wwPDB EM Validation Summary Report ⓘ

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PDB ID	:	5X5F
EMDB ID	:	EMD-6707
Title	:	Prefusion structure of MERS-CoV spike glycoprotein, conformation 2
Authors	:	Yuan, Y.; Cao, D.; Zhang, Y.; Ma, J.; Qi, J.; Wang, Q.; Lu, G.; Wu, Y.; Yan, J.; Shi, Y.; Zhang, X.; Gao, G.F.
Deposited on	:	2017-02-15
Resolution	:	4.20 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:

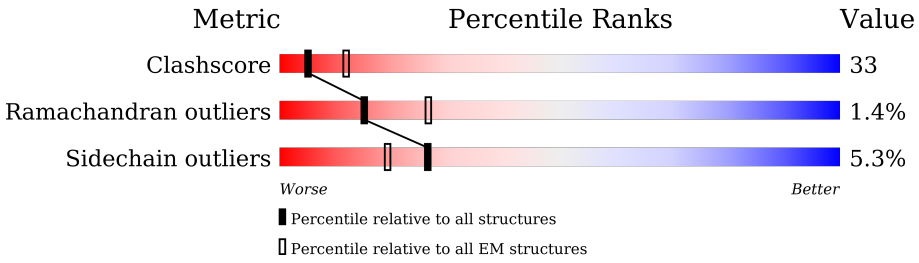
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 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	1323	55% 57% 24% • • 14%
1	B	1323	52% 57% 24% • • 14%
1	C	1323	54% 59% 23% • • 14%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 26422 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 S protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1141	Total	C	N	O	S	1	0
			8806	5599	1457	1699	51		
1	B	1141	Total	C	N	O	S	1	0
			8806	5599	1457	1699	51		
1	C	1141	Total	C	N	O	S	1	0
			8810	5601	1458	1700	51		

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	751	SER	ARG	engineered mutation	UNP W6A028
A	1020	GLN	ARG	engineered mutation	UNP W6A028
A	1295	GLU	-	expression tag	UNP W6A028
A	1296	PHE	-	expression tag	UNP W6A028
A	1297	ARG	-	expression tag	UNP W6A028
A	1298	LEU	-	expression tag	UNP W6A028
A	1299	VAL	-	expression tag	UNP W6A028
A	1300	PRO	-	expression tag	UNP W6A028
A	1301	ARG	-	expression tag	UNP W6A028
A	1302	GLY	-	expression tag	UNP W6A028
A	1303	SER	-	expression tag	UNP W6A028
A	1304	PRO	-	expression tag	UNP W6A028
A	1305	GLY	-	expression tag	UNP W6A028
A	1306	SER	-	expression tag	UNP W6A028
A	1307	GLY	-	expression tag	UNP W6A028
A	1308	TYR	-	expression tag	UNP W6A028
A	1309	ILE	-	expression tag	UNP W6A028
A	1310	PRO	-	expression tag	UNP W6A028
A	1311	GLU	-	expression tag	UNP W6A028
A	1312	ALA	-	expression tag	UNP W6A028
A	1313	PRO	-	expression tag	UNP W6A028
A	1314	ARG	-	expression tag	UNP W6A028
A	1315	ASP	-	expression tag	UNP W6A028
A	1316	GLY	-	expression tag	UNP W6A028

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1317	GLN	-	expression tag	UNP W6A028
A	1318	ALA	-	expression tag	UNP W6A028
A	1319	TYR	-	expression tag	UNP W6A028
A	1320	VAL	-	expression tag	UNP W6A028
A	1321	ARG	-	expression tag	UNP W6A028
A	1322	LYS	-	expression tag	UNP W6A028
A	1323	ASP	-	expression tag	UNP W6A028
A	1324	GLY	-	expression tag	UNP W6A028
A	1325	GLU	-	expression tag	UNP W6A028
A	1326	TRP	-	expression tag	UNP W6A028
A	1327	VAL	-	expression tag	UNP W6A028
A	1328	LEU	-	expression tag	UNP W6A028
A	1329	LEU	-	expression tag	UNP W6A028
A	1330	SER	-	expression tag	UNP W6A028
A	1331	THR	-	expression tag	UNP W6A028
A	1332	PHE	-	expression tag	UNP W6A028
A	1333	LEU	-	expression tag	UNP W6A028
A	1334	GLY	-	expression tag	UNP W6A028
A	1335	HIS	-	expression tag	UNP W6A028
A	1336	HIS	-	expression tag	UNP W6A028
A	1337	HIS	-	expression tag	UNP W6A028
A	1338	HIS	-	expression tag	UNP W6A028
A	1339	HIS	-	expression tag	UNP W6A028
A	1340	HIS	-	expression tag	UNP W6A028
B	751	SER	ARG	engineered mutation	UNP W6A028
B	1020	GLN	ARG	engineered mutation	UNP W6A028
B	1295	GLU	-	expression tag	UNP W6A028
B	1296	PHE	-	expression tag	UNP W6A028
B	1297	ARG	-	expression tag	UNP W6A028
B	1298	LEU	-	expression tag	UNP W6A028
B	1299	VAL	-	expression tag	UNP W6A028
B	1300	PRO	-	expression tag	UNP W6A028
B	1301	ARG	-	expression tag	UNP W6A028
B	1302	GLY	-	expression tag	UNP W6A028
B	1303	SER	-	expression tag	UNP W6A028
B	1304	PRO	-	expression tag	UNP W6A028
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B	1306	SER	-	expression tag	UNP W6A028
B	1307	GLY	-	expression tag	UNP W6A028
B	1308	TYR	-	expression tag	UNP W6A028
B	1309	ILE	-	expression tag	UNP W6A028
B	1310	PRO	-	expression tag	UNP W6A028

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1311	GLU	-	expression tag	UNP W6A028
B	1312	ALA	-	expression tag	UNP W6A028
B	1313	PRO	-	expression tag	UNP W6A028
B	1314	ARG	-	expression tag	UNP W6A028
B	1315	ASP	-	expression tag	UNP W6A028
B	1316	GLY	-	expression tag	UNP W6A028
B	1317	GLN	-	expression tag	UNP W6A028
B	1318	ALA	-	expression tag	UNP W6A028
B	1319	TYR	-	expression tag	UNP W6A028
B	1320	VAL	-	expression tag	UNP W6A028
B	1321	ARG	-	expression tag	UNP W6A028
B	1322	LYS	-	expression tag	UNP W6A028
B	1323	ASP	-	expression tag	UNP W6A028
B	1324	GLY	-	expression tag	UNP W6A028
B	1325	GLU	-	expression tag	UNP W6A028
B	1326	TRP	-	expression tag	UNP W6A028
B	1327	VAL	-	expression tag	UNP W6A028
B	1328	LEU	-	expression tag	UNP W6A028
B	1329	LEU	-	expression tag	UNP W6A028
B	1330	SER	-	expression tag	UNP W6A028
B	1331	THR	-	expression tag	UNP W6A028
B	1332	PHE	-	expression tag	UNP W6A028
B	1333	LEU	-	expression tag	UNP W6A028
B	1334	GLY	-	expression tag	UNP W6A028
B	1335	HIS	-	expression tag	UNP W6A028
B	1336	HIS	-	expression tag	UNP W6A028
B	1337	HIS	-	expression tag	UNP W6A028
B	1338	HIS	-	expression tag	UNP W6A028
B	1339	HIS	-	expression tag	UNP W6A028
B	1340	HIS	-	expression tag	UNP W6A028
C	751	SER	ARG	engineered mutation	UNP W6A028
C	1020	GLN	ARG	engineered mutation	UNP W6A028
C	1295	GLU	-	expression tag	UNP W6A028
C	1296	PHE	-	expression tag	UNP W6A028
C	1297	ARG	-	expression tag	UNP W6A028
C	1298	LEU	-	expression tag	UNP W6A028
C	1299	VAL	-	expression tag	UNP W6A028
C	1300	PRO	-	expression tag	UNP W6A028
C	1301	ARG	-	expression tag	UNP W6A028
C	1302	GLY	-	expression tag	UNP W6A028
C	1303	SER	-	expression tag	UNP W6A028
C	1304	PRO	-	expression tag	UNP W6A028

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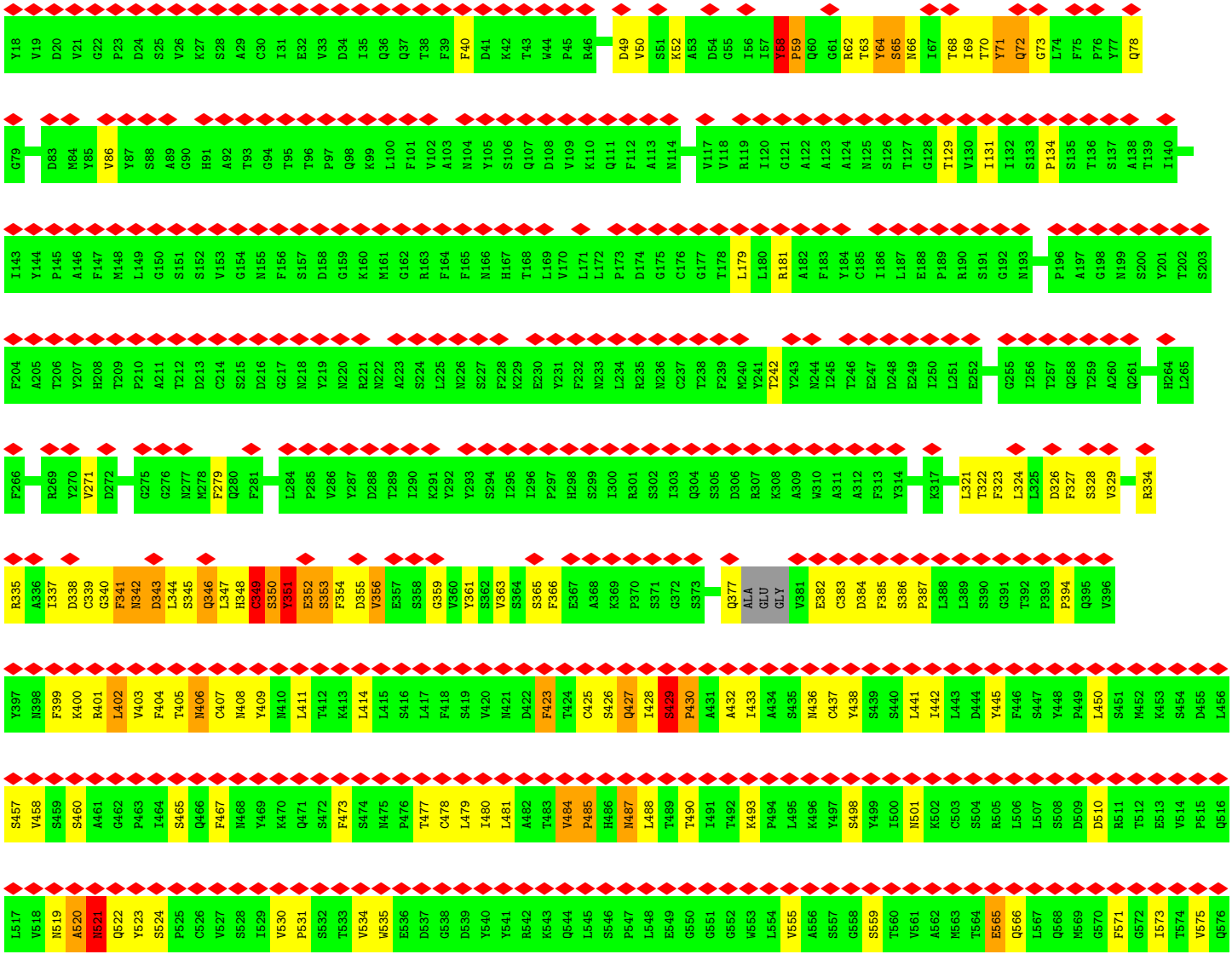
Chain	Residue	Modelled	Actual	Comment	Reference
C	1305	GLY	-	expression tag	UNP W6A028
C	1306	SER	-	expression tag	UNP W6A028
C	1307	GLY	-	expression tag	UNP W6A028
C	1308	TYR	-	expression tag	UNP W6A028
C	1309	ILE	-	expression tag	UNP W6A028
C	1310	PRO	-	expression tag	UNP W6A028
C	1311	GLU	-	expression tag	UNP W6A028
C	1312	ALA	-	expression tag	UNP W6A028
C	1313	PRO	-	expression tag	UNP W6A028
C	1314	ARG	-	expression tag	UNP W6A028
C	1315	ASP	-	expression tag	UNP W6A028
C	1316	GLY	-	expression tag	UNP W6A028
C	1317	GLN	-	expression tag	UNP W6A028
C	1318	ALA	-	expression tag	UNP W6A028
C	1319	TYR	-	expression tag	UNP W6A028
C	1320	VAL	-	expression tag	UNP W6A028
C	1321	ARG	-	expression tag	UNP W6A028
C	1322	LYS	-	expression tag	UNP W6A028
C	1323	ASP	-	expression tag	UNP W6A028
C	1324	GLY	-	expression tag	UNP W6A028
C	1325	GLU	-	expression tag	UNP W6A028
C	1326	TRP	-	expression tag	UNP W6A028
C	1327	VAL	-	expression tag	UNP W6A028
C	1328	LEU	-	expression tag	UNP W6A028
C	1329	LEU	-	expression tag	UNP W6A028
C	1330	SER	-	expression tag	UNP W6A028
C	1331	THR	-	expression tag	UNP W6A028
C	1332	PHE	-	expression tag	UNP W6A028
C	1333	LEU	-	expression tag	UNP W6A028
C	1334	GLY	-	expression tag	UNP W6A028
C	1335	HIS	-	expression tag	UNP W6A028
C	1336	HIS	-	expression tag	UNP W6A028
C	1337	HIS	-	expression tag	UNP W6A028
C	1338	HIS	-	expression tag	UNP W6A028
C	1339	HIS	-	expression tag	UNP W6A028
C	1340	HIS	-	expression tag	UNP W6A028

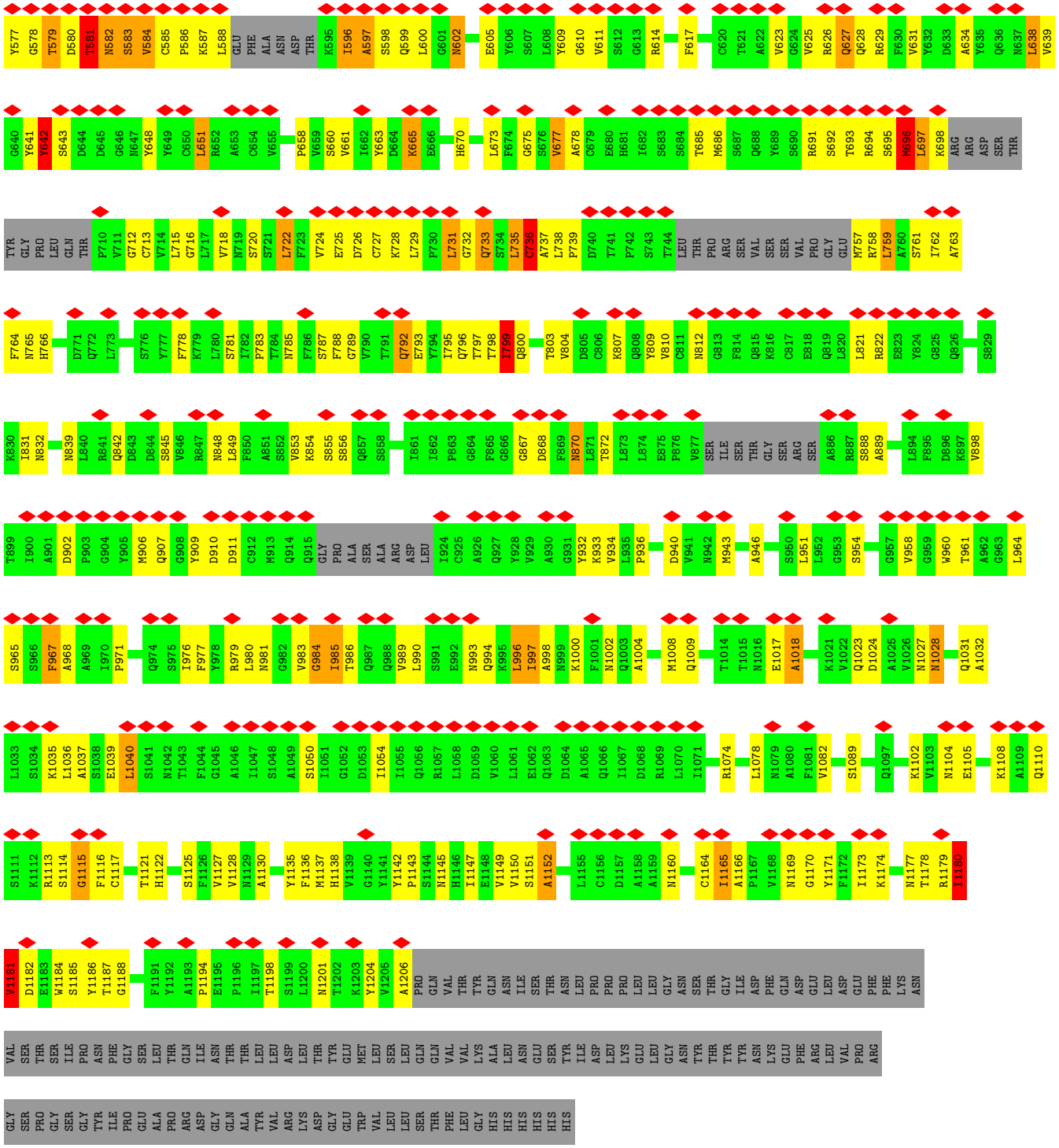
3 Residue-property plots (i)

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: S protein

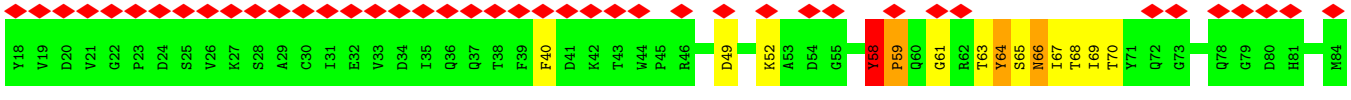
Chain A:

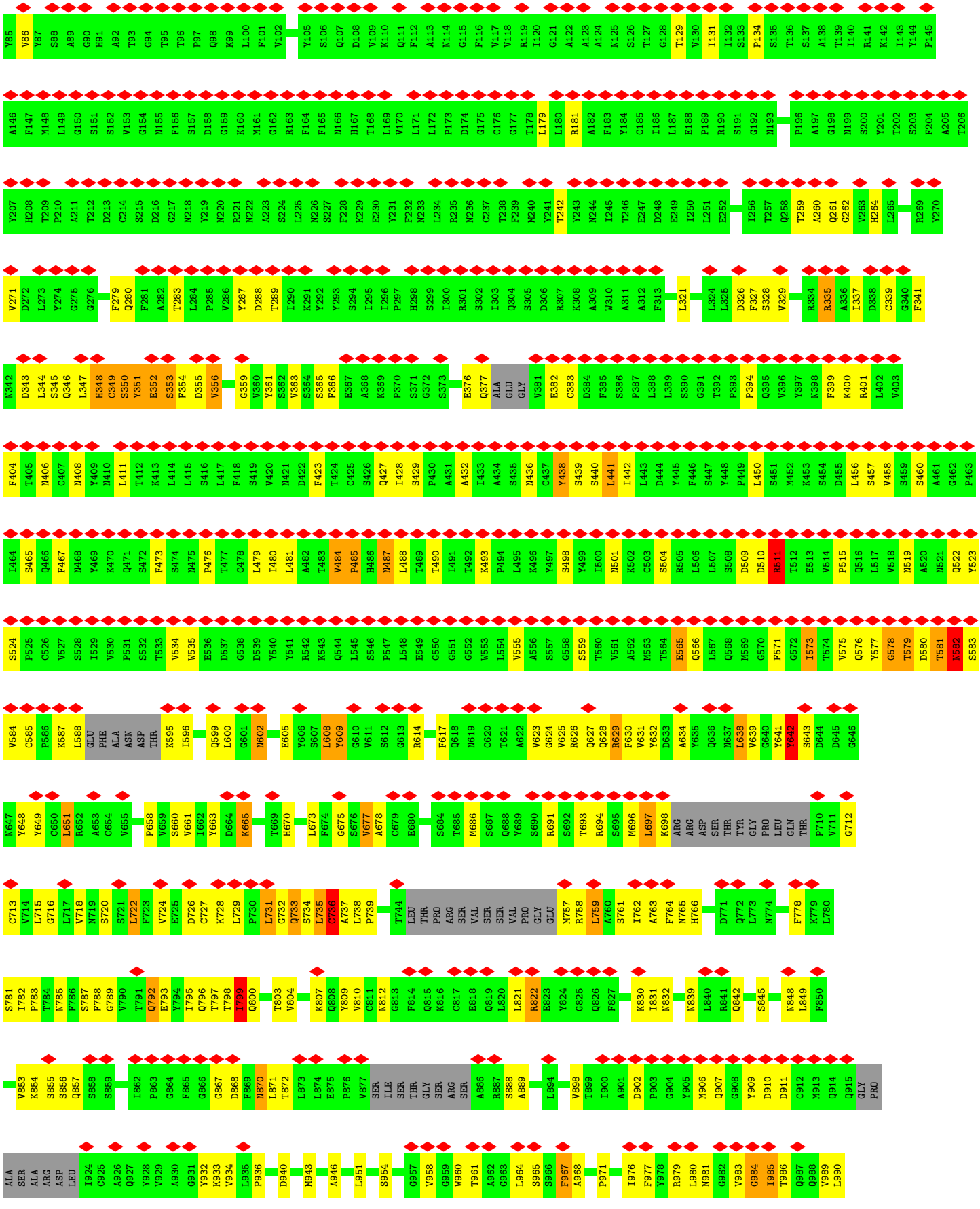


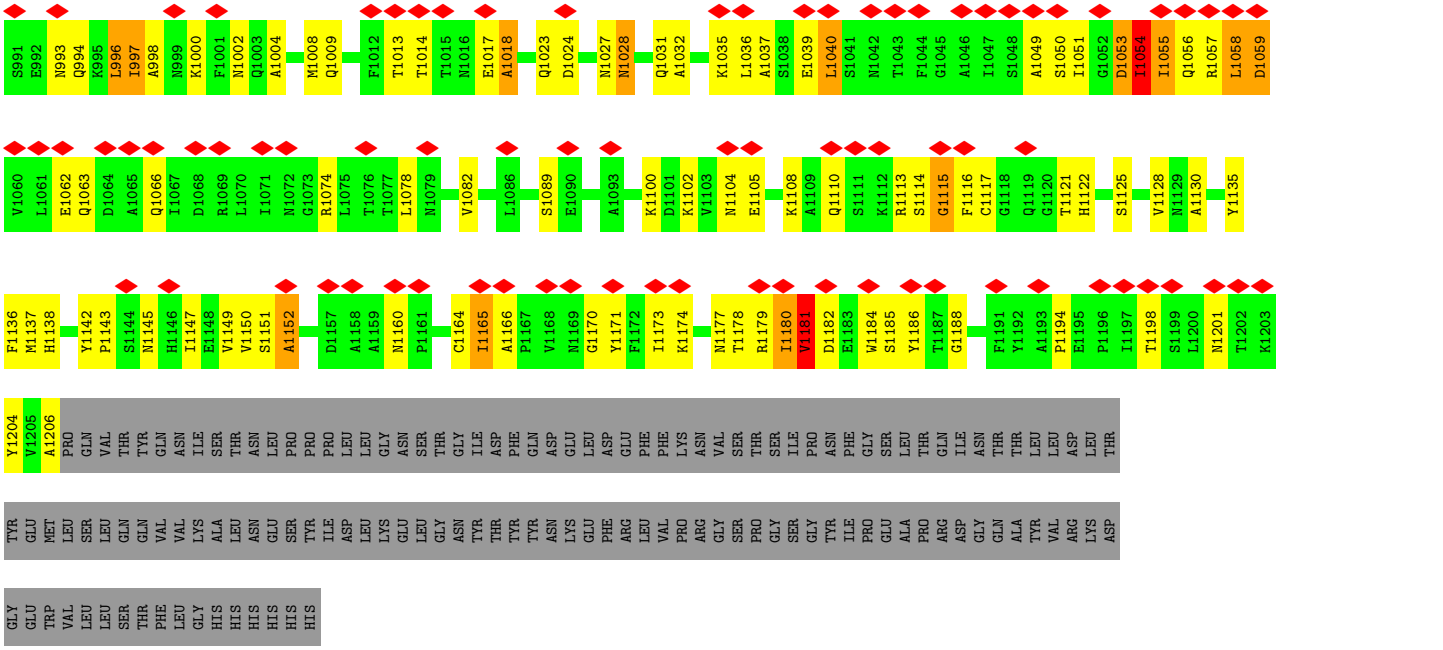


• Molecule 1: S protein

Chain B:

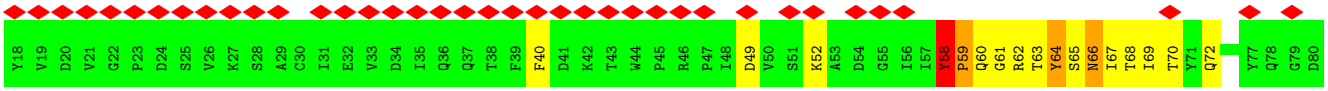


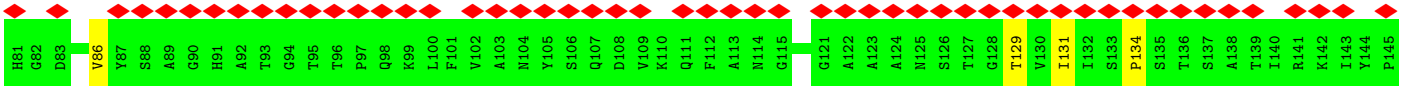

Y85 V86 Y87 S88 A89 G90 H91 A92 T93 G94 T95 T96 P97 Q98 K99 L100 F101 V102 Y105 S106 Q107 D108 V109 K110 Q111 F112 A113 N114 G115 F116 V117 V118 R119 I120 G121 A122 A123 A124 N125 S126 T127 G128 T129 V130 I131 I132 S133 P134 S135 T136 S137 A138 T139 I140 R141 K142 I143 Y144 P145
A146 F147 M148 L149 G150 S151 S152 V153 G154 N155 F156 S157 D158 G159 K160 M161 G162 R163 F164 F165 N166 H167 T168 L169 V170 L171 L172 P173 D174 G175 C176 G177 T178 L179 L180 R181 A182 F183 Y184 C185 I186 L187 E188 P189 R190 S191 G192 N193 P196 A197 G198 N199 S200 Y201 T202 S203 F204 A205 T206
Y207 H208 T209 P210 A211 T212 D213 C214 S215 D216 G217 N218 Y219 N220 R221 N222 A223 S224 L225 N226 S227 F228 K229 E230 Y231 F232 N233 L234 R235 N236 C237 T238 F239 M240 Y241 T242 Y243 N244 I245 T246 E247 D248 E249 I250 L251 E252 I256 T257 Q258 T259 A260 Q261 G262 Y263 H264 L265 R269 Y270
V271 D272 L273 Y274 G275 G276 F279 Q280 F281 A282 T283 L284 P285 V286 Y287 D288 T289 I290 K291 Y292 Y293 S294 I295 I296 P297 H298 S299 I300 R301 S302 I303 Q304 S305 D306 R307 K308 A309 W310 A311 A312 F313 L321 L324 L325 D326 F327 S328 V329 R334 R335 A336 I337 D338 C339 G340 F341
N342 D343 L344 S345 Q346 L347 H348 C349 S350 Y351 E352 S353 F354 D355 V356 G359 V360 Y361 S362 V363 S364 S365 F366 E367 A368 K369 P370 S371 G372 S373 E376 Q377 ALA GLU GLY V381 E382 C383 D384 F385 S386 P387 L388 L389 S390 G391 T392 P393 P394 Q395 V396 Y397 N398 F399 K400 R401 L402 V403
F404 T405 N406 C407 N408 Y409 N410 L411 T412 K413 L414 L415 S416 L417 F418 S419 V420 N421 D422 F423 T424 C425 S426 Q427 I428 S429 P430 A431 A432 I433 A434 S435 N436 C437 Y438 S439 S440 L441 I442 L443 D444 Y445 F446 S447 Y448 P449 L450 S451 M452 K453 S454 D455 L456 S457 V458 S459 S460 A461 G462 P463
I464 S465 Q466 F467 N468 Y469 K470 Q471 S472 F473 S474 N475 P476 T477 C478 L479 I480 L481 A482 T483 V484 P485 H486 N487 L488 T489 T490 I491 T492 K493 P494 L495 K496 Y497 S498 Y499 I500 N501 K502 C503 S504 R505 L506 L507 S508 D509 D510 R511 T512 E513 V514 P515 Q516 L517 V518 N519 A520 N521 Q522 Y523
S524 P525 C526 V527 S528 I529 V530 P531 S532 T533 V534 W535 E536 D537 G538 D539 Y540 Y541 R542 K543 Q544 L545 S546 P547 L548 E549 G550 G551 G552 W553 L554 V555 A556 S557 G558 S559 T560 V561 A562 M563 T564 E565 Q566 L567 Q568 M569 G570 F571 G572 I573 T574 V575 Q576 Y577 G578 T579 D580 T581 N582 S583
V584 C585 P586 K587 L588 GLU PHE ALA ASN ASP THR K595 I596 Q599 L600 G601 N602 E605 Y606 S607 L608 Y609 G610 V611 S612 G613 R614 F617 Q618 N619 C620 T621 A622 V623 G624 V625 R626 Q627 Q628 R629 F630 V631 Y632 D633 A634 Y635 Q636 N637 L638 V639 G640 Y641 Y642 S643 D644 D645 G646
N647 Y648 Y649 C650 L651 R652 A653 C654 V655 P658 V659 S660 V661 I662 Y663 D664 K665 T669 H670 L673 F674 G675 S676 V677 A678 C679 E680 S684 T685 M686 S687 Q688 Y689 S690 R691 S692 T693 R694 S695 M696 L697 K698 ARG ARG ASP SER THR TYR GLY PRO LEU GLN THR P710 V711 G712
C713 V714 L715 G716 L717 V718 N719 S720 S721 L722 F723 V724 E725 D726 C727 K728 L729 P730 L731 G732 Q733 S734 L735 C736 A737 L738 P739 T744 LEU THR PRO ARG SER VAL SER SER VAL PRO GLY GLU M757 R758 L759 A760 S761 I762 A763 F764 N765 H766 D771 Q772 L773 N774 F778 K779 L780
S781 I782 P783 T784 N785 F786 S787 F788 G789 V790 T791 Q792 E793 Y794 I795 Q796 T797 T798 T799 Q800 T803 V804 K807 Q808 Y809 V810 C811 N812 G813 F814 Q815 K816 C817 E818 Q819 L820 L821 R822 E823 Y824 G825 Q826 F827 K830 I831 N832 N839 L840 R841 Q842 S845 N848 L849 F850
V853 K854 S855 S856 Q857 S858 S859 I862 P863 G864 F865 G866 G867 D868 F869 N870 L871 T872 L873 L874 E875 P876 V877 SER ILE SER THR GLY SER ARG SER A886 R887 S888 A889 L894 V898 T899 I900 A901 D902 P903 G904 Y905 M906 Q907 G908 Y909 D910 D911 C912 M913 Q914 Q915 GLY PRO
ALA SER ALA ARG ASP LEU I924 C925 A926 Q927 Y928 V929 A930 G931 Y932 K933 V934 L935 P936 D940 M943 A946 L951 S954 G957 V958 G959 W960 T961 A962 G963 L964 S965 S966 F967 A968 P971 I976 F977 Y978 R979 L980 N981 G982 V983 G984 I985 T986 Q987 Q988 V989 L990

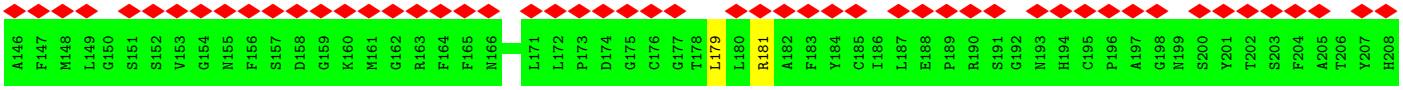


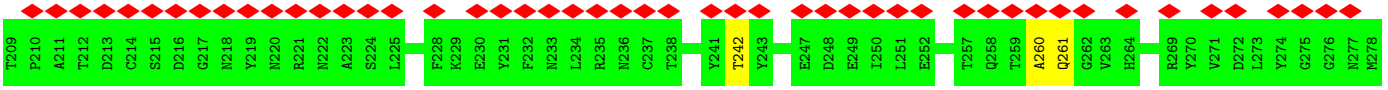
- Molecule 1: S protein

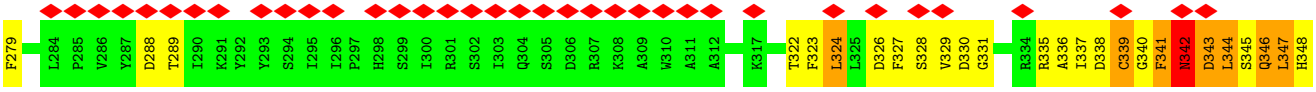
Chain C:

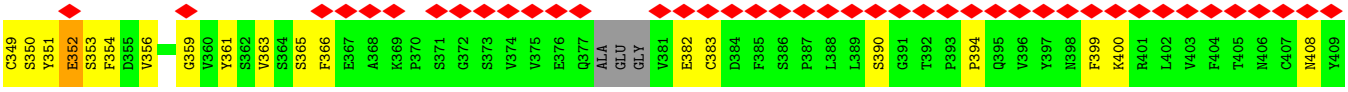


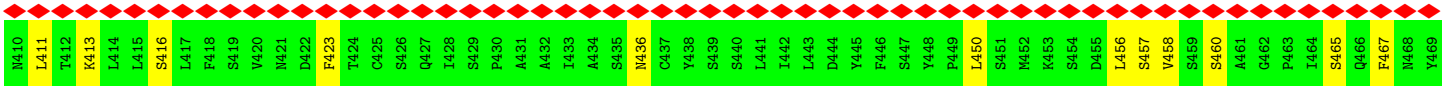


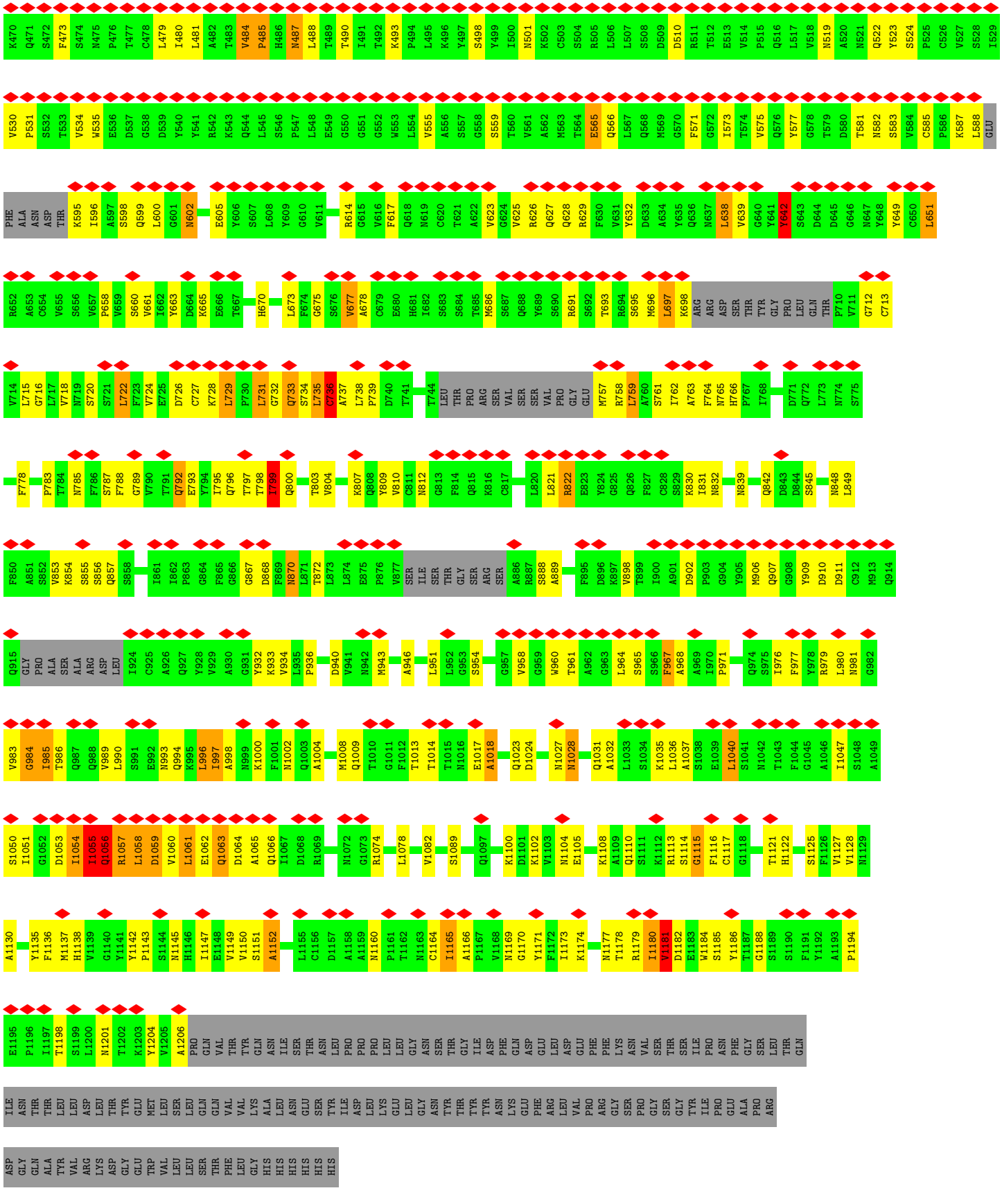











K470 Q471 S472 F473 S474 N475 P476 T477 C478 L479 I480 L481 A482 T483 V484 P485 H486 N487 L488 T489 T490 I491 T492 K493 P494 L495 K496 Y497 S498 Y499 I500 N501 K502 C503 S504 R505 L506 L507 S508 D509 D510 R511 T512 E513 V514 P515 Q516 L517 V518 N519 A520 N521 Q522 Y523 S524 P525 C526 V527 S528 I529
V530 P531 S532 T533 V534 W535 E536 D537 G538 D539 Y540 Y541 R542 K543 Q544 L545 S546 P547 L548 E549 G550 G551 G552 W553 L554 V555 A556 S557 G558 S559 T560 V561 A562 M563 T564 E565 Q566 L567 Q568 M569 G570 F571 G572 I573 T574 V575 Q576 Y577 G578 T579 D580 T581 N582 S583 V584 C585 P586 K587 L588 GLU
PHE ALA ASN ASP THR K595 I596 A597 S598 Q599 L600 G601 N602 E605 Y606 S607 L608 Y609 G610 V611 R614 G615 V616 F617 Q618 N619 C620 T621 A622 V623 G624 V625 R626 Q627 Q628 R629 F630 V631 Y632 D633 A634 Y635 Q636 N637 L638 V639 G640 Y641 Y642 S643 D644 D645 G646 N647 Y648 Y649 C650 L651
R652 A653 C654 V655 S656 V657 P658 V659 S660 V661 I662 Y663 D664 K665 E666 T667 H670 L673 F674 G675 S676 V677 A678 C679 E680 H681 I682 S683 S684 T685 M686 S687 Q688 Y689 S690 R691 S692 T693 R694 S695 M696 L697 K698 ARG ARG ASP SER THR TYR GLY PRO LEU GLN THR P710 V711 G712 C713
V714 L715 G716 L717 V718 N719 S720 S721 L722 F723 V724 E725 D726 C727 K728 L729 P730 L731 G732 Q733 S734 L735 C736 A737 L738 P739 D740 T741 T744 LEU THR PRO ARG SER VAL SER SER VAL PRO GLY GLU M757 R758 L759 A760 S761 I762 A763 F764 N765 H766 P767 I768 D771 Q772 L773 N774 S775
F778 P783 T784 N785 F786 S787 F788 G789 V790 T791 Q792 E793 Y794 I795 Q796 T797 T798 I799 Q800 T803 V804 K807 Q808 Y809 V810 C811 N812 G813 F814 Q815 K816 C817 L820 L821 R822 E823 Y824 G825 Q826 F827 C828 S829 K830 I831 N832 N839 Q842 D843 D844 S845 N848 L849
F850 A851 S852 V853 K854 S855 S856 Q857 S858 I861 I862 P863 G864 F865 G866 G867 D868 F869 N870 L871 T872 L873 L874 E875 P876 V877 SER ILE SER THR GLY SER ARG SER A886 R887 S888 A889 F895 D896 K897 V898 T899 I900 A901 D902 P903 G904 Y905 M906 Q907 G908 Y909 D910 D911 C912 M913 Q914
Q915 GLY PRO ALA SER ALA ARG ASP LEU I924 C925 A926 Q927 Y928 V929 A930 G931 Y932 K933 V934 L935 P936 D940 V941 N942 M943 A946 L951 L952 G953 S954 G957 V958 G959 W960 T961 A962 G963 L964 S965 S966 F967 A968 A969 I970 P971 Q974 S975 I976 F977 Y978 R979 L980 N981 G982
V983 G984 I985 T986 Q987 Q988 V989 L990 S991 E992 N993 Q994 K995 L996 I997 A998 N999 K1000 F1001 N1002 Q1003 A1004 M1008 Q1009 T1010 G1011 F1012 T1013 T1014 T1015 N1016 E1017 A1018 Q1023 D1024 N1027 N1028 Q1031 A1032 L1033 S1034 K1035 L1036 A1037 S1038 E1039 L1040 S1041 N1042 T1043 F1044 G1045 A1046 I1047 S1048 A1049
S1050 I1051 G1052 D1053 I1054 I1055 Q1056 R1057 L1058 D1059 V1060 L1061 E1062 Q1063 D1064 A1065 Q1066 I1067 D1068 R1069 N1072 G1073 R1074 L1078 V1082 S1089 Q1097 K1100 D1101 K1102 V1103 N1104 E1105 K1108 A1109 Q1110 S1111 K1112 R1113 S1114 G1115 F1116 C1117 G1118 T1121 H1122 S1125 F1126 V1127 V1128 N1129
A1130 Y1135 F1136 M1137 H1138 V1139 G1140 Y1141 Y1142 P1143 S1144 N1145 H1146 I1147 E1148 V1149 V1150 S1151 A1152 L1155 C1156 D1157 A1158 A1159 N1160 P1161 T1162 N1163 C1164 I1165 A1166 P1167 V1168 N1169 G1170 Y1171 F1172 I1173 K1174 N1177 T1178 R1179 I1180 V1181 D1182 E1183 W1184 S1185 Y1186 T1187 G1188 S1189 S1190 F1191 Y1192 A1193 P1194
E1195 P1196 I1197 T1198 S1199 L1200 N1201 T1202 K1203 Y1204 V1205 A1206 PRO GLN VAL THR TYR GLN ASN ILE SER THR ASN LEU PRO PRO PRO LEU LEU LEU GLY ASN SER THR GLY ILE ASP PHE GLN ASP GLU LEU ASP GLU PHE PHE LYS ASN VAL SER THR SER ILE PRO ASN PHE GLY SER LEU THR GLN
ILE ASN THR THR LEU LEU ASP LEU THR TYR GLU MET LEU SER LEU GLN GLN VAL VAL LYS ALA LEU ASN GLU SER TYR ILE ASP LEU LYS GLU LEU GLY ASN TYR THR GLY TYR TYR ASN LYS GLU PHE ARG LEU VAL PRO ARG GLY SER PRO GLY SER GLY TYR ILE PRO GLU ALA PRO ARG
ASP GLY GLN ALA TYR VAL ARG LYS ASP GLY GLU TRP VAL LEU LEU SER THR PHE LEU GLY HIS HIS HIS HIS HIS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	60000	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 ($e^-/Å^2$)	8	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.179	Depositor
Minimum map value	-0.093	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.0595	Depositor
Map size (Å)	260.0, 260.0, 260.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3, 1.3, 1.3	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	0.58	6/9006 (0.1%)	0.81	29/12245 (0.2%)
1	B	0.51	1/9006 (0.0%)	0.80	24/12245 (0.2%)
1	C	0.51	1/9010 (0.0%)	0.78	22/12250 (0.2%)
All	All	0.53	8/27022 (0.0%)	0.80	75/36740 (0.2%)

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	20
1	B	0	20
1	C	0	19
All	All	0	59

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	349	CYS	N-CA	-15.13	1.16	1.46
1	A	349	CYS	C-O	9.59	1.41	1.23
1	A	349	CYS	CB-SG	-8.35	1.68	1.82
1	A	696	MET	N-CA	6.67	1.59	1.46
1	A	59	PRO	N-CD	5.22	1.55	1.47

The worst 5 of 75 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	735	LEU	CA-CB-CG	11.61	142.00	115.30
1	B	735	LEU	CA-CB-CG	11.58	141.93	115.30
1	A	735	LEU	CA-CB-CG	11.51	141.78	115.30
1	A	349	CYS	O-C-N	-11.07	104.98	122.70
1	A	1040	LEU	CA-CB-CG	7.84	133.32	115.30

There are no chirality outliers.

5 of 59 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	520	ALA	Mainchain
1	A	639	VAL	Peptide
1	A	642	TYR	Peptide
1	A	65	SER	Peptide
1	A	733	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	8806	0	8507	678	0
1	B	8806	0	8504	766	0
1	C	8810	0	8512	581	0
All	All	26422	0	25523	1686	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 33.

The worst 5 of 1686 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:339:CYS:SG	1:C:349:CYS:HB2	1.35	1.62
1:B:344:LEU:CD2	1:B:670:HIS:HB3	1.16	1.61
1:A:583:SER:HB2	1:A:609:TYR:CE1	1.37	1.60
1:C:335:ARG:HB3	1:C:354:PHE:CE2	1.34	1.60
1:B:344:LEU:HD22	1:B:670:HIS:CB	1.16	1.58

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	1128/1323 (85%)	964 (86%)	147 (13%)	17 (2%)	10	46
1	B	1128/1323 (85%)	965 (86%)	147 (13%)	16 (1%)	11	47
1	C	1128/1323 (85%)	966 (86%)	147 (13%)	15 (1%)	12	48
All	All	3384/3969 (85%)	2895 (86%)	441 (13%)	48 (1%)	15	47

5 of 48 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	583	SER
1	A	584	VAL
1	A	596	ILE
1	A	597	ALA
1	A	797	THR

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	973/1143 (85%)	919 (94%)	54 (6%)	21	49
1	B	973/1143 (85%)	923 (95%)	50 (5%)	24	51
1	C	974/1143 (85%)	924 (95%)	50 (5%)	24	51
All	All	2920/3429 (85%)	2766 (95%)	154 (5%)	26	50

5 of 154 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	352	GLU
1	C	870	ASN
1	C	458	VAL
1	C	555	VAL
1	C	1059	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 62 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	599	GLN
1	C	848	ASN
1	B	839	ASN
1	C	842	GLN
1	C	1028	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.

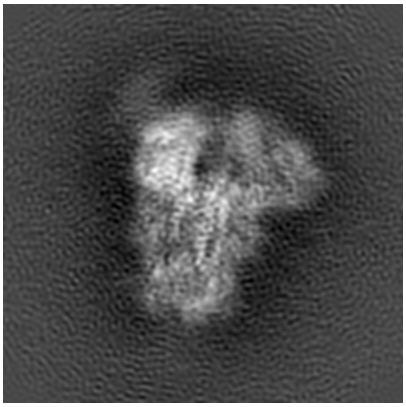
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-6707. These allow visual inspection of the internal detail of the map and identification of artifacts.

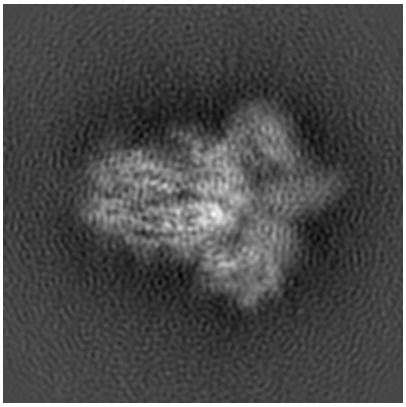
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

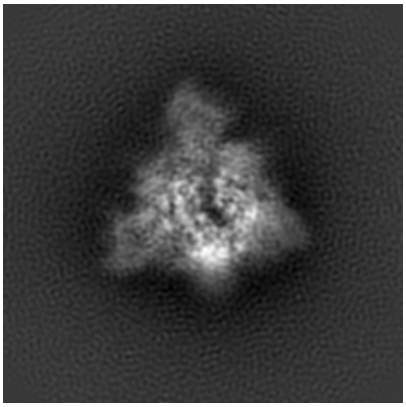
6.1.1 Primary map



X



Y

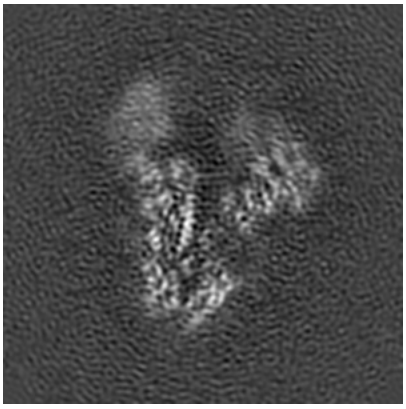


Z

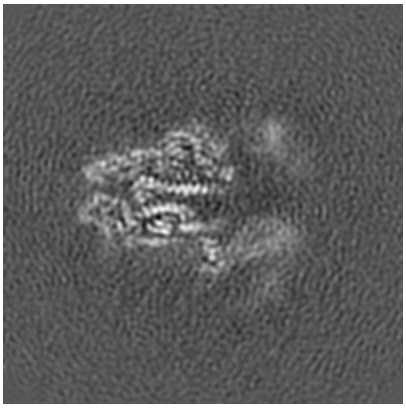
The images above show the map projected in three orthogonal directions.

6.2 Central slices

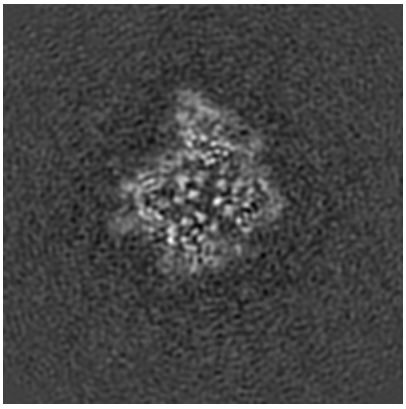
6.2.1 Primary map



X Index: 100



Y Index: 100

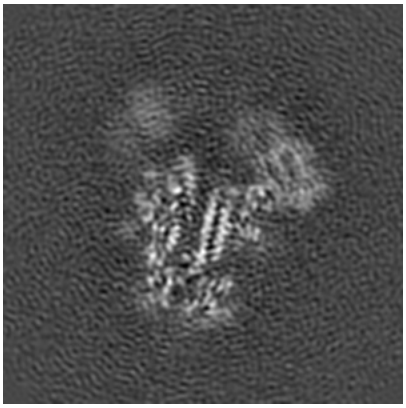


Z Index: 100

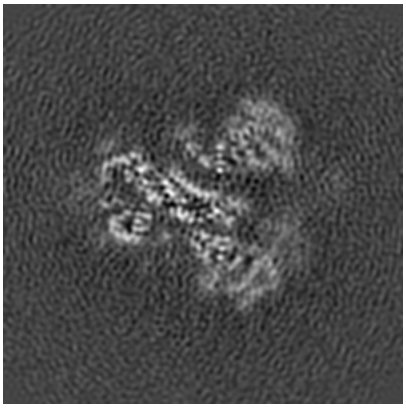
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

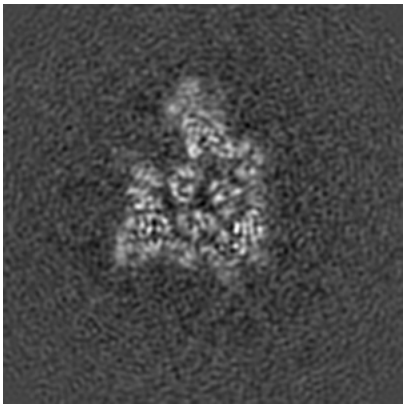
6.3.1 Primary map



X Index: 96



Y Index: 87



Z Index: 108

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 0.0595. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

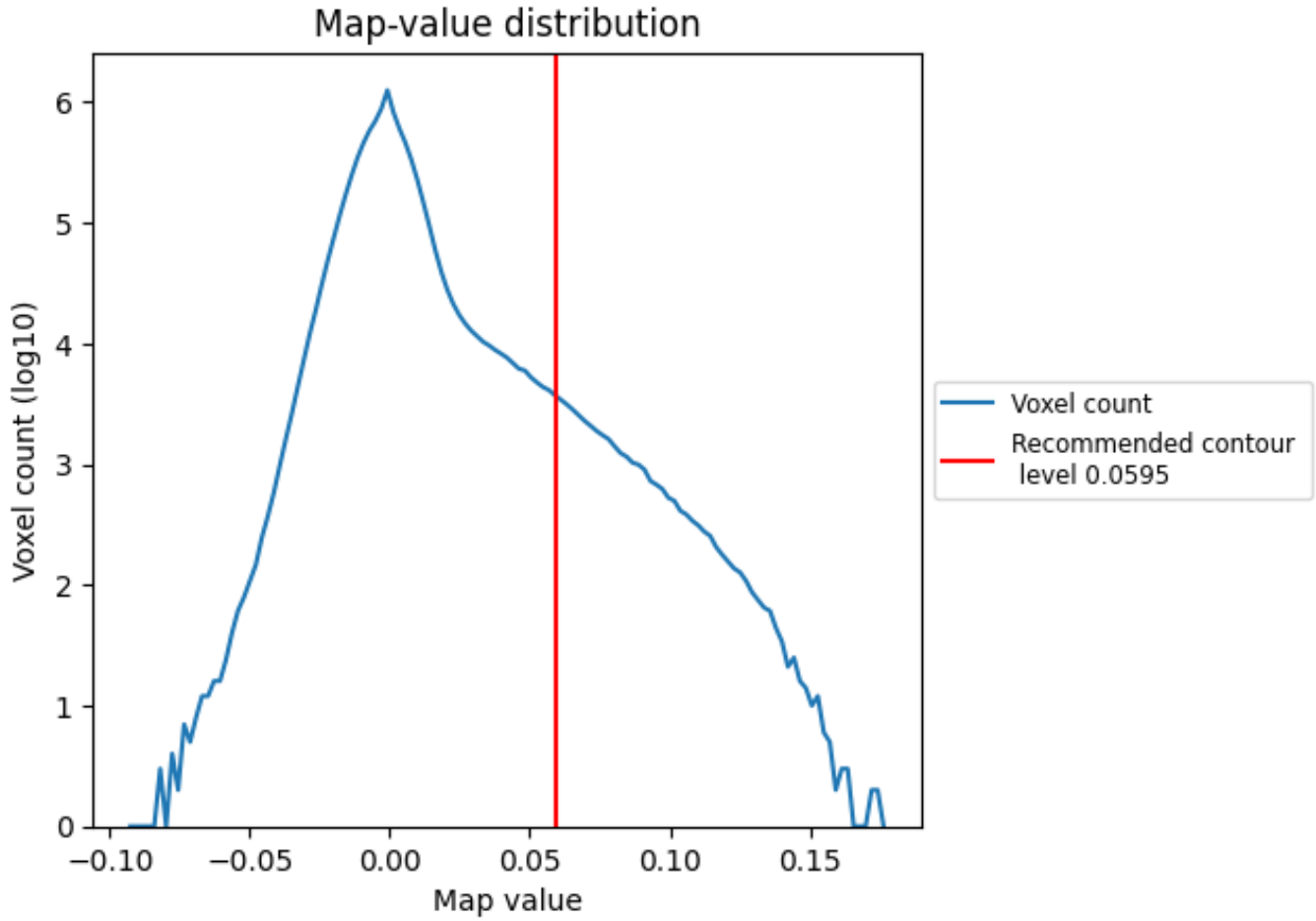
6.5 Mask visualisation (i)

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

7 Map analysis

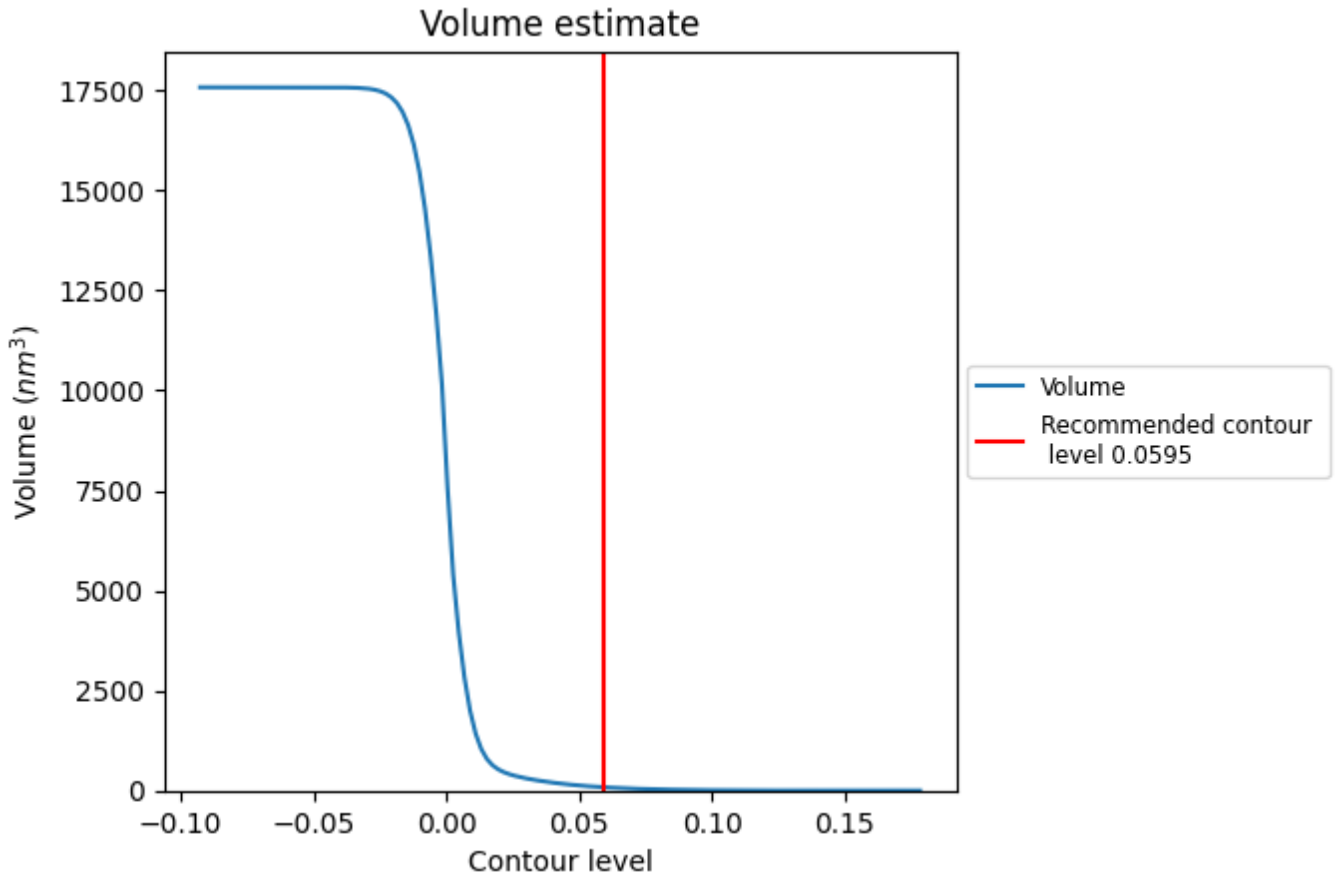
This section contains the results of statistical analysis of the map.

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.

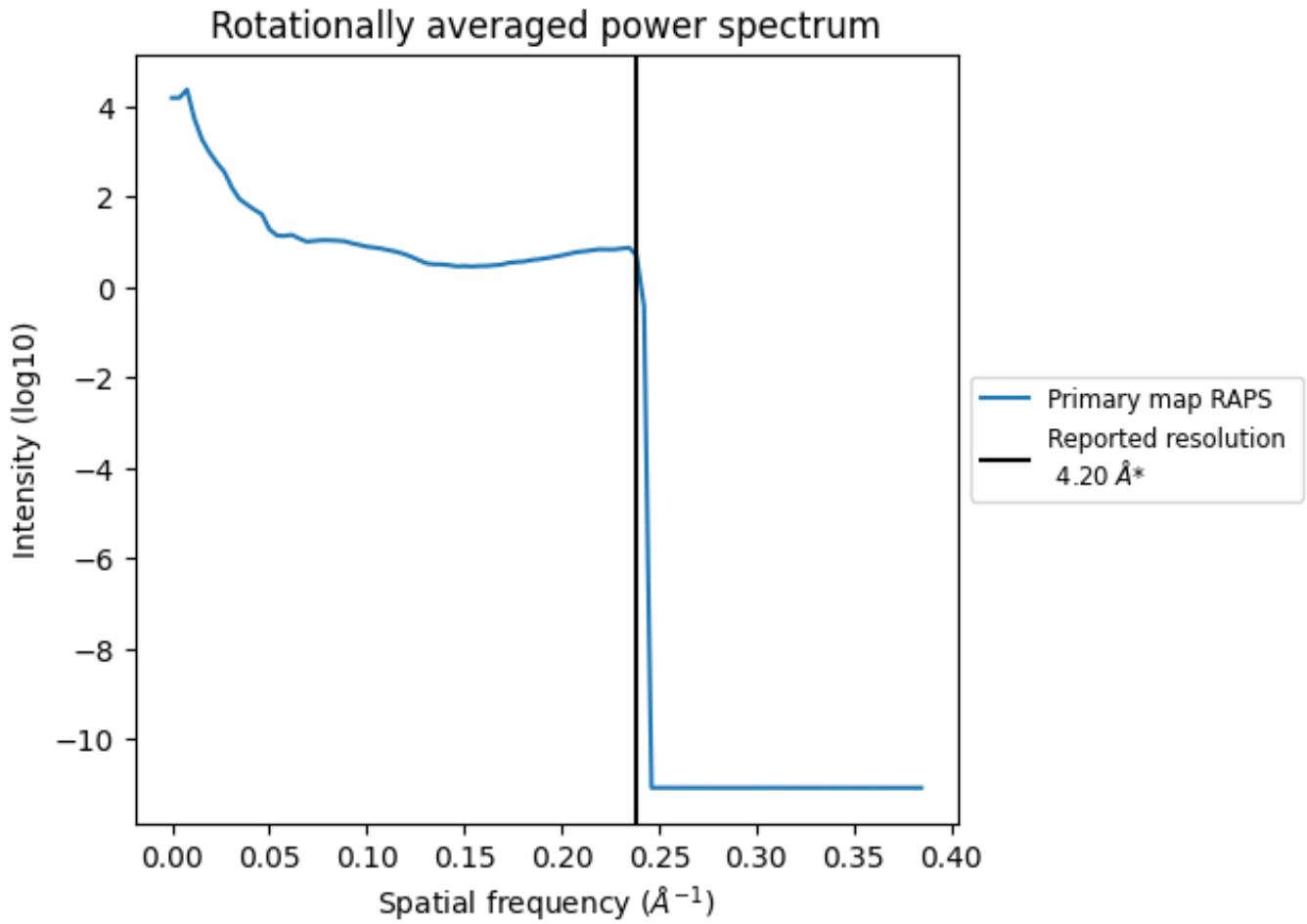
7.2 Volume estimate (i)



The volume at the recommended contour level is 82 nm^3; this corresponds to an approximate mass of 74 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}

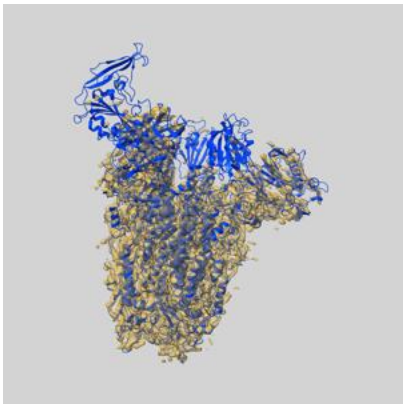
8 Fourier-Shell correlation (i)

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

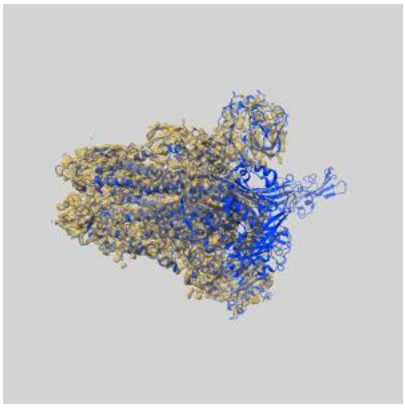
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-6707 and PDB model 5X5F. Per-residue inclusion information can be found in section 3 on page 7.

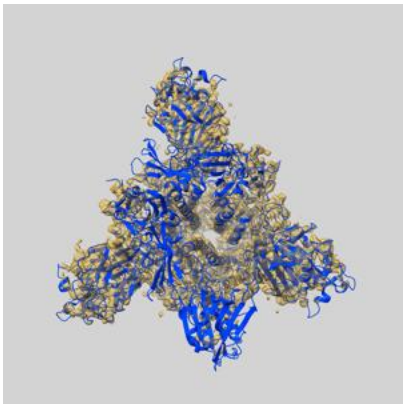
9.1 Map-model overlay



X



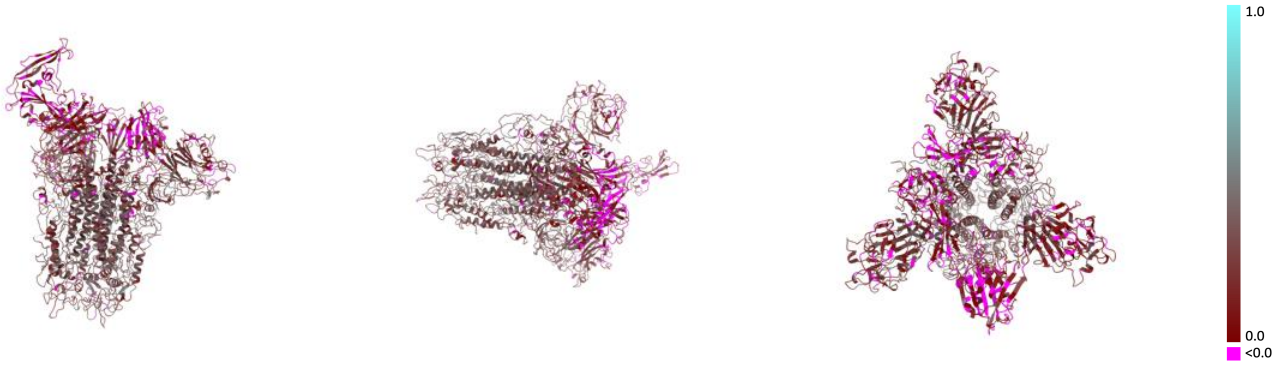
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0595 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.

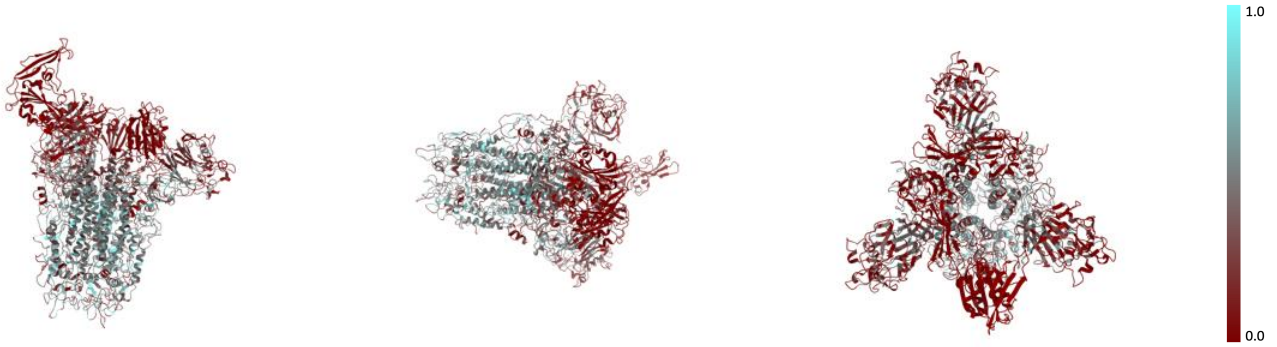
9.2 Q-score mapped to coordinate model (i)



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.

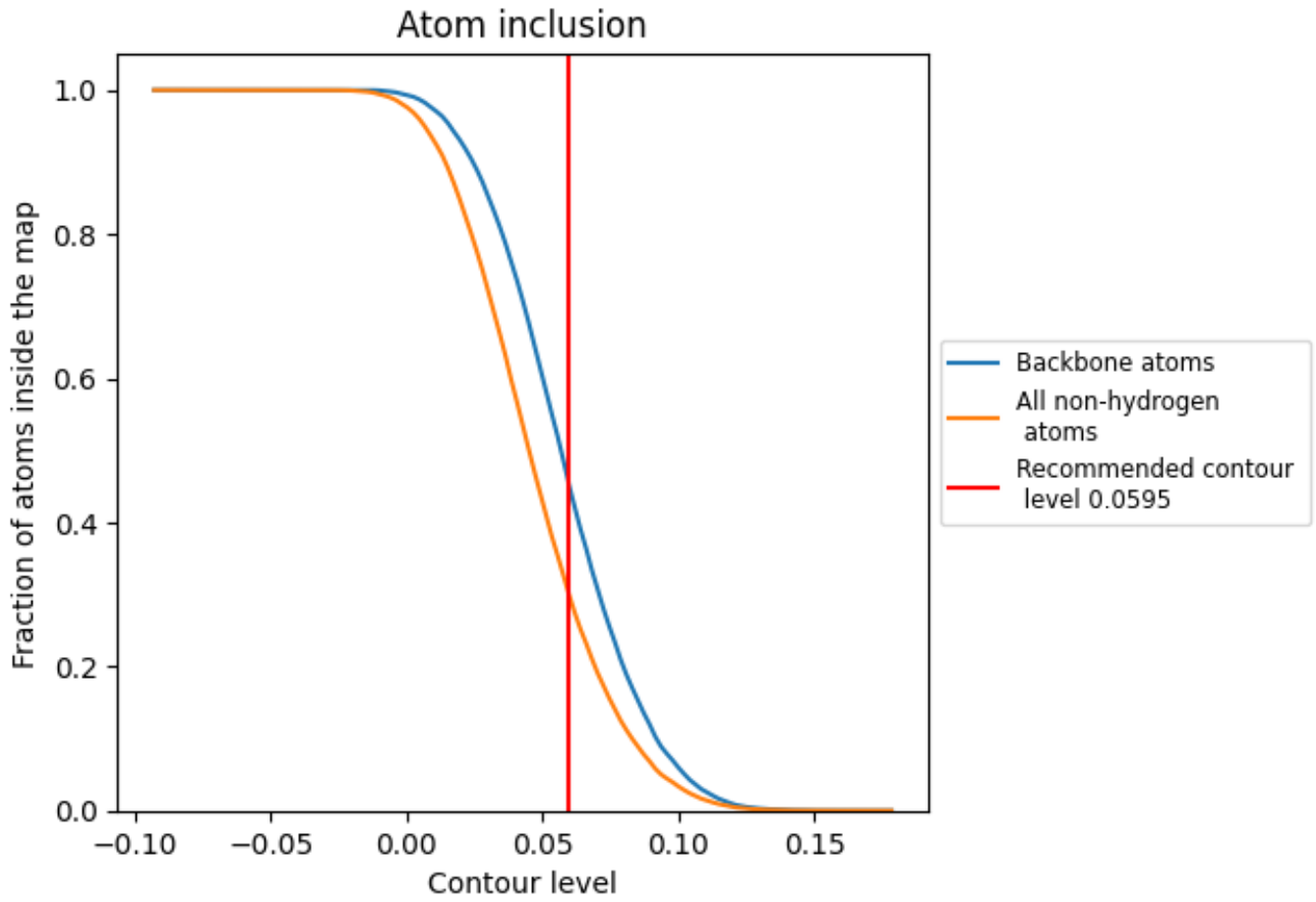
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0595).

9.4 Atom inclusion (i)



At the recommended contour level, 46% of all backbone atoms, 31% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0595) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3054	0.2240
A	0.2892	0.2110
B	0.3184	0.2350
C	0.3087	0.2270