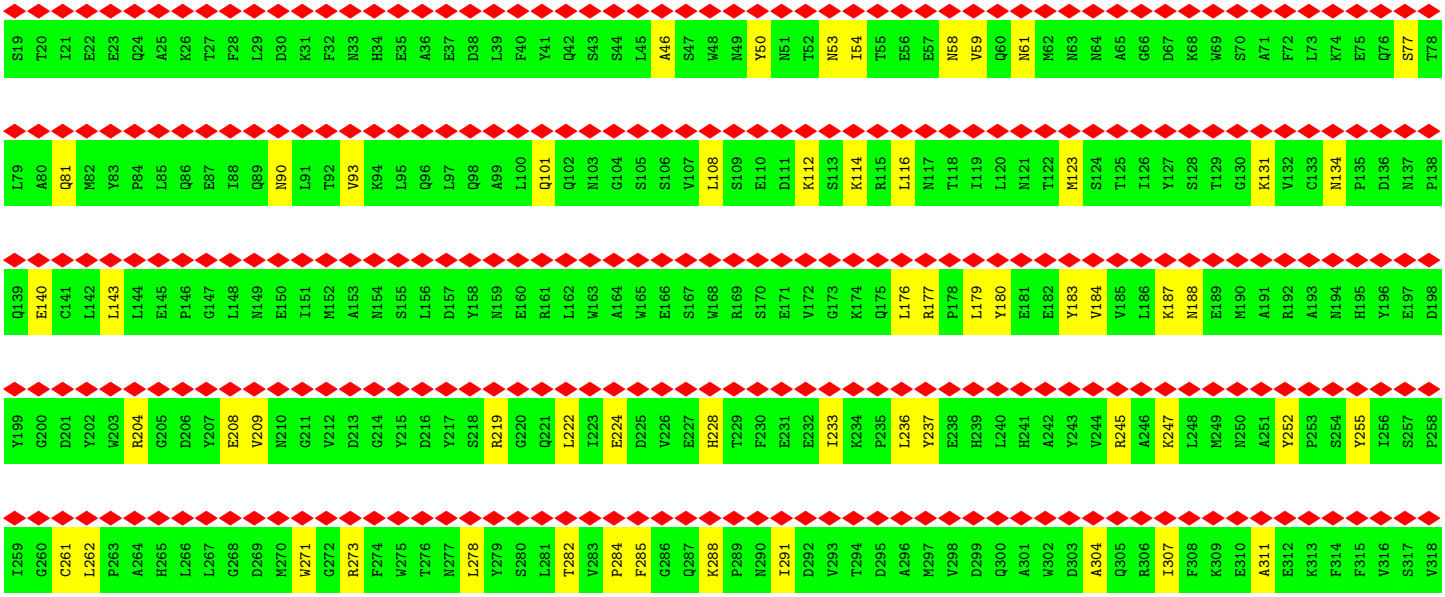


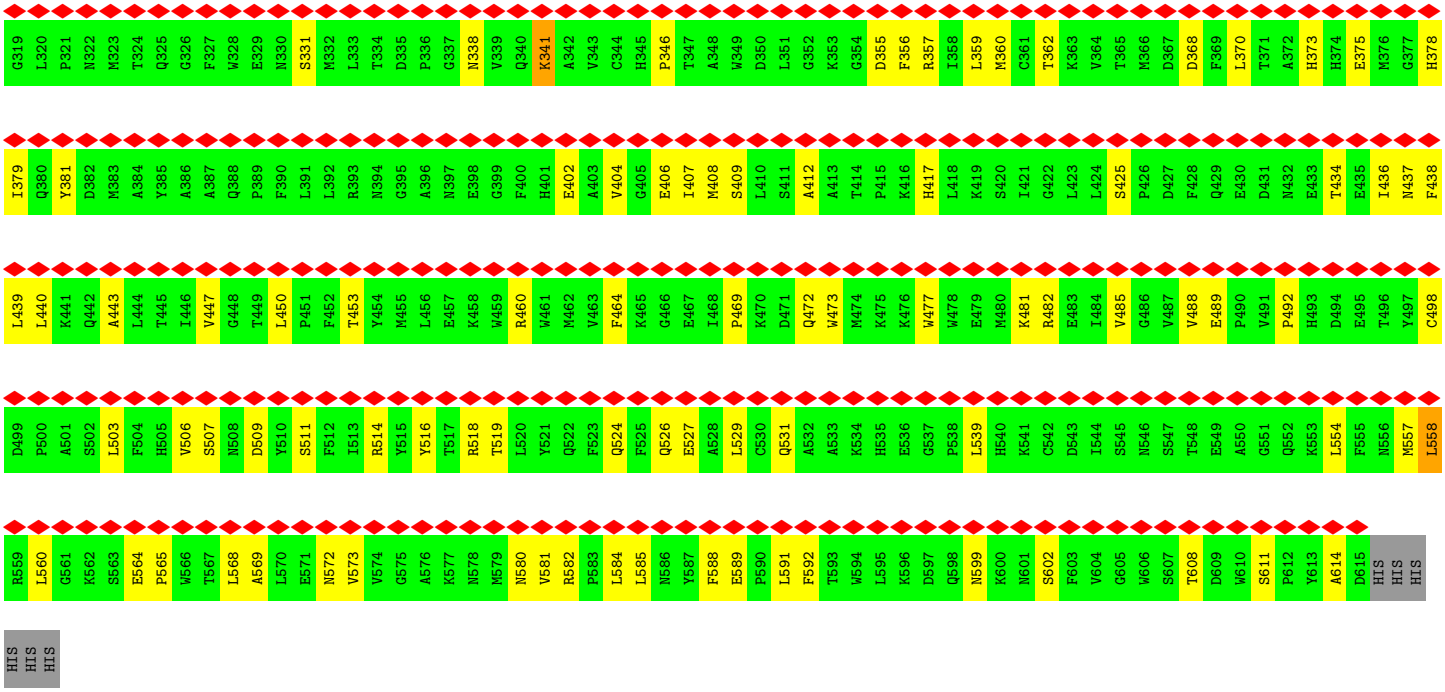


• Molecule 2: Angiotensin-converting enzyme 2

Chain D:






G319 L320 P321 N322 M323 T324 Q325 G326 F327 W328 E329 N330 S331 M332 L333 T334 D335 P336 G337 N338 V339 Q340 K341 A342 V343 C344 H345 P346 T347 A348 W349 D350 L351 G352 K353 G354 D355 F356 R357 I358 L359 M360 C361 T362 K363 V364 T365 M366 D367 D368 F369 L370 T371 A372 H373 H374 E375 M376 G377 H378
I379 Q380 Y381 D382 M383 A384 Y385 A386 A387 Q388 P389 F390 L391 L392 R393 N394 G395 A396 N397 E398 G399 F400 H401 E402 A403 V404 G405 E406 I407 M408 S409 L410 S411 A412 A413 T414 P415 K416 H417 L418 K419 S420 I421 G422 L423 L424 S425 P426 D427 F428 Q429 E430 D431 N432 E433 T434 E435 I436 N437 F438
L439 L440 K441 Q442 A443 L444 T445 I446 V447 G448 T449 L450 P451 F452 T453 Y454 M455 L456 E457 K458 W459 R460 W461 M462 V463 F464 K465 G466 E467 I468 P469 K470 D471 Q472 W473 M474 K475 K476 W477 W478 E479 M480 K481 R482 E483 I484 V485 G486 V487 V488 E489 P490 V491 P492 H493 D494 E495 T496 Y497 C498
D499 P500 A501 S502 L503 F504 H505 V506 S507 M508 D509 Y510 S511 F512 I513 R514 Y515 Y516 T517 R518 T519 L520 Y521 Q522 F523 Q524 F525 Q526 E527 A528 L529 C530 Q531 A532 A533 K534 H535 E536 G537 P538 L539 H540 K541 C542 D543 I544 S545 N546 S547 T548 E549 A550 G551 Q552 K553 L554 F555 N556 M557 L558
R559 L560 G561 K562 S563 E564 P565 W566 T567 L568 A569 L570 E571 N572 V573 V574 G575 A576 K577 N578 M579 N580 V581 R582 P583 L584 L585 N586 Y587 F588 E589 P590 L591 F592 T593 W594 L595 K596 D597 Q598 N599 K600 N601 S602 F603 V604 G605 W606 S607 T608 D609 W610 S611 P612 Y613 A614 D615 HIS HIS HIS
HIS HIS HIS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	53189	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)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	28.981	Depositor
Minimum map value	-13.647	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.921	Depositor
Recommended contour level	8.0	Depositor
Map size (Å)	380.16, 380.16, 380.16	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.32, 1.32, 1.32	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	0.55	3/8499 (0.0%)	0.75	6/11568 (0.1%)
1	B	0.55	0/8499	0.76	6/11568 (0.1%)
1	C	0.59	4/8435 (0.0%)	0.80	9/11477 (0.1%)
2	D	0.33	0/5007	0.58	3/6803 (0.0%)
All	All	0.53	7/30440 (0.0%)	0.74	24/41416 (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	A	0	17
1	B	0	17
1	C	0	19
2	D	0	2
All	All	0	55

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	677	TYR	CE2-CZ	-8.28	1.27	1.38
1	A	725	CYS	CB-SG	-6.81	1.70	1.82
1	A	731	CYS	CB-SG	-6.41	1.71	1.82
1	C	676	ALA	C-O	-5.93	1.12	1.23
1	A	411	LYS	C-N	-5.48	1.21	1.34

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	518	ASP	CB-CG-OD1	9.91	127.22	118.30
1	B	944	LEU	CA-CB-CG	9.05	136.12	115.30
1	A	557	ASP	CB-CG-OD1	8.32	125.78	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	966	LEU	CA-CB-CG	6.80	130.93	115.30
1	C	644	THR	CA-C-N	-6.62	102.64	117.20

There are no chirality outliers.

5 of 55 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	172	VAL	Peptide
1	A	206	VAL	Peptide
1	A	415	ASP	Peptide
1	A	416	PHE	Peptide
1	A	558	PHE	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	8302	0	8082	299	0
1	B	8302	0	8082	300	0
1	C	8241	0	8011	339	0
2	D	4870	0	4643	87	0
All	All	29715	0	28818	983	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 17.

The worst 5 of 983 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:C:656:ILE:CG1	1:C:677:TYR:O	1.89	1.21
1:C:678:THR:O	1:C:679:MET:HB2	1.43	1.18
1:C:656:ILE:HG12	1:C:677:TYR:O	1.00	1.17
1:C:647:GLU:O	1:C:648:CYS:CB	1.91	1.14
1:C:646:TYR:C	1:C:680:SER:OG	1.94	1.06

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	1057/1203 (88%)	850 (80%)	203 (19%)	4 (0%)	34	72
1	B	1057/1203 (88%)	836 (79%)	213 (20%)	8 (1%)	19	60
1	C	1045/1203 (87%)	834 (80%)	201 (19%)	10 (1%)	15	54
2	D	595/603 (99%)	565 (95%)	30 (5%)	0	100	100
All	All	3754/4212 (89%)	3085 (82%)	647 (17%)	22 (1%)	29	65

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	645	SER
1	C	648	CYS
1	C	675	VAL
1	C	676	ALA
1	C	679	MET

5.3.2 Protein sidechains

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	922/1048 (88%)	914 (99%)	8 (1%)	78	88
1	B	922/1048 (88%)	914 (99%)	8 (1%)	78	88
1	C	914/1048 (87%)	903 (99%)	11 (1%)	71	84
2	D	527/533 (99%)	522 (99%)	5 (1%)	78	88
All	All	3285/3677 (89%)	3253 (99%)	32 (1%)	77	86

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	114	LYS
2	D	273	ARG
1	B	760	THR
1	B	720	CYS
2	D	341	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 73 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	904	GLN
2	D	572	ASN
1	C	935	ASN
2	D	53	ASN
1	A	1005	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.

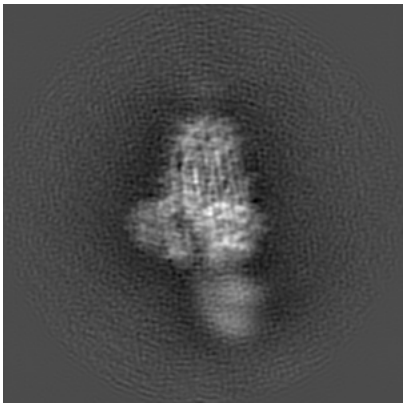
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-9591. These allow visual inspection of the internal detail of the map and identification of artifacts.

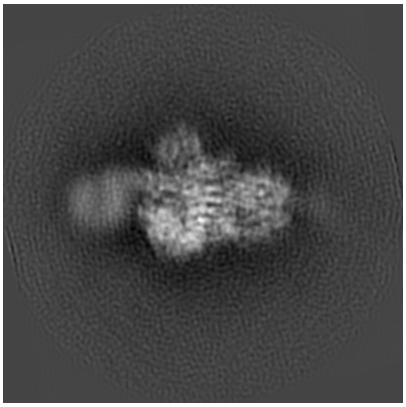
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

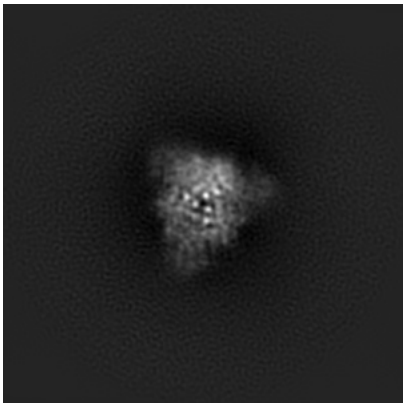
6.1.1 Primary map



X



Y

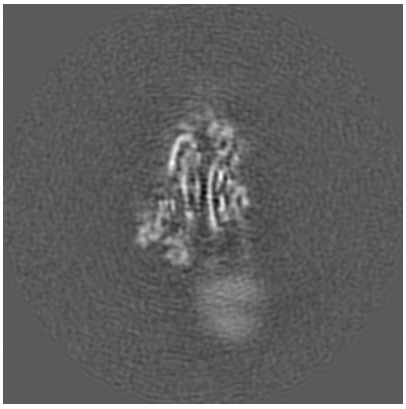


Z

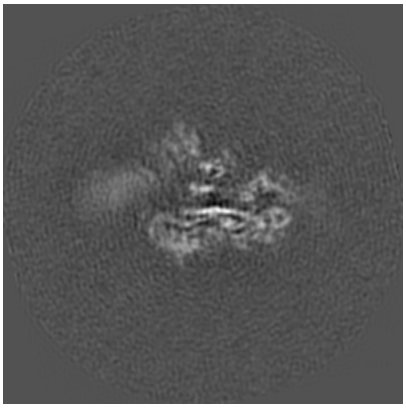
The images above show the map projected in three orthogonal directions.

6.2 Central slices

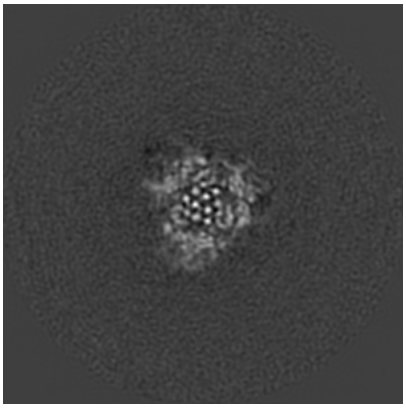
6.2.1 Primary map



X Index: 144



Y Index: 144

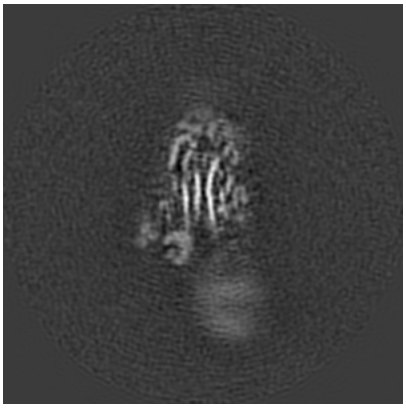


Z Index: 144

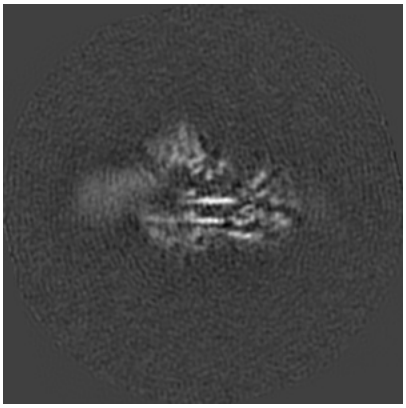
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

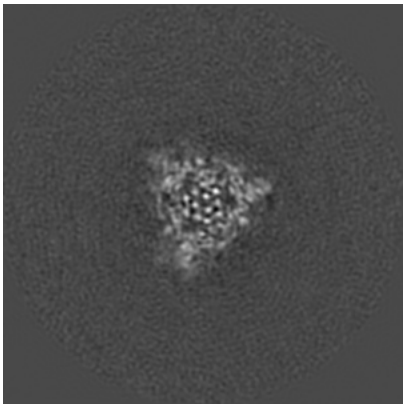
6.3.1 Primary map



X Index: 146



Y Index: 148



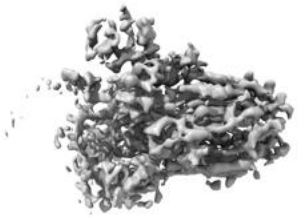
Z Index: 142

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

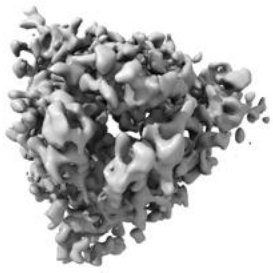
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 8.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

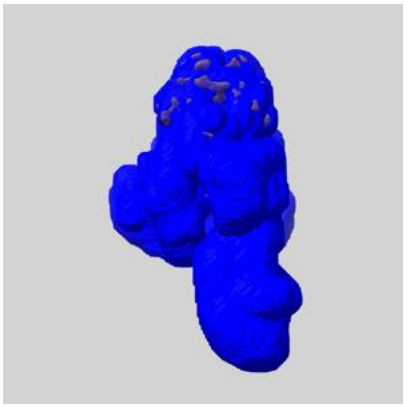
6.5 Mask visualisation (i)

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

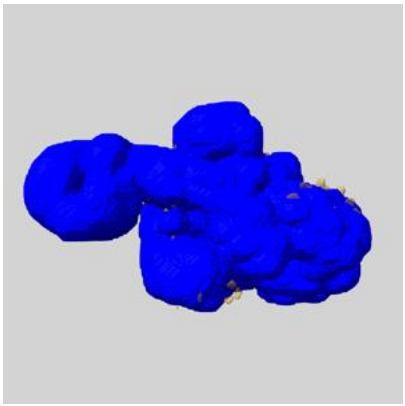
A mask typically either:

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

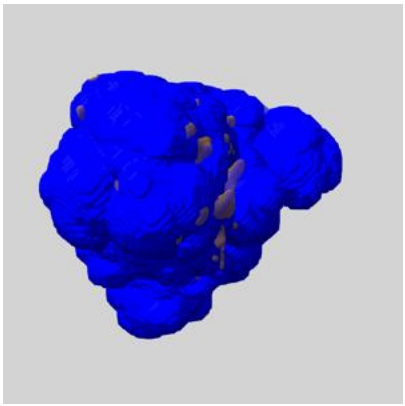
6.5.1 emd_9591_msk_1.map (i)



X



Y

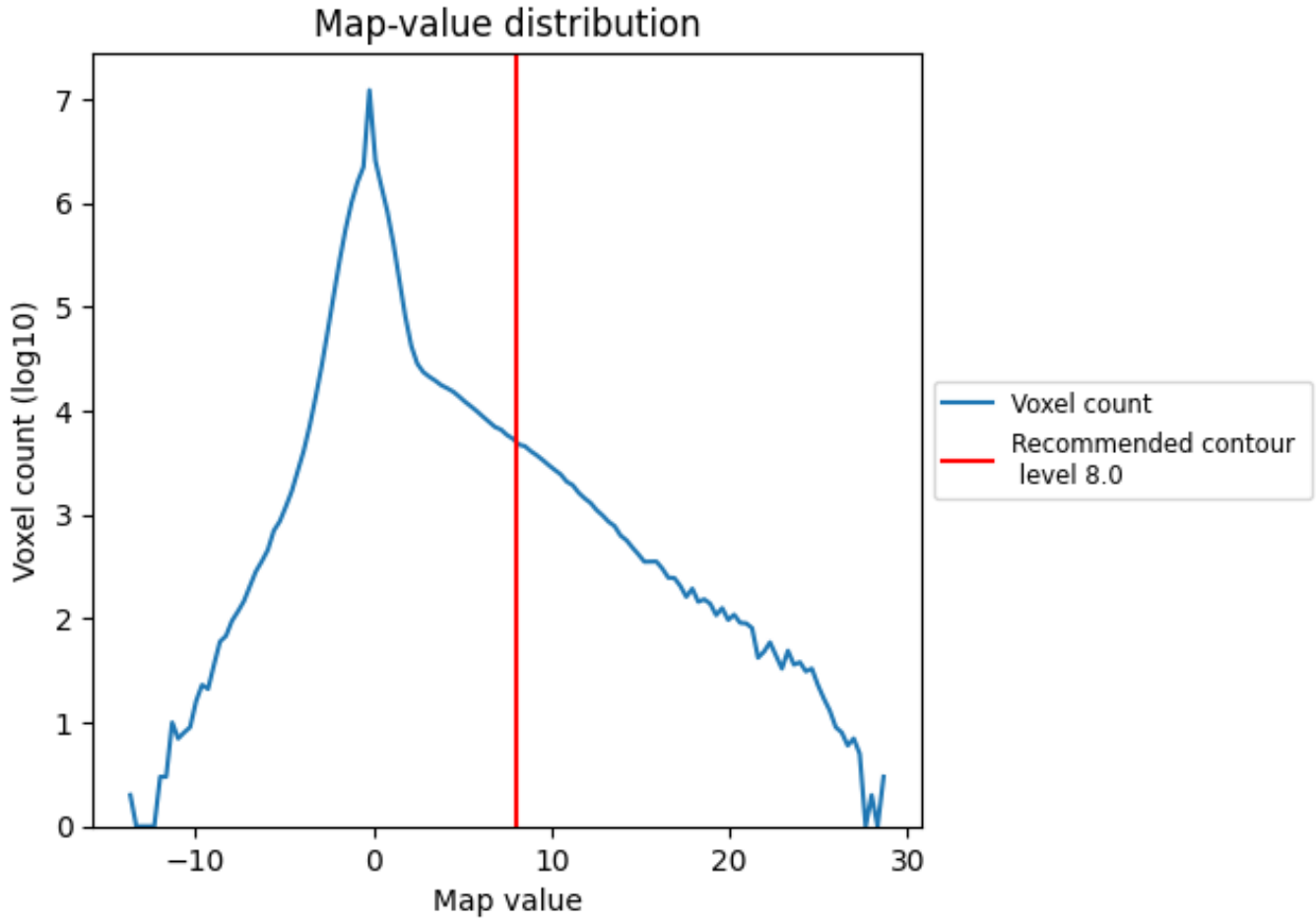


Z

7 Map analysis

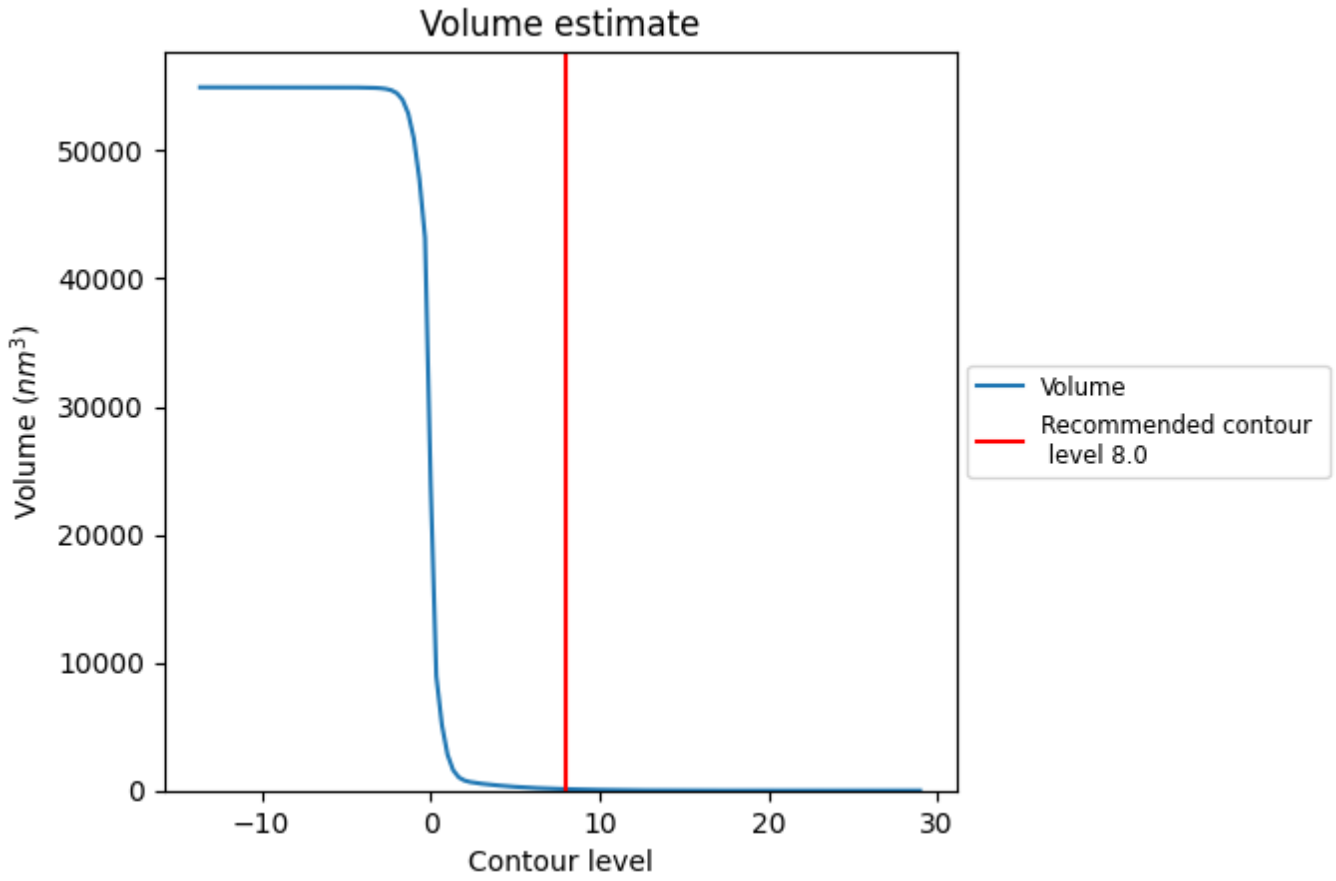
This section contains the results of statistical analysis of the map.

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.

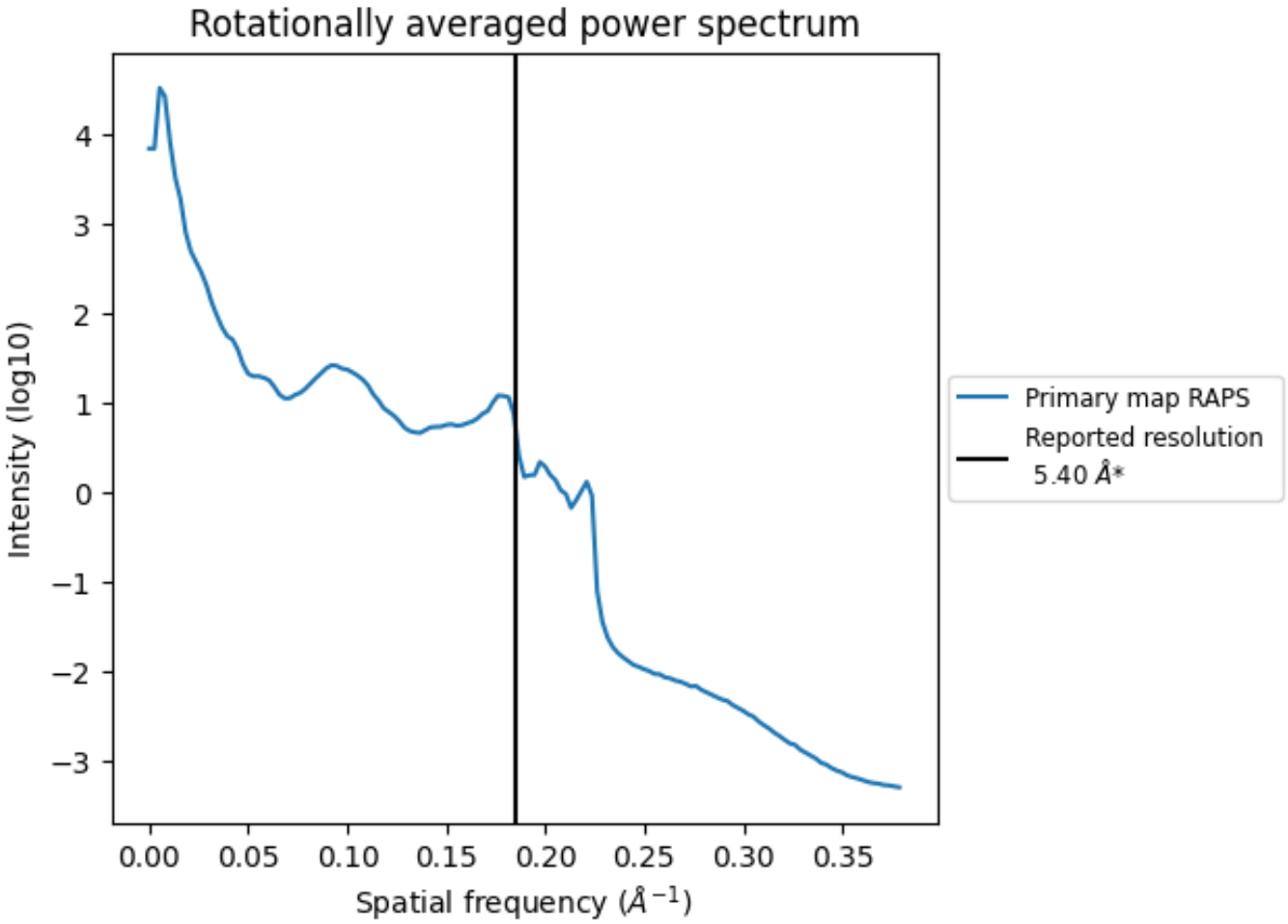
7.2 Volume estimate (i)



The volume at the recommended contour level is 114 nm^3; this corresponds to an approximate mass of 103 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)

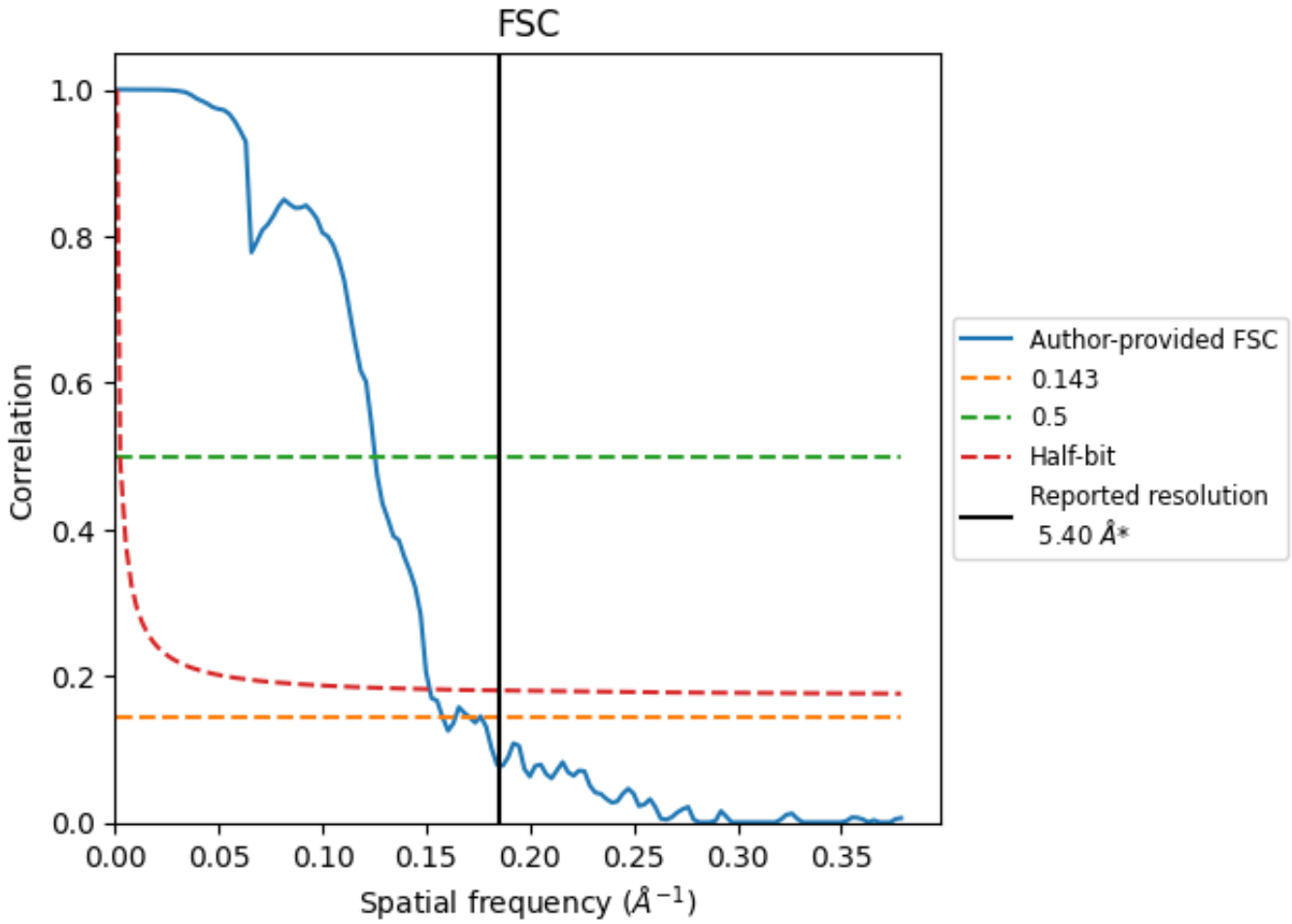


*Reported resolution corresponds to spatial frequency of 0.185 Å^{-1}

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 0.185 Å^{-1}

8.2 Resolution estimates (i)

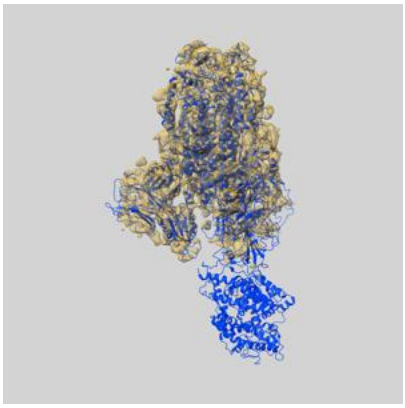
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.40	-	-
Author-provided FSC curve	6.33	7.98	6.59
Unmasked-calculated*	-	-	-

*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 6.33 differs from the reported value 5.4 by more than 10 %

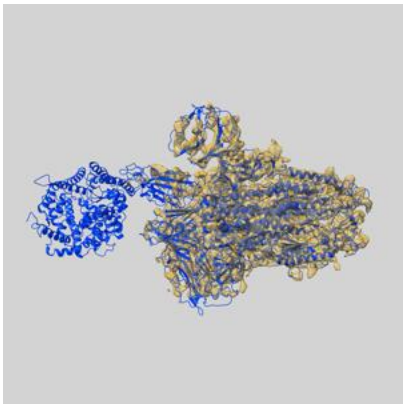
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-9591 and PDB model 6ACG. Per-residue inclusion information can be found in section 3 on page 5.

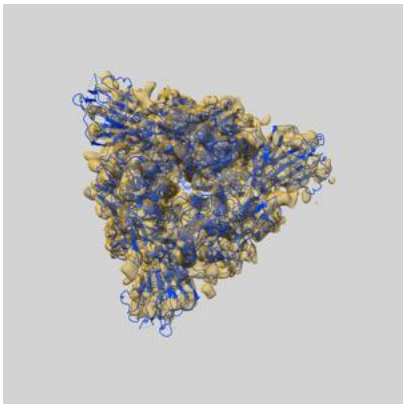
9.1 Map-model overlay



X



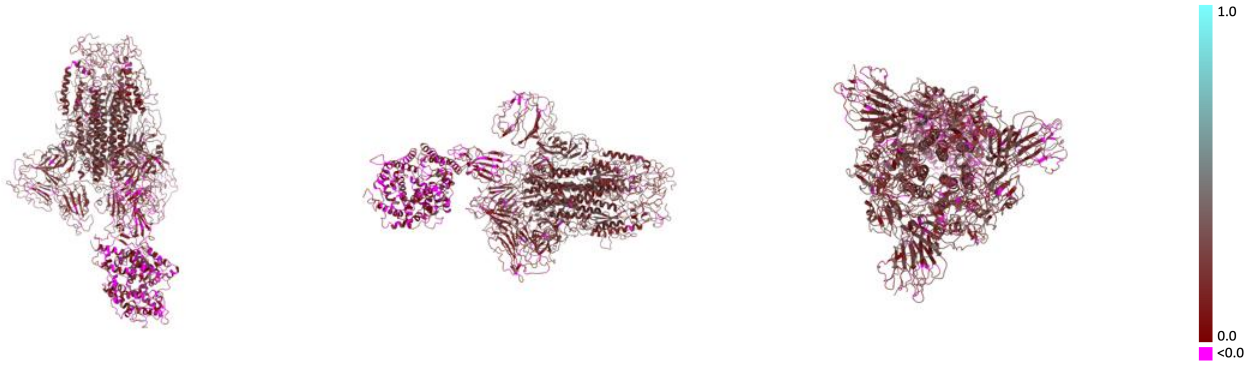
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 8.0 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.

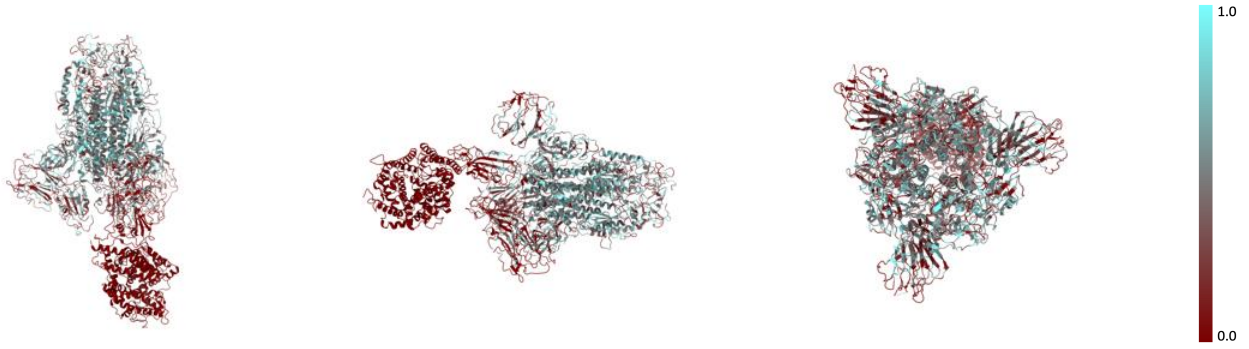
9.2 Q-score mapped to coordinate model (i)



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.

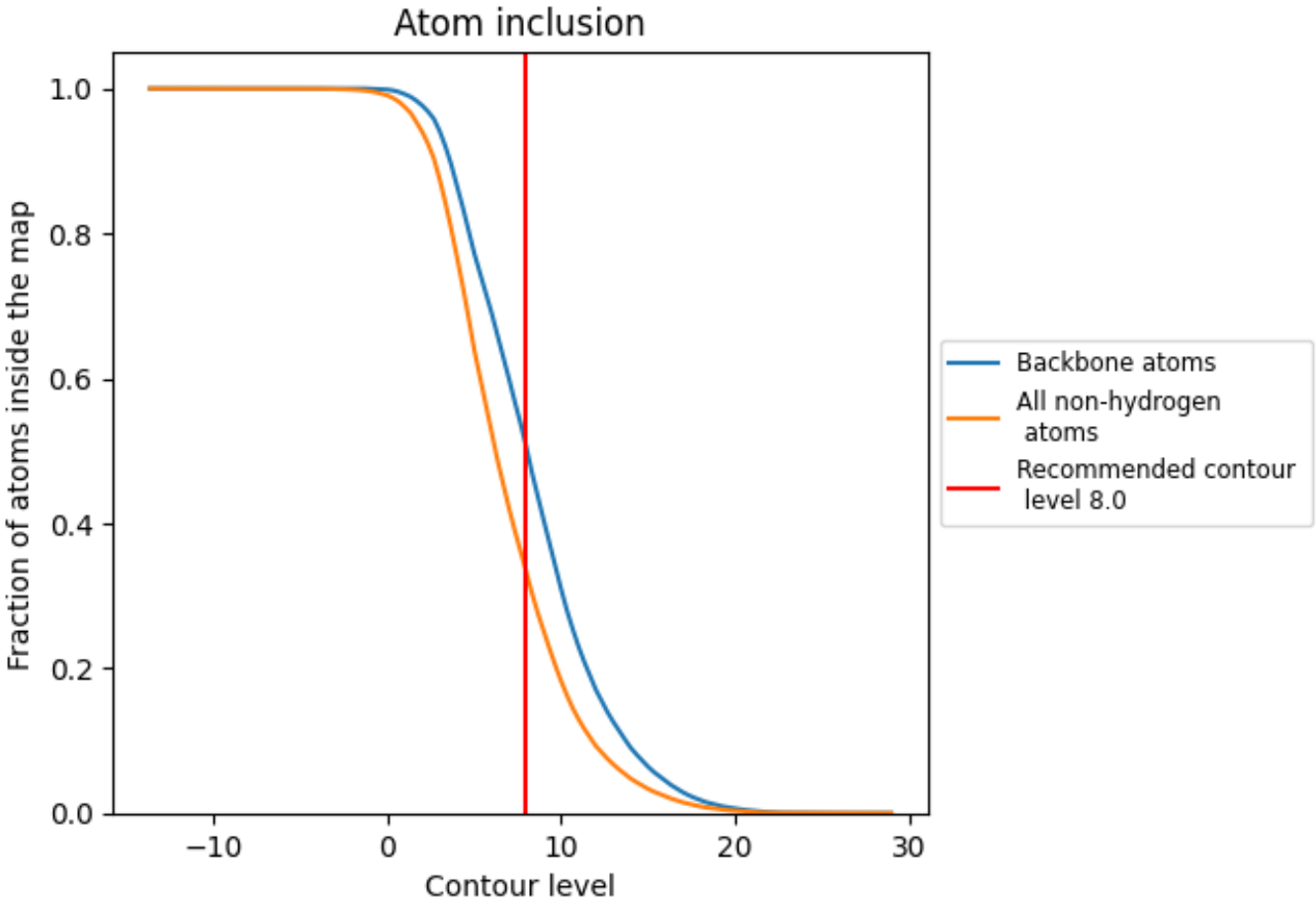
9.3 Atom inclusion mapped to coordinate model (i)



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 (8.0).

9.4 Atom inclusion (i)



At the recommended contour level, 50% of all backbone atoms, 33% 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 (8.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3320	0.2020
A	0.3872	0.2280
B	0.4303	0.2360
C	0.3731	0.2150
D	0.0004	0.0800