WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB EM Validation Summary Report (i)

Jun 10, 2024 – 08:45 AM JST

PDB ID	:	8Z9H
EMDB ID	:	EMD-39862
Title	:	Cryo-EM structure of Thogoto virus polymerase in a transcription elongation-reception conformation
Authors	:	Xue, L.; Chang, T.; Li, Z.; Zhao, H.; Li, M.; He, J.; Chen, X.; Xiong, X.
Deposited on	:	2024-04-23
Resolution	:	2.70 Å(reported)

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.70 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.

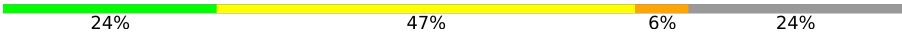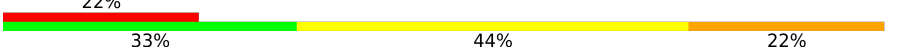| Metric	Percentile Ranks	Value
Clashscore		9
Ramachandran outliers		0
Sidechain outliers		0.1%
RNA backbone		0.57

Worse   *Better*

▌ Percentile relative to all structures

▯ Percentile relative to all EM structures
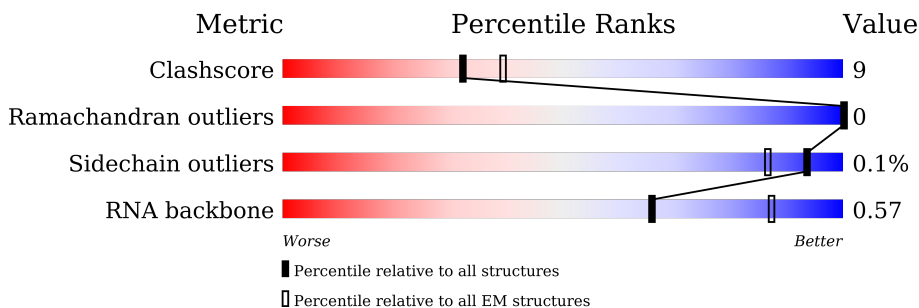
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	622	80% 20%
1	H	622	5% · 52% 20% 28%
2	B	710	72% 23% 5%
2	I	710	13% 56% 25% 18%
3	C	827	5% 71% 19% 10%
3	J	827	7% · 90%
4	D	18	22% 44% 33%

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Mol	Chain	Length	Quality of chain
5	E	17	12% 18% 71%
5	F	17	24% 47% 6% 24%
6	G	9	56% 44%
6	K	9	22% 33% 44% 22%

2 Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 26469 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 Polymerase acidic protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	621	Total	C	N	O	S	0	0
			5021	3172	874	947	28		
1	H	449	Total	C	N	O	S	0	0
			3616	2290	630	675	21		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	471	GLU	GLY	conflict	UNP P27194
H	471	GLU	GLY	conflict	UNP P27194

- Molecule 2 is a protein called RNA-directed RNA polymerase catalytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	676	Total	C	N	O	S	0	0
			5422	3447	943	996	36		
2	I	580	Total	C	N	O	S	0	0
			4631	2954	790	854	33		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	7	LEU	ARG	conflict	UNP O41353
B	230	TRP	CYS	conflict	UNP O41353
I	7	LEU	ARG	conflict	UNP O41353
I	230	TRP	CYS	conflict	UNP O41353

- Molecule 3 is a protein called Polymerase basic protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	748	Total	C	N	O	S	3	0
			6024	3812	1052	1125	35		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	J	79	649	422	109	116	2	0	0

There are 116 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	770	LEU	-	expression tag	UNP Q9YNA4
C	771	GLU	-	expression tag	UNP Q9YNA4
C	772	VAL	-	expression tag	UNP Q9YNA4
C	773	LEU	-	expression tag	UNP Q9YNA4
C	774	PHE	-	expression tag	UNP Q9YNA4
C	775	GLN	-	expression tag	UNP Q9YNA4
C	776	GLY	-	expression tag	UNP Q9YNA4
C	777	PRO	-	expression tag	UNP Q9YNA4
C	778	GLY	-	expression tag	UNP Q9YNA4
C	779	HIS	-	expression tag	UNP Q9YNA4
C	780	HIS	-	expression tag	UNP Q9YNA4
C	781	HIS	-	expression tag	UNP Q9YNA4
C	782	HIS	-	expression tag	UNP Q9YNA4
C	783	HIS	-	expression tag	UNP Q9YNA4
C	784	HIS	-	expression tag	UNP Q9YNA4
C	785	HIS	-	expression tag	UNP Q9YNA4
C	786	HIS	-	expression tag	UNP Q9YNA4
C	787	SER	-	expression tag	UNP Q9YNA4
C	788	ALA	-	expression tag	UNP Q9YNA4
C	789	ASP	-	expression tag	UNP Q9YNA4
C	790	TYR	-	expression tag	UNP Q9YNA4
C	791	LYS	-	expression tag	UNP Q9YNA4
C	792	ASP	-	expression tag	UNP Q9YNA4
C	793	ASP	-	expression tag	UNP Q9YNA4
C	794	ASP	-	expression tag	UNP Q9YNA4
C	795	ASP	-	expression tag	UNP Q9YNA4
C	796	LYS	-	expression tag	UNP Q9YNA4
C	797	GLY	-	expression tag	UNP Q9YNA4
C	798	GLY	-	expression tag	UNP Q9YNA4
C	799	TRP	-	expression tag	UNP Q9YNA4
C	800	SER	-	expression tag	UNP Q9YNA4
C	801	HIS	-	expression tag	UNP Q9YNA4
C	802	PRO	-	expression tag	UNP Q9YNA4
C	803	GLN	-	expression tag	UNP Q9YNA4
C	804	PHE	-	expression tag	UNP Q9YNA4
C	805	GLU	-	expression tag	UNP Q9YNA4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	806	LYS	-	expression tag	UNP Q9YNA4
C	807	GLY	-	expression tag	UNP Q9YNA4
C	808	GLY	-	expression tag	UNP Q9YNA4
C	809	GLY	-	expression tag	UNP Q9YNA4
C	810	SER	-	expression tag	UNP Q9YNA4
C	811	GLY	-	expression tag	UNP Q9YNA4
C	812	GLY	-	expression tag	UNP Q9YNA4
C	813	GLY	-	expression tag	UNP Q9YNA4
C	814	GLY	-	expression tag	UNP Q9YNA4
C	815	SER	-	expression tag	UNP Q9YNA4
C	816	GLY	-	expression tag	UNP Q9YNA4
C	817	GLY	-	expression tag	UNP Q9YNA4
C	818	SER	-	expression tag	UNP Q9YNA4
C	819	ALA	-	expression tag	UNP Q9YNA4
C	820	TRP	-	expression tag	UNP Q9YNA4
C	821	SER	-	expression tag	UNP Q9YNA4
C	822	HIS	-	expression tag	UNP Q9YNA4
C	823	PRO	-	expression tag	UNP Q9YNA4
C	824	GLN	-	expression tag	UNP Q9YNA4
C	825	PHE	-	expression tag	UNP Q9YNA4
C	826	GLU	-	expression tag	UNP Q9YNA4
C	827	LYS	-	expression tag	UNP Q9YNA4
J	761	LEU	-	expression tag	UNP Q9YNA4
J	762	GLU	-	expression tag	UNP Q9YNA4
J	763	VAL	-	expression tag	UNP Q9YNA4
J	764	LEU	-	expression tag	UNP Q9YNA4
J	765	PHE	-	expression tag	UNP Q9YNA4
J	766	GLN	-	expression tag	UNP Q9YNA4
J	767	GLY	-	expression tag	UNP Q9YNA4
J	768	PRO	-	expression tag	UNP Q9YNA4
J	769	GLY	-	expression tag	UNP Q9YNA4
J	770	HIS	-	expression tag	UNP Q9YNA4
J	771	HIS	-	expression tag	UNP Q9YNA4
J	772	HIS	-	expression tag	UNP Q9YNA4
J	773	HIS	-	expression tag	UNP Q9YNA4
J	774	HIS	-	expression tag	UNP Q9YNA4
J	775	HIS	-	expression tag	UNP Q9YNA4
J	776	HIS	-	expression tag	UNP Q9YNA4
J	777	HIS	-	expression tag	UNP Q9YNA4
J	778	SER	-	expression tag	UNP Q9YNA4
J	779	ALA	-	expression tag	UNP Q9YNA4
J	780	ASP	-	expression tag	UNP Q9YNA4

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Chain	Residue	Modelled	Actual	Comment	Reference
J	781	TYR	-	expression tag	UNP Q9YNA4
J	782	LYS	-	expression tag	UNP Q9YNA4
J	783	ASP	-	expression tag	UNP Q9YNA4
J	784	ASP	-	expression tag	UNP Q9YNA4
J	785	ASP	-	expression tag	UNP Q9YNA4
J	786	ASP	-	expression tag	UNP Q9YNA4
J	787	LYS	-	expression tag	UNP Q9YNA4
J	788	GLY	-	expression tag	UNP Q9YNA4
J	789	GLY	-	expression tag	UNP Q9YNA4
J	790	TRP	-	expression tag	UNP Q9YNA4
J	791	SER	-	expression tag	UNP Q9YNA4
J	792	HIS	-	expression tag	UNP Q9YNA4
J	793	PRO	-	expression tag	UNP Q9YNA4
J	794	GLN	-	expression tag	UNP Q9YNA4
J	795	PHE	-	expression tag	UNP Q9YNA4
J	796	GLU	-	expression tag	UNP Q9YNA4
J	797	LYS	-	expression tag	UNP Q9YNA4
J	798	GLY	-	expression tag	UNP Q9YNA4
J	799	GLY	-	expression tag	UNP Q9YNA4
J	800	GLY	-	expression tag	UNP Q9YNA4
J	801	SER	-	expression tag	UNP Q9YNA4
J	802	GLY	-	expression tag	UNP Q9YNA4
J	803	GLY	-	expression tag	UNP Q9YNA4
J	804	GLY	-	expression tag	UNP Q9YNA4
J	805	GLY	-	expression tag	UNP Q9YNA4
J	806	SER	-	expression tag	UNP Q9YNA4
J	807	GLY	-	expression tag	UNP Q9YNA4
J	808	GLY	-	expression tag	UNP Q9YNA4
J	809	SER	-	expression tag	UNP Q9YNA4
J	810	ALA	-	expression tag	UNP Q9YNA4
J	811	TRP	-	expression tag	UNP Q9YNA4
J	812	SER	-	expression tag	UNP Q9YNA4
J	813	HIS	-	expression tag	UNP Q9YNA4
J	814	PRO	-	expression tag	UNP Q9YNA4
J	815	GLN	-	expression tag	UNP Q9YNA4
J	816	PHE	-	expression tag	UNP Q9YNA4
J	817	GLU	-	expression tag	UNP Q9YNA4
J	818	LYS	-	expression tag	UNP Q9YNA4

- Molecule 4 is a RNA chain called RNA (5'-R(*AP*GP*AP*GP*AP*AP*AP*UP*CP*AP*
  AP*GP*GP*CP*AP*GP*UP*U)-3').

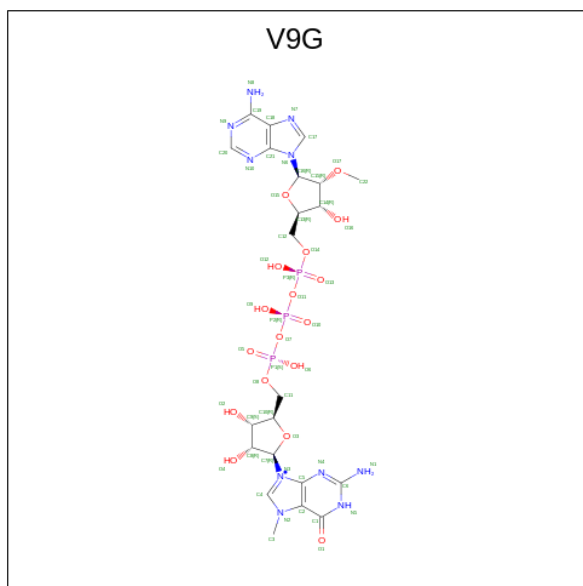| Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	12	Total	C	N	O	P	0	0
			260	118	55	76	11		

- Molecule 5 is a RNA chain called RNA (5'-R(*GP*AP*CP*UP*GP*CP*CP*UP*GP*UP*UP*UP*UP*UP*GP*CP*U)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	5	Total	C	N	O	P	0	0
			103	46	14	38	5		
5	F	13	Total	C	N	O	P	0	0
			269	120	38	98	13		

- Molecule 6 is a RNA chain called RNA (5'-R(P*GP*CP*AP*AP*AP*AP*AP*CP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	9	Total	C	N	O	P	0	0
			195	88	41	57	9		
6	K	9	Total	C	N	O	P	0	0
			195	88	41	57	9		

- Molecule 7 is 7-METHYL-GUANOSINE-5'-TRIPHOSPHATE-5'-(2'-O-METHYL)-ADENOSINE (three-letter code: V9G) (formula: $C_{22}H_{32}N_{10}O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).

V9G

Mol	Chain	Residues	Atoms					AltConf
7	G	1	Total	C	N	O	P	0
			52	22	10	17	3	

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
7	K	1	32	11	5	13	3	0

3 Residue-property plots ⓘ

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: Polymerase acidic protein

Chain A:

- Molecule 1: Polymerase acidic protein

Chain H:

L446 I447 A448 M451 K458 H462 S463 S466 V469 E470 E471 K472 S477 L478 K479 I480 T481 L488 R496 A502 V508 V509 L510 S511 R512 A513 A514 E515 N517 S518 L519 N520 L521 E522 V523 N524 P525 E526 I527 Q528 E532 G533 A534 Q535 L540

W543 I547 N558 N559 L566 R570 R571 L572 H577 M580 E581 R582 R583 F586 F589 E594 D595 K596 V597 N604 P605 I606 V607 W614 P618 Y621 Y622

• Molecule 2: RNA-directed RNA polymerase catalytic subunit

Chain B: 72%   23%   5%

M1 E9 I10 N11 P12 Y22 T23 G24 P25 A26 P27 Y30 G31 T32 R33 T34 I42 I60 H80 S83 L87 F92 M99 L102 K103 Y104 W105 K109 K112 L113 K114 Y115 L118 F127 N132 V143 E144 F145 L146 E147 Q148 N149

R152 P156 T157 L158 D167 D172 Y176 E177 G178 A179 R180 ASP PRO ARG PRO TRP ASP ILE GLN LEU GLU GLU ILE ASP SER ASP GLU GLU ASP PRO LEU PHE ARG GLN VAL GLY ARG GLU GLU T209 Y210 T211 R216 E217 Q222 M223 L226 M229 W230 K231 I243

A244 T245 P246 L249 G252 F253 I256 E263 I264 K280 L281 T289 F290 V294 T295 G296 E297 L298 R315 L325 E333 N336 I337 P338 E351 G352 L353 V354 K357 D363 R364 L376 I385 L389 M393 Y396 T399 S400 T401

L402 L403 I406 S407 R410 S420 S421 D422 C430 T442 T446 V450 L461 I462 S463 P464 A465 G466 I467 G468 A484 L487 L490 N493 M498 M503 N506 T514 G515 Q516 M517 N518 L519 C520 T521 I528 K534 R544 T555 P556

L557 A563 H567 S568 T571 E576 R581 E588 E589 T590 L591 R592 L595 N599 P600 K604 R612 I613 E614 P618 P627 S628 C629 R636 N637 R638 THR ILE GLN ASP LYS PRO H645 K646 E652 Q656 R657 V658 T659 S660 I661 I662 L665 F666

P667 E668 V669 L670 S675 A676 T679 E682 S683 L684 L688 V692 D696 E699 E700 R701 K702 K703 R704 R708 I709 F710

• Molecule 2: RNA-directed RNA polymerase catalytic subunit

Chain I: 13%   56%   25%   18%

M1 E9 I10 N11 P12 T13 T14 T15 Q16 L19 Y20 A21 Y22 P25 Y30 G31 T32 L38 E39 I42 R43 K50 L58 D59 T62 G63 C64 E68 D69 I70 N71 V72 E73 G74 F79 H80 T81 A82 L85 K86 L87 F91 F92 R93 K94 Y95 R96

M99 L102 K103 Y104 W105 I106 L107 V108 K109 L110 P111 K112 A116 E117 L118 S119 K120 G121 R122 Q123 L133 P134 A135 P136 I137 A138 L139 E140 E144 F145 L146 E147 Q148 N149 L150 R151 R152 K153 L159 S160 Y161 C162 Q163 A164 I165 A166 D167 V168 M169 E170 L171 D172 E173 T174

T175 Y176 E177 GLY ALA ARG ASP PRO ARG PRO TRP ASP ILE GLN LEU GLU GLU ILE ASP SER ASP GLU GLU ASP PRO LEU PHE ARG GLN VAL GLY ARG GLU GLU THR Y210 K213 F214 S215 R216 R224 R235 L238 N239 R240 T245 R251 G252 F253 V254 E258 K262

E263 I264 L265 E266 N267 G272 V273 P274 VAL GLY GLY GLU E279 K280 L281 A282 K283 L284 Q288 T289 F290 H291 T292 A293 V294 T295 L298 K304 F305 N306 E307 D310 P311 D312 A313 M314 R315 L316 M317 F321 L322 R323 K324 L325 P328 D329 W330 I331 M332 E333 L334 F335 N336

I337 P338 F339 M340 V341 F342 L346 M349 G350 E351 L366 G382 R388 M393 N397 T401 L402 L403 A404 L405 I406 S407 I408 E409 R410 E411 E412 L413 T414 G415 S416 H417 C430 M436 F437 K438 L447 K448 L449 V450 G451 I452 S465 P456 S457 K458 L461

A465 G466 I467 F470 H475 H476 R477 D478 F479 N482 V483 A484 T485 E486 A489 L490 V491 G494 T495 M496 P497 M498 T499 M503 T514 N518 L519 C520 T521 G522 A523 M526 M538 G541 V542 T543 R544 R545 F548 L557 N560 Q561 S568 F569

S570 T571 M572 H573 E576 V577 A578 R581 G584 L585 L586 D587 E588 R592 N599 P600 V601 T602 GLN LYS ASP PRO SER MET PHE ARG GLU ASN LYS MET PRO GLN ILE MET E622 D623 Y624 S625 F630 L634 S635 ARG ASN ARG THR ILE GLN ASP LYS PRO

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

ILE LEU SER ARG ILE PHE

• Molecule 3: Polymerase basic protein 2

Chain C:

MET ASP ARG GLU GLU PRO ALA E8 L13 R14 V17 E18 E19 A23 C24 K25 E26 F35 Y38 Y44 T45 T46 S47 L57 W65 P66 M69 S72 K73 E74 L77 V78 K83 L84 K85 D86 T87 I88 L89 D90 L91 G92 E93 S94 K95 R96 T97 R98

A99 N100 V103 K109 Y110 Q113 T114 V118 V119 N120 A121 I122 D127 Q131 F134 R142 Y143 G144 R145 M146 L147 R150 P157 N163 L171 C176 L182 D183 R186 H189 V206 E210 S211 A212 V213 H214 I215 T237 A238 E239

H249 L258 D265 E270 R274 R279 T284 N288 R297 P298 M299 V302 D305 L310 R317 S323 R331 S332 T333 K334 N339 S340 D341 R344 K348 K349 V350 F351 S352 L353 S354 P355 D356 V357 Q358 V359 T360 I361 P362 R365 F366

K371 Q375 N376 Q380 R388 I393 K394 E405 P406 Y413 G414 S415 F416 I417 F418 P419 E422 Q423 T424 F425 C426 F427 Y428 P429 A430 G431 K432 R433 E434 S438 M441 K458 L464 V481 Q489 N512 L517 I518 C519 P520 T521 L530 F541

I542 D543 I544 D547 N572 E576 Y577 E582 V585 Q586 T593 K599 Q603 I627 R635 D636 Q639 T667 T668 N669 R670 I671 I672 K683 G684 G685 P686 E687 V690 Q691 T692 G693 R700 C701 T706 P707 D708 H709 G710 M713 S716 R717

F718 C719 Q723 G724 R725 Y726 F727 Q728 Y729 I733 W736 E737 E738 D747 R750 D751 L752 K753 R754 R755 ARG ASP ILE GLU GLU MET VAL SER LYS ARG ARG ILE VAL LEU GLU VAL LEU PHE GLN GLY PRO GLY HIS HIS HIS HIS HIS HIS HIS HIS HIS SER ALA ASP TYR

LYS ASP ASP ASP LYS GLY TRP SER HIS PRO GLN PHE GLU LYS GLY GLY GLY SER GLY GLY GLY SER GLY GLY SER ALA TRP SER HIS PRO GLN PHE GLU LYS

• Molecule 3: Polymerase basic protein 2

Chain J:

MET ASP ARG GLU GLU PRO ALA GLU SER GLU CYS THR LEU ARG ALA LEU VAL GLU GLU TYR ASN GLY ALA CYS LYS GLU ALA PRO LYS GLU MET SER LYS GLN PHE THR ASP TYR ASN PHE LYS ARG TYR THR THR SER LYS LYS ASP HIS A43 L48 V49 Y50 K54 P55 W56

• Molecule 4: RNA (5'-R(*AP*GP*AP*GP*AP*AP*AP*UP*CP*AP*AP*GP*GP*CP*AP*GP*UP*U)-3')

Chain D:

| 22% | 44% | 33% |

• Molecule 5: RNA (5'-R(*GP*AP*CP*UP*GP*CP*CP*UP*GP*UP*UP*UP*UP*UP*GP*CP*U)-3')

Chain E:

| 12% | 18% | 71% |

• Molecule 5: RNA (5'-R(*GP*AP*CP*UP*GP*CP*CP*UP*GP*UP*UP*UP*UP*UP*GP*CP*U)-3')
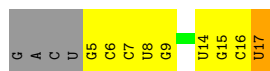
Chain F:

• Molecule 6: RNA (5'-R(P*GP*CP*AP*AP*AP*AP*AP*CP*A)-3')

Chain G:

• Molecule 6: RNA (5'-R(P*GP*CP*AP*AP*AP*AP*AP*CP*A)-3')

Chain K:
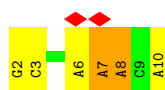
4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	80060	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	50	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.205	Depositor
Minimum map value	-0.071	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.017	Depositor
Map size (Å)	262.80002, 262.80002, 262.80002	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.095, 1.095, 1.095	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: V9G

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	0.24	0/5136	0.49	1/6967 (0.0%)
1	H	0.25	0/3697	0.50	0/5011
2	B	0.25	0/5532	0.51	1/7468 (0.0%)
2	I	0.25	0/4730	0.50	0/6396
3	C	0.25	0/6161	0.52	0/8332
3	J	0.25	0/666	0.51	0/905
4	D	0.18	0/293	0.72	0/456
5	E	0.17	0/113	0.68	0/173
5	F	0.18	0/297	0.77	0/459
6	G	0.20	0/219	0.66	0/339
6	K	0.20	0/219	0.71	0/339
All	All	0.25	0/27063	0.52	2/36845 (0.0%)

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
3	C	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	490	LEU	CA-CB-CG	6.33	129.86	115.30
1	A	109	PRO	CA-N-CD	-5.31	104.06	111.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

WORLDWIDE
wwPDB
PROTEIN DATA BANK

Mol	Chain	Res	Type	Group
3	C	418	GLU	Peptide

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	A	5021	0	4960	93	0
1	H	3616	0	3614	86	0
2	B	5422	0	5493	120	0
2	I	4631	0	4662	124	0
3	C	6024	0	6029	116	0
3	J	649	0	657	21	0
4	D	260	0	133	6	0
5	E	103	0	53	2	0
5	F	269	0	137	11	0
6	G	195	0	100	3	0
6	K	195	0	100	5	0
7	G	52	0	0	0	0
7	K	32	0	0	0	0
All	All	26469	0	25938	492	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 9.

The worst 5 of 492 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:I:253:PHE:HB3	2:I:338:PRO:HG3	1.57	0.86
1:A:396:THR:HG21	5:E:16:C:H41	1.40	0.85
2:B:656:GLN:NE2	3:C:44:TYR:O	2.17	0.77
2:I:102:LEU:HD23	2:I:264:ILE:HD13	1.68	0.75
2:I:538:MET:HB3	2:I:543:THR:HG21	1.68	0.74

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	619/622 (100%)	598 (97%)	21 (3%)	0	100	100
1	H	447/622 (72%)	426 (95%)	21 (5%)	0	100	100
2	B	670/710 (94%)	643 (96%)	27 (4%)	0	100	100
2	I	572/710 (81%)	547 (96%)	25 (4%)	0	100	100
3	C	748/827 (90%)	696 (93%)	52 (7%)	0	100	100
3	J	75/827 (9%)	75 (100%)	0	0	100	100
All	All	3131/4318 (72%)	2985 (95%)	146 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	560/561 (100%)	560 (100%)	0	100	100
1	H	403/561 (72%)	403 (100%)	0	100	100
2	B	600/633 (95%)	600 (100%)	0	100	100
2	I	513/633 (81%)	510 (99%)	3 (1%)	86	95
3	C	676/736 (92%)	675 (100%)	1 (0%)	93	98
3	J	73/736 (10%)	73 (100%)	0	100	100
All	All	2825/3860 (73%)	2821 (100%)	4 (0%)	93	98

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

Mol	Chain	Res	Type
3	C	145	ARG
2	I	213	LYS
2	I	283	LYS
2	I	438	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	528	GLN
1	H	535	GLN
2	I	476	HIS
2	B	656	GLN
1	A	577	HIS

5.3.3   RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	D	11/18 (61%)	2 (18%)	1 (9%)
5	E	4/17 (23%)	1 (25%)	0
5	F	12/17 (70%)	1 (8%)	0
6	G	8/9 (88%)	0	0
6	K	8/9 (88%)	3 (37%)	1 (12%)
All	All	43/70 (61%)	7 (16%)	2 (4%)

5 of 7 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	D	6	A
4	D	12	G
5	E	17	U
5	F	17	U
6	K	6	A

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	D	11	A
6	K	7	A

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

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

5.5　Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6　Ligand geometry ⓘ

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
7	V9G	G	1	6	46,57,57	4.10	21 (45%)	46,89,89	2.61	8 (17%)
7	V9G	K	1	6	26,34,57	3.98	9 (34%)	31,53,89	3.07	6 (19%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	V9G	G	1	6	-	11/26/94/94	0/6/6/6
7	V9G	K	1	6	-	9/20/40/94	0/3/3/6

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	1	V9G	C14-C15	-11.54	1.27	1.52
7	K	1	V9G	C14-C15	-11.47	1.27	1.52
7	G	1	V9G	O3-C7	11.38	1.57	1.41
7	K	1	V9G	O15-C16	11.12	1.56	1.41
7	G	1	V9G	O15-C16	11.09	1.56	1.41

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	K	1	V9G	C18-C19-N8	12.41	139.21	120.35
7	G	1	V9G	C18-C19-N8	12.38	139.17	120.35
7	K	1	V9G	N8-C19-N9	-8.56	100.80	118.57
7	G	1	V9G	N8-C19-N9	-8.54	100.85	118.57
7	K	1	V9G	N10-C20-N9	-5.54	120.02	128.68

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	G	1	V9G	O14-C12-C13-O15
7	G	1	V9G	C16-C15-O17-C22
7	G	1	V9G	C12-O14-P3-O13
7	G	1	V9G	C12-O14-P3-O12
7	K	1	V9G	C16-C15-O17-C22

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand V9G G 1

Bond lengths

Bond angles

Torsions

Rings

Ligand V9G K 1

Bond lengths

Bond angles

Torsions

Rings
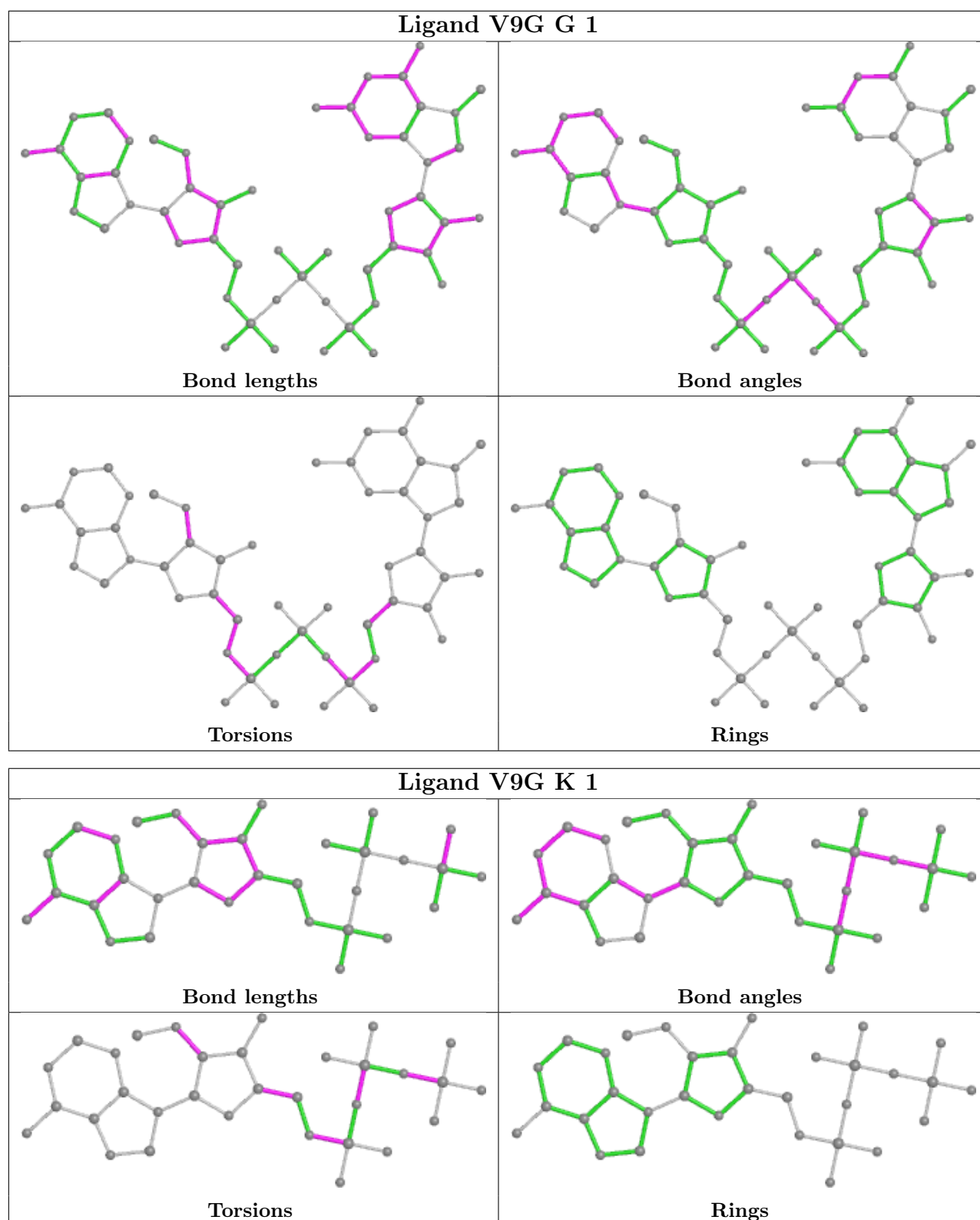
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6　Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-39862. 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 ⓘ
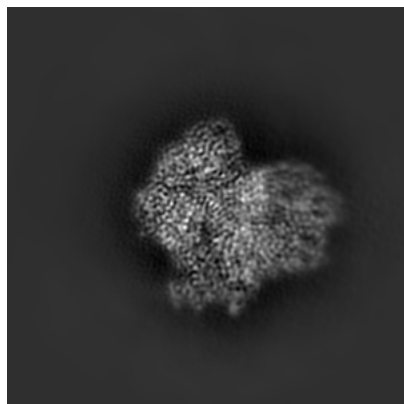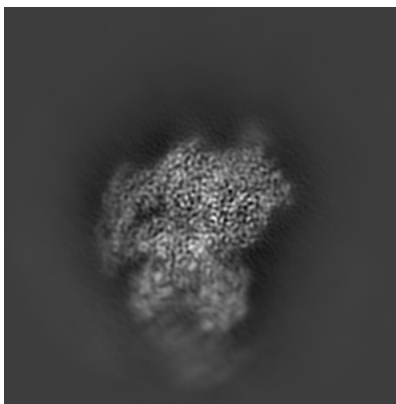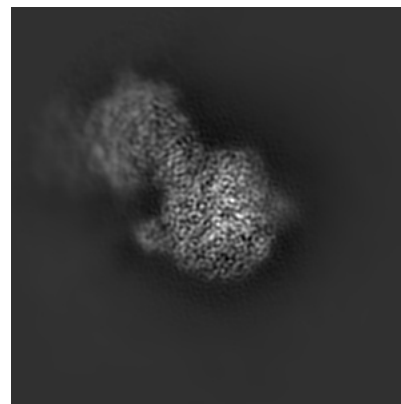
6.1.1　Primary map

X   Y   Z

6.1.2　Raw map

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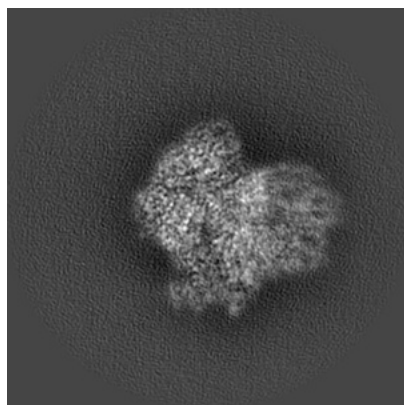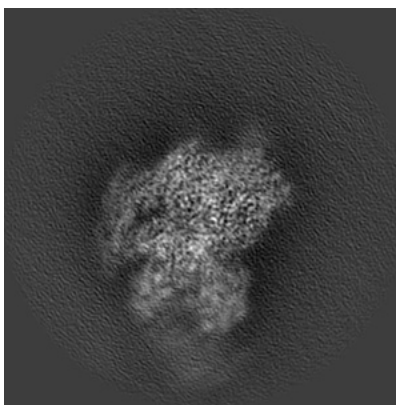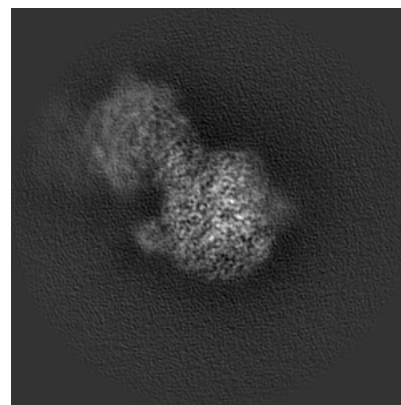
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ
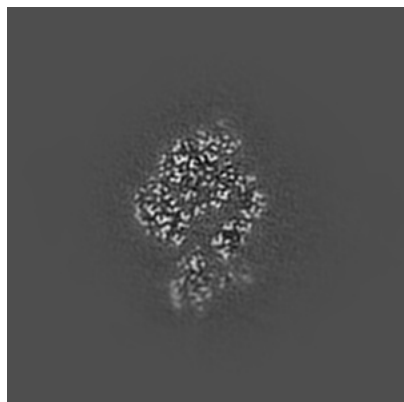
6.2.1 Primary map
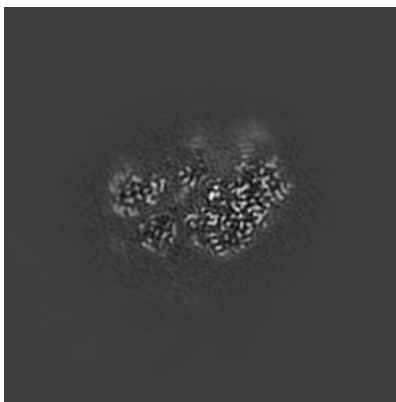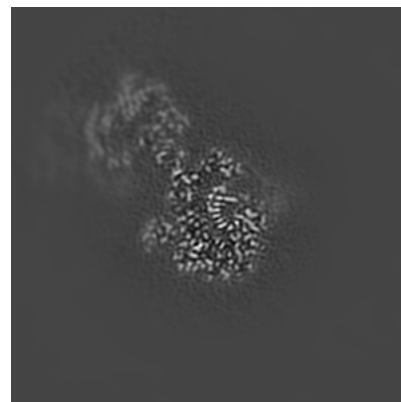
| X Index: 120 | Y Index: 120 | Z Index: 120 |

6.2.2 Raw map
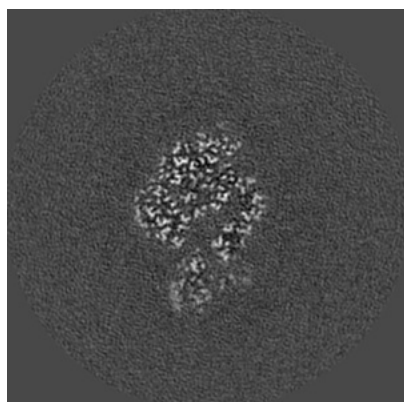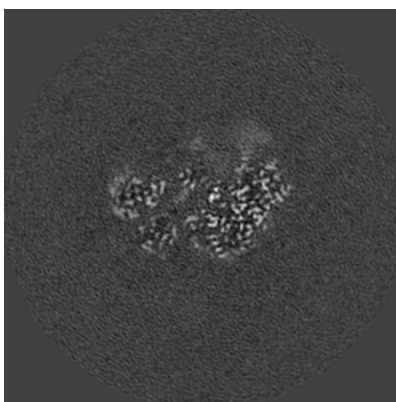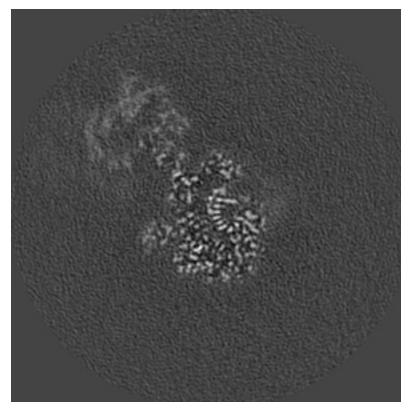
| X Index: 120 | Y Index: 120 | Z Index: 120 |

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

6.3 Largest variance slices ⓘ

6.3.1 Primary map
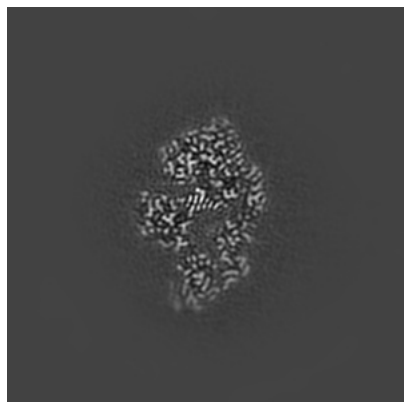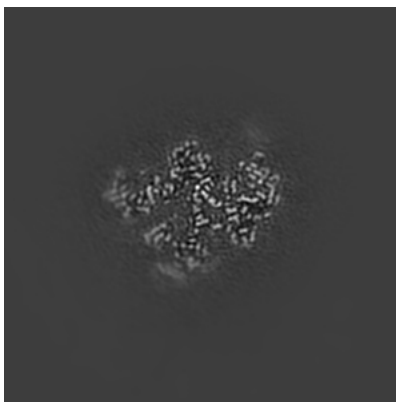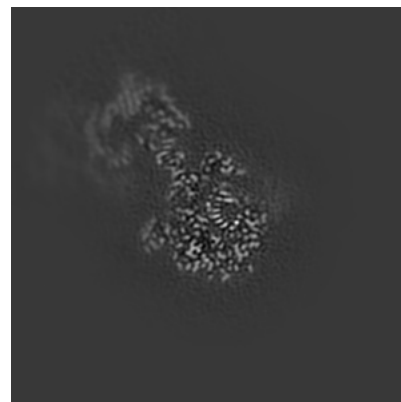
X Index: 124   Y Index: 109   Z Index: 119

6.3.2 Raw map
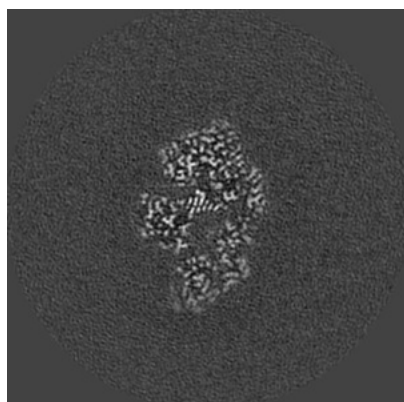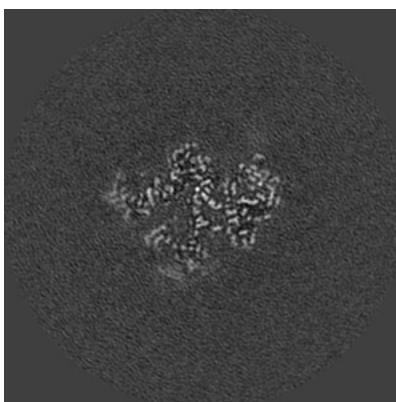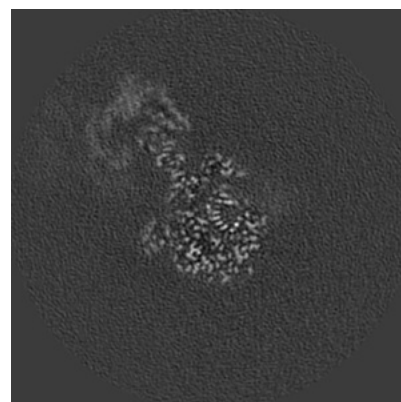
X Index: 124   Y Index: 109   Z Index: 119

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

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

6.4.1 Primary map
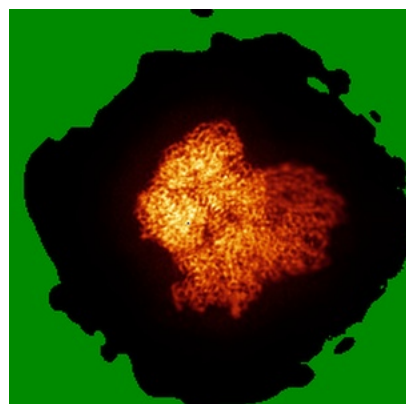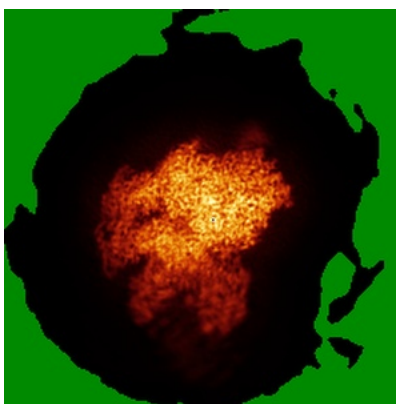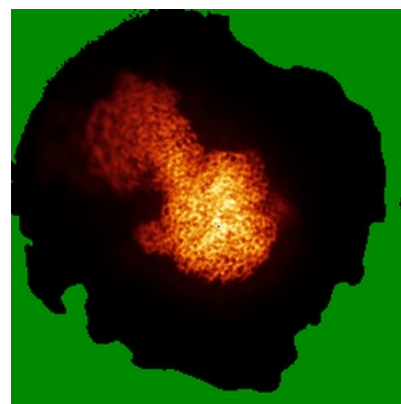
X   Y   Z

6.4.2 Raw map

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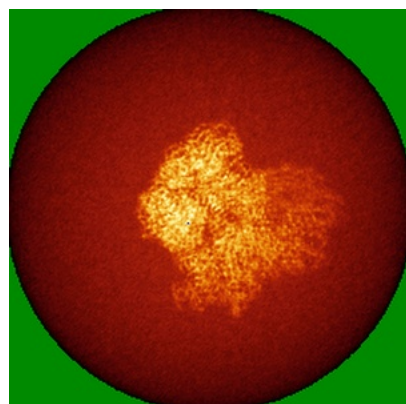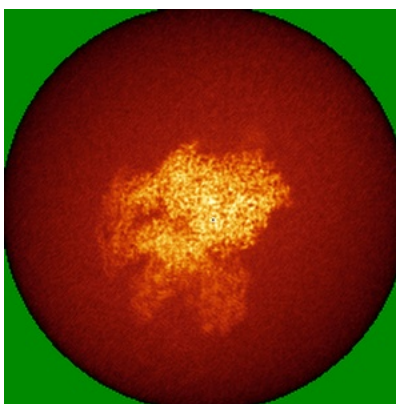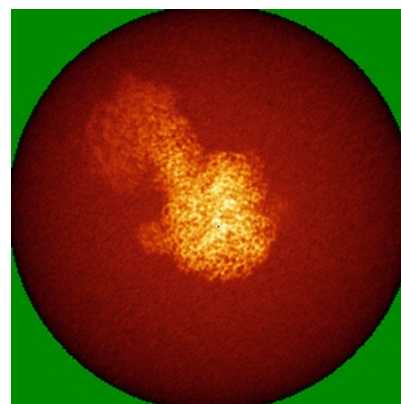
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5   Orthogonal surface views (i)

6.5.1   Primary map

| X | Y | Z |
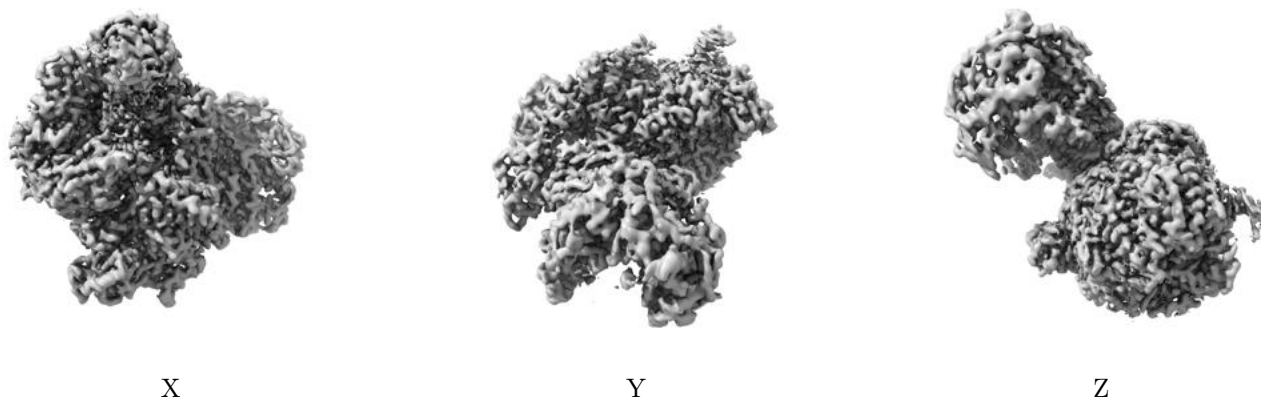
The images above show the 3D surface view of the map at the recommended contour level 0.017. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2   Raw map

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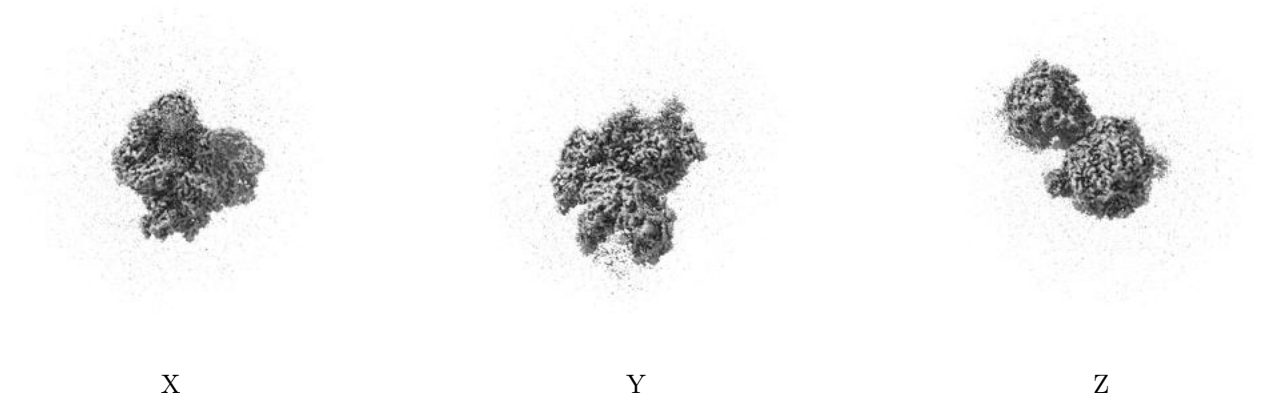
These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6   Mask visualisation ⓘ

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

A mask typically either:

- Encompasses the whole structure

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

6.6.1   emd_39862_msk_1.map ⓘ

X   Y   Z
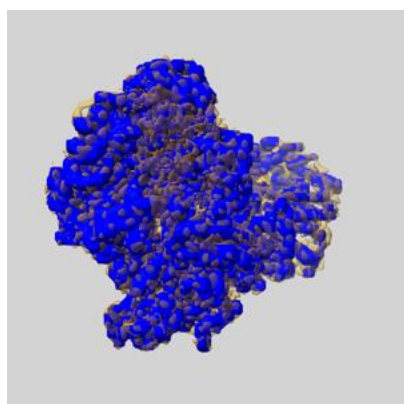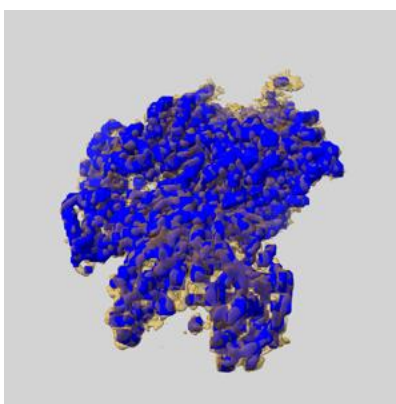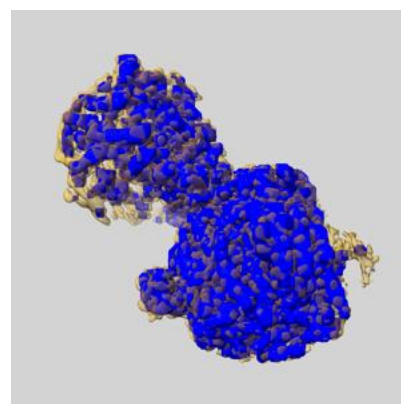
7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2   Volume estimate ⓘ
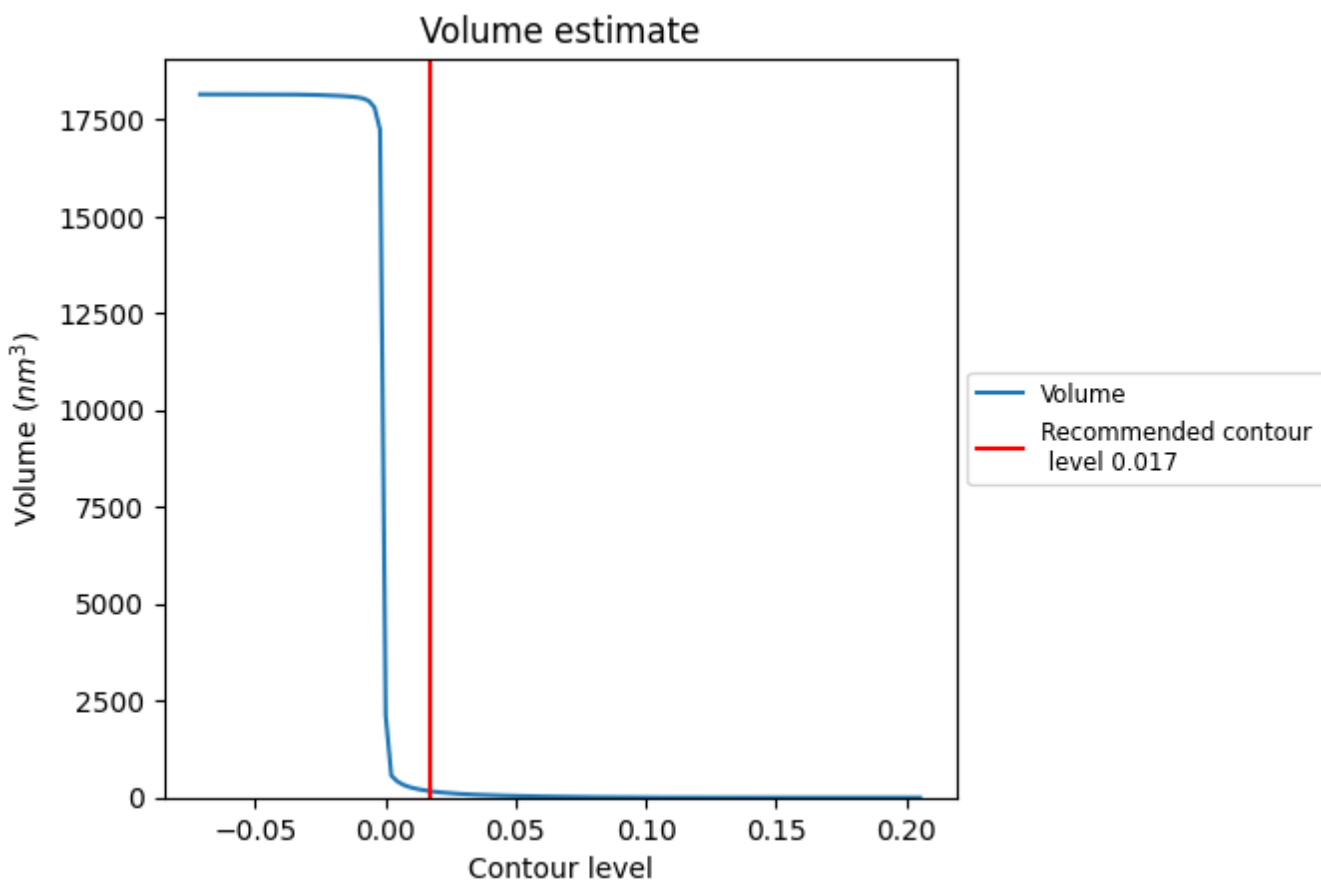
The volume at the recommended contour level is 167 nm^3; this corresponds to an approximate mass of 151 kDa.

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 ⓘ
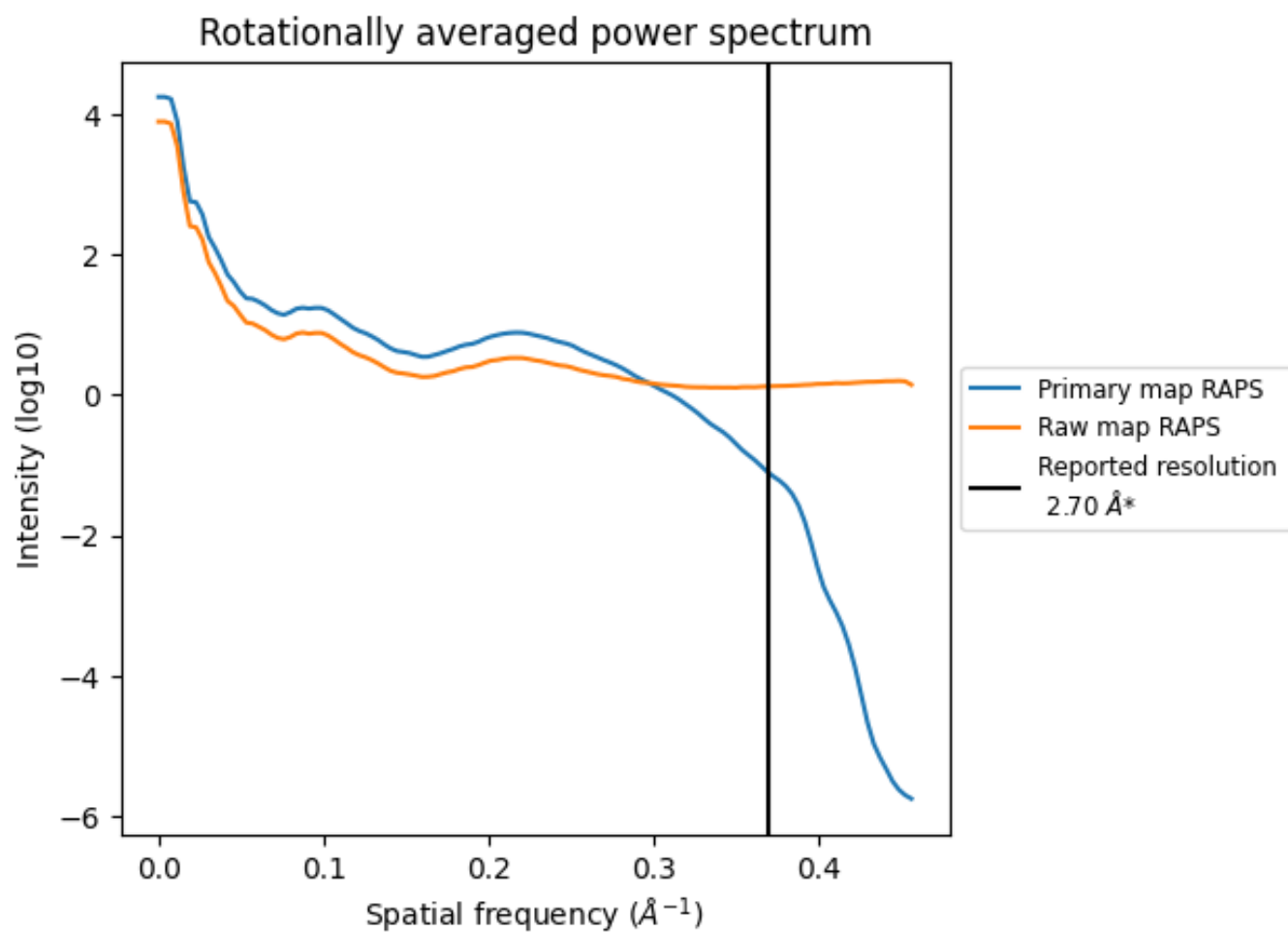
*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

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 ⓘ
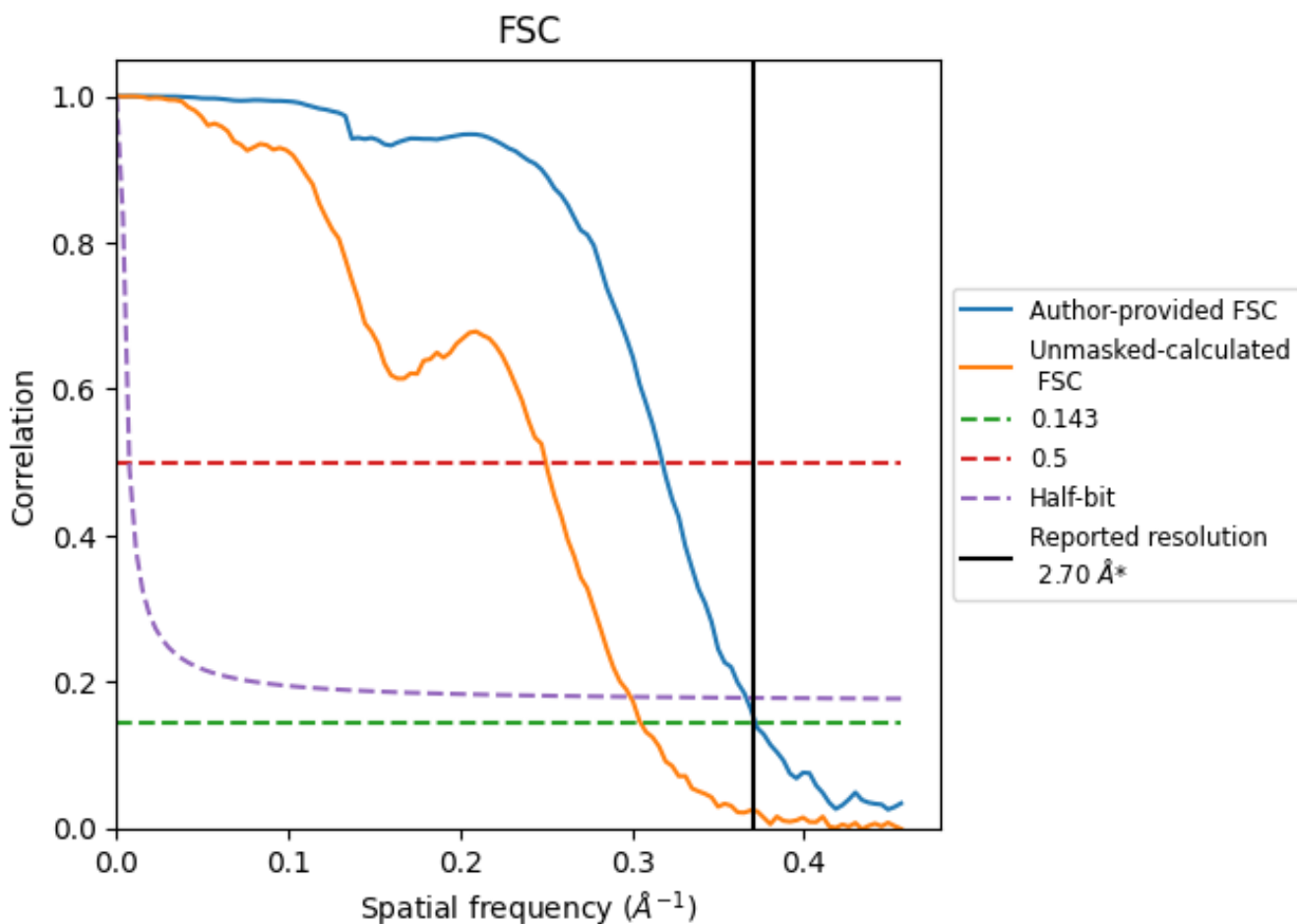
*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

8.2   Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.69	3.15	2.73
Unmasked-calculated*	3.28	4.00	3.34

*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 3.28 differs from the reported value 2.7 by more than 10 %

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-39862 and PDB model 8Z9H. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay ⓘ

X   Y   Z
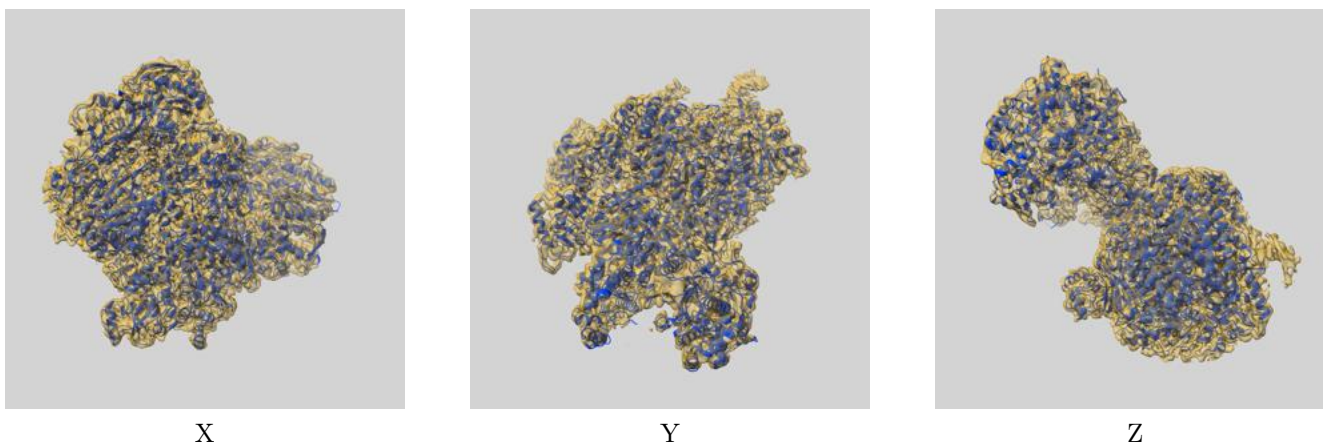
The images above show the 3D surface view of the map at the recommended contour level 0.017 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2   Q-score mapped to coordinate model   ⓘ

X   Y   Z
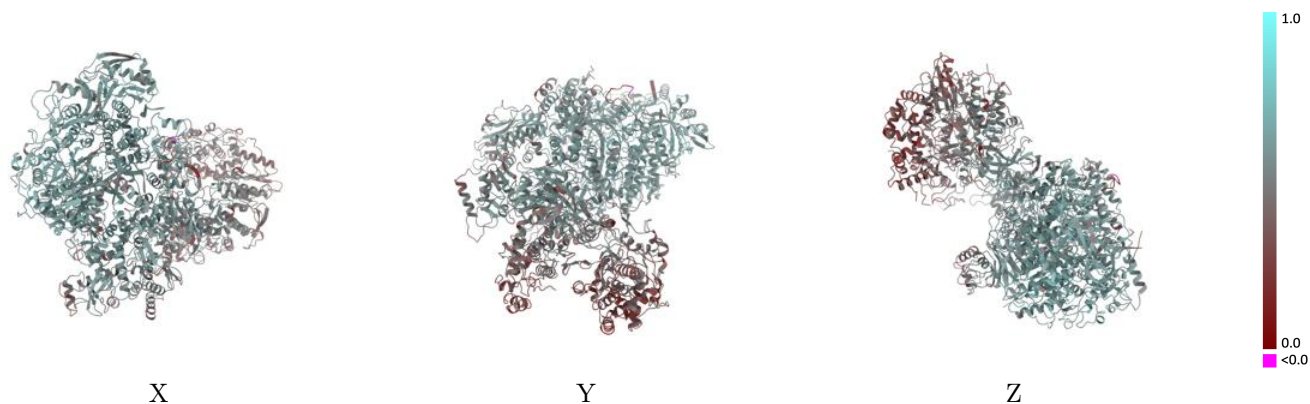
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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
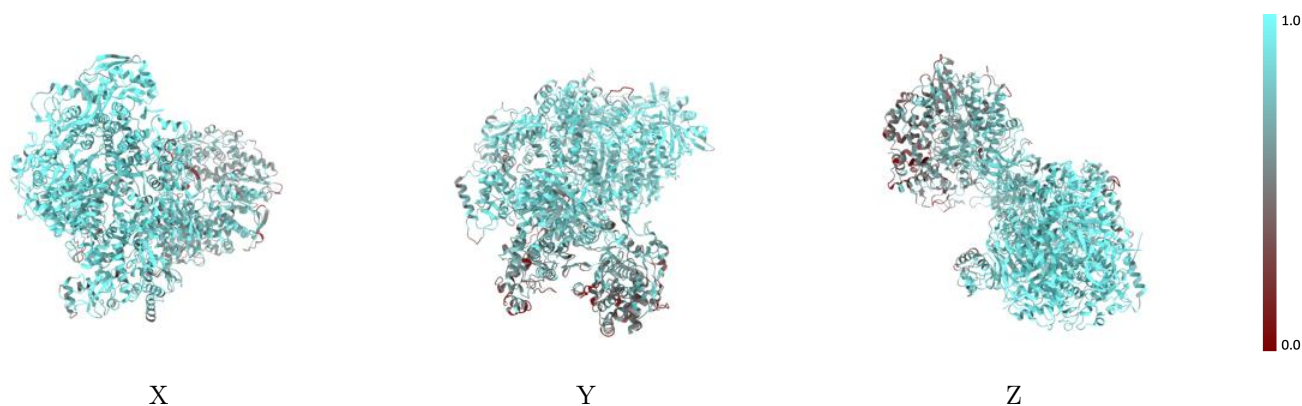
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.017).

9.4 Atom inclusion ⓘ
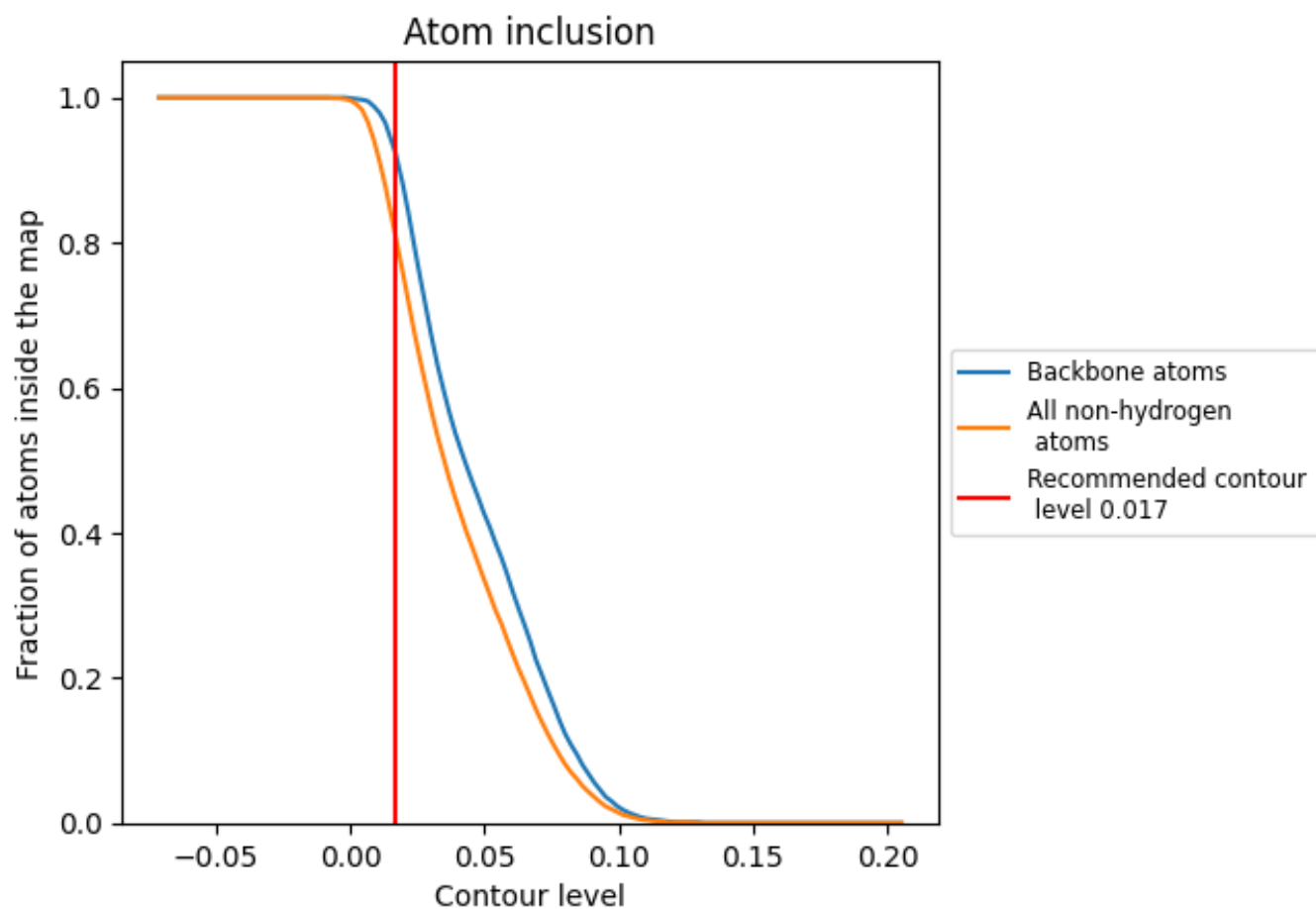
At the recommended contour level, 92% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.

9.5　Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.017) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8070	0.5140
A	0.9040	0.5750
B	0.9250	0.5900
C	0.8170	0.5210
D	0.9500	0.5480
E	0.9810	0.5880
F	0.9440	0.5730
G	0.9310	0.5730
H	0.7630	0.4900
I	0.6050	0.3820
J	0.4920	0.3430
K	0.8060	0.4780

1.0

0.0
<0.0