Full wwPDB EM Validation Report (i)

Oct 19, 2026 – 10:19 PM JST

PDB ID	:	9XRX / pdb_00009xrx
EMDB ID	:	EMD-67157
Title	:	Core-5RNA CCHFV
Authors	:	Zhu, H.; Gao, X.P.
Deposited on	:	2025-11-20
Resolution	:	3.32 Å(reported)

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 (i) 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 (i)) were used in the production of this report:

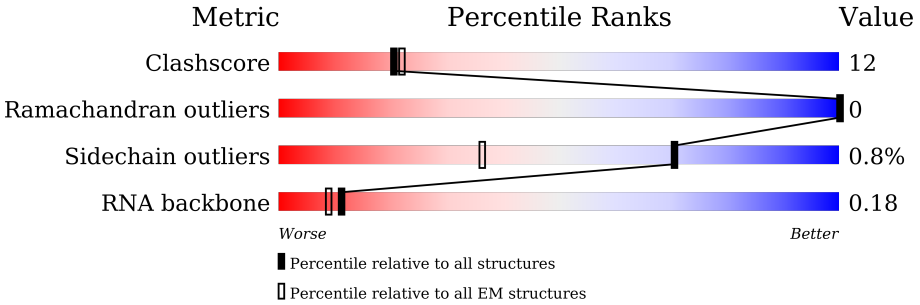
EMDB validation analysis	:	0.0.1.dev133
MolProbity	:	4-5-2 with Phenix2.2
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh &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

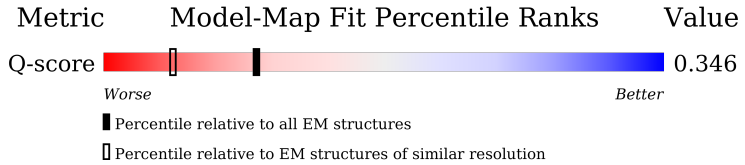
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.32 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	-
RNA backbone	8273	3508	-
Q-score	-	25397	14518 (2.82 - 3.82)

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	2341	22% 45% 16% 39%
2	B	18	17% 11% 11% 33% 44%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 11603 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 RNA-directed RNA polymerase L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1425	11390	7210	1968	2127	85	0	0

There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	916	MET	-	initiating methionine	UNP A0A1S6XXC8
A	917	HIS	-	expression tag	UNP A0A1S6XXC8
A	918	HIS	-	expression tag	UNP A0A1S6XXC8
A	919	HIS	-	expression tag	UNP A0A1S6XXC8
A	920	HIS	-	expression tag	UNP A0A1S6XXC8
A	921	HIS	-	expression tag	UNP A0A1S6XXC8
A	922	HIS	-	expression tag	UNP A0A1S6XXC8
A	923	GLY	-	expression tag	UNP A0A1S6XXC8
A	924	THR	-	expression tag	UNP A0A1S6XXC8
A	3229	TRP	-	expression tag	UNP A0A1S6XXC8
A	3230	SER	-	expression tag	UNP A0A1S6XXC8
A	3231	HIS	-	expression tag	UNP A0A1S6XXC8
A	3232	PRO	-	expression tag	UNP A0A1S6XXC8
A	3233	GLN	-	expression tag	UNP A0A1S6XXC8
A	3234	PHE	-	expression tag	UNP A0A1S6XXC8
A	3235	GLU	-	expression tag	UNP A0A1S6XXC8
A	3236	LYS	-	expression tag	UNP A0A1S6XXC8
A	3237	GLY	-	expression tag	UNP A0A1S6XXC8
A	3238	GLY	-	expression tag	UNP A0A1S6XXC8
A	3239	GLY	-	expression tag	UNP A0A1S6XXC8
A	3240	SER	-	expression tag	UNP A0A1S6XXC8
A	3241	GLY	-	expression tag	UNP A0A1S6XXC8
A	3242	GLY	-	expression tag	UNP A0A1S6XXC8
A	3243	GLY	-	expression tag	UNP A0A1S6XXC8
A	3244	SER	-	expression tag	UNP A0A1S6XXC8
A	3245	GLY	-	expression tag	UNP A0A1S6XXC8
A	3246	GLY	-	expression tag	UNP A0A1S6XXC8
A	3247	SER	-	expression tag	UNP A0A1S6XXC8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	3248	ALA	-	expression tag	UNP A0A1S6XXC8
A	3249	TRP	-	expression tag	UNP A0A1S6XXC8
A	3250	SER	-	expression tag	UNP A0A1S6XXC8
A	3251	HIS	-	expression tag	UNP A0A1S6XXC8
A	3252	PRO	-	expression tag	UNP A0A1S6XXC8
A	3253	GLN	-	expression tag	UNP A0A1S6XXC8
A	3254	PHE	-	expression tag	UNP A0A1S6XXC8
A	3255	GLU	-	expression tag	UNP A0A1S6XXC8
A	3256	LYS	-	expression tag	UNP A0A1S6XXC8

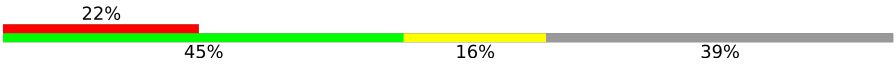
- Molecule 2 is a RNA chain called RNA (5'-R(*UP*CP*UP*CP*AP*AP*AP*GP*AP*AP*AP*UP*CP*GP*UP*UP*CP*C)-3').

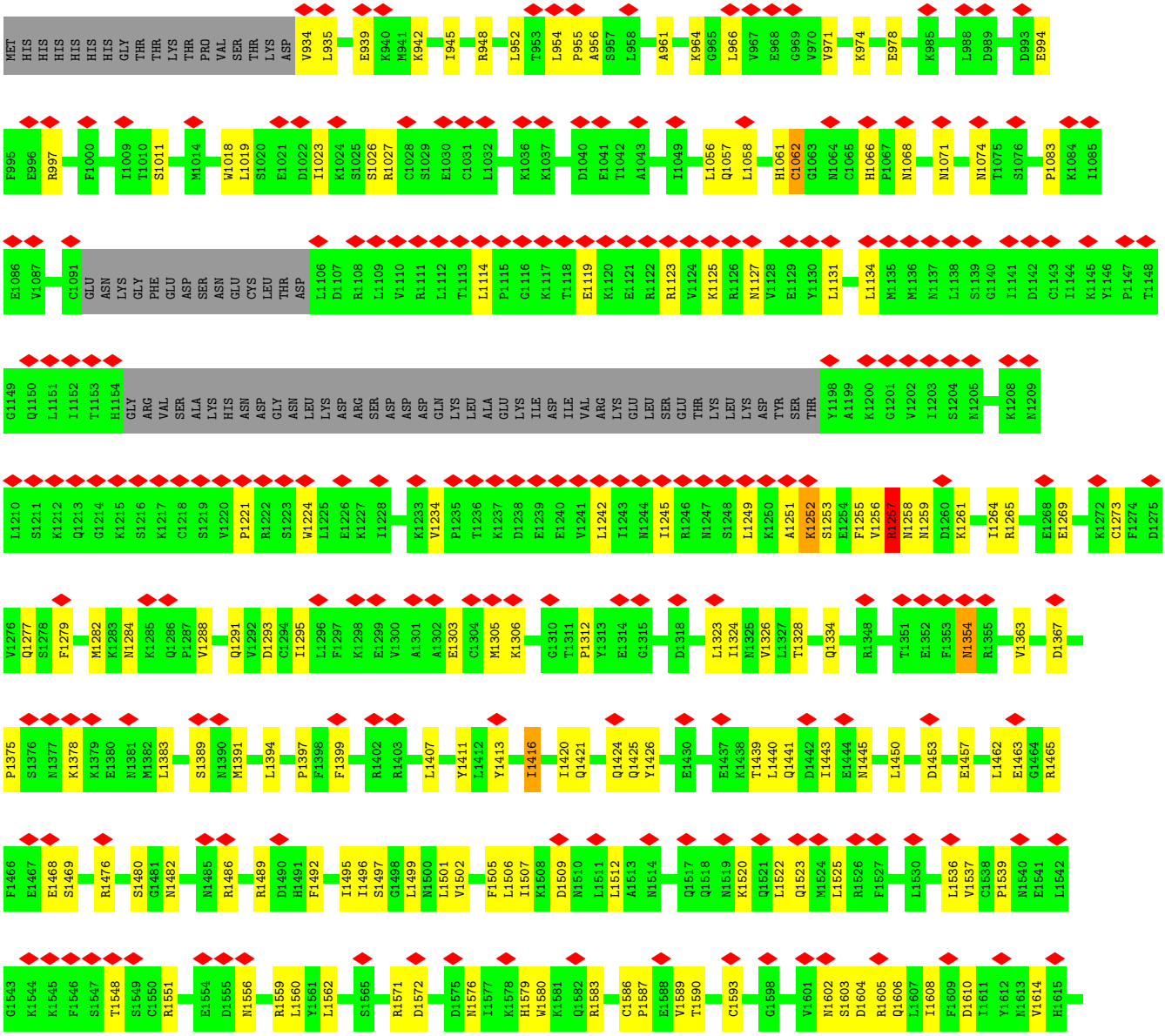
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	10	213	96	40	67	10	0	0

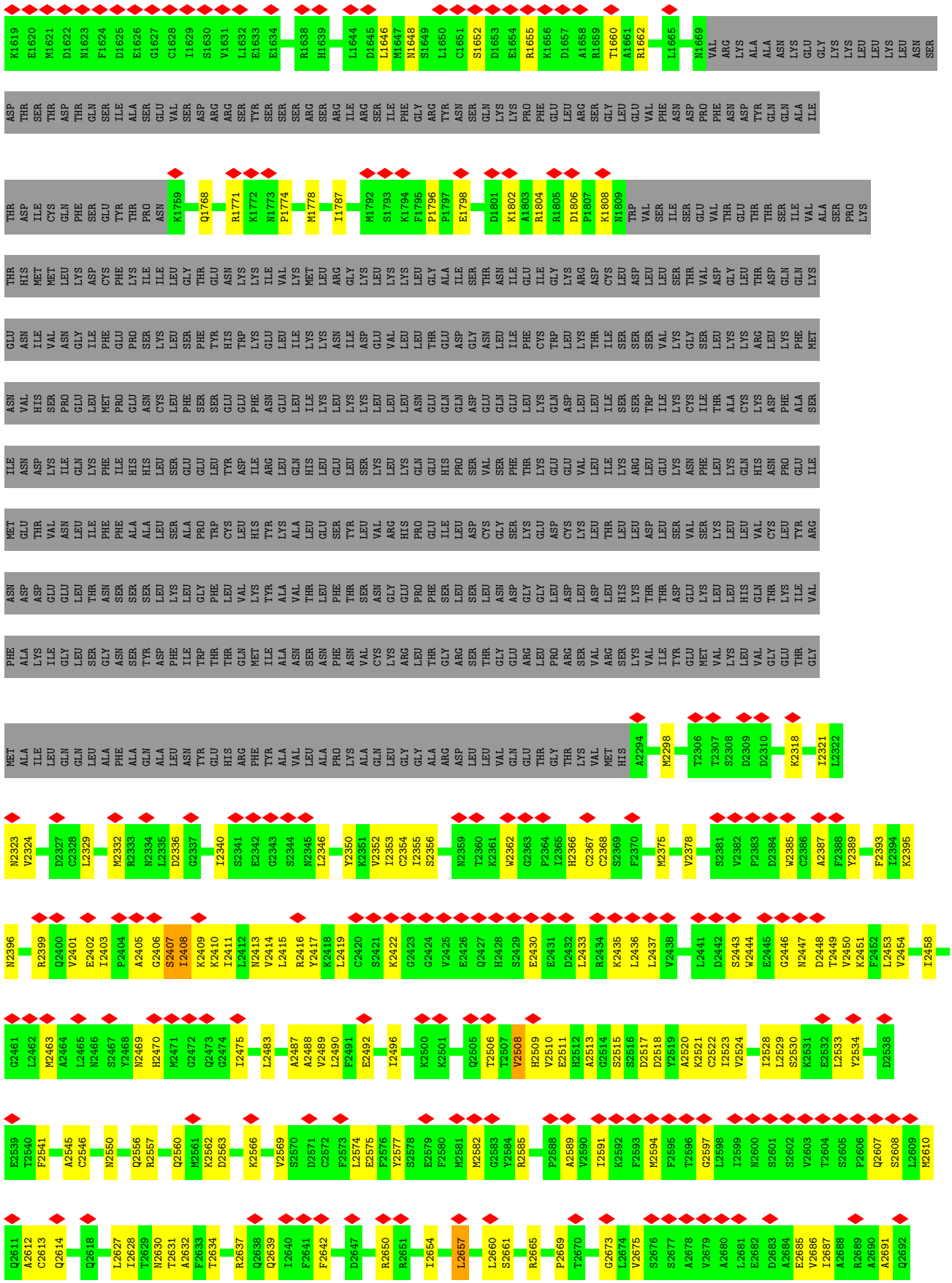
3 Residue-property plots (i)

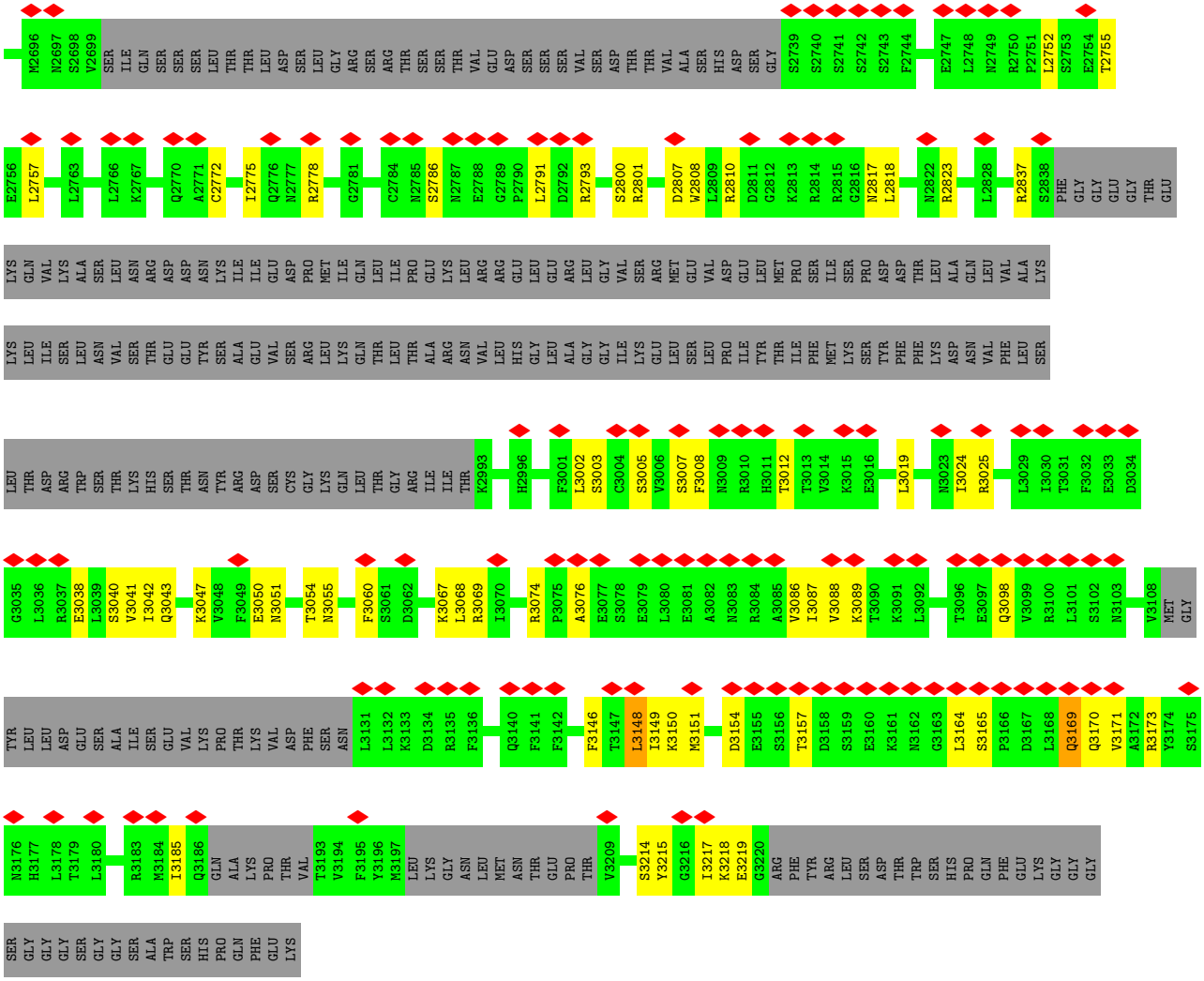
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

Chain A: 

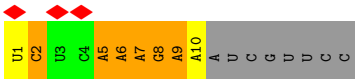



K1619 E1620 M1621 D1622 N1623 F1624 D1625 E1626 G1627 C1628 I1629 S1630 V1631 L1632 E1633 E1634 R1638 H1639 L1644 D1645 L1646 M1647 N1648 S1649 L1650 C1651 S1652 D1653 E1654 R1655 K1656 D1657 A1658 R1659 T1660 A1661 R1662 L1665 N1669
ASP THR SER THR ASP THR GLN SER ILE ALA SER GLU VAL SER ASP ARG ARG ARG SER TYR SER SER SER ARG SER ARG ILE ARG SER ILE PHE GLY ARG TYR ASN SER GLN LYS LYS PRO PHE GLU LEU ARG SER GLY LEU GLU VAL PHE ASN ASP PRO PHE ASN ASP TYR GLN GLN ALA ILE
THR ASP ILE CYS GLN PHE SER GLU TYR THR PRO ASN K1759 Q1768 R1771 K1772 N1773 P1774 M1778 I1787 M1792 S1793 K1794 F1795 P1796 P1797 E1798 D1801 K1802 A1803 R1804 R1805 D1806 P1807 K1808 N1809 TRP VAL SER ILE SER GLU VAL THR GLU THR THR SER ILE VAL ALA SER PRO LYS
THR HIS MET MET LEU LYS ASP CYS PHE LYS ILE ILE LEU GLY THR GLU ASN LYS LYS ILE VAL LYS MET LEU ARG GLY LYS LEU LYS LYS LEU GLY ALA ILE SER THR ASN ILE GLU ILE GLY LYS ARG ASP CYS LEU ASP LEU LEU SER THR VAL ASP GLY LEU THR ASP GLN GLN LYS
GLU ASN ILE VAL ASN GLY ILE PHE GLU PRO GLU SER LYS LEU SER PHE TYR HIS TRP LYS GLU LEU ILE LYS LYS ASN ILE ASP GLU VAL LEU LEU THR GLU ASP GLY ASN LEU ILE PHE CYS TRP LEU LYS THR ILE SER SER SER VAL LYS GLY SER LEU LYS LYS ARG LEU LYS PHE MET
ASN VAL HIS SER PRO GLU LEU MET PRO GLU ASN CYS LEU PHE SER SER GLU GLU PHE ASN GLU LEU LEU LYS LEU LYS LYS LEU LEU ASN GLU GLN GLN GLU GLU LEU LYS GLN ASP LEU LEU ILE SER SER SER TRP ILE LYS CYS ILE THR ALA CYS LYS ASP PHE ALA SER
ILE ASN ASP LYS ILE GLN LYS PHE ILE HIS HIS LEU SER GLU GLU LEU TYR ASP ILE ARG LEU GLN HIS LEU GLU LEU SER LYS LEU LYS LYS GLN GLU HIS PRO SER VAL SER PHE THR LYS GLU GLU VAL LEU ILE LYS ARG LEU GLU LYS ASN PHE LEU LYS GLN GLN PRO GLU
MET GLU THR VAL ASN LEU ILE PHE PHE ALA ALA LEU SER ALA PRO TRP CYS LEU HIS TYR LYS ALA LEU GLU SER TYR LEU VAL ARG HIS PRO GLU ILE LEU ASP CYS GLY SER LYS GLU ASP CYS LYS LEU THR LEU VAL SER LEU LEU LYS LEU LEU VAL CYS LEU TYR ARG
ASN ASP ASP GLU GLU LEU THR ASN SER SER SER LEU LYS LYS LEU SER ASN SER LEU LEU PHE THR LEU PHE THR SER ASN GLY GLU GLU ASP SER LEU ASN ASP GLY GLY LEU ASP LEU ASP LEU HIS LYS THR THR ASP GLU LYS LYS THR LYS ILE VAL
PHE ALA LYS ILE GLY LEU SER GLY ASN SER TYR ASP PHE ILE TRP THR THR GLN MET ILE ALA ASN SER ASN PHE ASN VAL CYS LYS ARG LEU THR GLY ARG SER THR GLY GLU ARG LEU PRO ARG SER VAL ARG SER LYS VAL ILE TYR GLU MET VAL LYS LEU VAL GLY GLU THR GLY
MET ALA ILE LEU GLN GLN LEU ALA PHE ALA GLN ALA LEU ASN TYR GLU HIS ARG PHE TYR ALA VAL LEU ALA PRO LYS ALA GLN LEU GLY GLY ALA ARG ASP LEU LEU VAL GLN GLN GLU THR GLY THR LYS VAL MET HIS A2294 M2298 T2306 T2307 S2308 D2309 D2310 K2318 I2321 L2322
N2323 V2324 D2327 C2328 L2329 M2332 R2333 N2334 L2335 D2336 G2337 I2340 S2341 E2342 G2343 S2344 N2345 L2346 Y2350 K2351 V2352 I2353 C2354 I2355 S2356 N2359 T2360 K2361 W2362 G2363 P2364 I2365 H2366 C2367 C2368 S2369 F2370 M2375 V2378 S2381 V2382 P2383 D2384 W2385 C2386 A2387 F2388 Y2389 F2393 I2394 K2395
N2396 R2399 Q2400 V2401 E2402 I2403 P2404 A2405 G2406 S2407 I2408 K2409 K2410 I2411 L2412 N2413 V2414 L2415 R2416 Y2417 K2418 L2419 C2420 S2421 K2422 G2423 G2424 V2425 E2426 Q2427 H2428 S2429 E2430 E2431 D2432 L2433 R2434 K2435 L2436 L2437 V2438 L2441 D2442 S2443 W2444 E2445 G2446 N2447 D2448 T2449 V2450 K2451 F2452 L2453 V2454 I2458
G2461 L2462 M2463 A2464 L2465 N2466 S2467 Y2468 N2469 H2470 M2471 G2472 Q2473 G2474 I2475 L2483 A2487 A2488 V2489 L2490 F2491 E2492 I2496 K2500 K2501 Q2505 T2506 T2507 V2508 H2509 V2510 E2511 H2512 A2513 G2514 S2515 S2516 D2517 D2518 Y2519 A2520 K2521 C2522 I2523 V2524 I2528 L2529 S2530 K2531 E2532 L2533 Y2534 D2538
E2539 T2540 F2541 A2545 C2546 N2550 Q2556 R2557 Q2560 M2561 K2562 D2563 K2566 V2569 S2570 D2571 C2572 F2573 L2574 E2575 F2576 Y2577 S2578 E2579 F2580 M2581 M2582 G2583 Y2584 R2585 P2588 A2589 V2590 I2591 K2592 F2593 M2594 F2595 T2596 G2597 L2598 I2599 N2600 S2601 S2602 V2603 T2604 S2605 P2606 Q2607 S2608 L2609 M2610
Q2611 A2612 C2613 Q2614 Q2618 L2627 I2628 T2629 N2630 T2631 A2632 F2633 T2634 R2637 Q2638 Q2639 I2640 F2641 F2642 D2647 R2650 R2651 I2654 L2657 L2660 S2661 R2665 P2669 T2670 G2673 L2674 V2675 S2676 S2677 A2678 V2679 A2680 L2681 E2682 D2683 A2684 E2685 V2686 I2687 A2688 R2689 A2690 A2691 Q2692



• Molecule 2: RNA (5'-R(*UP*CP*UP*CP*AP*AP*AP*GP*AP*AP*AP*UP*CP*GP*UP*UP*CP*C)-3')

Chain B:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	69639	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.972	Depositor
Minimum map value	-0.519	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.329	Depositor
Map size (Å)	298.8, 298.8, 298.8	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	0.32	0/11582	0.68	4/15614 (0.0%)
2	B	0.57	0/238	0.83	0/368
All	All	0.33	0/11820	0.69	4/15982 (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
1	A	0	9

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	971	VAL	N-CA-C	-8.02	105.50	113.20
1	A	2406	GLY	N-CA-C	-7.57	105.93	115.31
1	A	2321	ILE	N-CA-C	-5.50	107.08	111.81
1	A	3148	LEU	CA-CB-CG	5.03	133.92	116.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1062	CYS	Peptide
1	A	1234	VAL	Peptide
1	A	1257	ARG	Sidechain
1	A	2403	ILE	Peptide
1	A	2566	LYS	Peptide
1	A	3025	ARG	Peptide
1	A	3060	PHE	Peptide

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Mol	Chain	Res	Type	Group
1	A	3157	THR	Peptide
1	A	3169	GLN	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11390	0	11531	281	0
2	B	213	0	109	49	0
All	All	11603	0	11640	281	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 12.

All (281) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2414:VAL:HG22	2:B:7:A:C4	1.93	1.03
1:A:2450:VAL:HG11	2:B:6:A:N6	1.72	1.03
1:A:1255:PHE:CD2	2:B:7:A:C6	2.51	0.99
1:A:1255:PHE:CE2	2:B:7:A:C2	2.52	0.97
1:A:1255:PHE:CE2	2:B:7:A:N1	2.35	0.94
1:A:2444:TRP:CZ3	2:B:7:A:C2	2.56	0.94
1:A:2414:VAL:HG13	2:B:7:A:C5	2.02	0.93
1:A:1253:SER:HA	1:A:2417:TYR:HB3	1.50	0.93
1:A:2450:VAL:HG11	2:B:6:A:H62	1.33	0.92
1:A:2414:VAL:HG13	2:B:7:A:N7	1.87	0.90
1:A:1071:ASN:HD21	2:B:1:U:H5'	1.38	0.88
1:A:1255:PHE:CZ	2:B:7:A:C2	2.62	0.86
1:A:2444:TRP:CZ3	2:B:7:A:N1	2.47	0.82
1:A:1255:PHE:CD2	2:B:7:A:N1	2.48	0.81
1:A:1257:ARG:HE	1:A:2446:GLY:HA3	1.46	0.79
1:A:2450:VAL:CG1	2:B:6:A:N6	2.46	0.78
1:A:2450:VAL:CG1	2:B:6:A:H62	2.01	0.74
1:A:2444:TRP:CE3	2:B:7:A:N1	2.57	0.72
1:A:1257:ARG:HD3	2:B:5:A:H2'	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2411:ILE:HG13	2:B:6:A:C2	2.26	0.71
1:A:2414:VAL:CG1	2:B:7:A:C5	2.74	0.70
1:A:2353:ILE:HB	1:A:2523:ILE:HB	1.75	0.68
1:A:1536:LEU:HB2	1:A:2569:VAL:HB	1.75	0.68
1:A:1071:ASN:ND2	2:B:1:U:H5'	2.08	0.67
1:A:2368:CYS:HB3	1:A:2396:ASN:HD22	1.60	0.67
1:A:2414:VAL:CG2	2:B:7:A:C4	2.76	0.66
1:A:1259:ASN:OD1	2:B:5:A:N7	2.29	0.66
1:A:2444:TRP:HZ3	2:B:7:A:C2	2.15	0.65
1:A:1257:ARG:NE	1:A:2446:GLY:HA3	2.11	0.64
1:A:1265:ARG:HH21	1:A:1556:ASN:HB2	1.62	0.64
1:A:1323:LEU:HD11	1:A:1416:ILE:HG13	1.80	0.64
1:A:2393:PHE:HB2	1:A:2395:LYS:HG2	1.80	0.63
1:A:2416:ARG:HH21	1:A:2430:GLU:HB3	1.63	0.63
1:A:1261:LYS:NZ	1:A:1548:THR:O	2.32	0.62
1:A:1249:LEU:C	1:A:1251:ALA:H	2.07	0.62
1:A:1277:GLN:HG2	1:A:1505:PHE:HB3	1.82	0.62
1:A:1284:ASN:HD21	1:A:1334:GLN:HE22	1.46	0.61
1:A:2414:VAL:CG1	2:B:7:A:C6	2.83	0.61
1:A:1255:PHE:CG	2:B:7:A:C5	2.89	0.61
1:A:2414:VAL:HG22	2:B:7:A:C5	2.34	0.61
1:A:1324:ILE:HD11	1:A:1416:ILE:HD12	1.82	0.61
1:A:1399:PHE:CE2	2:B:9:A:H2	2.18	0.61
1:A:1383:LEU:HD11	1:A:1397:PRO:HB2	1.83	0.61
1:A:2496:ILE:HD13	1:A:2508:VAL:HG13	1.83	0.60
1:A:1027:ARG:HH12	1:A:1062:CYS:H	1.50	0.60
1:A:934:VAL:N	1:A:2387:ALA:O	2.34	0.60
1:A:1255:PHE:CD2	2:B:7:A:C2	2.88	0.60
1:A:1249:LEU:HD21	2:B:10:A:N6	2.17	0.59
1:A:2513:ALA:HB3	1:A:2520:ALA:H	1.67	0.59
1:A:1572:ASP:OD1	1:A:1572:ASP:N	2.34	0.59
1:A:1806:ASP:HB3	1:A:2298:MET:HE1	1.83	0.59
1:A:1551:ARG:HH22	2:B:5:A:P	2.26	0.58
1:A:1583:ARG:HD2	1:A:1587:PRO:HA	1.85	0.58
1:A:2585:ARG:NH1	1:A:3087:ILE:O	2.36	0.58
1:A:1399:PHE:CE2	2:B:9:A:C2	2.91	0.58
1:A:2489:VAL:HA	1:A:2492:GLU:HB2	1.86	0.58
1:A:2354:CYS:HB2	1:A:2574:LEU:HD13	1.85	0.58
1:A:2650:ARG:HH11	1:A:2793:ARG:HH12	1.52	0.58
1:A:1255:PHE:CG	2:B:7:A:C4	2.91	0.58
1:A:1509:ASP:OD1	1:A:1509:ASP:N	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2443:SER:O	2:B:7:A:N6	2.37	0.57
1:A:1604:ASP:HB2	1:A:2582:MET:HG3	1.84	0.57
1:A:2492:GLU:HA	1:A:2510:VAL:HG11	1.86	0.57
1:A:1027:ARG:NH1	1:A:1062:CYS:SG	2.76	0.57
1:A:2556:GLN:NE2	1:A:2563:ASP:OD2	2.38	0.57
1:A:3148:LEU:HB2	1:A:3150:LYS:HE3	1.87	0.57
1:A:1273:CYS:O	1:A:1277:GLN:NE2	2.38	0.57
1:A:1420:ILE:HD11	1:A:2632:ALA:HB2	1.87	0.57
1:A:2597:GLY:O	1:A:2637:ARG:NH1	2.36	0.57
1:A:2375:MET:HA	1:A:2378:VAL:HG12	1.87	0.56
1:A:2755:THR:OG1	1:A:3067:LYS:NZ	2.38	0.56
1:A:3041:VAL:HB	1:A:3043:GLN:HE21	1.71	0.56
1:A:1551:ARG:NH2	2:B:5:A:OP2	2.38	0.56
1:A:3005:SER:H	1:A:3038:GLU:HA	1.71	0.56
1:A:3170:GLN:O	1:A:3173:ARG:NH1	2.37	0.56
1:A:2354:CYS:HA	1:A:2522:CYS:HA	1.88	0.55
1:A:2414:VAL:HG11	2:B:7:A:C6	2.40	0.55
1:A:1798:GLU:OE1	1:A:1802:LYS:NZ	2.39	0.55
1:A:2443:SER:HB2	2:B:7:A:H62	1.70	0.55
1:A:1058:LEU:HD22	1:A:1066:HIS:HE1	1.70	0.55
1:A:3169:GLN:HA	1:A:3171:VAL:HG23	1.87	0.55
1:A:2366:HIS:O	1:A:2560:GLN:NE2	2.39	0.55
1:A:2346:LEU:HG	1:A:2528:ILE:HG22	1.88	0.55
1:A:2807:ASP:OD1	1:A:2810:ARG:NH2	2.39	0.54
1:A:1768:GLN:HA	1:A:1771:ARG:HE	1.72	0.54
1:A:3165:SER:HB2	1:A:3173:ARG:HH12	1.72	0.54
1:A:1255:PHE:CD2	2:B:7:A:C5	2.95	0.54
1:A:2591:ILE:HA	1:A:2594:MET:HE2	1.89	0.54
1:A:1265:ARG:NH1	1:A:1551:ARG:O	2.41	0.54
1:A:1421:GLN:HE22	1:A:2594:MET:HE1	1.72	0.54
1:A:1778:MET:O	1:A:2562:LYS:NZ	2.35	0.54
1:A:956:ALA:O	1:A:1662:ARG:NH2	2.41	0.54
1:A:1426:TYR:HH	1:A:1593:CYS:HG	1.54	0.54
1:A:2685:GLU:OE2	1:A:3069:ARG:NH2	2.41	0.54
1:A:2791:LEU:O	1:A:2817:ASN:ND2	2.41	0.54
1:A:1242:LEU:HD13	1:A:1245:ILE:HD11	1.89	0.53
1:A:2414:VAL:HG22	2:B:7:A:N9	2.22	0.53
1:A:1537:VAL:HG13	1:A:1539:PRO:HD3	1.89	0.53
1:A:2837:ARG:NH2	1:A:3024:ILE:O	2.41	0.53
1:A:1131:LEU:HA	1:A:1134:LEU:HB2	1.91	0.53
1:A:2837:ARG:NH1	1:A:3019:LEU:O	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1536:LEU:HD11	1:A:2546:CYS:HA	1.89	0.53
1:A:1288:VAL:O	1:A:1291:GLN:NE2	2.42	0.53
1:A:1502:VAL:HA	1:A:1506:LEU:HB2	1.91	0.53
1:A:1576:ASN:HA	1:A:1579:HIS:HB2	1.91	0.53
1:A:1796:PRO:HB2	1:A:1798:GLU:HG3	1.90	0.53
1:A:2660:LEU:HD21	1:A:2687:ILE:HD11	1.91	0.53
1:A:1123:ARG:HH21	1:A:1127:ASN:HB3	1.74	0.52
1:A:1399:PHE:HD2	2:B:2:C:O4'	1.93	0.52
1:A:2665:ARG:HH12	1:A:2686:VAL:HG21	1.74	0.52
1:A:1465:ARG:NH1	1:A:1468:GLU:OE1	2.42	0.52
1:A:1011:SER:HB2	1:A:1571:ARG:HA	1.91	0.52
1:A:3088:VAL:HG23	1:A:3089:LYS:HG2	1.90	0.52
1:A:1249:LEU:C	1:A:1251:ALA:N	2.64	0.52
1:A:2414:VAL:HG13	2:B:7:A:C6	2.43	0.52
1:A:2801:ARG:HB3	1:A:3003:SER:HA	1.91	0.52
1:A:1603:SER:HB3	1:A:1606:GLN:HG3	1.90	0.52
1:A:2329:LEU:HD13	1:A:2352:VAL:HG11	1.92	0.52
1:A:1480:SER:HA	1:A:1486:ARG:HH12	1.75	0.52
1:A:1502:VAL:HG22	1:A:1507:ILE:HG12	1.92	0.52
1:A:3150:LYS:HB2	1:A:3154:ASP:HA	1.92	0.51
1:A:1257:ARG:O	1:A:1258:ASN:C	2.53	0.51
1:A:1074:ASN:ND2	1:A:1269:GLU:OE2	2.44	0.51
1:A:1804:ARG:NH1	1:A:2385:TRP:O	2.43	0.51
1:A:961:ALA:HA	1:A:964:LYS:HG2	1.92	0.51
1:A:2340:ILE:HD11	1:A:2528:ILE:HG21	1.93	0.51
1:A:2454:VAL:HA	1:A:2458:ILE:HB	1.92	0.51
1:A:2488:ALA:O	1:A:2492:GLU:N	2.41	0.51
1:A:1312:PRO:HA	1:A:3076:ALA:HB2	1.92	0.51
1:A:2415:LEU:HD11	1:A:2436:LEU:HB3	1.92	0.51
1:A:1295:ILE:HG23	1:A:1413:TYR:HE1	1.76	0.51
1:A:2752:LEU:HD23	1:A:2757:LEU:HD23	1.93	0.51
1:A:1774:PRO:O	1:A:2557:ARG:NH2	2.44	0.50
1:A:2515:SER:OG	1:A:2518:ASP:N	2.42	0.50
1:A:2614:GLN:NE2	1:A:2673:GLY:O	2.44	0.50
1:A:1303:GLU:HB2	1:A:2657:LEU:HD13	1.94	0.50
1:A:1443:ILE:HG13	1:A:1497:SER:HB3	1.94	0.50
1:A:2511:GLU:HB3	1:A:2522:CYS:HB3	1.94	0.50
1:A:2367:CYS:HB3	1:A:2469:ASN:HA	1.94	0.50
1:A:1525:LEU:HD13	1:A:1562:LEU:HD11	1.93	0.50
1:A:945:ILE:O	1:A:948:ARG:NH2	2.44	0.50
1:A:2557:ARG:O	1:A:2562:LYS:NZ	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3164:LEU:HD13	1:A:3173:ARG:HB2	1.93	0.50
1:A:1023:ILE:HD13	1:A:1056:LEU:HD13	1.94	0.49
1:A:1279:PHE:HA	1:A:1282:MET:HE1	1.93	0.49
1:A:2433:LEU:HB3	1:A:2437:LEU:HD12	1.94	0.49
1:A:1252:LYS:HB2	1:A:2417:TYR:CD2	2.48	0.49
1:A:1252:LYS:HB2	1:A:2417:TYR:CE2	2.47	0.49
1:A:994:GLU:OE2	1:A:997:ARG:NH2	2.46	0.49
1:A:1439:THR:HB	1:A:1489:ARG:HH22	1.78	0.49
1:A:2613:CYS:HB3	1:A:2634:THR:HG23	1.95	0.49
1:A:1249:LEU:HD21	2:B:10:A:H61	1.76	0.48
1:A:1257:ARG:CZ	1:A:2446:GLY:HA3	2.43	0.48
1:A:2541:PHE:O	1:A:2545:ALA:N	2.43	0.48
1:A:2808:TRP:O	1:A:2823:ARG:NH1	2.45	0.48
1:A:954:LEU:HD12	1:A:955:PRO:HD2	1.96	0.48
1:A:1083:PRO:HB3	1:A:1394:LEU:HB3	1.96	0.48
1:A:2755:THR:O	1:A:3067:LYS:NZ	2.47	0.48
1:A:1407:LEU:O	1:A:1411:TYR:N	2.45	0.47
1:A:2612:ALA:HB1	1:A:2637:ARG:HH21	1.79	0.47
1:A:974:LYS:O	1:A:978:GLU:N	2.47	0.47
1:A:1114:LEU:HB2	1:A:1125:LYS:HD2	1.95	0.47
1:A:1221:PRO:HD2	1:A:1391:MET:HE1	1.96	0.47
1:A:1068:ASN:HB2	1:A:1256:VAL:HG11	1.96	0.47
1:A:3098:GLN:NE2	1:A:3185:ILE:O	2.40	0.47
1:A:1774:PRO:HG2	1:A:2557:ARG:CZ	2.44	0.47
1:A:1450:LEU:HB3	1:A:1501:LEU:HD22	1.97	0.47
1:A:1576:ASN:HB2	1:A:1589:VAL:HG23	1.97	0.47
1:A:2414:VAL:CG2	2:B:7:A:C5	2.97	0.47
1:A:3040:SER:OG	1:A:3041:VAL:N	2.48	0.47
1:A:2654:ILE:HA	1:A:2657:LEU:HD11	1.97	0.47
1:A:1492:PHE:HA	1:A:1495:ILE:HD12	1.96	0.46
1:A:1326:VAL:HG13	1:A:1440:LEU:HD21	1.96	0.46
1:A:1463:GLU:OE2	1:A:1465:ARG:NH2	2.48	0.46
1:A:2413:ASN:ND2	2:B:8:G:OP2	2.48	0.46
1:A:2775:ILE:HG23	1:A:2818:LEU:HD11	1.96	0.46
1:A:2419:LEU:HA	1:A:2422:LYS:HD3	1.98	0.46
1:A:1576:ASN:O	1:A:1580:TRP:N	2.42	0.46
1:A:2356:SER:HB3	1:A:2575:GLU:HG3	1.96	0.46
1:A:2435:LYS:HG2	1:A:2436:LEU:HD12	1.97	0.46
1:A:1305:MET:HG3	1:A:2778:ARG:HH11	1.81	0.46
1:A:2546:CYS:O	1:A:2550:ASN:ND2	2.47	0.46
1:A:2675:VAL:HG21	1:A:3068:LEU:HD21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1482:ASN:HD22	1:A:1586:CYS:HB2	1.81	0.45
1:A:1551:ARG:NH1	2:B:5:A:OP2	2.47	0.45
1:A:2405:ALA:C	1:A:2407:SER:H	2.23	0.45
1:A:2399:ARG:HH22	1:A:2475:ILE:HD13	1.81	0.45
1:A:2610:MET:HG2	1:A:2661:SER:HB2	1.99	0.45
1:A:1425:GLN:HG2	1:A:1605:ARG:HE	1.80	0.45
1:A:1520:LYS:HA	1:A:1523:GLN:HG2	1.98	0.45
1:A:1608:ILE:HG21	1:A:2589:ALA:HA	1.98	0.45
1:A:2800:SER:OG	1:A:3002:LEU:O	2.34	0.45
1:A:2407:SER:O	1:A:2410:LYS:N	2.49	0.45
1:A:2444:TRP:NE1	1:A:2447:ASN:OD1	2.43	0.45
1:A:1249:LEU:CD2	2:B:10:A:H61	2.30	0.45
1:A:1655:ARG:HD3	1:A:1660:THR:HG21	1.98	0.45
1:A:2530:SER:O	1:A:2534:TYR:N	2.41	0.45
1:A:2607:GLN:NE2	1:A:2608:SER:OG	2.49	0.45
1:A:3217:ILE:HG13	1:A:3218:LYS:HD3	1.99	0.45
1:A:952:LEU:HD13	1:A:1646:LEU:HG	1.99	0.45
1:A:3012:THR:HG21	1:A:3042:ILE:HG23	1.98	0.45
1:A:1306:LYS:NZ	1:A:2772:CYS:SG	2.89	0.45
1:A:1255:PHE:CE1	2:B:7:A:C2	3.05	0.45
1:A:1375:PRO:HG2	1:A:1378:LYS:HA	1.99	0.44
1:A:2407:SER:O	1:A:2408:ILE:C	2.57	0.44
1:A:2448:ASP:HA	1:A:2451:LYS:HB2	1.99	0.44
1:A:2450:VAL:HG12	1:A:2453:LEU:HD12	2.00	0.44
1:A:2407:SER:C	1:A:2409:LYS:N	2.74	0.44
1:A:1224:TRP:CD1	1:A:1391:MET:HG3	2.52	0.44
1:A:1808:LYS:HB3	1:A:2298:MET:HE3	2.00	0.44
1:A:1293:ASP:OD2	1:A:2786:SER:OG	2.27	0.44
1:A:1407:LEU:HD23	1:A:1512:LEU:HA	2.00	0.44
1:A:939:GLU:HA	1:A:942:LYS:HE2	1.99	0.43
1:A:1312:PRO:HG3	1:A:3074:ARG:HB2	1.98	0.43
1:A:1453:ASP:OD2	1:A:1476:ARG:NH2	2.51	0.43
1:A:1576:ASN:HB3	1:A:1590:THR:HG22	2.00	0.43
1:A:1457:GLU:HG3	1:A:1469:SER:HB2	1.98	0.43
1:A:3007:SER:OG	1:A:3008:PHE:N	2.51	0.43
1:A:1119:GLU:O	1:A:1123:ARG:N	2.47	0.43
1:A:1354:ASN:HD22	1:A:1354:ASN:HA	1.60	0.43
1:A:1522:LEU:HD23	1:A:1614:VAL:HG12	1.99	0.43
1:A:1774:PRO:HB2	1:A:2562:LYS:HE3	2.00	0.43
1:A:1018:TRP:HE1	1:A:1559:ARG:HH12	1.67	0.43
1:A:1443:ILE:HD12	1:A:1496:ILE:HG13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1496:ILE:HA	1:A:1499:LEU:HD12	2.01	0.43
1:A:2332:MET:HB3	1:A:2350:TYR:HD2	1.84	0.43
1:A:2410:LYS:NZ	2:B:8:G:O4'	2.51	0.43
1:A:2509:HIS:N	1:A:2524:VAL:O	2.45	0.43
1:A:2318:LYS:HD2	1:A:2577:TYR:HD2	1.83	0.43
1:A:2506:THR:HG22	1:A:2529:LEU:HD21	2.00	0.43
1:A:1606:GLN:O	1:A:1610:ASP:N	2.52	0.43
1:A:2332:MET:HB2	1:A:2336:ASP:HB2	2.00	0.43
1:A:1057:GLN:HA	1:A:1264:ILE:HG13	2.01	0.43
1:A:3086:VAL:HG21	1:A:3215:TYR:HE1	1.83	0.43
1:A:2411:ILE:HD13	1:A:2458:ILE:HG13	2.01	0.43
1:A:2353:ILE:O	1:A:2523:ILE:N	2.42	0.42
1:A:2405:ALA:C	1:A:2407:SER:N	2.75	0.42
1:A:3214:SER:HA	1:A:3219:GLU:HG3	2.00	0.42
1:A:1026:SER:O	1:A:1026:SER:OG	2.35	0.42
1:A:1655:ARG:HH11	1:A:1660:THR:HG21	1.84	0.42
1:A:2483:LEU:O	1:A:2487:ALA:N	2.50	0.42
1:A:3047:LYS:O	1:A:3051:ASN:ND2	2.52	0.42
1:A:1255:PHE:CB	2:B:7:A:C5	3.02	0.42
1:A:1323:LEU:HD13	1:A:1420:ILE:HG23	2.01	0.42
1:A:1462:LEU:HD13	1:A:1560:LEU:HD11	2.01	0.42
1:A:2402:GLU:HB2	1:A:2463:MET:HB3	2.02	0.42
1:A:2410:LYS:HB2	2:B:6:A:C2	2.53	0.42
1:A:2639:GLN:HA	1:A:2642:PHE:HB2	2.01	0.42
1:A:2517:ASP:OD1	1:A:2517:ASP:N	2.51	0.42
1:A:2631:THR:HG22	1:A:2669:PRO:HG2	2.02	0.42
1:A:1367:ASP:HB2	1:A:1389:SER:HB3	2.01	0.42
1:A:1018:TRP:CD1	1:A:1019:LEU:HD22	2.54	0.42
1:A:1328:THR:O	1:A:1334:GLN:NE2	2.51	0.42
1:A:2362:TRP:HB3	1:A:2517:ASP:HB3	2.02	0.42
1:A:2401:VAL:HB	1:A:2470:HIS:CD2	2.55	0.42
1:A:3151:MET:HE1	1:A:3164:LEU:HD11	2.02	0.42
1:A:1424:GLN:NE2	1:A:2628:ILE:HG23	2.35	0.42
1:A:2518:ASP:OD2	1:A:2577:TYR:N	2.47	0.42
1:A:935:LEU:HD13	1:A:966:LEU:HD12	2.02	0.41
1:A:1018:TRP:HE1	1:A:1559:ARG:NH1	2.17	0.41
1:A:1257:ARG:HE	1:A:2446:GLY:CA	2.24	0.41
1:A:2323:ASN:OD1	1:A:2324:VAL:N	2.53	0.41
1:A:1648:ASN:OD1	1:A:1652:SER:OG	2.36	0.41
1:A:3051:ASN:O	1:A:3055:ASN:ND2	2.53	0.41
1:A:3146:PHE:HD1	1:A:3149:ILE:H	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1252:LYS:HE2	1:A:1252:LYS:HB3	1.83	0.41
1:A:1804:ARG:HH22	1:A:2389:TYR:HB2	1.85	0.41
1:A:2627:LEU:HD12	1:A:2630:ASN:HB3	2.02	0.41
1:A:2529:LEU:HD12	1:A:2533:LEU:HD23	2.03	0.41
1:A:3050:GLU:O	1:A:3054:THR:N	2.51	0.41
1:A:2435:LYS:H	1:A:2435:LYS:HD2	1.86	0.41
1:A:1482:ASN:HA	1:A:1602:ASN:HD22	1.85	0.41
1:A:2657:LEU:H	1:A:2657:LEU:HG	1.63	0.41
1:A:1441:GLN:NE2	1:A:1445:ASN:OD1	2.54	0.40
1:A:2523:ILE:HD13	1:A:2523:ILE:HA	1.89	0.40
1:A:2355:ILE:N	1:A:2521:LYS:O	2.47	0.40
1:A:2449:THR:OG1	1:A:2450:VAL:N	2.55	0.40
1:A:2520:ALA:HB1	1:A:2574:LEU:HD11	2.03	0.40
1:A:1787:ILE:HG13	1:A:2490:LEU:HD12	2.02	0.40
1:A:3170:GLN:HG3	1:A:3173:ARG:HD2	2.04	0.40
1:A:2691:ALA:HB3	1:A:3050:GLU:HB3	2.02	0.40

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	A	1405/2341 (60%)	1225 (87%)	180 (13%)	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	A	1307/2138 (61%)	1297 (99%)	10 (1%)	73 78

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1061	HIS
1	A	1252	LYS
1	A	1257	ARG
1	A	1354	ASN
1	A	1363	VAL
1	A	1416	ILE
1	A	2407	SER
1	A	2408	ILE
1	A	2508	VAL
1	A	2657	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	987	ASN
1	A	1066	HIS
1	A	1150	GLN
1	A	1259	ASN
1	A	1334	GLN
1	A	1395	GLN
1	A	1421	GLN
1	A	1441	GLN
1	A	1445	ASN
1	A	1491	HIS
1	A	1518	GLN
1	A	1556	ASN
1	A	1618	ASN
1	A	2359	ASN
1	A	2376	GLN
1	A	2400	GLN
1	A	2428	HIS
1	A	2470	HIS
1	A	2556	GLN
1	A	2607	GLN

Continued on next page...

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Mol	Chain	Res	Type
1	A	2794	HIS
1	A	2822	ASN
1	A	3051	ASN
1	A	3057	ASN
1	A	3170	GLN
1	A	3177	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	9/18 (50%)	6 (66%)	0

All (6) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	2	C
2	B	5	A
2	B	6	A
2	B	7	A
2	B	8	G
2	B	9	A

There are no RNA pucker outliers to report.

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.

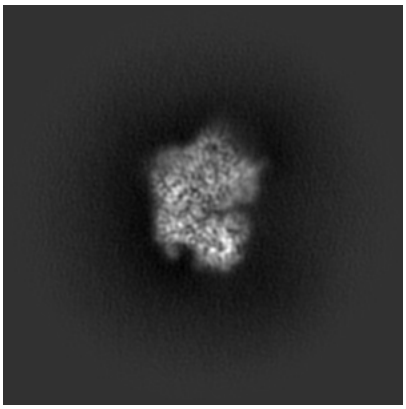
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-67157. These allow visual inspection of the internal detail of the map and identification of artifacts.

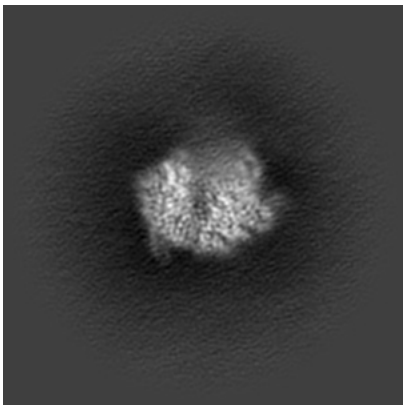
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

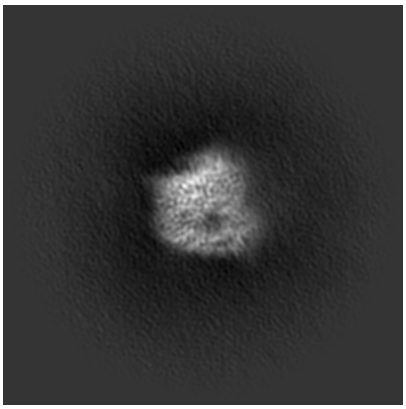
6.1.1 Primary map



X

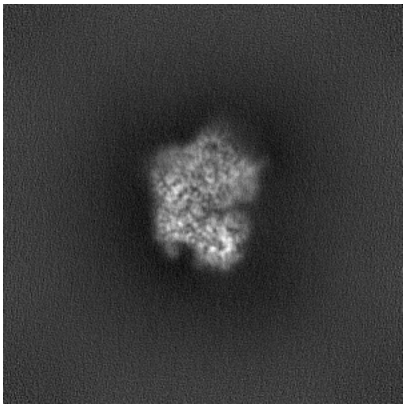


Y

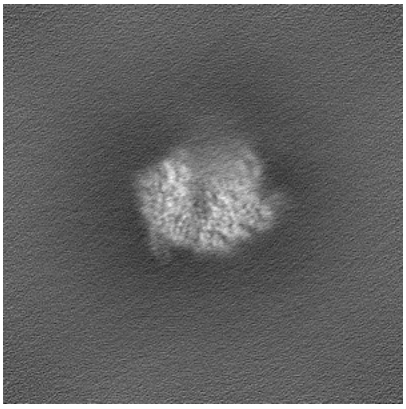


Z

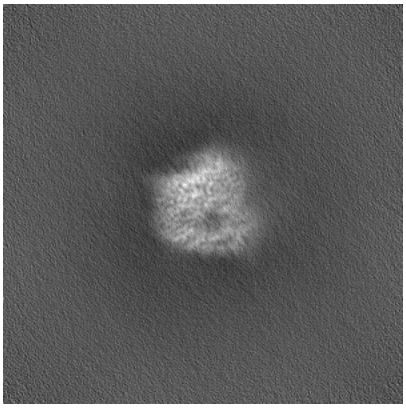
6.1.2 Raw map



X



Y

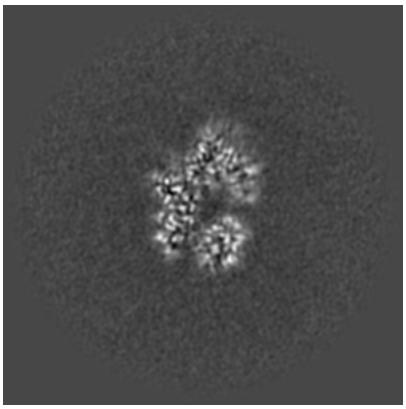


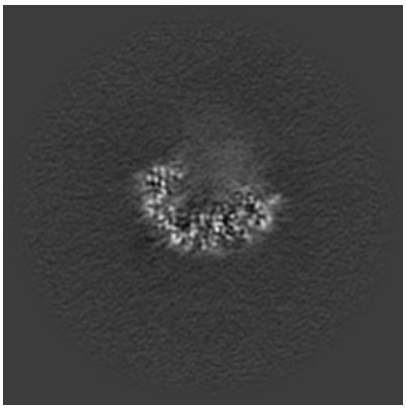
Z

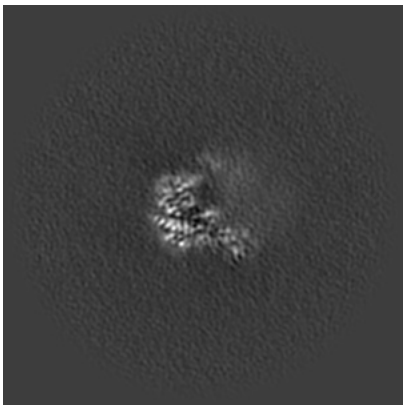
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

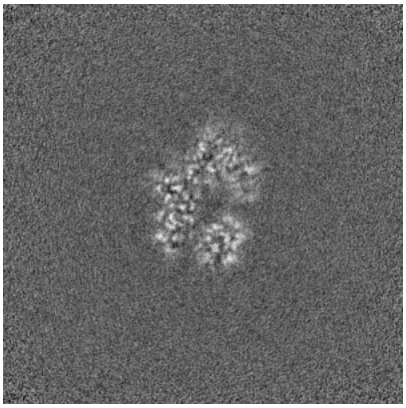
6.2.1 Primary map

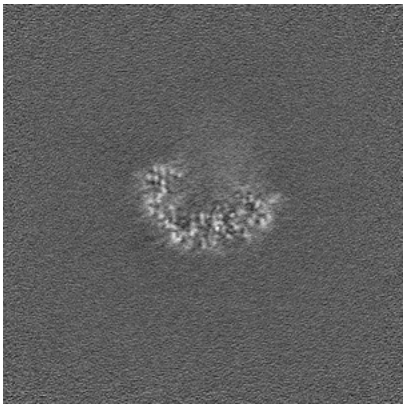

X Index: 180

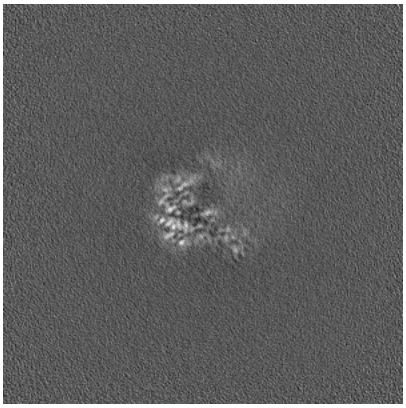

Y Index: 180


Z Index: 180

6.2.2 Raw map


X Index: 180

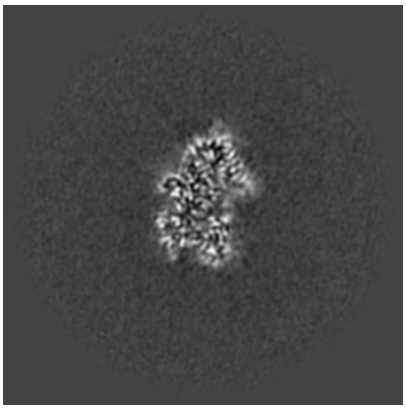

Y Index: 180


Z Index: 180

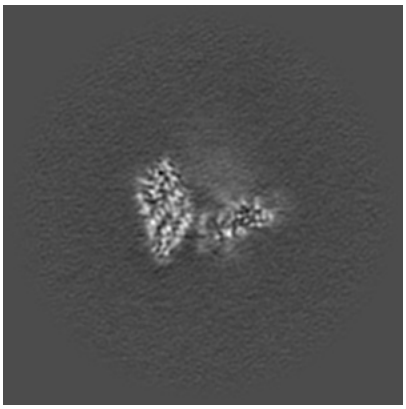
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

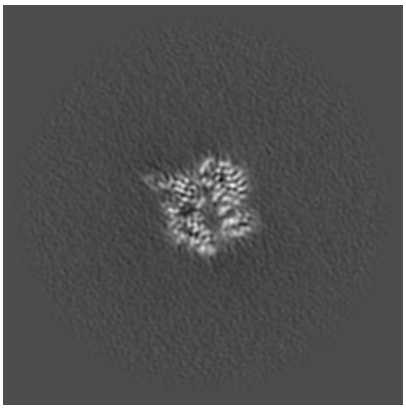
6.3.1 Primary map



X Index: 170

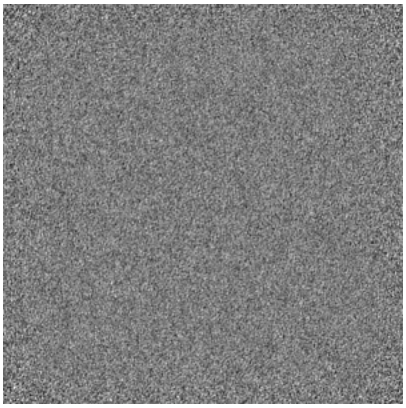


Y Index: 199

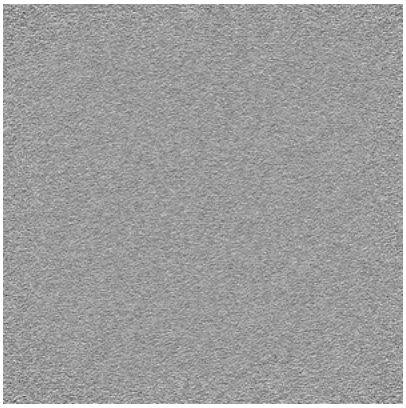


Z Index: 150

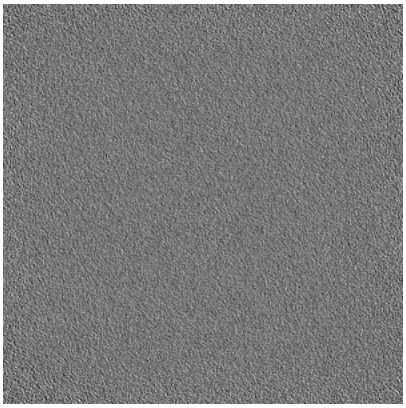
6.3.2 Raw map



X Index: 0



Y Index: 0

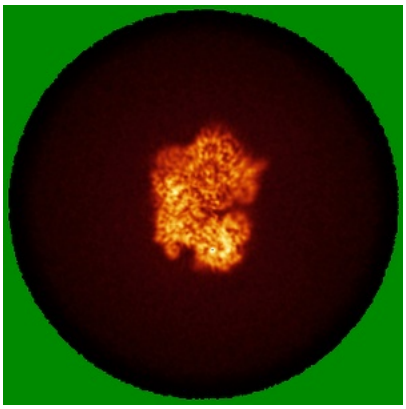


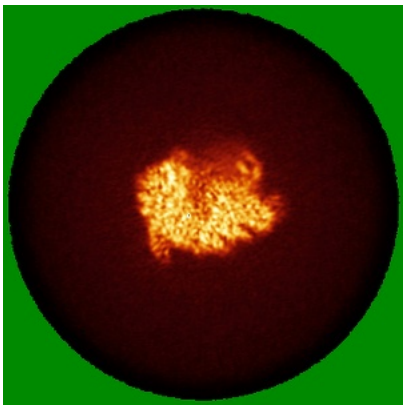
Z Index: 0

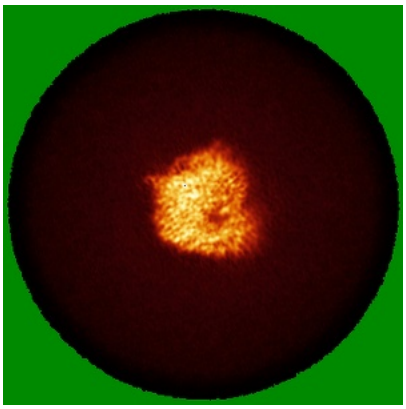
The images above show the largest variance slices of the map in three orthogonal directions.

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

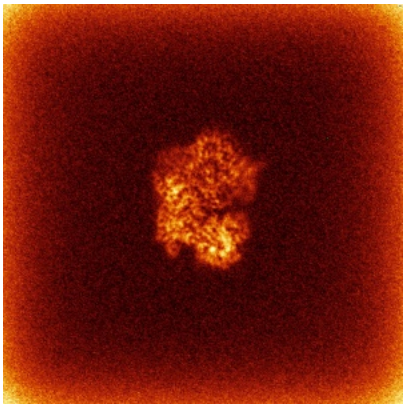
6.4.1 Primary map

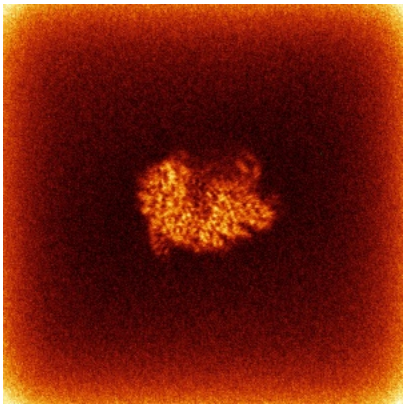

X

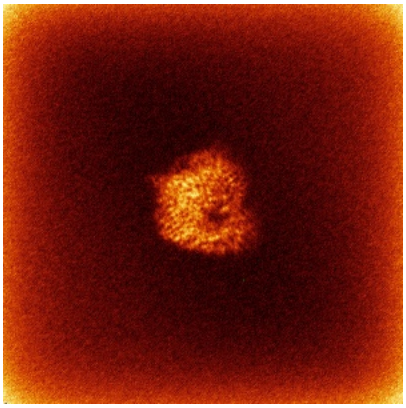

Y


Z

6.4.2 Raw map


X

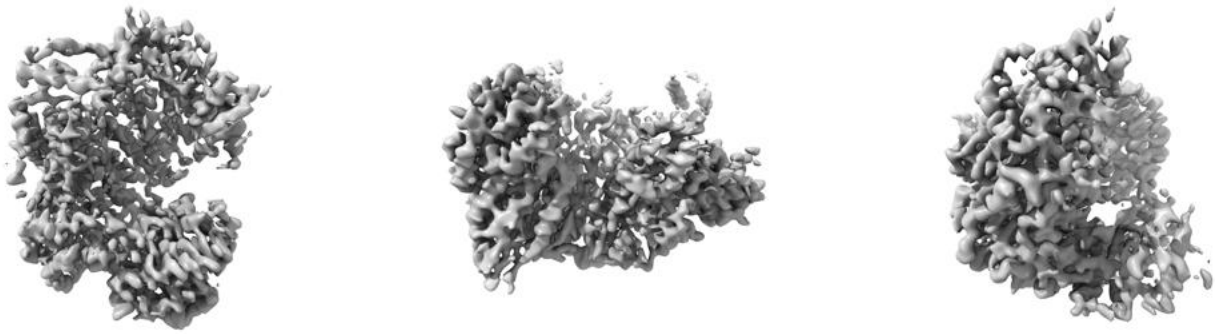

Y


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)

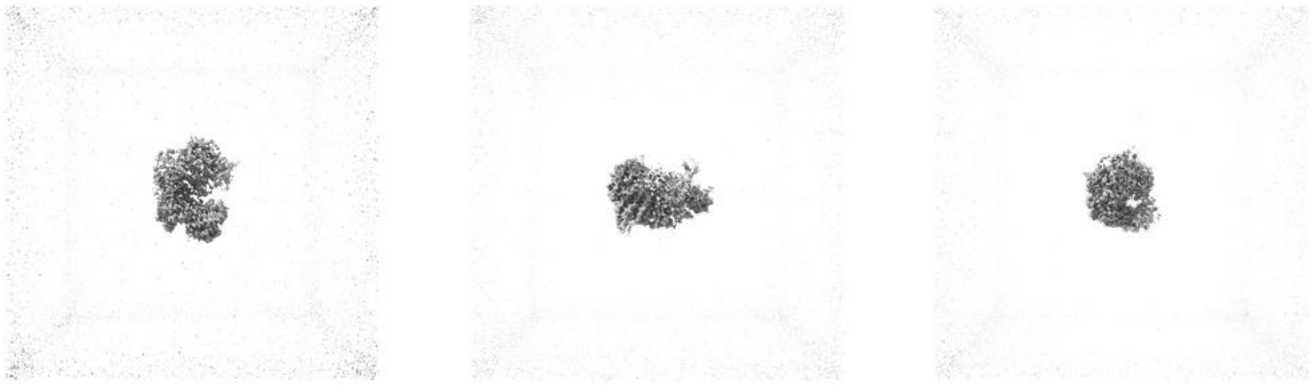
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.329. 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.

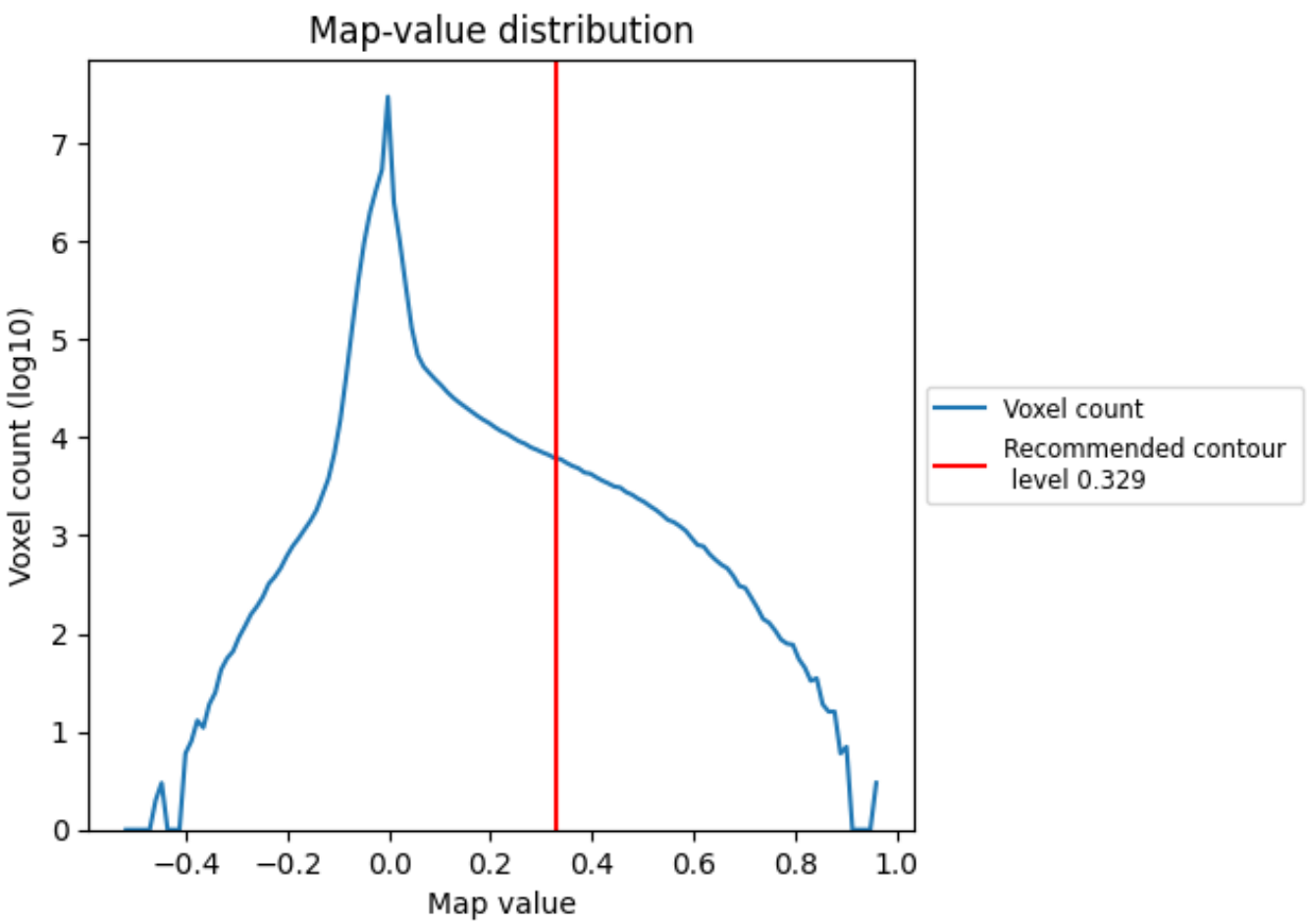
6.6 Mask visualisation (i)

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

7 Map analysis (i)

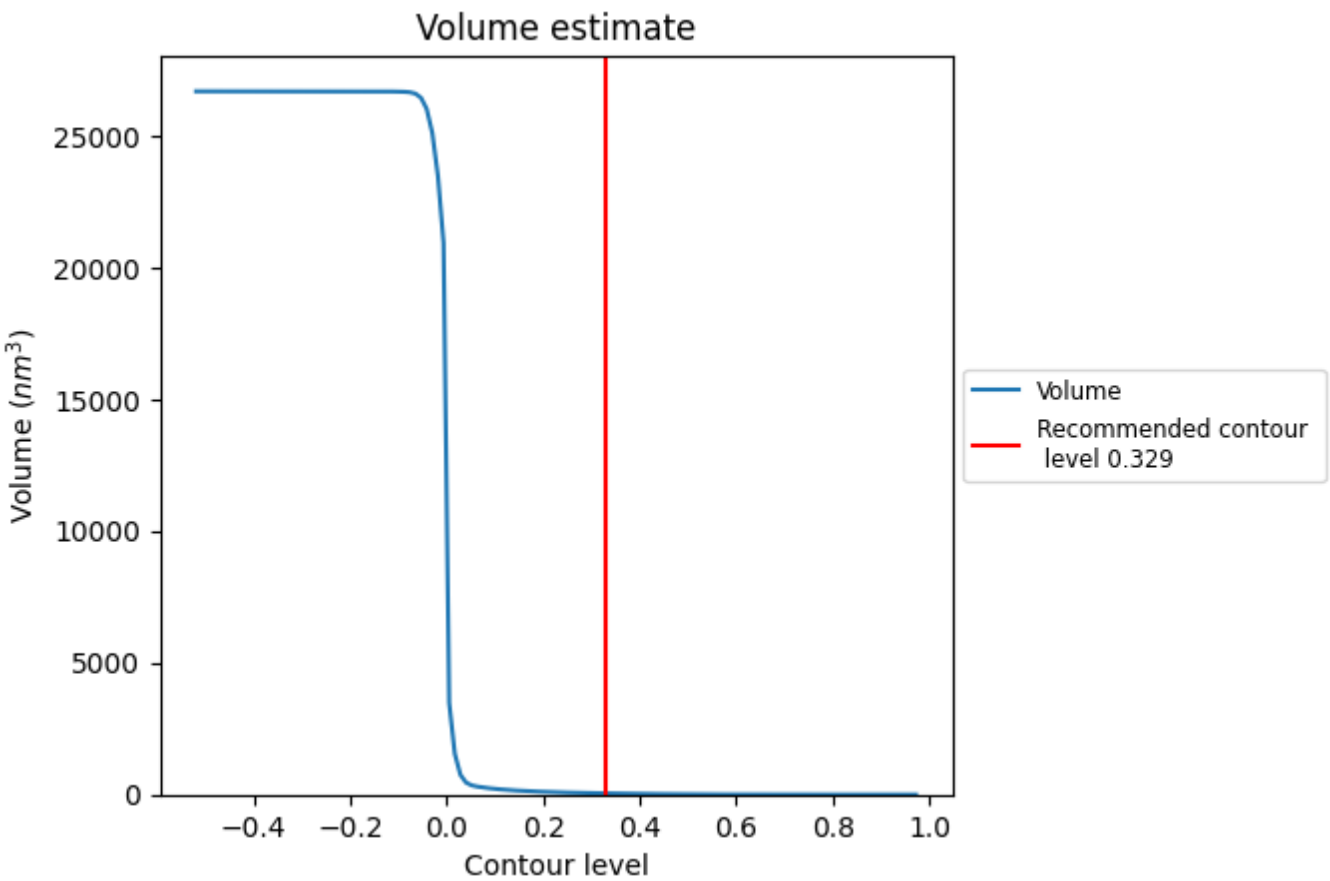
This section contains the results of statistical analysis of the map.

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.

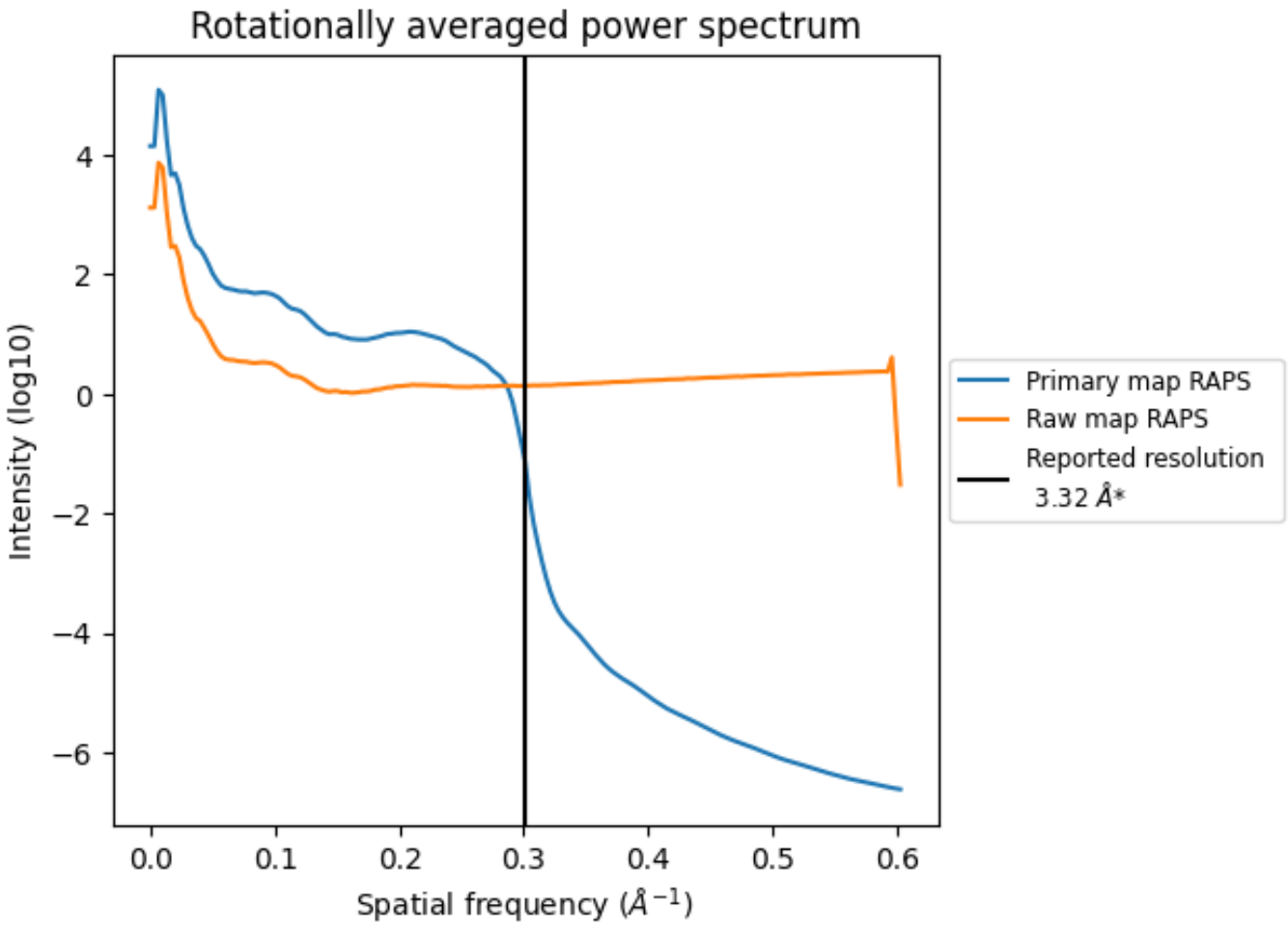
7.2 Volume estimate (i)



The volume at the recommended contour level is 46 nm^3; this corresponds to an approximate mass of 41 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)

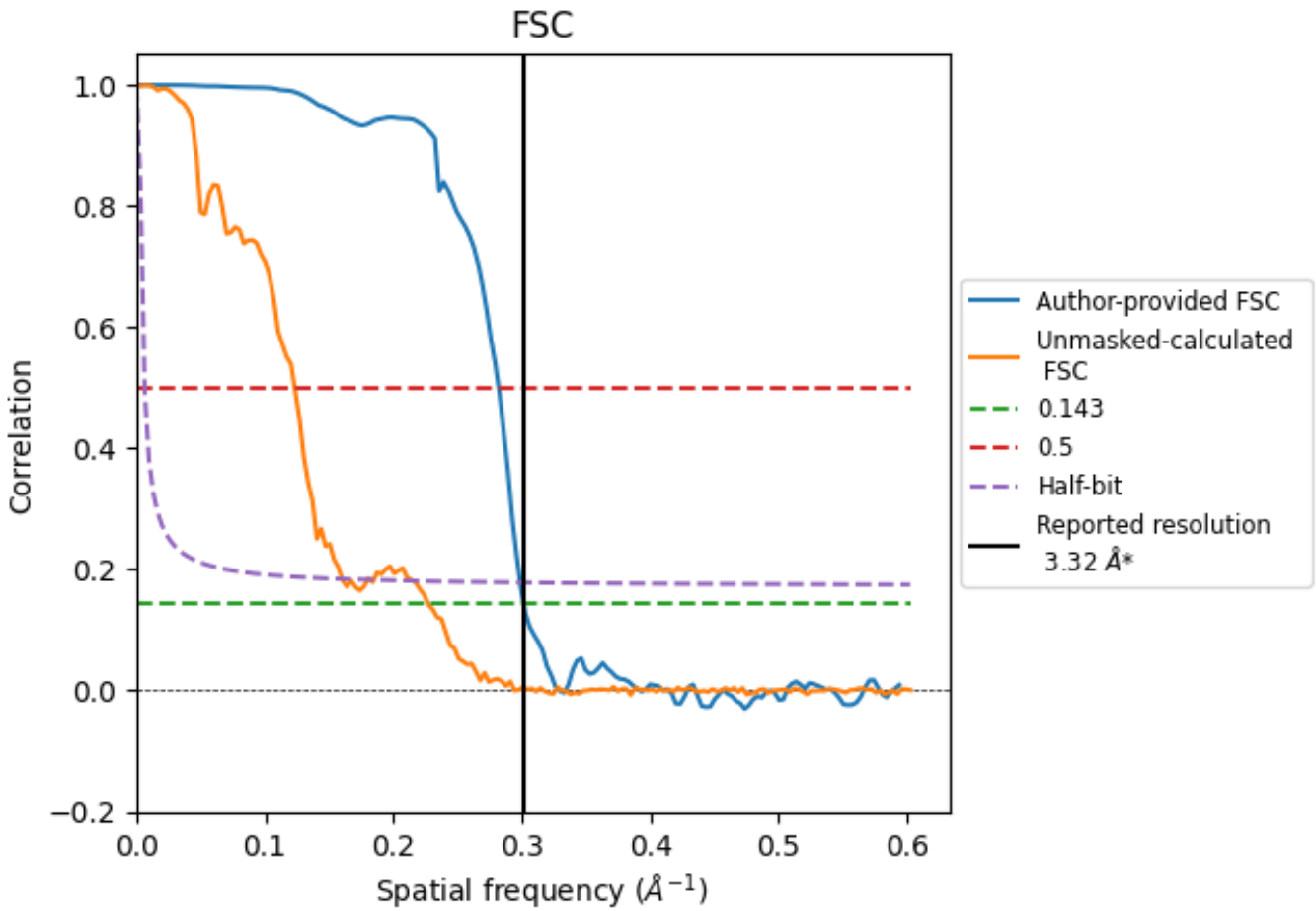


*Reported resolution corresponds to spatial frequency of 0.301 Å^{-1}

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 0.301 Å^{-1}

8.2 Resolution estimates (i)

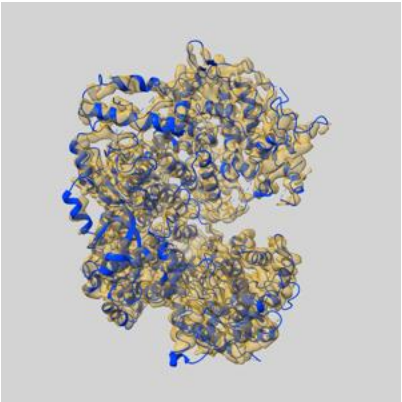
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.32	-	-
Author-provided FSC curve	3.32	3.54	3.35
Unmasked-calculated*	4.40	8.11	6.24

*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 4.40 differs from the reported value 3.32 by more than 10 %

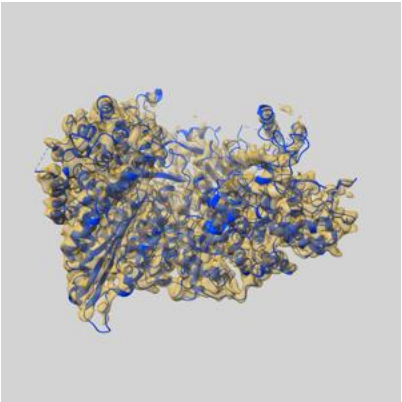
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-67157 and PDB model 9XRX. Per-residue inclusion information can be found in section 3 on page 5.

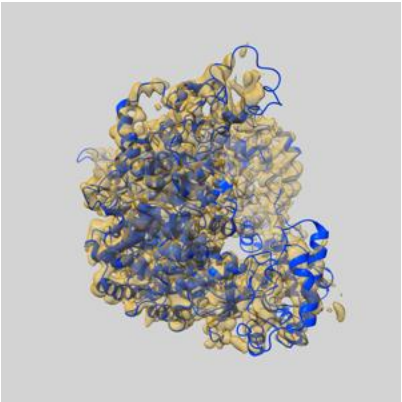
9.1 Map-model overlay (i)



X



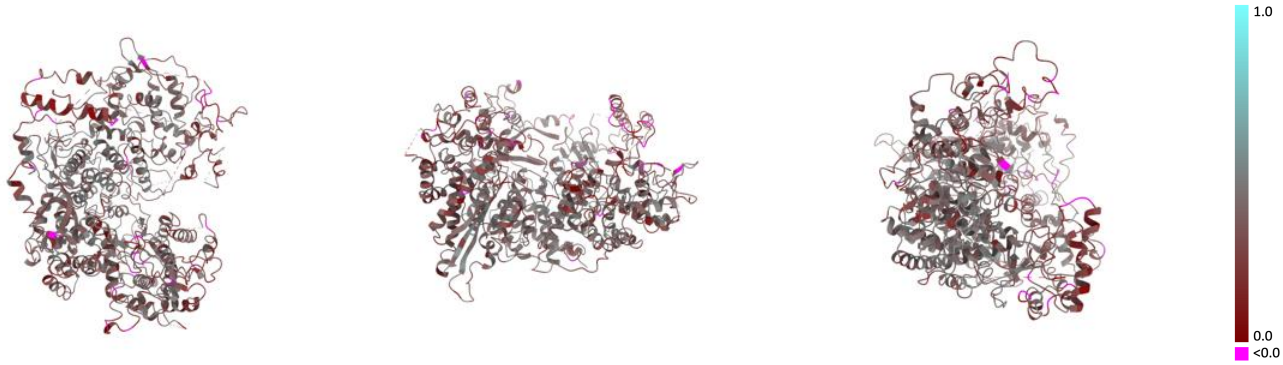
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.329 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

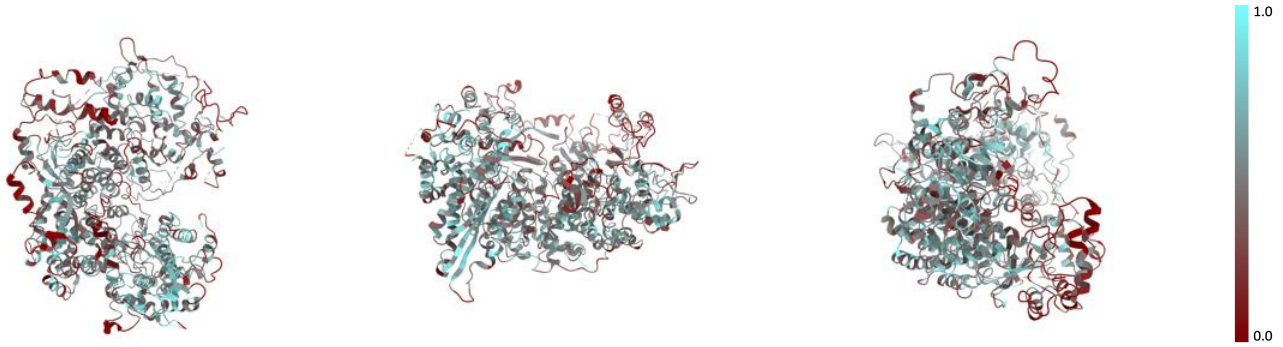
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

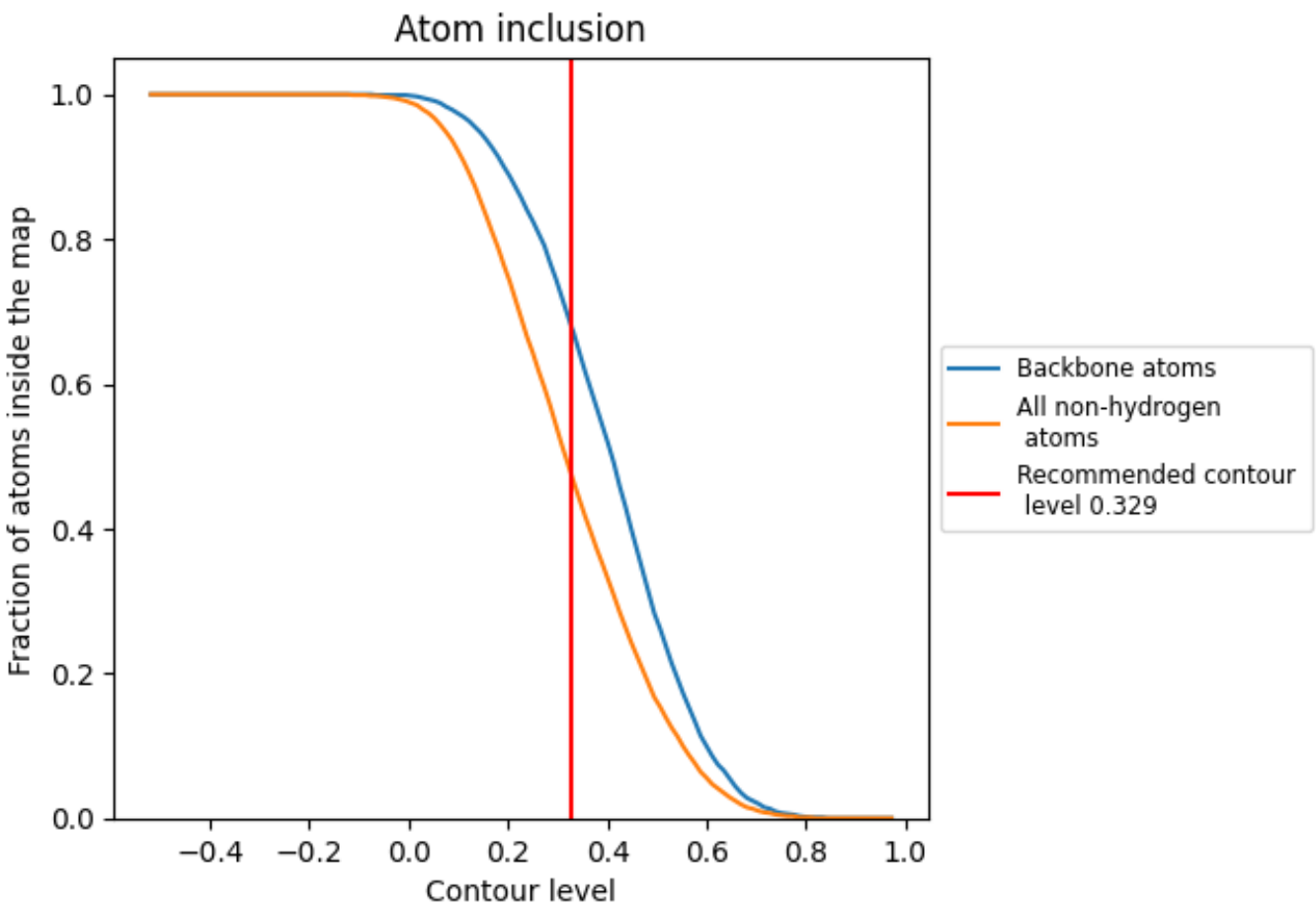
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.329).

9.4 Atom inclusion (i)



At the recommended contour level, 68% of all backbone atoms, 47% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.329) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4710	0.3460
A	0.4700	0.3460
B	0.5160	0.3460