wwPDB EM Validation Summary Report

Mar 13, 2024 – 12:23 PM JST

PDB ID	:	3DEG
EMDB ID	:	EMD-1524
Title	:	Complex of elongating Escherichia coli 70S ribosome and EF4(LepA)-GMPPNP
Authors	:	Connell, S.R.; Topf, M.; Qin, Y.; Wilson, D.N.; Mielke, T.; Fucini, P.; Nierhaus, K.H.; Spahn, C.M.T.
Deposited on	:	2008-06-10
Resolution	:	10.90 Å(reported)
Based on initial models	:	1GIX, 3CB4, 2I2P, 2J01, 2I2T

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

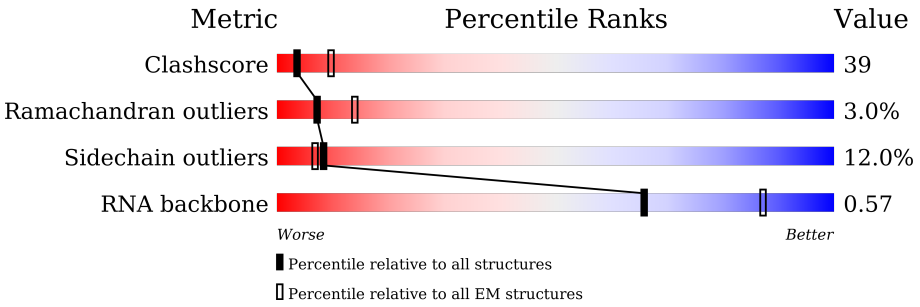
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 10.90 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	A	76	20% 28% 50% 12% 11%
2	B	77	10% 27% 48% 23% .
3	E	16	38% 56% 6%
4	F	12	8% 75% 25%
5	G	70	30% 56% 10% .
6	I	29	45% 55%
7	J	18	44% 50% 6%

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Mol	Chain	Length	Quality of chain
8	K	15	33% 60% 7%
9	C	545	28% 57% 34% 7%
10	D	123	29% 22% 58% 20%
11	H	141	11% 36% 55% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	M2G	A	26	-	-	X	-

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 12950 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 A/L-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	76	1652	746	294	536	76	0	0

- Molecule 2 is a RNA chain called P-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	77	1645	733	297	538	77	0	0

- Molecule 3 is a RNA chain called 30S RNA helix 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	E	16	345	154	65	110	16	0	0

- Molecule 4 is a RNA chain called 30S RNA helix 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	F	12	256	114	46	84	12	0	0

- Molecule 5 is a RNA chain called 50S RNA helix 42-44.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	G	70	1498	670	276	482	70	0	0

- Molecule 6 is a RNA chain called 50S RNA helix 95.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	I	29	625	278	116	202	29	0	0

- Molecule 7 is a RNA chain called 50S RNA helix 71.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	18	Total	C	N	O	P	0	0
			384	171	67	128	18		

- Molecule 8 is a RNA chain called 50S RNA helix 92.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	K	15	Total	C	N	O	P	0	0
			316	141	52	108	15		

- Molecule 9 is a protein called GTP-binding protein lepA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	545	Total	C	N	O	S	0	0
			4242	2671	726	824	21		

- Molecule 10 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

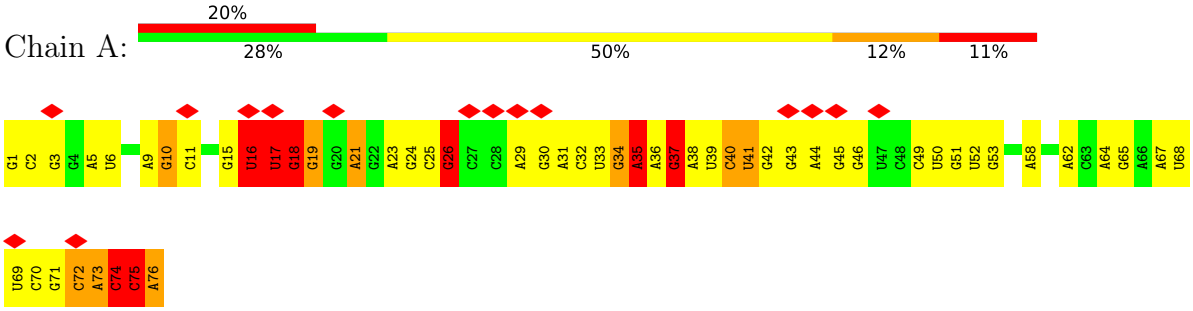
- Molecule 11 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	H	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

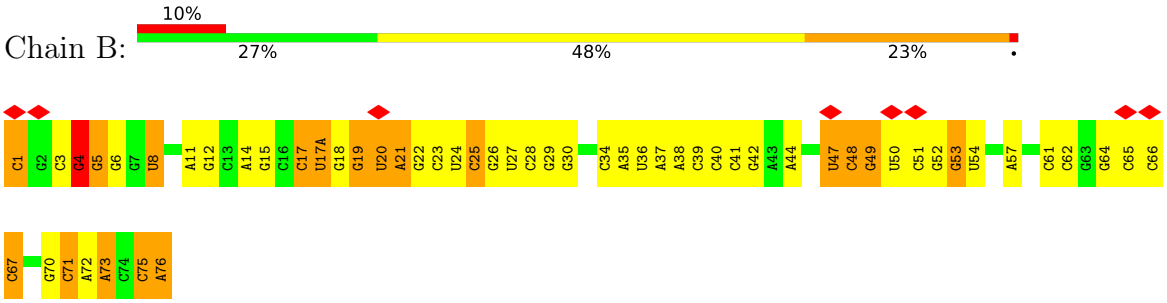
3 Residue-property plots (i)

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: A/L-tRNA

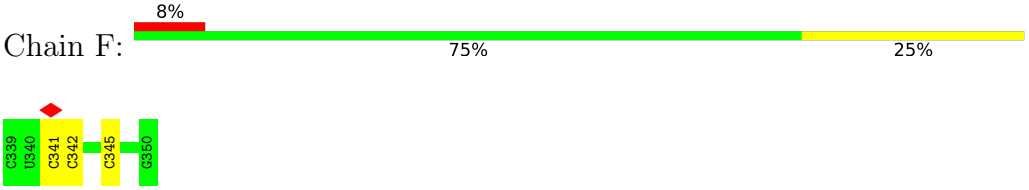


- Molecule 2: P-tRNA



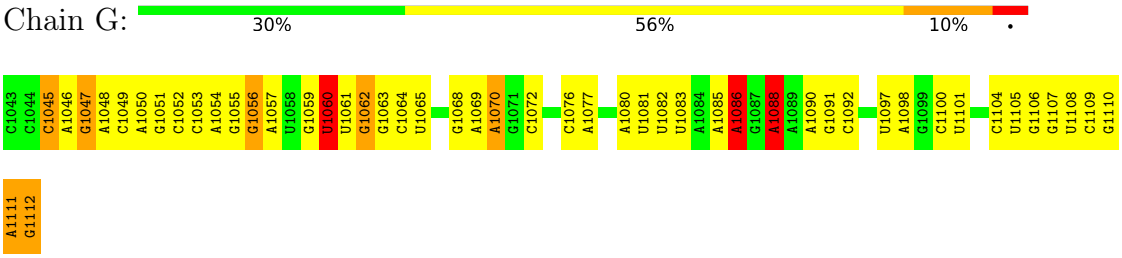
- Molecule 3: 30S RNA helix 8

- Molecule 4: 30S RNA helix 14



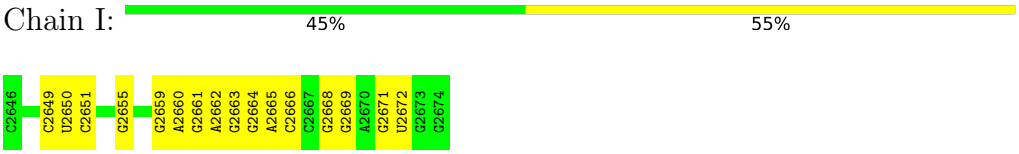
- Molecule 5: 50S RNA helix 42-44

Chain G:



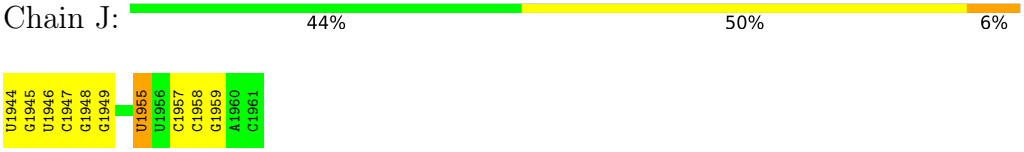
• Molecule 6: 50S RNA helix 95

Chain I:



• Molecule 7: 50S RNA helix 71

Chain J:

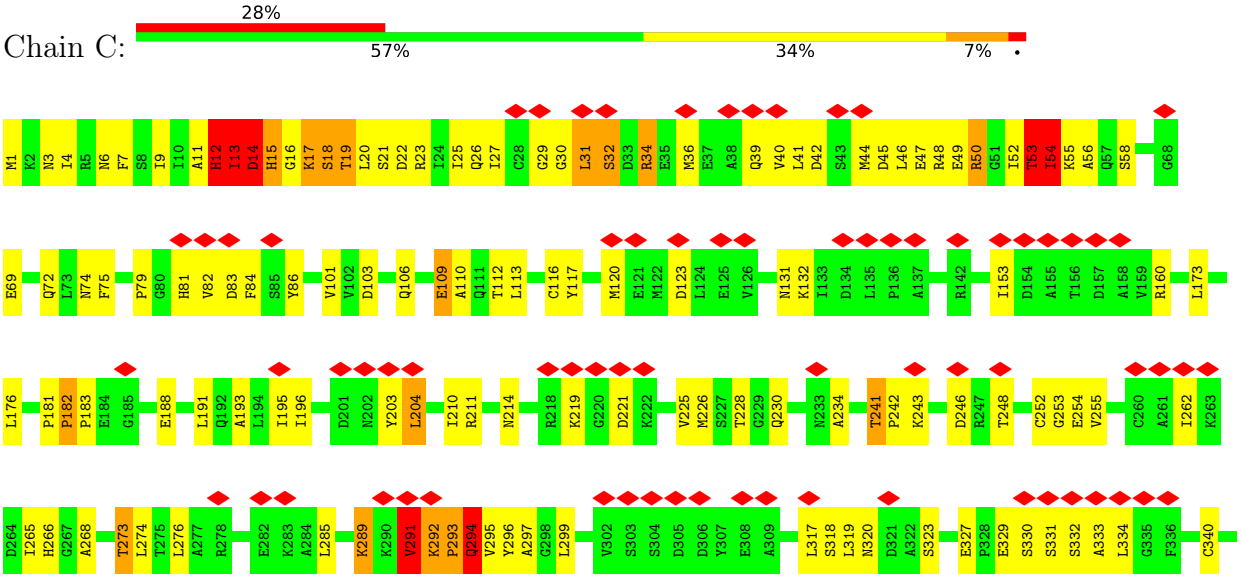


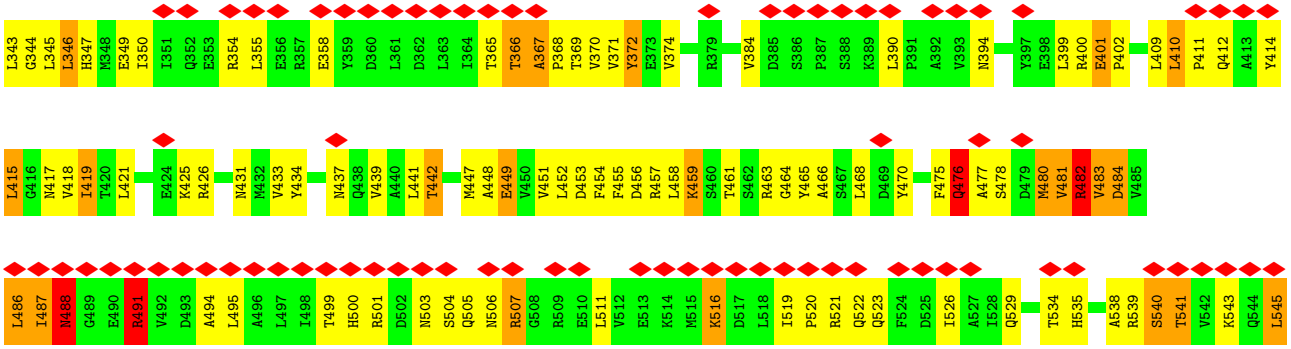
• Molecule 8: 50S RNA helix 92

Chain K:

• Molecule 9: GTP-binding protein lepA

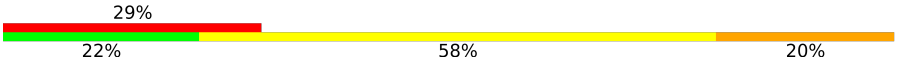
Chain C:

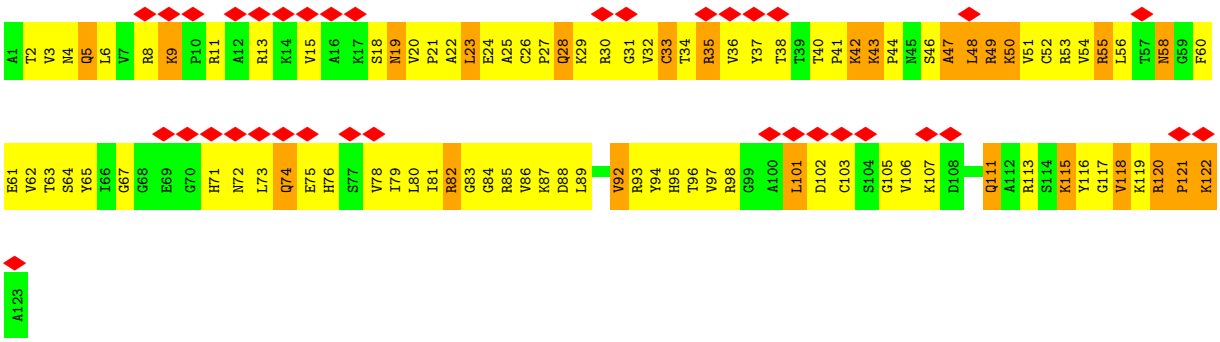




• Molecule 10: 30S ribosomal protein S12

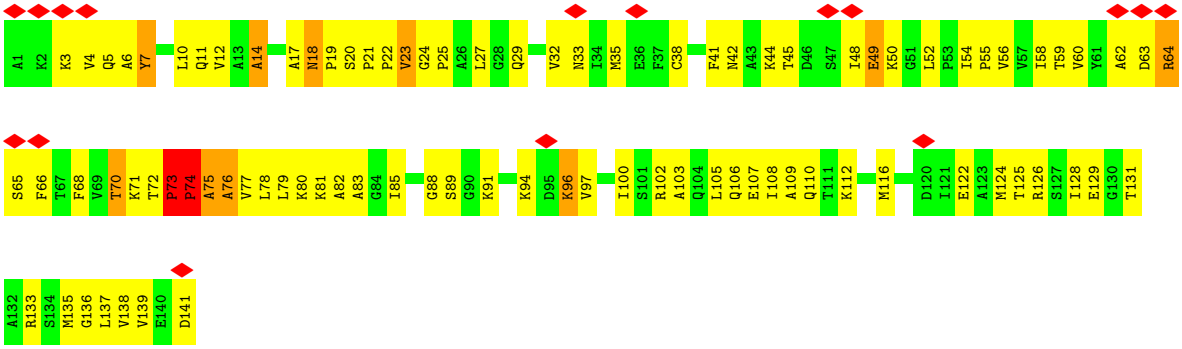
Chain D:





• Molecule 11: 50S ribosomal protein L11

Chain H:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	41294	Depositor
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3900	Depositor
Magnification	39000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	11.559	Depositor
Minimum map value	-5.058	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1.0	Depositor
Map size (Å)	378, 378, 378	wwPDB
Map dimensions	150, 150, 150	wwPDB
Map angles (°)	90, 90, 90	wwPDB
Pixel spacing (Å)	2.52, 2.52, 2.52	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: 1MA, PSU, H2U, 7MG, 2MG, 5MC, OMG, OMC, YG, M2G, 5MU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.97	2/1486 (0.1%)	1.34	8/2311 (0.3%)
2	B	0.52	1/1814 (0.1%)	0.72	0/2825
3	E	0.21	0/386	0.71	0/600
4	F	0.27	0/285	0.76	0/442
5	G	0.67	5/1677 (0.3%)	0.82	8/2612 (0.3%)
6	I	0.27	0/699	0.74	0/1089
7	J	0.24	0/428	0.72	0/665
8	K	0.23	0/351	0.75	0/544
9	C	0.60	4/4312 (0.1%)	1.04	45/5844 (0.8%)
10	D	0.22	0/969	0.46	0/1300
11	H	0.63	5/1046 (0.5%)	0.74	5/1410 (0.4%)
All	All	0.59	17/13453 (0.1%)	0.92	66/19642 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	7	3
2	B	0	2
5	G	0	4
9	C	1	11
11	H	0	1
All	All	8	21

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	34	OMG	O3'-P	19.74	1.84	1.61
5	G	1086	A	C5-C6	-16.32	1.26	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	1088	A	C6-N1	-10.50	1.28	1.35
9	C	480	MET	C-N	8.63	1.53	1.34
5	G	1060	U	C2-N3	7.75	1.43	1.37

The worst 5 of 66 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	35	A	P-O3'-C3'	41.08	168.99	119.70
1	A	34	OMG	O3'-P-O5'	19.74	141.51	104.00
9	C	14	ASP	CB-CA-C	17.60	145.59	110.40
9	C	13	ILE	C-N-CA	-17.05	79.07	121.70
9	C	13	ILE	N-CA-C	12.32	144.26	111.00

5 of 8 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	73	A	C2'
1	A	74	C	C1',C4'
1	A	75	C	C3',C4',C2'
1	A	76	A	C4'
9	C	13	ILE	CA

5 of 21 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	18	G	Sidechain
1	A	19	G	Sidechain
1	A	62	A	Sidechain
2	B	25	C	Sidechain
2	B	4	G	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1652	0	857	153	0
2	B	1645	0	838	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	345	0	174	12	0
4	F	256	0	131	1	0
5	G	1498	0	757	64	0
6	I	625	0	314	23	0
7	J	384	0	193	27	0
8	K	316	0	161	9	0
9	C	4242	0	4236	417	0
10	D	955	0	1019	126	0
11	H	1032	0	1088	122	0
All	All	12950	0	9768	893	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 39.

The worst 5 of 893 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:G:P	9:C:543:LYS:HE3	1.19	1.65
9:C:110:ALA:HB2	9:C:465:TYR:CD2	1.11	1.63
1:A:69:U:C5'	9:C:539:ARG:HD2	1.22	1.56
9:C:26:GLN:CG	9:C:34:ARG:HB3	1.40	1.47
9:C:26:GLN:CD	9:C:34:ARG:HG2	1.31	1.45

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
9	C	543/545 (100%)	507 (93%)	31 (6%)	5 (1%)	17 57
10	D	121/123 (98%)	80 (66%)	30 (25%)	11 (9%)	1 11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
11	H	139/141 (99%)	115 (83%)	16 (12%)	8 (6%)	1 18
All	All	803/809 (99%)	702 (87%)	77 (10%)	24 (3%)	7 28

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	C	488	ASN
10	D	42	LYS
11	H	18	ASN
9	C	291	VAL
9	C	293	PRO

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
9	C	465/465 (100%)	407 (88%)	58 (12%)	4 19
10	D	103/103 (100%)	83 (81%)	20 (19%)	1 8
11	H	109/109 (100%)	106 (97%)	3 (3%)	43 65
All	All	677/677 (100%)	596 (88%)	81 (12%)	8 20

5 of 81 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	C	545	LEU
10	D	72	ASN
10	D	9	LYS
10	D	48	LEU
10	D	115	LYS

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

Mol	Chain	Res	Type
11	H	29	GLN
11	H	93	ASN
9	C	505	GLN
9	C	523	GLN
10	D	28	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	74/76 (97%)	16 (21%)	6 (8%)
2	B	76/77 (98%)	18 (23%)	0
3	E	15/16 (93%)	1 (6%)	0
4	F	11/12 (91%)	1 (9%)	0
5	G	69/70 (98%)	9 (13%)	0
6	I	28/29 (96%)	0	0
7	J	17/18 (94%)	1 (5%)	0
8	K	14/15 (93%)	1 (7%)	0
All	All	304/313 (97%)	47 (15%)	6 (1%)

5 of 47 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	C
1	A	3	G
1	A	17	H2U
1	A	18	G
1	A	19	G

5 of 6 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	73	A
1	A	74	C
1	A	75	C
1	A	18	G
1	A	16	H2U

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

15 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	A	10	1	18,26,27	1.09	2 (11%)	16,38,41	0.75	0
1	5MC	A	49	1	18,22,23	0.76	0	26,32,35	0.73	1 (3%)
1	M2G	A	26	1	20,27,28	1.20	2 (10%)	22,40,43	0.77	0
1	YG	A	37	1	31,42,43	0.91	1 (3%)	33,62,65	2.59	10 (30%)
1	7MG	A	46	1	22,26,27	1.11	2 (9%)	29,39,42	1.22	3 (10%)
1	PSU	A	55	1	18,21,22	0.73	0	22,30,33	0.85	0
1	OMC	A	32	1	19,22,23	0.47	0	26,31,34	0.57	0
1	H2U	A	16	1	18,21,22	0.75	1 (5%)	21,30,33	1.13	2 (9%)
1	5MU	A	54	1	19,22,23	0.53	0	28,32,35	0.66	0
1	1MA	A	58	1	16,25,26	2.81	4 (25%)	18,37,40	2.21	5 (27%)
1	H2U	A	17	1	18,21,22	0.66	1 (5%)	21,30,33	0.99	2 (9%)
1	PSU	A	39	1	18,21,22	0.70	0	22,30,33	0.68	0
1	OMG	A	34	1	18,26,27	1.05	2 (11%)	19,38,41	0.86	1 (5%)
1	5MC	A	40	1	18,22,23	0.45	0	26,32,35	0.71	1 (3%)
2	5MU	B	54	2	19,22,23	0.25	0	28,32,35	0.39	0

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	A	10	1	-	0/5/27/28	0/3/3/3
1	5MC	A	49	1	-	0/7/25/26	0/2/2/2
1	M2G	A	26	1	-	0/7/29/30	0/3/3/3
1	YG	A	37	1	-	8/20/42/43	0/3/4/4
1	7MG	A	46	1	-	2/7/37/38	0/3/3/3
1	PSU	A	55	1	-	0/7/25/26	0/2/2/2
1	OMC	A	32	1	-	0/9/27/28	0/2/2/2
1	H2U	A	16	1	-	4/7/38/39	0/2/2/2
1	5MU	A	54	1	-	0/7/25/26	0/2/2/2
1	1MA	A	58	1	-	0/3/25/26	0/3/3/3
1	H2U	A	17	1	-	1/7/38/39	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	A	39	1	-	0/7/25/26	0/2/2/2
1	OMG	A	34	1	-	1/5/27/28	0/3/3/3
1	5MC	A	40	1	-	1/7/25/26	0/2/2/2
2	5MU	B	54	2	-	0/7/25/26	0/2/2/2

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	58	1MA	C6-N6	7.96	1.48	1.27
1	A	58	1MA	C2-N3	6.86	1.37	1.29
1	A	46	7MG	C4-N9	3.14	1.41	1.37
1	A	26	M2G	C5-C6	-3.06	1.41	1.47
1	A	10	2MG	C5-C6	-2.96	1.41	1.47

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	37	YG	C11-C12-N1	8.57	111.36	106.53
1	A	37	YG	C24-O23-C21	6.25	123.05	115.66
1	A	58	1MA	CM1-N1-C6	-5.20	112.39	120.27
1	A	37	YG	C3-N3-C4	4.97	125.53	116.71
1	A	58	1MA	CM1-N1-C2	4.55	130.12	120.55

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	16	H2U	O4'-C1'-N1-C2
1	A	16	H2U	O4'-C1'-N1-C6
1	A	16	H2U	C2'-C1'-N1-C6
1	A	37	YG	C12-C13-C14-C15
1	A	37	YG	C15-C16-O18-C19

There are no ring outliers.

10 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	10	2MG	1	0
1	A	26	M2G	13	0
1	A	37	YG	7	0
1	A	32	OMC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	16	H2U	3	0
1	A	17	H2U	3	0
1	A	39	PSU	1	0
1	A	34	OMG	1	0
1	A	40	5MC	3	0
2	B	54	5MU	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	44:A	O3'	45:G	P	2.49
1	A	34:OMG	O3'	35:A	P	1.84
1	A	33:U	O3'	34:OMG	P	1.32

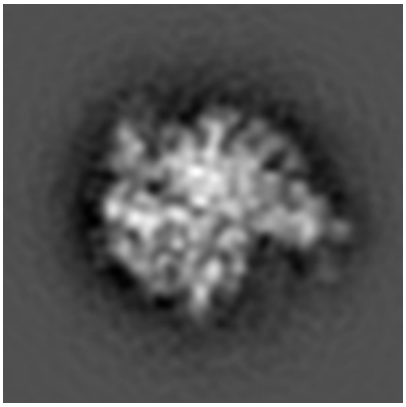
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-1524. These allow visual inspection of the internal detail of the map and identification of artifacts.

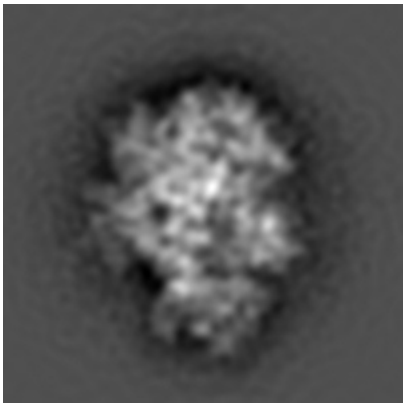
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

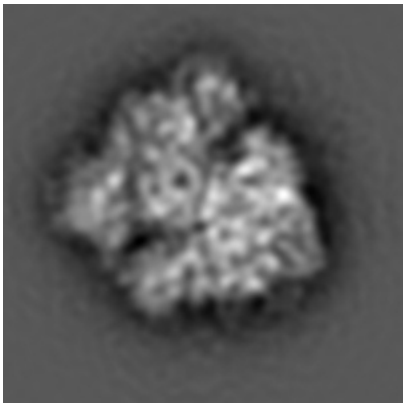
6.1.1 Primary map



X



Y

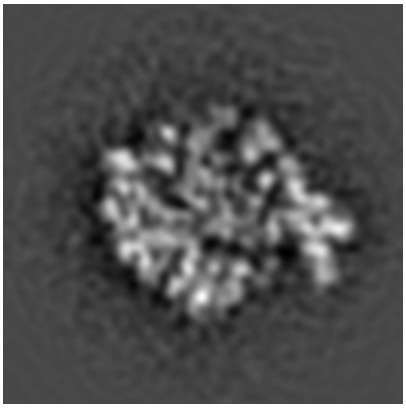


Z

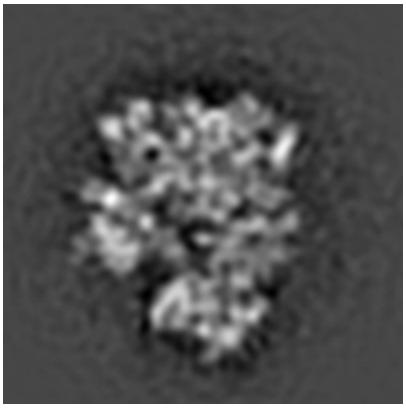
The images above show the map projected in three orthogonal directions.

6.2 Central slices

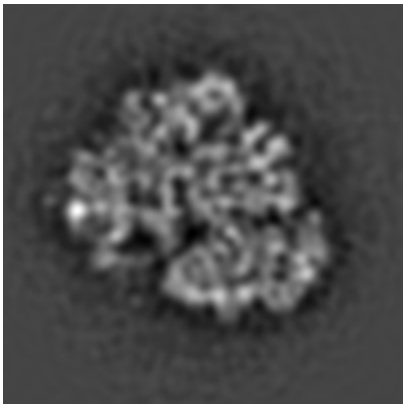
6.2.1 Primary map



X Index: 75



Y Index: 75

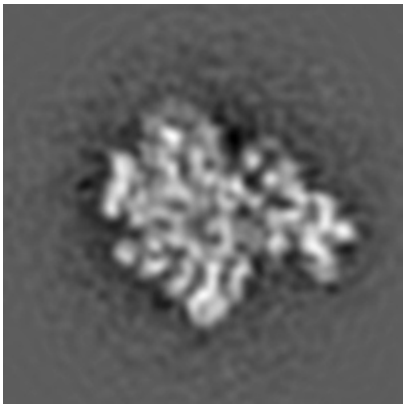


Z Index: 75

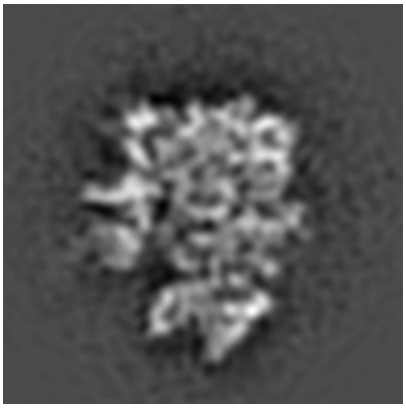
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

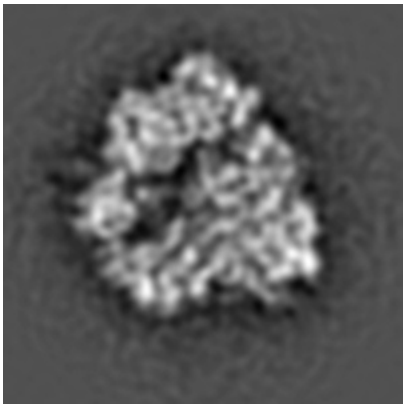
6.3.1 Primary map



X Index: 78



Y Index: 78

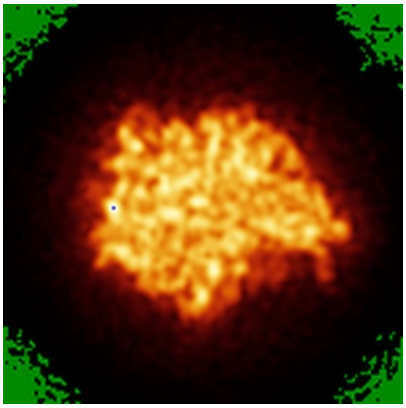


Z Index: 68

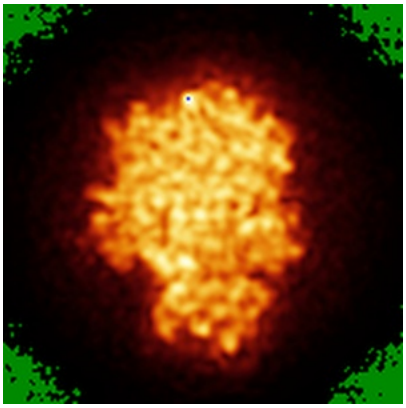
The images above show the largest variance slices of the map in three orthogonal directions.

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

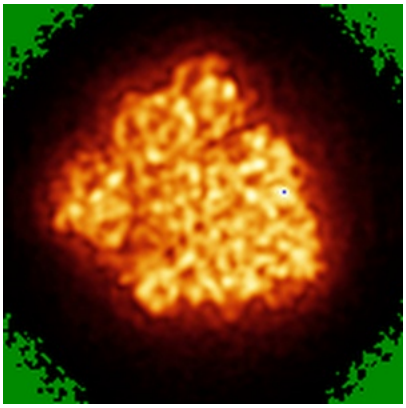
6.4.1 Primary map



X



Y

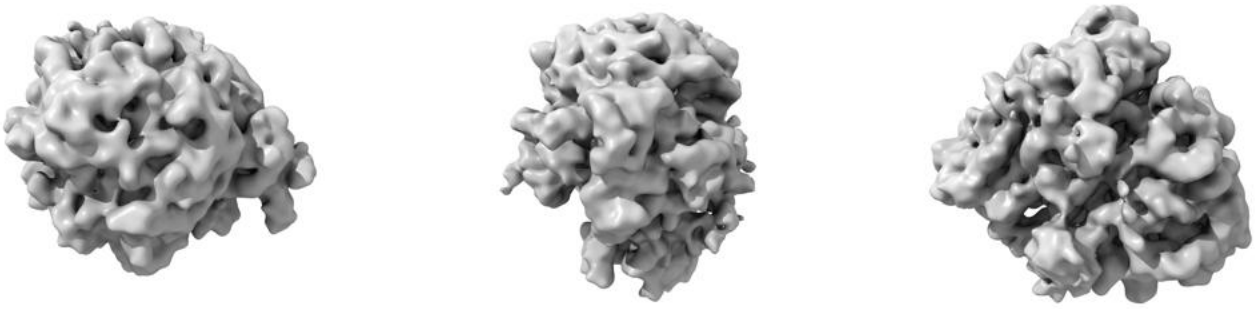


Z

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

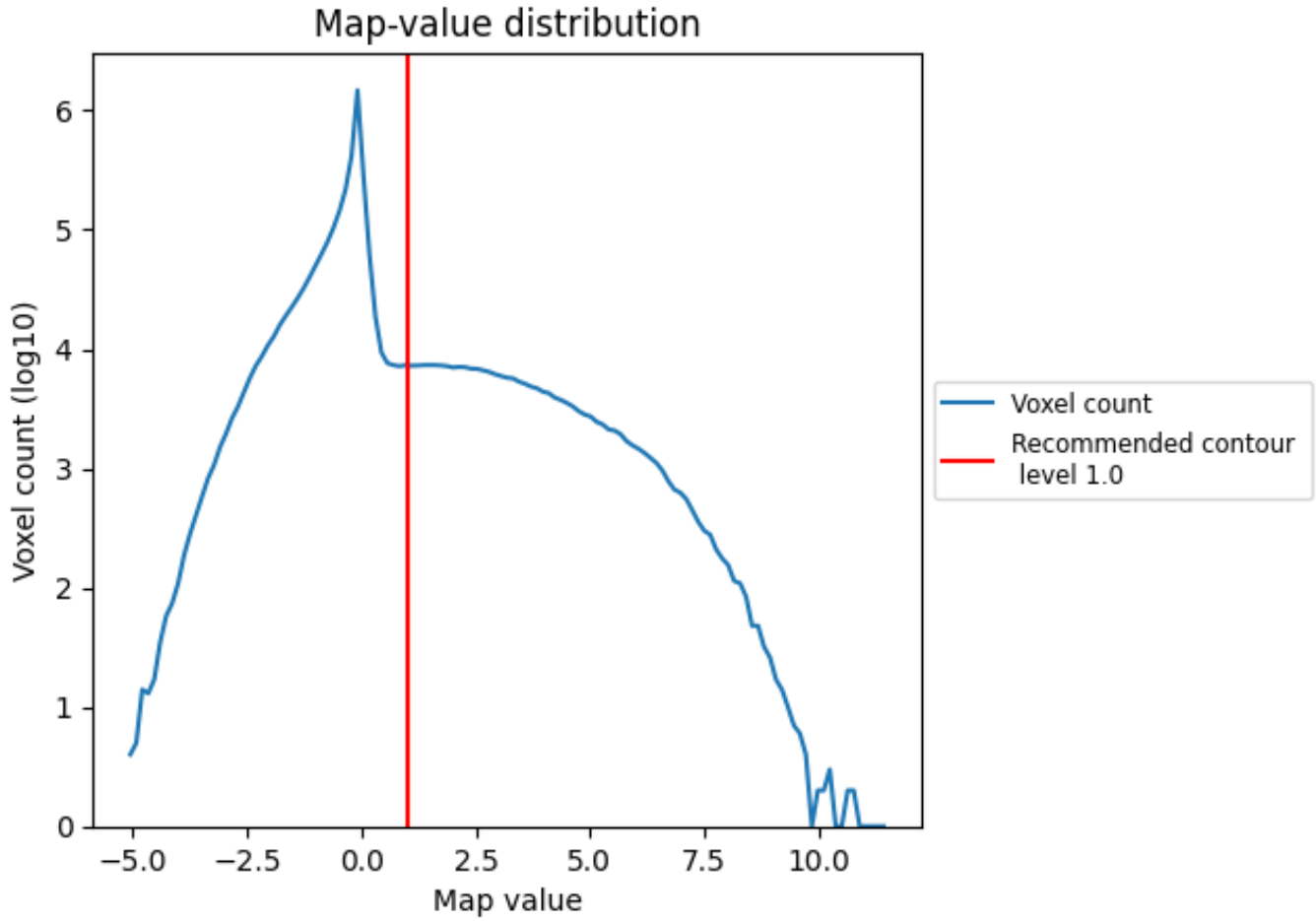
6.6 Mask visualisation (i)

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

7 Map analysis

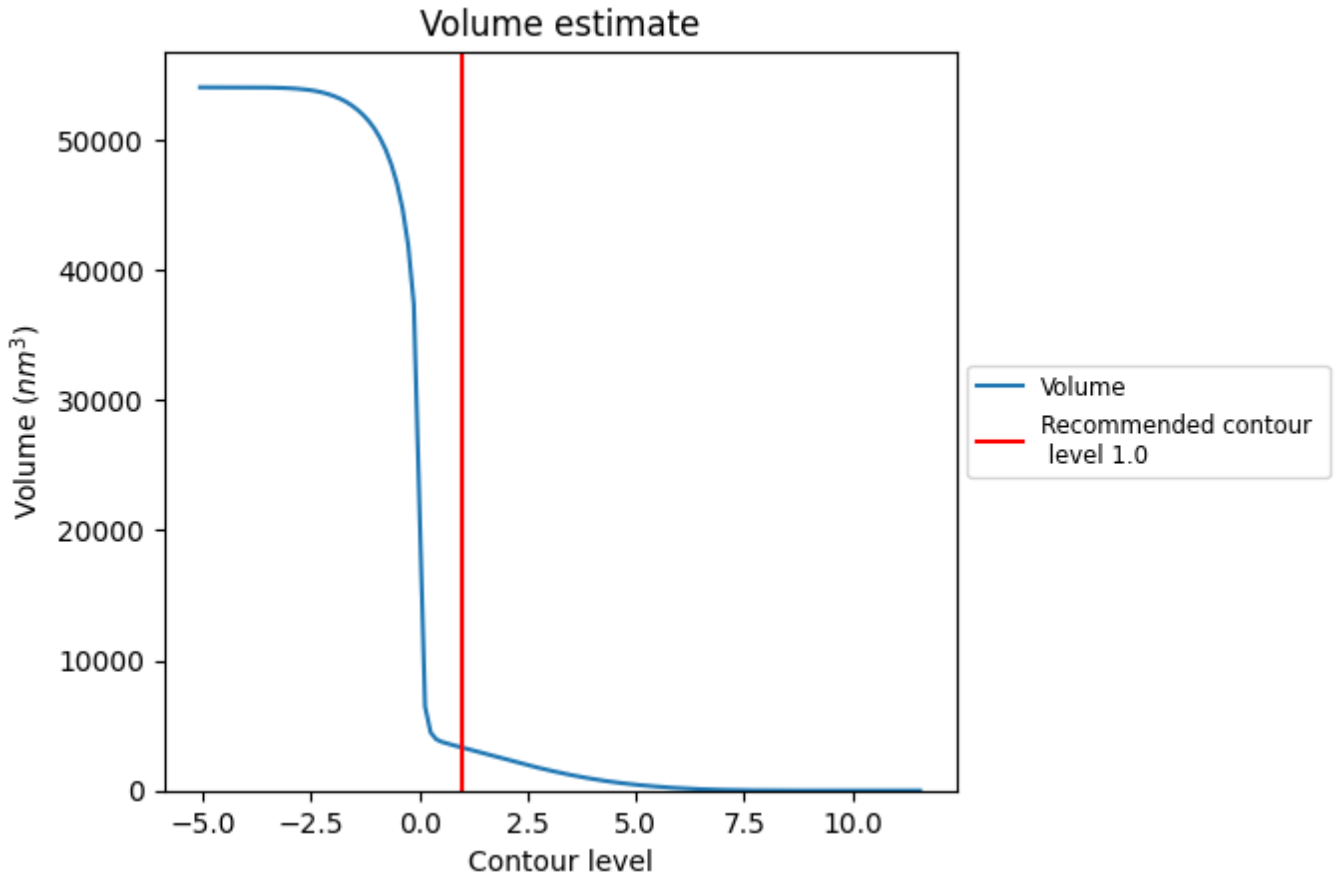
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

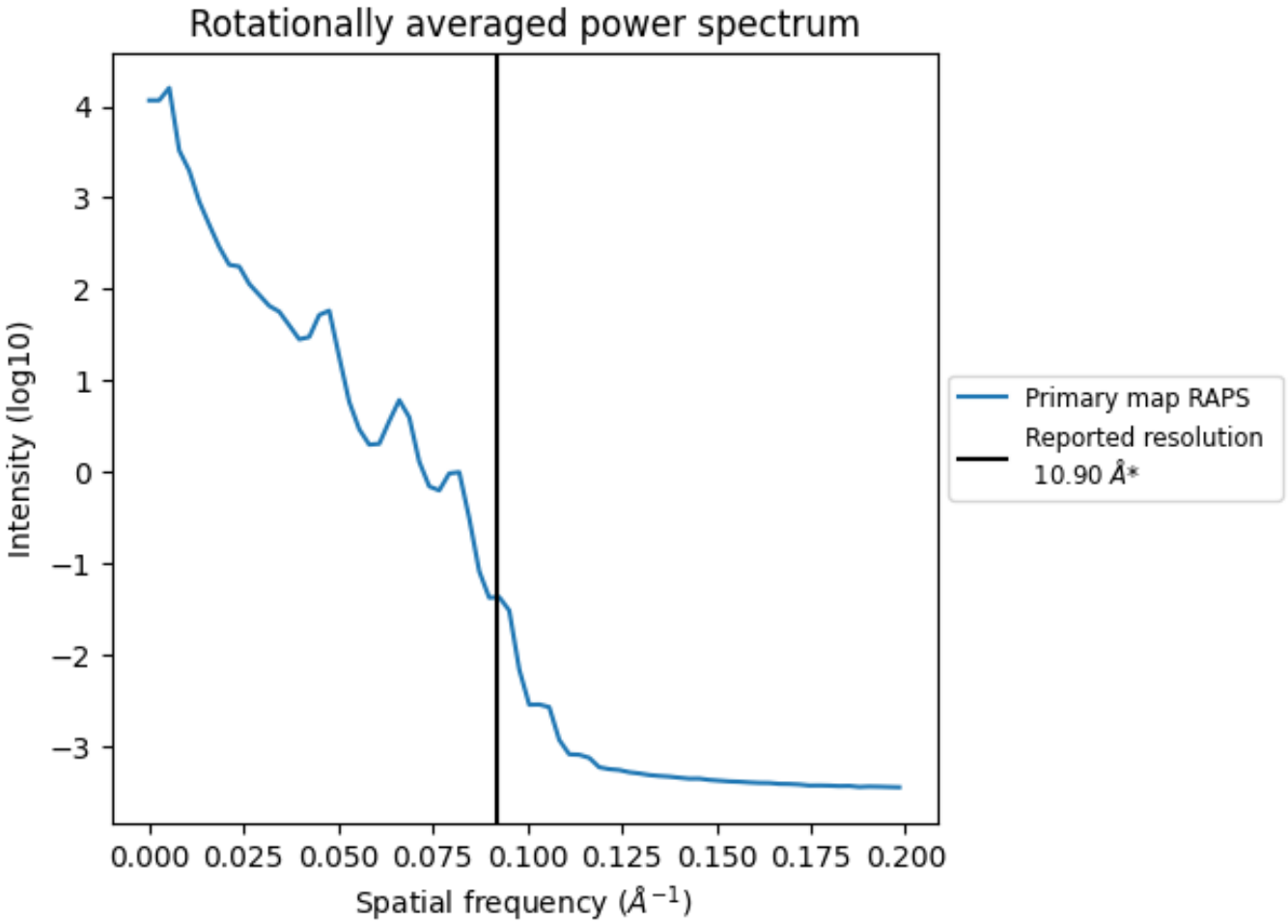
7.2 Volume estimate (i)



The volume at the recommended contour level is 3292 nm^3; this corresponds to an approximate mass of 2974 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 0.092 Å^{-1}

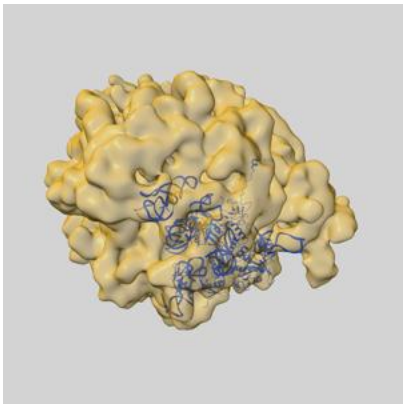
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

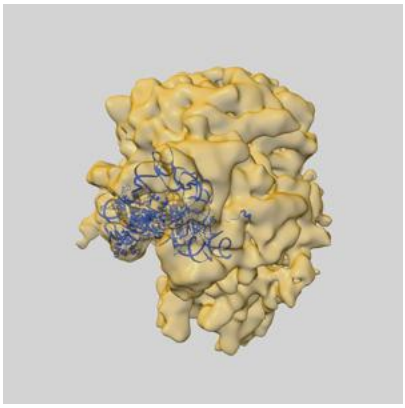
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-1524 and PDB model 3DEG. Per-residue inclusion information can be found in section 3 on page 6.

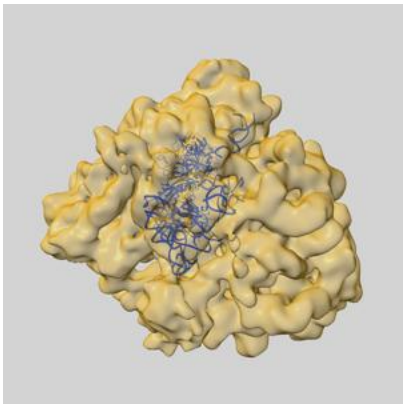
9.1 Map-model overlay



X



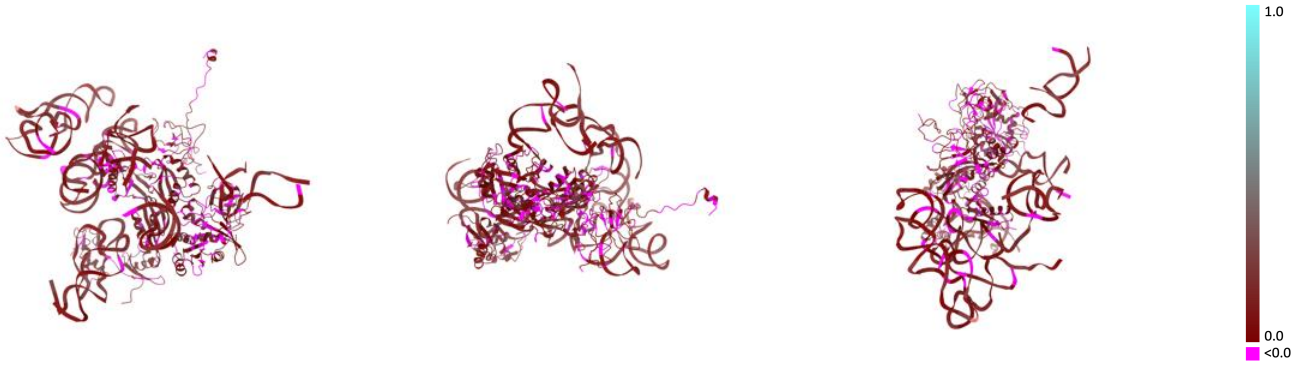
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.0 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.

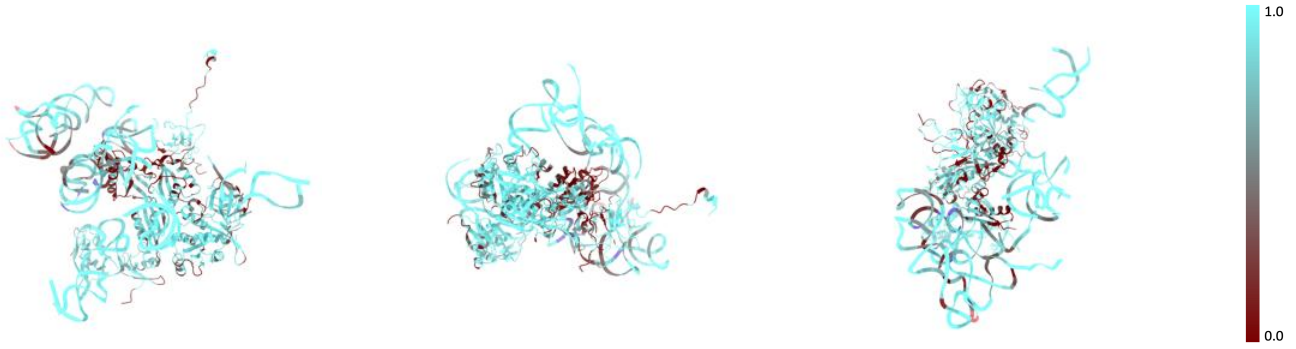
9.2 Q-score mapped to coordinate model (i)



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.

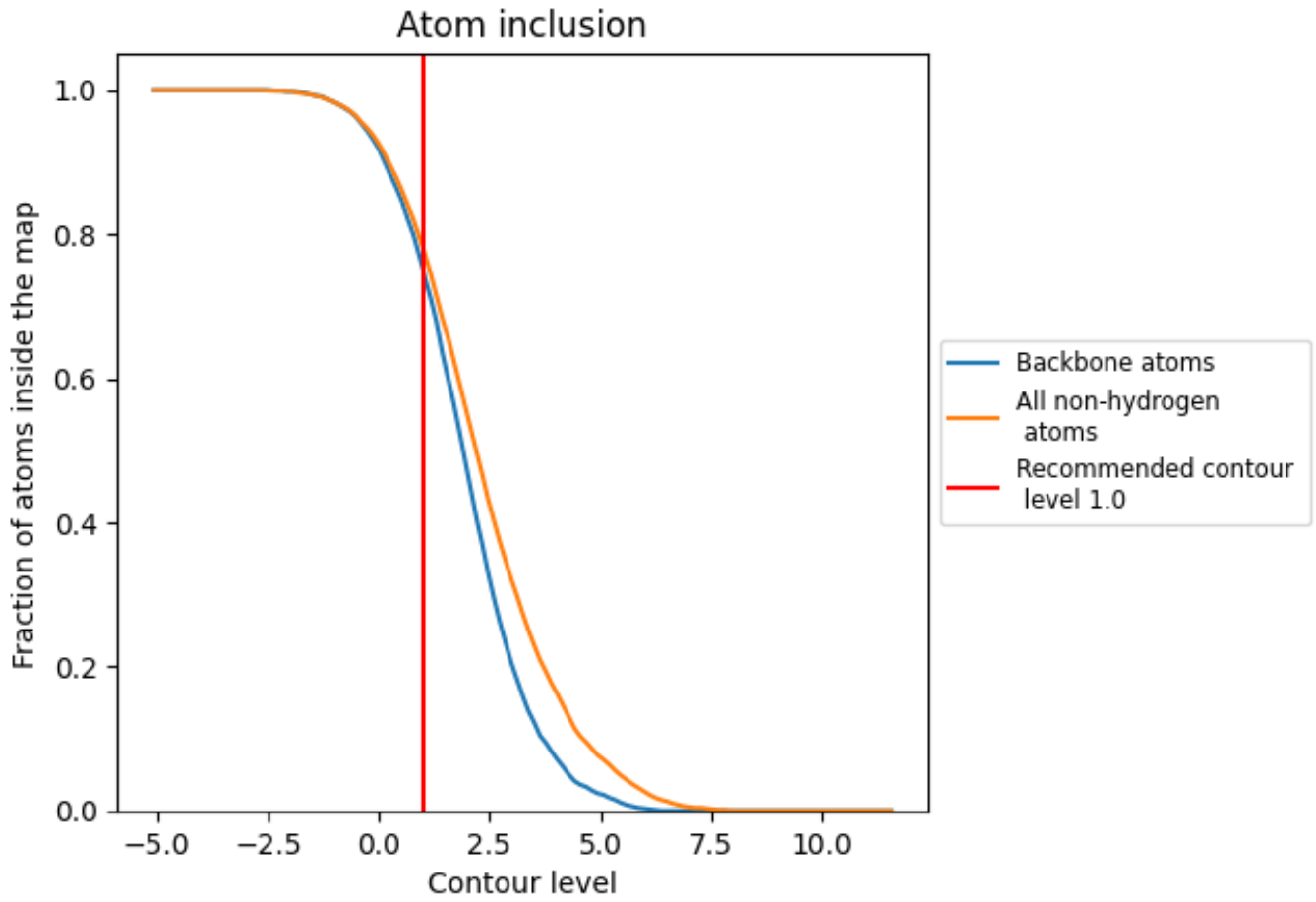
9.3 Atom inclusion mapped to coordinate model (i)



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 (1.0).

9.4 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (1.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7810	0.0790
A	0.7310	0.0830
B	0.7780	0.0950
C	0.6810	0.0630
D	0.6730	0.0370
E	0.9070	0.1280
F	0.8360	0.1000
G	0.9750	0.0960
H	0.8200	0.0690
I	0.9810	0.1090
J	0.9450	0.1070
K	0.8770	0.0980