Full wwPDB EM Validation Report ⓘ

Oct 27, 2026 – 06:09 PM EDT

PDB ID	:	36PU / pdb_000036pu
EMDB ID	:	EMD-77747
Title	:	Cryo-EM Structure of RSV Polymerase (L:P) Bound to Tr3-mimic RNA (TrC12-4U-Tr3), Unreacted Tr3-mimic Form B
Authors	:	Cao, D.; Liang, B.
Deposited on	:	2026-06-25
Resolution	:	3.48 Å(reported)
Based on initial model	:	9PFR

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

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

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

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

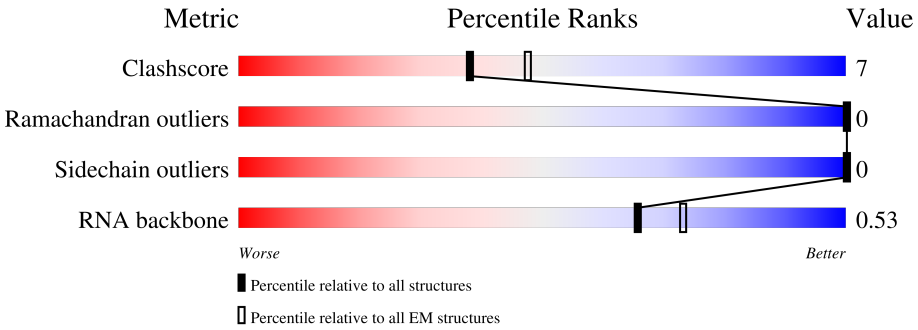
EMDB validation analysis	:	0.0.1.dev133
MolProbity	:	4-5-2 with Phenix2.2
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh &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

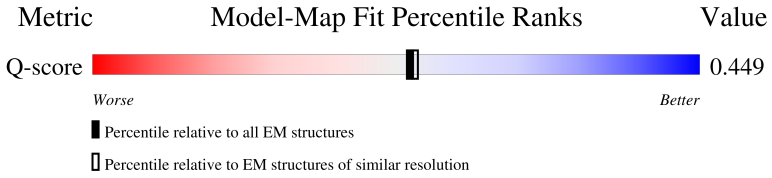
1 Overall quality at a glance

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

The reported resolution of this entry is 3.48 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	13672 (2.98 - 3.98)

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	B	241	22% 76%
1	C	241	18% 78%
1	D	241	20% 76%

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Mol	Chain	Length	Quality of chain
1	E	241	37% 8% 55%
2	P	3	100%
3	T	12	58% 25% 17%
4	A	2165	51% 13% 36%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13686 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 Phosphoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	58	Total	C	N	O	S	0	0
			444	273	81	86	4		
1	C	54	Total	C	N	O	S	0	0
			414	254	77	80	3		
1	D	58	Total	C	N	O	S	0	0
			456	279	86	87	4		
1	E	108	Total	C	N	O	S	0	0
			839	508	149	176	6		

- Molecule 2 is a RNA chain called RNA (5'-R(P*AP*CP*G)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	3	Total	C	N	O	P	0	0
			65	29	13	20	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	T	10	Total	C	N	O	P	0	0
			203	91	25	77	10		

- Molecule 4 is a protein called RNA-directed RNA polymerase L.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	1381	Total	C	N	O	S	0	0
			11265	7261	1886	2061	57		

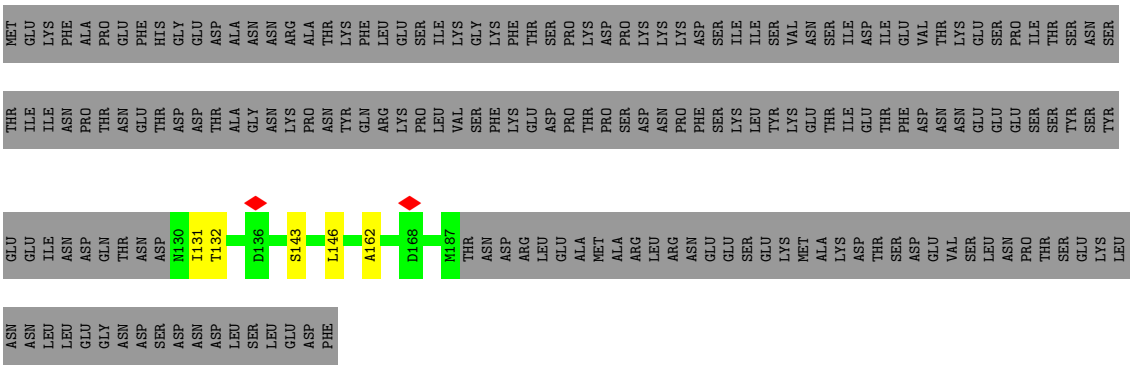
3 Residue-property plots (i)

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: Phosphoprotein

Chain B:

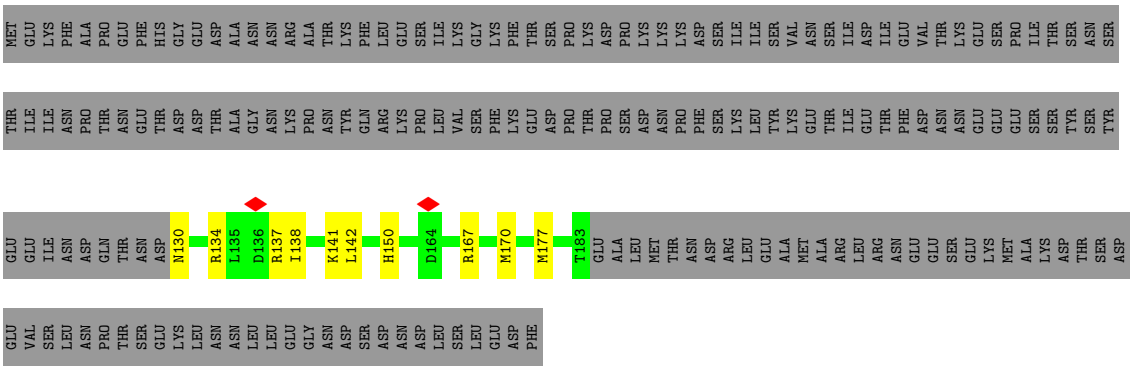




• Molecule 1: Phosphoprotein

Chain C:



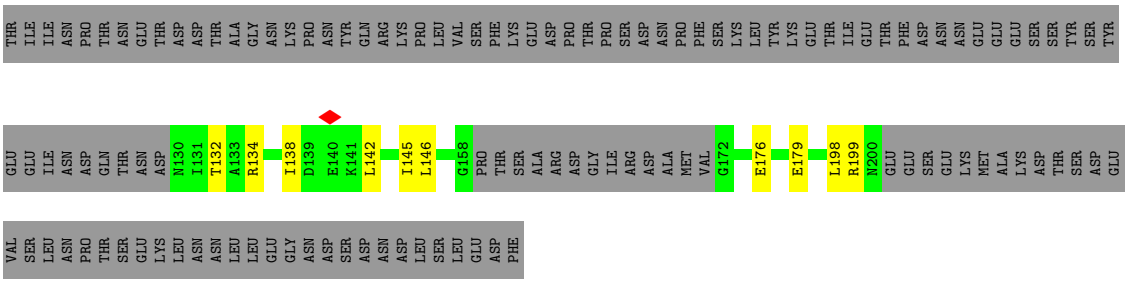


• Molecule 1: Phosphoprotein

Chain D:



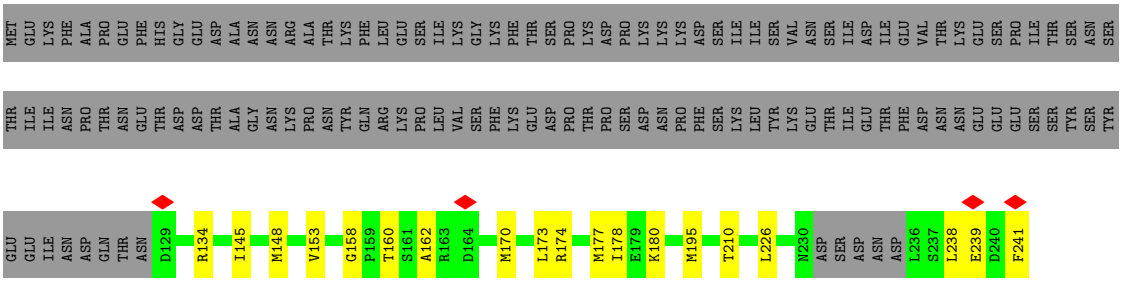




• Molecule 1: Phosphoprotein

Chain E:





• Molecule 2: RNA (5'-R(P*AP*CP*G)-3')

Chain P:

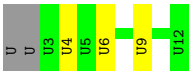


There are no outlier residues recorded for this chain.

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

Chain T:

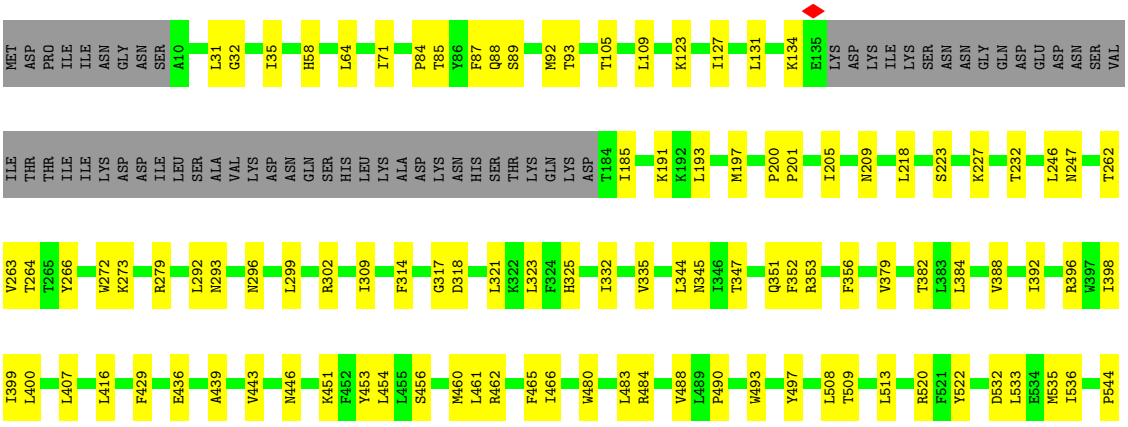


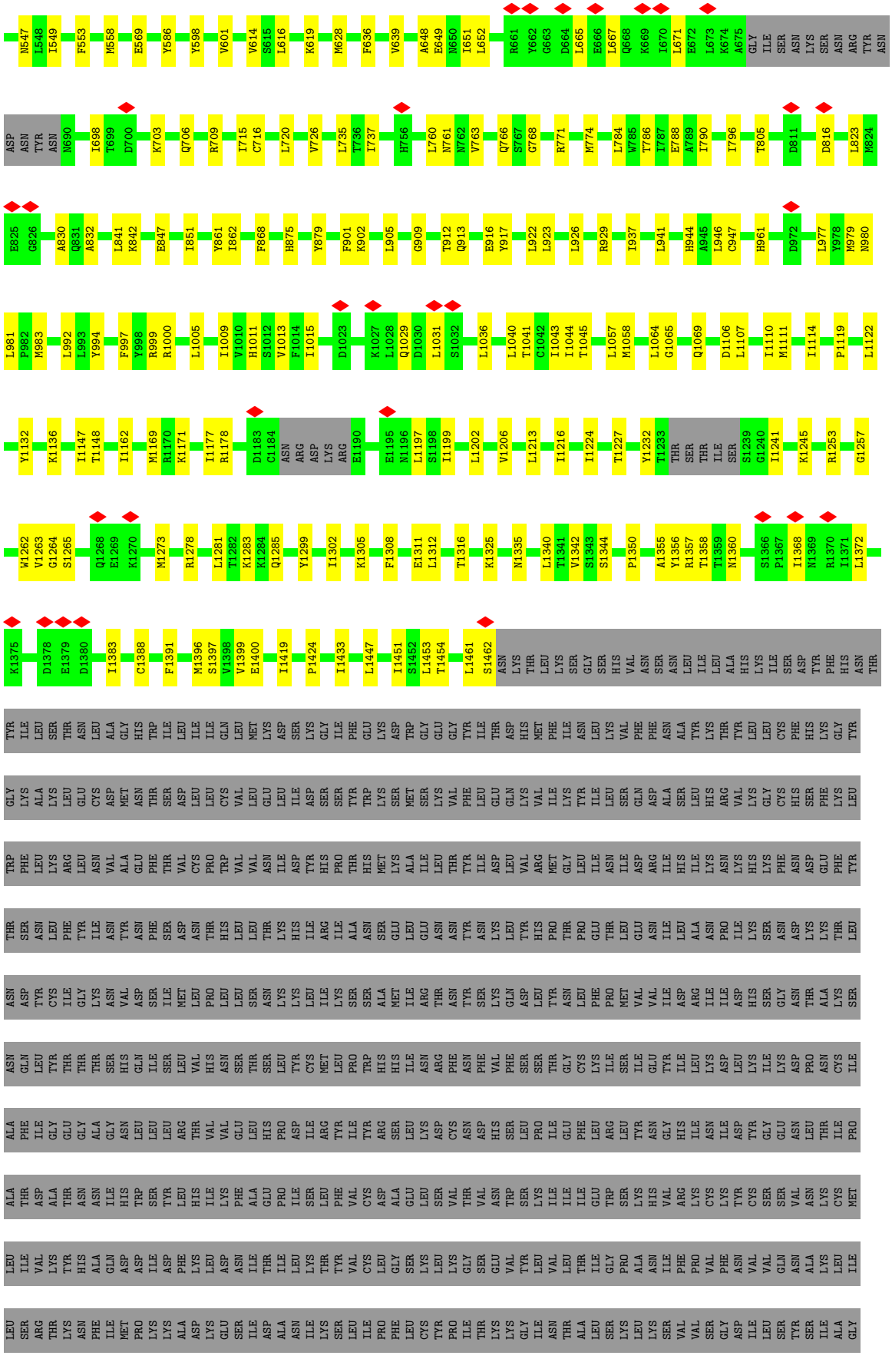


• Molecule 4: RNA-directed RNA polymerase L

Chain A:






N547 L548 I549 F553 M558 E569 Y586 Y598 V601 V614 S615 L616 K619 M628 F636 V639 A648 E649 N650 I651 L652 R661 Y662 G663 D664 L665 E666 L667 Q668 K669 I670 L671 E672 L673 K674 A675 GLY ILE SER ASN LYS SER ASN ARG TYR ASN
ASP ASN TYR ASN N690 I698 T699 D700 K703 Q706 R709 I715 C716 L720 V726 L735 T736 I737 H756 L760 N761 N762 V763 Q766 S767 G768 R771 M774 L784 W785 T786 I787 E788 A789 I790 I796 T805 D811 D816 L823 N824
E825 G826 A830 Q831 A832 L841 K842 E847 I851 Y861 I862 F868 H875 Y879 F901 K902 L905 G909 T912 Q913 E916 Y917 L922 L923 L926 R929 I937 L941 H944 A945 L946 C947 H961 D972 L977 Y978 M979 N980
L981 P982 M983 L992 L993 Y994 F997 Y998 R999 R1000 L1005 I1009 V1010 H1011 S1012 V1013 F1014 I1015 D1023 K1027 L1028 Q1029 D1030 L1031 S1032 L1036 L1040 T1041 C1042 I1043 I1044 T1045 L1057 M1058 L1064 G1065 Q1069 D1106 L1107 I1110 M1111 I1114 P1119 L1122
Y1132 K1136 I1147 T1148 I1162 M1169 R1170 K1171 I1177 R1178 D1183 C1184 ASN ARG ASP LYS ARG E1190 E1195 N1196 L1197 S1198 I1199 L1202 V1206 L1213 I1216 I1224 T1227 Y1232 T1233 THR SER THR ILE SER S1239 G1240 I1241 K1245 R1253 G1257
W1262 V1263 G1264 S1265 Q1268 E1269 K1270 M1273 R1278 L1281 T1282 K1283 K1284 Q1285 Y1299 I1302 K1305 F1308 E1311 L1312 T1316 K1325 N1335 L1340 T1341 V1342 S1343 S1344 P1350 A1355 Y1356 R1357 T1358 T1359 N1360 S1366 P1367 I1368 N1369 R1370 I1371 L1372
K1375 D1378 E1379 D1380 I1383 C1388 F1391 M1396 S1397 V1398 V1399 E1400 I1419 P1424 I1433 L1447 I1451 S1452 L1453 T1454 L1461 S1462 ASN LYS THR LEU LYS SER GLY SER HIS VAL ASN SER ASN LEU ILE LEU ALA HIS LYS ILE SER ASP TYR PHE HIS ASN THR
TYR ILE LEU SER THR ASN LEU ALA GLY HIS TRP ILE LEU ILE ILE GLN LEU MET LYS ASP SER LYS GLY ILE PHE GLU LYS ASP TRP GLY GLU GLY TYR ILE THR ASP HIS MET PHE ILE ASN LEU LYS VAL PHE PHE ASN ALA TYR LYS THR TYR LEU LEU CYS PHE HIS LYS GLY TYR
GLY LYS ALA LYS LEU GLU CYS ASP MET ASN THR SER ASP LEU LEU CYS VAL LEU GLU LEU ILE ASP SER TYR TRP LYS SER MET SER LYS VAL PHE LEU GLU GLN LYS VAL ILE LYS TYR ILE LEU SER GLN ASP ALA SER LEU HIS ARG VAL LYS LYS GLY CYS HIS SER PHE LYS LEU
TRP PHE LEU LYS ARG LEU ASN VAL ALA GLU PHE THR VAL CYS PRO TRP VAL VAL ASN ILE ASP TYR HIS PRO THR HIS MET LYS ALA ILE LEU THR TYR ILE ASP LEU VAL ARG MET GLY LEU ILE ASN ILE ASP ARG ILE HIS ILE LYS ASN LYS HIS LYS PHE ASN ASP GLU PHE TYR
THR SER ASN LEU PHE TYR ILE ASN TYR ASN PHE SER ASP ASN THR HIS LEU LEU THR LYS HIS ILE ARG ILE ALA ASN SER GLU LEU GLU GLU ASN GLY ASN ASN TYR ASN LYS LEU TYR HIS PRO THR PRO GLU THR LEU GLU ASN ILE LEU ALA ASN PRO ILE LYS SER ASN ASP LYS LYS THR LEU
ASN ASP TYR CYS ILE GLY LYS ASN VAL ASP SER ILE MET LEU PRO LEU LEU SER ASN LYS LYS LEU ILE LYS SER SER ALA MET LEU VAL ASN ARG THR ILE LYS GLN ASP LEU TYR ASN LEU PHE PRO MET VAL VAL ILE ASP ARG ILE LYS ILE ASP HIS SER GLY ASN THR ALA LYS SER
ASN GLN LEU TYR THR SER HIS GLN ILE SER LEU VAL HIS ASN SER THR SER LEU TYR CYS MET LEU PRO TRP HIS HIS ILE ASN ARG PHE ASN PHE VAL PHE VAL SER SER LEU ILE GLU TYR ILE LEU LYS ASP LEU LYS ILE LYS ASP PRO ASN CYS ILE
ALA PHE ILE GLY GLU GLY LEU LEU LEU ARG THR VAL VAL GLU LEU HIS PRO ASP ILE ARG TYR ILE TYR ARG SER LEU LYS ASP CYS ASN ASP HIS SER LEU PRO ILE GLU PHE LEU ARG LEU TYR ASN GLY HIS ILE ASN ASN ILE ASP TYR CYS GLY GLU ASN LEU PRO ILE
ALA THR ASP ALA THR ASN ASN ILE HIS TRP SER TYR LEU HIS ILE LYS PHE ALA GLU PRO ILE SER LEU PHE VAL CYS ASP ALA GLU LEU SER VAL THR VAL ASN TRP SER LYS ILE ILE ILE GLU TRP SER LYS HIS VAL ARG LYS CYS LYS ILE SER VAL ASN LEU TYR CYS SER SER VAL ASN CYS MET
LEU ILE VAL LYS TYR HIS ALA GLN ASP ASP ILE ASP PHE LYS LEU ASP ASN ILE THR ILE LEU LYS THR TYR VAL CYS LEU GLY SER LYS LEU LYS GLY SER GLU VAL TYR LEU VAL LEU THR ILE GLY PRO ALA ASN VAL PHE PRO VAL VAL SER GLN ASN ASN ILE ASP VAL VAL SER ASN ALA LEU ILE
LEU SER ARG THR LYS ASN PHE ILE MET PRO LYS LYS ALA ASP LYS GLU SER ILE ASP ALA ASN ILE LYS SER LEU ILE CYS TYR PRO ILE THR LYS LYS GLY ILE LEU ASN THR ALA LEU SER LYS LEU LYS SER VAL VAL SER GLY ASP ILE LEU SER TYR SER ILE ALA GLY


ARG ASN GLU VAL PHE SER ASN LYS LEU ILE ASN HIS LYS HIS MET ASN ILE LEU LYS TRP PHE ASN HIS VAL LEU ASN PHE ARG SER THR GLU LEU ASN TYR ASN HIS LEU TYR MET VAL GLU SER THR TYR PRO TYR LEU SER GLU LEU LEU ASN SER LEU THR THR ASN GLU LEU LYS

LYS LEU ILE LYS ILE THR GLY SER LEU LEU TYR ASN PHE HIS ASN GLU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	36361	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 ($e^-/Å^2$)	53.52	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.846	Depositor
Minimum map value	-1.257	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.067	Depositor
Recommended contour level	0.187	Depositor
Map size (Å)	220.064, 220.064, 220.064	wwPDB
Map dimensions	208, 208, 208	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.058, 1.058, 1.058	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	B	0.11	0/445	0.28	0/596
1	C	0.13	0/415	0.30	0/556
1	D	0.11	0/455	0.27	0/606
1	E	0.11	0/841	0.29	0/1127
2	P	0.26	0/72	0.67	0/110
3	T	0.18	0/223	0.62	0/343
4	A	0.15	0/11499	0.33	0/15562
All	All	0.15	0/13950	0.33	0/18900

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	B	444	0	466	5	0
1	C	414	0	435	9	0
1	D	456	0	479	9	0
1	E	839	0	842	15	0
2	P	65	0	34	0	0
3	T	203	0	104	1	0
4	A	11265	0	11469	180	0
All	All	13686	0	13829	203	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (203) 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)
4:A:302:ARG:HG2	4:A:1253:ARG:HD3	1.69	0.75
4:A:698:ILE:HG21	4:A:868:PHE:HB3	1.73	0.70
4:A:532:ASP:HB3	4:A:535:MET:HG2	1.73	0.70
4:A:698:ILE:HB	4:A:861:TYR:HB2	1.72	0.69
4:A:796:ILE:HG12	4:A:847:GLU:HG3	1.81	0.62
4:A:446:ASN:HD22	4:A:703:LYS:HD3	1.65	0.61
4:A:649:GLU:HG2	4:A:1283:LYS:HD2	1.82	0.61
4:A:774:MET:HE1	1:E:158:GLY:HA2	1.81	0.61
4:A:232:THR:HG23	4:A:247:ASN:HB2	1.83	0.60
4:A:439:ALA:HB3	4:A:628:MET:HE2	1.84	0.60
4:A:382:THR:HG23	4:A:384:LEU:H	1.65	0.60
4:A:1281:LEU:HD22	4:A:1285:GLN:HG2	1.84	0.60
4:A:484:ARG:HD3	4:A:520:ARG:HB3	1.83	0.60
4:A:1245:LYS:HB2	4:A:1396:MET:HE1	1.84	0.60
4:A:841:LEU:HD11	4:A:862:ILE:HD11	1.84	0.59
4:A:345:ASN:HA	4:A:353:ARG:HB2	1.82	0.59
1:B:162:ALA:HB2	4:A:735:LEU:HD23	1.84	0.59
4:A:1029:GLN:HG3	4:A:1031:LEU:HD22	1.85	0.59
1:C:134:ARG:HD3	1:C:137:ARG:HH12	1.67	0.58
1:E:170:MET:HE1	1:E:180:LYS:HE3	1.86	0.58
4:A:323:LEU:HD22	4:A:400:LEU:HD13	1.86	0.58
4:A:614:VAL:HG21	4:A:737:ILE:HD12	1.85	0.58
4:A:461:LEU:HD23	4:A:715:ILE:HD11	1.85	0.58
1:B:143:SER:HB2	1:C:141:LYS:HZ3	1.69	0.57
4:A:1241:ILE:HG13	4:A:1388:CYS:SG	2.45	0.57
4:A:200:PRO:HB2	4:A:205:ILE:HD11	1.86	0.57
4:A:636:PHE:HA	4:A:639:VAL:HG12	1.87	0.57
4:A:1224:ILE:HG21	4:A:1388:CYS:HA	1.86	0.57
1:E:160:THR:HG22	1:E:162:ALA:H	1.70	0.56
4:A:1311:GLU:HG3	4:A:1433:ILE:HG23	1.88	0.56
4:A:1273:MET:HG3	4:A:1278:ARG:HH22	1.71	0.56
1:D:142:LEU:HD23	1:D:145:ILE:HD12	1.88	0.56
4:A:88:GLN:O	4:A:92:MET:HG2	2.06	0.56
4:A:1342:VAL:HG12	4:A:1344:SER:H	1.70	0.56
1:B:131:ILE:HD12	1:B:131:ILE:H	1.71	0.55
4:A:396:ARG:HD2	4:A:399:ILE:HD13	1.88	0.55
4:A:1213:LEU:HD12	4:A:1216:ILE:HD11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:443:VAL:HG22	4:A:706:GLN:HE22	1.72	0.54
4:A:89:SER:HA	4:A:318:ASP:HB3	1.89	0.54
4:A:1232:TYR:OH	4:A:1399:VAL:HG21	2.07	0.54
4:A:89:SER:O	4:A:93:THR:HG22	2.07	0.54
4:A:351:GLN:HG3	4:A:352:PHE:HD1	1.73	0.54
4:A:902:LYS:HG3	4:A:983:MET:HE3	1.90	0.54
4:A:1005:LEU:HD13	4:A:1064:LEU:HD11	1.88	0.54
4:A:87:PHE:HE2	4:A:262:THR:HG23	1.73	0.54
4:A:1057:LEU:HD12	4:A:1119:PRO:HB3	1.90	0.54
4:A:553:PHE:HB2	4:A:558:MET:HE2	1.89	0.54
4:A:549:ILE:HG21	4:A:760:LEU:HD11	1.90	0.53
4:A:913:GLN:HB3	4:A:917:TYR:CE2	2.43	0.53
4:A:1253:ARG:HB2	4:A:1357:ARG:HH22	1.74	0.53
1:C:170:MET:HA	1:C:170:MET:HE2	1.92	0.52
1:C:138:ILE:O	1:C:142:LEU:HG	2.10	0.52
4:A:1009:ILE:HG21	4:A:1199:ILE:HD11	1.92	0.52
4:A:1368:ILE:O	4:A:1372:LEU:HG	2.10	0.52
4:A:536:ILE:HD12	4:A:586:TYR:HE2	1.74	0.52
4:A:842:LYS:HG2	1:E:210:THR:HG21	1.91	0.52
4:A:1316:THR:HA	4:A:1447:LEU:HD22	1.92	0.52
4:A:201:PRO:O	4:A:205:ILE:HG12	2.10	0.51
4:A:1132:TYR:CZ	4:A:1136:LYS:HD2	2.46	0.51
4:A:1197:LEU:HD11	4:A:1202:LEU:HD12	1.92	0.51
4:A:1224:ILE:HA	4:A:1227:THR:HG22	1.93	0.51
4:A:1257:GLY:HA3	4:A:1360:ASN:HA	1.91	0.51
1:C:130:ASN:O	1:C:134:ARG:HG2	2.11	0.51
4:A:1273:MET:HE2	4:A:1278:ARG:HH12	1.76	0.50
1:D:132:THR:HB	1:E:134:ARG:HH12	1.76	0.50
4:A:443:VAL:HG22	4:A:706:GLN:NE2	2.27	0.50
4:A:490:PRO:HD2	4:A:493:TRP:HB2	1.92	0.50
4:A:905:LEU:HD12	4:A:983:MET:HE1	1.93	0.50
4:A:1011:HIS:O	4:A:1015:ILE:HG12	2.11	0.50
4:A:901:PHE:H	4:A:1169:MET:HE3	1.77	0.50
4:A:1335:ASN:HA	4:A:1424:PRO:HG3	1.93	0.50
4:A:416:LEU:HD21	4:A:875:HIS:NE2	2.27	0.49
4:A:246:LEU:HD11	4:A:266:TYR:HD1	1.77	0.49
1:B:146:LEU:HG	4:A:488:VAL:HG23	1.93	0.49
4:A:716:CYS:HB2	4:A:788:GLU:OE2	2.12	0.49
3:T:9:U:O4	4:A:619:LYS:NZ	2.40	0.49
4:A:784:LEU:O	4:A:788:GLU:HG2	2.13	0.49
4:A:1041:THR:O	4:A:1045:THR:HG22	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:992:LEU:HB2	4:A:994:TYR:HD1	1.78	0.49
4:A:1000:ARG:HG3	4:A:1350:PRO:HD2	1.95	0.49
4:A:484:ARG:HG2	4:A:522:TYR:CD1	2.48	0.49
4:A:127:ILE:O	4:A:131:LEU:HG	2.13	0.49
4:A:456:SER:O	4:A:460:MET:HG3	2.13	0.49
4:A:1005:LEU:HD22	4:A:1064:LEU:HD21	1.94	0.48
4:A:109:LEU:HD23	4:A:205:ILE:HD13	1.95	0.48
4:A:547:ASN:HB3	4:A:569:GLU:HG2	1.95	0.48
4:A:1107:LEU:HA	4:A:1110:ILE:HD12	1.95	0.48
4:A:1340:LEU:HG	4:A:1342:VAL:HG23	1.94	0.48
4:A:601:VAL:HG22	4:A:726:VAL:HG21	1.94	0.48
4:A:292:LEU:HD22	4:A:299:LEU:HD22	1.95	0.47
4:A:912:THR:HG21	4:A:929:ARG:HB2	1.97	0.47
4:A:64:LEU:HD11	4:A:232:THR:HG21	1.95	0.47
4:A:87:PHE:CE2	4:A:262:THR:HG23	2.49	0.47
4:A:398:ILE:HG13	1:E:226:LEU:HD12	1.96	0.47
4:A:760:LEU:HA	4:A:763:VAL:HG12	1.97	0.47
4:A:1454:THR:HA	1:D:199:ARG:HG3	1.96	0.47
1:D:134:ARG:O	1:D:138:ILE:HG12	2.15	0.47
4:A:32:GLY:HA2	4:A:263:VAL:HG21	1.97	0.47
4:A:1065:GLY:H	4:A:1069:GLN:HG2	1.80	0.47
4:A:1355:ALA:HA	4:A:1358:THR:HG22	1.96	0.47
4:A:651:ILE:HD12	4:A:720:LEU:HD22	1.96	0.47
4:A:31:LEU:O	4:A:35:ILE:HG12	2.15	0.46
4:A:937:ILE:HD12	4:A:979:MET:SD	2.56	0.46
4:A:1253:ARG:HB2	4:A:1357:ARG:NH2	2.30	0.46
4:A:1383:ILE:HD12	4:A:1419:ILE:HD11	1.96	0.46
4:A:1397:SER:O	4:A:1400:GLU:HG3	2.15	0.46
4:A:223:SER:O	4:A:227:LYS:HG2	2.15	0.46
4:A:323:LEU:HG	4:A:392:ILE:HD11	1.98	0.46
4:A:946:LEU:HD22	4:A:1162:ILE:HD12	1.97	0.46
4:A:131:LEU:HD13	4:A:1399:VAL:HG22	1.97	0.46
4:A:1040:LEU:HA	4:A:1043:ILE:HG22	1.98	0.46
1:E:148:MET:HE3	1:E:148:MET:HB2	1.88	0.46
1:B:132:THR:HG23	1:C:134:ARG:HH12	1.81	0.45
4:A:88:GLN:HB2	4:A:272:TRP:NE1	2.31	0.45
4:A:85:THR:HG21	4:A:325:HIS:HA	1.97	0.45
4:A:344:LEU:HA	4:A:347:THR:HG22	1.98	0.45
4:A:465:PHE:CG	4:A:716:CYS:HB3	2.52	0.45
4:A:105:THR:HG21	4:A:209:ASN:HB2	1.98	0.45
4:A:805:THR:HG23	4:A:816:ASP:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:123:LYS:HB2	4:A:926:LEU:HD21	1.99	0.45
4:A:1263:VAL:HG13	4:A:1265:SER:H	1.82	0.45
4:A:299:LEU:HD21	4:A:923:LEU:HD23	1.98	0.45
4:A:667:LEU:O	4:A:671:LEU:HG	2.17	0.45
4:A:830:ALA:C	4:A:832:ALA:H	2.25	0.45
4:A:508:LEU:HD12	4:A:509:THR:H	1.81	0.44
4:A:1058:MET:HG2	4:A:1122:LEU:HB3	1.99	0.44
4:A:544:PRO:HG2	4:A:549:ILE:HA	1.98	0.44
4:A:84:PRO:HG3	4:A:264:THR:HG22	2.00	0.44
4:A:944:HIS:HB3	4:A:947:CYS:O	2.18	0.44
4:A:1462:SER:HA	1:D:198:LEU:HD21	1.98	0.44
4:A:454:LEU:HA	1:E:153:VAL:HG23	2.00	0.44
4:A:35:ILE:HG22	4:A:71:ILE:HD11	1.99	0.44
4:A:616:LEU:HD13	4:A:628:MET:HG3	2.00	0.44
1:C:150:HIS:CD2	1:D:176:GLU:HG2	2.53	0.44
4:A:400:LEU:HD12	1:E:241:PHE:CG	2.52	0.44
4:A:218:LEU:HD22	4:A:273:LYS:HE2	2.00	0.44
4:A:344:LEU:HD12	4:A:356:PHE:CD2	2.53	0.44
4:A:648:ALA:HA	4:A:652:LEU:HD12	2.01	0.43
4:A:879:TYR:HB3	4:A:1356:TYR:CD1	2.53	0.43
1:E:153:VAL:HG13	1:E:177:MET:HG3	1.99	0.43
4:A:309:ILE:HG23	4:A:407:LEU:HD11	2.00	0.43
4:A:453:TYR:HE1	4:A:851:ILE:O	2.02	0.43
4:A:761:ASN:C	4:A:771:ARG:HH21	2.27	0.43
4:A:134:LYS:HE2	4:A:134:LYS:HB2	1.84	0.43
1:D:146:LEU:HD22	1:E:145:ILE:HD11	1.99	0.43
1:E:174:ARG:O	1:E:178:ILE:HG12	2.19	0.43
4:A:88:GLN:HB2	4:A:272:TRP:HE1	1.83	0.43
4:A:786:THR:O	4:A:790:ILE:HG12	2.19	0.43
4:A:1147:ILE:HG22	4:A:1148:THR:H	1.84	0.43
1:E:173:LEU:O	1:E:177:MET:HG2	2.18	0.43
4:A:436:GLU:HA	4:A:628:MET:HE1	2.00	0.43
4:A:462:ARG:O	4:A:466:ILE:HG12	2.19	0.43
4:A:766:GLN:HG2	4:A:768:GLY:H	1.84	0.43
4:A:1111:MET:HE3	4:A:1114:ILE:HG13	2.00	0.43
4:A:1171:LYS:HE2	4:A:1178:ARG:HH12	1.84	0.43
4:A:483:LEU:H	4:A:483:LEU:HD23	1.84	0.43
4:A:823:LEU:HD23	4:A:823:LEU:HA	1.90	0.43
4:A:1013:VAL:HG22	4:A:1036:LEU:HD11	2.01	0.42
4:A:193:LEU:HG	4:A:197:MET:CE	2.49	0.42
4:A:480:TRP:CE2	4:A:497:TYR:HA	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1299:TYR:HB3	4:A:1302:ILE:HG13	2.01	0.42
4:A:332:ILE:O	4:A:335:VAL:HG12	2.19	0.42
4:A:484:ARG:HG2	4:A:522:TYR:CE1	2.53	0.42
4:A:1325:LYS:HE3	4:A:1325:LYS:HB3	1.87	0.42
1:C:167:ARG:HG3	1:C:167:ARG:HH11	1.83	0.42
4:A:317:GLY:HA3	4:A:429:PHE:CE1	2.55	0.42
4:A:1111:MET:HE1	4:A:1299:TYR:CZ	2.54	0.42
4:A:31:LEU:HD12	4:A:58:HIS:CD2	2.55	0.42
4:A:317:GLY:O	4:A:321:LEU:HD23	2.19	0.42
4:A:1302:ILE:HB	4:A:1305:LYS:HB2	2.01	0.42
4:A:598:TYR:HA	4:A:601:VAL:HG12	2.02	0.42
4:A:1106:ASP:O	4:A:1110:ILE:HG13	2.19	0.42
4:A:508:LEU:HD21	4:A:513:LEU:HD13	2.02	0.42
4:A:909:GLY:O	4:A:913:GLN:HG2	2.20	0.42
1:C:177:MET:HE2	1:C:177:MET:HA	2.02	0.41
4:A:916:GLU:OE1	4:A:922:LEU:HA	2.20	0.41
4:A:665:LEU:HD13	4:A:999:ARG:NH2	2.35	0.41
4:A:944:HIS:HE2	4:A:1169:MET:HE1	1.86	0.41
4:A:1041:THR:HA	4:A:1044:ILE:HG22	2.02	0.41
4:A:1461:LEU:HD23	4:A:1461:LEU:HA	1.90	0.41
1:E:238:LEU:O	1:E:239:GLU:HG2	2.20	0.41
4:A:85:THR:OG1	4:A:321:LEU:HB3	2.21	0.41
4:A:185:ILE:HG22	4:A:191:LYS:HG3	2.02	0.41
4:A:293:ASN:HA	4:A:296:ASN:O	2.20	0.41
4:A:379:VAL:HG21	4:A:388:VAL:HG21	2.03	0.41
4:A:997:PHE:HB3	4:A:1391:PHE:HD1	1.85	0.41
4:A:1453:LEU:HD23	1:D:199:ARG:HD3	2.02	0.41
4:A:533:LEU:HD13	4:A:536:ILE:HD11	2.03	0.41
4:A:941:LEU:HD23	4:A:941:LEU:HA	1.91	0.41
1:E:178:ILE:HG23	1:E:195:MET:SD	2.60	0.41
4:A:321:LEU:HD21	4:A:332:ILE:HG13	2.03	0.41
4:A:1308:PHE:CZ	4:A:1312:LEU:HD11	2.56	0.41
4:A:901:PHE:CE2	4:A:905:LEU:HD11	2.55	0.41
4:A:1202:LEU:O	4:A:1206:VAL:HG23	2.21	0.41
4:A:1262:TRP:CZ2	4:A:1264:GLY:HA2	2.56	0.40
4:A:977:LEU:O	4:A:981:LEU:HG	2.20	0.40
1:D:176:GLU:O	1:D:179:GLU:HG3	2.21	0.40
4:A:279:ARG:HG2	4:A:314:PHE:CD2	2.56	0.40
4:A:1285:GLN:NE2	4:A:1451:ILE:HG13	2.37	0.40
4:A:451:LYS:HE2	4:A:709:ARG:NH2	2.36	0.40
4:A:532:ASP:O	4:A:536:ILE:HG12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:961:HIS:NE2	4:A:1177:ILE:HA	2.35	0.40
4:A:980:ASN:O	4:A:1015:ILE:HG13	2.22	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	B	56/241 (23%)	55 (98%)	1 (2%)	0	100	100
1	C	52/241 (22%)	52 (100%)	0	0	100	100
1	D	54/241 (22%)	54 (100%)	0	0	100	100
1	E	104/241 (43%)	102 (98%)	2 (2%)	0	100	100
4	A	1371/2165 (63%)	1323 (96%)	48 (4%)	0	100	100
All	All	1637/3129 (52%)	1586 (97%)	51 (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	B	48/220 (22%)	48 (100%)	0	100	100
1	C	45/220 (20%)	45 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	49/220 (22%)	49 (100%)	0	100	100
1	E	94/220 (43%)	94 (100%)	0	100	100
4	A	1281/2012 (64%)	1281 (100%)	0	100	100
All	All	1517/2892 (52%)	1517 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	224	ASN
4	A	290	ASN
4	A	604	GLN
4	A	706	GLN
4	A	766	GLN
4	A	827	GLN
4	A	930	ASN
4	A	1438	GLN
1	D	189	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	P	2/3 (66%)	0	0
3	T	9/12 (75%)	2 (22%)	0
All	All	11/15 (73%)	2 (18%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	T	4	U
3	T	6	U

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.

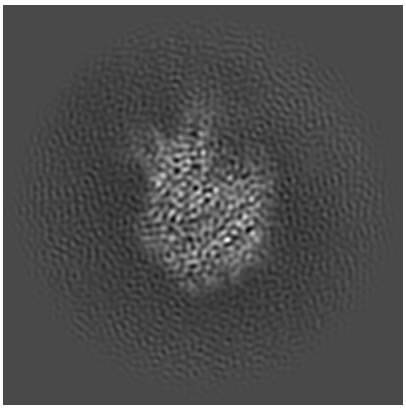
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-77747. These allow visual inspection of the internal detail of the map and identification of artifacts.

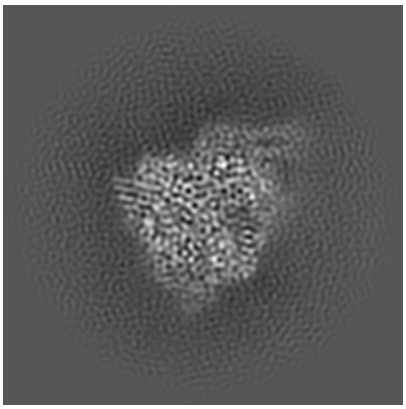
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

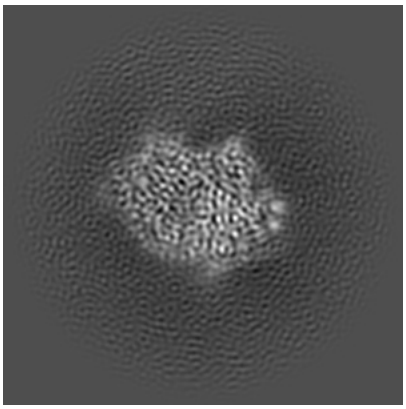
6.1.1 Primary map



X

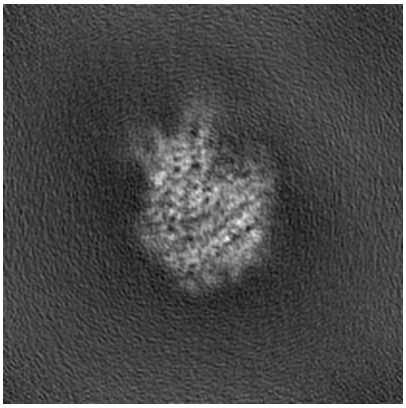


Y

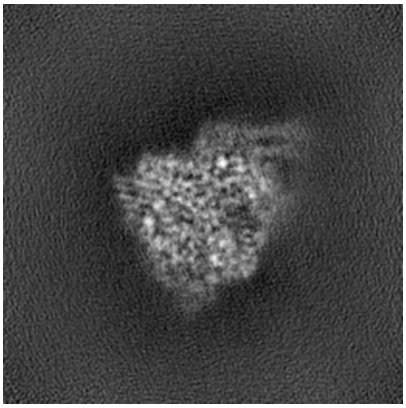


Z

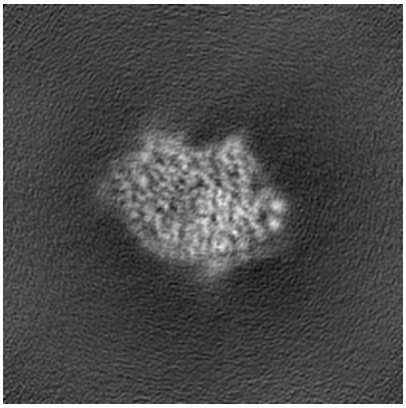
6.1.2 Raw map



X



Y

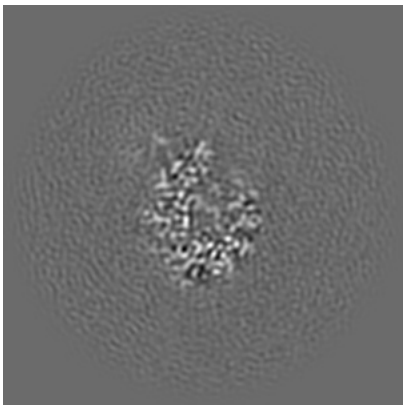


Z

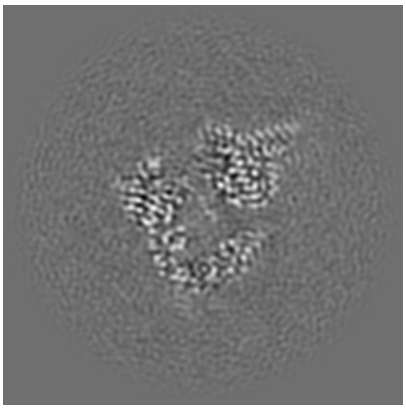
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

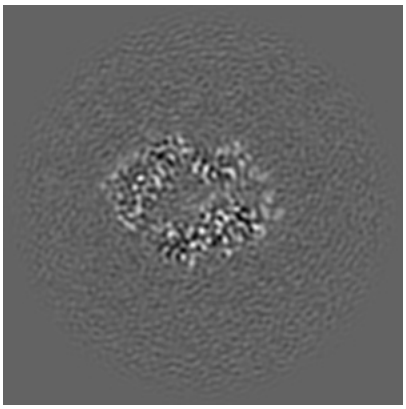
6.2.1 Primary map



X Index: 104

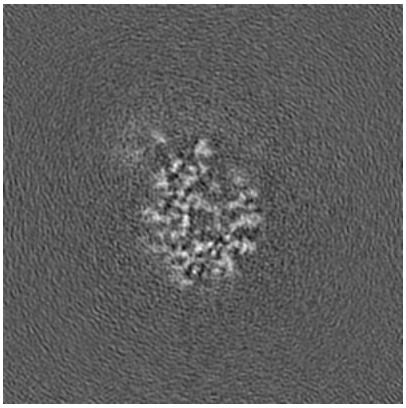


Y Index: 104

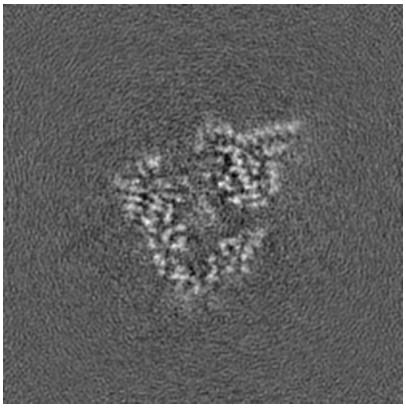


Z Index: 104

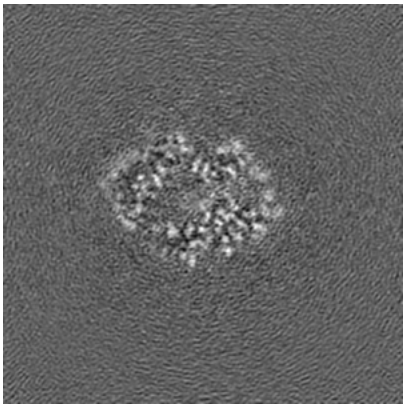
6.2.2 Raw map



X Index: 104



Y Index: 104

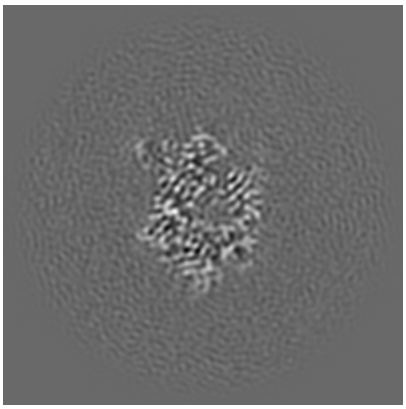


Z Index: 104

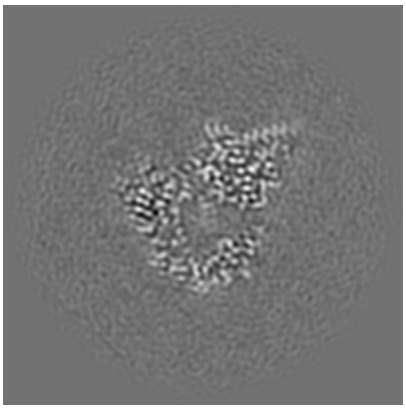
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

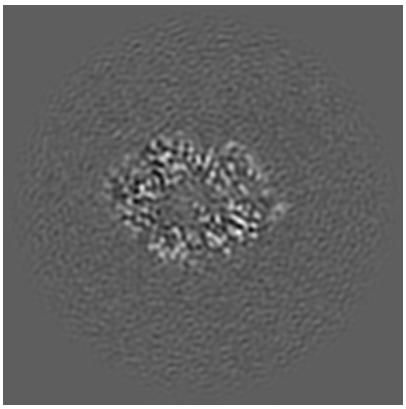
6.3.1 Primary map



X Index: 115

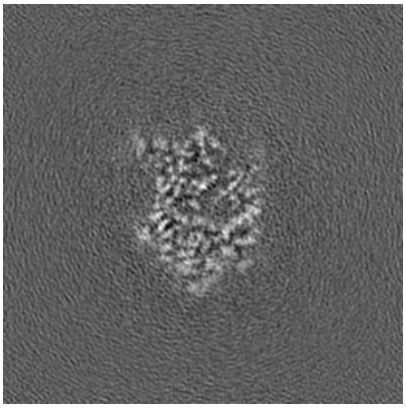


Y Index: 102

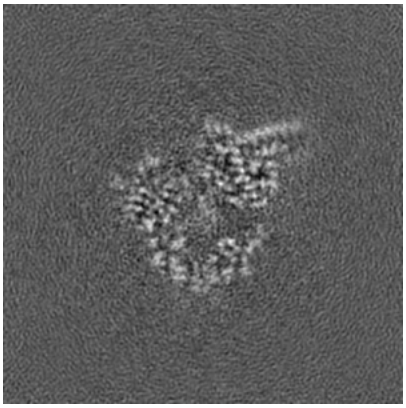


Z Index: 106

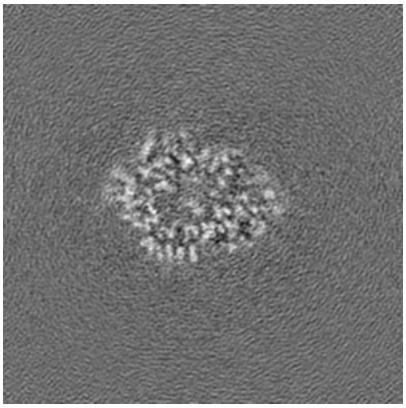
6.3.2 Raw map



X Index: 114



Y Index: 103

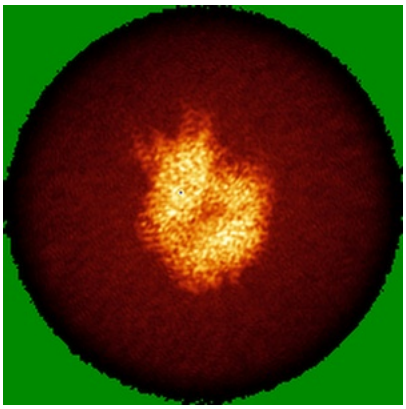


Z Index: 109

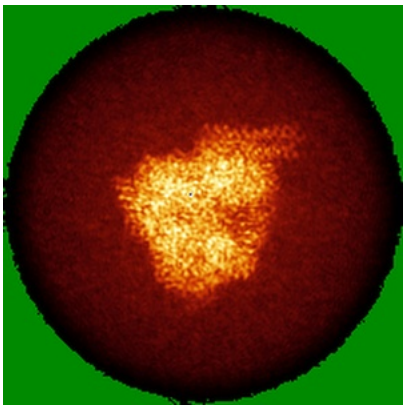
The images above show the largest variance slices of the map in three orthogonal directions.

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

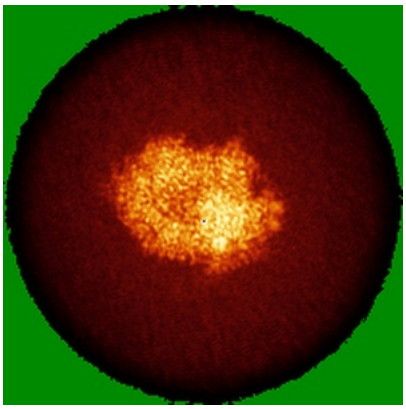
6.4.1 Primary map



X

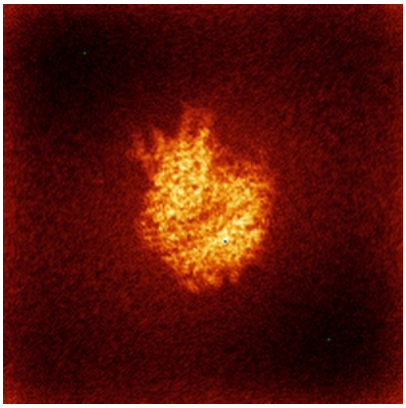


Y

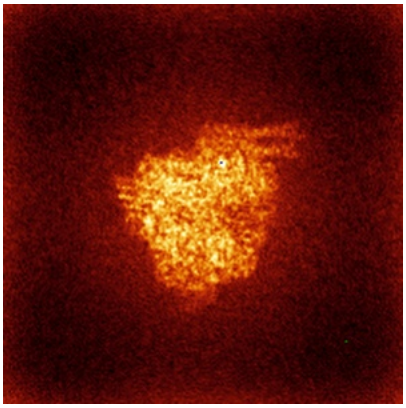


Z

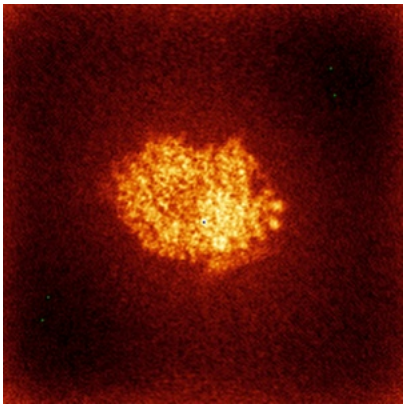
6.4.2 Raw map



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 0.187. 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.

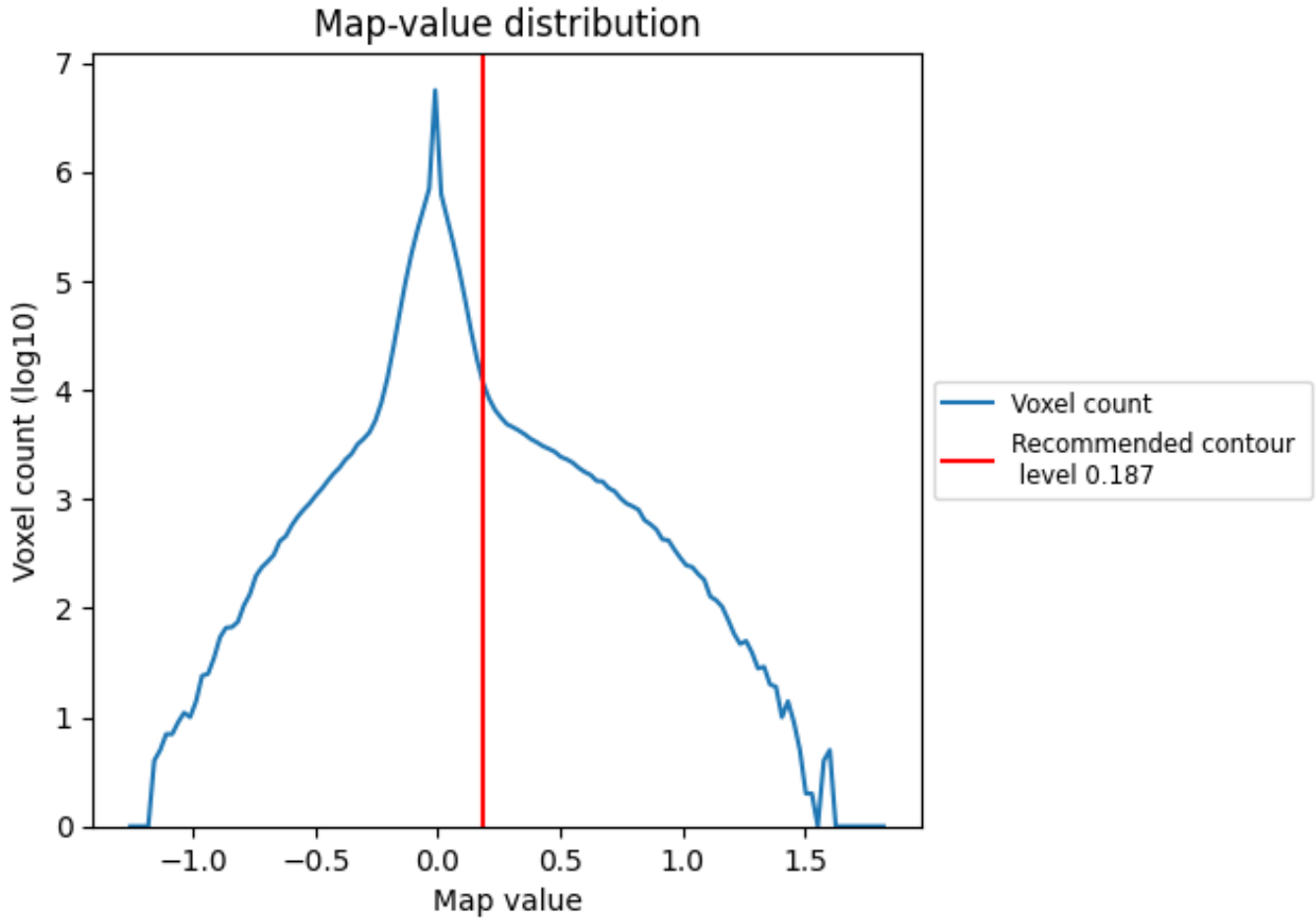
6.6 Mask visualisation (i)

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

7 Map analysis

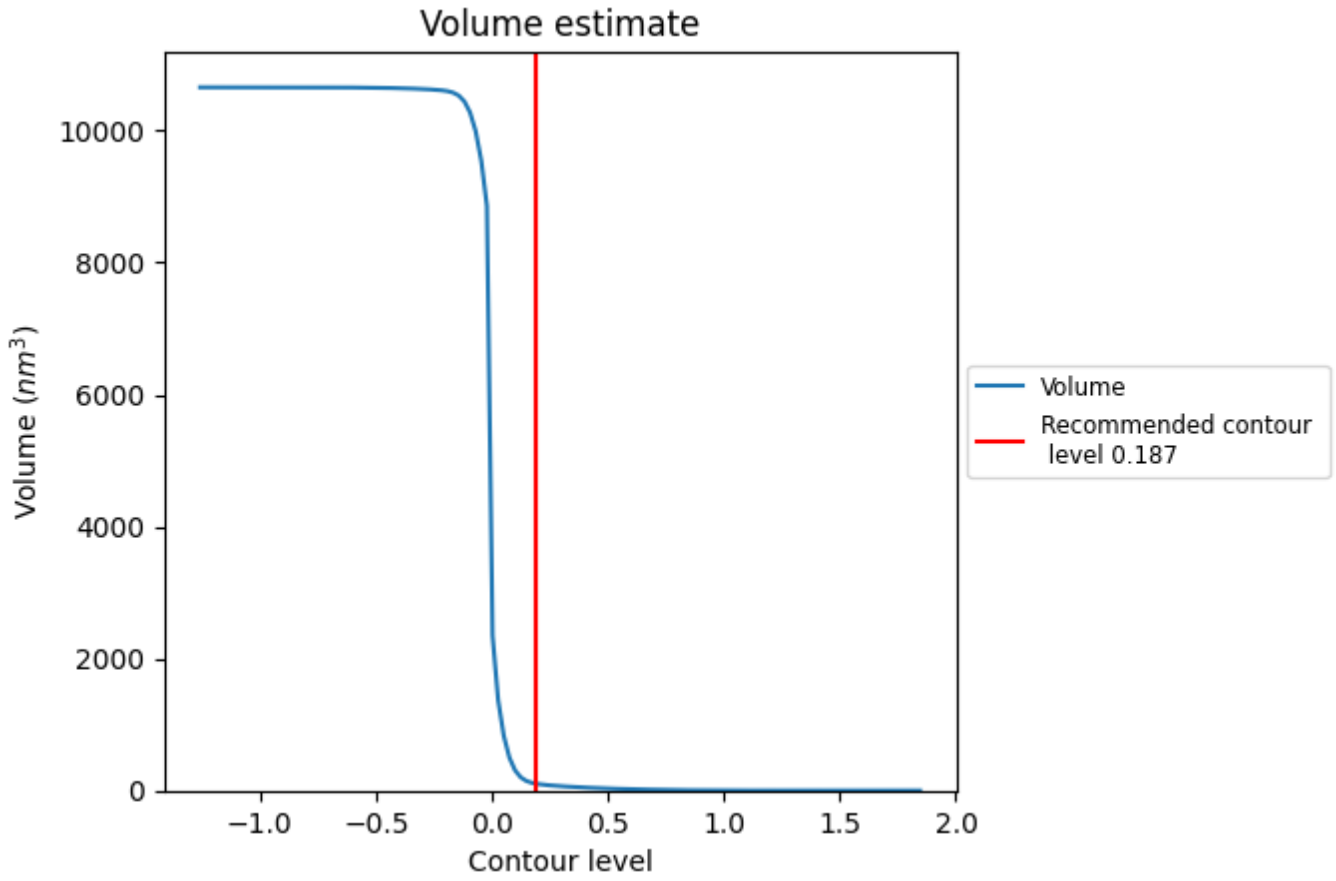
This section contains the results of statistical analysis of the map.

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.

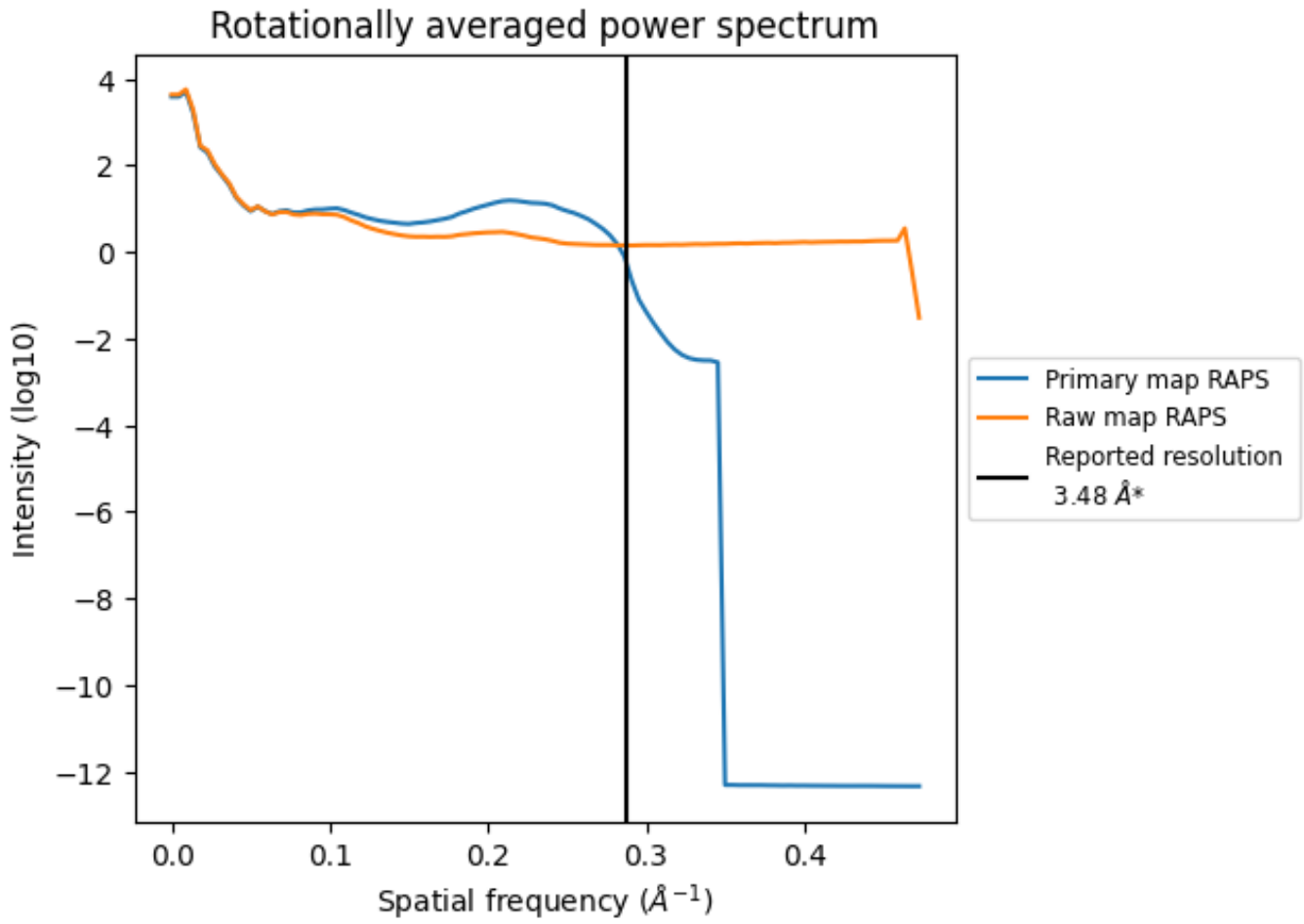
7.2 Volume estimate



The volume at the recommended contour level is 107 nm^3; this corresponds to an approximate mass of 97 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)

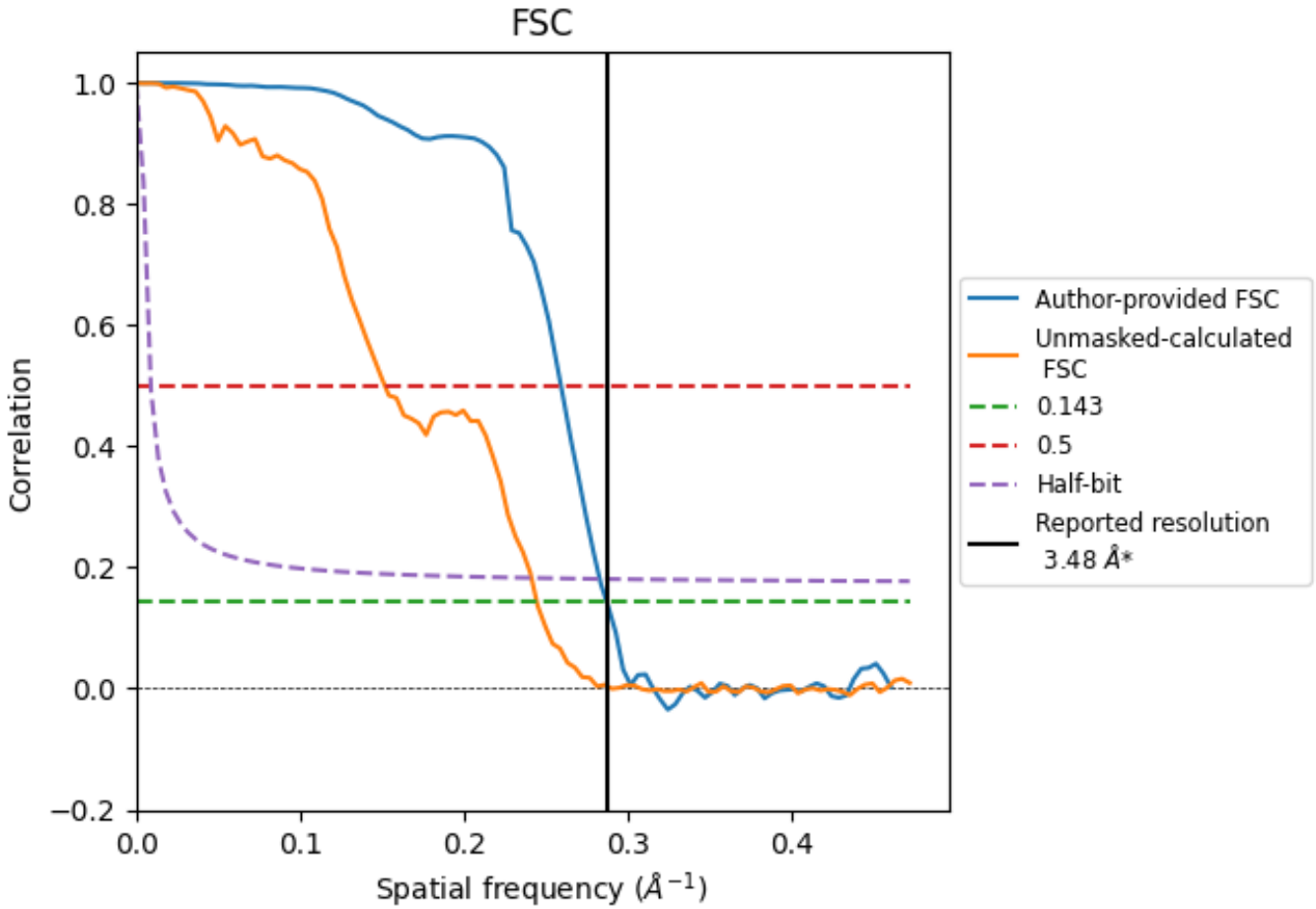


*Reported resolution corresponds to spatial frequency of 0.287 Å^{-1}

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 0.287 Å^{-1}

8.2 Resolution estimates (i)

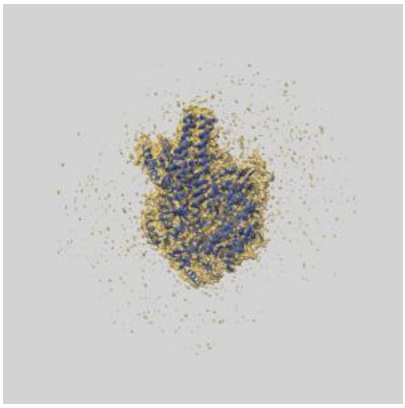
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.48	-	-
Author-provided FSC curve	3.48	3.85	3.53
Unmasked-calculated*	4.08	6.58	4.14

*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 4.08 differs from the reported value 3.48 by more than 10 %

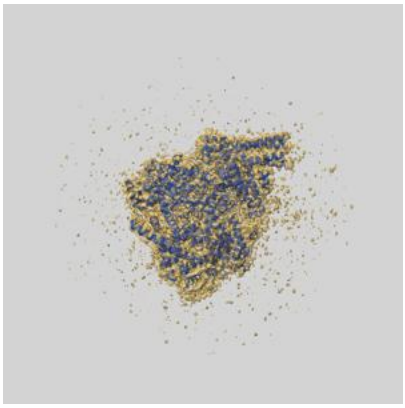
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-77747 and PDB model 36PU. Per-residue inclusion information can be found in section 3 on page 5.

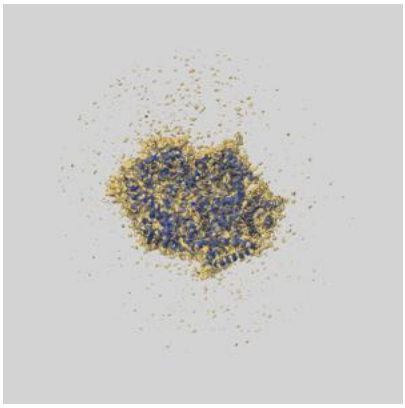
9.1 Map-model overlay



X



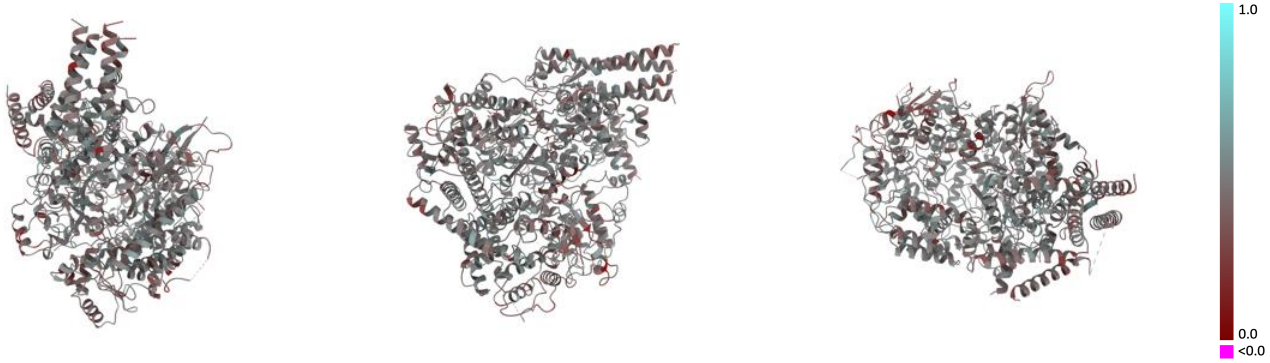
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.187 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.

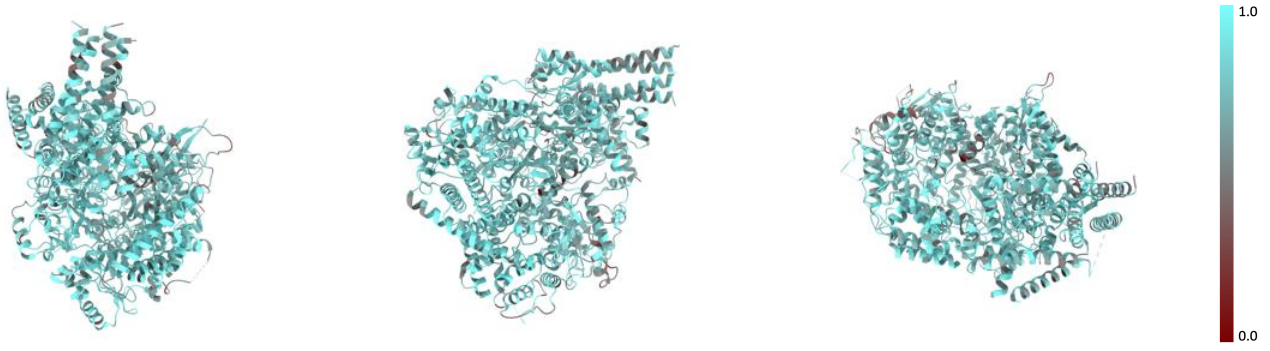
9.2 Q-score mapped to coordinate model



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.

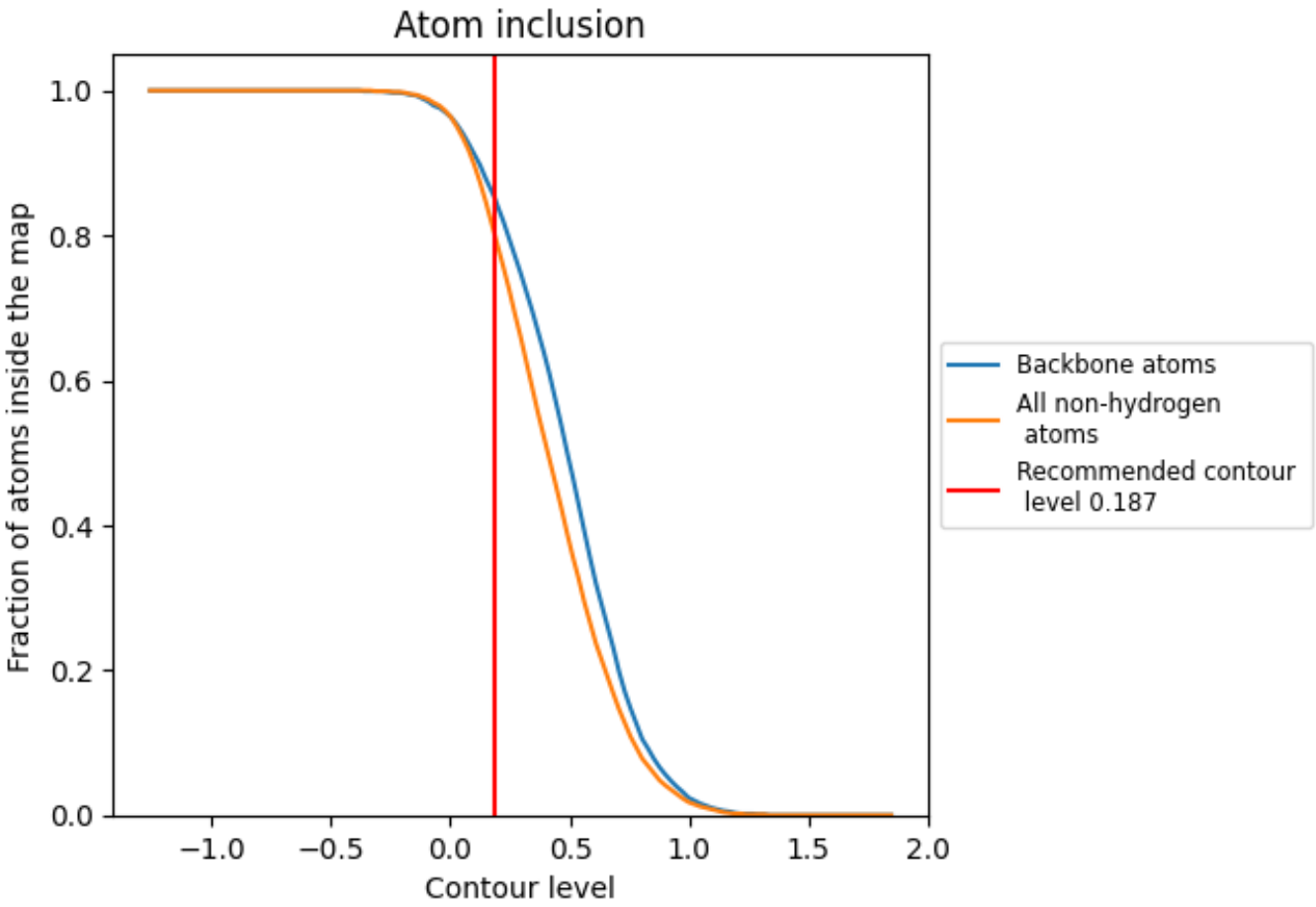
9.3 Atom inclusion mapped to coordinate model



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 (0.187).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 80% 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 (0.187) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8000	0.4490
A	0.8100	0.4530
B	0.7920	0.4580
C	0.7440	0.4150
D	0.7290	0.4050
E	0.7310	0.4290
P	0.7230	0.4050
T	0.8670	0.4730

