



Full wwPDB EM Validation Report ⓘ

Mar 19, 2026 – 08:37 PM UTC

PDB ID : 6MHG / pdb_00006mhg
EMDB ID : EMD-9114
Title : Cryo-EM structure of the circumsporozoite protein of Plasmodium falciparum with a vaccine-elicited antibody reveals maturation of inter-antibody contacts
Authors : Cottrell, C.A.; Torres, J.L.; Ward, A.B.
Deposited on : 2018-09-17
Resolution : 3.57 Å(reported)
Based on initial model : 6AXK

This is a Full wwPDB EM Validation 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.dev132
MolProbity : 4-5-2 with Phenix2.0
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) : 2.49

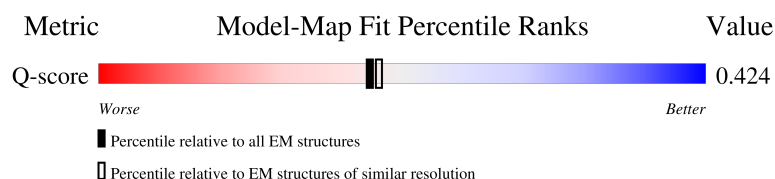
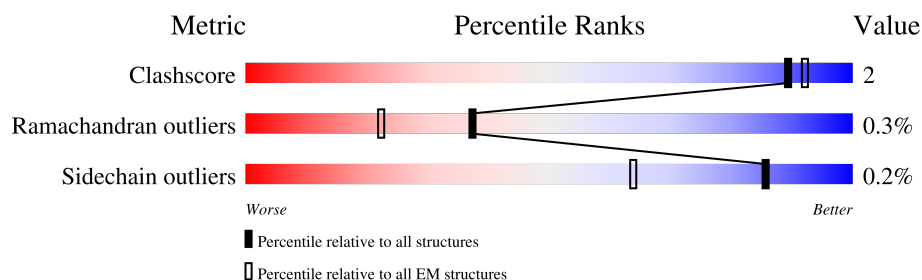
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.57 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.



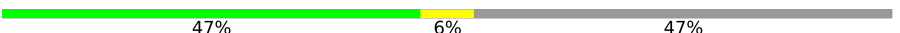
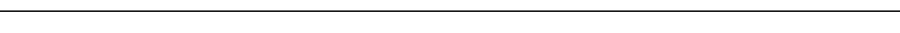
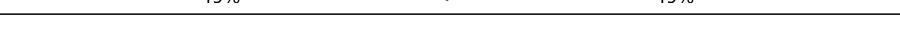
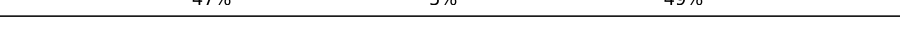
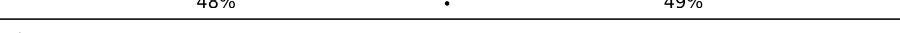
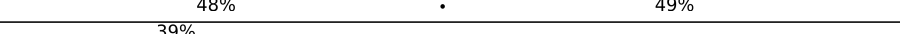
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12682 (3.07 - 4.07)

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 $\leq 5\%$. 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	E	278	26% 6% 68%
2	A	225	52% 47%
2	B	225	50% 47%
2	C	225	52% 47%

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Mol	Chain	Length	Quality of chain
2	D	225	
2	F	225	
2	G	225	
2	H	225	
2	I	225	
2	J	225	
2	K	225	
2	M	225	
3	L	218	
3	N	218	
3	O	218	
3	P	218	
3	Q	218	
3	R	218	
3	S	218	
3	T	218	
3	U	218	
3	V	218	
3	W	218	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19931 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 circumsporozoite protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	E	90	Total	C	N	O	0	0
			637	367	131	139		

- Molecule 2 is a protein called Fab311 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	120	Total	C	N	O	S	0	0
			937	594	161	178	4		
2	A	120	Total	C	N	O	S	0	0
			937	594	161	178	4		
2	B	120	Total	C	N	O	S	0	0
			937	594	161	178	4		
2	C	120	Total	C	N	O	S	0	0
			937	594	161	178	4		
2	D	120	Total	C	N	O	S	0	0
			937	594	161	178	4		
2	F	120	Total	C	N	O	S	0	0
			937	594	161	178	4		
2	G	120	Total	C	N	O	S	0	0
			937	594	161	178	4		
2	I	120	Total	C	N	O	S	0	0
			937	594	161	178	4		
2	J	120	Total	C	N	O	S	0	0
			937	594	161	178	4		
2	K	120	Total	C	N	O	S	0	0
			937	594	161	178	4		
2	M	120	Total	C	N	O	S	0	0
			937	594	161	178	4		

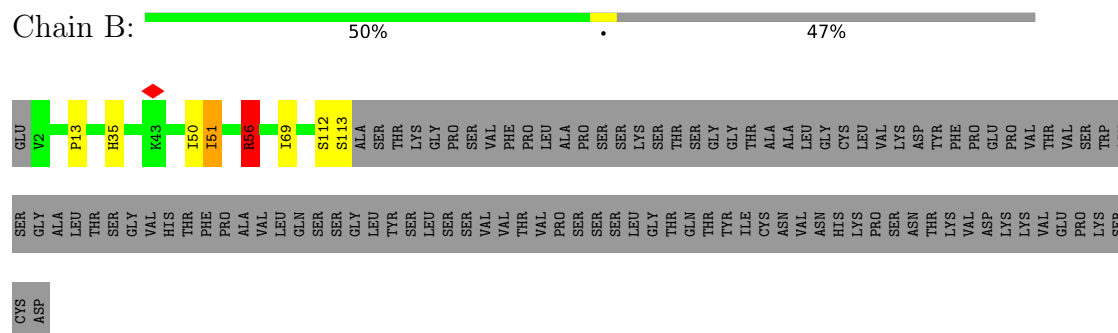
- Molecule 3 is a protein called Fab311 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	112	Total	C	N	O	S	0	0
			817	510	140	165	2		

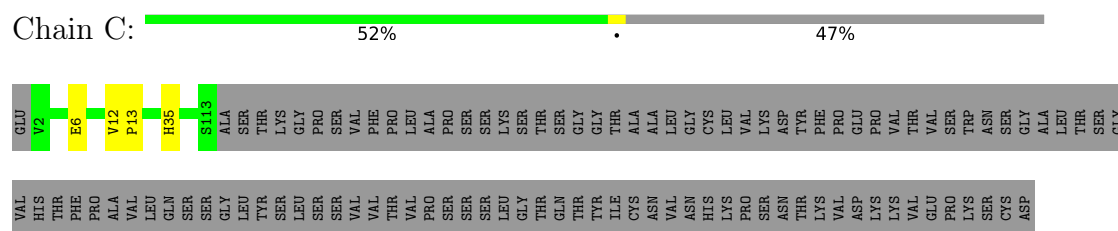
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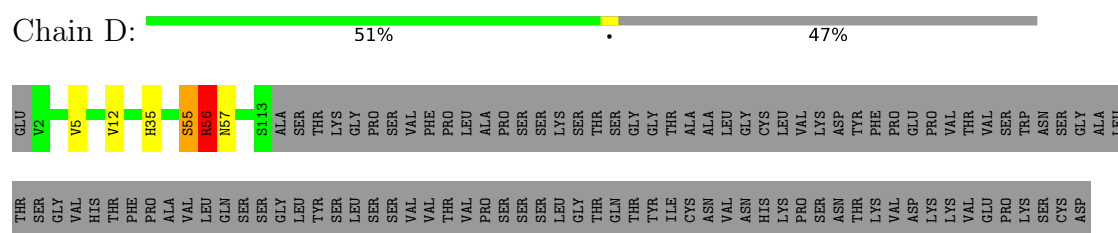
Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	112	Total 817	C 510	N 140	O 165	S 2	0	0
3	O	112	Total 817	C 510	N 140	O 165	S 2	0	0
3	P	112	Total 817	C 510	N 140	O 165	S 2	0	0
3	Q	112	Total 817	C 510	N 140	O 165	S 2	0	0
3	R	112	Total 817	C 510	N 140	O 165	S 2	0	0
3	S	112	Total 817	C 510	N 140	O 165	S 2	0	0
3	T	112	Total 817	C 510	N 140	O 165	S 2	0	0
3	U	112	Total 817	C 510	N 140	O 165	S 2	0	0
3	V	112	Total 817	C 510	N 140	O 165	S 2	0	0
3	W	112	Total 817	C 510	N 140	O 165	S 2	0	0



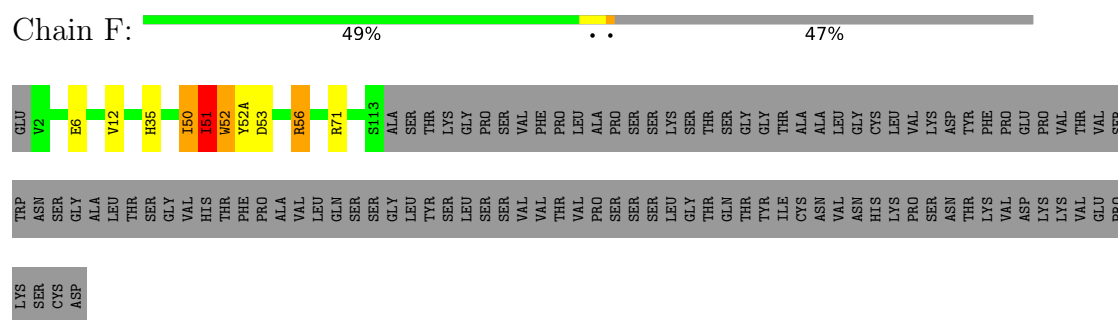
- Molecule 2: Fab311 heavy chain



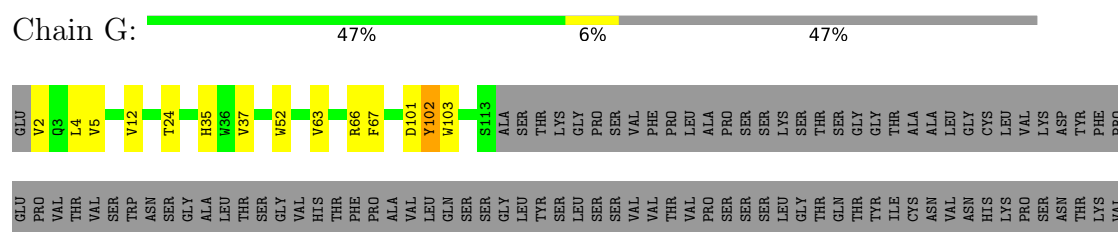
- Molecule 2: Fab311 heavy chain



- Molecule 2: Fab311 heavy chain

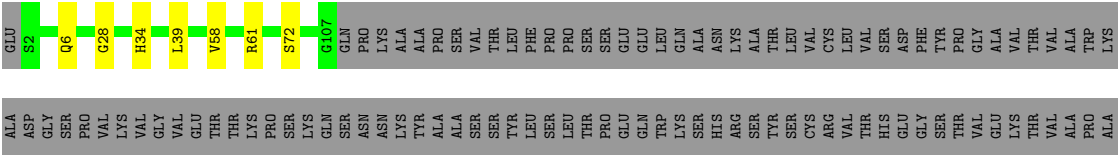


- Molecule 2: Fab311 heavy chain



VAL
ALA
PRO
ALA
GLU
CYS
SER

• Molecule 3: Fab311 light chain



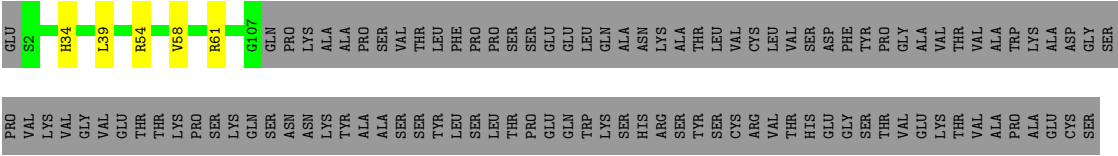
GLU
CYS
SER

• Molecule 3: Fab311 light chain

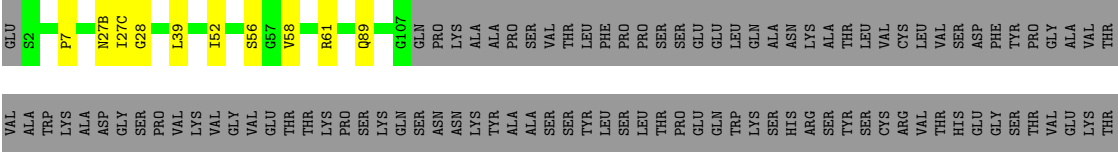


GLU
CYS
SER

• Molecule 3: Fab311 light chain



• Molecule 3: Fab311 light chain



VAL
ALA
PRO
ALA
GLU
CYS
SER

• Molecule 3: Fab311 light chain

[illegible]

Position	Residue	Conservation	Feature
1	SER	0.00	
2	THR	0.00	
3	VAL	0.00	
4	GLU	0.00	
5	LYS	0.00	
6	THR	0.00	
7	VAL	0.00	
8	ALA	0.00	
9	PRO	0.00	
10	ALA	0.00	
11	GLU	0.00	
12	CYS	0.00	
13	SER	0.00	
14	GLU	0.00	
15	THR	0.00	
16	VAL	0.00	
17	THR	0.00	
18	GLY	0.00	
19	THR	0.00	
20	THR	0.00	
21	THR	0.00	
22	LYS	0.00	
23	ASN	0.00	
24	ASN	0.00	
25	LYS	0.00	
26	TYR	0.00	
27	ALA	0.00	
28	ALA	0.00	
29	SER	0.00	
30	SER	0.00	
31	TYR	0.00	
32	LEU	0.00	
33	SER	0.00	
34	LEU	0.00	
35	THR	0.00	
36	PRO	0.00	
37	GLU	0.00	
38	GLN	0.00	
39	TRP	0.00	
40	LYS	0.00	
41	SER	0.00	
42	HIS	0.00	
43	ARG	0.00	
44	SER	0.00	
45	TYR	0.00	
46	SER	0.00	
47	CYS	0.00	
48	ARG	0.00	
49	VAL	0.00	
50	THR	0.00	
51	HIS	0.00	
52	GLU	0.00	
53	GLY	0.00	
54	ASP	0.00	
55	PRO	0.00	
56	LEU	0.00	
57	VAL	0.00	
58	CYS	0.00	
59	LEU	0.00	
60	THR	0.00	
61	ALA	0.00	
62	ASN	0.00	
63	ALA	0.00	
64	GLN	0.00	
65	GLU	0.00	
66	SER	0.00	
67	SER	0.00	
68	PRO	0.00	
69	PHE	0.00	
70	LEU	0.00	
71	THR	0.00	
72	VAL	0.00	
73	SER	0.00	
74	PRO	0.00	
75	ALA	0.00	
76	LYS	0.00	
77	PRO	0.00	
78	GLN	0.00	
79	G107	0.00	Conserved
80	L106A	0.00	Conserved
81	V106	0.00	Conserved
82	E83	0.00	Conserved
83	SER	0.00	
84	PRO	0.00	
85	LYS	0.00	
86	ASN	0.00	
87	SER	0.00	
88	SER	0.00	
89	GLN	0.00	
90	LYS	0.00	
91	THR	0.00	
92	THR	0.00	
93	THR	0.00	
94	Q79	0.00	Conserved
95	R61	0.00	
96	GLY	0.00	
97	VAL	0.00	
98	GLY	0.00	
99	VAL	0.00	
100	LYS	0.00	
101	VAL	0.00	
102	ASP	0.00	
103	GLY	0.00	
104	SER	0.00	
105	L47	0.00	Conserved
106	L39	0.00	Conserved
107	Q17	0.00	Conserved
108	ALA	0.00	
109	TRP	0.00	
110	VAL	0.00	
111	THR	0.00	
112	VAL	0.00	
113	ALA	0.00	
114	S12	0.00	Conserved
115	P7	0.00	Conserved
116	Q6	0.00	Conserved
117	GLY	0.00	
118	PRO	0.00	
119	S2	0.00	Conserved
120	GLU	0.00	

Chain W:

39%

48%

49%

GLU S2 V3 L4 T5 Q6 P7 P8 S9 V11 S12 G13 A14 P15 G16 Q17 T18 V19 T20 I21 S22 C23 G28 A29 D32 W35 Y36 Q37 Q38 L39 P40 G41 T42 A43 P44 K45 L46 I47 N51 I52 N53 R54 P55 S56 G57 V58 P59 D60 R61 P62 S63 G64 S65 K66 S67 G68

T69 S70 A71 S72 L73 A74 T75 T76 T77 L78 Q79 A80 E81 D82 E83 A84 D85 Y86 Y87 C88 R93 R94 F98 G99 G100 G101 T102 K103 L104 T105 V106 A106A G107 G108 G109 G110 G111 G112 G113 G114 G115 G116 G117 G118 G119 G120 G121 G122 G123 G124 G125 G126 G127 G128 G129 G130 G131 G132 G133 G134 G135 G136 G137 G138 G139 G140 G141 G142 G143 G144 G145 G146 G147 G148 G149 G150 G151 G152 G153 G154 G155 G156 G157 G158 G159 G160 G161 G162 G163 G164 G165 G166 G167 G168 G169 G170 G171 G172 G173 G174 G175 G176 G177 G178 G179 G180 G181 G182 G183 G184 G185 G186 G187 G188 G189 G190 G191 G192 G193 G194 G195 G196 G197 G198 G199 G200 G201 G202 G203 G204 G205 G206 G207 G208 G209 G210 G211 G212 G213 G214 G215 G216 G217 G218 G219 G220 G221 G222 G223 G224 G225 G226 G227 G228 G229 G230 G231 G232 G233 G234 G235 G236 G237 G238 G239 G240 G241 G242 G243 G244 G245 G246 G247 G248 G249 G250 G251 G252 G253 G254 G255 G256 G257 G258 G259 G260 G261 G262 G263 G264 G265 G266 G267 G268 G269 G270 G271 G272 G273 G274 G275 G276 G277 G278 G279 G280 G281 G282 G283 G284 G285 G286 G287 G288 G289 G290 G291 G292 G293 G294 G295 G296 G297 G298 G299 G300 G301 G302 G303 G304 G305 G306 G307 G308 G309 G310 G311 G312 G313 G314 G315 G316 G317 G318 G319 G320 G321 G322 G323 G324 G325 G326 G327 G328 G329 G330 G331 G332 G333 G334 G335 G336 G337 G338 G339 G340 G341 G342 G343 G344 G345 G346 G347 G348 G349 G350 G351 G352 G353 G354 G355 G356 G357 G358 G359 G360 G361 G362 G363 G364 G365 G366 G367 G368 G369 G370 G371 G372 G373 G374 G375 G376 G377 G378 G379 G380 G381 G382 G383 G384 G385 G386 G387 G388 G389 G390 G391 G392 G393 G394 G395 G396 G397 G398 G399 G400 G401 G402 G403 G404 G405 G406 G407 G408 G409 G410 G411 G412 G413 G414 G415 G416 G417 G418 G419 G420 G421 G422 G423 G424 G425 G426 G427 G428 G429 G430 G431 G432 G433 G434 G435 G436 G437 G438 G439 G440 G441 G442 G443 G444 G445 G446 G447 G448 G449 G450 G451 G452 G453 G454 G455 G456 G457 G458 G459 G460 G461 G462 G463 G464 G465 G466 G467 G468 G469 G470 G471 G472 G473 G474 G475 G476 G477 G478 G479 G480 G481 G482 G483 G484 G485 G486 G487 G488 G489 G490 G491 G492 G493 G494 G495 G496 G497 G498 G499 G500 G501 G502 G503 G504 G505 G506 G507 G508 G509 G510 G511 G512 G513 G514 G515 G516 G517 G518 G519 G520 G521 G522 G523 G524 G525 G526 G527 G528 G529 G530 G531 G532 G533 G534 G535 G536 G537 G538 G539 G540 G541 G542 G543 G544 G545 G546 G547 G548 G549 G550 G551 G552 G553 G554 G555 G556 G557 G558 G559 G560 G561 G562 G563 G564 G565 G566 G567 G568 G569 G570 G571 G572 G573 G574 G575 G576 G577 G578 G579 G580 G581 G582 G583 G584 G585 G586 G587 G588 G589 G590 G591 G592 G593 G594 G595 G596 G597 G598 G599 G600 G601 G602 G603 G604 G605 G606 G607 G608 G609 G610 G611 G612 G613 G614 G615 G616 G617 G618 G619 G620 G621 G622 G623 G624 G625 G626 G627 G628 G629 G630 G631 G632 G633 G634 G635 G636 G637 G638 G639 G640 G641 G642 G643 G644 G645 G646 G647 G648 G649 G650 G651 G652 G653 G654 G655 G656 G657 G658 G659 G660 G661 G662 G663 G664 G665 G666 G667 G668 G669 G670 G671 G672 G673 G674 G675 G676 G677 G678 G679 G680 G681 G682 G683 G684 G685 G686 G687 G688 G689 G690 G691 G692 G693 G694 G695 G696 G697 G698 G699 G700 G701 G702 G703 G704 G705 G706 G707 G708 G709 G710 G711 G712 G713 G714 G715 G716 G717 G718 G719 G720 G721 G722 G723 G724 G725 G726 G727 G728 G729 G730 G731 G732 G733 G734 G735 G736 G737 G738 G739 G740 G741 G742 G743 G744 G745 G746 G747 G748 G749 G750 G751 G752 G753 G754 G755 G756 G757 G758 G759 G760 G761 G762 G763 G764 G765 G766 G767 G768 G769 G770 G771 G772 G773 G774 G775 G776 G777 G778 G779 G780 G781 G782 G783 G784 G785 G786 G787 G788 G789 G790 G791 G792 G793 G794 G795 G796 G797 G798 G799 G800 G801 G802 G803 G804 G805 G806 G807 G808 G809 G810 G811 G812 G813 G814 G815 G816 G817 G818 G819 G820 G821 G822 G823 G824 G825 G826 G827 G828 G829 G830 G831 G832 G833 G834 G835 G836 G837 G838 G839 G840 G841 G842 G843 G844 G845 G846 G847 G848 G849 G850 G851 G852 G853 G854 G855 G856 G857 G858 G859 G860 G861 G862 G863 G864 G865 G866 G867 G868 G869 G870 G871 G872 G873 G874 G875 G876 G877 G878 G879 G880 G881 G882 G883 G884 G885 G886 G887 G888 G889 G890 G891 G892 G893 G894 G895 G896 G897 G898 G899 G900 G901 G902 G903 G904 G905 G906 G907 G908 G909 G910 G911 G912 G913 G914 G915 G916 G917 G918 G919 G920 G921 G922 G923 G924 G925 G926 G927 G928 G929 G930 G931 G932 G933 G934 G935 G936 G937 G938 G939 G940 G941 G942 G943 G944 G945 G946 G947 G948 G949 G950 G951 G952 G953 G954 G955 G956 G957 G958 G959 G960 G961 G962 G963 G964 G965 G966 G967 G968 G969 G970 G971 G972 G973 G974 G97

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	206990	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 ($e^-/\text{\AA}^2$)	62	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	29000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	5.606	Depositor
Minimum map value	-2.844	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.221	Depositor
Recommended contour level	0.81	Depositor
Map size (Å)	296.63998, 296.63998, 296.63998	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	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	E	1.31	0/659	1.55	12/931 (1.3%)
2	A	1.18	2/962 (0.2%)	1.23	1/1308 (0.1%)
2	B	1.21	2/962 (0.2%)	1.22	3/1308 (0.2%)
2	C	1.25	2/962 (0.2%)	1.22	3/1308 (0.2%)
2	D	1.24	1/962 (0.1%)	1.22	5/1308 (0.4%)
2	F	1.22	3/962 (0.3%)	1.20	2/1308 (0.2%)
2	G	1.24	2/962 (0.2%)	1.20	5/1308 (0.4%)
2	H	1.07	1/962 (0.1%)	1.25	3/1308 (0.2%)
2	I	1.20	1/962 (0.1%)	1.18	1/1308 (0.1%)
2	J	1.15	2/962 (0.2%)	1.20	2/1308 (0.2%)
2	K	1.09	1/962 (0.1%)	1.20	3/1308 (0.2%)
2	M	1.07	2/962 (0.2%)	1.23	2/1308 (0.2%)
3	L	0.98	0/836	1.37	15/1139 (1.3%)
3	N	1.01	0/836	1.28	10/1139 (0.9%)
3	O	1.05	2/836 (0.2%)	1.32	13/1139 (1.1%)
3	P	1.07	1/836 (0.1%)	1.36	15/1139 (1.3%)
3	Q	1.12	1/836 (0.1%)	1.37	10/1139 (0.9%)
3	R	1.14	2/836 (0.2%)	1.33	11/1139 (1.0%)
3	S	1.14	2/836 (0.2%)	1.32	8/1139 (0.7%)
3	T	1.09	1/836 (0.1%)	1.33	9/1139 (0.8%)
3	U	1.09	1/836 (0.1%)	1.30	10/1139 (0.9%)
3	V	1.00	1/836 (0.1%)	1.29	11/1139 (1.0%)
3	W	0.95	0/836	1.41	14/1139 (1.2%)
All	All	1.13	30/20437 (0.1%)	1.28	168/27848 (0.6%)

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
2	B	0	1
2	D	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	F	0	1
All	All	0	3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	35	HIS	CB-CG	-8.04	1.38	1.50
2	K	35	HIS	CB-CG	-7.76	1.39	1.50
2	J	35	HIS	CB-CG	-7.64	1.39	1.50
2	G	35	HIS	CB-CG	-7.42	1.39	1.50
2	C	6	GLU	CG-CD	-7.11	1.34	1.52
2	A	35	HIS	CB-CG	-7.10	1.40	1.50
2	A	6	GLU	CG-CD	-7.03	1.34	1.52
2	F	6	GLU	CG-CD	-6.90	1.34	1.52
2	B	35	HIS	CB-CG	-6.68	1.40	1.50
2	B	51	ILE	CB-CG1	-6.62	1.40	1.53
2	M	6	GLU	CG-CD	-6.45	1.35	1.52
2	F	35	HIS	CB-CG	-6.44	1.41	1.50
2	I	35	HIS	CB-CG	-6.33	1.41	1.50
2	C	35	HIS	CB-CG	-6.30	1.41	1.50
2	D	35	HIS	CB-CG	-6.12	1.41	1.50
2	F	51	ILE	C-O	-5.90	1.17	1.24
2	J	6	GLU	CG-CD	-5.68	1.37	1.52
3	Q	34	HIS	CG-CD2	-5.62	1.29	1.35
3	R	34	HIS	CG-CD2	-5.60	1.29	1.35
3	S	34	HIS	CG-CD2	-5.43	1.29	1.35
2	G	102	TYR	C-O	-5.43	1.17	1.23
3	U	34	HIS	CG-CD2	-5.36	1.29	1.35
3	R	34	HIS	CB-CG	-5.34	1.42	1.50
3	T	89	GLN	CG-CD	-5.30	1.38	1.52
3	S	34	HIS	CB-CG	-5.25	1.42	1.50
3	O	34	HIS	CG-CD2	-5.23	1.30	1.35
2	M	47	TRP	NE1-CE2	-5.15	1.31	1.37
3	P	34	HIS	CG-CD2	-5.06	1.30	1.35
3	O	34	HIS	CB-CG	-5.02	1.43	1.50
3	V	47	LEU	CB-CG	-5.01	1.43	1.53

All (168) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	61	ARG	N-CA-C	-12.09	100.83	114.62
3	S	61	ARG	N-CA-C	-10.95	102.14	114.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	V	61	ARG	N-CA-C	-10.60	102.54	114.62
3	R	61	ARG	N-CA-C	-10.19	101.91	114.75
3	P	61	ARG	N-CA-C	-10.05	102.08	114.75
3	T	61	ARG	N-CA-C	-9.82	102.38	114.75
3	U	61	ARG	N-CA-C	-9.64	102.60	114.75
1	E	42	PRO	N-CA-C	-9.05	97.64	111.13
2	G	12	VAL	CA-C-N	8.22	125.66	119.66
2	G	12	VAL	C-N-CA	8.22	125.66	119.66
1	E	5	ASN	CA-C-N	8.17	129.72	120.98
1	E	5	ASN	C-N-CA	8.17	129.72	120.98
2	D	12	VAL	CA-C-N	8.05	125.54	119.66
2	D	12	VAL	C-N-CA	8.05	125.54	119.66
1	E	1	ASP	CA-C-N	7.62	127.33	119.56
1	E	1	ASP	C-N-CA	7.62	127.33	119.56
2	C	12	VAL	CA-C-N	7.54	125.16	119.66
2	C	12	VAL	C-N-CA	7.54	125.16	119.66
2	J	12	VAL	CA-C-N	7.26	124.96	119.66
2	J	12	VAL	C-N-CA	7.26	124.96	119.66
3	W	54	ARG	CA-C-N	7.23	127.23	119.78
3	W	54	ARG	C-N-CA	7.23	127.23	119.78
3	W	61	ARG	N-CA-C	-6.97	105.97	114.75
3	W	39	LEU	N-CA-C	-6.93	100.84	109.64
2	M	12	VAL	CA-C-N	6.71	124.56	119.66
2	M	12	VAL	C-N-CA	6.71	124.56	119.66
1	E	9	ASP	CA-C-N	6.71	128.23	119.84
1	E	9	ASP	C-N-CA	6.71	128.23	119.84
3	W	28	GLY	CA-C-N	6.57	129.73	120.28
3	W	28	GLY	C-N-CA	6.57	129.73	120.28
3	O	39	LEU	N-CA-C	-6.53	101.90	110.39
3	T	52	ILE	N-CA-C	6.52	119.46	113.20
3	T	58	VAL	CA-C-N	6.50	126.46	120.03
3	T	58	VAL	C-N-CA	6.50	126.46	120.03
2	B	13	PRO	N-CA-C	-6.44	104.28	110.47
3	W	39	LEU	CA-C-N	6.39	126.08	119.56
3	W	39	LEU	C-N-CA	6.39	126.08	119.56
2	D	55	SER	CA-C-N	-6.39	111.95	122.11
2	D	55	SER	C-N-CA	-6.39	111.95	122.11
3	N	39	LEU	CA-C-N	6.37	126.86	119.47
3	N	39	LEU	C-N-CA	6.37	126.86	119.47
3	W	6	GLN	CA-C-N	6.37	124.25	119.66
3	W	6	GLN	C-N-CA	6.37	124.25	119.66
3	N	6	GLN	CA-C-N	6.36	124.24	119.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	6	GLN	C-N-CA	6.36	124.24	119.66
3	R	39	LEU	CA-C-N	6.34	126.83	119.47
3	R	39	LEU	C-N-CA	6.34	126.83	119.47
3	P	39	LEU	CA-C-N	6.34	126.83	119.47
3	P	39	LEU	C-N-CA	6.34	126.83	119.47
3	L	54	ARG	CA-C-N	6.33	126.30	119.78
3	L	54	ARG	C-N-CA	6.33	126.30	119.78
2	H	12	VAL	CA-C-N	6.30	124.26	119.66
2	H	12	VAL	C-N-CA	6.30	124.26	119.66
3	P	58	VAL	CA-C-N	6.23	126.20	120.03
3	P	58	VAL	C-N-CA	6.23	126.20	120.03
2	G	24	THR	N-CA-C	6.23	118.77	108.99
3	L	58	VAL	CA-C-N	6.21	126.18	119.78
3	L	58	VAL	C-N-CA	6.21	126.18	119.78
2	F	12	VAL	CA-C-N	6.18	124.11	119.66
2	F	12	VAL	C-N-CA	6.18	124.11	119.66
3	W	58	VAL	CA-C-N	6.14	126.11	119.78
3	W	58	VAL	C-N-CA	6.14	126.11	119.78
3	U	39	LEU	CA-C-N	6.08	126.52	119.47
3	U	39	LEU	C-N-CA	6.08	126.52	119.47
3	L	61	ARG	N-CA-C	-6.08	104.67	114.09
2	K	13	PRO	N-CA-C	-6.08	103.29	110.70
3	L	39	LEU	CA-C-N	6.04	126.48	119.47
3	L	39	LEU	C-N-CA	6.04	126.48	119.47
3	L	39	LEU	N-CA-C	-6.02	101.47	109.84
3	Q	39	LEU	CA-C-N	6.02	126.45	119.47
3	Q	39	LEU	C-N-CA	6.02	126.45	119.47
3	R	42	THR	N-CA-C	6.00	116.01	108.45
3	V	39	LEU	N-CA-C	-5.99	102.61	110.39
3	R	6	GLN	CA-C-N	5.98	123.96	119.66
3	R	6	GLN	C-N-CA	5.98	123.96	119.66
3	N	39	LEU	N-CA-C	-5.94	101.88	110.08
2	G	5	VAL	N-CA-C	5.92	116.69	107.28
3	V	39	LEU	CA-C-N	5.88	126.29	119.47
3	V	39	LEU	C-N-CA	5.88	126.29	119.47
3	O	39	LEU	CA-C-N	5.87	126.28	119.47
3	O	39	LEU	C-N-CA	5.87	126.28	119.47
3	P	72	SER	N-CA-C	5.82	118.13	108.99
3	N	42	THR	N-CA-C	5.78	115.73	108.45
3	N	52	ILE	N-CA-C	5.77	119.19	113.71
3	O	58	VAL	CA-C-N	5.77	125.68	119.85
3	O	58	VAL	C-N-CA	5.77	125.68	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	V	58	VAL	CA-C-N	5.77	125.67	119.85
3	V	58	VAL	C-N-CA	5.77	125.67	119.85
3	P	28	GLY	N-CA-C	-5.77	107.77	115.32
3	Q	58	VAL	CA-C-N	5.74	125.72	120.03
3	Q	58	VAL	C-N-CA	5.74	125.72	120.03
3	R	58	VAL	CA-C-N	5.73	125.70	120.03
3	R	58	VAL	C-N-CA	5.73	125.70	120.03
3	T	39	LEU	CA-C-N	5.70	126.09	119.47
3	T	39	LEU	C-N-CA	5.70	126.09	119.47
3	Q	6	GLN	CA-C-N	5.70	123.76	119.66
3	Q	6	GLN	C-N-CA	5.70	123.76	119.66
3	S	39	LEU	CA-C-N	5.69	126.07	119.47
3	S	39	LEU	C-N-CA	5.69	126.07	119.47
3	R	54	ARG	CA-C-N	5.68	125.63	119.78
3	R	54	ARG	C-N-CA	5.68	125.63	119.78
1	E	85	ASN	CA-C-N	5.64	126.58	120.83
1	E	85	ASN	C-N-CA	5.64	126.58	120.83
1	E	81	ASN	N-CA-C	5.63	122.26	109.81
3	W	42	THR	N-CA-C	5.63	115.54	108.45
3	W	28	GLY	N-CA-C	-5.61	107.37	114.16
3	U	42	THR	N-CA-C	5.60	115.51	108.45
3	P	54	ARG	CA-C-N	5.60	125.55	119.78
3	P	54	ARG	C-N-CA	5.60	125.55	119.78
3	U	58	VAL	CA-C-N	5.59	125.56	120.03
3	U	58	VAL	C-N-CA	5.59	125.56	120.03
3	O	42	THR	N-CA-C	5.53	115.42	108.45
2	I	5	VAL	N-CA-C	5.52	115.94	107.77
3	N	58	VAL	CA-C-N	5.48	125.42	119.78
3	N	58	VAL	C-N-CA	5.48	125.42	119.78
3	T	39	LEU	N-CA-C	-5.47	103.23	110.40
2	B	51	ILE	CB-CA-C	-5.42	102.61	110.63
3	L	6	GLN	CA-C-N	5.39	123.54	119.66
3	L	6	GLN	C-N-CA	5.39	123.54	119.66
3	S	58	VAL	CA-C-N	5.39	125.37	120.03
3	S	58	VAL	C-N-CA	5.39	125.37	120.03
3	O	72	SER	N-CA-C	5.39	117.27	108.76
3	U	72	SER	N-CA-C	5.39	117.27	108.76
3	P	6	GLN	CA-C-N	5.35	123.51	119.66
3	P	6	GLN	C-N-CA	5.35	123.51	119.66
3	S	54	ARG	CA-C-N	5.35	125.29	119.78
3	S	54	ARG	C-N-CA	5.35	125.29	119.78
3	V	7	PRO	N-CA-C	-5.35	104.86	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	41	ASN	CA-C-N	5.33	125.80	120.52
1	E	41	ASN	C-N-CA	5.33	125.80	120.52
2	B	50	ILE	N-CA-C	5.30	116.30	108.45
2	C	13	PRO	N-CA-C	-5.30	105.38	110.47
3	P	28	GLY	CA-C-N	5.29	127.90	120.28
3	P	28	GLY	C-N-CA	5.29	127.90	120.28
2	K	108	LEU	N-CA-C	5.29	117.87	109.24
3	O	6	GLN	CA-C-N	5.26	123.45	119.66
3	O	6	GLN	C-N-CA	5.26	123.45	119.66
3	Q	72	SER	N-CA-C	5.25	117.06	108.76
3	P	42	THR	N-CA-C	5.25	115.22	108.34
3	Q	28	GLY	CA-C-N	5.24	127.83	120.28
3	Q	28	GLY	C-N-CA	5.24	127.83	120.28
2	D	5	VAL	N-CA-C	5.23	116.03	107.24
2	A	66	ARG	N-CA-C	-5.22	107.57	114.04
2	H	35	HIS	N-CA-C	5.21	117.74	109.50
3	S	39	LEU	N-CA-C	-5.20	102.59	110.39
3	V	54	ARG	CA-C-N	5.20	125.13	119.78
3	V	54	ARG	C-N-CA	5.20	125.13	119.78
2	G	66	ARG	N-CA-C	-5.17	107.64	114.04
3	L	28	GLY	CA-C-N	5.14	128.83	120.60
3	L	28	GLY	C-N-CA	5.14	128.83	120.60
3	O	43	ALA	CA-C-N	5.13	126.26	119.84
3	O	43	ALA	C-N-CA	5.13	126.26	119.84
3	L	102	THR	CA-C-N	-5.12	115.39	122.30
3	L	102	THR	C-N-CA	-5.12	115.39	122.30
3	T	28	GLY	N-CA-C	-5.12	109.04	114.67
3	U	54	ARG	CA-C-N	5.11	125.04	119.78
3	U	54	ARG	C-N-CA	5.11	125.04	119.78
3	T	7	PRO	N-CA-C	-5.10	105.12	110.58
3	V	6	GLN	CA-C-N	5.08	123.32	119.66
3	V	6	GLN	C-N-CA	5.08	123.32	119.66
3	N	72	SER	N-CA-C	5.05	116.92	108.99
3	R	39	LEU	N-CA-C	-5.05	103.60	110.36
3	P	39	LEU	N-CA-C	-5.04	103.84	110.39
2	K	71	ARG	N-CA-C	5.04	117.04	109.23
3	L	7	PRO	N-CA-C	-5.03	105.20	110.58
3	U	7	PRO	N-CA-C	-5.01	105.22	110.58
3	O	54	ARG	CA-C-N	5.01	124.94	119.78
3	O	54	ARG	C-N-CA	5.01	124.94	119.78

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	56	ARG	Sidechain
2	D	56	ARG	Sidechain
2	F	50	ILE	Mainchain

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	E	637	0	547	11	0
2	A	937	0	883	1	0
2	B	937	0	883	5	0
2	C	937	0	883	0	0
2	D	937	0	883	9	0
2	F	937	0	883	27	0
2	G	937	0	883	12	0
2	H	937	0	883	2	0
2	I	937	0	883	0	0
2	J	937	0	883	0	0
2	K	937	0	883	0	0
2	M	937	0	883	0	0
3	L	817	0	785	11	0
3	N	817	0	785	1	0
3	O	817	0	785	0	0
3	P	817	0	785	0	0
3	Q	817	0	785	0	0
3	R	817	0	785	0	0
3	S	817	0	785	0	0
3	T	817	0	785	1	0
3	U	817	0	785	0	0
3	V	817	0	785	0	0
3	W	817	0	785	0	0
All	All	19931	0	18895	71	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (71) 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:G:37:VAL:HG21	2:G:103:TRP:HZ3	1.33	0.93
3:L:25:GLY:HA3	3:L:27(C):ILE:HG13	1.53	0.90
2:F:52(A):TYR:CE2	2:F:53:ASP:HB3	2.07	0.90
3:L:27(C):ILE:HG21	3:L:69:THR:O	1.74	0.88
2:F:52(A):TYR:CD2	2:F:53:ASP:N	2.43	0.86
2:G:37:VAL:HG21	2:G:103:TRP:CZ3	2.14	0.82
2:D:56:ARG:NH2	2:D:56:ARG:HG2	1.97	0.77
3:L:27(C):ILE:HG22	3:L:69:THR:HA	1.66	0.76
3:L:27(C):ILE:HG21	3:L:69:THR:C	2.14	0.73
2:G:101:ASP:N	2:G:101:ASP:OD1	2.17	0.72
2:B:56:ARG:HG2	2:B:56:ARG:NH1	2.04	0.71
2:F:52(A):TYR:HE2	2:F:53:ASP:HB3	1.51	0.70
2:F:51:ILE:HD13	2:F:71:ARG:HD2	1.72	0.70
2:D:56:ARG:O	2:D:57:ASN:CG	2.36	0.69
1:E:84:ALA:HB3	2:H:52:TRP:CH2	2.29	0.68
2:F:56:ARG:CB	2:F:56:ARG:HH11	2.08	0.66
1:E:84:ALA:HB3	2:H:52:TRP:HH2	1.59	0.66
2:F:51:ILE:CD1	2:F:71:ARG:HD2	2.26	0.64
2:B:56:ARG:HG2	2:B:56:ARG:HH11	1.62	0.62
1:E:46:PRO:HA	2:F:52:TRP:NE1	2.14	0.62
1:E:48:ALA:HA	2:F:52(A):TYR:CE1	2.35	0.62
2:F:52(A):TYR:HD2	2:F:53:ASP:N	1.98	0.60
2:D:55:SER:O	2:D:56:ARG:HG3	2.01	0.60
2:D:55:SER:C	2:D:56:ARG:HG3	2.27	0.60
2:F:52(A):TYR:CD2	2:F:53:ASP:HB3	2.37	0.60
1:E:46:PRO:HA	2:F:52:TRP:CD1	2.36	0.60
2:F:56:ARG:HH11	2:F:56:ARG:HB3	1.67	0.59
3:L:27(C):ILE:CG2	3:L:69:THR:HA	2.34	0.58
2:F:51:ILE:O	2:F:51:ILE:HG23	2.03	0.58
2:F:52(A):TYR:CD2	2:F:52(A):TYR:C	2.82	0.56
2:G:4:LEU:CD1	2:G:102:TYR:O	2.54	0.56
2:F:50:ILE:HG12	2:F:51:ILE:N	2.20	0.56
2:G:103:TRP:CD1	2:G:103:TRP:N	2.73	0.55
2:F:51:ILE:HD11	2:F:71:ARG:CD	2.36	0.55
2:G:2:VAL:HG21	2:G:102:TYR:CE2	2.42	0.55
2:F:50:ILE:CG1	2:F:51:ILE:N	2.70	0.55
2:D:55:SER:O	2:D:56:ARG:CG	2.55	0.55
2:F:51:ILE:CD1	2:F:71:ARG:CD	2.85	0.54
2:F:51:ILE:O	2:F:52:TRP:O	2.26	0.54
2:F:56:ARG:HH11	2:F:56:ARG:CG	2.22	0.53
3:L:27(C):ILE:CG2	3:L:69:THR:C	2.82	0.52
2:B:56:ARG:NH1	2:B:56:ARG:CG	2.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:106(A):LEU:O	3:L:107:GLY:C	2.52	0.52
2:G:4:LEU:HD12	2:G:102:TYR:O	2.11	0.51
2:D:56:ARG:HG2	2:D:56:ARG:HH21	1.75	0.50
2:D:56:ARG:NH2	2:D:56:ARG:CG	2.73	0.49
3:T:27(B):ASN:OD1	3:T:27(C):ILE:N	2.47	0.48
2:D:56:ARG:O	2:D:57:ASN:ND2	2.47	0.47
1:E:44:ALA:HB3	2:F:52:TRP:HZ2	1.80	0.47
1:E:12:ALA:O	1:E:14:PRO:HD3	2.15	0.47
1:E:38:PRO:HA	2:G:52:TRP:NE1	2.29	0.46
2:F:52(A):TYR:CE2	2:F:53:ASP:CB	2.88	0.46
1:E:81:ASN:N	1:E:82:PRO:CD	2.79	0.45
3:L:31:TYR:O	3:L:66:LYS:NZ	2.49	0.45
2:F:51:ILE:O	2:F:52:TRP:C	2.58	0.45
3:L:95:LEU:HG	3:L:95(B):GLY:H	1.81	0.45
2:F:52(A):TYR:CD2	2:F:53:ASP:CB	3.01	0.43
3:N:55:PRO:O	3:N:57:GLY:N	2.52	0.43
2:F:56:ARG:CG	2:F:56:ARG:NH1	2.79	0.43
3:L:27(C):ILE:HG22	3:L:69:THR:CA	2.45	0.43
2:D:55:SER:C	2:D:56:ARG:CG	2.93	0.41
2:A:102:TYR:CD2	2:A:102:TYR:C	2.98	0.41
3:L:27(C):ILE:CG2	3:L:69:THR:CA	2.99	0.41
2:B:51:ILE:HG13	2:B:69:ILE:HD12	2.02	0.41
2:G:63:VAL:HB	2:G:67:PHE:CD1	2.56	0.41
2:F:52(A):TYR:HD2	2:F:52(A):TYR:C	2.28	0.41
2:G:103:TRP:N	2:G:103:TRP:HD1	2.17	0.41
1:E:38:PRO:HA	2:G:52:TRP:CE2	2.56	0.40
2:G:2:VAL:HG21	2:G:102:TYR:CD2	2.56	0.40
2:B:112:SER:O	2:B:113:SER:C	2.64	0.40
1:E:46:PRO:HA	2:F:52:TRP:CE2	2.57	0.40

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	E	88/278 (32%)	71 (81%)	13 (15%)	4 (4%)	2	17
2	A	61/225 (27%)	60 (98%)	1 (2%)	0	100	100
2	B	42/225 (19%)	42 (100%)	0	0	100	100
2	C	91/225 (40%)	88 (97%)	3 (3%)	0	100	100
2	D	118/225 (52%)	116 (98%)	2 (2%)	0	100	100
2	F	118/225 (52%)	114 (97%)	2 (2%)	2 (2%)	7	35
2	G	118/225 (52%)	115 (98%)	3 (2%)	0	100	100
2	H	118/225 (52%)	115 (98%)	2 (2%)	1 (1%)	16	49
2	I	118/225 (52%)	115 (98%)	3 (2%)	0	100	100
2	J	118/225 (52%)	115 (98%)	3 (2%)	0	100	100
2	K	118/225 (52%)	115 (98%)	3 (2%)	0	100	100
2	M	118/225 (52%)	115 (98%)	3 (2%)	0	100	100
3	L	107/218 (49%)	101 (94%)	6 (6%)	0	100	100
3	N	92/218 (42%)	89 (97%)	3 (3%)	0	100	100
3	O	65/218 (30%)	60 (92%)	5 (8%)	0	100	100
3	P	110/218 (50%)	104 (94%)	6 (6%)	0	100	100
3	Q	46/218 (21%)	44 (96%)	2 (4%)	0	100	100
3	R	110/218 (50%)	105 (96%)	5 (4%)	0	100	100
3	S	110/218 (50%)	103 (94%)	7 (6%)	0	100	100
3	T	110/218 (50%)	105 (96%)	4 (4%)	1 (1%)	14	46
3	U	110/218 (50%)	105 (96%)	5 (4%)	0	100	100
3	V	110/218 (50%)	105 (96%)	5 (4%)	0	100	100
3	W	110/218 (50%)	104 (94%)	6 (6%)	0	100	100
All	All	2306/5151 (45%)	2206 (96%)	92 (4%)	8 (0%)	37	65

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	16	VAL
2	F	52	TRP
3	T	56	SER
1	E	81	ASN
1	E	7	ASN
1	E	13	ASN
2	H	52(A)	TYR

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Mol	Chain	Res	Type
2	F	51	ILE

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	E	71/240 (30%)	71 (100%)	0	100	100
2	A	97/188 (52%)	97 (100%)	0	100	100
2	B	97/188 (52%)	96 (99%)	1 (1%)	68	75
2	C	97/188 (52%)	97 (100%)	0	100	100
2	D	97/188 (52%)	96 (99%)	1 (1%)	68	75
2	F	97/188 (52%)	95 (98%)	2 (2%)	47	65
2	G	97/188 (52%)	97 (100%)	0	100	100
2	H	97/188 (52%)	97 (100%)	0	100	100
2	I	97/188 (52%)	97 (100%)	0	100	100
2	J	97/188 (52%)	97 (100%)	0	100	100
2	K	97/188 (52%)	97 (100%)	0	100	100
2	M	97/188 (52%)	97 (100%)	0	100	100
3	L	88/179 (49%)	88 (100%)	0	100	100
3	N	88/179 (49%)	88 (100%)	0	100	100
3	O	88/179 (49%)	88 (100%)	0	100	100
3	P	88/179 (49%)	88 (100%)	0	100	100
3	Q	88/179 (49%)	88 (100%)	0	100	100
3	R	88/179 (49%)	88 (100%)	0	100	100
3	S	88/179 (49%)	88 (100%)	0	100	100
3	T	88/179 (49%)	88 (100%)	0	100	100
3	U	88/179 (49%)	88 (100%)	0	100	100
3	V	88/179 (49%)	88 (100%)	0	100	100
3	W	88/179 (49%)	88 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2106/4277 (49%)	2102 (100%)	4 (0%)	85 85

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	56	ARG
2	D	56	ARG
2	F	51	ILE
2	F	56	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	3	GLN
2	H	73	ASN
2	C	57	ASN
2	C	105	GLN
2	D	57	ASN
2	F	81	GLN
2	G	81	GLN
2	I	73	ASN
2	J	57	ASN
2	J	105	GLN
3	V	34	HIS
2	M	3	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.

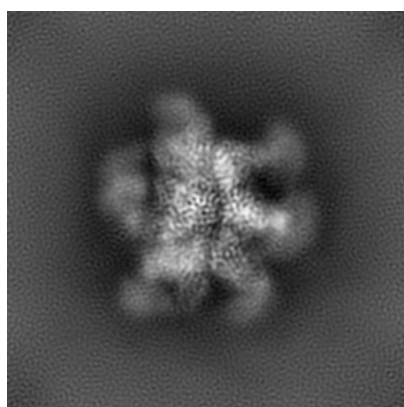
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9114. These allow visual inspection of the internal detail of the map and identification of artifacts.

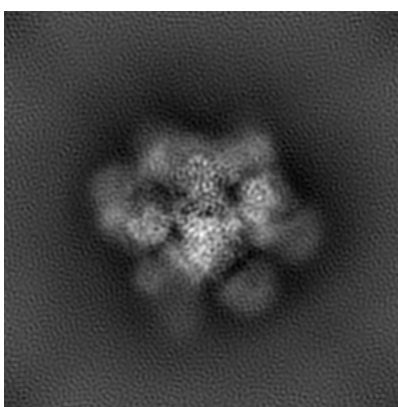
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

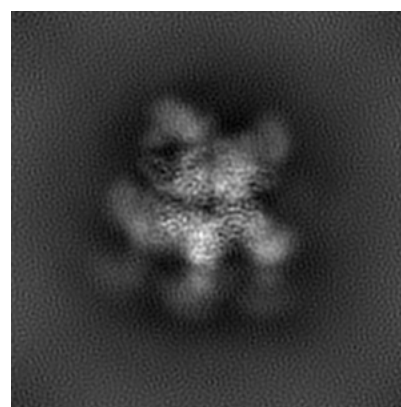
6.1.1 Primary map



X



Y

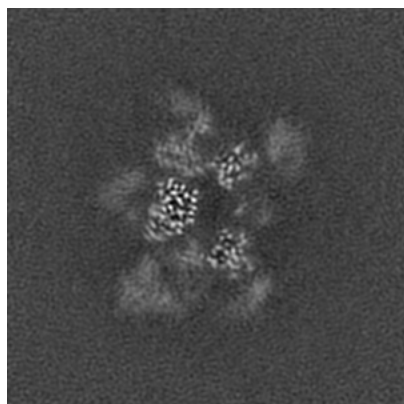


Z

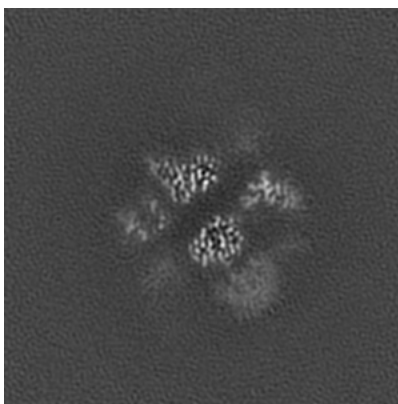
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

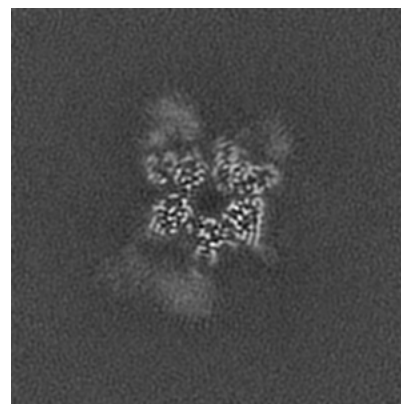
6.2.1 Primary map



X Index: 144



Y Index: 144

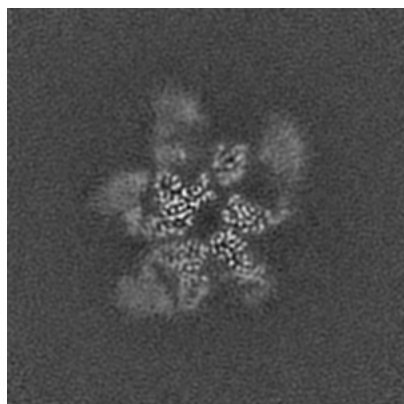


Z Index: 144

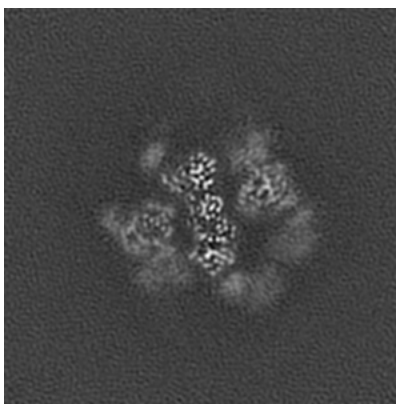
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

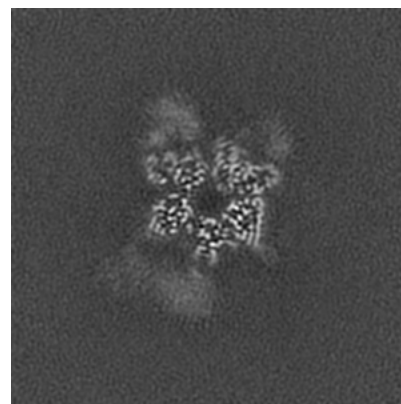
6.3.1 Primary map



X Index: 136



Y Index: 134

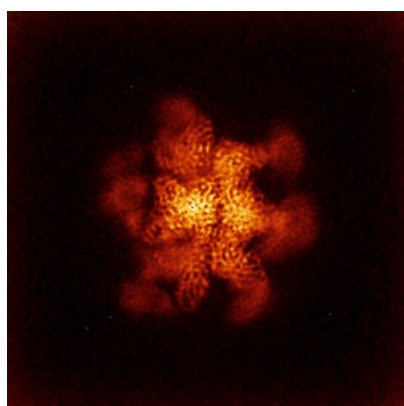


Z Index: 144

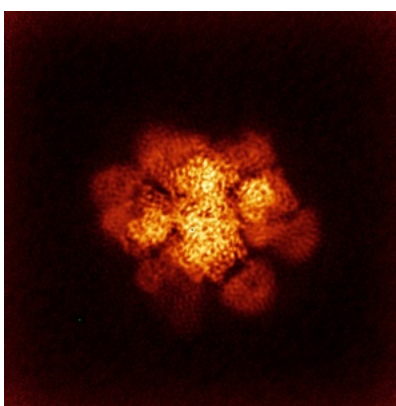
The images above show the largest variance slices of the map in three orthogonal directions.

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

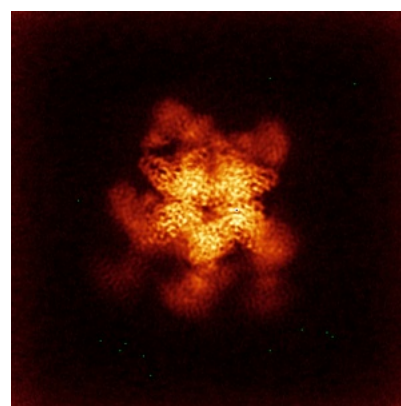
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views

This section was not generated.

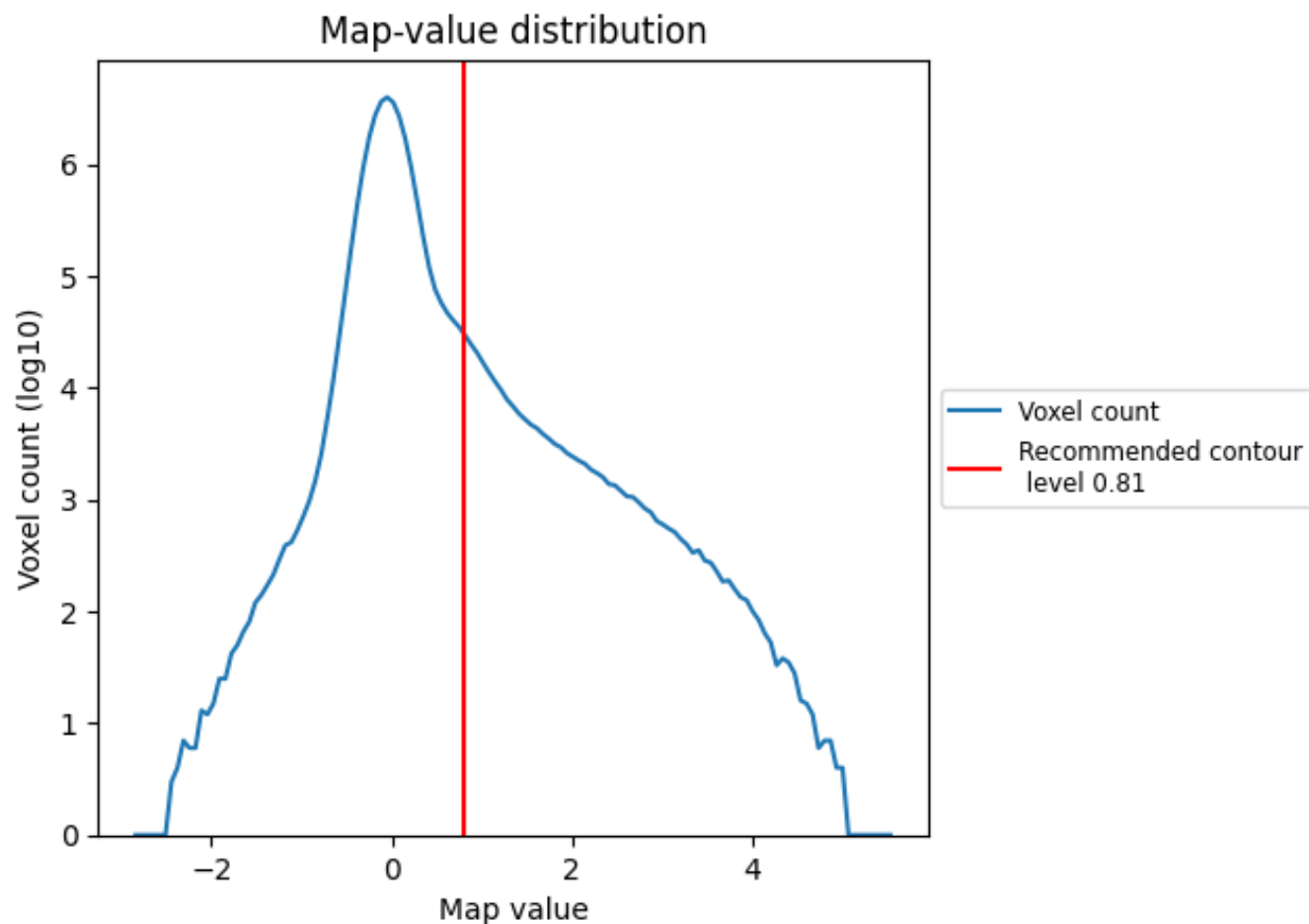
6.6 Mask visualisation

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

7 Map analysis [i](#)

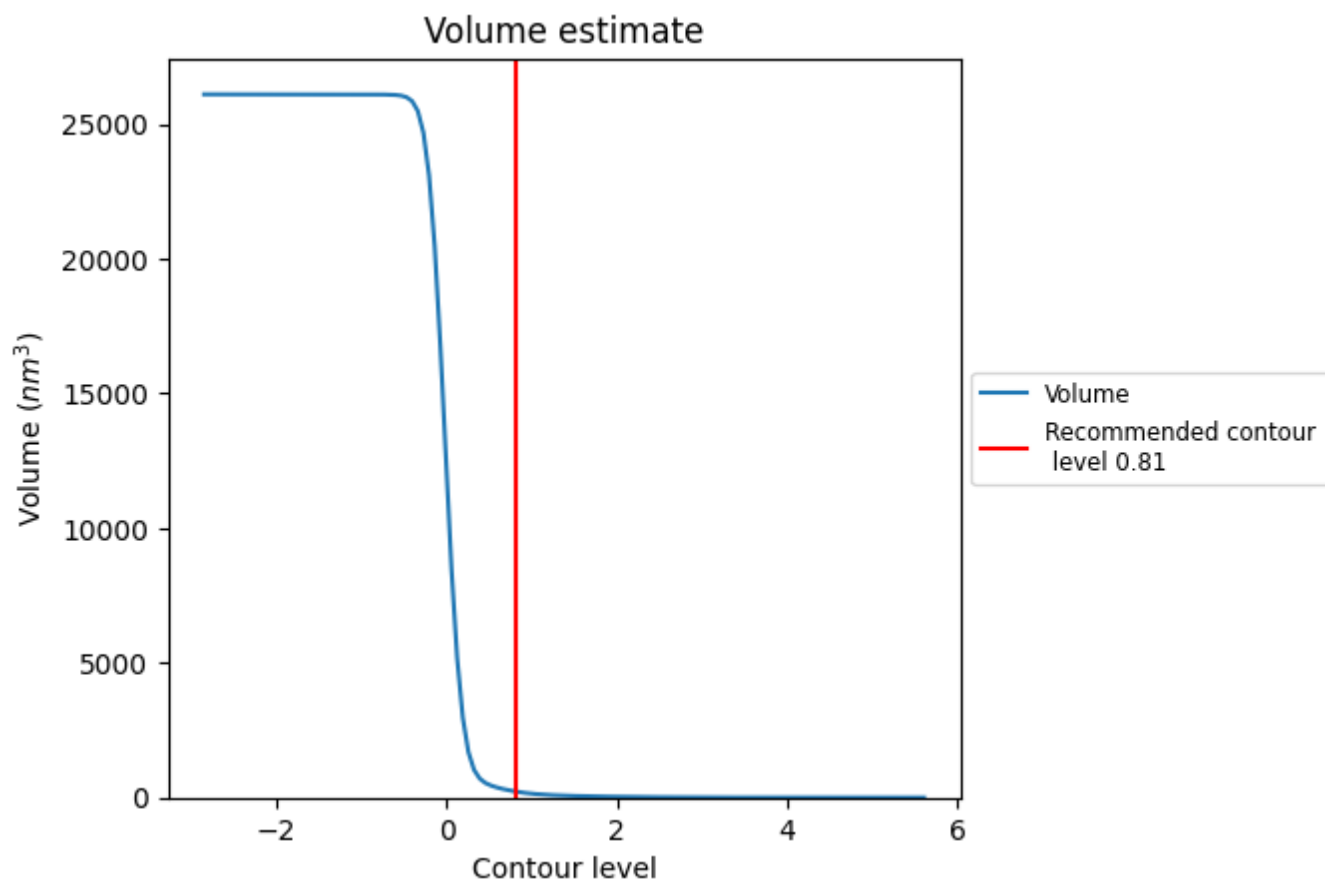
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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.

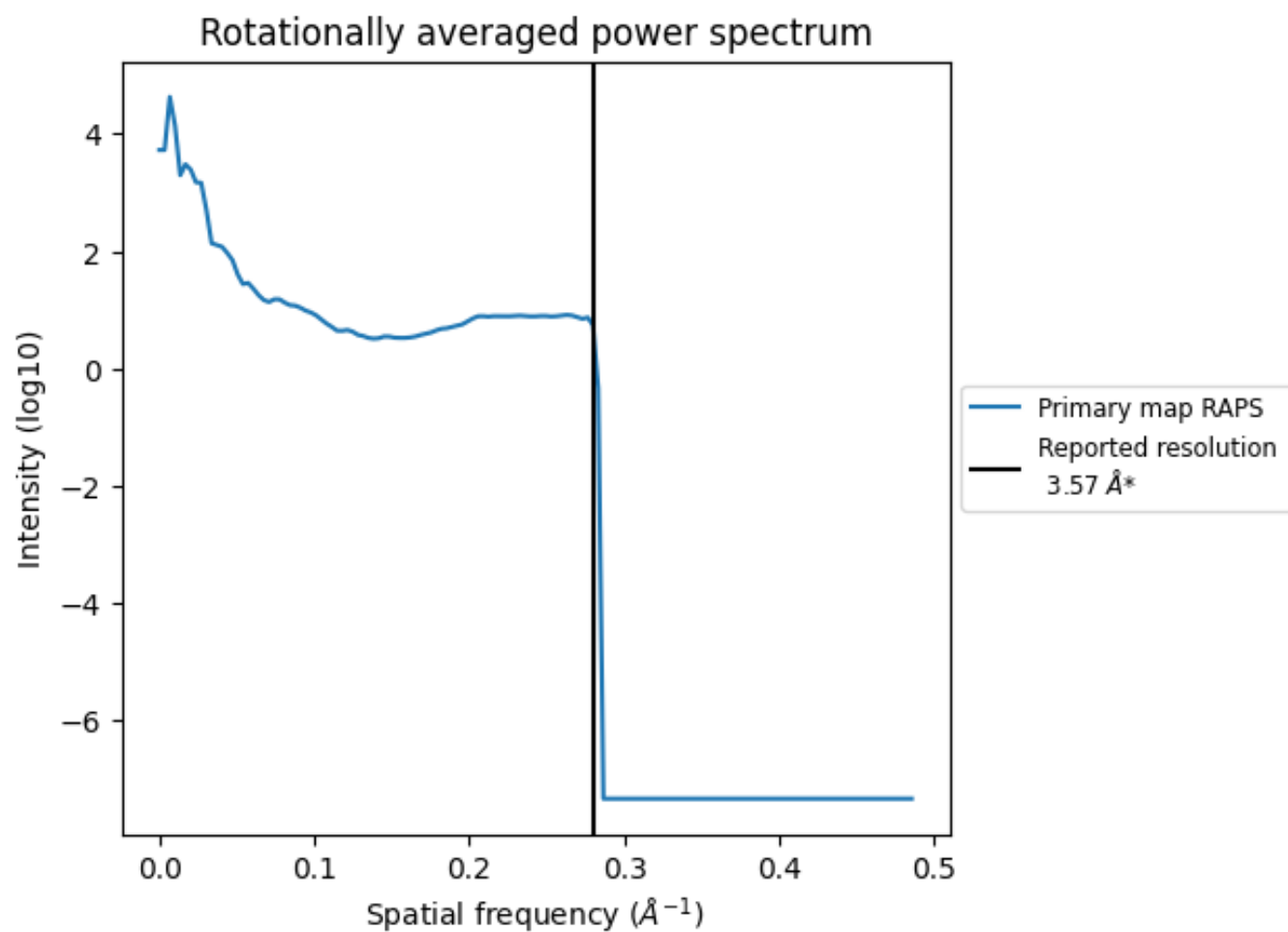
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 225 nm³; this corresponds to an approximate mass of 204 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 ⓘ

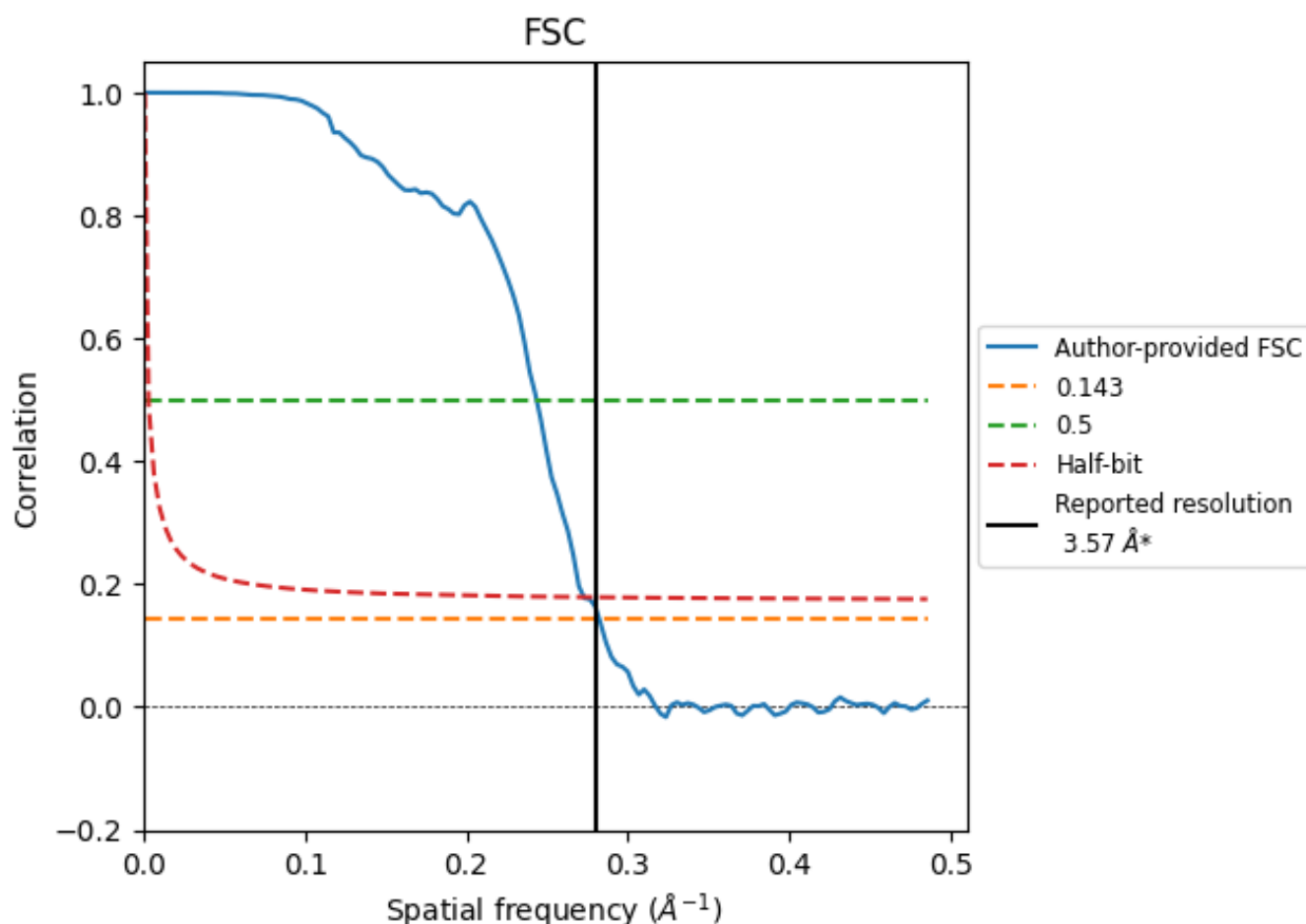


*Reported resolution corresponds to spatial frequency of 0.280 Å⁻¹

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.280 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.57	-	-
Author-provided FSC curve	3.54	4.11	3.67
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

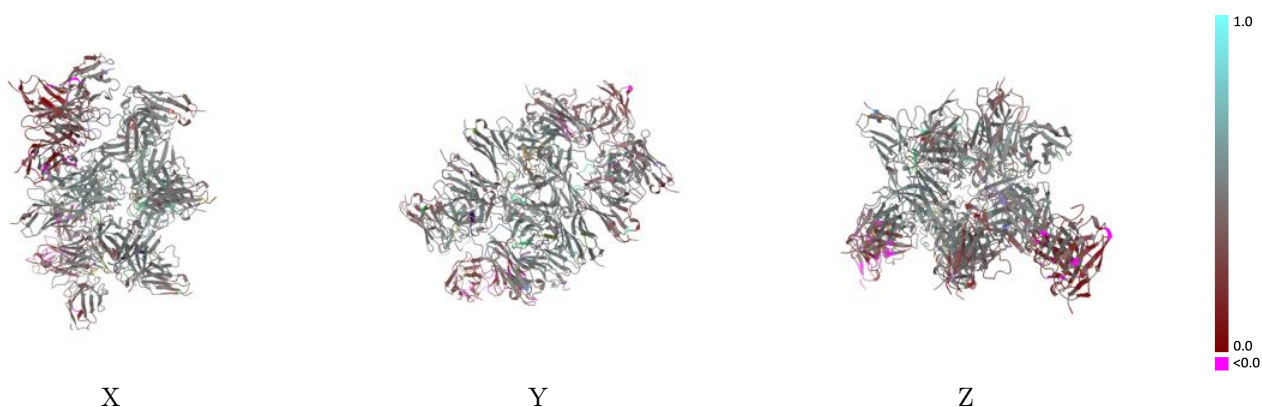
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9114 and PDB model 6MHG. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)

This section was not generated.

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

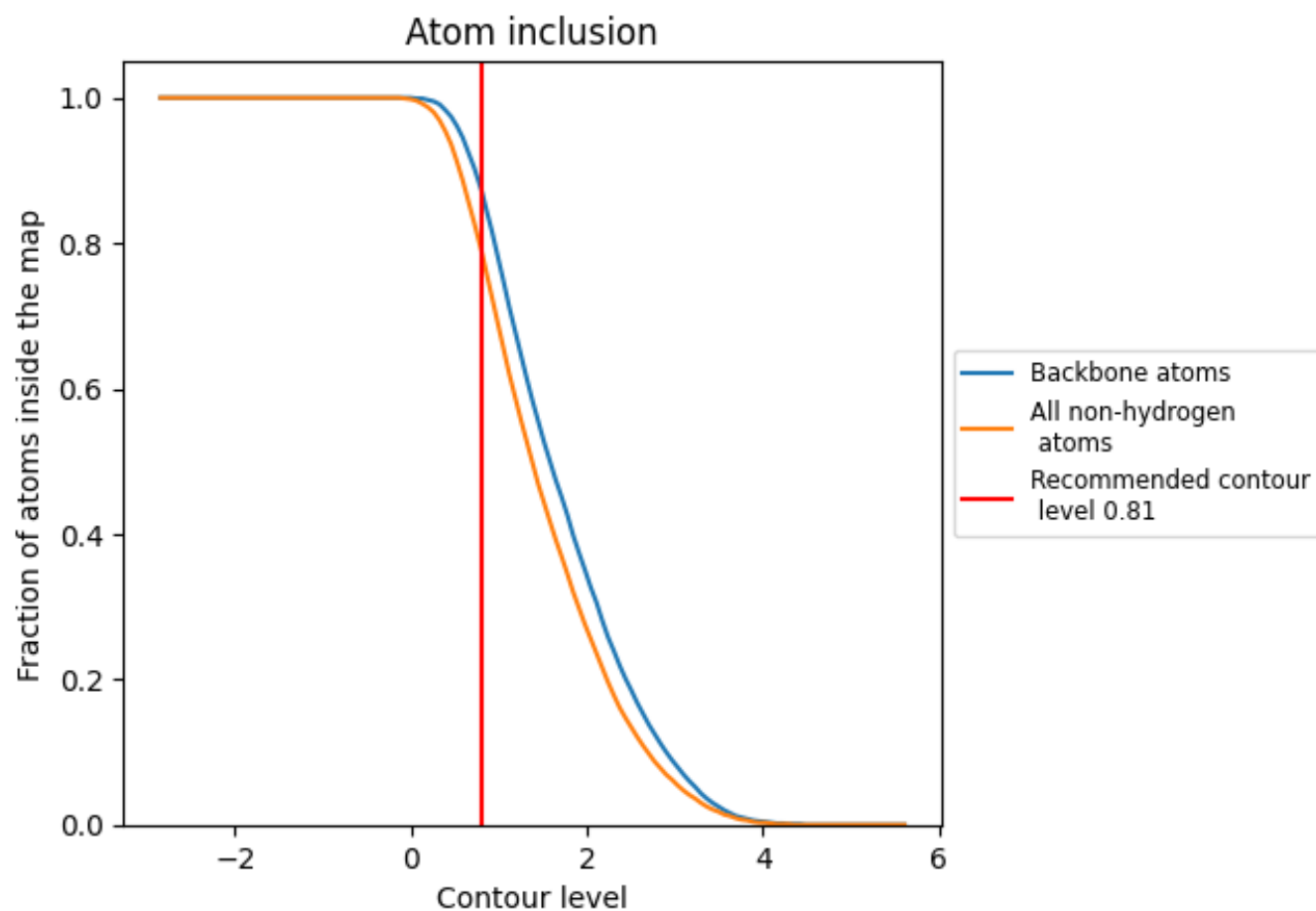


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 78% 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 (0.81) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7850	 0.4240
A	 0.8520	 0.4190
B	 0.8990	 0.4710
C	 0.9100	 0.4940
D	 0.9220	 0.5070
E	 0.8790	 0.4490
F	 0.9210	 0.5110
G	 0.9140	 0.5160
H	 0.5790	 0.2870
I	 0.9030	 0.5030
J	 0.8730	 0.4790
K	 0.7960	 0.4100
L	 0.3920	 0.2350
M	 0.3450	 0.2290
N	 0.7810	 0.3790
O	 0.8560	 0.4350
P	 0.8730	 0.4560
Q	 0.8790	 0.4790
R	 0.8900	 0.4890
S	 0.8890	 0.4940
T	 0.8860	 0.4800
U	 0.8540	 0.4520
V	 0.7520	 0.3830
W	 0.1860	 0.1710

