wwPDB EM Validation Summary Report (i)

Sep 17, 2026 – 05:58 AM EDT

PDB ID	:	10QM / pdb_000010qm
EMDB ID	:	EMD-75389
Title	:	E.coli 50S ribosomal subunit bound to compound 48a
Authors	:	Raskar, T.; Lee, I.
Deposited on	:	2026-02-01
Resolution	:	2.49 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 (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 (1)) were used in the production of this report:

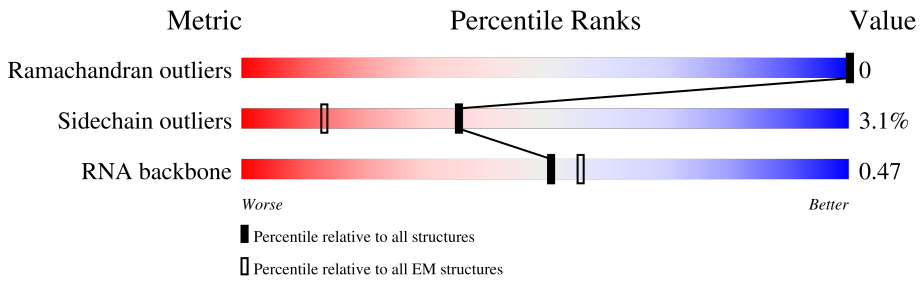
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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

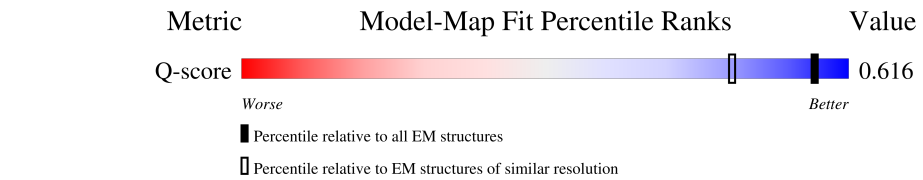
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.49 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))
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	6237 (2.00 - 2.99)

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	I	2904	17% 83% 17%
2	J	120	48% 83% 15% •
3	K	273	11% 97% • •
4	L	209	18% 98% •

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Mol	Chain	Length	Quality of chain
5	M	201	43% 99%
6	N	179	99% 95%
7	O	177	84% 95% 5%
8	P	149	93% 98%
9	Q	134	100% 98%
10	R	142	11% 98%
11	S	123	28% 98%
12	T	144	27% 97%
13	U	136	22% 96%
14	V	127	7% 93% 6%
15	W	117	75% 96%
16	X	115	27% 96%
17	Y	118	8% 98%
18	Z	103	38% 95%
19	a	110	13% 97%
20	b	100	34% 92% 7%
21	c	104	60% 97%
22	d	94	57% 96%
23	e	85	11% 86% 12%
24	f	77	29% 100%
25	g	62	74% 97%
26	h	58	16% 98%
27	i	56	27% 98%
28	j	50	64% 96%
29	k	46	96%

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Mol	Chain	Length	Quality of chain
30	l	64	6% 97%
31	m	38	24% 92% 8%

2 Entry composition (i)

There are 36 unique types of molecules in this entry. The entry contains 107784 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 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	I	2898	62229	27768	11448	20115	2898	0	0

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	J	118	2529	1126	464	821	118	0	0

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	K	271	2093	1294	427	365	7	1	0

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	L	209	1565	979	288	294	4	0	0

- Molecule 5 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	M	201	1552	974	283	290	5	0	0

- Molecule 6 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	N	177	1410	899	249	256	6	0	0

- Molecule 7 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	O	176	1323	832	243	246	2	0	0

- Molecule 8 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	P	149	1110	699	197	213	1	0	0

- Molecule 9 is a protein called Large ribosomal subunit protein uL11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	Q	134	979	619	169	185	6	0	0

- Molecule 10 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	R	142	1129	714	212	199	4	0	0

- Molecule 11 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	S	122	938	587	180	165	6	0	0

- Molecule 12 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	T	144	1053	654	207	190	2	0	0

- Molecule 13 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	U	136	1075	686	205	178	6	0	0

- Molecule 14 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	V	120	960	593	196	166	5	0	0

- Molecule 15 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
15	W	116	892	552	178	162	0	0

- Molecule 16 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	X	114	917	574	179	163	1	0	0

- Molecule 17 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
17	Y	117	947	604	192	151	0	0

- Molecule 18 is a protein called Ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	Z	103	816	516	153	145	2	0	0

- Molecule 19 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	a	110	857	532	166	156	3	0	0

- Molecule 20 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	b	93	738	466	139	131	2	0	0

- Molecule 21 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
21	c	102	779	492	146	141	0	0

- Molecule 22 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	d	94	753	479	137	134	3	0	0

- Molecule 23 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	e	75	575	356	116	102	1	0	0

- Molecule 24 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	f	77	625	388	129	106	2	0	0

- Molecule 25 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	g	62	501	308	98	94	1	0	0

- Molecule 26 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	h	58	449	281	87	79	2	0	0

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	i	56	444	269	94	80	1	0	0

- Molecule 28 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
28	j	50	409	263	75	71	0	0

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	k	46	377	228	90	57	2	0	0

- Molecule 30 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	l	64	504	323	105	74	2	0	0

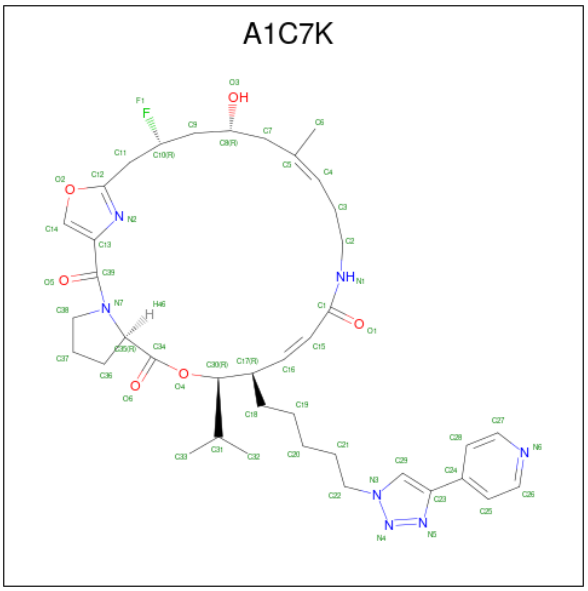
- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	m	38	302	185	65	48	4	0	0

- Molecule 32 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
32	I	183	183	183	0
32	J	1	1	1	0
32	V	1	1	1	0

- Molecule 33 is (3R,4R,5E,11E,14R,16R,23R,26aR)-16-fluoro-14-hydroxy-12-methyl-3-(propan-2-yl)-4-{5-[4-(pyridin-4-yl)-1H-1,2,3-triazol-1-yl]pentyl}-3,4,8,9,10,13,14,15,16,17,24,25,26,26a-tetradecahydro-1H,7H,22H-21,18-(azeno)pyrrolo[2,1-c][1,8,4,19]dioxadiazacyclotetracosine-1,7,22-trione (CCD ID: A1C7K) (formula: $C_{39}H_{52}FN_7O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	F	N	O	
33	I	1	53	39	1	7	6	0

- Molecule 34 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
			Total	Na	
34	K	1	1	1	0

- Molecule 35 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
35	m	1	1	1	0

- Molecule 36 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
36	I	11897	11897	11897	0
			Total	O	
36	J	549	549	549	0
			Total	O	
36	K	253	253	253	0
			Total	O	
36	L	221	221	221	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	O	
36	M	201	201	201	0
			Total	O	
36	N	274	274	274	0
			Total	O	
36	O	292	292	292	0
			Total	O	
36	P	430	430	430	0
			Total	O	
36	Q	359	359	359	0
			Total	O	
36	R	142	142	142	0
			Total	O	
36	S	120	120	120	0
			Total	O	
36	T	142	142	142	0
			Total	O	
36	U	143	143	143	0
			Total	O	
36	V	101	101	101	0
			Total	O	
36	W	147	147	147	0
			Total	O	
36	X	153	153	153	0
			Total	O	
36	Y	95	95	95	0
			Total	O	
36	Z	112	112	112	0
			Total	O	
36	a	106	106	106	0
			Total	O	
36	b	115	115	115	0
			Total	O	
36	c	161	161	161	0
			Total	O	
36	d	123	123	123	0
			Total	O	
36	e	76	76	76	0
			Total	O	
36	f	86	86	86	0
			Total	O	
36	g	92	92	92	0

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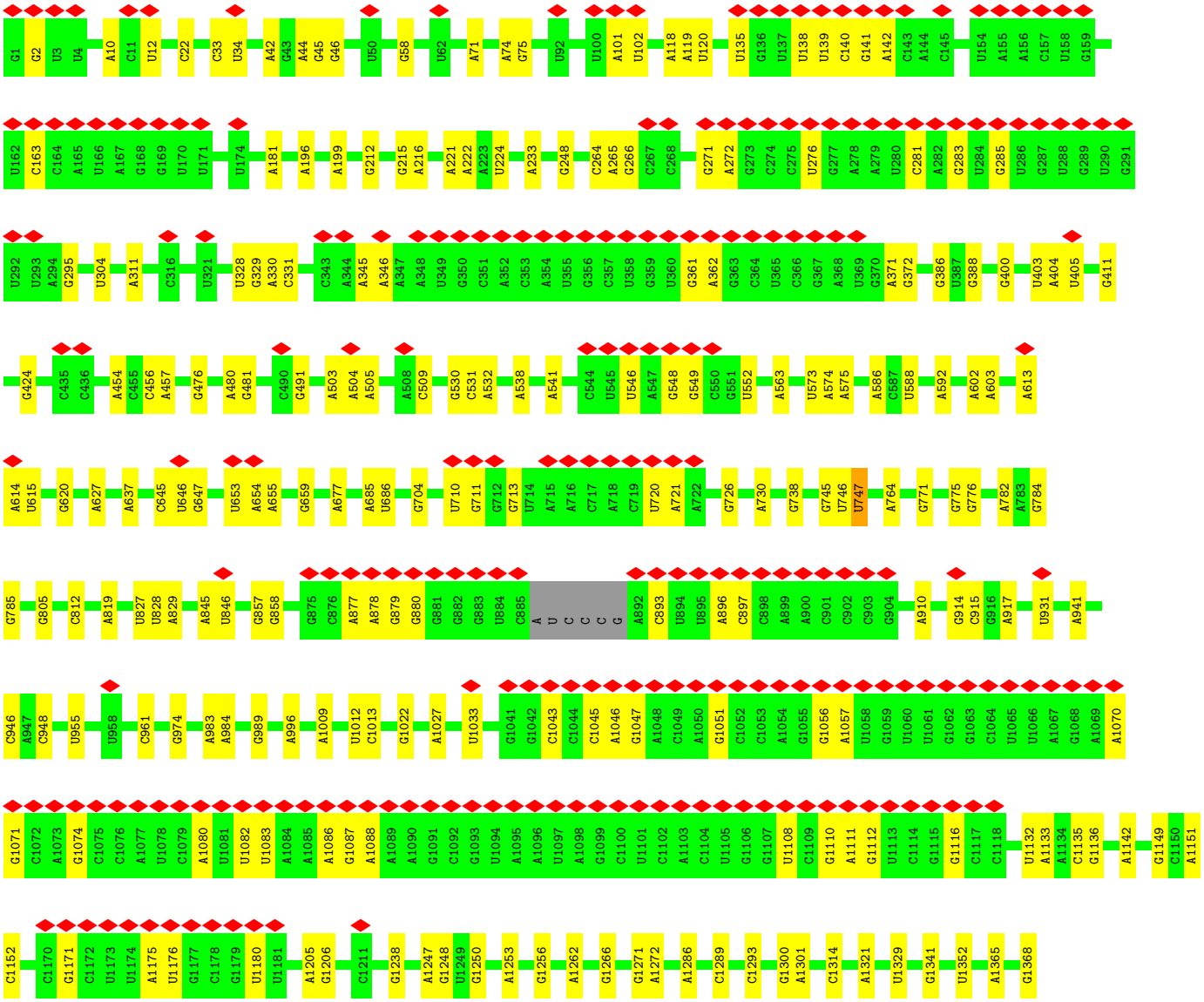
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
36	h	58	58	58	0
			Total	O	
36	i	70	70	70	0
			Total	O	
36	j	61	61	61	0
			Total	O	
36	k	59	59	59	0
			Total	O	
36	l	46	46	46	0
			Total	O	
36	m	30	30	30	0

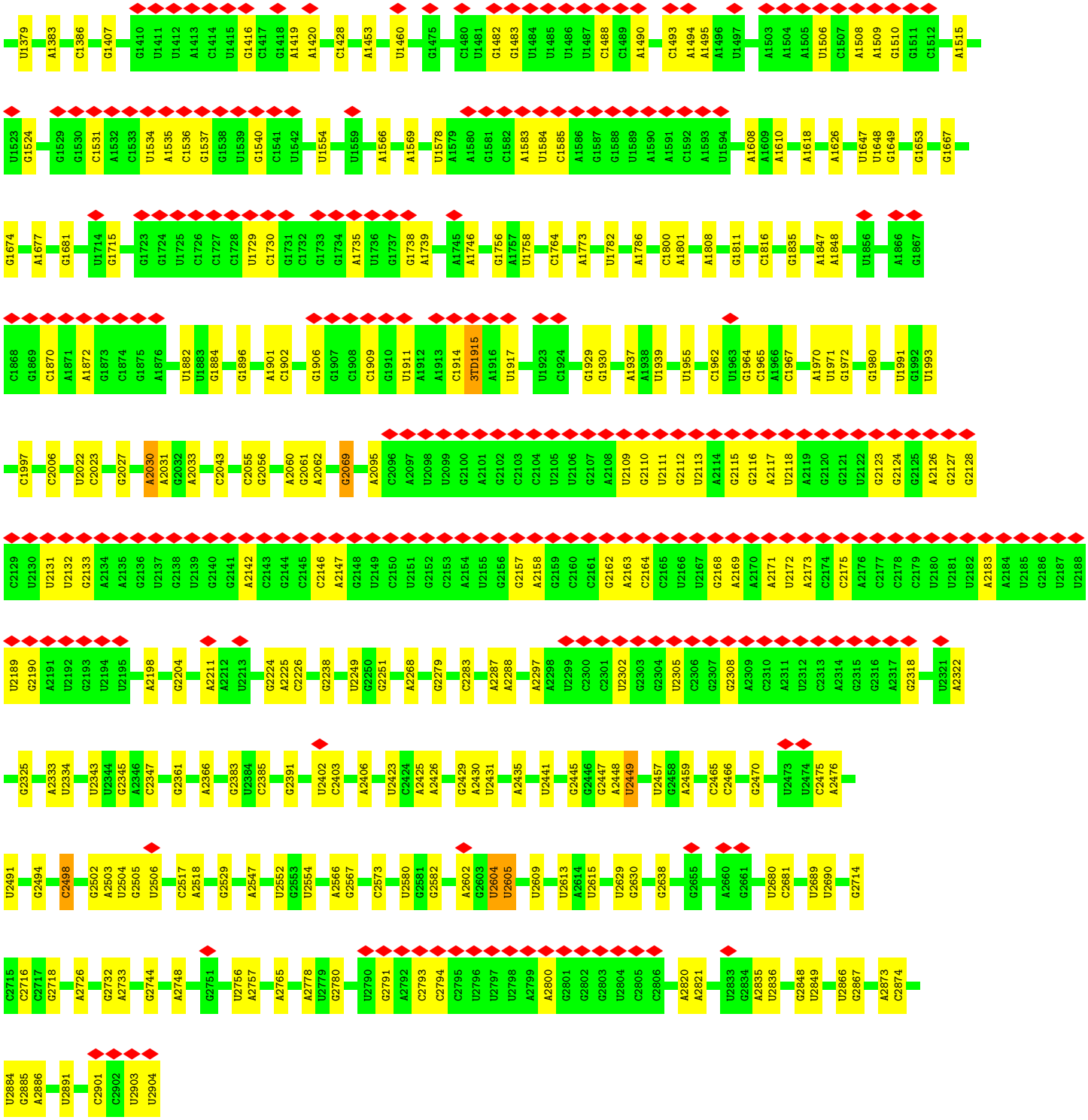
3 Residue-property plots (i)

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: 23S ribosomal RNA

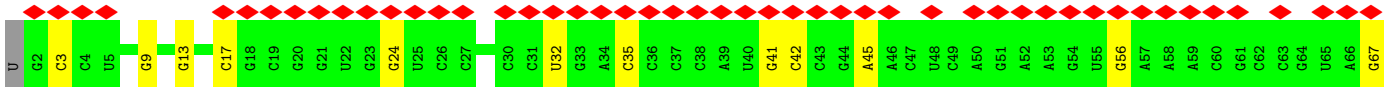
Chain I:

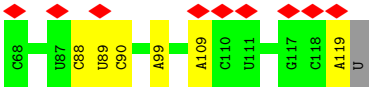




- Molecule 2: 5S ribosomal RNA

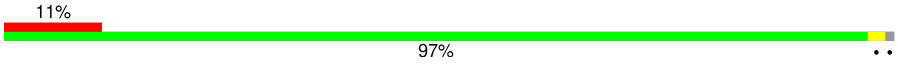
Chain J:

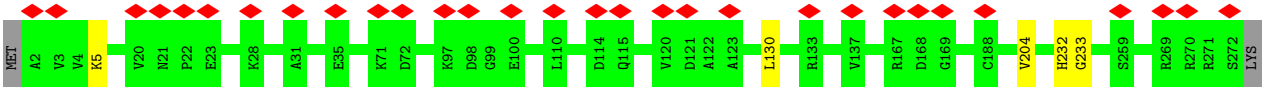




• Molecule 3: 50S ribosomal protein L2

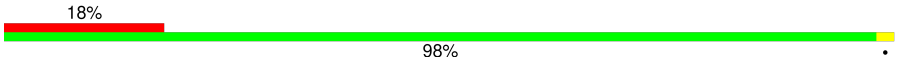
Chain K:

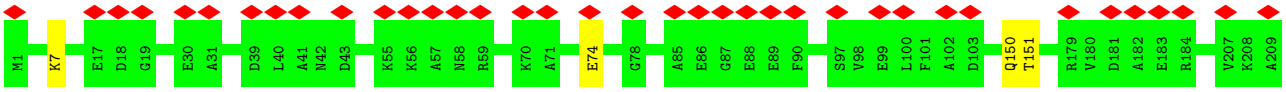




• Molecule 4: 50S ribosomal protein L3

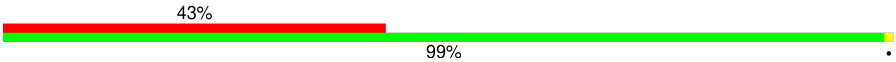
Chain L:

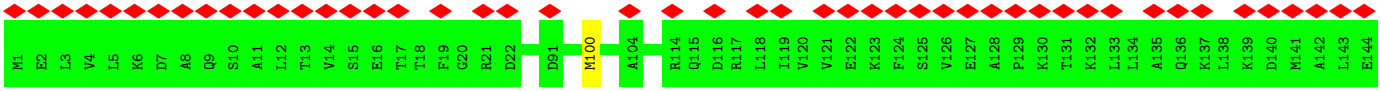


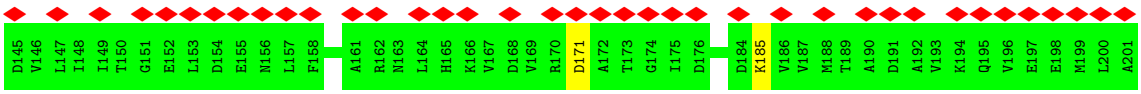


• Molecule 5: Large ribosomal subunit protein uL4

Chain M:

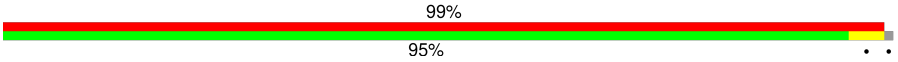






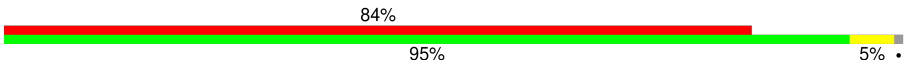
• Molecule 6: Large ribosomal subunit protein uL5

Chain N:



• Molecule 7: Large ribosomal subunit protein uL6

Chain O:



MET S2 R3 V4 A5 K6 A7 P8 V9 V10 V11 P12 A13 G14 V15 D16 V17 K18 I19 N20 G21 Q22 V23 I24 T25 I26 K27 G28 K29 N30 G31 E32 L33 T34 R35 T36 L37 N38 D39 A40 V41 E42 V43 K44 H45 A46 D47 N48 T49 L50 T51 F52 G53 P54 R55 D56 G57 Y58 A59 D60

G61 W62 A63 Q64 A65 A68 R69 A70 L71 L72 N73 S74 M75 V76 I77 G78 V79 T80 E81 T84 K85 K86 L87 Q88 G91 V92 G93 Y94 R95 A96 A97 V98 K99 G100 N101 V102 I103 N104 L105 S106 L107 G108 F109 S110 H111 P112 V113 D114 H115 Q116 L117 P118 A119 G120 I121 T122 A123

E124 C125 P126 T127 Q128 T129 E130 I131 V132 L133 K134 G135 A136 D137 K138 Q139 D147 L148 R149 A150 Y151 R152 R153 P154 E155 P156 Y157 K158 G159 K160 R163 Y164 A165 D166 E167 V168 V169 R170 T171 K172 E173 A174 K175 K176 K177

- Molecule 8: Large ribosomal subunit protein bL9

Chain P: 93% 98%

M1 Q2 V3 I4 L5 L6 D7 K8 V9 A10 N11 L12 G13 S14 L15 G16 D17 Q18 V19 N20 V21 K22 F29 Q33 G34 K35 A36 V37 P38 A39 T40 K41 K42 N43 I44 E45 F46 F47 E48 A49 R50 R51 A52 E53 L54 E55 A56 K57 L58 A59 E60 V61 L62 A63 A64 A65 N66 A67

R68 A69 E70 K71 I72 N73 A74 L75 E76 T77 V78 T79 I80 A81 S82 K83 A84 G85 D86 E87 G88 K89 L90 F91 G92 S93 I94 G95 T96 R97 D98 I99 A100 D101 A102 V103 T104 A105 A106 G107 V108 E109 V110 A111 K112 S113 E114 V115 R116 L117 P118 N119 G120 V121 L122 R123 T124 T125 G126 E127

H128 E129 V130 S131 F132 Q133 V134 H135 S136 E137 V138 F139 A140 K141 V142 I143 V144 N145 V146 V147 A148 E149

- Molecule 9: Large ribosomal subunit protein uL11

Chain Q: 100% 98%

Y8 V9 K10 L11 Q12 V13 A14 A15 G16 M17 A18 N19 P20 S21 P22 P23 V24 G25 P26 A27 L28 G29 Q30 Q31 G32 V33 N34 I35 M36 E37 F38 C39 K40 A41 F42 N43 A44 K45 T46 D47 S48 I49 E50 K51 G52 L53 P54 I55 P56 V57 V58 I59 T60 V61 Y62 A63 D64 R65 S66 F67

T68 F69 V70 T71 K72 T73 P74 P75 A76 A77 V78 L79 L80 K81 K82 A83 A84 G85 I86 K87 S88 G89 S90 G91 K92 P93 N94 K95 D96 K97 V98 G99 K100 I101 S102 R103 A104 Q105 L106 Q107 E108 I109 A110 Q111 T112 K113 A114 A115 D116 M117 T118 G119 A120 D121 I122 E123 A124 M125 T126 R127

S128 I129 E130 G131 T132 A133 R134 S135 M136 G137 L138 V139 V140 E141

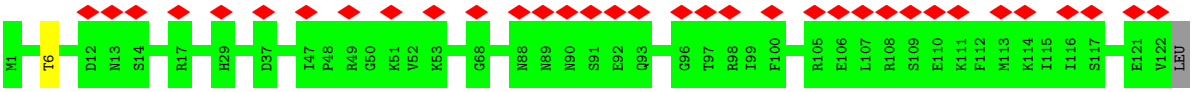
- Molecule 10: Large ribosomal subunit protein uL13

Chain R: 11% 98%

M1 K2 E9 T10 V11 K12 D19 D71 E90 R95 R96 N128 E129 H130 N131 Q136 P137 Q138 D141 I142

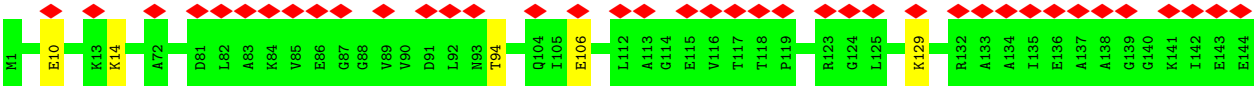
- Molecule 11: Large ribosomal subunit protein uL14

Chain S: 28% 98%



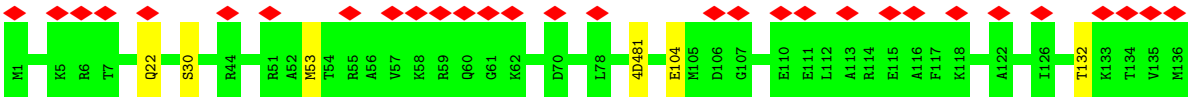
• Molecule 12: Large ribosomal subunit protein uL15

Chain T: 27% 97%



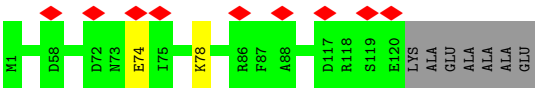
• Molecule 13: 50S ribosomal protein L16

Chain U: 22% 96%



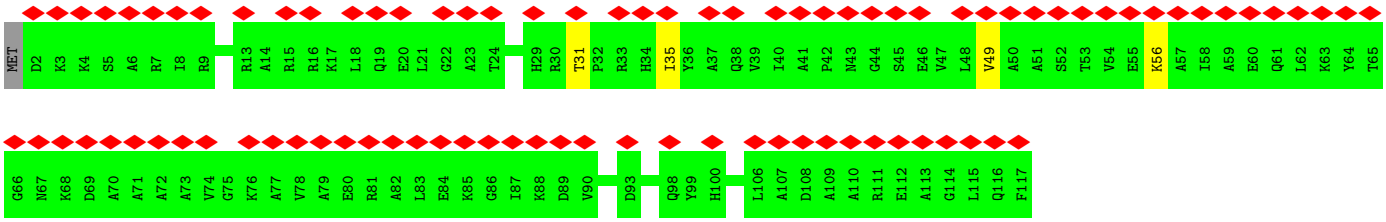
• Molecule 14: Large ribosomal subunit protein bL17

Chain V: 7% 93% 6%



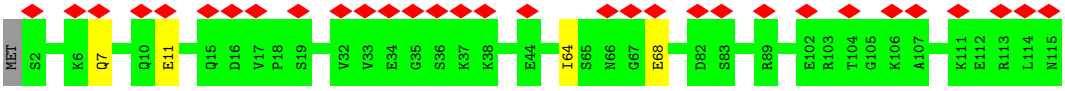
• Molecule 15: Large ribosomal subunit protein uL18

Chain W: 75% 96%



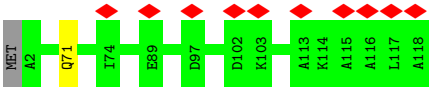
• Molecule 16: Large ribosomal subunit protein bL19

Chain X: 27% 96%



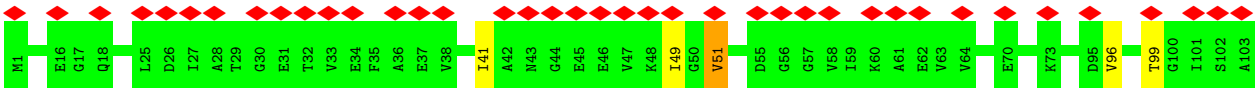
• Molecule 17: 50S ribosomal protein L20

Chain Y: 8% 98%



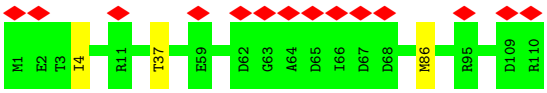
• Molecule 18: Ribosomal protein L21

Chain Z: 38% 95%



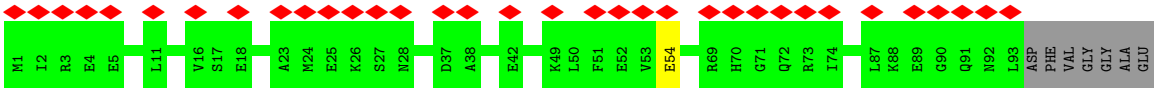
• Molecule 19: 50S ribosomal protein L22

Chain a: 13% 97%



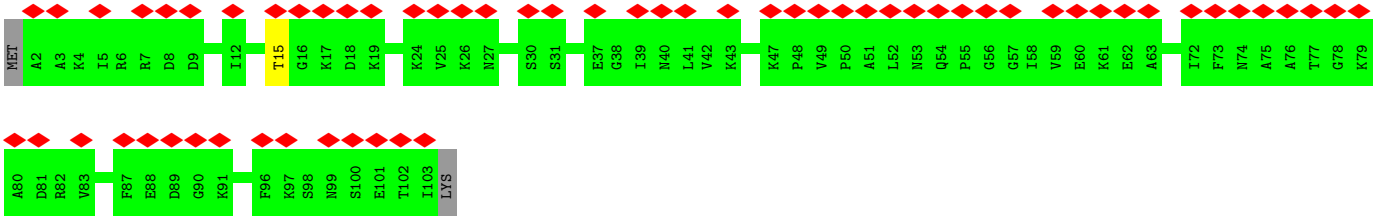
• Molecule 20: 50S ribosomal protein L23

Chain b: 34% 92% 7%



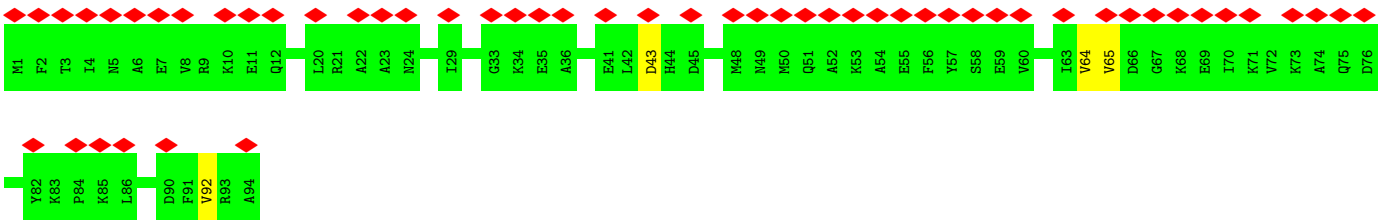
• Molecule 21: 50S ribosomal protein L24

Chain c: 60% 97%



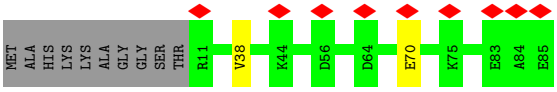
• Molecule 22: Large ribosomal subunit protein bL25

Chain d: 57% 96%



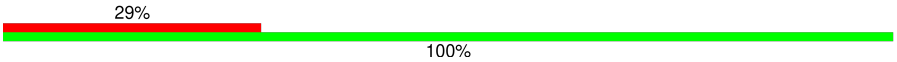
- Molecule 23: 50S ribosomal protein L27

Chain e:



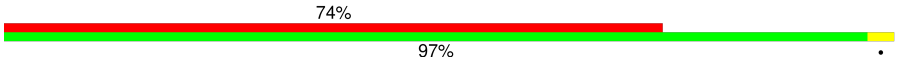
- Molecule 24: 50S ribosomal protein L28

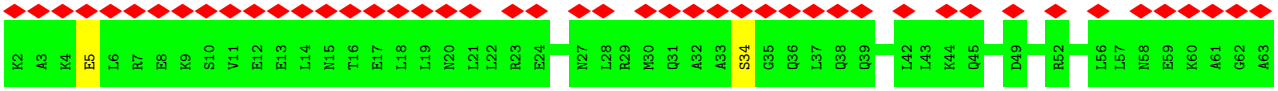
Chain f:



- Molecule 25: Large ribosomal subunit protein uL29

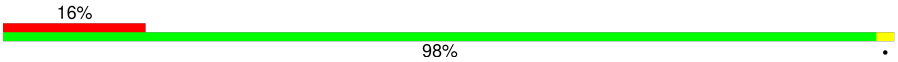
Chain g:

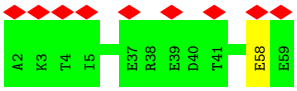




- Molecule 26: 50S ribosomal protein L30

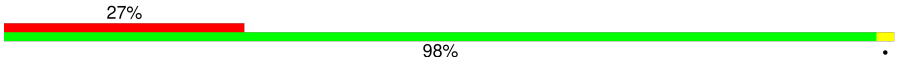
Chain h:

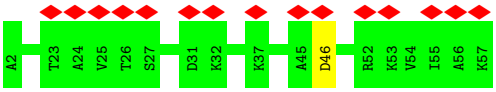




- Molecule 27: 50S ribosomal protein L32

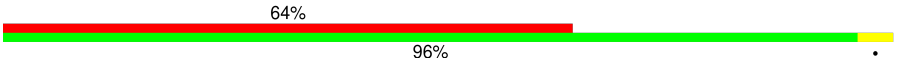
Chain i:

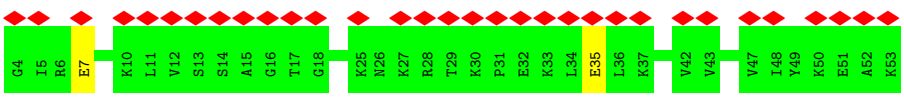




- Molecule 28: Large ribosomal subunit protein bL33

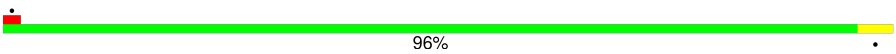
Chain j:

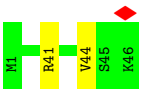




- Molecule 29: 50S ribosomal protein L34

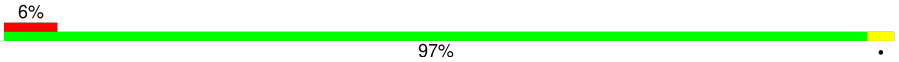
Chain k:

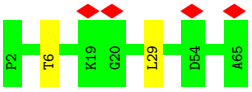




• Molecule 30: Large ribosomal subunit protein bL35

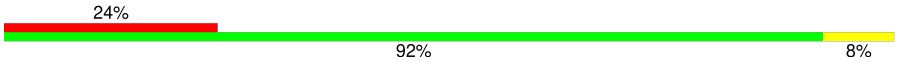
Chain l:

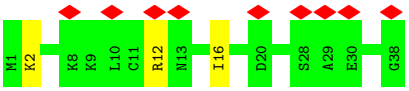




• Molecule 31: 50S ribosomal protein L36

Chain m:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	569471	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.266	Depositor
Minimum map value	-1.344	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.057	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	429.24002, 429.24002, 429.24002	wwPDB
Map dimensions	588, 588, 588	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.73, 0.73, 0.73	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: ZN, 1MG, NA, OMU, H2U, G7M, 3TD, OMC, 5MU, A1C7K, 4D4, 6MZ, 2MG, OMG, PSU, 5MC, 2MA, 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	I	0.46	0/69121	0.42	0/107828
2	J	0.34	0/2828	0.34	0/4410
3	K	0.38	0/2132	0.53	1/2866 (0.0%)
4	L	0.38	0/1586	0.48	0/2134
5	M	0.35	0/1571	0.47	0/2113
6	N	0.26	0/1434	0.54	0/1926
7	O	0.27	0/1343	0.51	2/1816 (0.1%)
8	P	0.20	0/1121	0.49	0/1515
9	Q	0.21	0/993	0.50	0/1341
10	R	0.35	0/1152	0.43	0/1551
11	S	0.36	0/947	0.47	0/1268
12	T	0.36	0/1062	0.52	0/1413
13	U	0.35	0/1081	0.47	0/1443
14	V	0.39	0/973	0.50	0/1301
15	W	0.30	0/902	0.45	0/1209
16	X	0.34	0/929	0.45	0/1242
17	Y	0.38	0/960	0.44	0/1278
18	Z	0.36	0/829	0.46	0/1107
19	a	0.36	0/864	0.48	0/1156
20	b	0.32	0/744	0.44	0/994
21	c	0.34	0/787	0.49	0/1051
22	d	0.31	0/766	0.41	0/1025
23	e	0.35	0/582	0.48	0/769
24	f	0.32	0/635	0.46	0/848
25	g	0.28	0/502	0.44	0/667
26	h	0.34	0/453	0.42	0/605
27	i	0.37	0/450	0.48	0/599
28	j	0.30	0/416	0.47	0/554
29	k	0.41	0/380	0.55	0/498
30	l	0.39	0/513	0.50	0/676
31	m	0.36	0/303	0.46	0/397

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
All	All	0.43	0/98359	0.43	3/147600 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	K	0	1
9	Q	0	1
18	Z	0	1
All	All	0	3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	O	154	PRO	CA-C-N	-6.69	111.04	123.55
7	O	154	PRO	C-N-CA	-6.69	111.04	123.55
3	K	233	GLY	N-CA-C	5.21	120.56	111.50

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	K	232	HIS	Peptide
9	Q	19	ASN	Peptide
18	Z	51	VAL	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	
3	K	270/273 (99%)	255 (94%)	15 (6%)	0	100	100
4	L	207/209 (99%)	195 (94%)	12 (6%)	0	100	100
5	M	199/201 (99%)	191 (96%)	8 (4%)	0	100	100
6	N	175/179 (98%)	155 (89%)	20 (11%)	0	100	100
7	O	174/177 (98%)	163 (94%)	11 (6%)	0	100	100
8	P	147/149 (99%)	136 (92%)	11 (8%)	0	100	100
9	Q	132/134 (98%)	109 (83%)	23 (17%)	0	100	100
10	R	140/142 (99%)	139 (99%)	1 (1%)	0	100	100
11	S	120/123 (98%)	116 (97%)	4 (3%)	0	100	100
12	T	142/144 (99%)	140 (99%)	2 (1%)	0	100	100
13	U	133/136 (98%)	128 (96%)	5 (4%)	0	100	100
14	V	118/127 (93%)	113 (96%)	5 (4%)	0	100	100
15	W	114/117 (97%)	107 (94%)	7 (6%)	0	100	100
16	X	112/115 (97%)	109 (97%)	3 (3%)	0	100	100
17	Y	115/118 (98%)	115 (100%)	0	0	100	100
18	Z	101/103 (98%)	93 (92%)	8 (8%)	0	100	100
19	a	108/110 (98%)	102 (94%)	6 (6%)	0	100	100
20	b	91/100 (91%)	84 (92%)	7 (8%)	0	100	100
21	c	100/104 (96%)	92 (92%)	8 (8%)	0	100	100
22	d	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
23	e	73/85 (86%)	72 (99%)	1 (1%)	0	100	100
24	f	75/77 (97%)	72 (96%)	3 (4%)	0	100	100
25	g	60/62 (97%)	56 (93%)	4 (7%)	0	100	100
26	h	56/58 (97%)	54 (96%)	2 (4%)	0	100	100
27	i	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
28	j	48/50 (96%)	46 (96%)	2 (4%)	0	100	100
29	k	44/46 (96%)	44 (100%)	0	0	100	100
30	l	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
31	m	36/38 (95%)	36 (100%)	0	0	100	100
All	All	3298/3391 (97%)	3123 (95%)	175 (5%)	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	
3	K	217/218 (100%)	214 (99%)	3 (1%)	59	81
4	L	164/164 (100%)	160 (98%)	4 (2%)	43	70
5	M	165/165 (100%)	162 (98%)	3 (2%)	51	77
6	N	148/150 (99%)	141 (95%)	7 (5%)	23	47
7	O	137/138 (99%)	130 (95%)	7 (5%)	21	43
8	P	114/114 (100%)	111 (97%)	3 (3%)	40	68
9	Q	104/104 (100%)	102 (98%)	2 (2%)	50	76
10	R	116/116 (100%)	113 (97%)	3 (3%)	40	68
11	S	103/104 (99%)	102 (99%)	1 (1%)	68	86
12	T	103/103 (100%)	98 (95%)	5 (5%)	22	45
13	U	108/108 (100%)	103 (95%)	5 (5%)	24	48
14	V	100/103 (97%)	98 (98%)	2 (2%)	48	75
15	W	86/87 (99%)	82 (95%)	4 (5%)	23	47
16	X	99/100 (99%)	95 (96%)	4 (4%)	28	54
17	Y	89/90 (99%)	88 (99%)	1 (1%)	65	84
18	Z	84/84 (100%)	79 (94%)	5 (6%)	17	36
19	a	93/93 (100%)	90 (97%)	3 (3%)	34	62
20	b	80/84 (95%)	79 (99%)	1 (1%)	61	82
21	c	83/85 (98%)	82 (99%)	1 (1%)	63	83
22	d	78/78 (100%)	74 (95%)	4 (5%)	21	43
23	e	57/63 (90%)	55 (96%)	2 (4%)	32	58
24	f	67/67 (100%)	67 (100%)	0	100	100
25	g	54/54 (100%)	52 (96%)	2 (4%)	30	57
26	h	48/48 (100%)	47 (98%)	1 (2%)	47	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	i	47/47 (100%)	46 (98%)	1 (2%)	47	74
28	j	45/45 (100%)	43 (96%)	2 (4%)	25	50
29	k	38/38 (100%)	36 (95%)	2 (5%)	20	42
30	l	51/51 (100%)	49 (96%)	2 (4%)	28	55
31	m	34/34 (100%)	31 (91%)	3 (9%)	9	20
All	All	2712/2735 (99%)	2629 (97%)	83 (3%)	36	62

5 of 83 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	Z	96	VAL
25	g	34	SER
19	a	4	ILE
22	d	64	VAL
28	j	35	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
25	g	20	ASN
26	h	20	HIS
11	S	5	GLN
9	Q	111	GLN
29	k	26	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	I	2896/2904 (99%)	464 (16%)	22 (0%)
2	J	117/120 (97%)	18 (15%)	0
All	All	3013/3024 (99%)	482 (15%)	22 (0%)

5 of 482 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	I	2	G
1	I	10	A
1	I	12	U

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Mol	Chain	Res	Type
1	I	22	C
1	I	33	C

5 of 22 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	I	2425	A
1	I	2680	U
1	I	2447	G
1	I	2756	U
1	I	984	A

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

25 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	2MG	I	1835	1	23,26,27	0.91	1 (4%)	33,38,41	2.03	8 (24%)
1	G7M	I	2069	1	23,26,27	0.67	0	34,39,42	0.87	1 (2%)
1	6MZ	I	2030	1	22,25,26	1.21	3 (13%)	29,36,39	2.34	9 (31%)
1	PSU	I	2605	1	18,21,22	1.32	3 (16%)	21,30,33	2.23	6 (28%)
1	2MA	I	2503	32,1	22,25,26	1.41	4 (18%)	32,37,40	2.01	7 (21%)
1	2MG	I	2445	1	23,26,27	1.16	3 (13%)	33,38,41	2.26	10 (30%)
1	PSU	I	2604	1	18,21,22	1.31	3 (16%)	21,30,33	2.32	6 (28%)
1	PSU	I	2457	1	18,21,22	1.32	3 (16%)	21,30,33	2.33	4 (19%)
1	PSU	I	2580	1	18,21,22	1.38	4 (22%)	21,30,33	2.27	7 (33%)
1	1MG	I	745	1	23,26,27	1.18	3 (13%)	33,39,42	1.74	6 (18%)
1	5MU	I	1939	1	19,22,23	1.47	4 (21%)	27,32,35	2.24	6 (22%)
1	PSU	I	746	1	18,21,22	1.38	4 (22%)	21,30,33	2.11	5 (23%)
1	H2U	I	2449	1	18,21,22	0.62	0	19,30,33	1.11	1 (5%)
1	OMC	I	2498	32,1	19,22,23	1.05	2 (10%)	25,31,34	1.08	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	6MZ	I	1618	1	22,25,26	1.27	2 (9%)	29,36,39	2.20	8 (27%)
1	3TD	I	1915	1	19,22,23	1.23	4 (21%)	23,32,35	1.93	3 (13%)
1	PSU	I	2504	1	18,21,22	1.28	3 (16%)	21,30,33	2.15	4 (19%)
13	4D4	U	81	13	9,11,12	0.92	0	7,13,15	1.58	2 (28%)
1	PSU	I	955	1	18,21,22	1.32	3 (16%)	21,30,33	2.18	4 (19%)
1	PSU	I	1911	1	18,21,22	0.98	1 (5%)	21,30,33	2.06	4 (19%)
1	OMG	I	2251	1	23,26,27	0.99	2 (8%)	32,38,41	1.88	7 (21%)
1	PSU	I	1917	1	18,21,22	1.04	2 (11%)	21,30,33	2.02	3 (14%)
1	5MC	I	1962	1	19,22,23	1.39	3 (15%)	26,32,35	1.11	2 (7%)
1	OMU	I	2552	1	19,22,23	1.39	4 (21%)	25,31,34	2.07	6 (24%)
1	5MU	I	747	1	19,22,23	1.30	3 (15%)	27,32,35	1.92	5 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MG	I	1835	1	-	0/9/27/28	0/3/3/3
1	G7M	I	2069	1	-	1/7/25/26	0/3/3/3
1	6MZ	I	2030	1	-	2/9/27/28	0/3/3/3
1	PSU	I	2605	1	-	2/7/25/26	0/2/2/2
1	2MA	I	2503	32,1	-	1/7/25/26	0/3/3/3
1	2MG	I	2445	1	-	2/9/27/28	0/3/3/3
1	PSU	I	2604	1	-	2/7/25/26	0/2/2/2
1	PSU	I	2457	1	-	0/7/25/26	0/2/2/2
1	PSU	I	2580	1	-	0/7/25/26	0/2/2/2
1	1MG	I	745	1	-	0/7/25/26	0/3/3/3
1	5MU	I	1939	1	-	0/7/25/26	0/2/2/2
1	PSU	I	746	1	-	0/7/25/26	0/2/2/2
1	H2U	I	2449	1	-	1/7/38/39	0/2/2/2
1	OMC	I	2498	32,1	-	1/9/27/28	0/2/2/2
1	6MZ	I	1618	1	-	0/9/27/28	0/3/3/3
1	3TD	I	1915	1	-	2/7/25/26	0/2/2/2
1	PSU	I	2504	1	-	2/7/25/26	0/2/2/2
13	4D4	U	81	13	-	0/11/12/14	-
1	PSU	I	955	1	-	0/7/25/26	0/2/2/2
1	PSU	I	1911	1	-	0/7/25/26	0/2/2/2
1	OMG	I	2251	1	-	1/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	I	1917	1	-	0/7/25/26	0/2/2/2
1	5MC	I	1962	1	-	2/7/25/26	0/2/2/2
1	OMU	I	2552	1	-	0/9/27/28	0/2/2/2
1	5MU	I	747	1	-	0/7/25/26	0/2/2/2

The worst 5 of 64 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	2503	2MA	C5-N7	-3.59	1.32	1.39
1	I	1962	5MC	C5-C4	-3.52	1.41	1.44
1	I	1962	5MC	C2-N1	-3.41	1.32	1.40
1	I	2503	2MA	C6-N1	3.39	1.39	1.35
1	I	1939	5MU	C2-N1	-3.39	1.33	1.38

The worst 5 of 126 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	2445	2MG	C2-N3-C4	7.42	121.28	112.00
1	I	1835	2MG	C2-N3-C4	6.87	120.59	112.00
1	I	2604	PSU	N1-C2-N3	6.72	122.26	115.17
1	I	2457	PSU	N1-C2-N3	6.70	122.24	115.17
1	I	2605	PSU	N1-C2-N3	6.61	122.14	115.17

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	I	1915	3TD	O4'-C4'-C5'-O5'
1	I	2251	OMG	C1'-C2'-O2'-CM2
1	I	1915	3TD	C3'-C4'-C5'-O5'
1	I	2504	PSU	O4'-C4'-C5'-O5'
1	I	2604	PSU	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 188 ligands modelled in this entry, 187 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
33	A1C7K	I	3184	-	55,57,57	3.90	25 (45%)	67,77,77	1.94	14 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	A1C7K	I	3184	-	-	13/60/70/70	0/4/5/5

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	I	3184	A1C7K	C39-N7	9.79	1.48	1.34
33	I	3184	A1C7K	C4-C5	8.61	1.52	1.33
33	I	3184	A1C7K	C7-C5	-8.24	1.35	1.51
33	I	3184	A1C7K	O6-C34	8.04	1.41	1.21
33	I	3184	A1C7K	C25-C26	7.72	1.53	1.38

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	I	3184	A1C7K	O2-C12-N2	-6.17	107.42	114.09
33	I	3184	A1C7K	C3-C4-C5	-5.38	115.31	127.62
33	I	3184	A1C7K	C36-C35-N7	4.75	109.98	103.02
33	I	3184	A1C7K	O2-C14-C13	-4.53	104.77	108.12
33	I	3184	A1C7K	C30-O4-C34	3.60	123.74	117.76

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

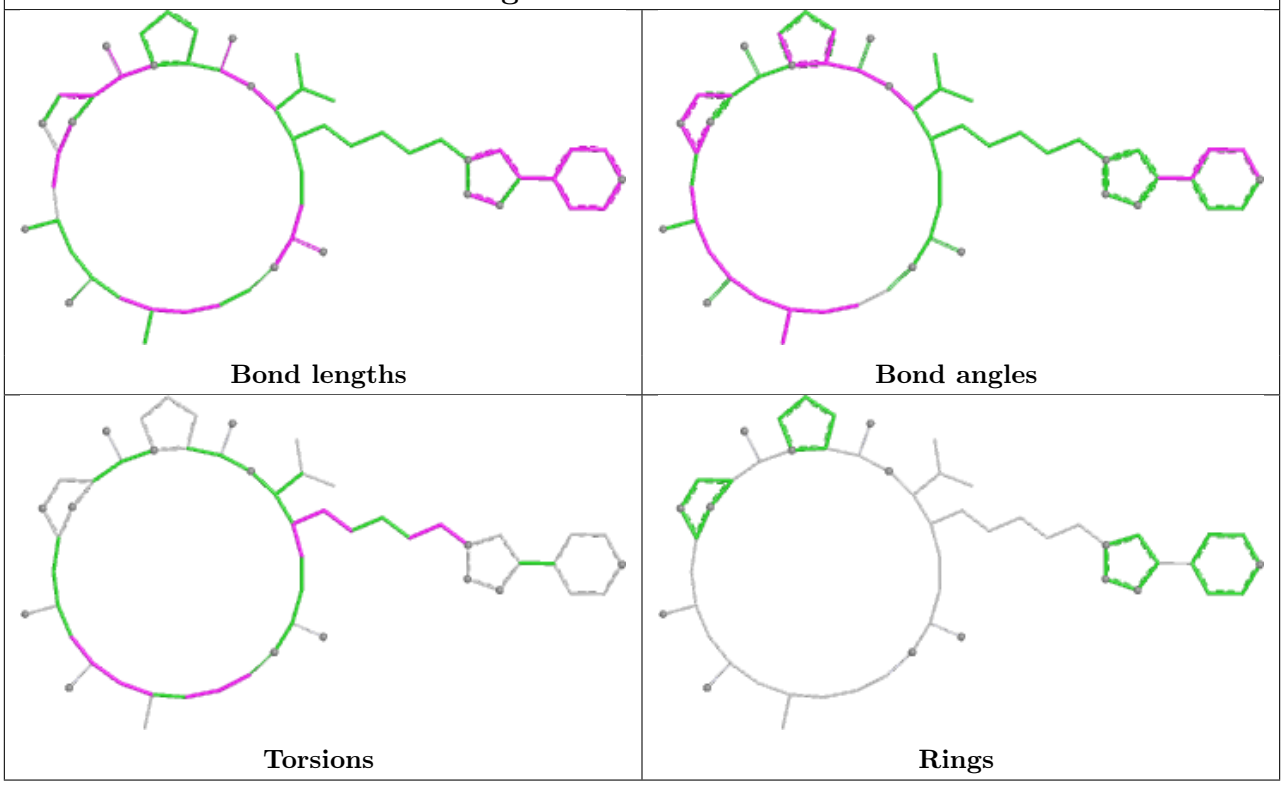
Mol	Chain	Res	Type	Atoms
33	I	3184	A1C7K	C4-C5-C7-C8
33	I	3184	A1C7K	C6-C5-C7-C8
33	I	3184	A1C7K	C5-C7-C8-C9
33	I	3184	A1C7K	C5-C7-C8-O3
33	I	3184	A1C7K	C15-C16-C17-C18

There are no ring outliers.

No monomer is involved in short contacts.

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

Ligand A1C7K I 3184



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.

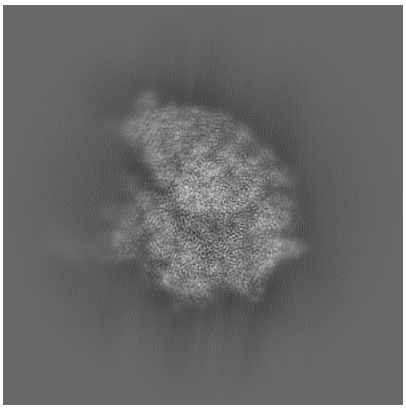
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-75389. 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



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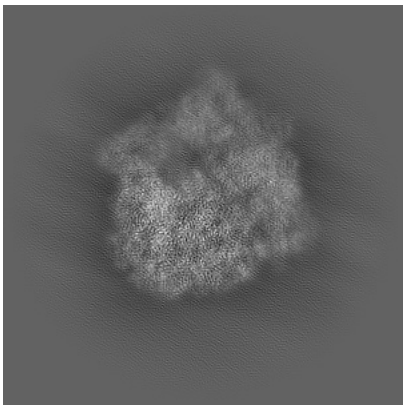

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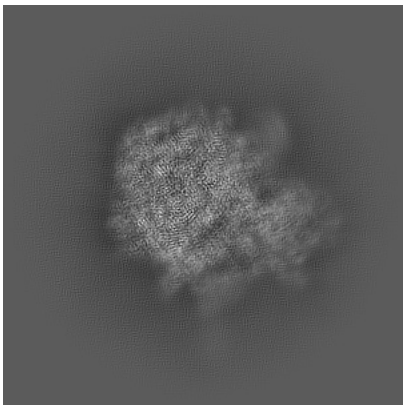
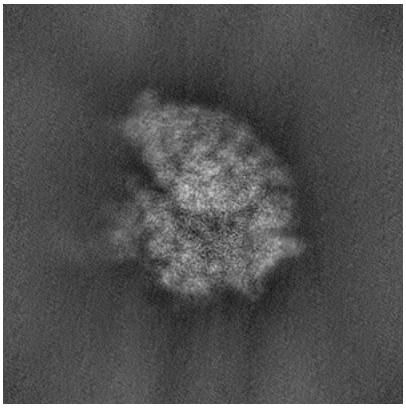


Z

6.1.2 Raw map



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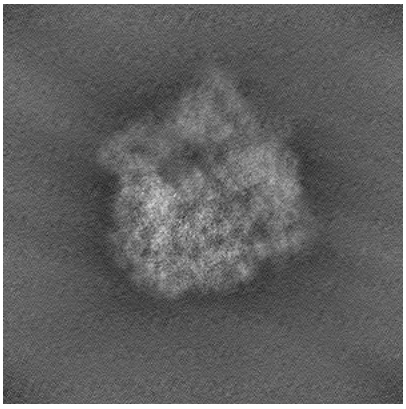
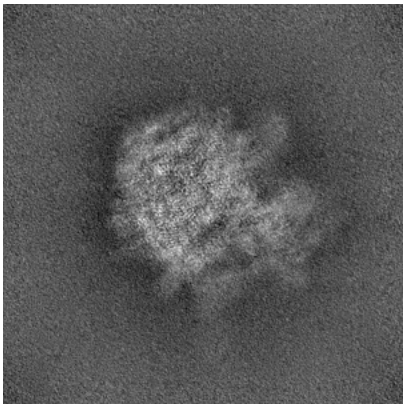


Y

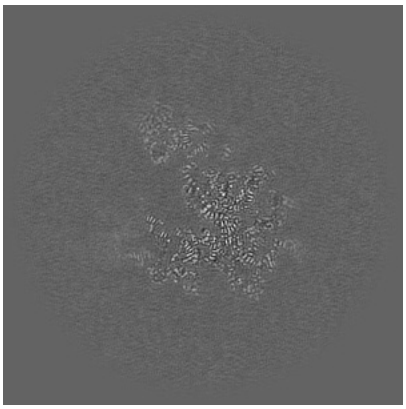


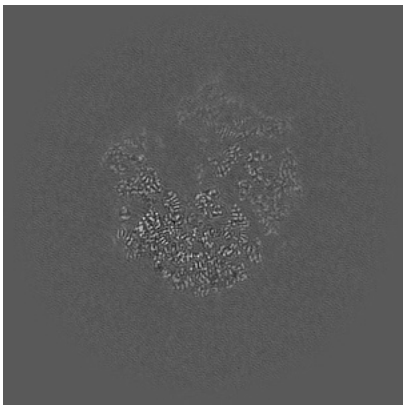
Z

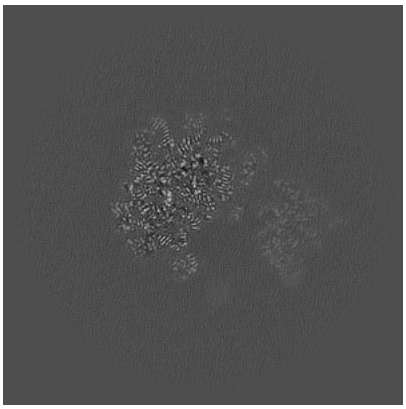
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

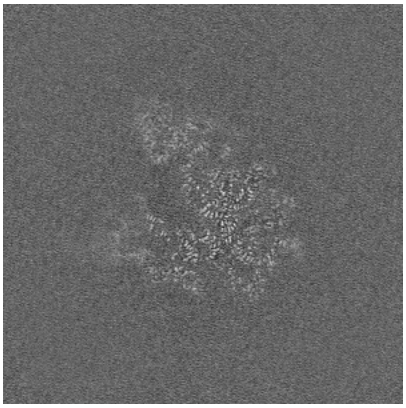
6.2.1 Primary map

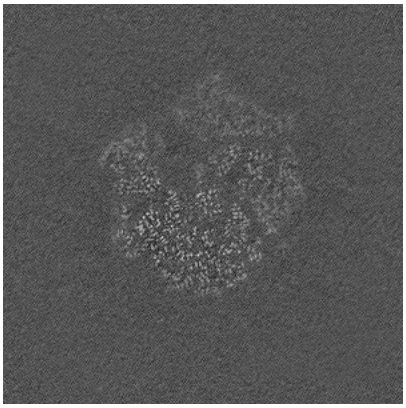

X Index: 294


Y Index: 294


Z Index: 294

6.2.2 Raw map


X Index: 294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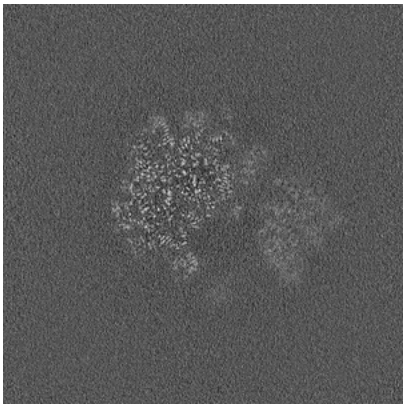
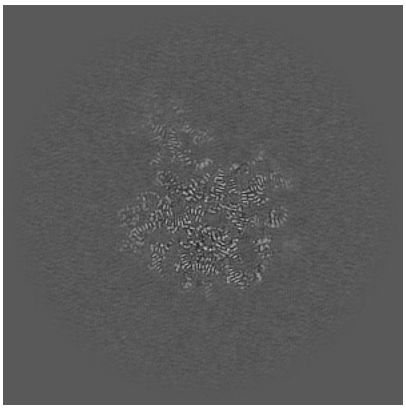

Z Index: 294

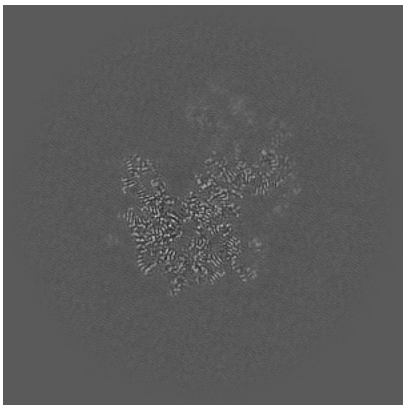
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

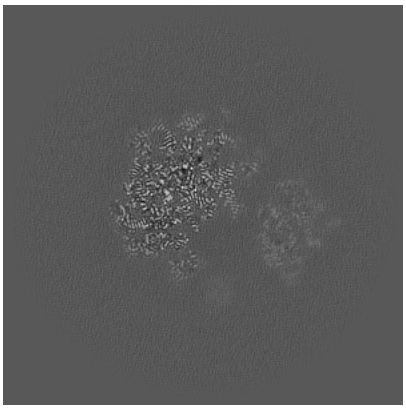
6.3.1 Primary map



X Index: 258

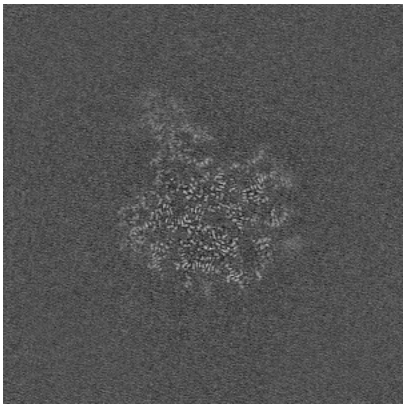


Y Index: 314



Z Index: 290

6.3.2 Raw map



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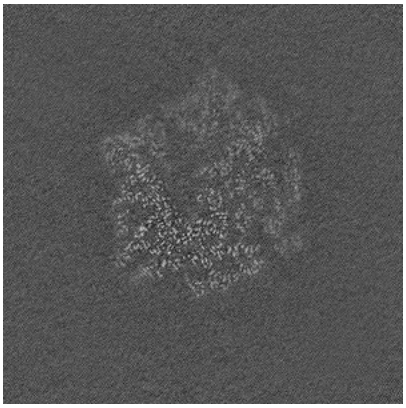

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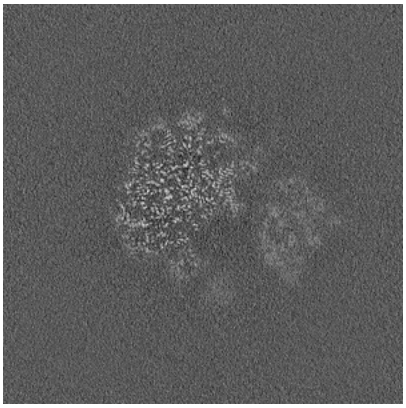
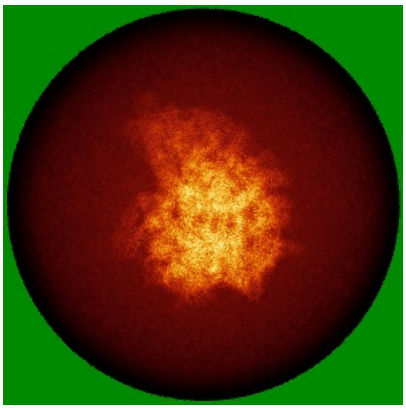


Z Index: 290

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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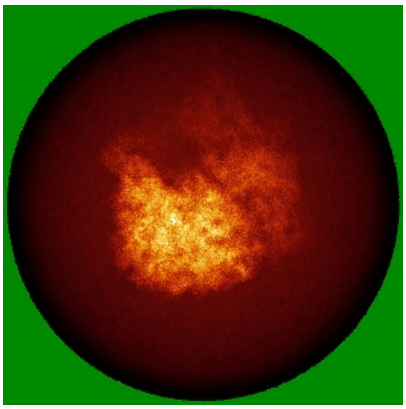
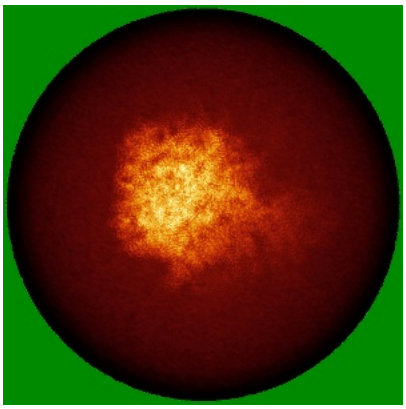
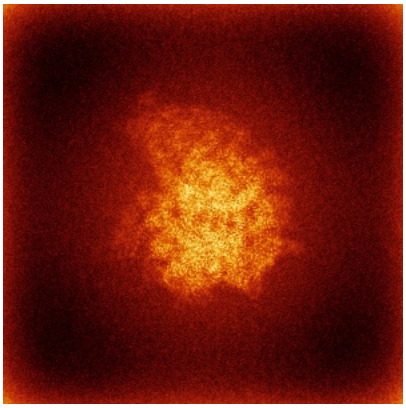
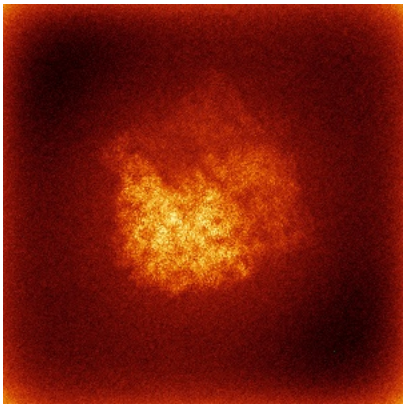
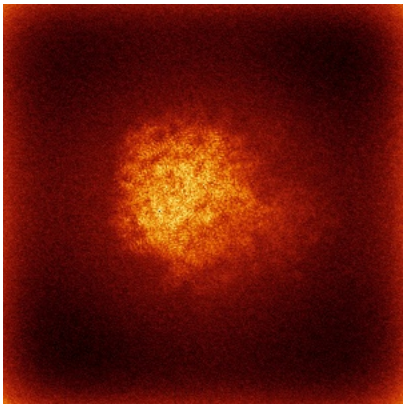

Y


Z

6.4.2 Raw map


X

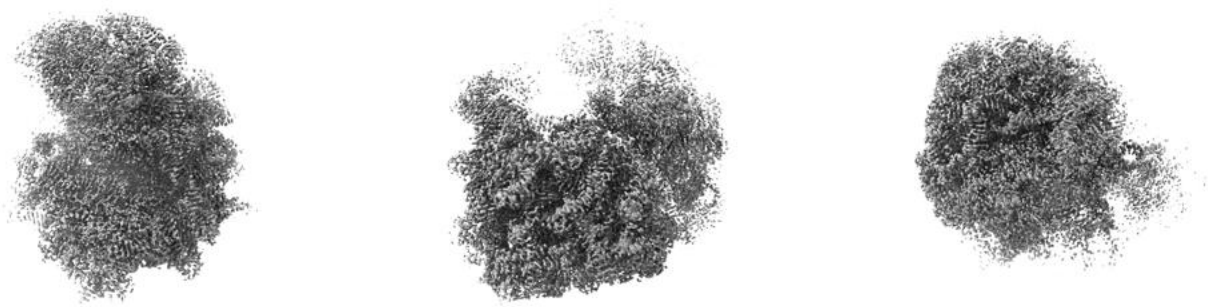

Y


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

6.5.2 Raw map

X Y Z

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

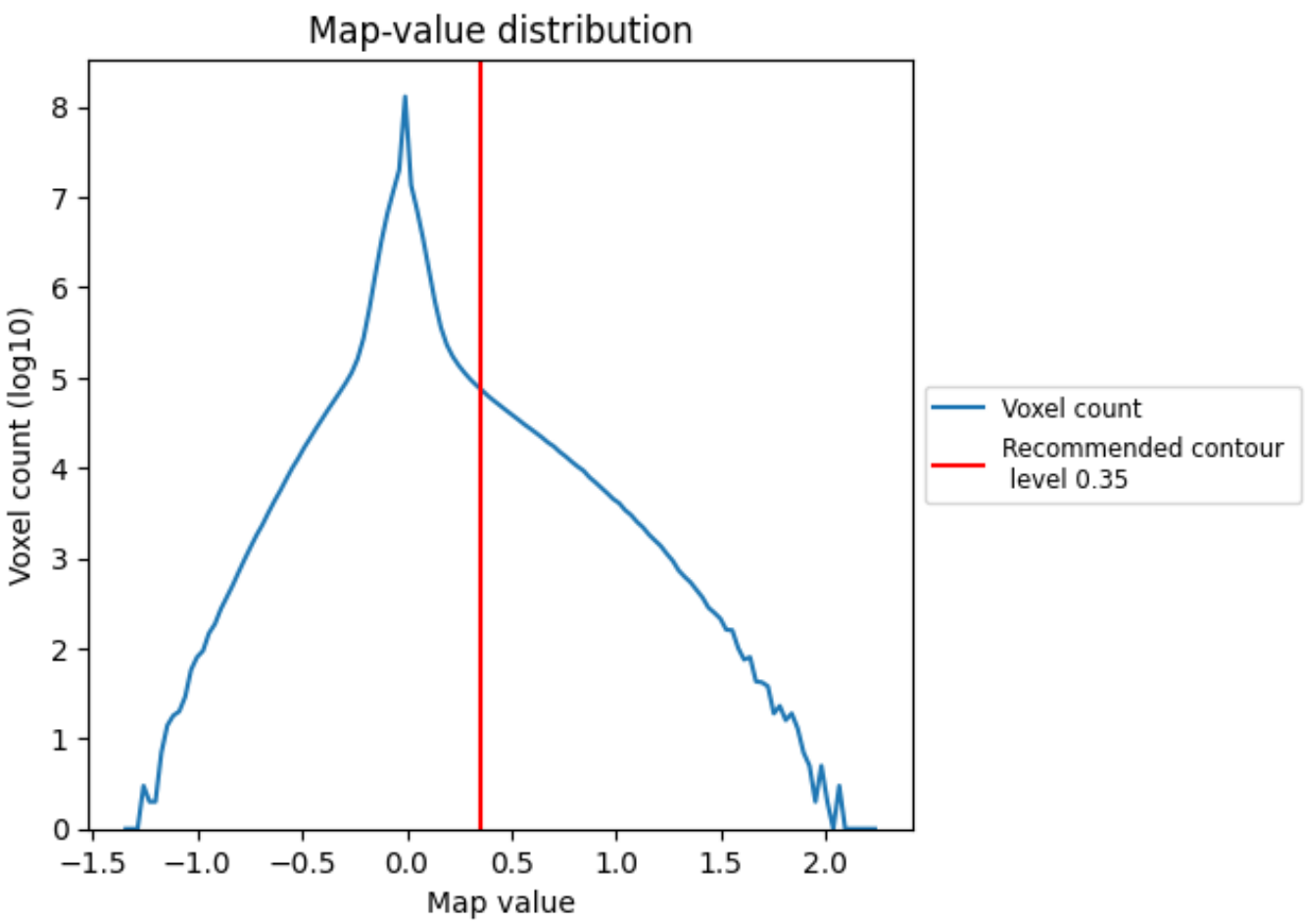
6.6 Mask visualisation (i)

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

7 Map analysis (i)

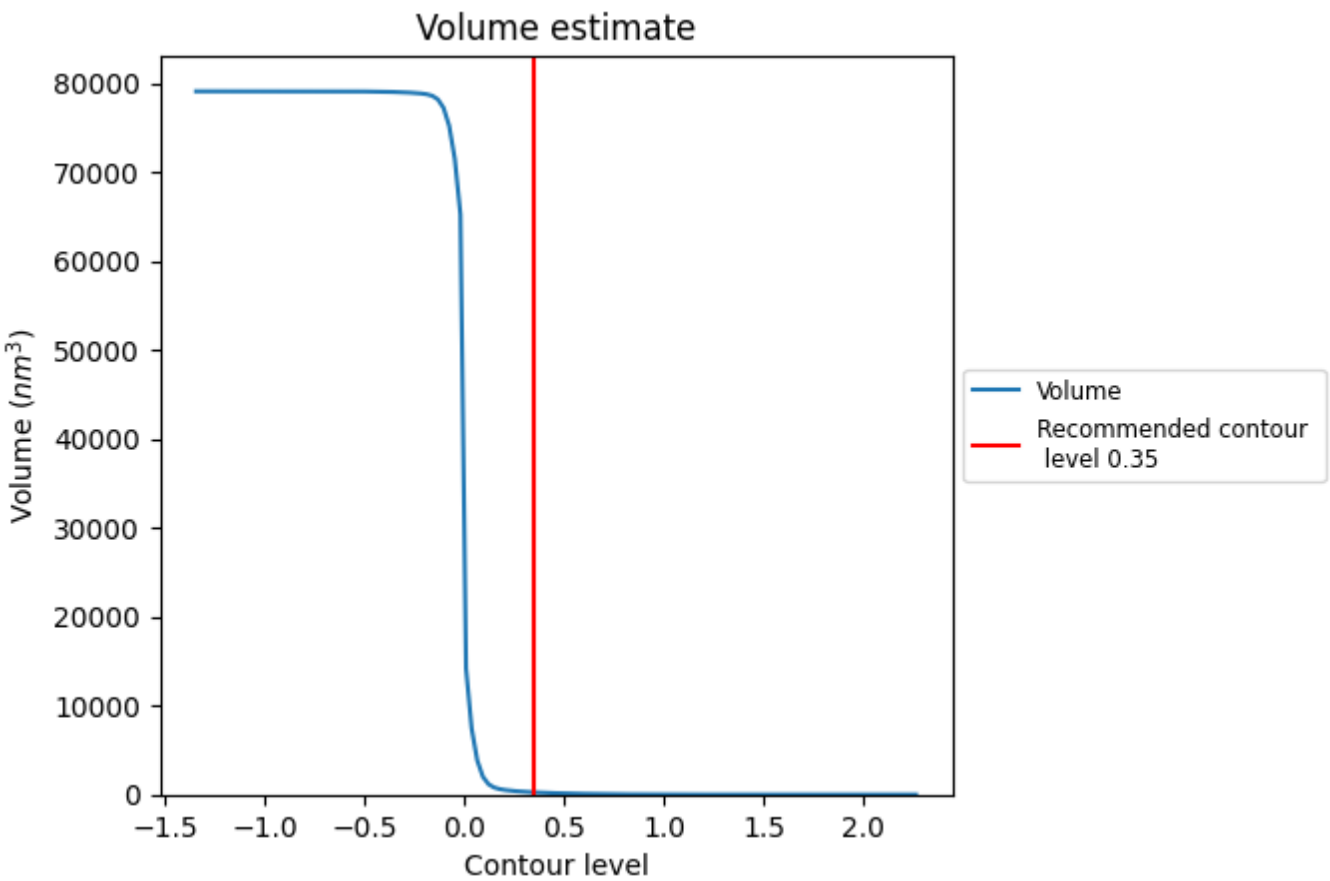
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

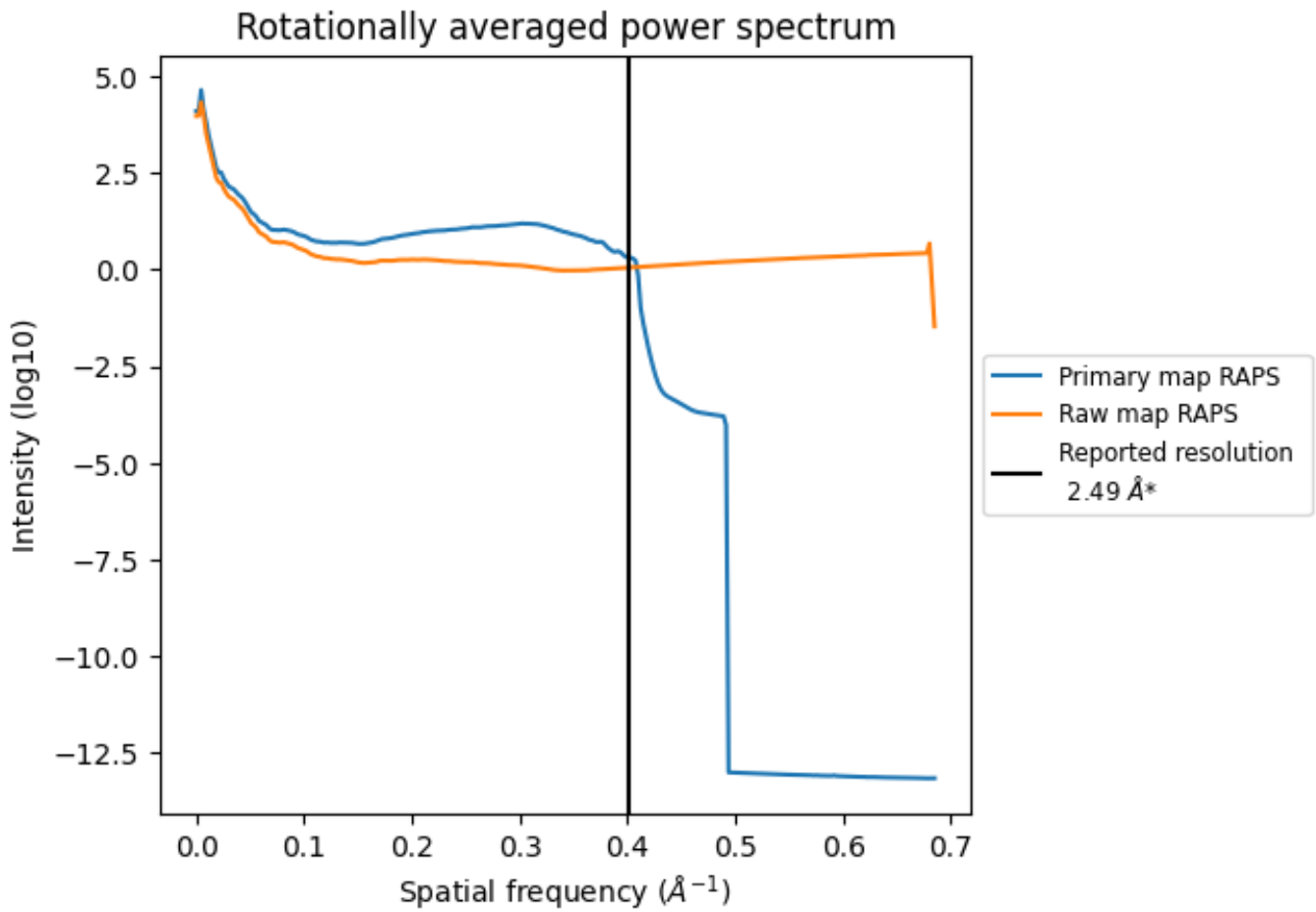
7.2 Volume estimate (i)



The volume at the recommended contour level is 251 nm^3; this corresponds to an approximate mass of 226 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)

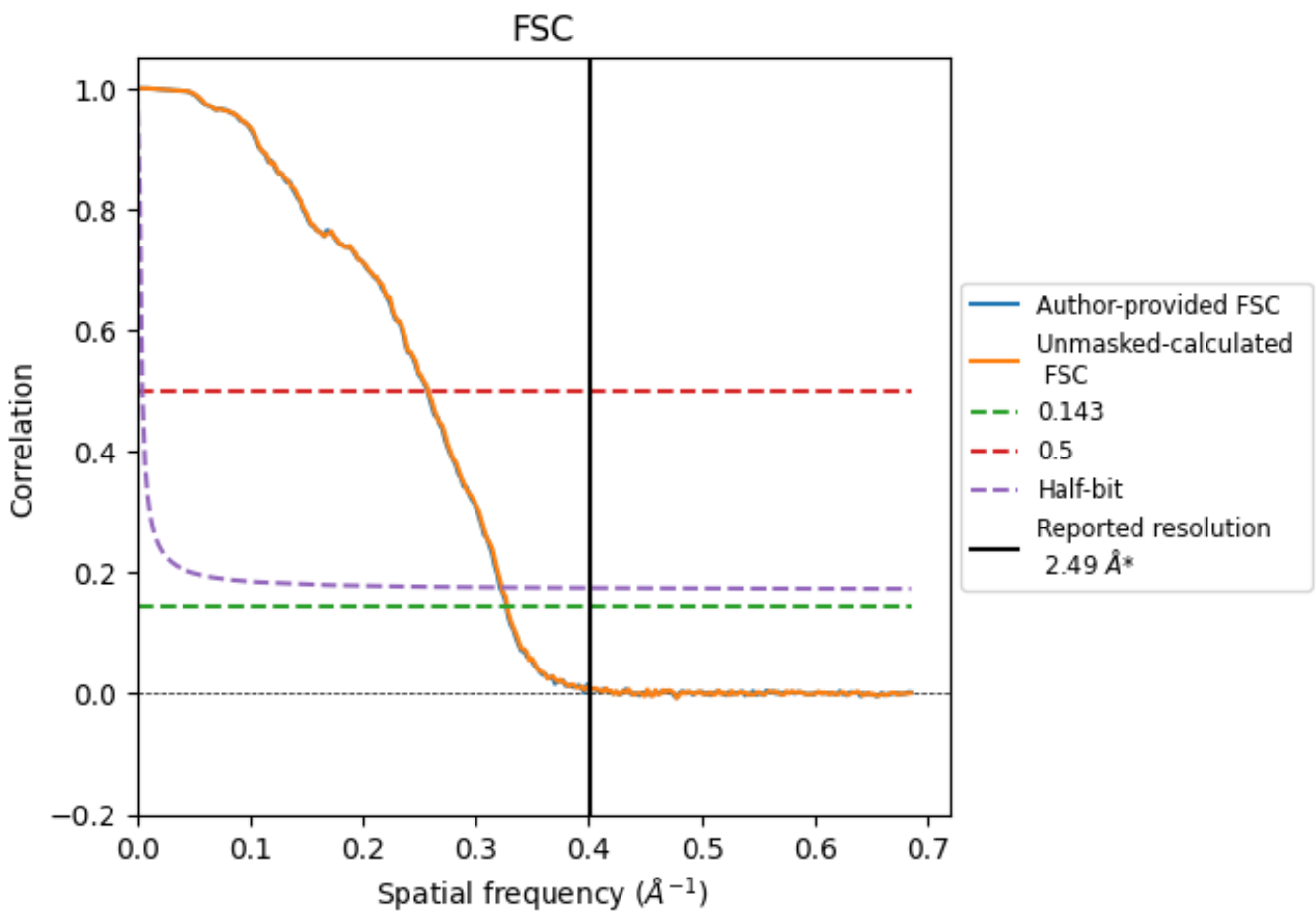


*Reported resolution corresponds to spatial frequency of 0.402 Å^{-1}

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 0.402 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.49	-	-
Author-provided FSC curve	3.06	3.89	3.11
Unmasked-calculated*	3.05	3.88	3.10

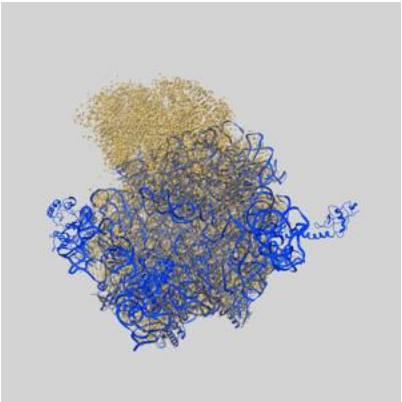
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.06 differs from the reported value 2.49 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.05 differs from the reported value 2.49 by more than 10 %

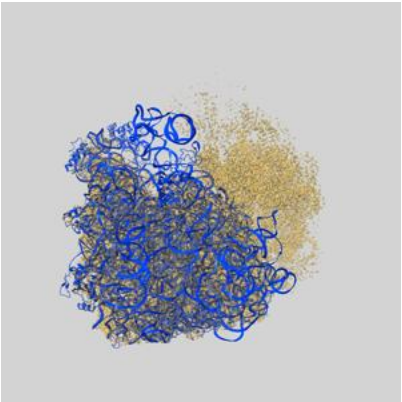
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-75389 and PDB model 10QM. Per-residue inclusion information can be found in section 3 on page 13.

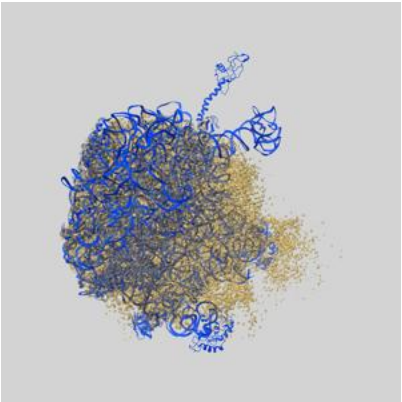
9.1 Map-model overlay (i)



X



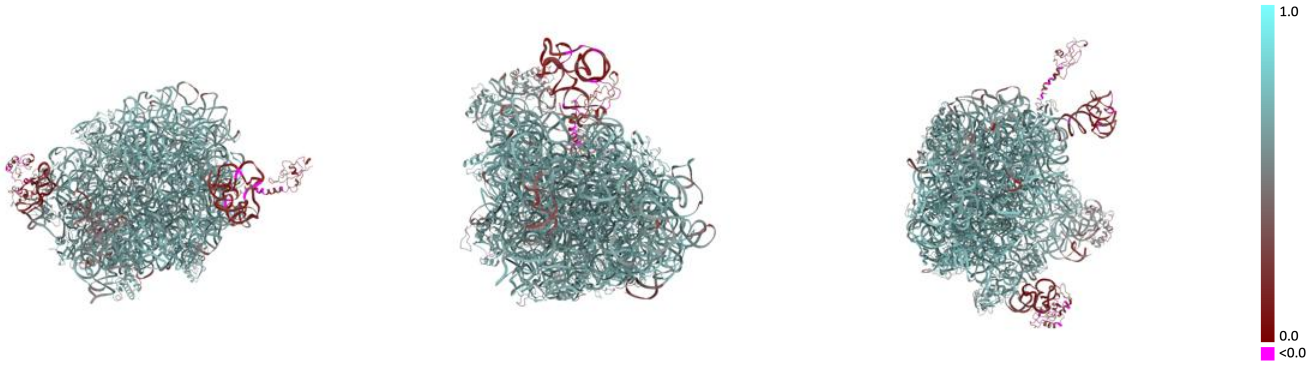
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.35 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.

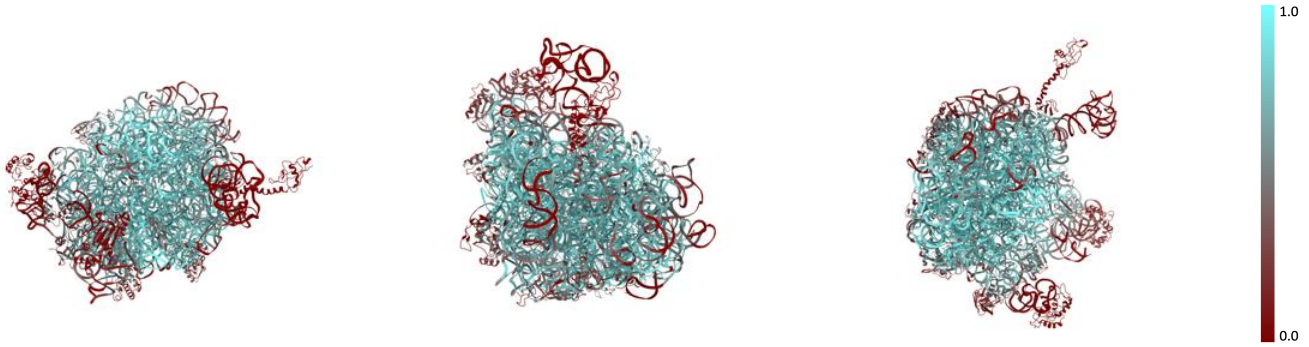
9.2 Q-score mapped to coordinate model (i)



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.

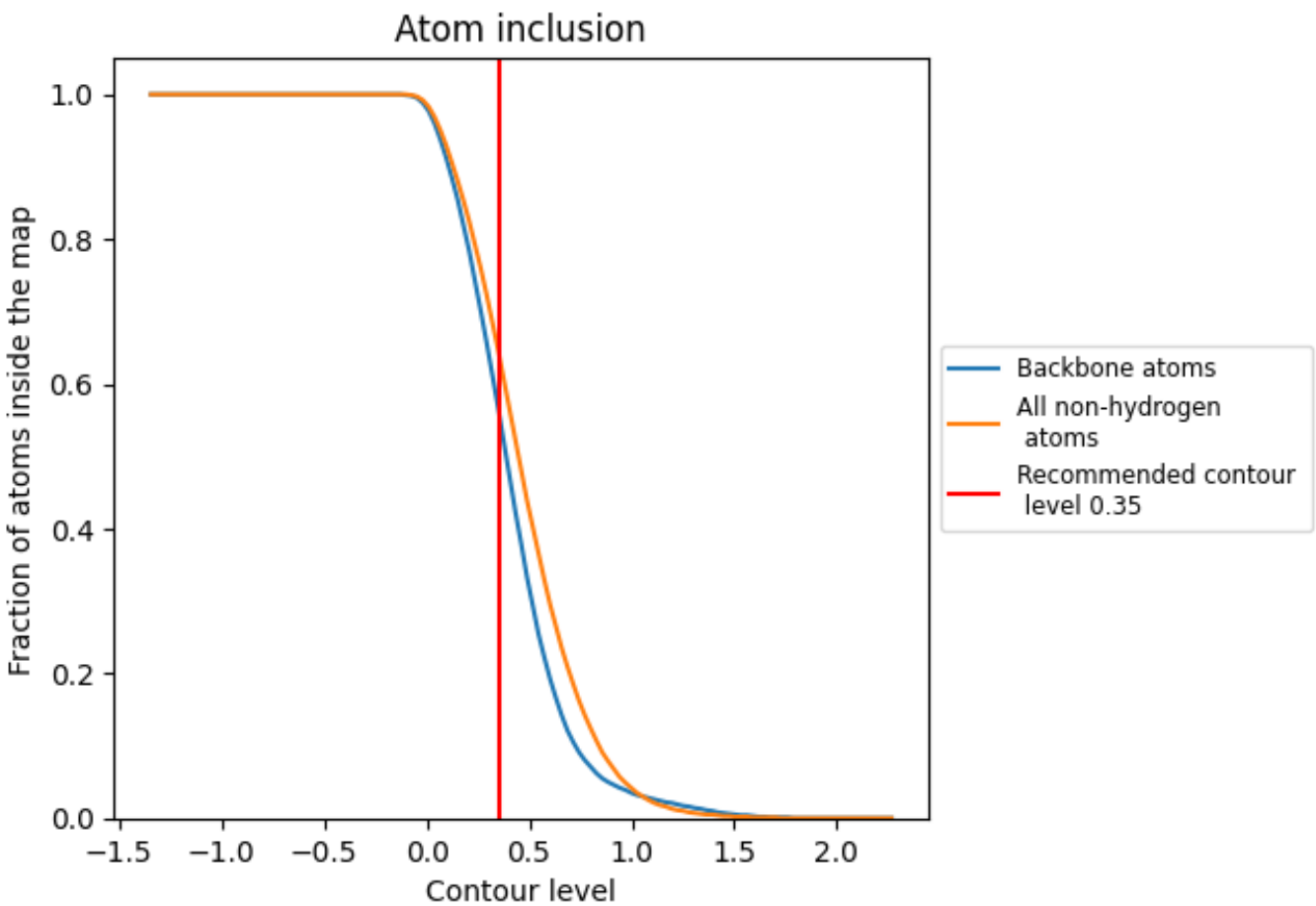
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.35).

9.4 Atom inclusion (i)



At the recommended contour level, 56% of all backbone atoms, 64% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6450	0.6160
I	0.7110	0.6220
J	0.4630	0.6030
K	0.7330	0.6750
L	0.6910	0.6690
M	0.4920	0.6290
N	0.0160	0.4160
O	0.1710	0.5680
P	0.0570	0.2780
Q	0.0000	0.1950
R	0.7290	0.6750
S	0.6070	0.6670
T	0.6250	0.6560
U	0.6160	0.6650
V	0.7790	0.6750
W	0.2740	0.5920
X	0.5740	0.6550
Y	0.7850	0.6850
Z	0.5620	0.6380
a	0.6940	0.6640
b	0.5230	0.6210
c	0.3450	0.5890
d	0.4000	0.6280
e	0.7100	0.6630
f	0.6020	0.6590
g	0.2740	0.5940
h	0.6340	0.6500
i	0.6610	0.6620
j	0.3620	0.6300
k	0.8560	0.6860
l	0.7960	0.6830
m	0.6040	0.6580