Full wwPDB EM Validation Report (i)

Jun 1, 2024 – 11:20 AM EDT

PDB ID	:	7UIM
EMDB ID	:	EMD-26549
Title	:	CryoEM Structure of an Group II Intron Retroelement (apo-complex)
Authors	:	Chung, K.; Xu, L.
Deposited on	:	2022-03-29
Resolution	:	3.10 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:

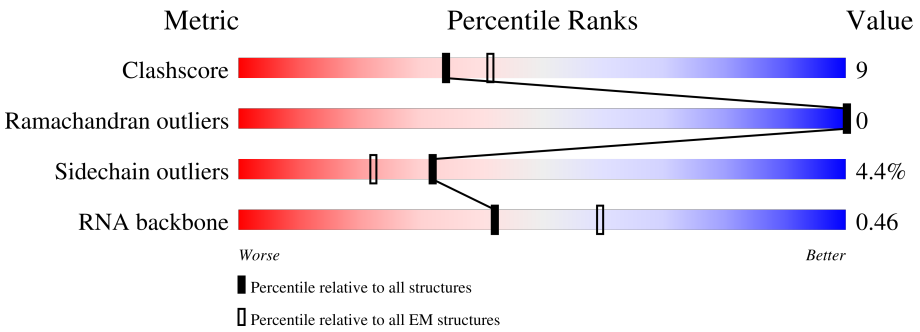
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.10 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	638	15% 44% 32% 9% 15%
2	D	427	62% 64% 25% • 9%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 14772 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 RNA chain called E.r IIC Intron.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	B	541	11624	5197	2167	3724	536	0	0

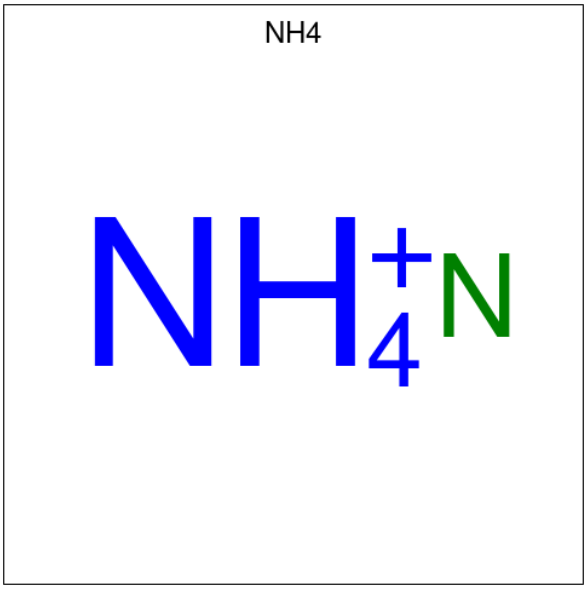
- Molecule 2 is a protein called Group II intron reverse transcriptase/maturase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	387	3133	1987	567	558	21	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
3	B	13	13	13	0

- Molecule 4 is AMMONIUM ION (three-letter code: NH4) (formula: H_4N) (labeled as "Ligand of Interest" by depositor).



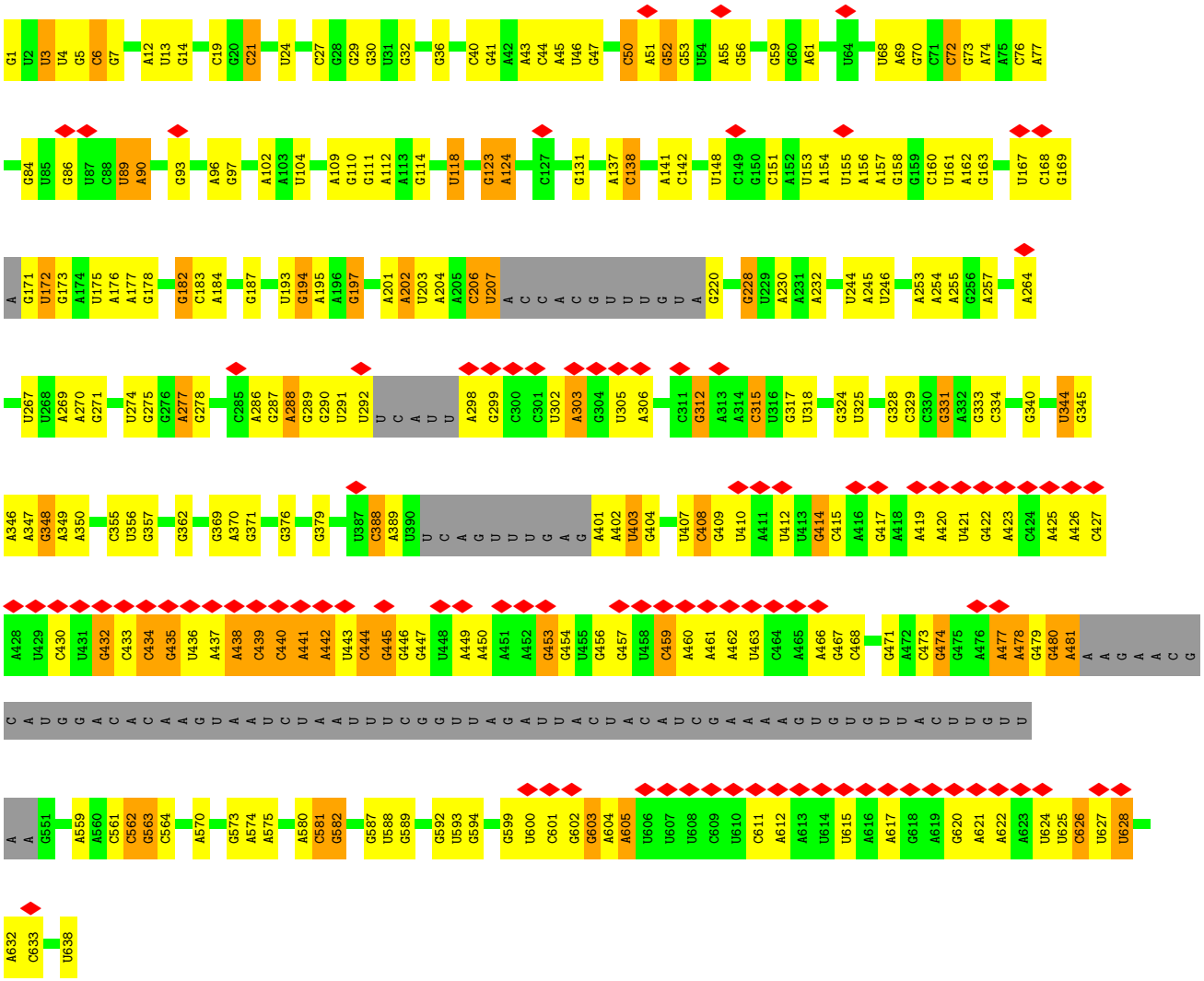
Mol	Chain	Residues	Atoms		AltConf
			Total	N	
4	B	1	1	1	0
			Total	N	
4	B	1	1	1	0

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: E.r IIC Intron

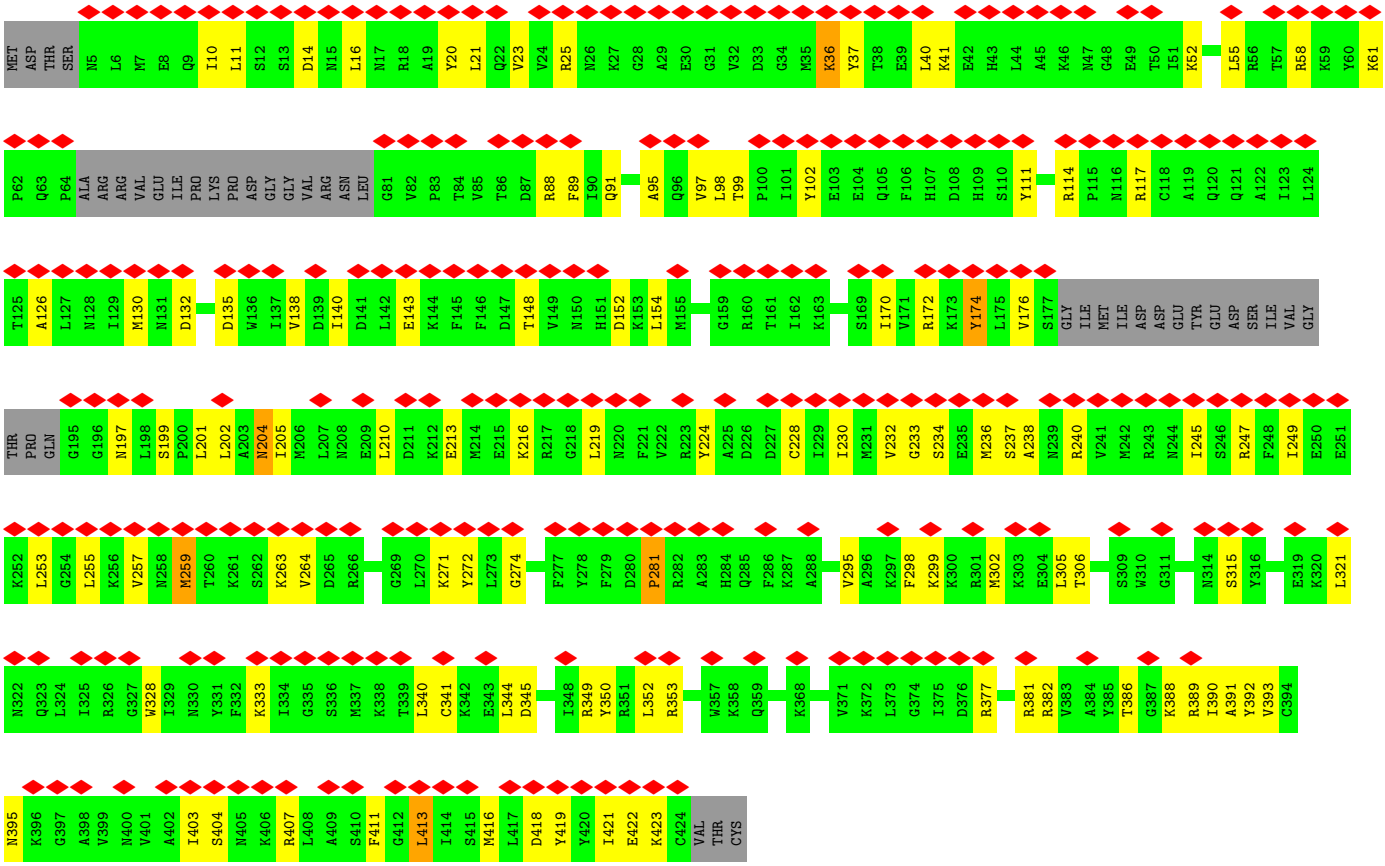
Chain B: 15% 44% 32% 9% 15%



- Molecule 2: Group II intron reverse transcriptase/maturase

Chain D:

62%
64%
25%
9%


MET ASP THR SER N5 L6 M7 E8 Q9 I10 L11 S12 S13 D14 N15 L16 N17 R18 A19 Y20 L21 Q22 V23 V24 R25 N26 K27 G28 A29 E30 G31 V32 D33 G34 M35 K36 Y37 T38 E39 L40 K41 E42 H43 L44 A45 K46 N47 G48 E49 T50 I51 K52 L55 R56 T57 R58 K59 Y60 K61
P62 Q63 P64 ALA ARG ARG VAL GLU ILE PRO LYS PRO ASP GLY GLY VAL ARG ASN LEU G81 V82 P83 T84 V85 T86 D87 R88 F89 I90 Q91 A95 Q96 V97 L98 T99 P100 I101 Y102 E103 E104 Q105 F106 H107 D108 H109 S110 Y111 R114 P115 N116 R117 C118 A119 Q120 Q121 A122 I123 L124
T125 A126 L127 N128 I129 M130 N131 D132 D135 W136 I137 V138 D139 I140 D141 L142 E143 K144 F145 F146 D147 T148 V149 N150 H151 D152 K153 L154 M155 G159 R160 T161 I162 K163 S169 I170 V171 R172 K173 Y174 L175 V176 S177 GLY ILE MET ILE ASP ASP GLU TYR GLU ASP SER ILE VAL GLY
THR PRO GLN G195 G196 N197 L198 S199 P200 L201 L202 A203 N204 I205 M206 L207 N208 E209 L210 D211 K212 E213 M214 E215 K216 R217 G218 L219 N220 F221 V222 R223 Y224 A225 D226 D227 C228 I229 I230 M231 V232 G233 S234 E235 M236 S237 A238 N239 R240 V241 M242 R243 N244 I245 S246 R247 F248 I249 E250 E251
K252 L253 G254 L255 K256 V257 N258 M259 T260 K261 S262 K263 V264 D265 R266 G269 L270 K271 Y272 L273 G274 F277 Y278 F279 D280 P281 R282 A283 H284 Q285 F286 K287 A288 V295 A296 K297 F298 K299 K300 R301 M302 K303 E304 L305 T306 S309 W310 G311 N314 S315 Y316 E319 K320 L321
N322 Q323 L324 I325 R326 G327 W328 I329 N330 Y331 F332 K333 I334 G335 S336 M337 K338 T339 L340 C341 K342 E343 L344 D345 I348 R349 Y350 R351 L352 R353 W357 K358 Q359 K368 V371 K372 L373 G374 I375 D376 R377 R381 R382 V383 A384 Y385 T386 G387 K388 R389 I390 A391 Y392 V393 C394
N395 K396 G397 A398 V399 N400 V401 A402 I403 S404 N405 K406 R407 L408 A409 S410 F411 G412 L413 I414 S415 M416 L417 D418 Y419 Y420 I421 E422 K423 C424 VAL THR CYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	434467	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50.3	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	0.425	Depositor
Minimum map value	-0.145	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	319.488, 319.488, 319.488	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.832, 0.832, 0.832	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NH4, MG

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	0.50	0/13028	0.98	27/20316 (0.1%)
2	D	0.34	0/3186	0.69	4/4273 (0.1%)
All	All	0.47	0/16214	0.94	31/24589 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	1

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	138	C	N1-C2-O2	7.84	123.60	118.90
1	B	27	C	C5-C6-N1	7.14	124.57	121.00
1	B	110	G	C4-N9-C1'	7.09	135.71	126.50
1	B	3	U	N3-C2-O2	-6.88	117.38	122.20
1	B	3	U	N1-C2-O2	6.66	127.47	122.80
2	D	36	LYS	CA-CB-CG	6.44	127.56	113.40
1	B	408	C	C2-N1-C1'	6.39	125.83	118.80
1	B	408	C	N1-C2-O2	6.32	122.69	118.90
1	B	27	C	C6-N1-C2	-6.21	117.82	120.30
1	B	3	U	C2-N1-C1'	6.15	125.08	117.70
1	B	110	G	C8-N9-C1'	-6.04	119.15	127.00
1	B	138	C	N3-C2-O2	-5.84	117.81	121.90
1	B	110	G	N3-C4-C5	-5.81	125.69	128.60
1	B	110	G	N3-C4-N9	5.77	129.46	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	142	C	N1-C2-O2	5.53	122.22	118.90
1	B	315	C	N1-C2-O2	5.52	122.21	118.90
1	B	626	C	C5-C6-N1	5.47	123.73	121.00
1	B	355	C	C2-N1-C1'	5.38	124.72	118.80
1	B	151	C	N1-C2-O2	5.36	122.11	118.90
1	B	459	C	N1-C2-O2	5.34	122.10	118.90
1	B	160	C	N1-C2-O2	5.31	122.08	118.90
1	B	602	G	N3-C4-N9	5.30	129.18	126.00
2	D	413	LEU	CA-CB-CG	5.21	127.29	115.30
1	B	267	U	N1-C2-O2	5.21	126.45	122.80
1	B	331	G	O4'-C1'-N9	5.20	112.36	108.20
1	B	142	C	C2-N1-C1'	5.16	124.48	118.80
2	D	152	ASP	CB-CG-OD2	5.16	122.94	118.30
1	B	50	C	C2-N1-C1'	5.10	124.41	118.80
2	D	281	PRO	CA-N-CD	-5.06	104.42	111.50
1	B	21	C	N1-C2-O2	5.00	121.90	118.90
1	B	267	U	N3-C2-O2	-5.00	118.70	122.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	281	PRO	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	B	11624	0	5848	120	0
2	D	3133	0	3219	67	0
3	B	13	0	0	0	0
4	B	2	0	0	0	0
All	All	14772	0	9067	184	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (184) 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:B:401:A:H3'	1:B:480:G:H1	1.21	1.03
1:B:303:A:H62	1:B:312:G:H21	1.21	0.88
1:B:444:C:H2'	1:B:445:G:C8	2.08	0.87
1:B:434:C:H42	1:B:445:G:H1	1.21	0.84
1:B:477:A:H2'	1:B:478:A:O4'	1.90	0.71
1:B:436:U:H3'	1:B:437:A:H8	1.56	0.71
1:B:434:C:N4	1:B:445:G:H1	1.91	0.68
1:B:288:A:H61	1:B:302:U:H3	1.40	0.67
1:B:430:C:H42	1:B:453:G:H1	1.43	0.67
1:B:479:G:H2'	1:B:480:G:C8	2.30	0.66
1:B:70:G:HO2'	1:B:257:A:HO2'	1.38	0.66
1:B:303:A:H62	1:B:312:G:N2	1.91	0.65
1:B:442:A:H4'	1:B:444:C:C5	2.32	0.64
1:B:437:A:H3'	1:B:438:A:C2	2.31	0.64
2:D:135:ASP:H	2:D:233:GLY:HA2	1.62	0.64
1:B:401:A:H61	1:B:480:G:H3'	1.63	0.63
2:D:236:MET:SD	2:D:240:ARG:NH2	2.72	0.62
1:B:436:U:H2'	1:B:437:A:O4'	2.00	0.62
1:B:444:C:H2'	1:B:445:G:H8	1.64	0.61
1:B:440:C:H4'	1:B:441:A:O5'	2.00	0.61
2:D:219:LEU:HD21	2:D:230:ILE:HG23	1.82	0.61
1:B:436:U:H3'	1:B:437:A:C8	2.36	0.60
2:D:386:THR:HG22	2:D:390:ILE:HG21	1.82	0.60
1:B:438:A:H1'	1:B:439:C:C2	2.36	0.60
2:D:102:TYR:HE2	2:D:205:ILE:HD11	1.65	0.59
1:B:445:G:C2	1:B:446:G:C8	2.91	0.59
1:B:24:U:O2'	1:B:68:U:O2	2.20	0.58
2:D:391:ALA:O	2:D:395:ASN:ND2	2.35	0.58
1:B:40:C:H2'	1:B:41:G:H8	1.68	0.57
1:B:401:A:N6	1:B:480:G:H3'	2.19	0.57
2:D:353:ARG:NE	2:D:403:ILE:O	2.37	0.57
2:D:11:LEU:HB3	2:D:52:LYS:HE3	1.86	0.57
1:B:228:G:OP1	2:D:299:LYS:NZ	2.37	0.57
1:B:73:G:O2'	1:B:118:U:O4	2.23	0.57
2:D:382:ARG:O	2:D:386:THR:OG1	2.19	0.56
1:B:89:U:H2'	1:B:90:A:H8	1.70	0.56
1:B:438:A:H1'	1:B:439:C:O2	2.06	0.56
1:B:175:U:O2	1:B:197:G:O6	2.24	0.56
1:B:131:G:O2'	1:B:195:A:N3	2.35	0.56
1:B:6:C:H2'	1:B:7:G:H8	1.71	0.55
1:B:427:C:H42	1:B:456:G:H1	1.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:U:H3	1:B:298:A:H61	1.55	0.54
2:D:148:THR:HB	2:D:255:LEU:HA	1.89	0.54
1:B:141:A:N1	1:B:232:A:O2'	2.38	0.54
1:B:421:U:H2'	1:B:422:G:H8	1.72	0.54
1:B:153:U:O2'	1:B:232:A:N1	2.39	0.54
2:D:126:ALA:O	2:D:130:MET:HG2	2.08	0.54
1:B:175:U:C2	1:B:197:G:O6	2.61	0.53
2:D:249:ILE:HG21	2:D:257:VAL:HG23	1.88	0.53
2:D:390:ILE:HB	2:D:393:VAL:HB	1.90	0.53
1:B:414:G:H2'	1:B:415:C:C6	2.43	0.53
1:B:440:C:H6	1:B:444:C:C5	2.27	0.53
1:B:201:A:H5'	1:B:202:A:H5'	1.91	0.53
2:D:352:LEU:HD11	2:D:413:LEU:HD13	1.91	0.53
1:B:435:G:H3'	1:B:436:U:C6	2.44	0.52
1:B:442:A:O3'	1:B:443:U:H3'	2.09	0.52
2:D:418:ASP:HA	2:D:421:ILE:HG12	1.91	0.52
2:D:138:VAL:HG22	2:D:264:VAL:HG12	1.92	0.52
1:B:72:C:H2'	1:B:73:G:C8	2.45	0.52
1:B:435:G:C2	1:B:436:U:H1'	2.45	0.52
2:D:388:LYS:HD2	2:D:389:ARG:HH11	1.74	0.52
1:B:580:A:OP1	1:B:582:G:O2'	2.27	0.52
2:D:295:VAL:HG11	2:D:340:LEU:HD21	1.90	0.52
2:D:11:LEU:HD22	2:D:52:LYS:HG2	1.91	0.51
2:D:23:VAL:HG21	2:D:89:PHE:HA	1.92	0.51
1:B:303:A:N6	1:B:312:G:H21	1.99	0.51
1:B:468:C:OP1	2:D:58:ARG:NH1	2.44	0.51
1:B:277:A:OP2	1:B:324:G:N1	2.44	0.50
2:D:353:ARG:HG2	2:D:403:ILE:HB	1.93	0.50
2:D:14:ASP:N	2:D:14:ASP:OD1	2.44	0.50
2:D:11:LEU:HD21	2:D:55:LEU:HD12	1.93	0.49
2:D:234:SER:O	2:D:238:ALA:N	2.45	0.49
1:B:1:G:OP2	1:B:632:A:O2'	2.29	0.49
1:B:401:A:H2'	1:B:480:G:H22	1.78	0.49
2:D:210:LEU:HB2	2:D:253:LEU:HD21	1.95	0.49
1:B:437:A:N1	1:B:439:C:H1'	2.27	0.49
2:D:377:ARG:NH1	2:D:381:ARG:HB2	2.28	0.49
2:D:114:ARG:NH2	2:D:204:ASN:OD1	2.39	0.49
2:D:170:ILE:O	2:D:174:TYR:HB2	2.12	0.49
1:B:603:G:H2'	1:B:604:A:C8	2.48	0.49
1:B:438:A:H4'	1:B:439:C:OP1	2.13	0.48
1:B:89:U:H2'	1:B:90:A:C8	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:432:G:H1'	1:B:450:A:H61	1.79	0.48
1:B:402:A:C4	1:B:481:A:H2	2.31	0.48
2:D:234:SER:HB2	2:D:237:SER:HB2	1.96	0.48
2:D:298:PHE:HB2	2:D:328:TRP:CZ2	2.48	0.48
1:B:289:G:H2'	1:B:290:G:C4	2.49	0.47
2:D:140:ILE:HB	2:D:228:CYS:HB2	1.96	0.47
2:D:345:ASP:O	2:D:349:ARG:HG2	2.15	0.47
2:D:11:LEU:HA	2:D:16:LEU:HD21	1.95	0.47
1:B:40:C:H2'	1:B:41:G:C8	2.48	0.47
1:B:84:G:H1	1:B:104:U:H3	1.61	0.47
1:B:441:A:H1'	1:B:443:U:C5	2.49	0.47
1:B:403:U:H3'	1:B:404:G:H8	1.80	0.47
1:B:435:G:C6	1:B:436:U:C2	3.03	0.47
2:D:230:ILE:HD13	2:D:245:ILE:HD13	1.97	0.47
1:B:43:A:H2'	1:B:44:C:H6	1.80	0.47
1:B:50:C:OP1	1:B:52:G:N1	2.48	0.47
1:B:43:A:H2'	1:B:44:C:C6	2.49	0.46
1:B:194:G:HO2'	1:B:195:A:H8	1.61	0.46
2:D:91:GLN:NE2	2:D:174:TYR:OH	2.42	0.46
2:D:10:ILE:HG12	2:D:97:VAL:HG11	1.97	0.46
2:D:271:LYS:HE3	2:D:274:GLY:H	1.81	0.46
1:B:76:C:H2'	1:B:77:A:C8	2.50	0.46
1:B:168:C:H42	1:B:220:G:H1	1.64	0.46
2:D:36:LYS:HD2	2:D:37:TYR:N	2.31	0.46
1:B:286:A:H2'	1:B:287:G:H8	1.80	0.45
1:B:437:A:H5"	1:B:438:A:N1	2.31	0.45
1:B:442:A:OP2	1:B:444:C:N4	2.48	0.45
2:D:333:LYS:HD3	2:D:423:LYS:HB3	1.97	0.45
1:B:345:G:O2'	1:B:348:G:O2'	2.28	0.45
2:D:61:LYS:HE2	2:D:61:LYS:HB2	1.77	0.45
2:D:213:GLU:HG2	2:D:216:LYS:HE3	1.97	0.45
1:B:436:U:C2	1:B:437:A:H1'	2.52	0.44
2:D:95:ALA:O	2:D:99:THR:HG23	2.17	0.44
2:D:259:MET:O	2:D:263:LYS:NZ	2.34	0.44
1:B:401:A:C3'	1:B:480:G:H1	2.09	0.44
1:B:445:G:N1	1:B:446:G:N7	2.66	0.44
1:B:171:G:H2'	1:B:172:U:H4'	1.99	0.44
1:B:182:G:N7	2:D:392:TYR:HB3	2.32	0.44
1:B:287:G:H2'	1:B:288:A:H8	1.82	0.44
2:D:305:LEU:HD23	2:D:321:LEU:HD23	2.00	0.43
1:B:603:G:H2'	1:B:604:A:H8	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:403:U:C4	1:B:404:G:C5	3.05	0.43
1:B:76:C:H2'	1:B:77:A:H8	1.81	0.43
1:B:344:U:H2'	1:B:345:G:H8	1.84	0.43
1:B:349:A:H2'	1:B:350:A:H8	1.84	0.43
1:B:479:G:H2'	1:B:480:G:H8	1.82	0.43
1:B:627:U:H2'	1:B:628:U:H6	1.83	0.43
1:B:44:C:H2'	1:B:45:A:H8	1.83	0.43
1:B:625:U:H2'	1:B:626:C:C6	2.53	0.43
2:D:37:TYR:O	2:D:40:LEU:HB3	2.18	0.43
1:B:356:U:H2'	1:B:357:G:C8	2.53	0.43
1:B:421:U:H2'	1:B:422:G:C8	2.51	0.43
1:B:466:A:H3'	1:B:467:G:H8	1.83	0.43
2:D:111:TYR:HA	2:D:117:ARG:HD2	1.99	0.43
1:B:604:A:H2'	1:B:605:A:C8	2.54	0.43
2:D:154:LEU:HD21	2:D:202:LEU:HD22	2.01	0.43
1:B:44:C:H2'	1:B:45:A:C8	2.53	0.43
1:B:178:G:H1	1:B:193:U:H3	1.67	0.43
1:B:274:U:H2'	1:B:275:G:C8	2.53	0.43
1:B:563:G:O6	1:B:588:U:O2	2.37	0.43
1:B:427:C:N3	1:B:456:G:N2	2.63	0.42
1:B:401:A:H61	1:B:480:G:H5"	1.83	0.42
1:B:422:G:H2'	1:B:423:A:C8	2.53	0.42
2:D:299:LYS:HE2	2:D:344:LEU:HD11	2.01	0.42
1:B:123:G:O2'	1:B:124:A:OP2	2.28	0.42
2:D:52:LYS:HB3	2:D:52:LYS:HE2	1.74	0.42
1:B:206:C:H2'	1:B:207:U:C6	2.55	0.42
2:D:201:LEU:HA	2:D:201:LEU:HD23	1.80	0.42
1:B:473:C:H2'	1:B:474:G:C8	2.54	0.42
2:D:388:LYS:HB2	2:D:388:LYS:HE2	1.88	0.42
1:B:401:A:N1	1:B:480:G:H3'	2.34	0.42
1:B:402:A:C8	1:B:480:G:N3	2.88	0.42
2:D:302:MET:O	2:D:306:THR:HG22	2.20	0.42
1:B:611:C:H2'	1:B:612:A:H8	1.84	0.42
1:B:562:C:H5"	1:B:638:U:H4'	2.02	0.42
1:B:230:A:O2'	1:B:232:A:OP1	2.37	0.41
2:D:20:TYR:CE1	2:D:41:LYS:HB2	2.54	0.41
2:D:98:LEU:HD23	2:D:98:LEU:HA	1.91	0.41
2:D:10:ILE:HG12	2:D:97:VAL:HG21	2.01	0.41
2:D:224:TYR:N	2:D:272:TYR:OH	2.52	0.41
2:D:232:VAL:HG11	2:D:238:ALA:HA	2.02	0.41
2:D:345:ASP:OD2	2:D:416:MET:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:G:N2	1:B:203:U:O2	2.38	0.41
1:B:277:A:H3'	1:B:278:G:H8	1.86	0.41
2:D:114:ARG:HD2	2:D:117:ARG:HD2	2.01	0.41
1:B:401:A:C6	1:B:480:G:H3'	2.56	0.41
2:D:388:LYS:HD2	2:D:389:ARG:NH1	2.34	0.41
1:B:287:G:H2'	1:B:288:A:C8	2.55	0.41
1:B:344:U:H2'	1:B:345:G:C8	2.56	0.41
1:B:435:G:H2'	1:B:436:U:O4'	2.20	0.41
1:B:441:A:C8	1:B:443:U:C2	3.07	0.41
2:D:21:LEU:O	2:D:25:ARG:HG3	2.21	0.41
1:B:161:U:H2'	1:B:162:A:C8	2.56	0.40
1:B:187:G:H5"	1:B:575:A:H61	1.86	0.40
1:B:388:C:H2'	1:B:389:A:H8	1.86	0.40
1:B:564:C:OP2	1:B:581:C:O2'	2.37	0.40
2:D:172:ARG:O	2:D:176:VAL:HG23	2.22	0.40
1:B:620:G:H2'	1:B:621:A:C8	2.56	0.40
2:D:249:ILE:HG23	2:D:255:LEU:HB2	2.03	0.40
2:D:404:SER:H	2:D:407:ARG:HD2	1.86	0.40
1:B:68:U:H2'	1:B:69:A:C8	2.56	0.40
1:B:627:U:H2'	1:B:628:U:C6	2.56	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
2	D	381/427 (89%)	367 (96%)	14 (4%)	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
2	D	341/376 (91%)	326 (96%)	15 (4%)	28 61

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	88	ARG
2	D	132	ASP
2	D	143	GLU
2	D	174	TYR
2	D	197	ASN
2	D	199	SER
2	D	204	ASN
2	D	247	ARG
2	D	259	MET
2	D	315	SER
2	D	341	CYS
2	D	350	TYR
2	D	411	PHE
2	D	419	TYR
2	D	422	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B	535/638 (83%)	162 (30%)	7 (1%)

All (162) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	B	3	U

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Mol	Chain	Res	Type
1	B	4	U
1	B	5	G
1	B	6	C
1	B	12	A
1	B	13	U
1	B	14	G
1	B	19	C
1	B	21	C
1	B	29	G
1	B	30	G
1	B	32	G
1	B	36	G
1	B	47	G
1	B	51	A
1	B	52	G
1	B	53	G
1	B	55	A
1	B	56	G
1	B	61	A
1	B	72	C
1	B	74	A
1	B	86	G
1	B	90	A
1	B	93	G
1	B	96	A
1	B	97	G
1	B	102	A
1	B	109	A
1	B	111	G
1	B	112	A
1	B	114	G
1	B	118	U
1	B	123	G
1	B	124	A
1	B	137	A
1	B	138	C
1	B	148	U
1	B	154	A
1	B	155	U
1	B	156	A
1	B	157	A
1	B	158	G

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Mol	Chain	Res	Type
1	B	163	G
1	B	167	U
1	B	169	G
1	B	172	U
1	B	173	G
1	B	176	A
1	B	177	A
1	B	182	G
1	B	183	C
1	B	184	A
1	B	194	G
1	B	197	G
1	B	202	A
1	B	204	A
1	B	206	C
1	B	207	U
1	B	228	G
1	B	244	U
1	B	245	A
1	B	246	U
1	B	253	A
1	B	254	A
1	B	255	A
1	B	264	A
1	B	269	A
1	B	270	A
1	B	271	G
1	B	277	A
1	B	288	A
1	B	291	U
1	B	299	G
1	B	303	A
1	B	305	U
1	B	306	A
1	B	312	G
1	B	315	C
1	B	317	G
1	B	318	U
1	B	325	U
1	B	328	G
1	B	329	C
1	B	331	G

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Mol	Chain	Res	Type
1	B	334	C
1	B	340	G
1	B	344	U
1	B	346	A
1	B	347	A
1	B	348	G
1	B	362	G
1	B	369	G
1	B	370	A
1	B	371	G
1	B	376	G
1	B	379	G
1	B	388	C
1	B	403	U
1	B	407	U
1	B	408	C
1	B	409	G
1	B	410	U
1	B	412	U
1	B	414	G
1	B	417	G
1	B	419	A
1	B	420	A
1	B	425	A
1	B	426	A
1	B	432	G
1	B	433	C
1	B	434	C
1	B	435	G
1	B	438	A
1	B	439	C
1	B	440	C
1	B	441	A
1	B	442	A
1	B	444	C
1	B	445	G
1	B	447	G
1	B	449	A
1	B	453	G
1	B	454	G
1	B	457	G
1	B	459	C

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Mol	Chain	Res	Type
1	B	460	A
1	B	461	A
1	B	462	A
1	B	463	U
1	B	471	G
1	B	474	G
1	B	477	A
1	B	478	A
1	B	480	G
1	B	481	A
1	B	559	A
1	B	561	C
1	B	562	C
1	B	563	G
1	B	570	A
1	B	573	G
1	B	574	A
1	B	581	C
1	B	582	G
1	B	587	G
1	B	589	G
1	B	592	G
1	B	593	U
1	B	594	G
1	B	599	G
1	B	600	U
1	B	601	C
1	B	603	G
1	B	605	A
1	B	615	U
1	B	617	A
1	B	622	A
1	B	624	U
1	B	628	U
1	B	633	C

All (7) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	B	46	U
1	B	89	U
1	B	123	G

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Mol	Chain	Res	Type
1	B	206	C
1	B	333	G
1	B	438	A
1	B	480	G

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 13 are monoatomic and 2 are modelled with single atom - 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.

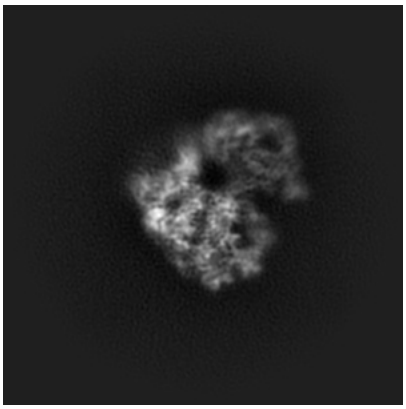
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-26549. These allow visual inspection of the internal detail of the map and identification of artifacts.

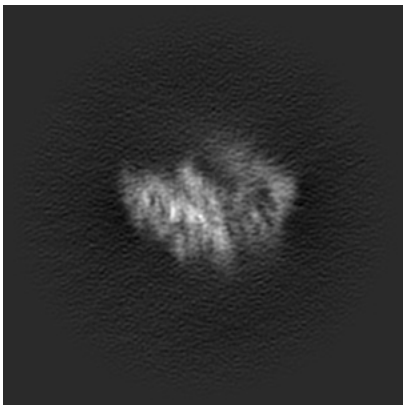
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

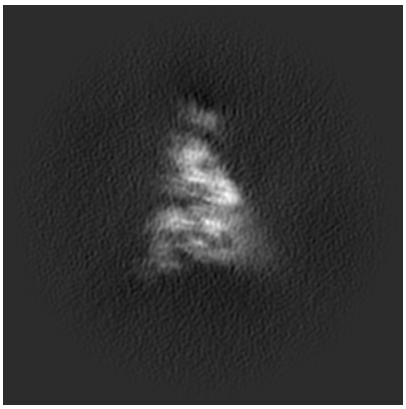
6.1.1 Primary map



X

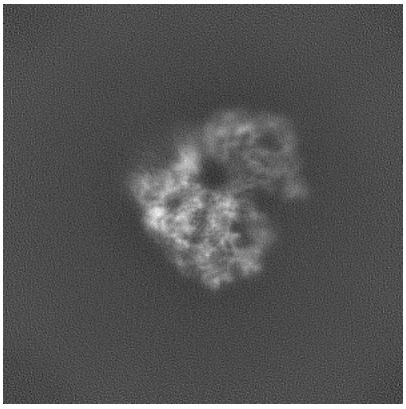


Y

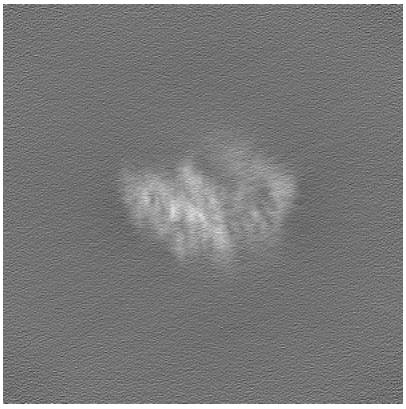


Z

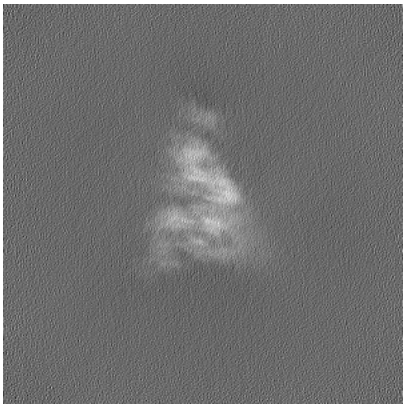
6.1.2 Raw map



X



Y

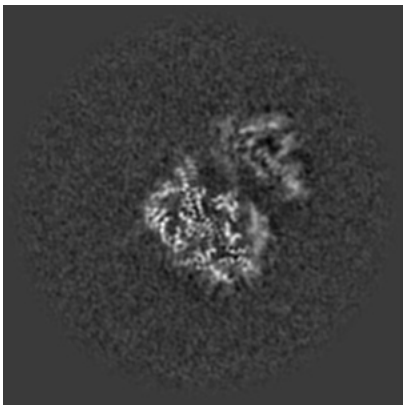


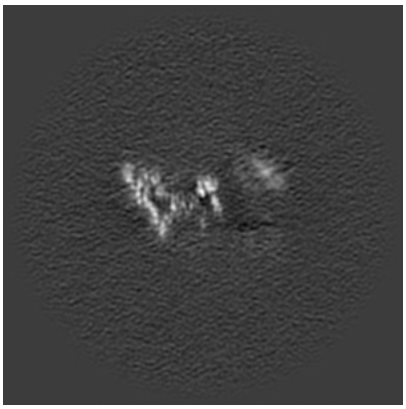
Z

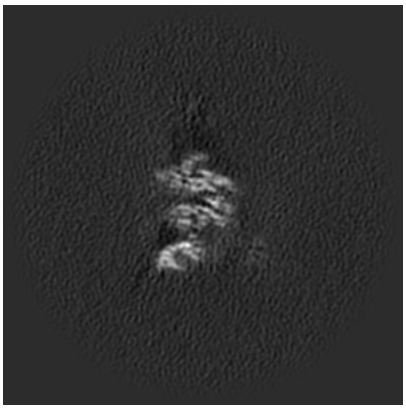
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

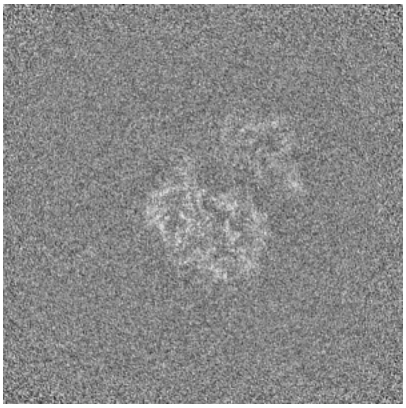
6.2.1 Primary map

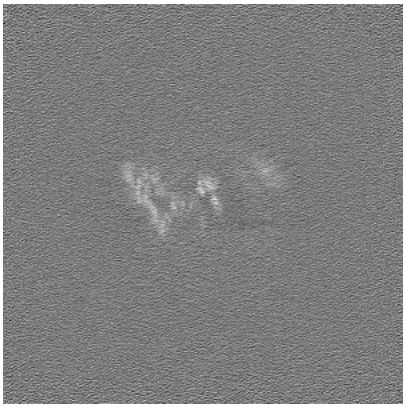

X Index: 192

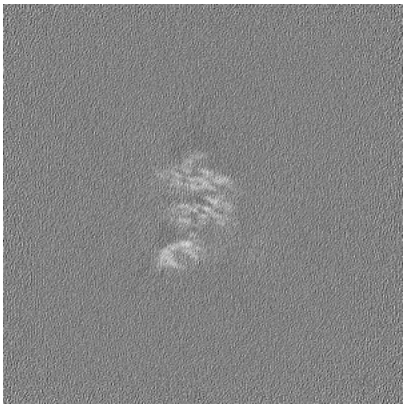

Y Index: 192


Z Index: 192

6.2.2 Raw map


X Index: 192

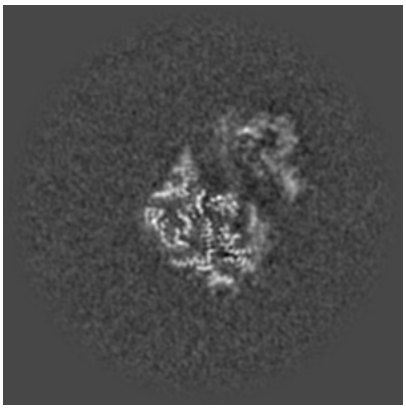

Y Index: 192

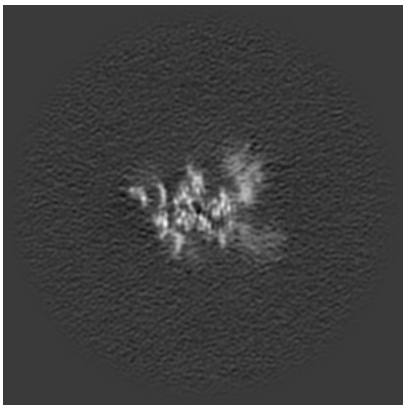

Z Index: 192

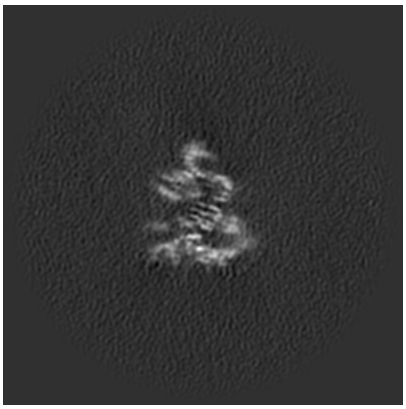
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

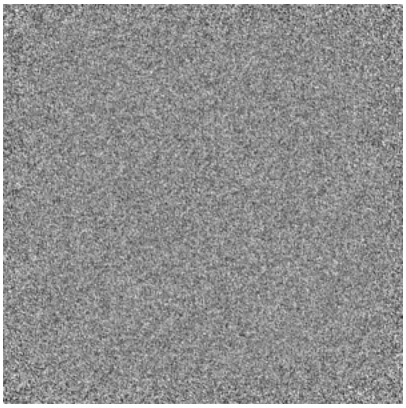
6.3.1 Primary map

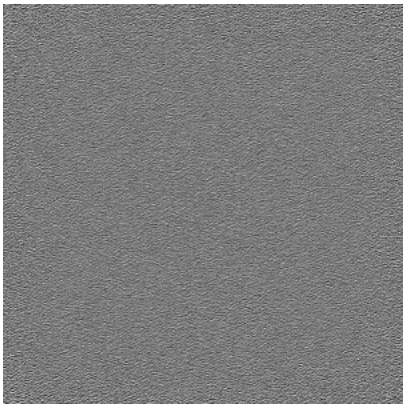

X Index: 195

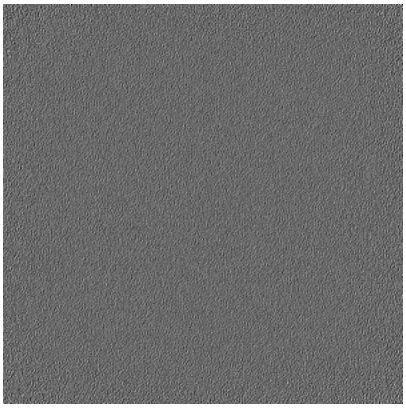

Y Index: 175


Z Index: 181

6.3.2 Raw map


X Index: 0

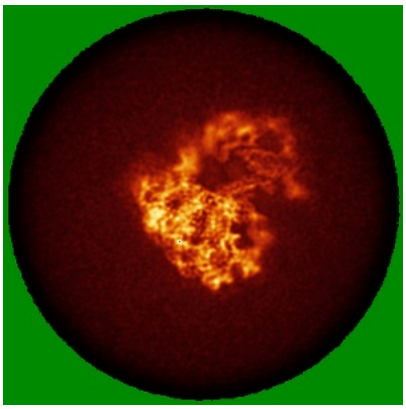

Y Index: 0

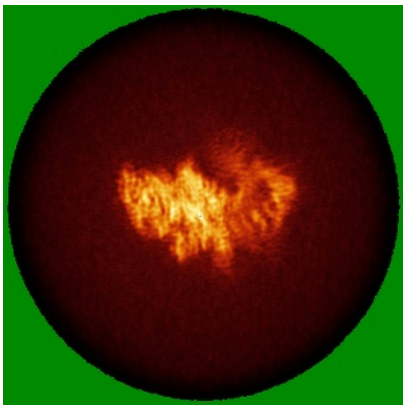

Z Index: 0

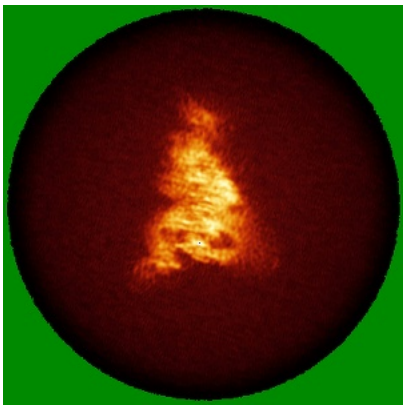
The images above show the largest variance slices of the map in three orthogonal directions.

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

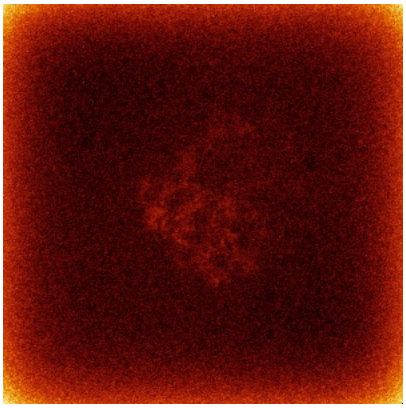
6.4.1 Primary map

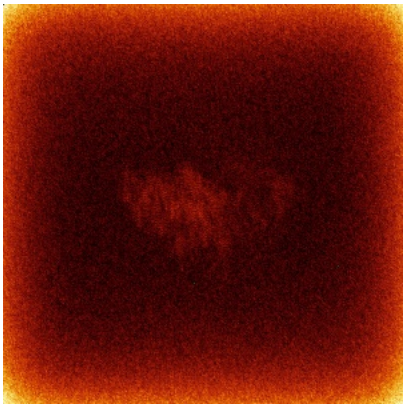

X

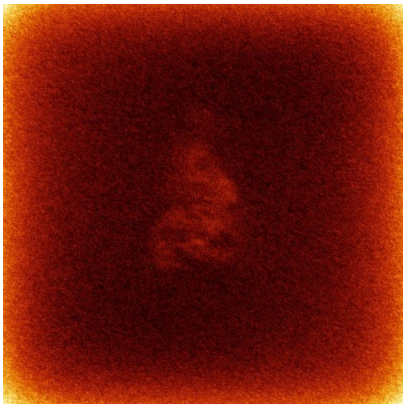

Y


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 0.12. 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.

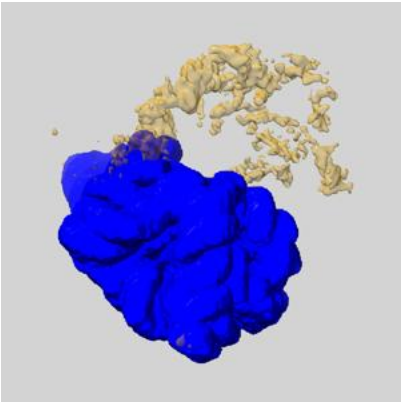
6.6 Mask visualisation (i)

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

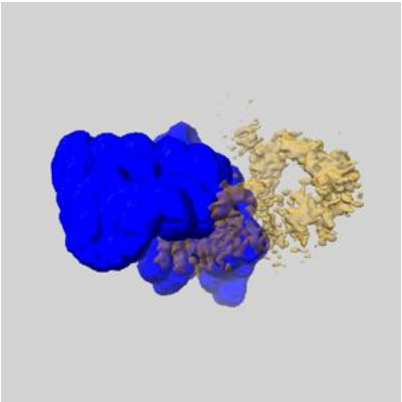
A mask typically either:

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

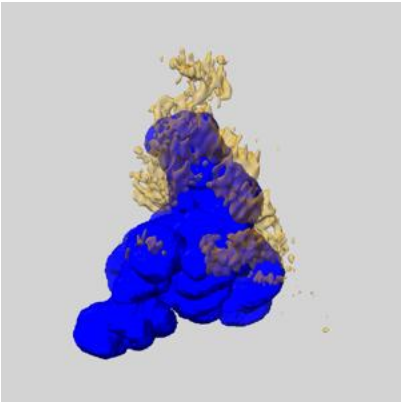
6.6.1 emd_26549_msk_1.map (i)



X

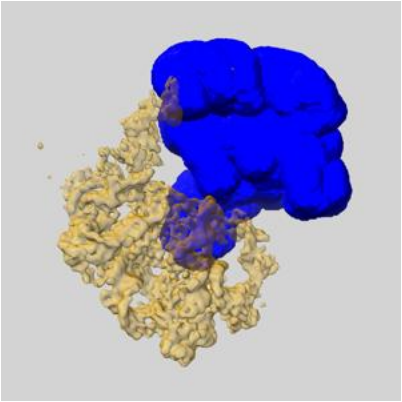


Y

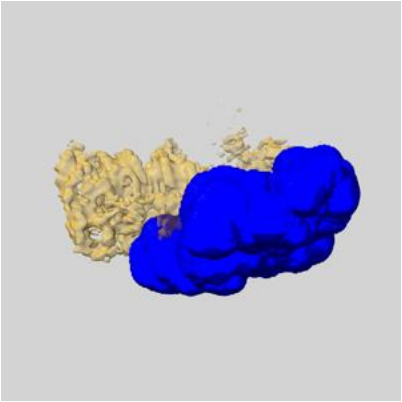


Z

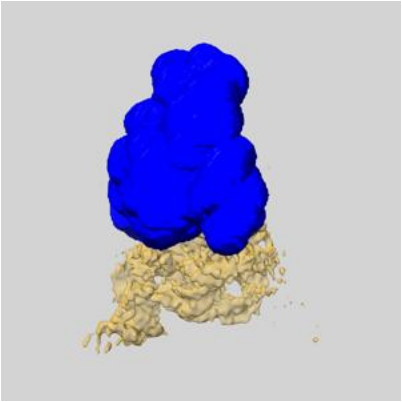
6.6.2 emd_26549_msk_2.map (i)



X



Y

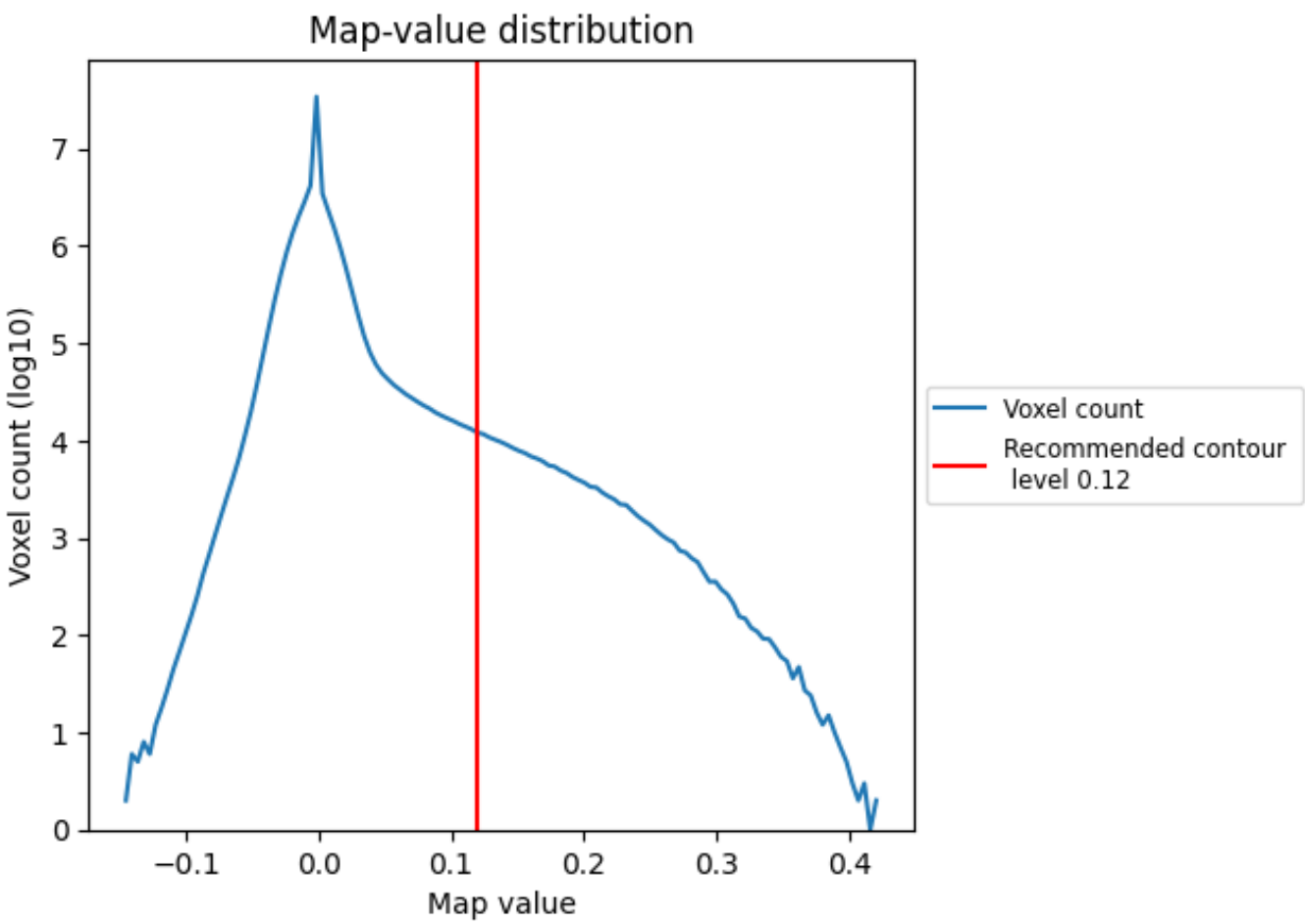


Z

7 Map analysis (i)

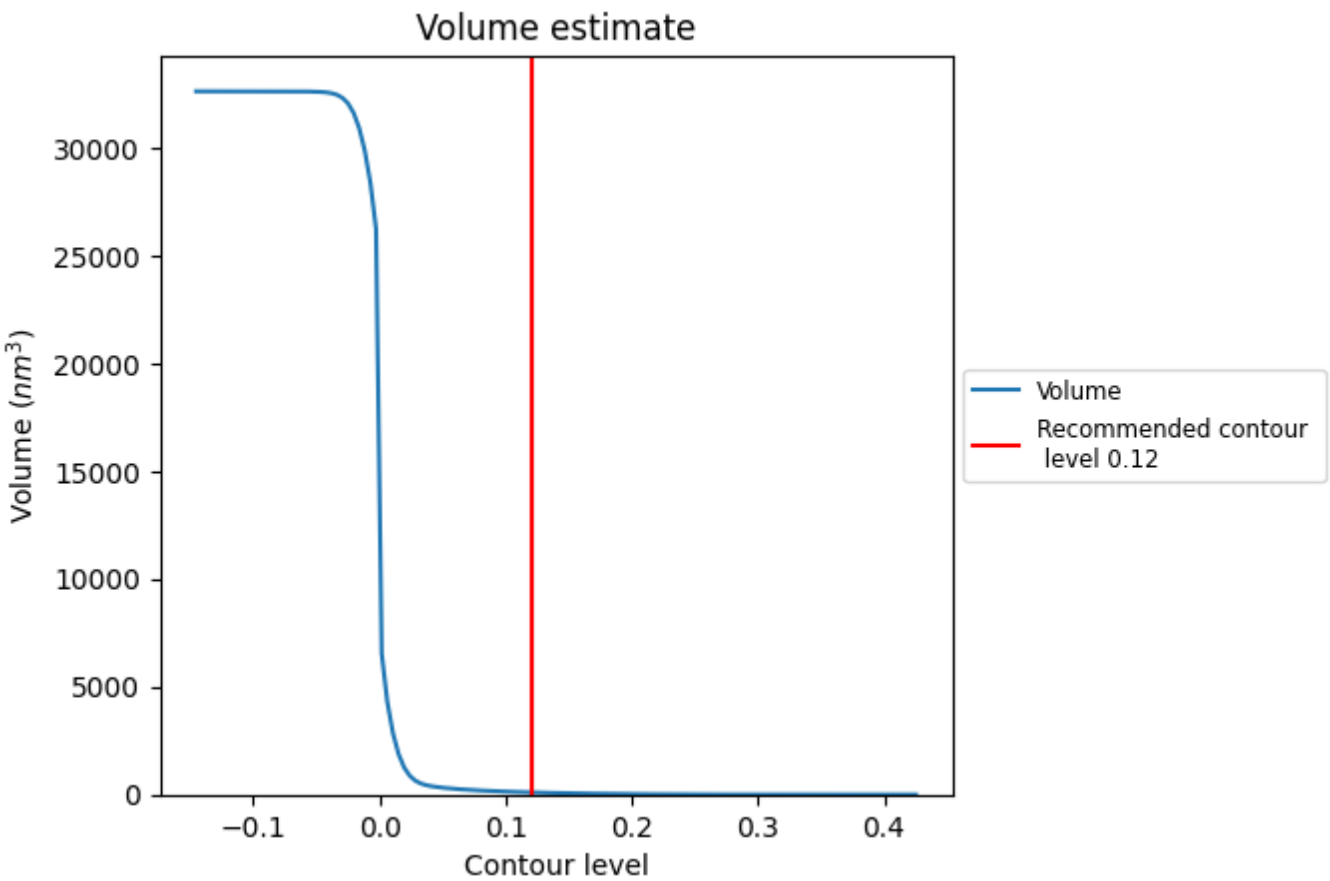
This section contains the results of statistical analysis of the map.

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.

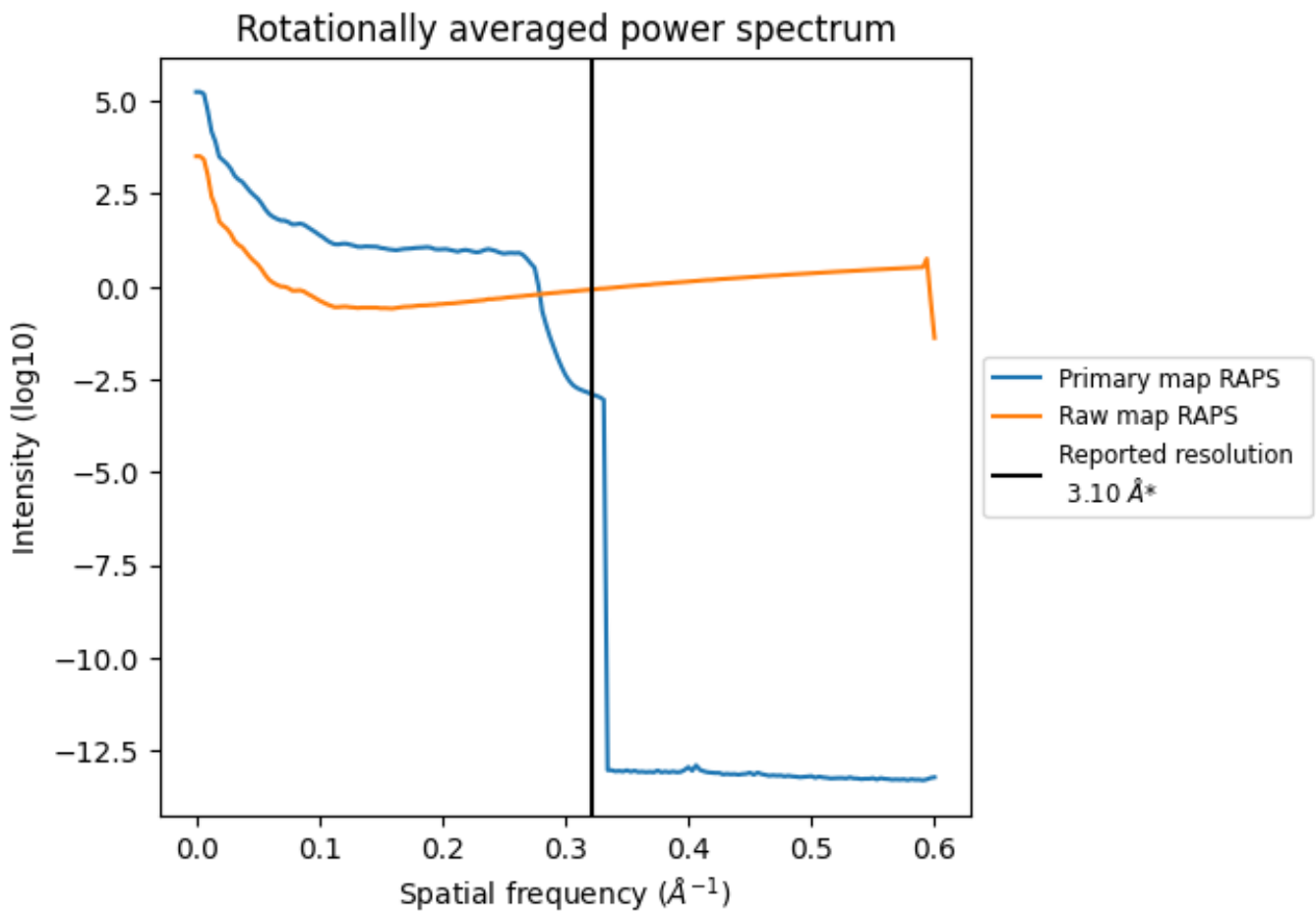
7.2 Volume estimate (i)



The volume at the recommended contour level is 100 nm^3; this corresponds to an approximate mass of 90 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)

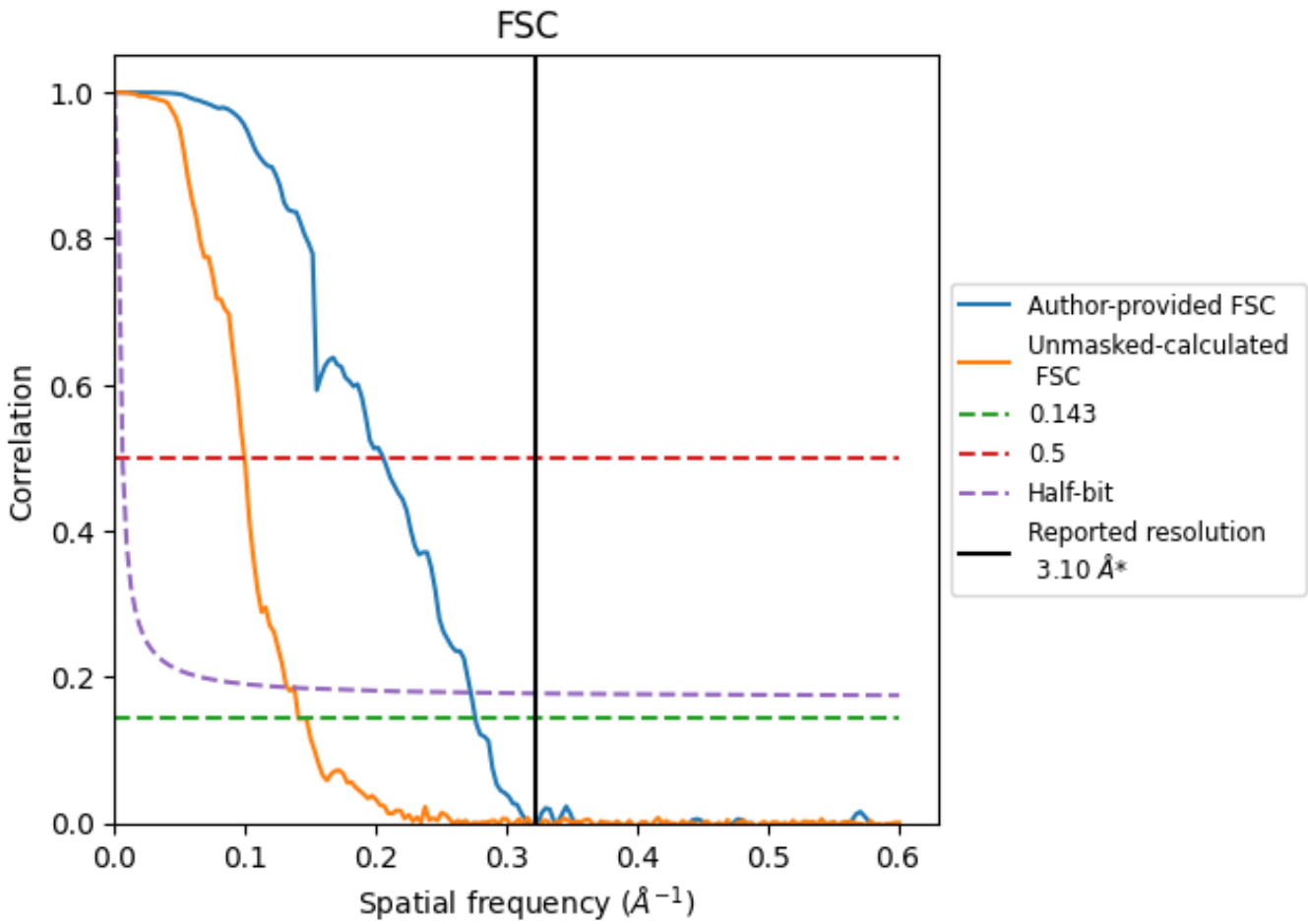


*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

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 0.323 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.62	4.86	3.66
Unmasked-calculated*	7.10	10.05	7.55

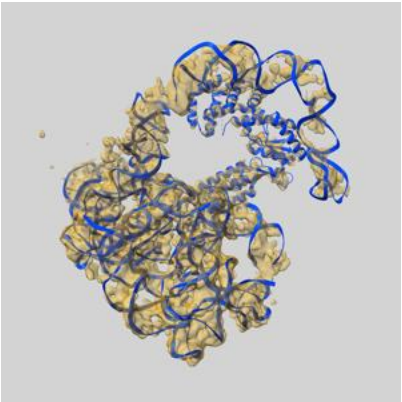
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.62 differs from the reported value 3.1 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.10 differs from the reported value 3.1 by more than 10 %

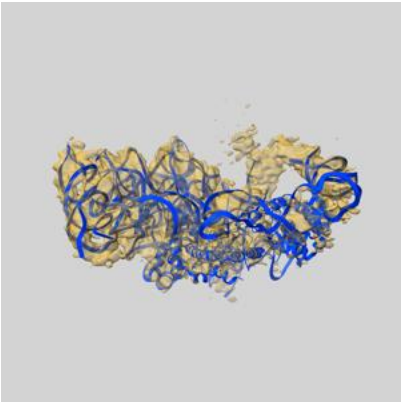
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-26549 and PDB model 7UIM. Per-residue inclusion information can be found in section 3 on page 5.

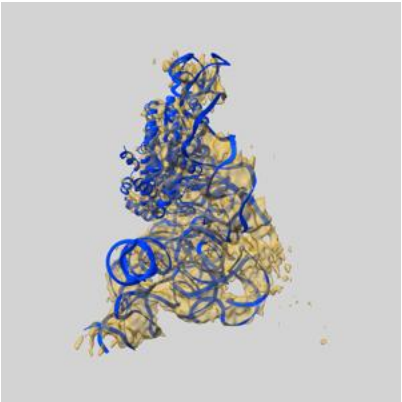
9.1 Map-model overlay (i)



X



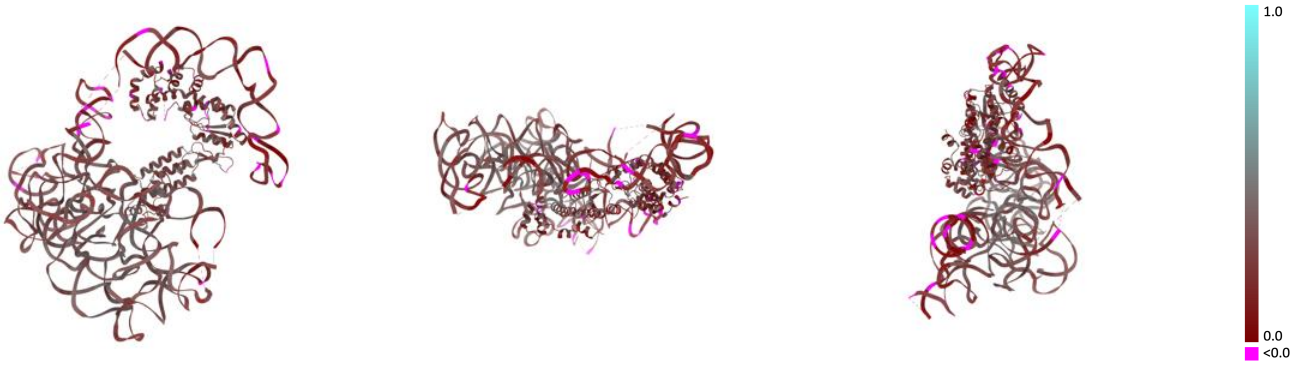
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.12 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.

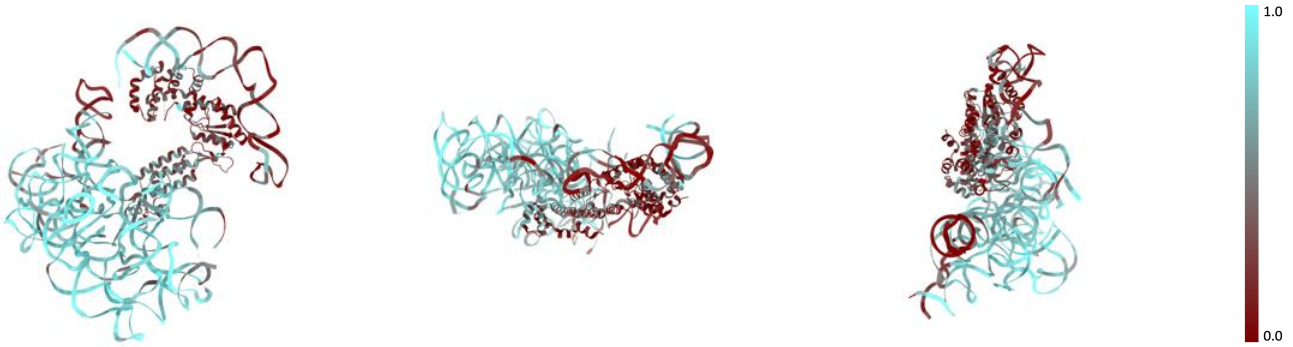
9.2 Q-score mapped to coordinate model (i)



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.

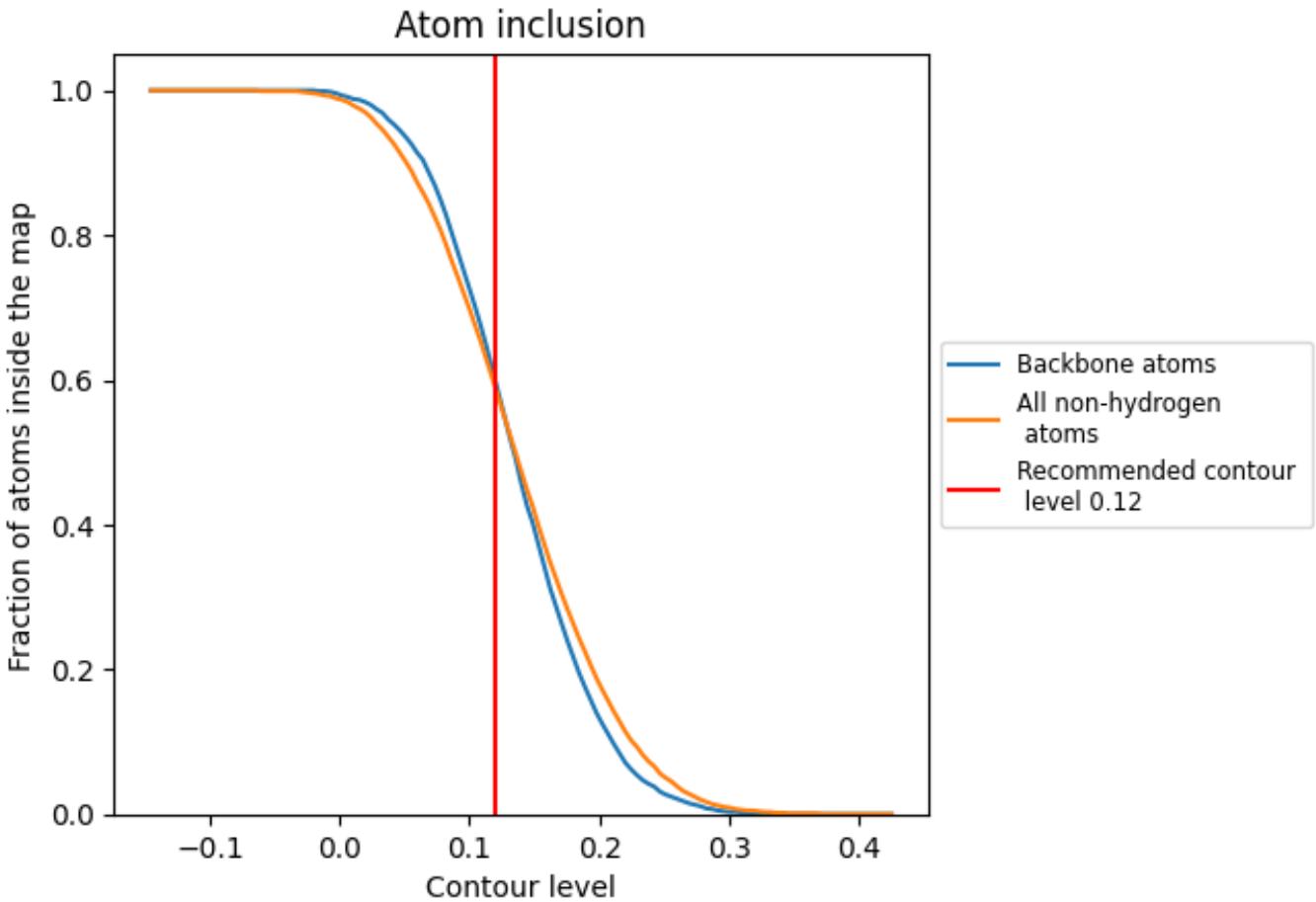
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.12).

9.4 Atom inclusion (i)



At the recommended contour level, 60% of all backbone atoms, 59% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5890	0.2620
B	0.6700	0.2700
D	0.2800	0.2310