wwPDB EM Validation Summary Report ⓘ

Sep 27, 2026 – 01:29 AM JST

PDB ID	:	25XL / pdb_000025xl
EMDB ID	:	EMD-80447
Title	:	Cryo-EM structure of the Crimean-Congo hemorrhagic fever virus L protein (apo form)
Authors	:	Jia, H.; Liu, S.; Gong, P.
Deposited on	:	2026-04-22
Resolution	:	2.88 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

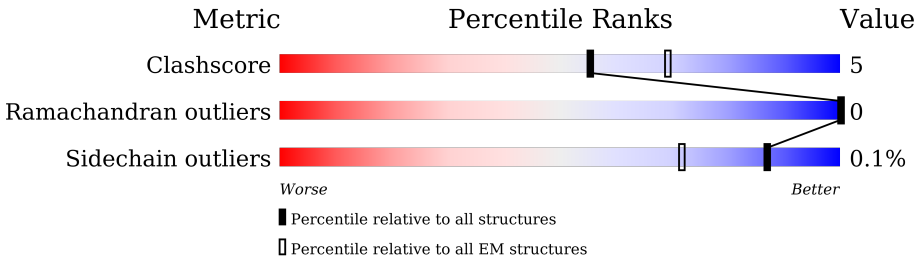
EMDB validation analysis	:	0.0.1.dev133
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

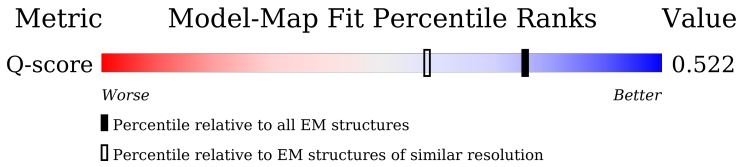
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.88 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	12111 (2.38 - 3.38)

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	3989	30% · 66%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10152 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	1363	10149	6468	1775	1835	71	1	0

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-43	MET	-	initiating methionine	UNP A0A068JD44
A	-42	TRP	-	expression tag	UNP A0A068JD44
A	-41	SER	-	expression tag	UNP A0A068JD44
A	-40	HIS	-	expression tag	UNP A0A068JD44
A	-39	PRO	-	expression tag	UNP A0A068JD44
A	-38	GLN	-	expression tag	UNP A0A068JD44
A	-37	PHE	-	expression tag	UNP A0A068JD44
A	-36	GLU	-	expression tag	UNP A0A068JD44
A	-35	LYS	-	expression tag	UNP A0A068JD44
A	-34	GLY	-	expression tag	UNP A0A068JD44
A	-33	GLY	-	expression tag	UNP A0A068JD44
A	-32	GLY	-	expression tag	UNP A0A068JD44
A	-31	SER	-	expression tag	UNP A0A068JD44
A	-30	GLY	-	expression tag	UNP A0A068JD44
A	-29	GLY	-	expression tag	UNP A0A068JD44
A	-28	GLY	-	expression tag	UNP A0A068JD44
A	-27	SER	-	expression tag	UNP A0A068JD44
A	-26	GLY	-	expression tag	UNP A0A068JD44
A	-25	GLY	-	expression tag	UNP A0A068JD44
A	-24	GLY	-	expression tag	UNP A0A068JD44
A	-23	SER	-	expression tag	UNP A0A068JD44
A	-22	TRP	-	expression tag	UNP A0A068JD44
A	-21	SER	-	expression tag	UNP A0A068JD44
A	-20	HIS	-	expression tag	UNP A0A068JD44
A	-19	PRO	-	expression tag	UNP A0A068JD44
A	-18	GLN	-	expression tag	UNP A0A068JD44
A	-17	PHE	-	expression tag	UNP A0A068JD44
A	-16	GLU	-	expression tag	UNP A0A068JD44

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	LYS	-	expression tag	UNP A0A068JD44
A	-14	GLY	-	expression tag	UNP A0A068JD44
A	-13	SER	-	expression tag	UNP A0A068JD44
A	-12	SER	-	expression tag	UNP A0A068JD44
A	-11	SER	-	expression tag	UNP A0A068JD44
A	-10	HIS	-	expression tag	UNP A0A068JD44
A	-9	HIS	-	expression tag	UNP A0A068JD44
A	-8	HIS	-	expression tag	UNP A0A068JD44
A	-7	HIS	-	expression tag	UNP A0A068JD44
A	-6	HIS	-	expression tag	UNP A0A068JD44
A	-5	HIS	-	expression tag	UNP A0A068JD44
A	-4	HIS	-	expression tag	UNP A0A068JD44
A	-3	HIS	-	expression tag	UNP A0A068JD44
A	-2	GLY	-	expression tag	UNP A0A068JD44
A	-1	SER	-	expression tag	UNP A0A068JD44
A	0	SER	-	expression tag	UNP A0A068JD44
A	1	SER	-	expression tag	UNP A0A068JD44

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
2	A	2	Total	Zn	0
			2	2	

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	O	0
			1	1	

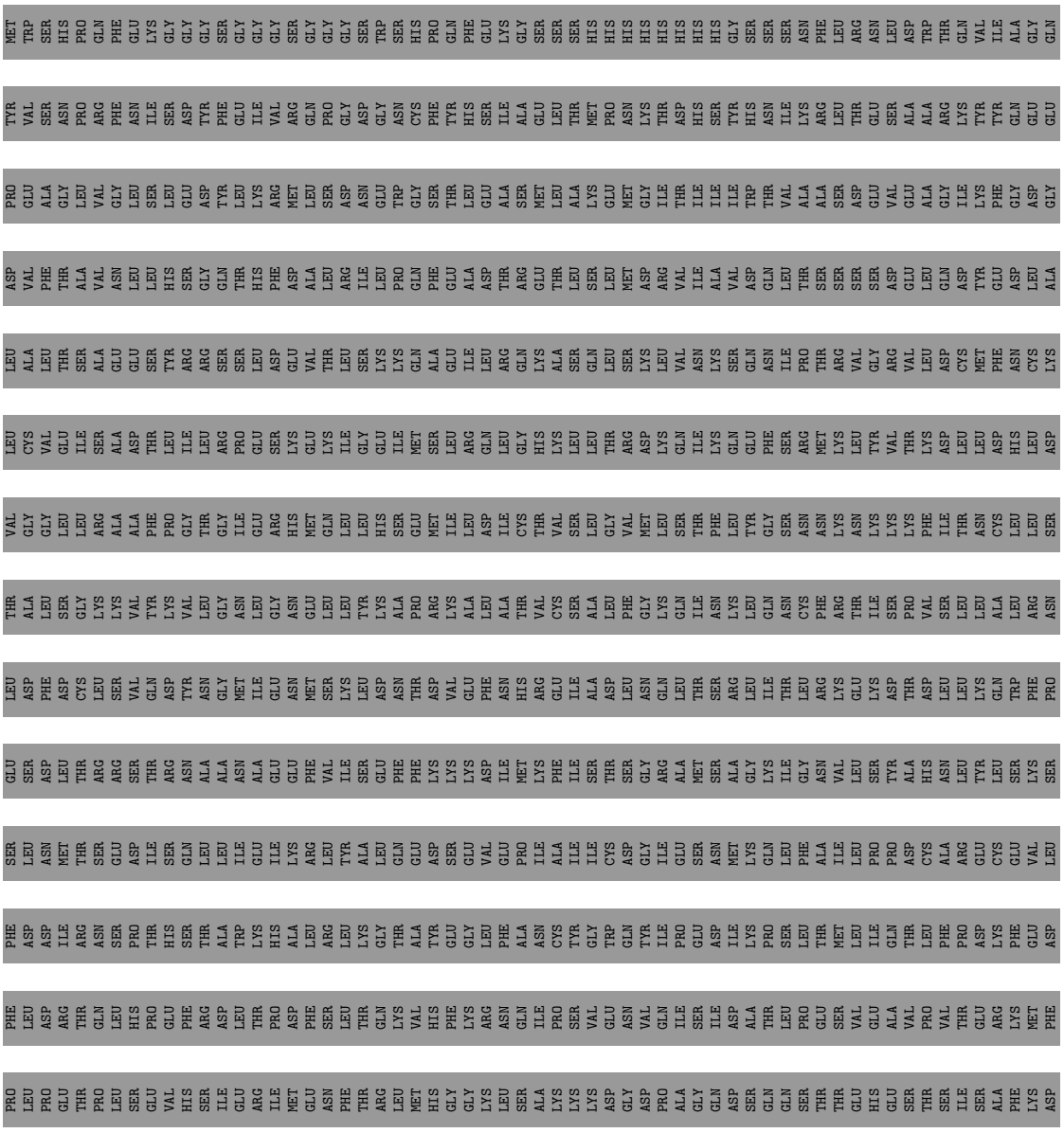
3 Residue-property plots (i)

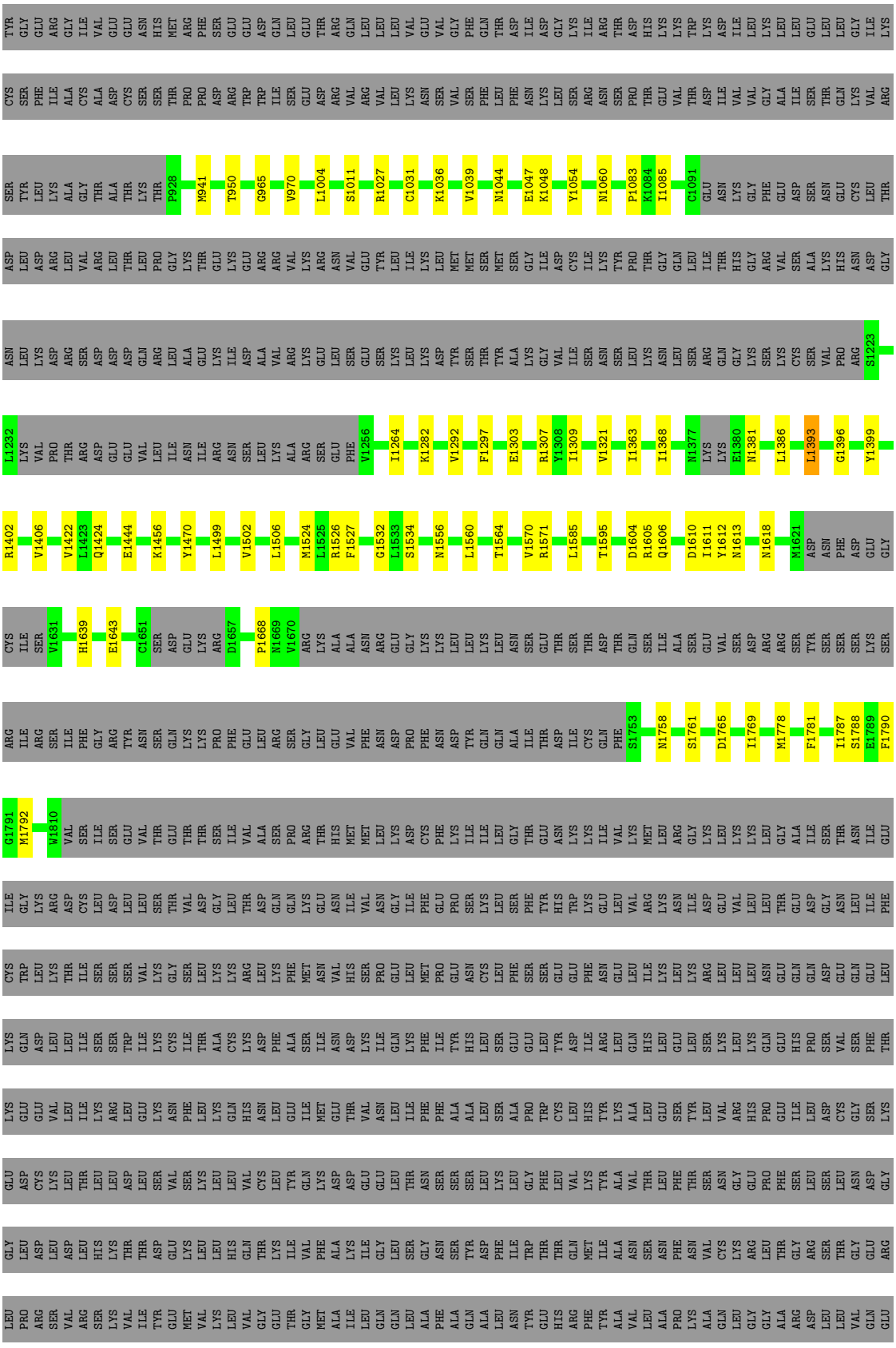
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

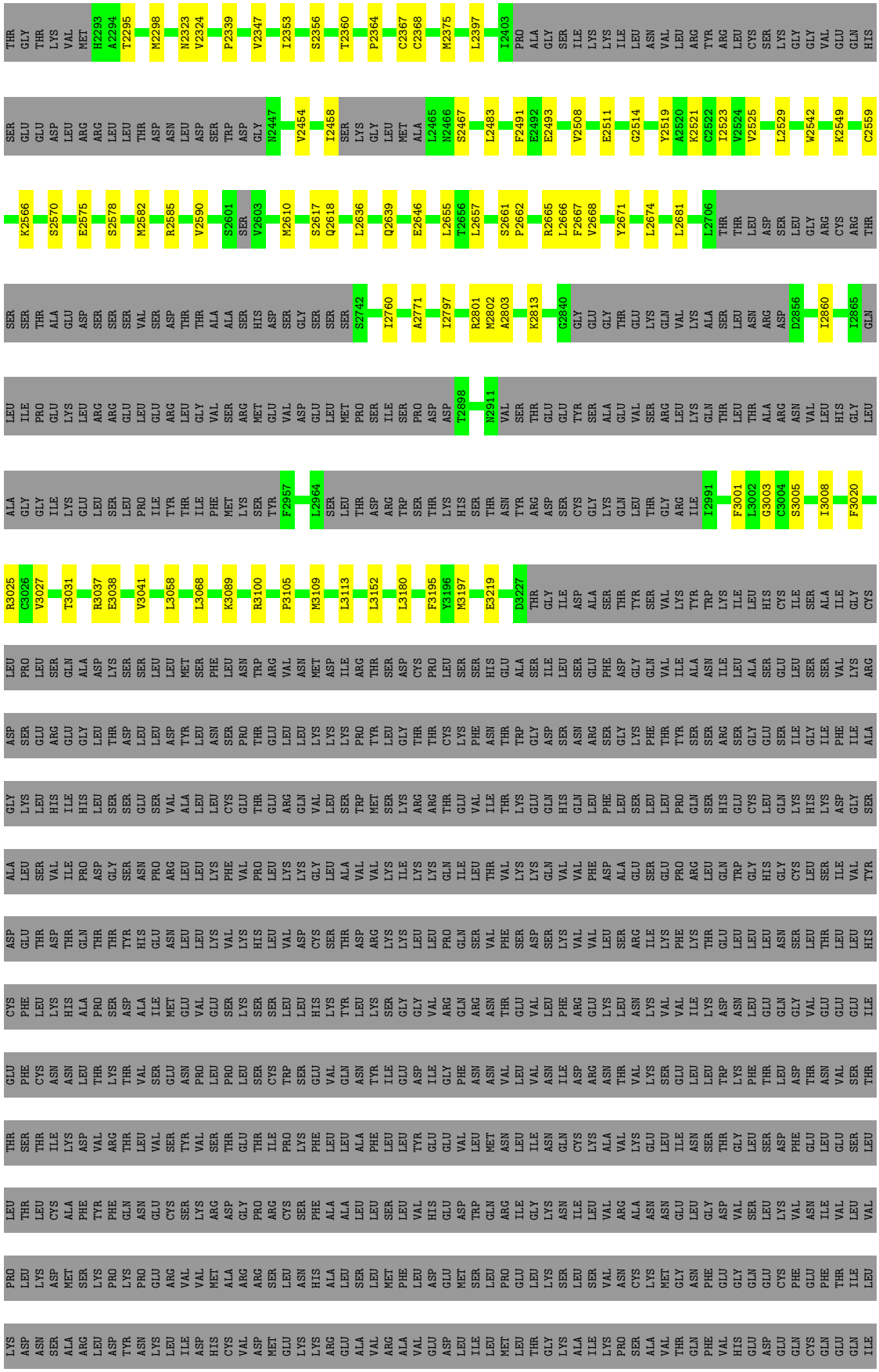
- Molecule 1: RNA-directed RNA polymerase L

Chain A:






TYR GLY GLU ARG GLY ILE VAL GLU GLU ASN HIS MET ARG PHE SER GLU GLU ASP GLN LEU LEU GLU THR ARG GLN LEU LEU LEU VAL GLU VAL GLY PHE GLN THR ASP ILE ASP GLY LYS ILE ARG THR ASP HIS LYS LYS TRP LYS ASP ILE LEU LYS LEU LEU GLU LEU LEU GLY ILE LYS
CYS SER PHE ILE ALA CYS ALA ASP CYS SER SER THR PRO PRO ASP ARG TRP TRP ILE SER GLU ASP ARG VAL ARG VAL LEU LYS ASN SER VAL SER PHE LEU PHE ASN LYS LEU GLN GLY PHE GLY ALA ILE SER THR GLN LYS VAL ARG
SER TYR LEU LYS ALA GLY THR ALA THR LYS THR P928 M941 T950 G965 V970 L1004 S1011 R1027 C1031 K1036 V1039 N1044 E1047 K1048 Y1054 N1060 P1083 K1084 I1085 C1091 GLU ASN LYS GLY PHE GLU ASP SER ASN GLU CYS LEU THR
ASP LEU ASP ARG LEU VAL ARG LEU THR LEU PRO GLY LYS THR GLU LYS GLU ARG ARG VAL LYS ARG ASN VAL GLU TYR LEU ILE LYS LEU MET MET SER MET SER GLY ILE ASP CYS ILE LYS TYR PRO THR GLY GLN LEU ILE THR HIS GLY ARG VAL SER ALA LYS HIS ASN ASP GLY
ASN LEU LYS ASP ARG SER ASP ASP ASP GLN ARG LEU ALA GLU LYS ILE ASP ALA VAL ARG LYS GLU LEU SER GLU SER LYS LEU LYS ASP TYR SER THR TYR ALA LYS GLY VAL ILE SER ASN SER LEU LYS ASN LEU SER ARG GLN GLY GLY LYS SER LYS CYS SER VAL PRO ARG S1223
L1232 LYS VAL PRO THR ARG ASP GLU GLU VAL LEU ILE ASN ILE ARG ASN SER LEU LYS ALA ARG SER GLU PHE V1256 I1264 K1282 V1292 F1297 E1303 R1307 Y1308 I1309 V1321 I1363 I1368 N1377 LYS LYS E1380 N1381 L1386 L1393 G1396 Y1399
R1402 V1406 V1422 L1423 Q1424 E1444 K1456 Y1470 L1499 V1502 L1506 M1524 L1525 R1526 F1527 G1532 L1533 S1534 N1556 L1560 T1564 V1570 R1571 L1585 T1595 D1604 R1605 Q1606 D1610 I1611 Y1612 N1613 N1618 M1621 ASP ASN PHE ASP GLU GLY
CYS ILE SER V1631 H1639 E1643 C1651 SER ASP GLU LYS ARG D1657 P1668 N1669 V1670 ARG LYS ALA ALA ASN ARG GLU GLY LYS LYS LEU LEU LYS LEU ASN SER GLU THR SER THR ASP THR GLN SER ILE ALA SER GLU VAL PHE ARG ARG ARG SER LYS
ARG ILE ARG SER ILE PHE GLY ARG TYR ASN SER GLN LYS LYS PRO PHE GLU LEU GLU VAL PHE ASN ASP PRO PHE ASN ASP TYR GLN GLN ALA ILE THR ASP ILE CYS GLN PHE S1753 N1758 S1761 D1765 I1769 M1778 F1781 I1787 S1788 E1789 F1790
G1791 M1792 W1810 VAL SER ILE SER GLU VAL THR GLU THR THR SER ILE VAL ALA SER PRO ARG 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 LYS ASN ILE ASP GLU LYS LYS SER THR ASN ILE GLU
ILE GLY LYS ARG ASP CYS LEU ASP LEU LEU SER THR VAL ASP GLY LEU THR ASP GLN LYS GLU ASN ILE VAL ASN GLY ILE PHE GLU PRO SER LYS LEU GLY PHE TYR HIS TRP LYS GLU LEU VAL ARG LYS ASN LEU LEU LEU THR GLU ASP GLU VAL LEU LEU LEU GLY ALA ILE SER ASN LEU LEU PHE
CYS TRP LEU LYS THR ILE SER SER SER VAL LYS GLY SER LEU LYS PHE MET ASN VAL HIS SER PRO GLU LEU MET PRO GLU ASN CYS LEU PHE SER SER TYR HIS LEU LEU SER GLU GLY PHE ASN GLU LEU ILE LYS LEU LYS ARG LEU LEU LEU ASN GLU GLN GLN GLU ASP GLN ASP GLU LEU
LYS GLN ASP LEU LEU ILE SER SER TRP ILE LYS CYS LYS ASP PHE ILE THR ALA CYS LYS ASP PHE ALA SER ILE ASN ASP LYS ILE GLN LYS PHE ILE TYR HIS LEU SER GLU LYS ILE ARG LEU GLN HIS LEU GLU LEU SER LYS LEU GLU LEU HIS PRO SER VAL SER PHE THR
LYS GLU GLU VAL LEU ILE LYS ARG LEU GLU LYS ASN PHE LEU LYS GLN HIS ASN LEU GLU THR VAL ASN LEU ILE PHE PHE ALA ALA LEU SER GLU ALA PRO TRP CYS LEU HIS TYR LYS ALA LEU GLU SER TYR LEU VAL ARG HIS PRO GLU ILE LEU ASP CYS SER VAL SER LYS
GLU ASP CYS LYS LEU THR LEU LEU ASP LEU SER SER VAL GLY LEU TYR GLN LYS ASP LEU GLU GLU LEU THR ASN SER SER LEU LYS PHE LEU VAL LYS TYR TYR ALA VAL THR LEU PHE THR SER ASN GLY GLU PRO PHE SER LEU ASN ASP GLY
GLY LEU ASP LEU ASP LEU HIS LYS THR THR ASP GLU LYS LEU LEU HIS GLN 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 GLU LEU THR GLY ARG SER THR GLY GLU ARG
LEU PRO ARG SER VAL LYS VAL THR 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 GLU


THR GLY THR LYS VAL MET H2293 A2294 T2295 M2298 N2323 V2324 P2339 V2347 I2353 S2356 T2360 P2364 C2367 C2368 M2375 L2397 I2403 PRO ALA GLY SER ILE LYS LYS ILE LEU ASN VAL LEU ARG TYR ARG LEU CYS SER LYS GLY GLY VAL GLU GLN HIS
SER GLU GLU ASP LEU ARG ARG LEU LEU THR ASP ASN LEU ASP SER TRP ASP GLY N2447 V2454 I2458 SER LYS GLY LEU MET ALA L2465 N2466 S2467 L2483 F2491 E2492 E2493 V2508 E2511 G2514 Y2519 A2520 K2521 C2522 I2523 V2524 V2525 L2529 W2542 K2549 C2559
K2566 S2570 E2575 S2578 M2582 R2585 V2590 S2601 SER V2603 M2610 S2617 Q2618 L2636 Q2639 E2646 L2655 T2656 L2657 S2661 P2662 R2665 L2666 F2667 V2668 Y2671 L2674 L2681 L2706 THR THR LEU ASP SER LEU GLY ARG CYS ARG THR
SER SER THR ALA GLU ASP SER SER SER VAL SER ASP THR THR ALA ALA SER HIS ASP SER GLY SER SER SER S2742 I2760 A2771 I2797 R2801 M2802 A2803 K2813 G2840 GLY GLU GLY THR GLU LYS GLN VAL LYS ALA SER LEU ASN ARG ASP D2856 I2860 I2865 GLN
LEU ILE PRO GLU LYS LEU ARG ARG GLU LEU GLU GLU ARG LEU GLY VAL SER ARG MET GLU VAL ASP GLU LEU MET PRO SER ILE SER PRO ASP ASP T2898 N2911 VAL SER THR GLU GLU TYR SER ALA GLU VAL SER ARG LEU LYS GLN THR LEU THR ALA ARG ASN VAL LEU HIS GLY LEU
ALA GLY GLY ILE LYS GLU LEU PRO ILE TYR THR ILE PHE MET LYS SER TYR F2957 L2964 SER LEU THR ASP ARG TRP SER THR ASN TYR ARG ASP SER CYS GLY LYS GLN LEU THR GLY ARG ILE I2991 F3001 L3002 G3003 C3004 S3005 I3008 F3020
R3025 C3026 V3027 T3031 R3037 E3038 V3041 L3058 L3068 K3089 R3100 P3105 M3109 L3113 L3152 L3180 F3195 Y3196 M3197 E3219 D3227 THR GLY ILE ASP ALA SER THR TYR SER VAL LYS TYR TRP LYS ILE LEU HIS CYS ILE SER ALA ILE GLY CYS
LEU PRO LEU SER GLN ALA ASP LYS SER SER LEU LEU MET SER PHE LEU ASN TRP ARG VAL ASN MET ASP ILE ARG THR SER ASP CYS PRO LEU SER SER HIS GLU ALA SER ILE LEU SER GLU PHE ASP GLY GLN VAL ILE ALA ASN ILE LEU ALA SER GLU GLU VAL SER LYS
ASP SER GLU ARG GLU GLY LEU THR ASP LEU LEU ASP TYR LEU SER LYS LYS PRO TYR LEU GLY THR THR CYS LYS PHE ASN THR TRP GLY ASP SER ASN ARG SER GLY LYS PHE THR TYR SER SER ARG SER GLY GLU LEU SER ILE GLY ILE PHE ILE ALA
GLY LYS LEU HIS ILE HIS LEU SER SER GLU SER VAL ALA LEU LEU LEU CYS GLU GLY THR GLU VAL ILE THR LYS GLU GLN HIS GLN LEU PHE LEU SER SER LEU LEU PRO GLN SER HIS GLU CYS LEU GLN LYS HIS LYS ASP GLY SER
ALA LEU SER VAL ILE PRO ASP GLY SER ASN PRO ARG LEU LEU LYS PHE VAL PRO LEU LYS LYS GLY LEU ALA VAL VAL LYS ILE LYS LYS LEU ILE LEU THR VAL LYS LYS GLN VAL VAL PHE ASP ALA GLU SER GLU PRO ARG LEU GLN ILE SER GLY HIS GLY CYS LEU SER ILE VAL TYR
ASP GLU THR ASP THR GLN THR THR TYR HIS GLU ASN LEU LEU LYS VAL LYS HIS LEU VAL ASP CYS SER THR ASP ARG LYS LYS LEU PRO GLN SER VAL PHE SER ASP SER LYS VAL LEU SER ARG SER ILE LYS VAL PHE LYS THR GLU LEU LEU LEU ASN SER LEU THR LEU LEU HIS
CYS PHE LEU LYS HIS ALA PRO SER ASP ALA ILE MET GLU VAL GLU SER LYS SER LEU LEU HIS LYS TYR LEU LYS SER GLY GLY VAL ARG GLN ARG ASN THR GLU VAL LEU LYS LEU ASN LYS VAL VAL ILE LYS ASP ASN LEU GLN GLN GLY VAL GLU GLU GLU ILE
GLU PHE CYS ASN ASN LEU THR LYS THR VAL SER GLU ASN PRO LEU PRO LEU SER CYS TRP SER GLU VAL GLN ASN TYR ILE GLU ASP ILE GLY PHE ASN LEU VAL ASN ILE ASP ARG ASN THR VAL LYS SER GLU LEU LEU TRP LYS PHE THR LEU ASP ASN SER VAL ASP THR ASN
THR SER THR ILE LYS ASP VAL ARG THR LEU VAL SER TYR VAL SER THR GLU GLU ILE PRO LYS PHE LEU LEU ALA ALA PHE LEU LEU TYR GLU GLU VAL SER LEU ILE LEU ASN GLN CYS LYS ALA VAL LYS GLU VAL LEU MET ASN LEU ILE ASN GLN CYS LYS ALA VAL LYS GLU LEU ILE ASN SER THR GLY LEU SER ASP PHE GLU LEU GLU SER LEU
LEU THR LEU CYS ALA PHE TYR PHE GLN ASN GLU CYS SER LYS ARG ASP GLY PRO ARG CYS SER PHE ALA ALA LEU LEU SER LEU MET PHE LEU ASP GLU MET SER LEU GLN ARG ILE GLY LYS ASN ILE LEU GLY ASP VAL SER LEU LEU LYS VAL ASN ILE VAL LEU VAL
PRO LEU LYS ASP MET SER HIS ALA ALA LEU SER LEU ASN HIS LEU SER VAL ASN CYS LYS MET GLY ASN PHE GLU GLN GLU CYS PHE GLU PHE THR ILE LEU
LYS ASP ASN SER ALA ARG GLU ALA VAL ARG ALA VAL GLU ASP LEU ILE LEU LEU MET LEU THR GLY LYS ALA ILE LYS PRO SER ALA VAL THR GLN PHE VAL HIS GLU GLU ASP GLN CYS GLN GLU ILE

SER
LEU
ASP
ASP
LEU
MET
ALA
ASN
ASP
THR
VAL
THR
ASP
LEU
PRO
ASP
ARG
GLU
ALA
GLU
ALA
LEU
ARG
THR
GLY
ASN
LEU
GLY
PHE
ASN
TRP
ASP
SER
ASP

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	136867	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.731	Depositor
Minimum map value	-0.336	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.11	Depositor
Map size (Å)	342.0, 342.0, 342.0	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.95, 0.95, 0.95	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.08	0/10324	0.23	0/14022

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10149	0	9633	98	0
2	A	2	0	0	0	0
3	A	1	0	0	0	0
All	All	10152	0	9633	98	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 5.

The worst 5 of 98 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:2323:ASN:HD21	1:A:3089:LYS:HE3	1.54	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1534:SER:HA	1:A:2570:SER:HB2	1.75	0.68
1:A:1502:VAL:HA	1:A:1506:LEU:HB2	1.78	0.64
1:A:2657:LEU:HD22	1:A:2666:LEU:HB2	1.81	0.62
1:A:1792:MET:HA	1:A:1792:MET:HE3	1.81	0.62

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	1332/3989 (33%)	1296 (97%)	36 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1031/3633 (28%)	1030 (100%)	1 (0%)	88	97

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1393	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2639	GLN
1	A	3186	GLN
1	A	1606	GLN
1	A	1613	ASN
1	A	1618	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

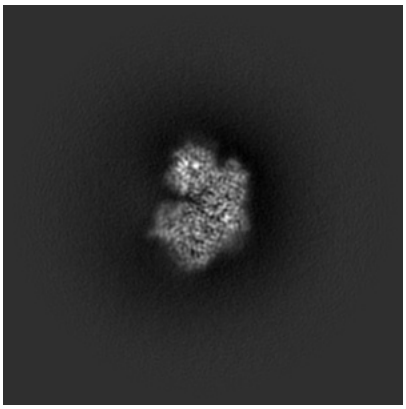
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-80447. These allow visual inspection of the internal detail of the map and identification of artifacts.

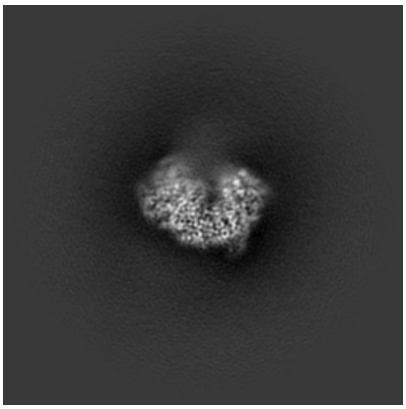
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

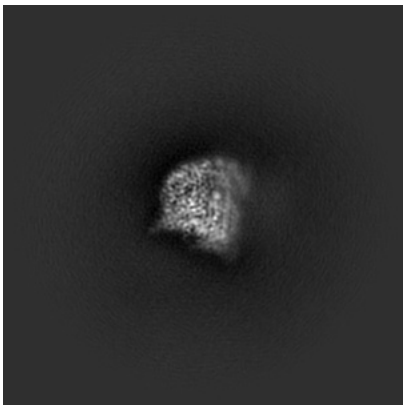
6.1.1 Primary map



X

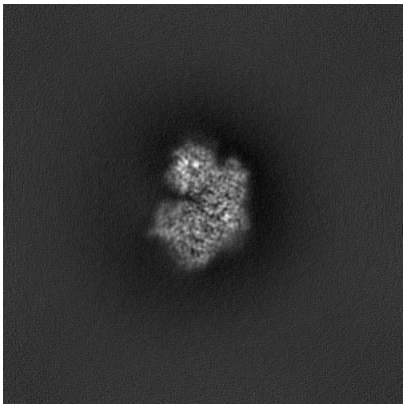


Y

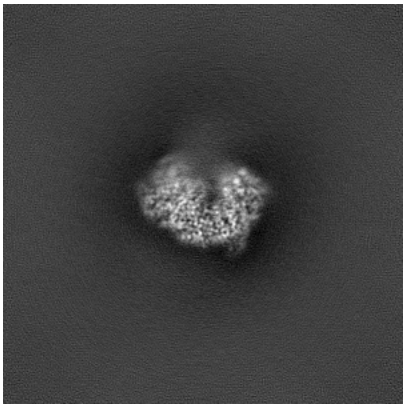


Z

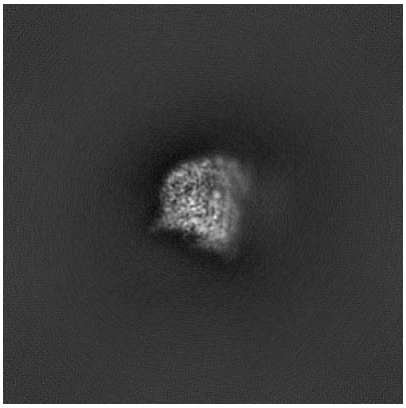
6.1.2 Raw map



X



Y

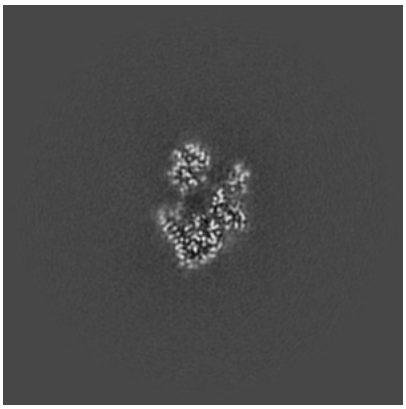


Z

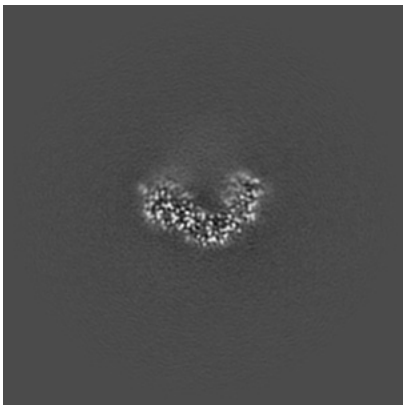
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

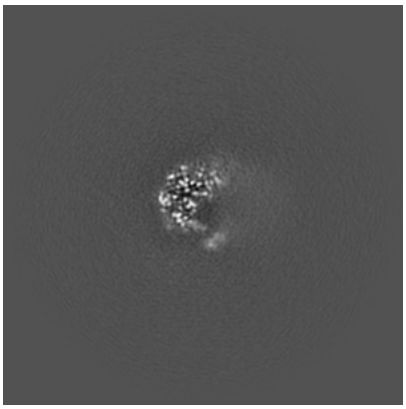
6.2.1 Primary map



X Index: 180

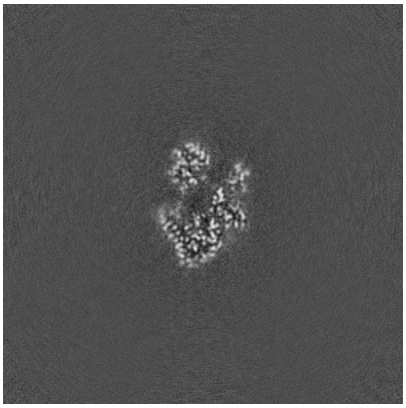


Y Index: 180

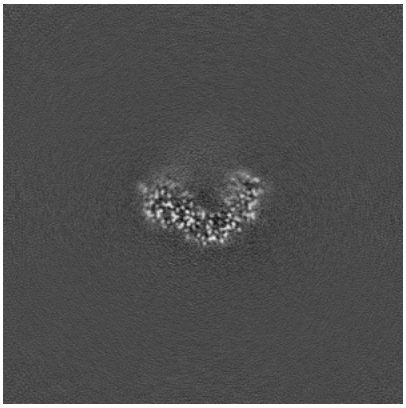


Z Index: 180

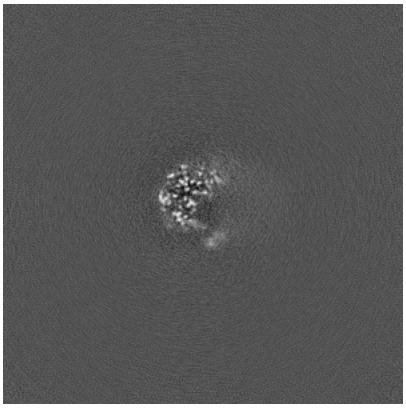
6.2.2 Raw map



X Index: 180



Y Index: 180

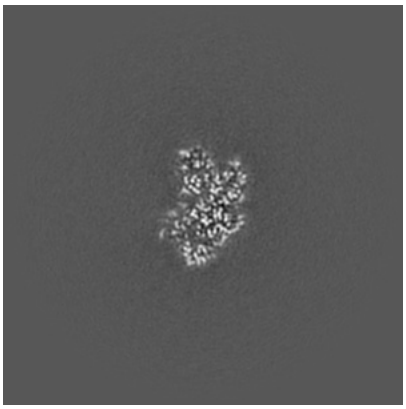


Z Index: 180

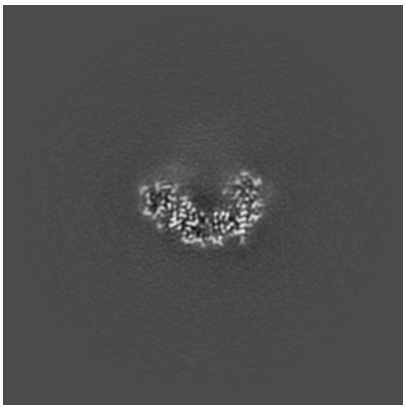
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

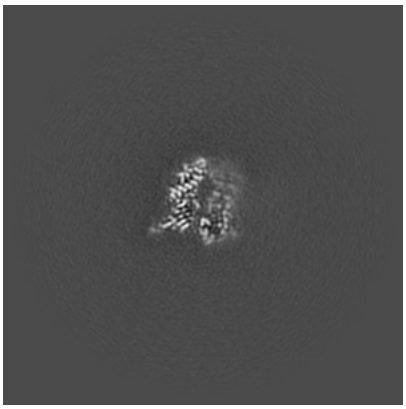
6.3.1 Primary map



X Index: 172

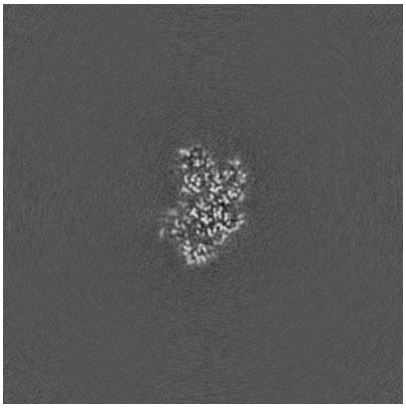


Y Index: 175

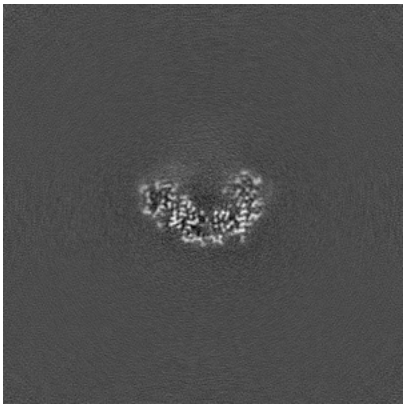


Z Index: 207

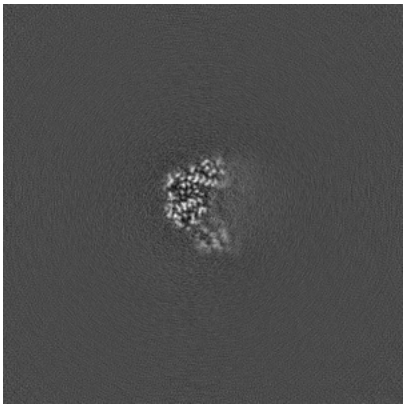
6.3.2 Raw map



X Index: 172



Y Index: 175

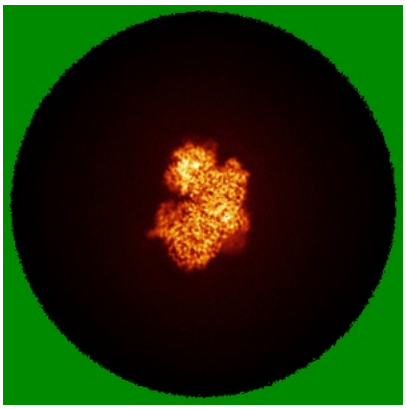


Z Index: 167

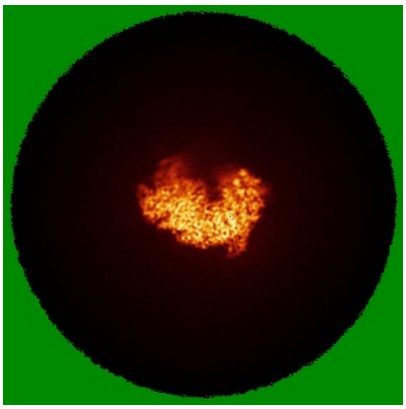
The images above show the largest variance slices of the map in three orthogonal directions.

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

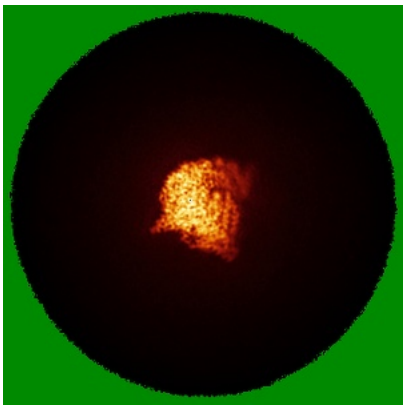
6.4.1 Primary map



X

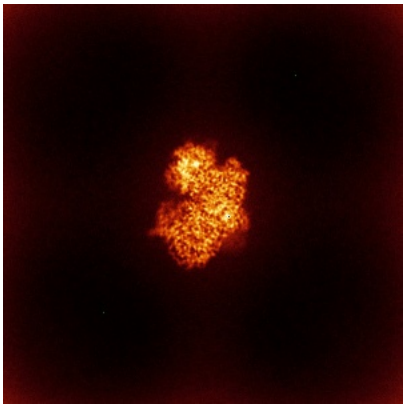


Y

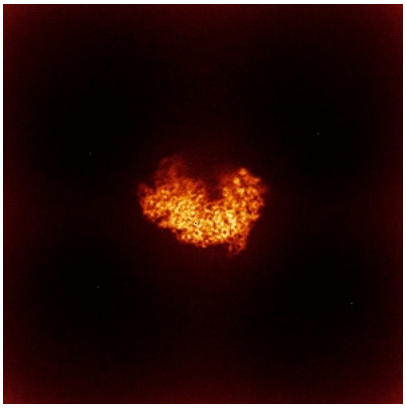


Z

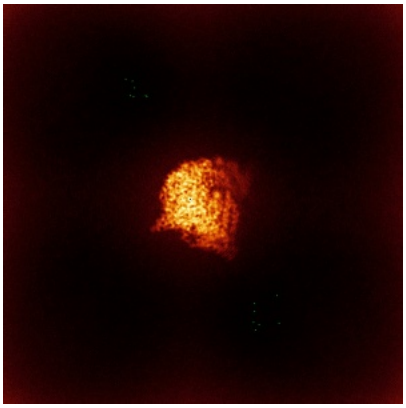
6.4.2 Raw map



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

6.5.2 Raw map



X Y Z

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

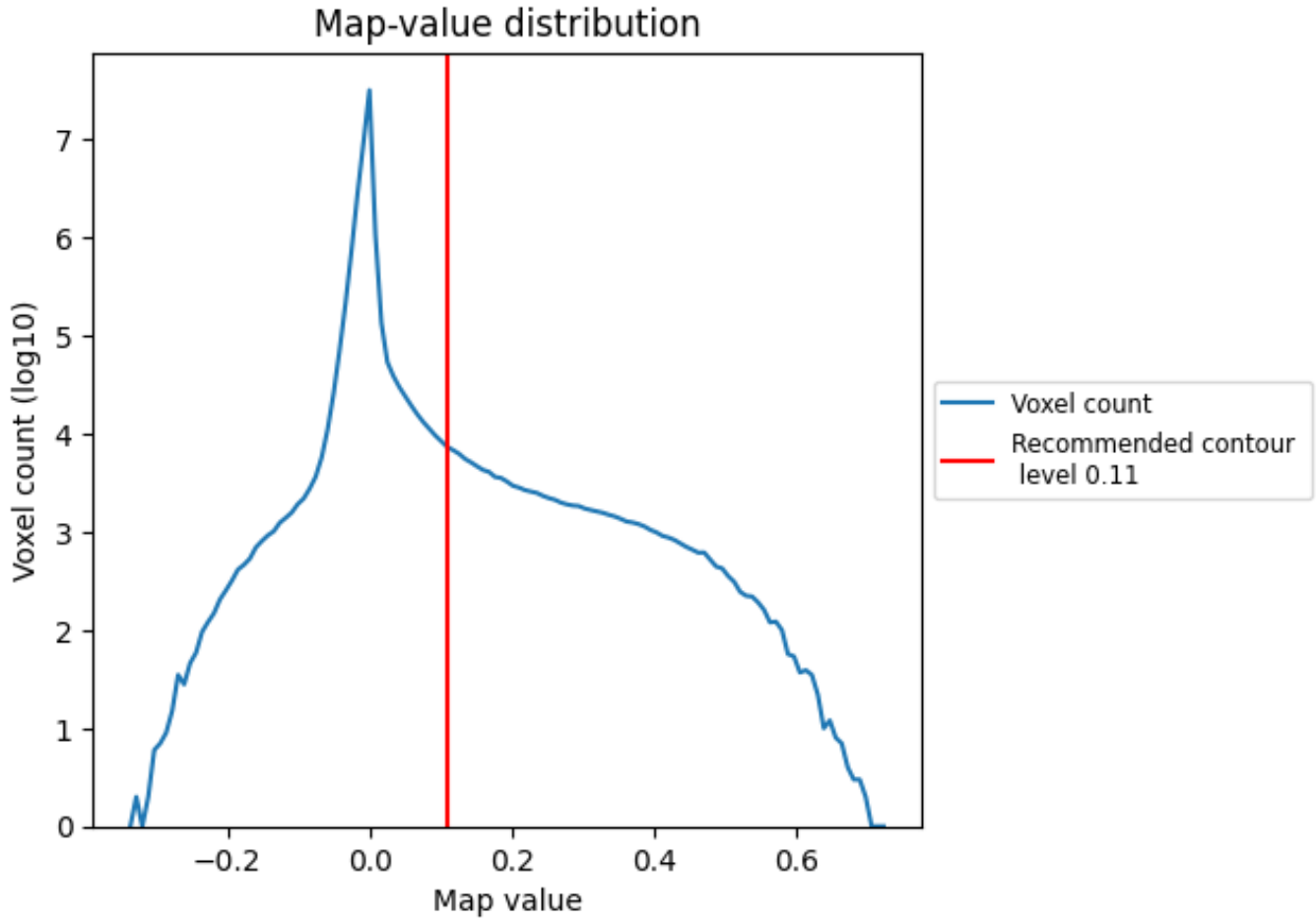
6.6 Mask visualisation (i)

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

7 Map analysis

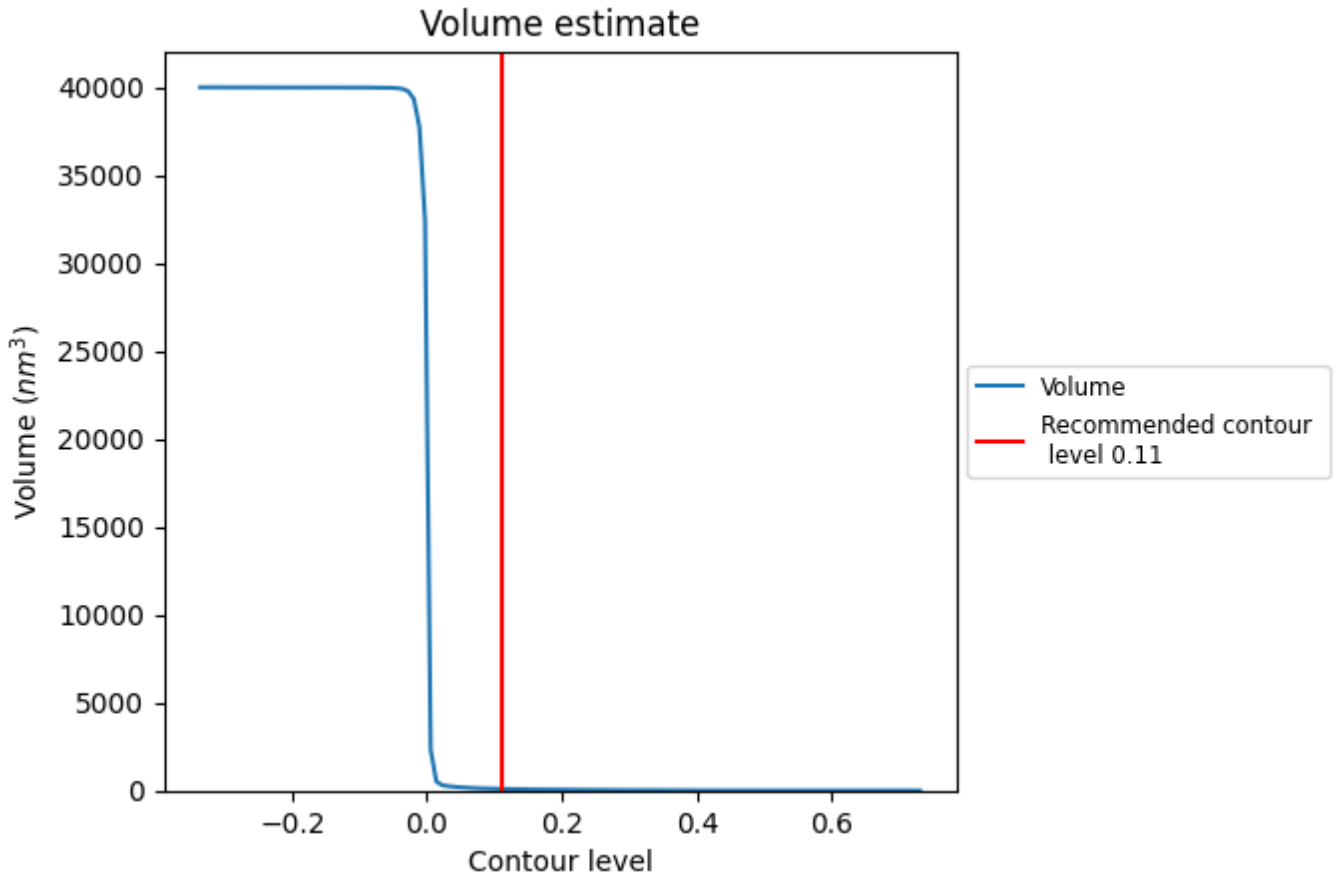
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

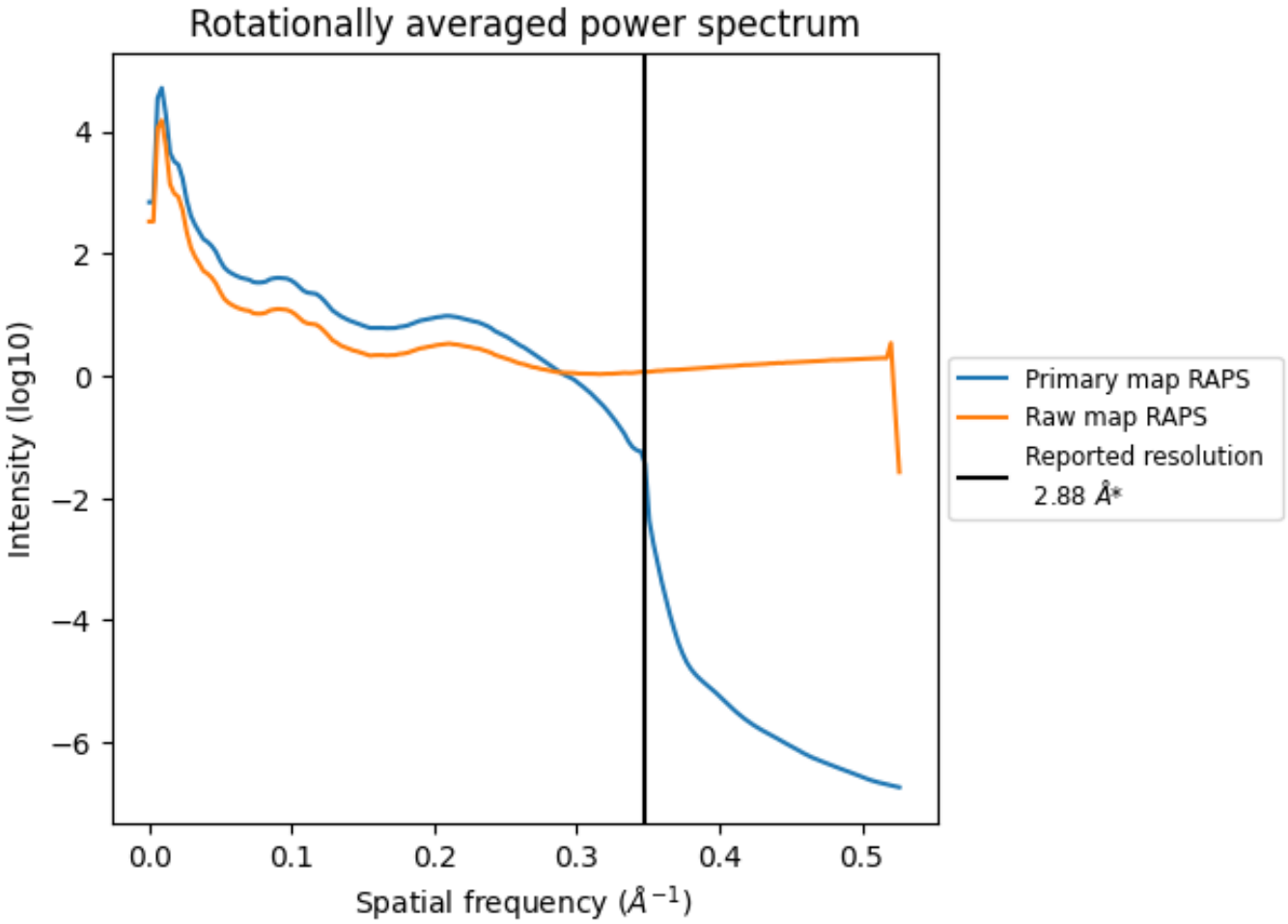
7.2 Volume estimate (i)



The volume at the recommended contour level is 94 nm^3; this corresponds to an approximate mass of 85 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)

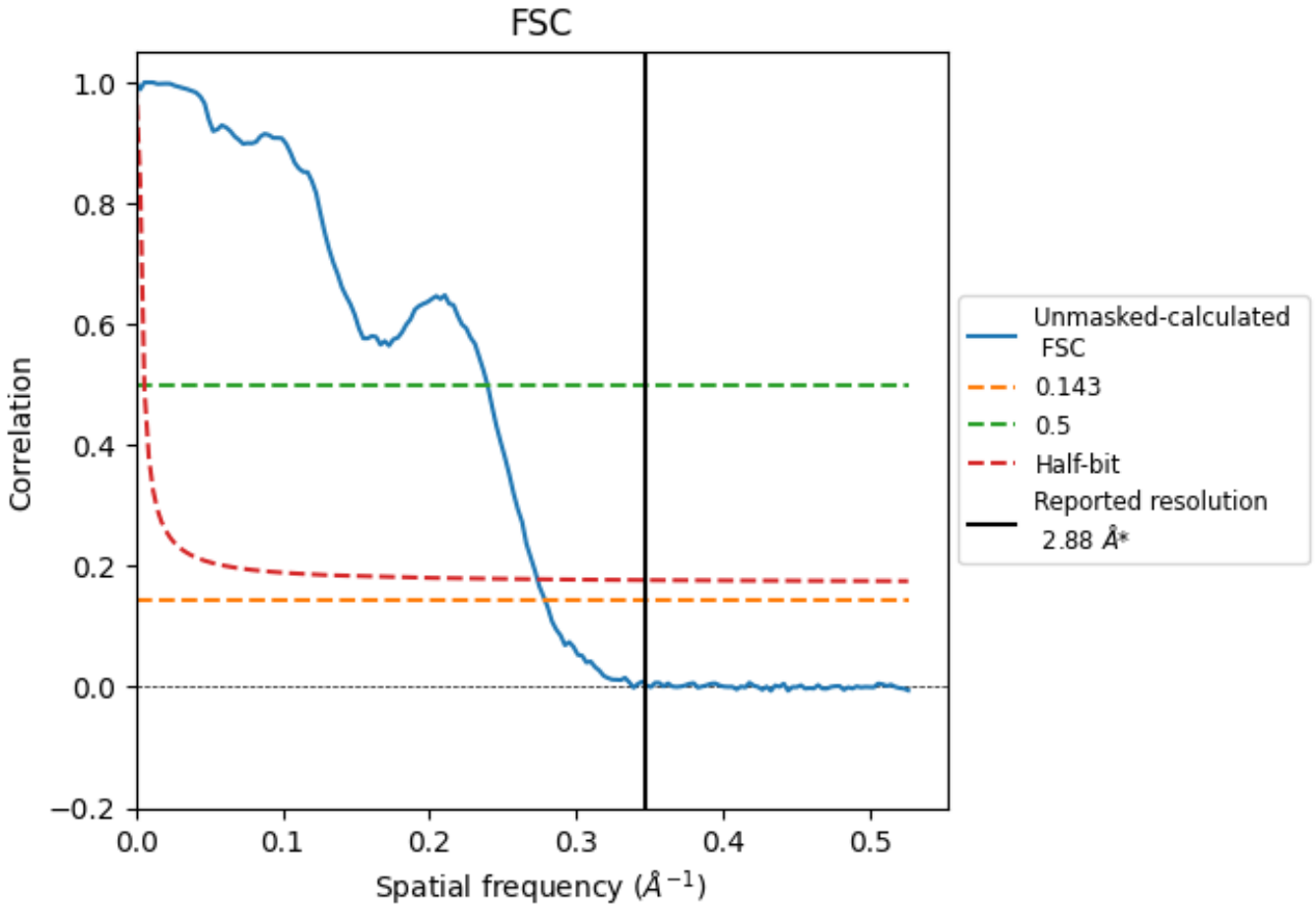


*Reported resolution corresponds to spatial frequency of 0.347 Å^{-1}

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 0.347 Å^{-1}

8.2 Resolution estimates (i)

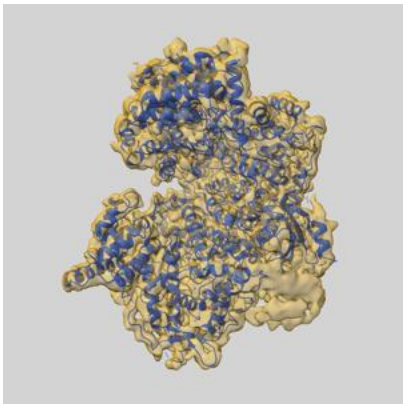
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.88	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.59	4.18	3.66

*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 3.59 differs from the reported value 2.88 by more than 10 %

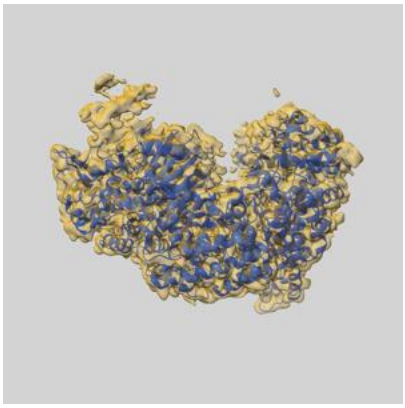
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-80447 and PDB model 25XL. Per-residue inclusion information can be found in section 3 on page 5.

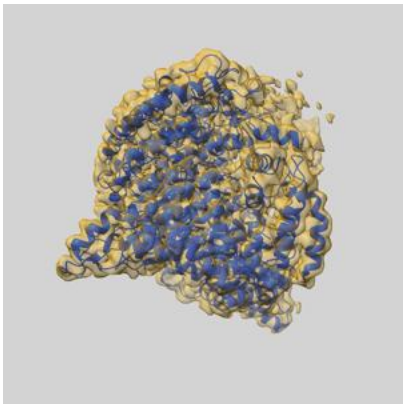
9.1 Map-model overlay



X



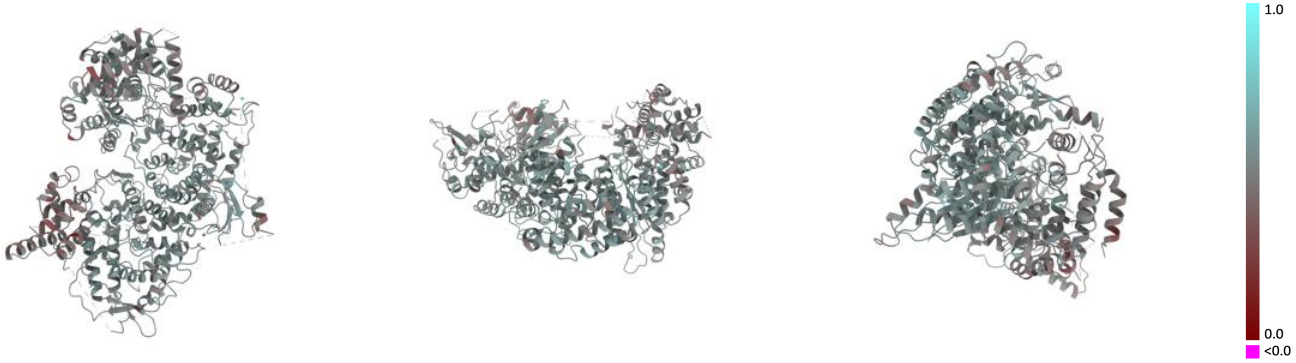
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.11 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.

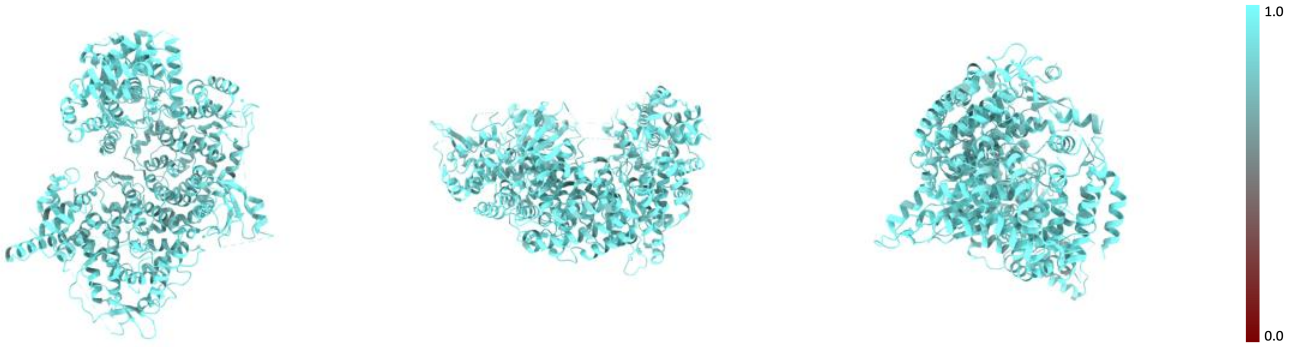
9.2 Q-score mapped to coordinate model



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.

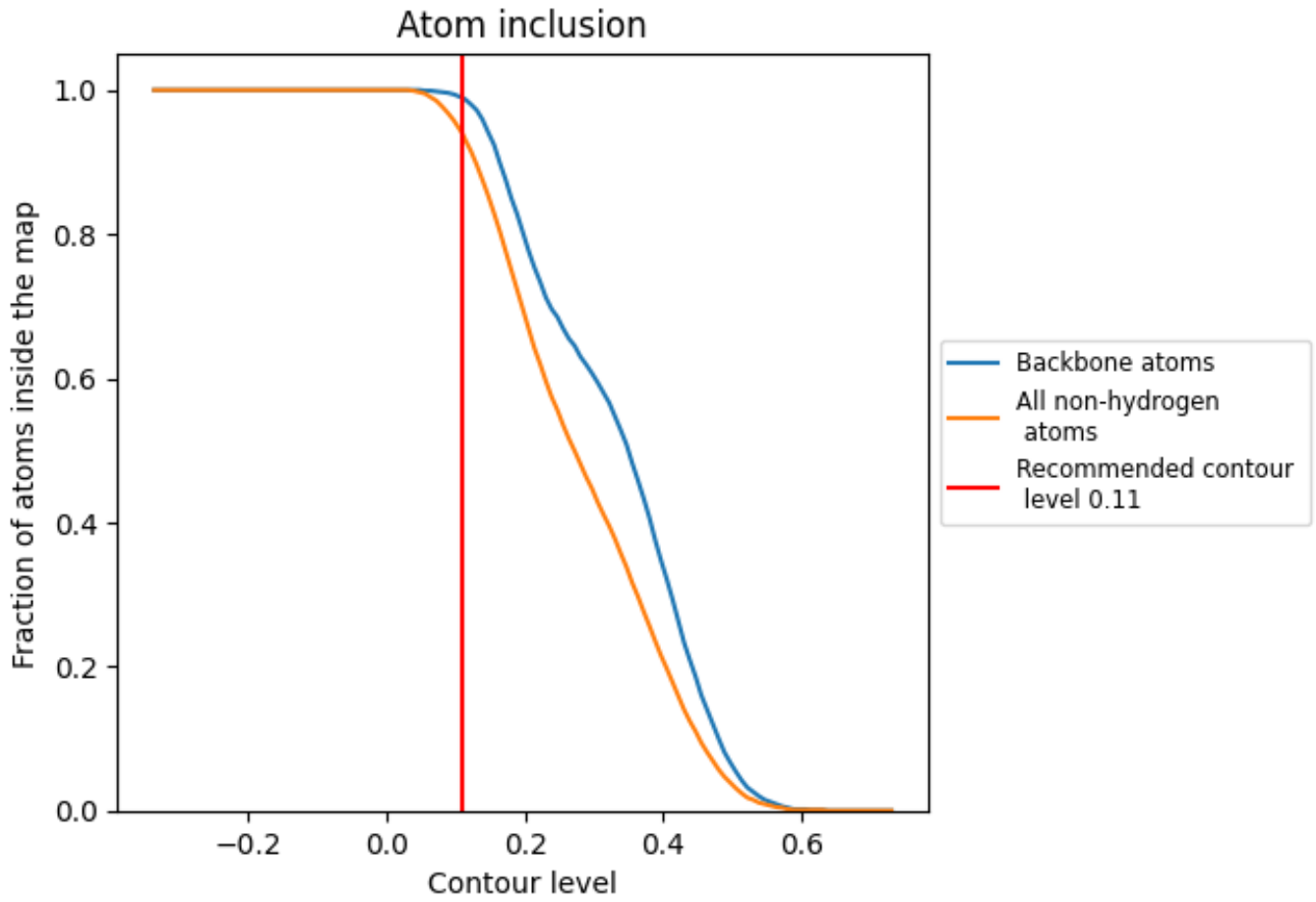
9.3 Atom inclusion mapped to coordinate model



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 (0.11).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 94% 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 (0.11) and Q-score for the entire model and for each chain.



Chain	Atom inclusion	Q-score
All	0.9390	0.5220
A	0.9390	0.5220