wwPDB EM Validation Summary Report

Oct 26, 2026 – 02:25 PM EDT

PDB ID	:	9O5R / pdb_00009o5r
EMDB ID	:	EMD-70147
Title	:	VAR2CSA in complex with V2C.044 Fab
Authors	:	Raghavan, S.S.R.; Ward, A.B.
Deposited on	:	2025-04-10
Resolution	:	3.50 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:

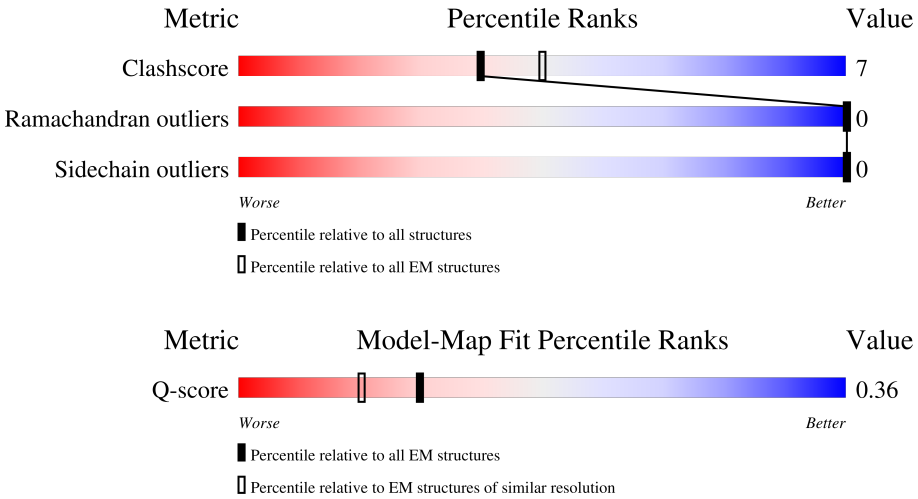
EMDB validation analysis	:	0.0.1.dev133
MolProbity	:	4-5-2 with Phenix2.2
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 3.50 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

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	H	120	14% 81% 19%
2	L	108	6% 69% 31%
3	A	2683	31% 51% 11% 38%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 15461 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 V2C.044 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	H	120	Total	C	N	O	S	0	0
			933	593	151	184	5		

- Molecule 2 is a protein called V2C.044 Light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	108	Total	C	N	O	S	0	0
			817	517	138	160	2		

- Molecule 3 is a protein called Erythrocyte membrane protein 1, PfEMP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	1671	Total	C	N	O	S	0	0
			13711	8622	2335	2659	95		

There are 55 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP A0A024V5I6
A	-18	LYS	-	expression tag	UNP A0A024V5I6
A	-17	LEU	-	expression tag	UNP A0A024V5I6
A	-16	CYS	-	expression tag	UNP A0A024V5I6
A	-15	ILE	-	expression tag	UNP A0A024V5I6
A	-14	LEU	-	expression tag	UNP A0A024V5I6
A	-13	LEU	-	expression tag	UNP A0A024V5I6
A	-12	ALA	-	expression tag	UNP A0A024V5I6
A	-11	VAL	-	expression tag	UNP A0A024V5I6
A	-10	VAL	-	expression tag	UNP A0A024V5I6
A	-9	ALA	-	expression tag	UNP A0A024V5I6
A	-8	PHE	-	expression tag	UNP A0A024V5I6
A	-7	VAL	-	expression tag	UNP A0A024V5I6
A	-6	GLY	-	expression tag	UNP A0A024V5I6
A	-5	LEU	-	expression tag	UNP A0A024V5I6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	SER	-	expression tag	UNP A0A024V5I6
A	-3	LEU	-	expression tag	UNP A0A024V5I6
A	-2	GLY	-	expression tag	UNP A0A024V5I6
A	-1	GLY	-	expression tag	UNP A0A024V5I6
A	0	THR	-	expression tag	UNP A0A024V5I6
A	2510	GLY	GLU	conflict	UNP A0A024V5I6
A	2630	GLY	-	expression tag	UNP A0A024V5I6
A	2631	SER	-	expression tag	UNP A0A024V5I6
A	2632	GLU	-	expression tag	UNP A0A024V5I6
A	2633	ASN	-	expression tag	UNP A0A024V5I6
A	2634	LEU	-	expression tag	UNP A0A024V5I6
A	2635	TYR	-	expression tag	UNP A0A024V5I6
A	2636	PHE	-	expression tag	UNP A0A024V5I6
A	2637	GLN	-	expression tag	UNP A0A024V5I6
A	2638	SER	-	expression tag	UNP A0A024V5I6
A	2639	ALA	-	expression tag	UNP A0A024V5I6
A	2640	SER	-	expression tag	UNP A0A024V5I6
A	2641	GLY	-	expression tag	UNP A0A024V5I6
A	2642	LEU	-	expression tag	UNP A0A024V5I6
A	2643	ASN	-	expression tag	UNP A0A024V5I6
A	2644	ASP	-	expression tag	UNP A0A024V5I6
A	2645	ILE	-	expression tag	UNP A0A024V5I6
A	2646	PHE	-	expression tag	UNP A0A024V5I6
A	2647	GLU	-	expression tag	UNP A0A024V5I6
A	2648	ALA	-	expression tag	UNP A0A024V5I6
A	2649	GLN	-	expression tag	UNP A0A024V5I6
A	2650	LYS	-	expression tag	UNP A0A024V5I6
A	2651	ILE	-	expression tag	UNP A0A024V5I6
A	2652	GLU	-	expression tag	UNP A0A024V5I6
A	2653	TRP	-	expression tag	UNP A0A024V5I6
A	2654	HIS	-	expression tag	UNP A0A024V5I6
A	2655	GLU	-	expression tag	UNP A0A024V5I6
A	2656	HIS	-	expression tag	UNP A0A024V5I6
A	2657	HIS	-	expression tag	UNP A0A024V5I6
A	2658	HIS	-	expression tag	UNP A0A024V5I6
A	2659	HIS	-	expression tag	UNP A0A024V5I6
A	2660	HIS	-	expression tag	UNP A0A024V5I6
A	2661	HIS	-	expression tag	UNP A0A024V5I6
A	2662	HIS	-	expression tag	UNP A0A024V5I6
A	2663	HIS	-	expression tag	UNP A0A024V5I6

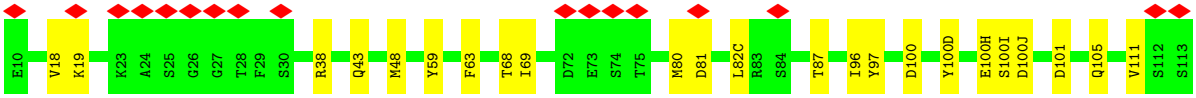
3 Residue-property plots (i)

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: V2C.044 heavy chain

Chain H:

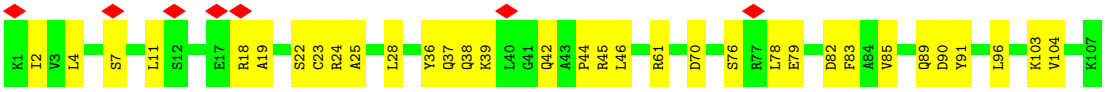




- Molecule 2: V2C.044 Light chain

Chain L:

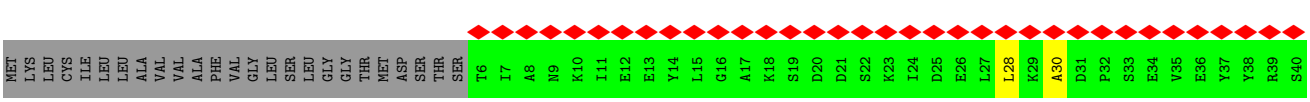


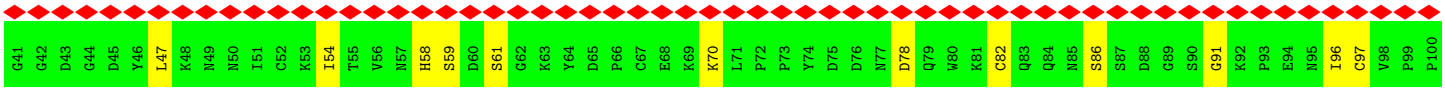


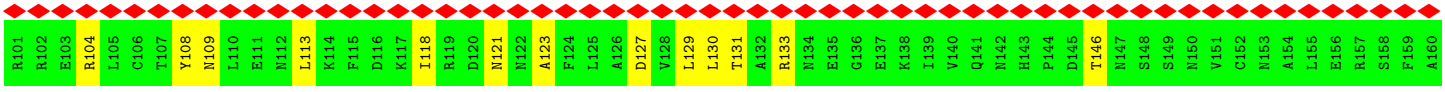
- Molecule 3: Erythrocyte membrane protein 1, PfEMP1

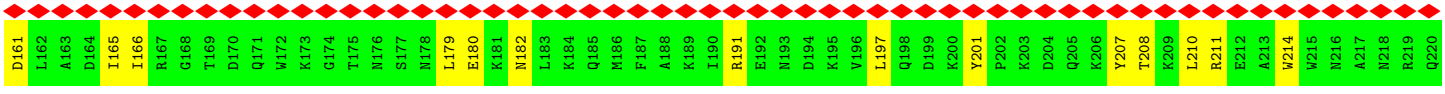
Chain A:

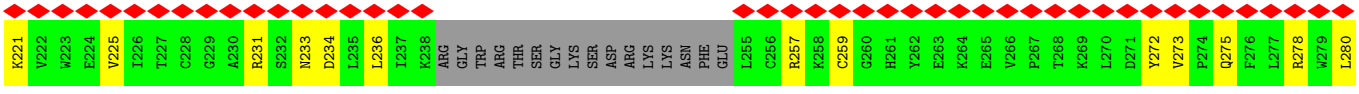


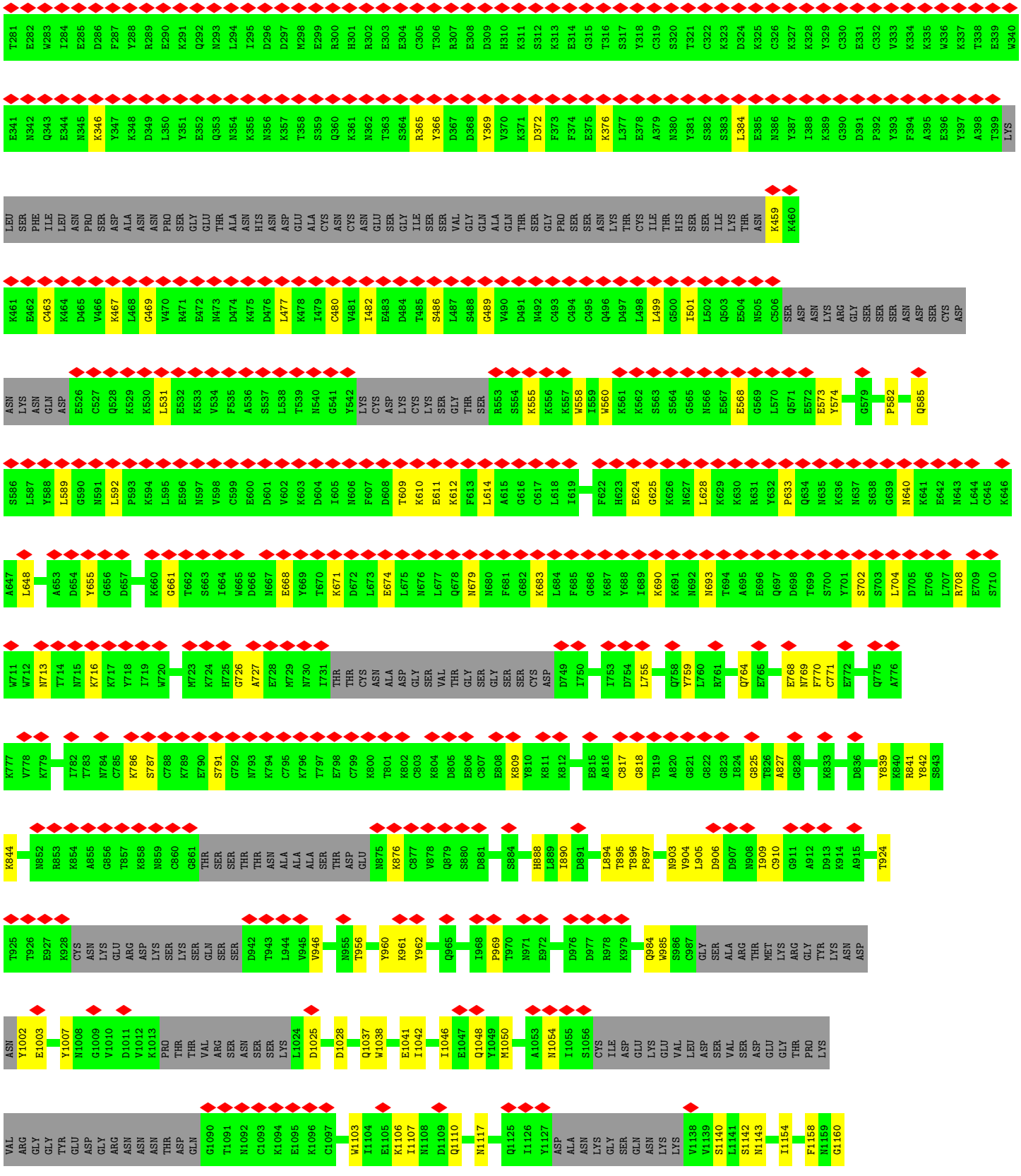


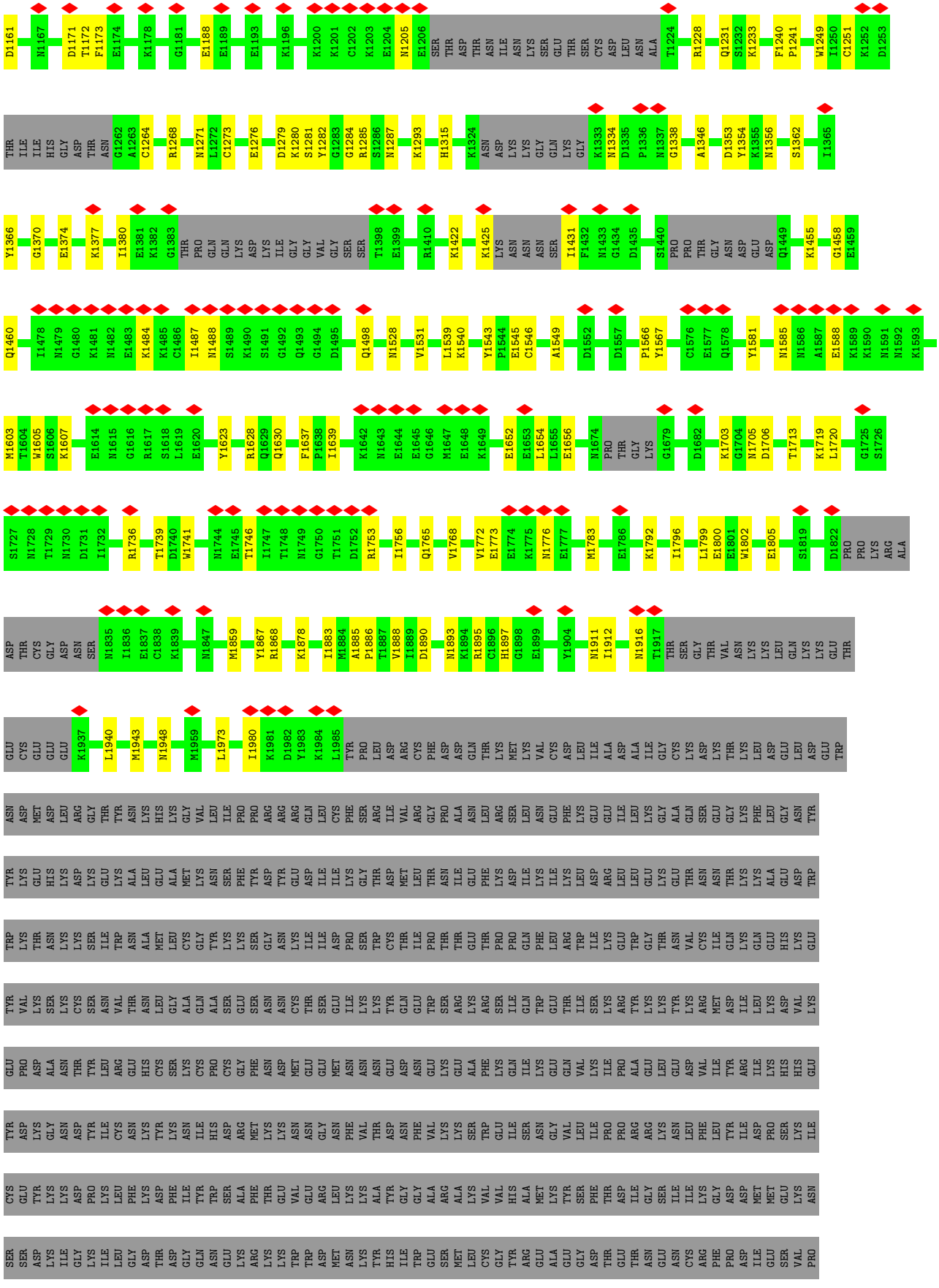









T281 E282 W283 I284 E285 D286 F287 Y288 R289 E290 K291 Q292 N293 L294 I295 D296 D297 M298 E299 R300 H301 R302 E303 E304 C305 T306 R307 E308 D309 H310 K311 S312 K313 E314 G315 T316 S317 Y318 C319 S320 T321 C322 K323 D324 K325 C326 K327 K328 Y329 C330 E331 C332 V333 K334 K335 W336 K337 T338 E339 W340
E341 N342 Q343 E344 N345 K346 Y347 K348 D349 L350 Y351 E352 Q353 N354 K355 N356 K357 T358 S359 Q360 K361 N362 T363 S364 R365 Y366 D367 D368 Y369 V370 K371 D372 F373 F374 E375 K376 L377 E378 A379 N380 Y381 S382 S383 L384 E385 N386 Y387 I388 K389 G390 D391 P392 Y393 F394 A395 E396 Y397 A398 T399 LYS
LEU SER PHE ILE LEU ASN PRO SER ASP ALA ASN ASN PRO SER GLY GLU THR ALA ASN HIS ASN ASP GLU ALA CYS ASN CYS ASN GLU SER GLY ILE SER SER VAL GLY GLN ALA GLN THR SER GLY PRO SER SER ASN LYS THR CYS ILE THR HIS SER SER ILE LYS THR ASN K459 K460
K461 E462 C463 K464 D465 V466 K467 L468 G469 V470 R471 E472 N473 D474 K475 D476 L477 K478 I479 C480 V481 I482 E483 D484 T485 S486 L487 S488 G489 V490 D491 N492 C493 C494 C495 Q496 D497 L498 L499 G500 I501 L502 Q503 E504 N505 C506 SER ASP ASN LYS ARG GLY SER SER SER ASN ASP SER CYS ASP
ASN LYS ASN GLN ASP E526 C527 Q528 K529 K530 L531 E532 K533 V534 F535 A536 S537 L538 T539 N540 G541 Y542 LYS CYS ASP LYS CYS LYS SER GLY THR SER R553 S554 K555 K556 K557 W558 I559 W560 K561 K562 S563 S564 G565 N566 E567 E568 G569 L570 Q571 E572 E573 Y574 G579 P582 Q585
S586 L587 Y588 L589 G590 N591 L592 P593 K594 L595 E596 N597 V598 C599 E600 D601 V602 K603 D604 I605 N606 F607 D608 T609 K610 E611 K612 F613 L614 A615 G616 C617 L618 I619 F622 H623 E624 G625 K626 N627 L628 K629 K630 R631 Y632 P633 Q634 N635 K636 N637 S638 G639 N640 K641 E642 N643 L644 C645 K646
A647 L648 A653 D654 Y655 G656 D657 K660 G661 T662 S663 I664 W665 D666 N667 E668 Y669 T670 K671 D672 L673 E674 L675 N676 L677 Q678 N679 N680 F681 G682 K683 L684 F685 G686 K687 Y688 I689 K690 K691 N692 N693 T694 A695 E696 Q697 D698 T699 S700 Y701 S702 S703 L704 D705 E706 L707 R708 E709 S710
W711 W712 N713 T714 N715 K716 K717 Y718 I719 W720 M723 K724 H725 G726 A727 E728 M729 N730 I731 THR THR CYS ASN ALA ASP GLY SER VAL THR GLY SER GLY SER SER CYS ASP D749 I750 I753 D754 L755 Q758 Y759 L760 R761 Q764 E765 E768 N769 F770 C771 E772 Q775 A776
K777 V778 K779 I782 T783 N784 C785 K786 S787 C788 K789 E790 S791 G792 N793 K794 C795 K796 T797 E798 C799 K800 T801 K802 C803 K804 D805 E806 C807 E808 K809 Y810 K811 K812 E815 A816 C817 G818 T819 A820 G821 G822 G823 I824 G825 T826 A827 G828 K833 D836 Y839 K840 R841 Y842 S843
K844 N852 R853 K854 A855 G856 T857 K858 N859 C860 G861 THR SER SER THR THR ASN ALA ALA ALA SER THR ASP GLU N875 K876 C877 V878 Q879 S880 D881 S884 H888 L889 I890 D891 L894 T895 T896 P897 N903 V904 L905 D906 D907 N908 I909 C910 G911 A912 D913 K914 A915 T924
T925 T926 E927 K928 CYS ASN LYS GLU ARG ASP LYS SER LYS SER GLN SER SER D942 T943 L944 V945 V946 N955 T956 Y960 K961 Y962 Q965 I968 P969 T970 N971 E972 D976 D977 R978 K979 Q984 W985 S986 C987 GLY SER ALA ARG THR MET LYS ARG GLY TYR LYS ASN ASP
ASN Y1002 E1003 Y1007 N1008 G1009 V1010 D1011 V1012 K1013 PRO THR THR VAL ARG SER ASN SER SER SER LYS L1024 D1025 D1028 Q1037 W1038 E1041 I1042 I1046 E1047 Q1048 Y1049 M1050 A1053 N1054 I1055 S1056 CYS ILE ASP GLU LYS GLU VAL LEU ASP SER VAL SER ASP GLU GLY THR PRO LYS
VAL ARG GLY GLY TYR GLU ASP GLY ARG ASN ASN ASN THR ASP GLN G1090 T1091 N1092 C1093 K1094 E1095 K1096 C1097 W1103 I1104 E1105 K1106 I1107 N1108 D1109 Q1110 N1117 Q1125 I1126 Y1127 ASP ALA ASN LYS GLY SER GLN ASN LYS LYS V1138 V1139 S1140 L1141 S1142 N1143 I1154 F1158 N1159 G1160


D1161 N1167 D1171 T1172 F1173 E1174 K1178 G1181 E1188 E1189 E1193 K1196 K1200 K1201 C1202 K1203 E1204 N1205 E1206 SER THR ASP THR ASN ILE ASN LYS SER GLU THR SER CYS ASP LEU ASN ALA T1224 R1228 Q1231 S1232 K1233 F1240 P1241 W1249 I1250 C1251 K1252 D1253
THR ILE ILE HIS GLY ASP THR ASN G1262 A1263 C1264 R1268 N1271 L1272 C1273 E1276 D1279 K1280 S1281 Y1282 G1283 G1284 R1285 S1286 N1287 K1293 H1315 K1324 ASN ASP LYS LYS GLY GLN LYS GLY K1333 N1334 D1335 P1336 N1337 G1338 A1346 D1353 Y1354 K1385 N1356 S1362 I1365
Y1366 G1370 E1374 K1377 I1380 E1381 K1382 G1383 THR PRO GLN GLN LYS ASP LYS ILE GLY GLY VAL GLY SER SER T1398 E1399 R1410 K1422 K1425 LYS ASN ASN ASN SER I1431 F1432 N1433 G1434 D1435 S1440 PRO PRO THR GLY ASN ASP GLU ASP Q1449 K1455 G1458 E1459
Q1460 I1478 N1479 G1480 K1481 N1482 E1483 K1484 K1485 C1486 I1487 N1488 S1489 K1490 S1491 G1492 Q1493 G1494 D1495 Q1498 N1528 V1531 L1539 K1540 Y1543 P1544 E1545 C1546 A1549 D1552 D1557 P1566 Y1567 C1576 E1577 Q1578 Y1581 N1585 N1586 A1587 E1588 K1589 K1590 N1591 N1592 K1593
M1603 T1604 W1605 S1606 K1607 E1614 N1615 G1616 R1617 S1618 L1619 E1620 Y1623 R1628 Q1629 Q1630 F1637 P1638 I1639 K1642 N1643 E1644 E1645 G1646 M1647 E1648 K1649 E1652 E1653 L1654 L1655 E1656 N1674 PRO THR GLY LYS G1679 D1682 K1703 G1704 N1705 D1706 T1713 K1719 L1720 G1725 S1726
S1727 N1728 T1729 N1730 D1731 I1732 R1736 T1739 D1740 W1741 N1744 E1745 T1746 I1747 T1748 N1749 G1750 T1751 D1752 R1753 I1756 Q1765 V1768 V1772 E1773 E1774 K1775 N1776 E1777 M1783 E1786 K1792 I1796 L1799 E1800 E1801 W1802 E1805 S1819 D1822 PRO PRO LYS ARG ALA
ASP THR CYS GLY ASP ASN SER N1835 I1836 E1837 C1838 K1839 N1847 M1859 Y1867 R1868 K1878 I1883 M1884 A1885 P1886 T1887 V1888 I1889 D1890 N1893 K1894 R1895 C1896 H1897 G1898 E1899 Y1904 N1911 I1912 N1916 T1917 THR SER GLY THR VAL ASN LYS LYS LEU GLN LYS LYS GLU THR
GLU CYS GLU GLU GLU K1937 L1940 M1943 N1948 M1959 L1973 T1980 K1981 D1982 Y1983 K1984 L1985 TYR PRO LEU ASP ARG CYS PHE ASP ASP GLN THR LYS MET LYS VAL CYS ASP LEU ILE ALA ASP ALA ILE GLY CYS LYS ASP LYS THR LYS LEU ASP GLU LEU ASP GLU TRP
ASN ASP MET ASP LEU ARG GLY THR TYR ASN LYS HIS LYS GLY VAL LEU ILE PRO PRO ARG ARG ARG LEU CYS PHE SER ARG ILE VAL ARG GLY PRO ALA ASN LEU ARG SER LEU ASN GLU GLU PHE LYS GLU GLU ILE LEU LYS GLY ALA GLN SER GLU GLY LYS PHE LEU GLY ASN TYR
TYR LYS GLU HIS LYS ASP LYS GLU LYS ALA LEU GLU ALA MET LYS ASN SER PHE TYR ASP TYR GLU ASP ILE ILE LYS GLY PHE THR ASN ILE GLU GLU PHE LYS ASP ILE LYS LYS LEU ASP ARG LEU LEU ASP MET LEU THR GLU GLU LYS GLY GLU THR ASN ASN THR LYS LYS ALA GLU ASP TRP
TRP LYS THR ASN LYS LYS SER ILE TRP ASN ALA MET LEU CYS LYS SER GLY ASN LYS ILE ILE ASP PRO SER TRP CYS THR ILE PRO THR THR GLU GLU THR PRO PRO GLN PHE LEU ARG TRP ILE LYS GLU TRP GLY THR ASN VAL CYS ILE GLN LYS GLN GLU HIS LYS GLU
TYR VAL LYS SER LYS CYS SER ASN VAL THR ASN LEU GLY ALA GLN ALA SER GLU SER ASN ASN CYS THR SER GLU ILE LYS LYS TYR GLN GLU TRP SER ARG LYS ILE GLN TRP GLU THR ILE SER LYS ARG TYR LYS LYS TYR LYS ARG ARG MET ASP ILE LEU LYS ASP VAL LYS
GLU PRO ASP ALA ASN THR TYR LEU ARG GLU HIS CYS SER LYS CYS PRO CYS GLY PHE ASN ASP MET GLU GLU MET ASN ASN ASN GLU ASP ASN GLU LYS GLU ALA PHE LYS GLN ILE LYS GLU GLN VAL LYS ILE PRO ALA GLU LEU GLU ASP VAL ILE ILE TYR ARG ILE LYS HIS HIS GLU
TYR ASP LYS GLY ASN ASP TYR ILE CYS ASN LYS TYR LYS ASN ASN GLY ASN PHE VAL THR ASP ASN PHE VAL LYS LYS SER TRP GLU ILE SER ASN GLY VAL LEU ILE PRO PRO ARG ARG LYS ASN LEU PHE LEU TYR ILE ASP PRO SER LYS ILE
CYS GLU TYR LYS LYS ASP PRO LYS LEU PHE LYS ASP PHE ILE TYR TRP SER ALA PHE THR GLU VAL GLU ARG LEU LYS LYS ALA TYR GLY GLY ALA ARG ALA LYS VAL VAL HIS ALA MET LYS TYR SER PHE THR ASP ILE GLY SER ILE ILE LYS GLY ASP ASP MET MET GLU LYS ASN
SER SER ASP LYS ILE GLY ASP THR ASP GLY GLN ASN GLU LYS ARG LYS LYS TRP TRP ASP MET ASN LYS TYR HIS ILE TRP GLU SER MET LEU CYS GLY TYR ARG GLU ALA GLU GLY ASP THR GLU THR ASN GLU ASN CYS ARG PHE PRO ASP ILE GLU SER VAL PRO

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

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

LYS SER LYS CYS ASP CYS PRO GLY SER GLU ASN LEU TYR PHE GLN SER ALA SER GLY LEU ASN ASP ILE PHE GLU ALA GLN LYS ILE GLU TRP HIS GLU HIS HIS HIS 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	58296	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	48	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.282	Depositor
Minimum map value	-0.161	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.045	Depositor
Map size (Å)	371.2, 371.2, 371.2	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.725, 0.725, 0.725	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	H	0.21	0/956	0.38	0/1298
2	L	0.19	0/836	0.40	0/1135
3	A	0.14	0/13978	0.26	0/18769
All	All	0.14	0/15770	0.28	0/21202

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	933	0	880	22	0
2	L	817	0	805	19	0
3	A	13711	0	13279	182	0
All	All	15461	0	14964	215	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 7.

The worst 5 of 215 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)
2:L:89:GLN:HE21	2:L:96:LEU:HD13	1.52	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1251:CYS:HB3	3:A:1264:CYS:HA	1.73	0.69
3:A:894:LEU:HD11	3:A:903:ASN:HD22	1.56	0.69
3:A:1911:ASN:ND2	3:A:1916:ASN:OD1	2.29	0.66
1:H:68:THR:HB	1:H:81:ASP:HB3	1.77	0.65

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	H	118/120 (98%)	109 (92%)	9 (8%)	0	100	100
2	L	106/108 (98%)	99 (93%)	7 (7%)	0	100	100
3	A	1629/2683 (61%)	1593 (98%)	36 (2%)	0	100	100
All	All	1853/2911 (64%)	1801 (97%)	52 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	98/98 (100%)	98 (100%)	0	100	100
2	L	88/88 (100%)	88 (100%)	0	100	100
3	A	1514/2429 (62%)	1514 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1700/2615 (65%)	1700 (100%)	0	100 100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
3	A	1844	ASN
3	A	1804	ASN
3	A	1205	ASN
3	A	1337	ASN
3	A	1110	GLN

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 oligosaccharides 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.

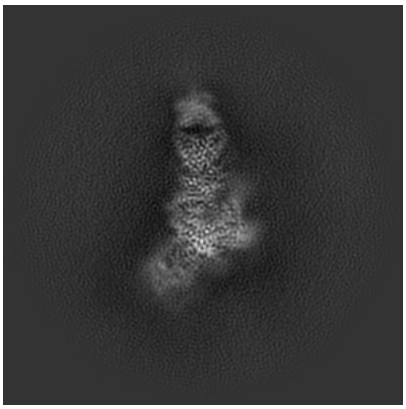
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-70147. These allow visual inspection of the internal detail of the map and identification of artifacts.

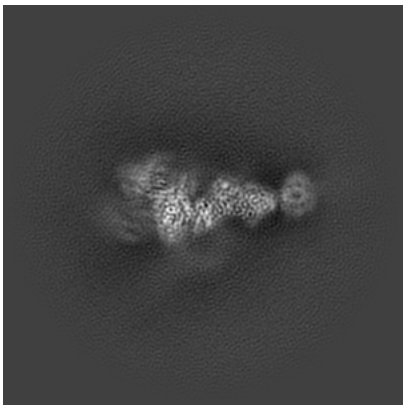
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

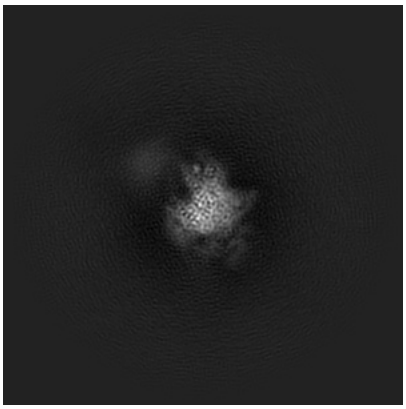
6.1.1 Primary map



X

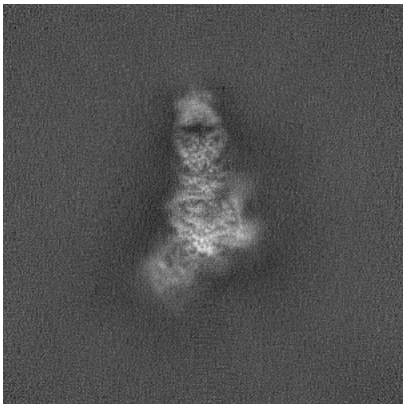


Y

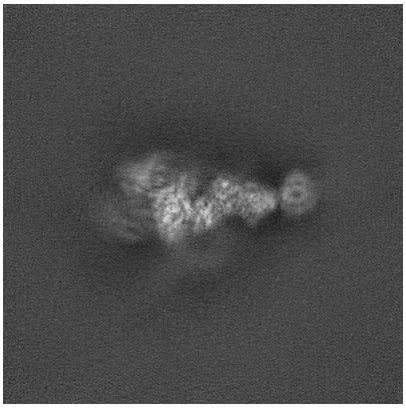


Z

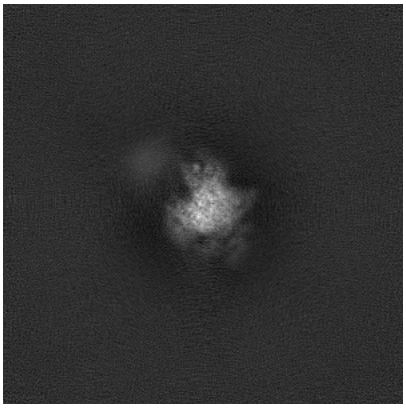
6.1.2 Raw map



X



Y

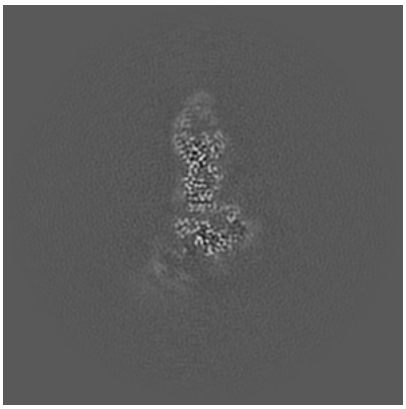


Z

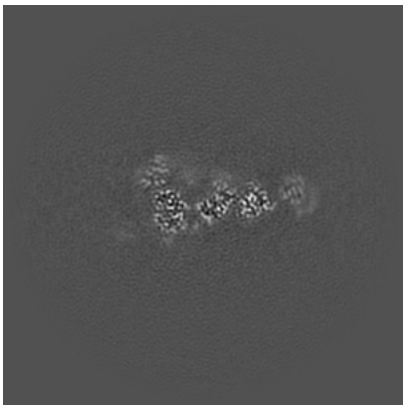
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

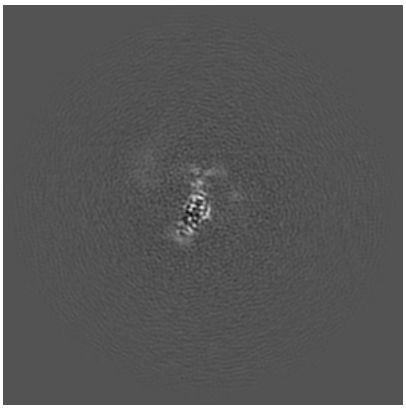
6.2.1 Primary map



X Index: 256

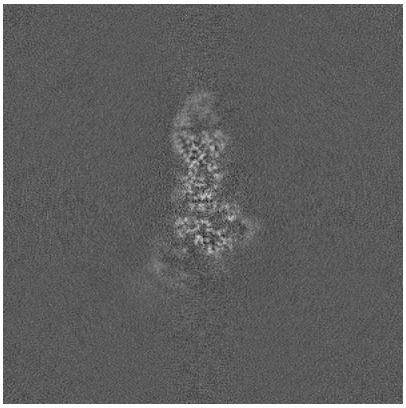


Y Index: 256

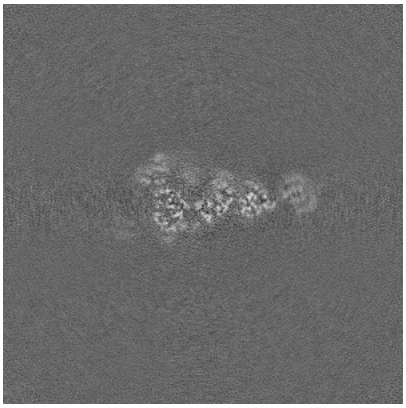


Z Index: 256

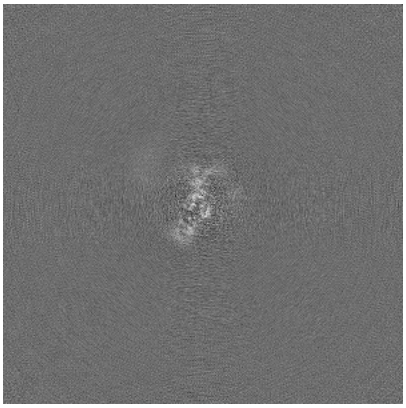
6.2.2 Raw map



X Index: 256



Y Index: 256

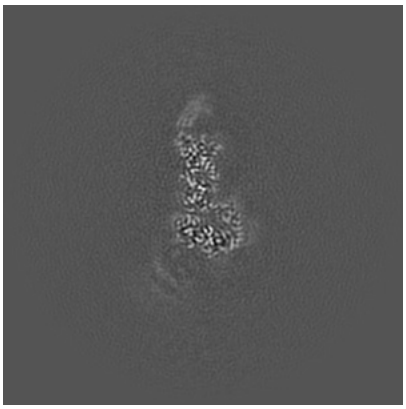


Z Index: 256

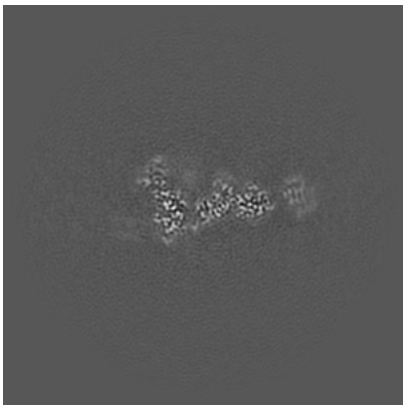
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

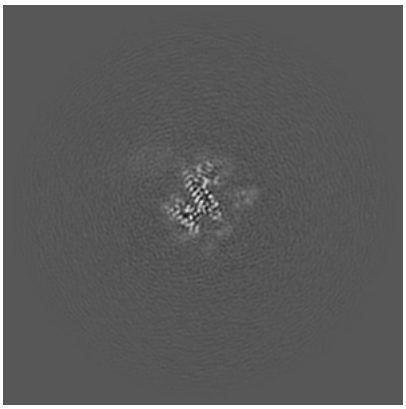
6.3.1 Primary map



X Index: 250

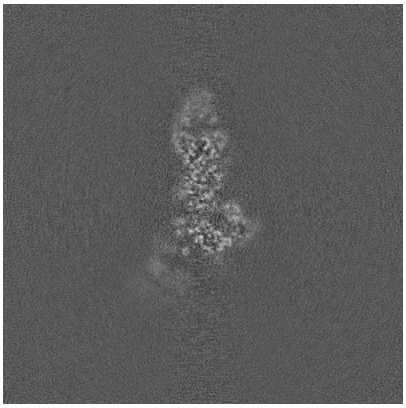


Y Index: 254

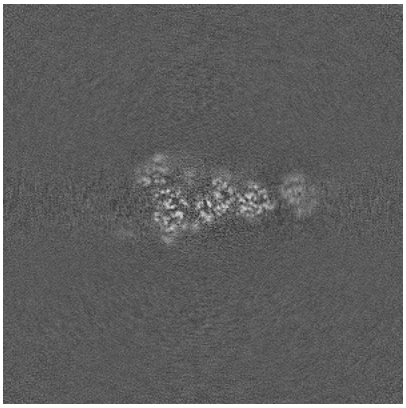


Z Index: 211

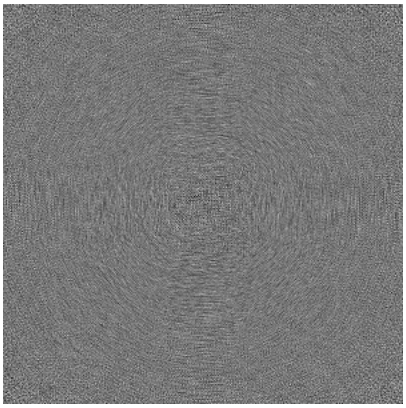
6.3.2 Raw map



X Index: 258



Y Index: 255

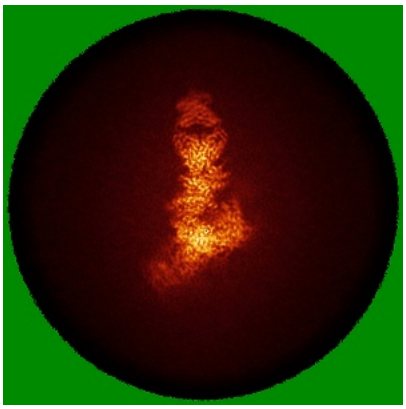


Z Index: 0

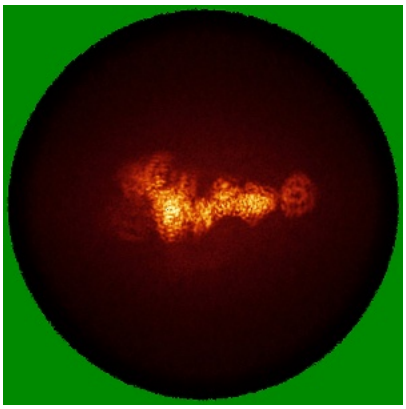
The images above show the largest variance slices of the map in three orthogonal directions.

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

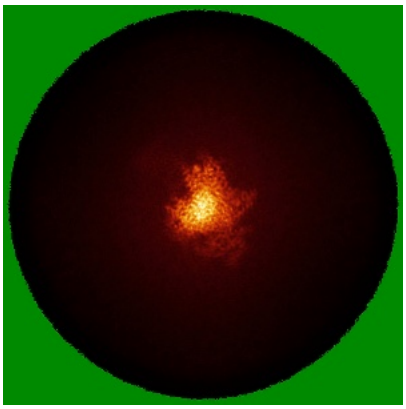
6.4.1 Primary map



X

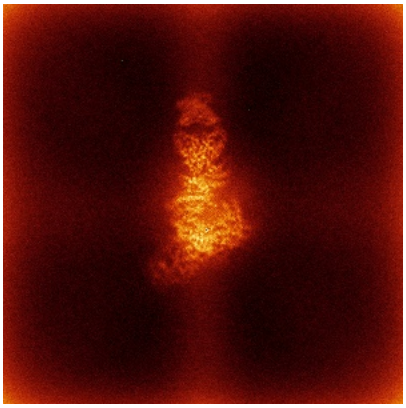


Y

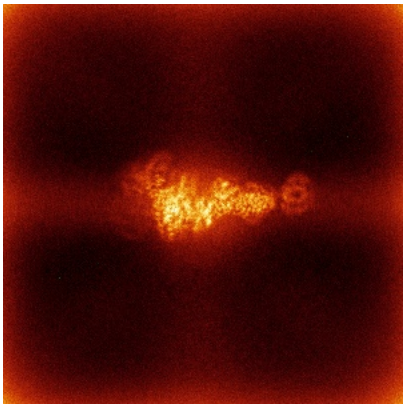


Z

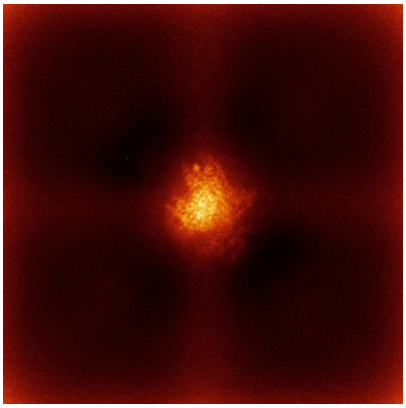
6.4.2 Raw map



X



Y

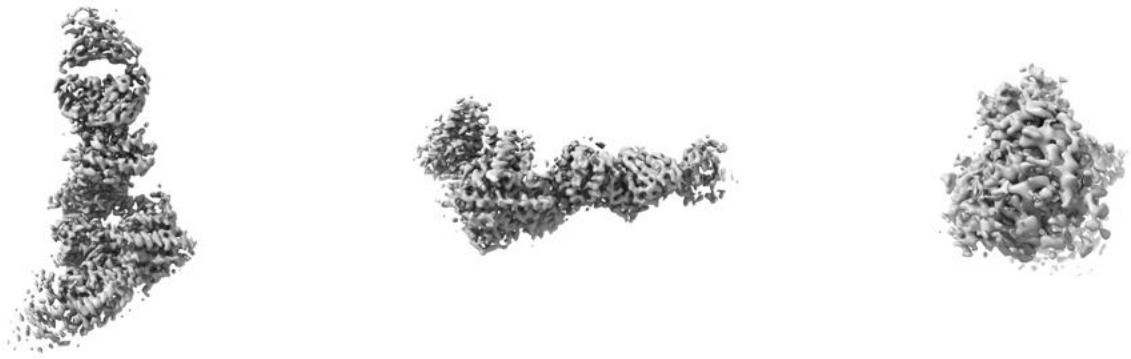


Z

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 0.045. 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.

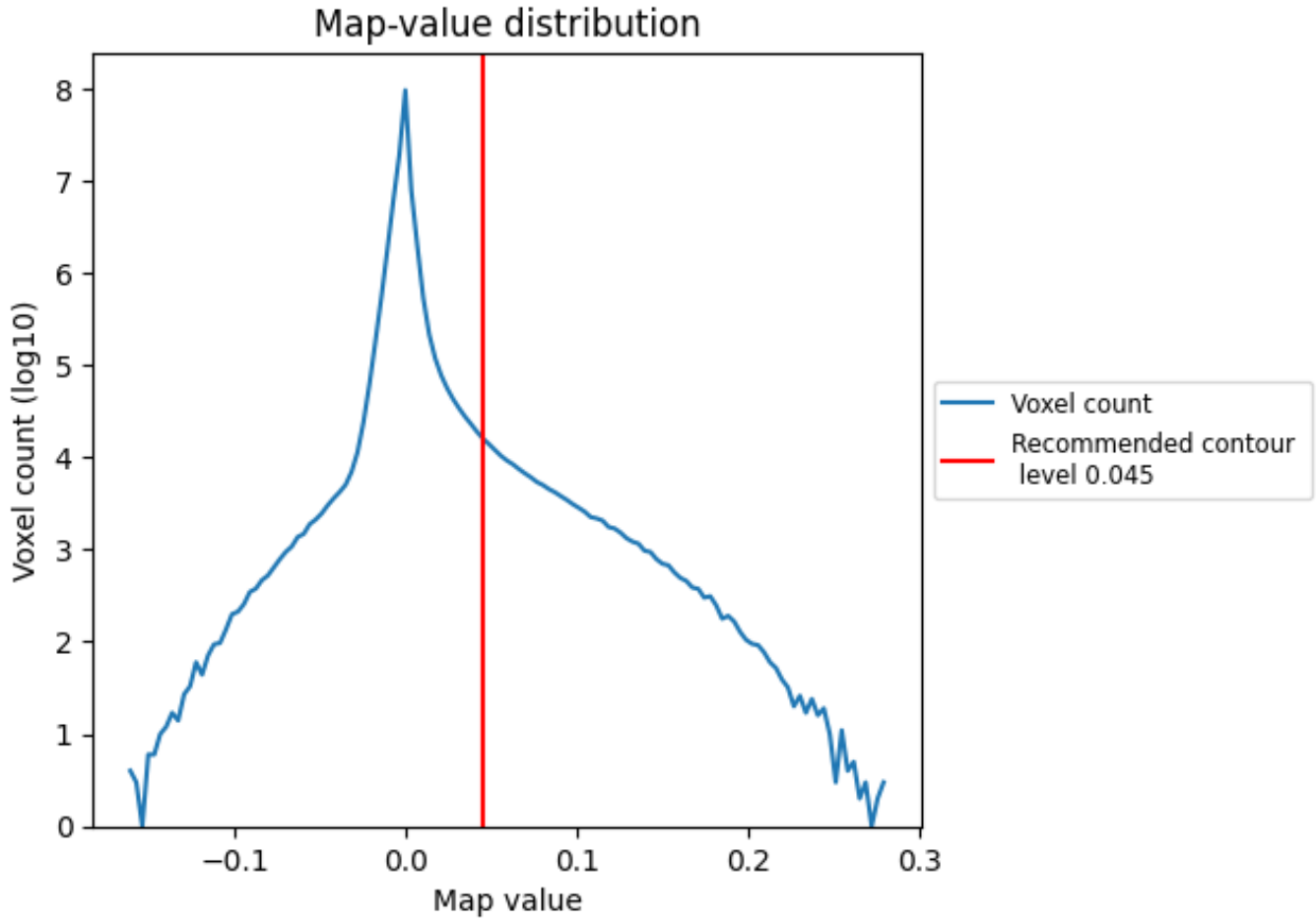
6.6 Mask visualisation (i)

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

7 Map analysis

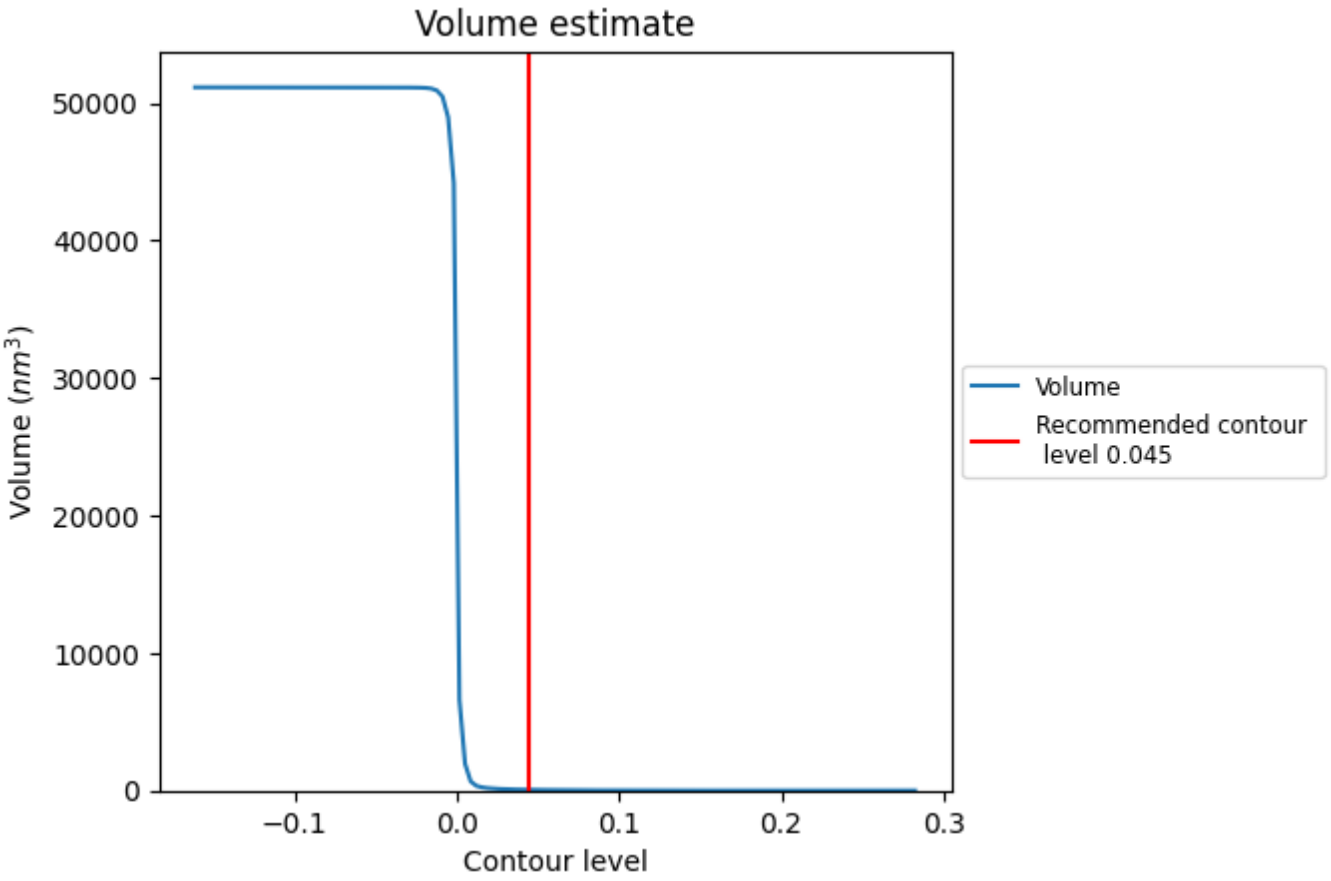
This section contains the results of statistical analysis of the map.

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.

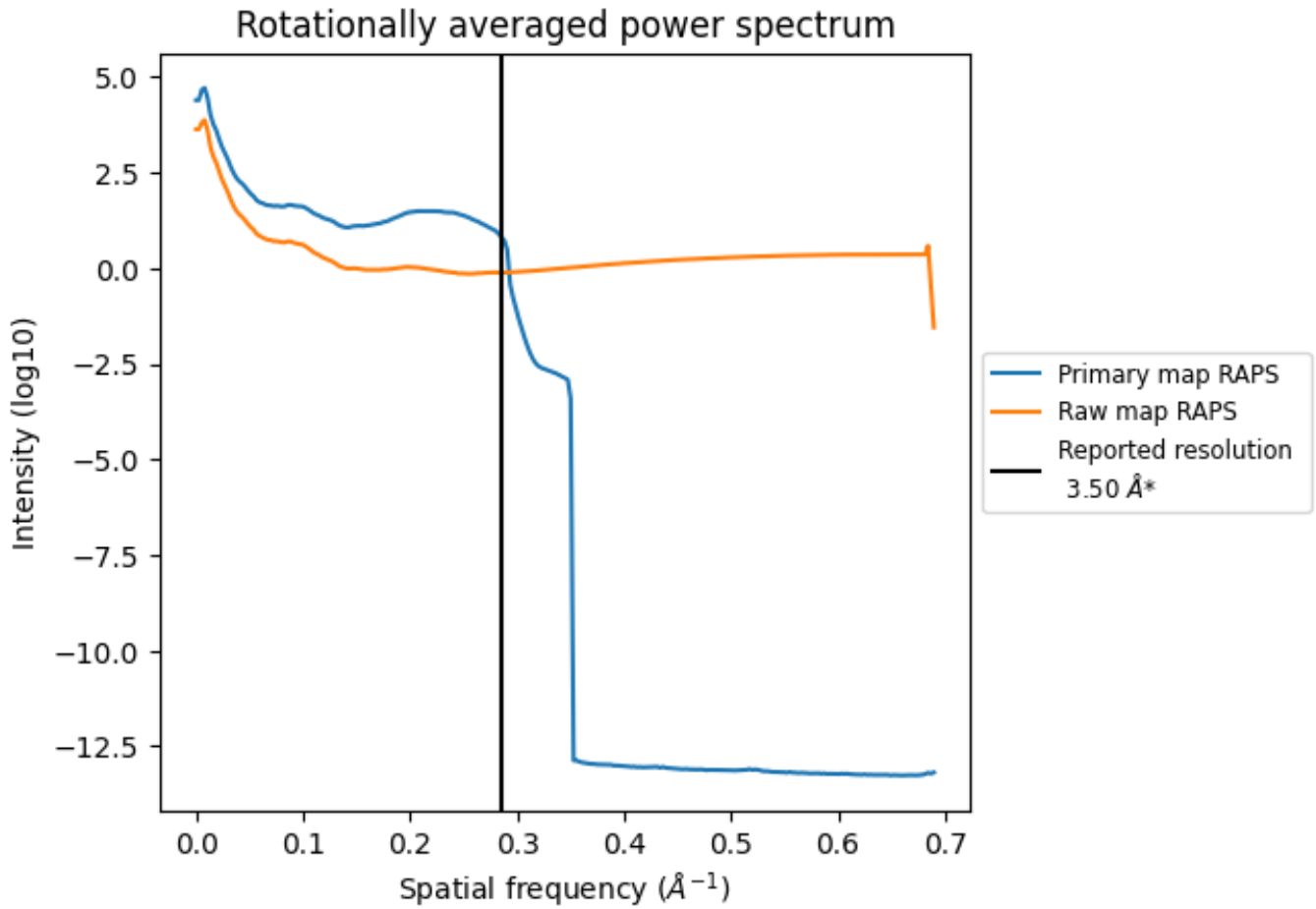
7.2 Volume estimate (i)



The volume at the recommended contour level is 57 nm^3; this corresponds to an approximate mass of 51 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)

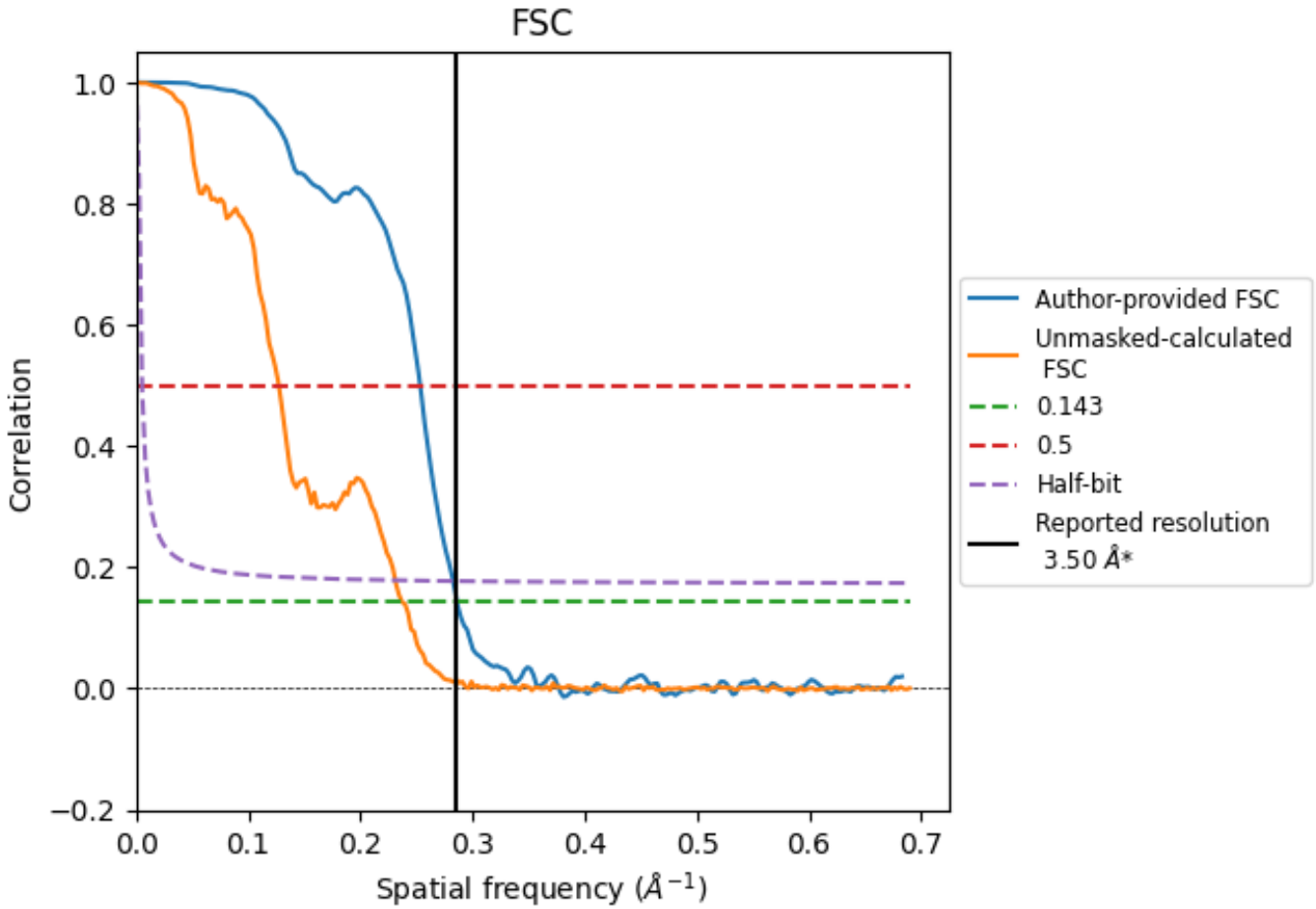


*Reported resolution corresponds to spatial frequency of 0.286 $Å^{-1}$

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 0.286 Å^{-1}

8.2 Resolution estimates (i)

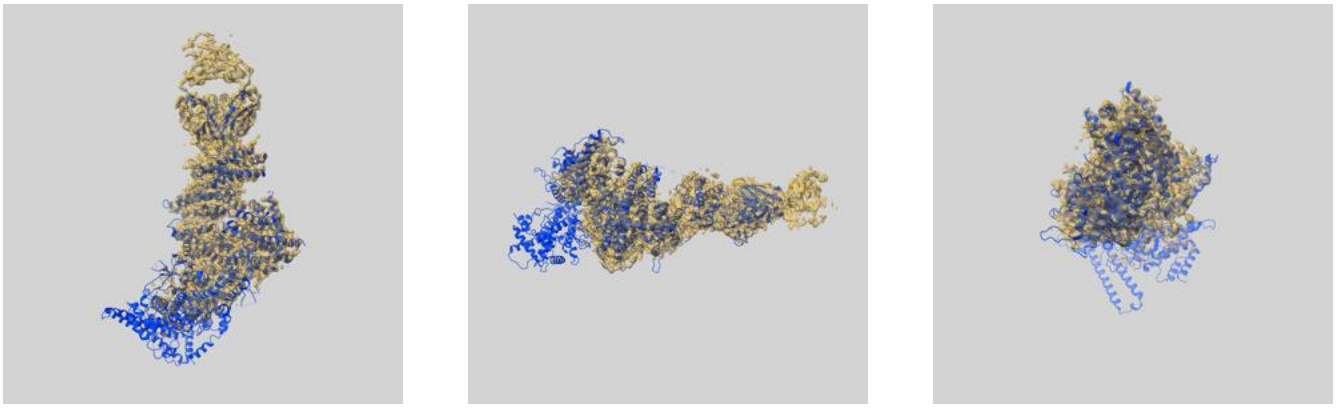
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.49	3.95	3.54
Unmasked-calculated*	4.22	7.86	4.33

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.22 differs from the reported value 3.5 by more than 10 %

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-70147 and PDB model 9O5R. Per-residue inclusion information can be found in section 3 on page 5.

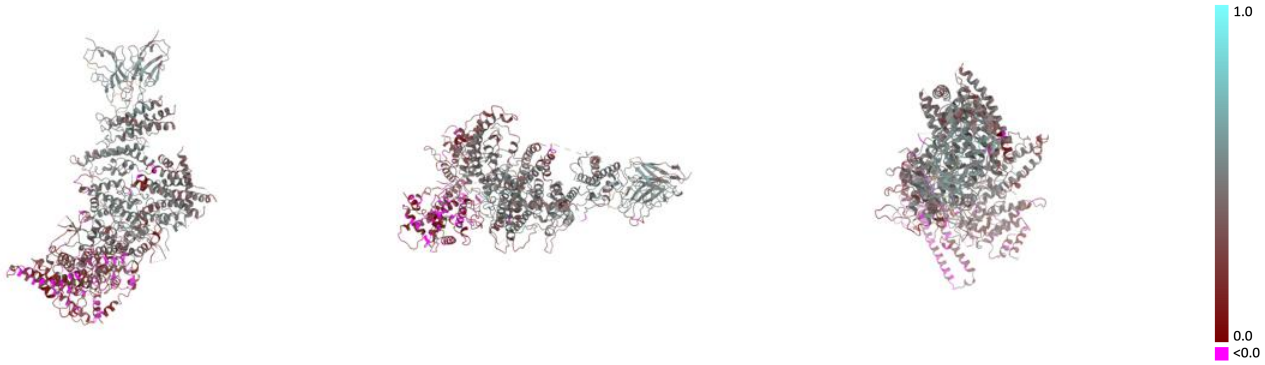
9.1 Map-model overlay



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.045 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.

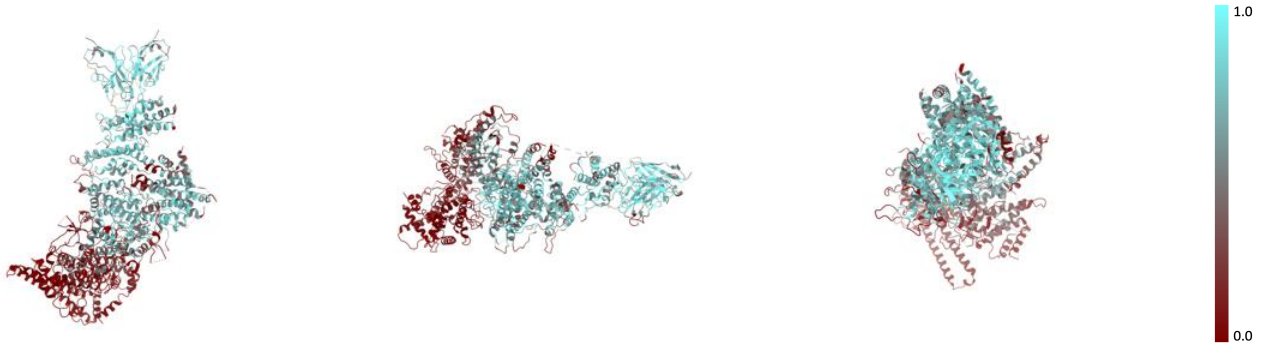
9.2 Q-score mapped to coordinate model



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.

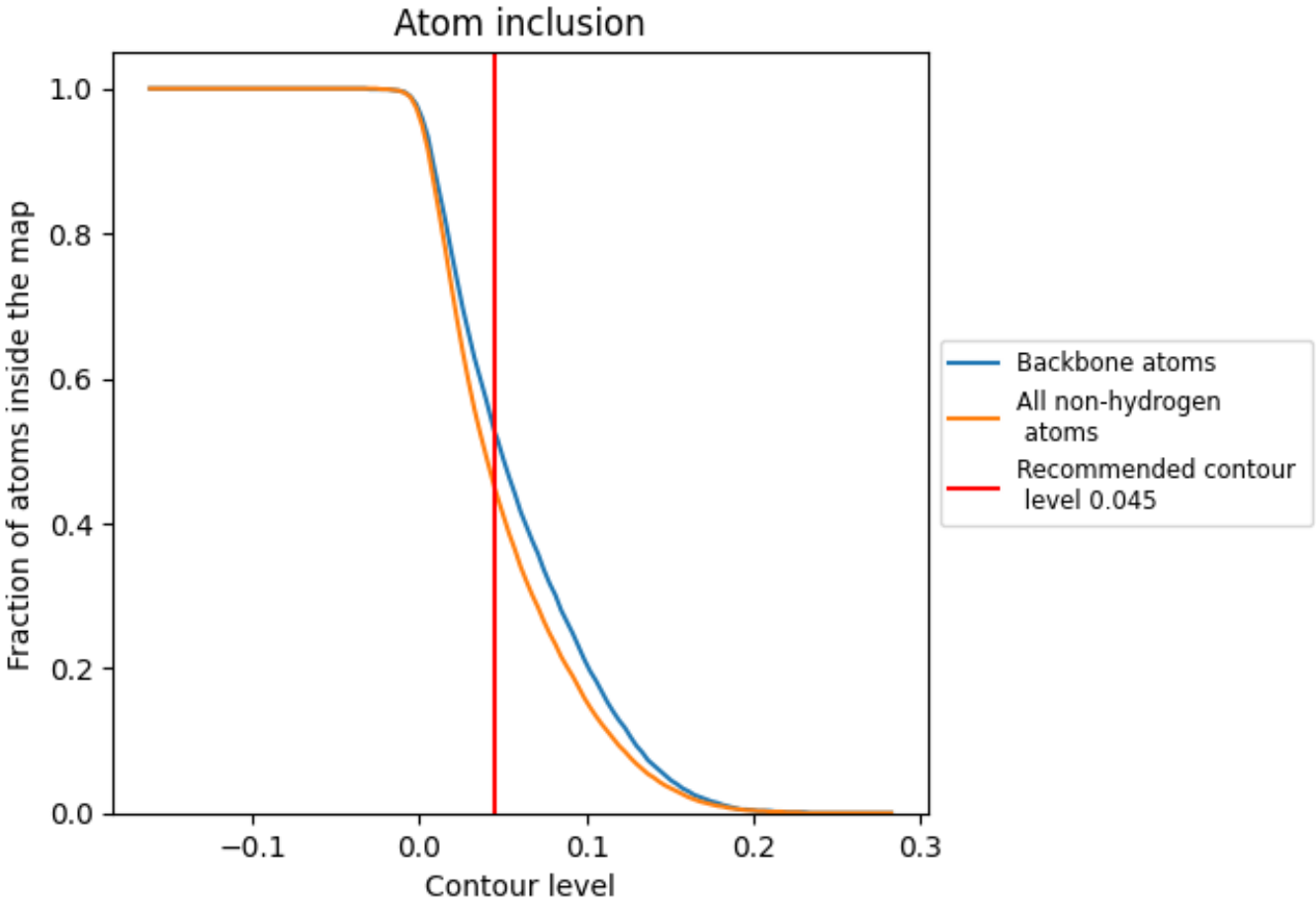
9.3 Atom inclusion mapped to coordinate model



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 (0.045).

9.4 Atom inclusion (i)



At the recommended contour level, 53% of all backbone atoms, 45% 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 (0.045) and Q-score for the entire model and for each chain.



Chain	Atom inclusion	Q-score
All	0.4490	0.3600
A	0.4130	0.3430
H	0.7170	0.4840
L	0.7430	0.4940