



## wwPDB EM Validation Summary Report ⓘ

Mar 3, 2024 – 12:46 PM EST

PDB ID : 6AWC  
EMDB ID : EMD-7015  
Title : Structure of 30S ribosomal subunit and RNA polymerase complex in rotated state  
Authors : Demo, G.; Rasouly, A.; Vasilyev, N.; Loveland, A.B.; Diaz-Avalos, R.; Grigorieff, N.; Nudler, E.; Korostelev, A.A.  
Deposited on : 2017-09-05  
Resolution : 7.90 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

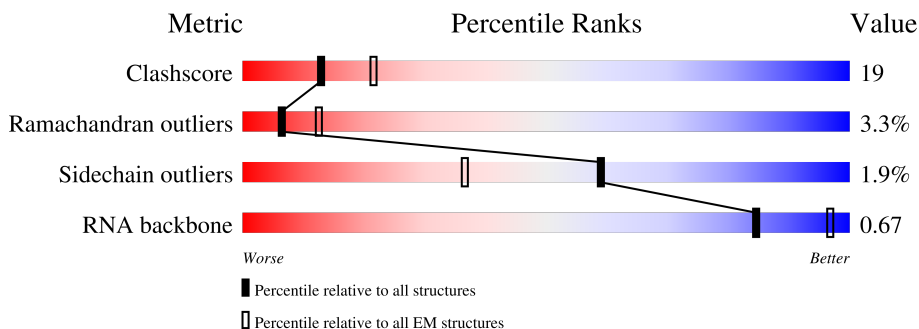
EMDB validation analysis : 0.0.1.dev70  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP)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

# 1 Overall quality at a glance

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

The reported resolution of this entry is 7.90 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.



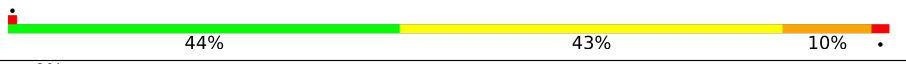


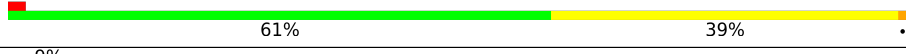
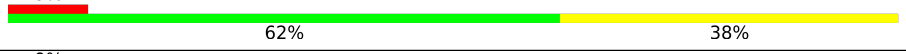






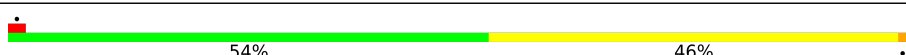
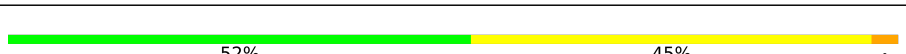
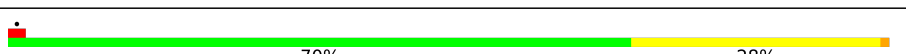
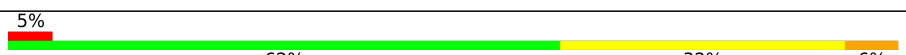
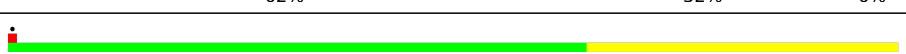

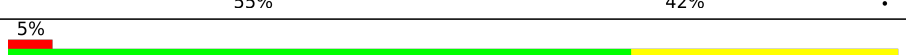
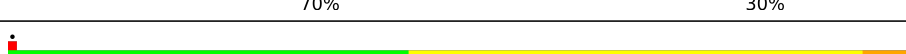

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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  $\geq 3$ , 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  $\leq 5\%$ . 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	1539	
2	01	229	
2	02	229	
3	03	1340	
4	04	1369	
5	05	59	
6	B	153	

Continued on next page...

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Mol	Chain	Length	Quality of chain
7	E	218	 44% 43% 10% 9%
8	F	206	 67% 31% 9%
9	G	205	 56% 40%
10	H	157	 61% 39% 9%
11	I	100	 62% 38% 9%
12	J	151	 60% 38% 9%
13	K	129	 62% 36% 7%
14	L	127	 49% 49% 7%
15	M	98	 58% 40% 7%
16	N	116	 57% 41% 7%
17	O	123	 66% 33% 7%
18	P	114	 54% 46% 9%
19	Q	100	 52% 45%
20	R	88	 70% 28% 9%
21	S	82	 62% 32% 6% 5%
22	T	80	 65% 35% 9%
23	U	65	 55% 42% 8%
24	V	79	 70% 30% 5%
25	W	85	 45% 51% 5% 9%
26	X	65	 57% 34% 8% 9%

## 2 Entry composition [i](#)

There are 26 unique types of molecules in this entry. The entry contains 75169 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 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	1443	30955	13808	5681	10024	1442	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	01	227	1753	1091	311	345	6	0	0
2	02	227	1757	1094	311	346	6	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	03	1327	10272	6441	1787	2001	43	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	04	1345	10372	6508	1853	1962	49	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	05	59	458	283	86	88	1	0	0

- Molecule 6 is a protein called 30S ribosomal protein S1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	B	153	774	463	154	157	0	0

- Molecule 7 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	E	218	1705	1081	305	312	7	0	0

- Molecule 8 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	F	206	1625	1028	305	289	3	0	0

- Molecule 9 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	G	205	1643	1026	315	298	4	0	0

- Molecule 10 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	H	157	1157	719	218	214	6	0	0

- Molecule 11 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	I	100	818	515	148	149	6	0	0

- Molecule 12 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	J	151	1182	735	227	216	4	0	0

- Molecule 13 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	K	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 14 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 15 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	M	98	Total	C	N	O	S	0	0
			787	493	150	143	1		

- Molecule 16 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	N	116	Total	C	N	O	S	0	0
			870	535	173	159	3		

- Molecule 17 is a protein called 30S ribosomal protein S12.

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

- Molecule 18 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	P	114	Total	C	N	O	S	0	0
			884	546	178	157	3		

- Molecule 19 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Q	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 20 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	R	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 21 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	S	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 22 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	T	80	Total	C	N	O	S	0	0
			649	411	121	114	3		

- Molecule 23 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	U	65	Total	C	N	O	S	0	0
			536	339	100	96	1		

- Molecule 24 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	V	79	Total	C	N	O	S	0	0
			638	408	120	108	2		

- Molecule 25 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	W	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

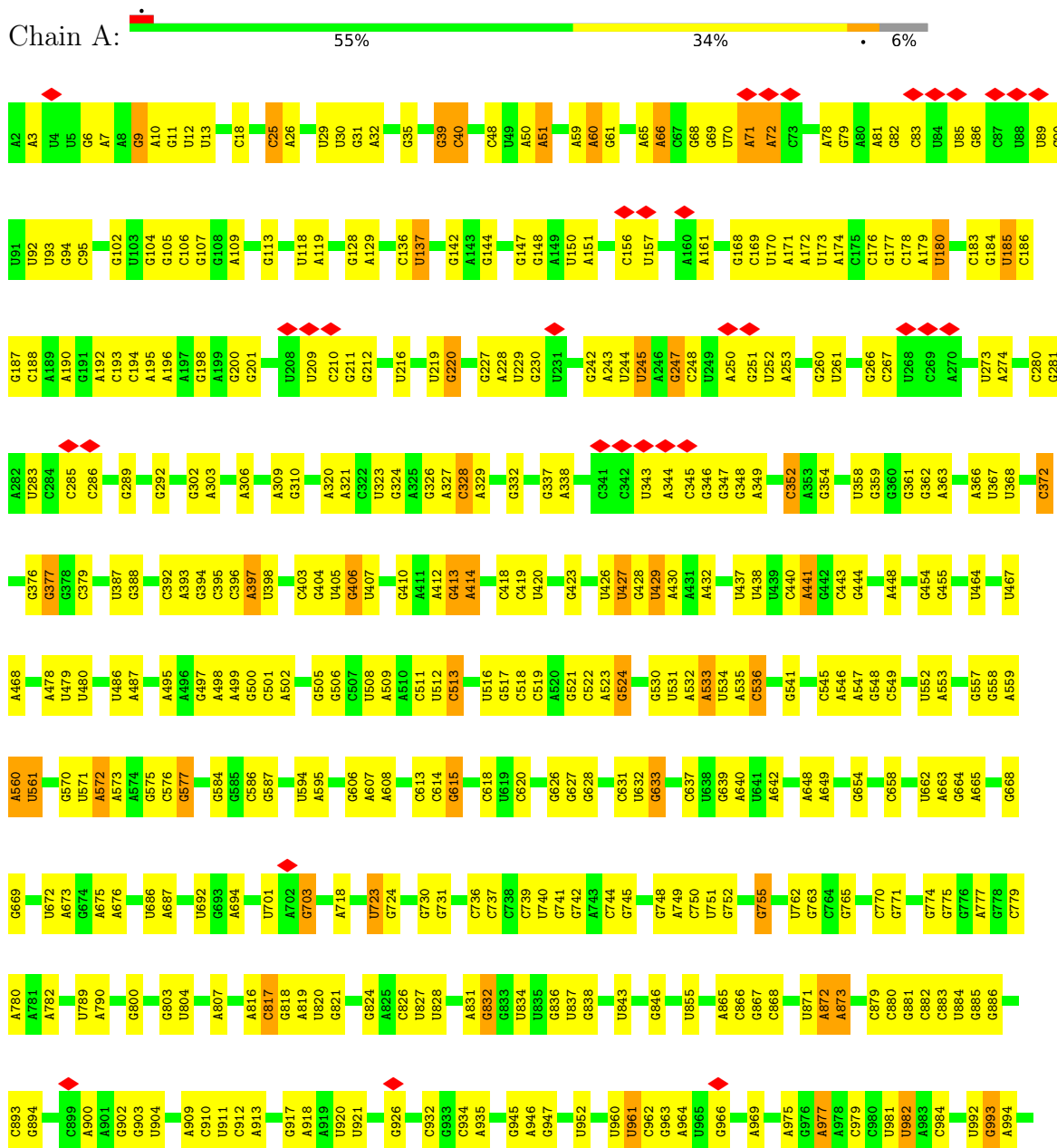
- Molecule 26 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	X	65	Total	C	N	O	S	0	0
			545	335	117	92	1		

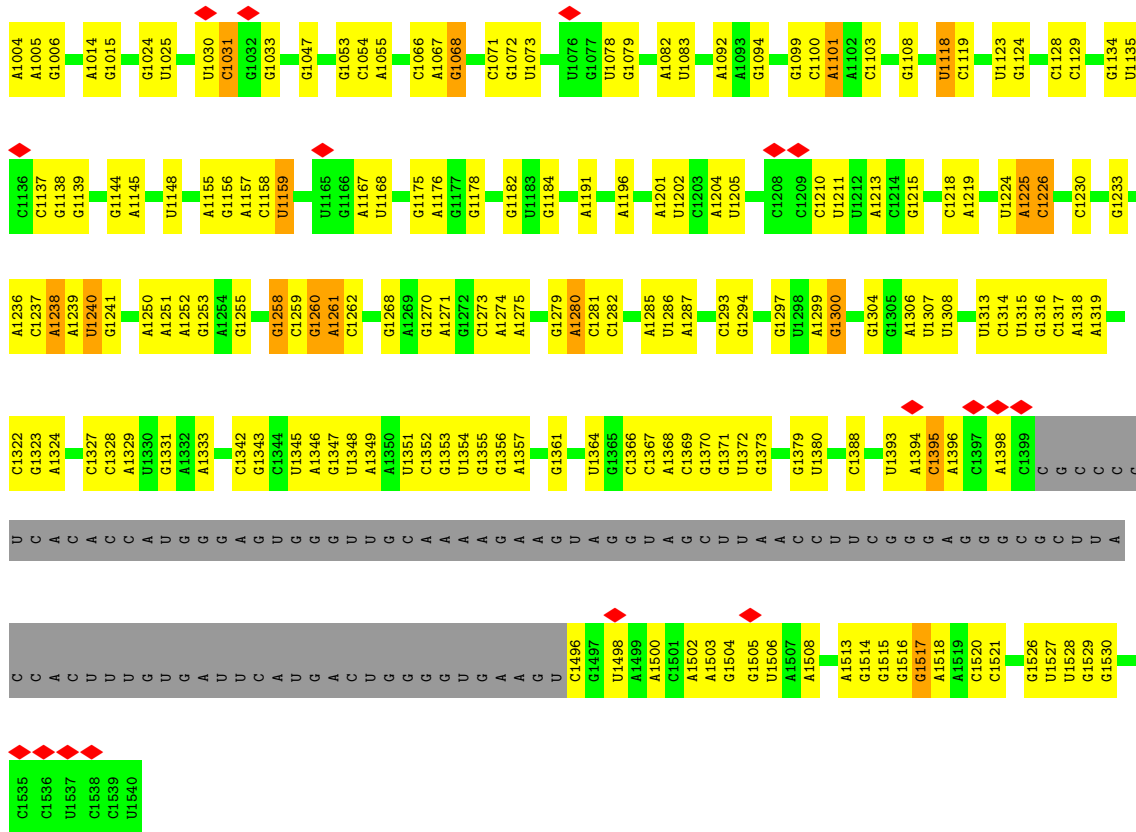
### 3 Residue-property plots

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: 16S rRNA



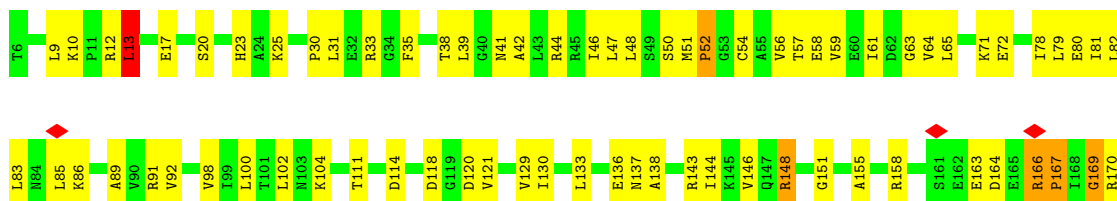


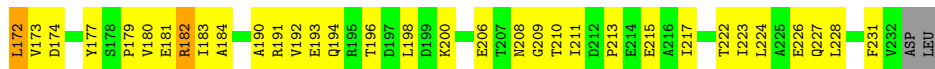


• Molecule 2: DNA-directed RNA polymerase subunit alpha

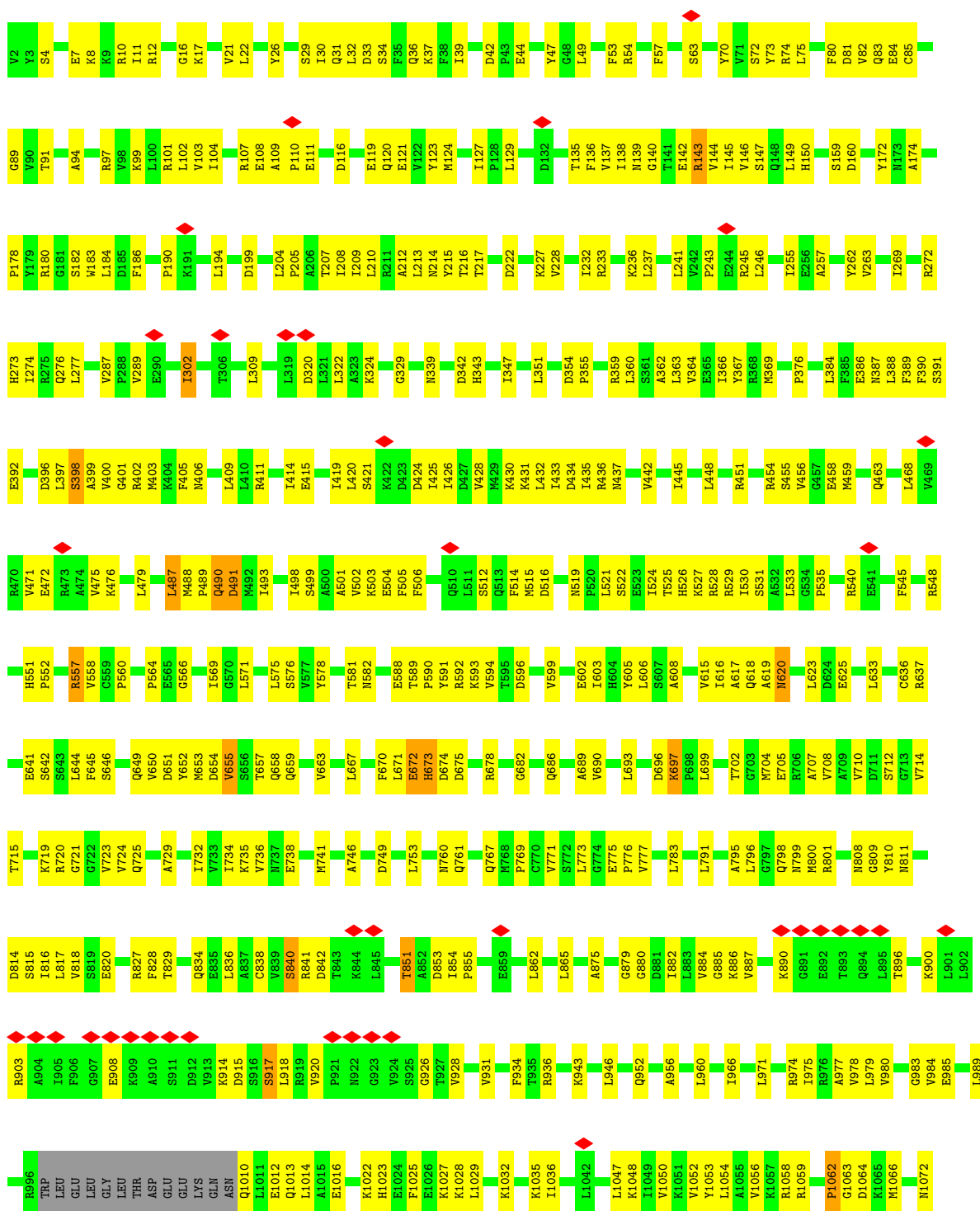


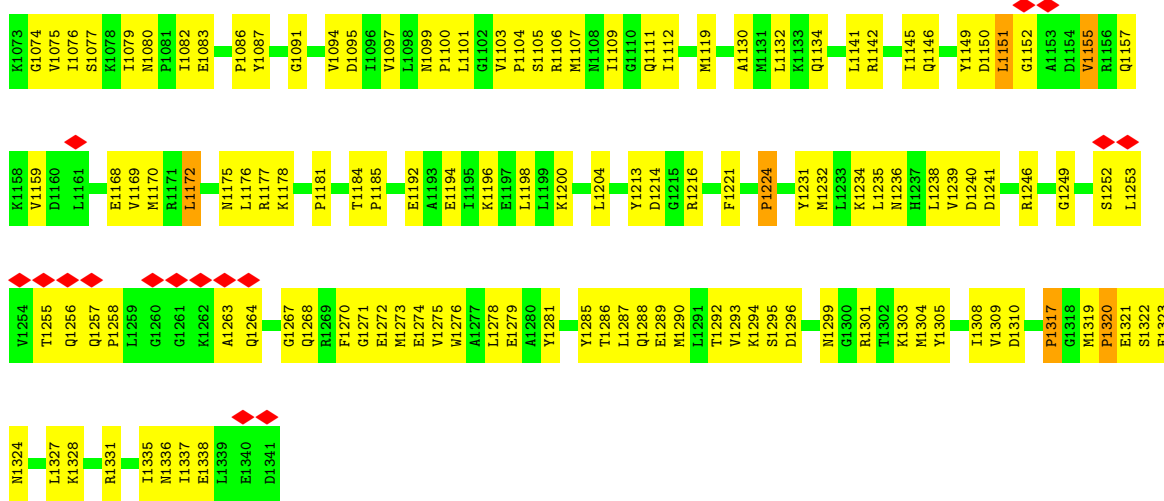
• Molecule 2: DNA-directed RNA polymerase subunit alpha



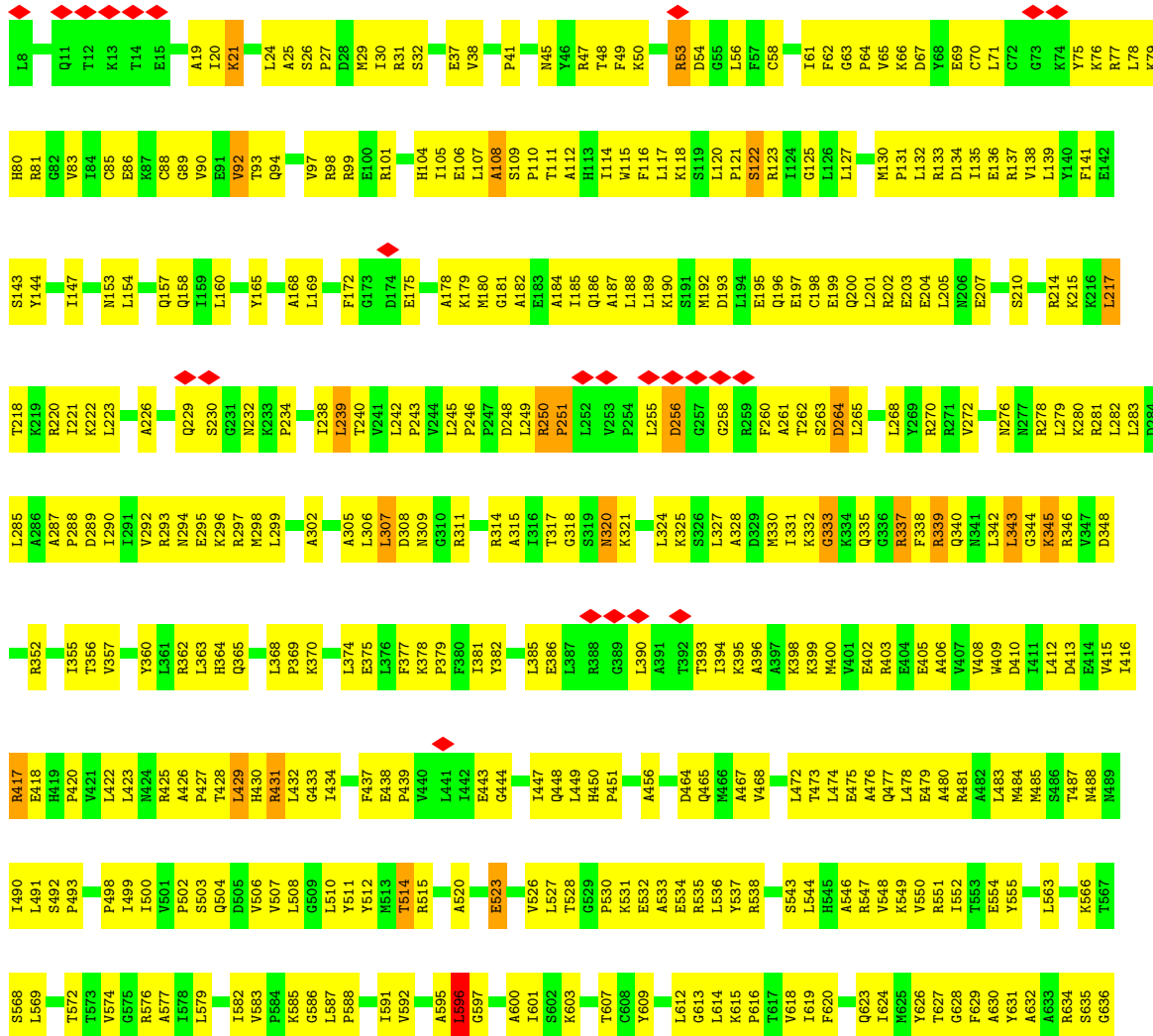


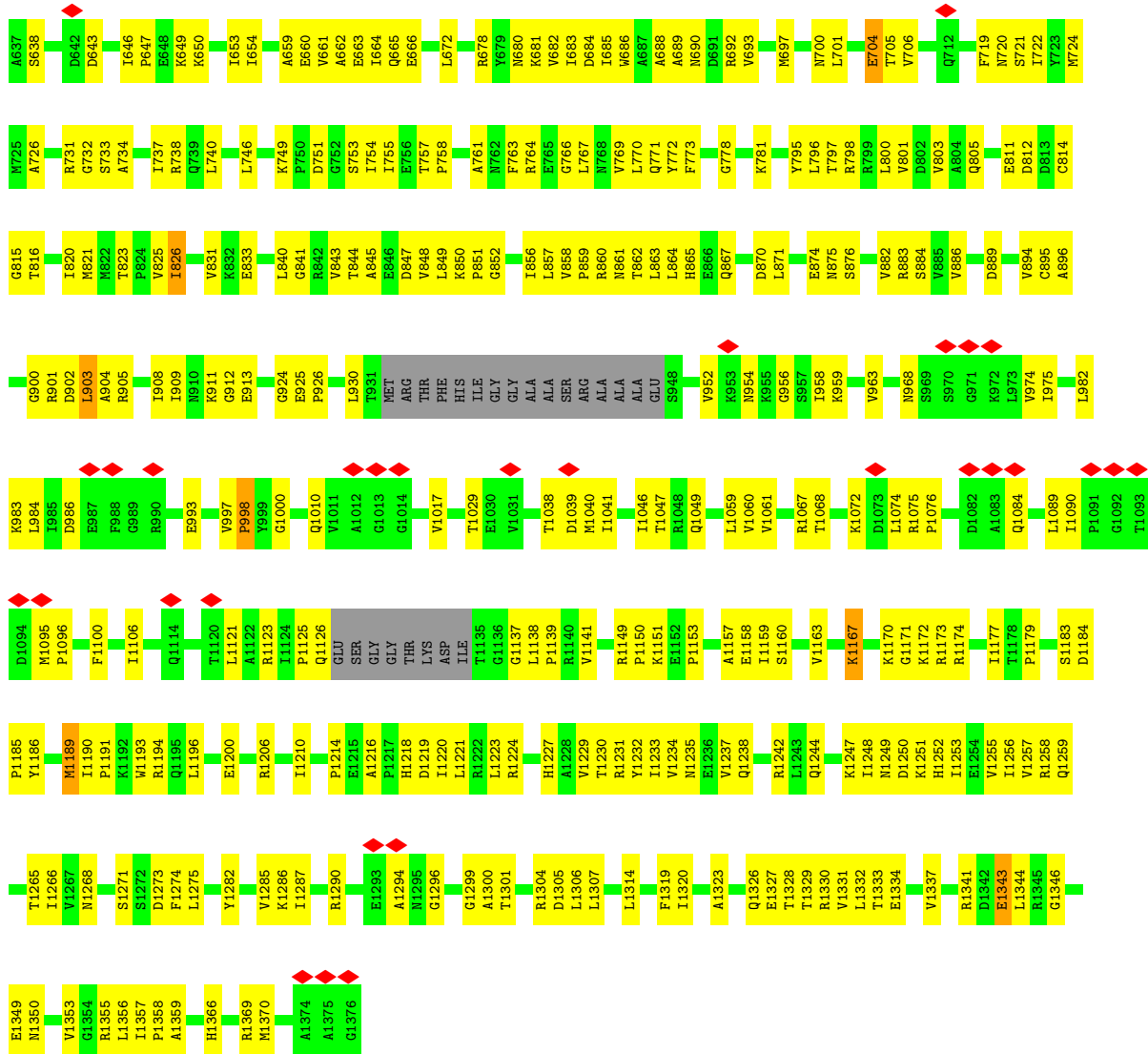
• Molecule 3: DNA-directed RNA polymerase subunit beta



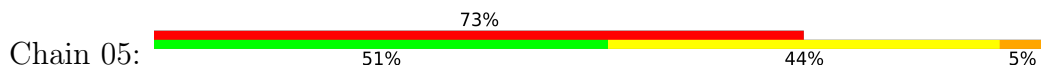


• Molecule 4: DNA-directed RNA polymerase subunit beta'

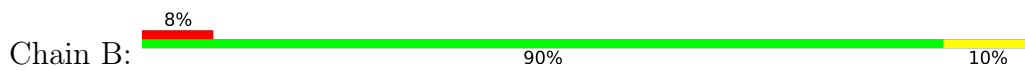




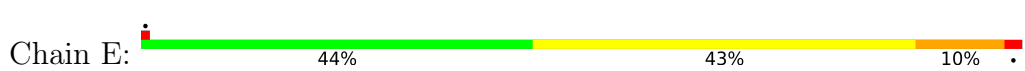
• Molecule 5: DNA-directed RNA polymerase subunit omega

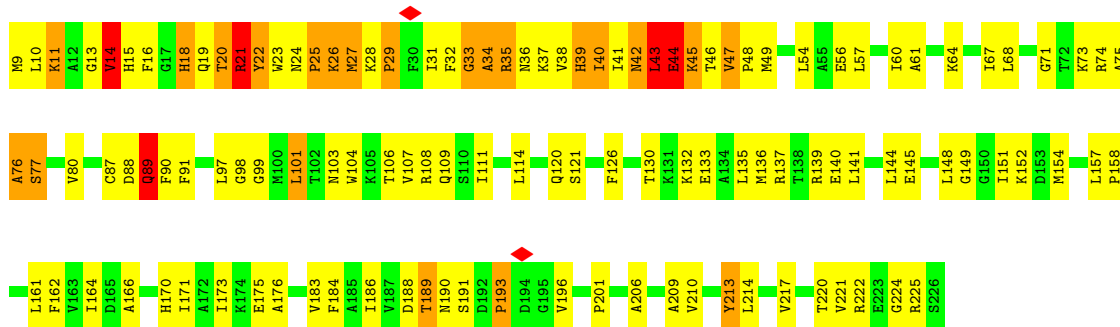


• Molecule 6: 30S ribosomal protein S1

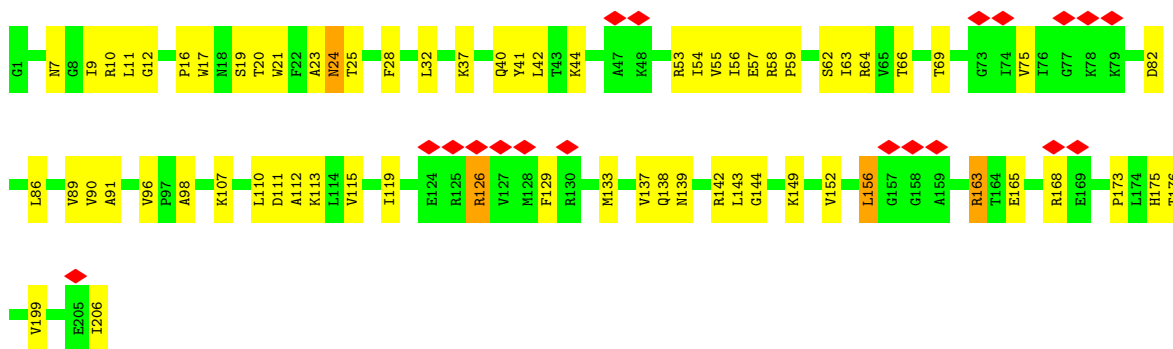


• Molecule 7: 30S ribosomal protein S2





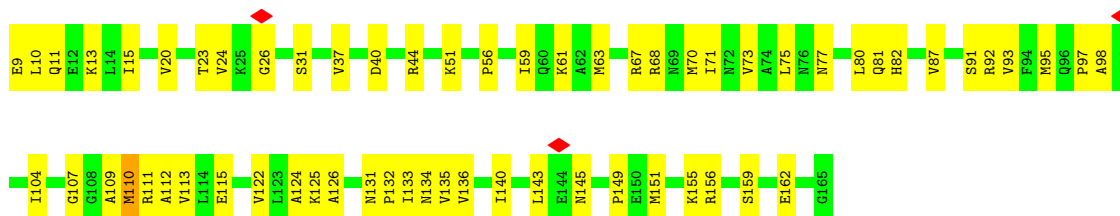
• Molecule 8: 30S ribosomal protein S3



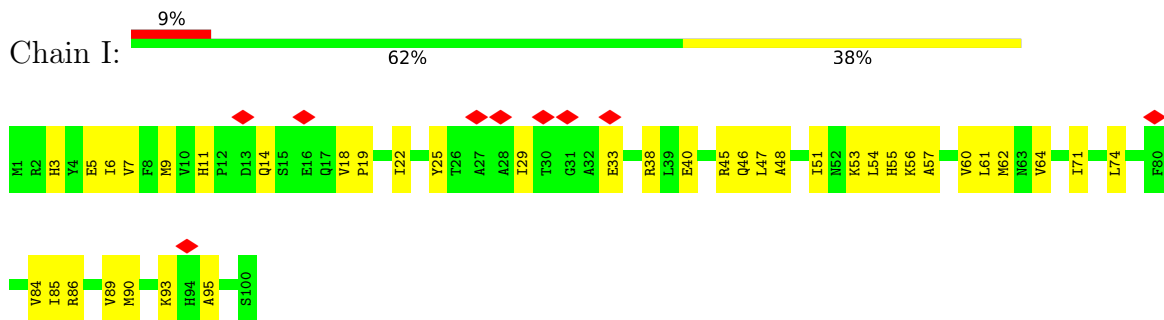
• Molecule 9: 30S ribosomal protein S4



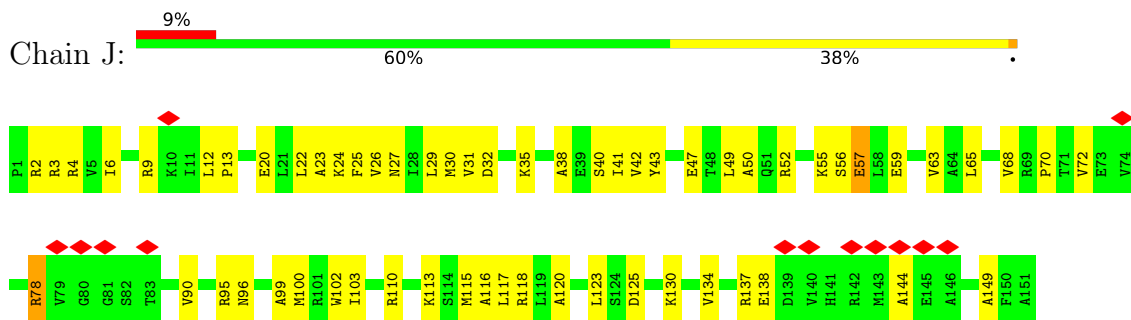
• Molecule 10: 30S ribosomal protein S5



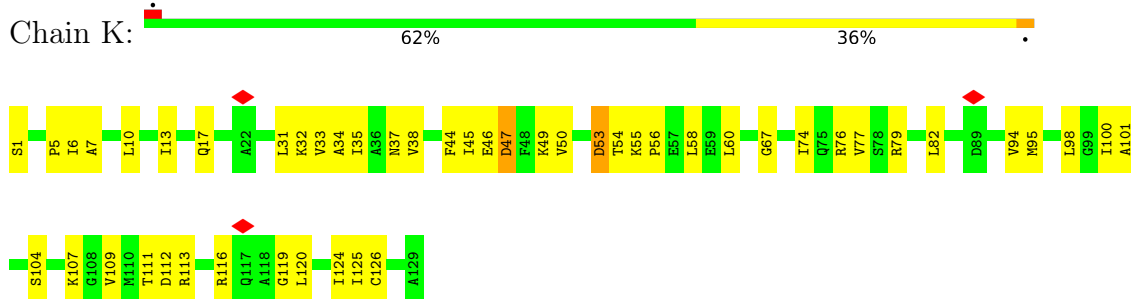
• Molecule 11: 30S ribosomal protein S6



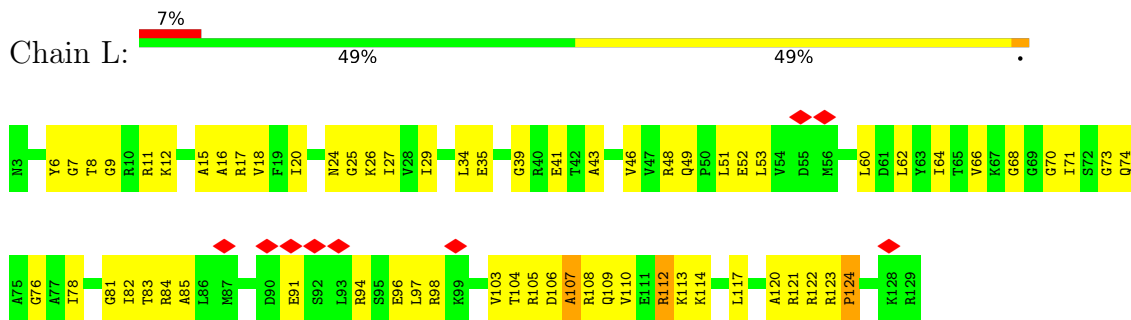
• Molecule 12: 30S ribosomal protein S7



• Molecule 13: 30S ribosomal protein S8

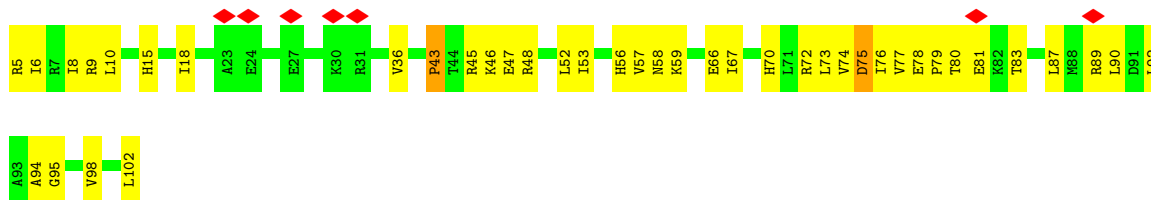


• Molecule 14: 30S ribosomal protein S9

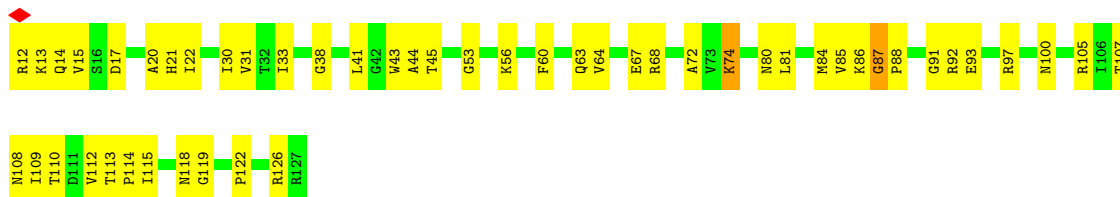


• Molecule 15: 30S ribosomal protein S10

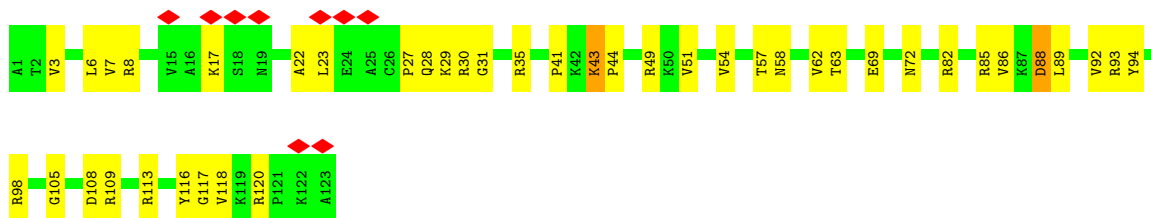




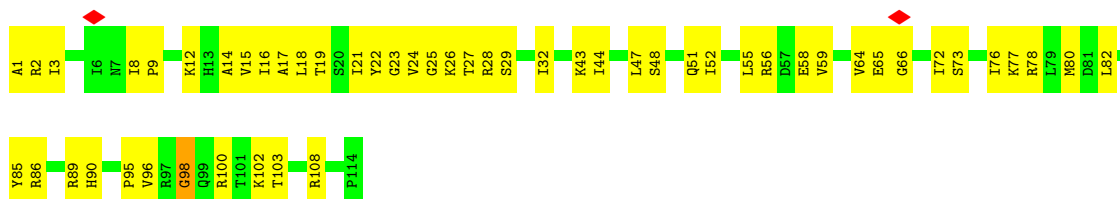
- Molecule 16: 30S ribosomal protein S11



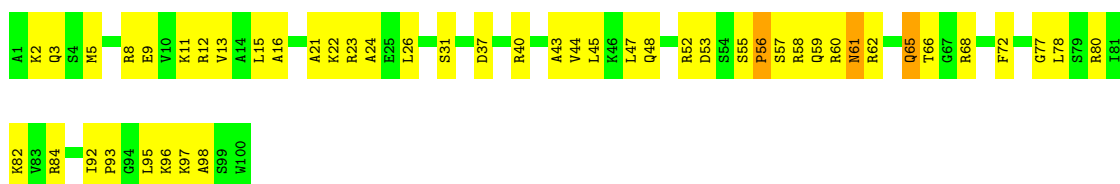
- Molecule 17: 30S ribosomal protein S12



- Molecule 18: 30S ribosomal protein S13



- Molecule 19: 30S ribosomal protein S14



- Molecule 20: 30S ribosomal protein S15

Chain R:  70% 28%



- Molecule 21: 30S ribosomal protein S16

Chain S:  5% 62% 32% 6%



- Molecule 22: 30S ribosomal protein S17

Chain T:  65% 35%



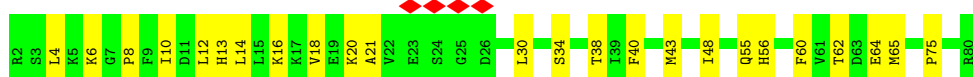
- Molecule 23: 30S ribosomal protein S18

Chain U:  8% 55% 42%



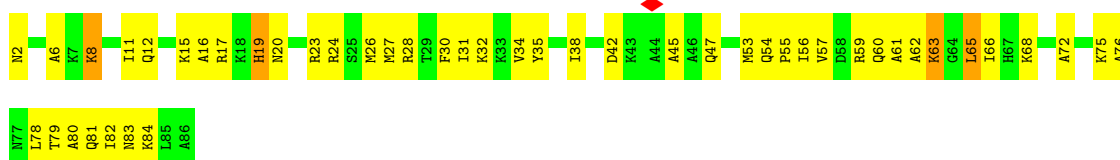
- Molecule 24: 30S ribosomal protein S19

Chain V:  5% 70% 30%



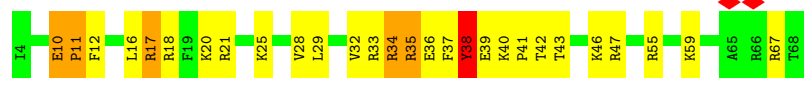
- Molecule 25: 30S ribosomal protein S20

Chain W:  45% 51% 5%



- Molecule 26: 30S ribosomal protein S21





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	10090	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 ( $e^-/\text{\AA}^2$ )	40.0	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	25000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	9.739	Depositor
Minimum map value	-3.633	Depositor
Average map value	-0.011	Depositor
Map value standard deviation	0.655	Depositor
Recommended contour level	2.0	Depositor
Map size ( $\text{\AA}$ )	459.98398, 459.98398, 459.98398	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.6428, 1.6428, 1.6428	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.25	0/34660	0.66	0/54067
2	01	0.25	0/1774	0.62	0/2405
2	02	0.28	0/1779	0.70	0/2411
3	03	0.28	0/10433	0.67	1/14101 (0.0%)
4	04	0.28	0/10528	0.68	2/14224 (0.0%)
5	05	0.28	0/460	0.73	1/620 (0.2%)
6	B	0.43	0/65	0.60	0/86
7	E	0.36	0/1736	0.82	3/2338 (0.1%)
8	F	0.26	0/1652	0.58	0/2225
9	G	0.26	0/1665	0.59	0/2227
10	H	0.27	0/1170	0.57	0/1573
11	I	0.28	0/836	0.64	0/1128
12	J	0.27	0/1196	0.61	0/1602
13	K	0.29	0/989	0.68	1/1326 (0.1%)
14	L	0.26	0/1034	0.56	0/1375
15	M	0.27	0/797	0.61	1/1077 (0.1%)
16	N	0.28	0/886	0.62	0/1195
17	O	0.26	0/969	0.64	1/1300 (0.1%)
18	P	0.25	0/893	0.60	0/1193
19	Q	0.28	0/817	0.58	0/1088
20	R	0.26	0/722	0.58	0/964
21	S	0.30	0/659	0.60	0/884
22	T	0.27	0/658	0.60	0/881
23	U	0.31	0/545	0.70	0/731
24	V	0.29	0/653	0.60	0/877
25	W	0.29	0/671	0.58	0/888
26	X	0.39	0/551	0.65	0/728
All	All	0.27	0/78798	0.66	10/113514 (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
1	A	0	3
7	E	0	1
All	All	0	4

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	E	26	LYS	N-CA-C	-9.24	86.05	111.00
4	04	339	ARG	N-CA-C	-6.41	93.70	111.00
7	E	44	GLU	N-CA-C	5.60	126.12	111.00
4	04	1296	GLY	N-CA-C	-5.41	99.57	113.10
13	K	67	GLY	N-CA-C	-5.32	99.81	113.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	25	C	Sidechain
1	A	872	A	Sidechain
1	A	9	G	Sidechain
7	E	22	TYR	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	30955	0	15586	432	0
2	01	1753	0	1780	96	0
2	02	1757	0	1778	95	0
3	03	10272	0	10138	477	0
4	04	10372	0	10512	614	0
5	05	458	0	476	31	0
6	B	774	0	201	9	0
7	E	1705	0	1732	163	0
8	F	1625	0	1699	49	0
9	G	1643	0	1710	71	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	H	1157	0	1199	48	0
11	I	818	0	808	36	0
12	J	1182	0	1240	48	0
13	K	979	0	1034	37	0
14	L	1022	0	1070	62	0
15	M	787	0	828	34	0
16	N	870	0	878	36	0
17	O	955	0	1019	31	0
18	P	884	0	944	51	0
19	Q	805	0	847	53	0
20	R	714	0	737	23	0
21	S	649	0	666	25	0
22	T	649	0	691	21	0
23	U	536	0	552	21	0
24	V	638	0	665	29	0
25	W	665	0	714	60	0
26	X	545	0	579	39	0
All	All	75169	0	60083	2504	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 19.

The worst 5 of 2504 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)
7:E:25:PRO:HB2	7:E:28:LYS:HB2	1.30	1.13
25:W:54:GLN:HA	25:W:57:VAL:HG12	1.39	1.03
7:E:23:TRP:CZ3	7:E:25:PRO:HB3	1.96	1.00
3:03:979:LEU:HD21	3:03:989:LEU:HD22	1.43	0.99
7:E:19:GLN:H	7:E:40:ILE:HA	1.27	0.98

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	01	225/229 (98%)	192 (85%)	30 (13%)	3 (1%)	12	48
2	02	225/229 (98%)	176 (78%)	36 (16%)	13 (6%)	1	18
3	03	1323/1340 (99%)	1076 (81%)	209 (16%)	38 (3%)	4	29
4	04	1339/1369 (98%)	1128 (84%)	167 (12%)	44 (3%)	4	26
5	05	57/59 (97%)	46 (81%)	9 (16%)	2 (4%)	3	25
6	B	6/153 (4%)	6 (100%)	0	0	100	100
7	E	216/218 (99%)	159 (74%)	31 (14%)	26 (12%)	0	6
8	F	204/206 (99%)	185 (91%)	17 (8%)	2 (1%)	15	55
9	G	203/205 (99%)	166 (82%)	32 (16%)	5 (2%)	5	32
10	H	155/157 (99%)	123 (79%)	28 (18%)	4 (3%)	5	31
11	I	98/100 (98%)	82 (84%)	14 (14%)	2 (2%)	7	38
12	J	149/151 (99%)	133 (89%)	14 (9%)	2 (1%)	12	48
13	K	127/129 (98%)	105 (83%)	20 (16%)	2 (2%)	9	44
14	L	125/127 (98%)	98 (78%)	25 (20%)	2 (2%)	9	44
15	M	96/98 (98%)	72 (75%)	19 (20%)	5 (5%)	2	19
16	N	114/116 (98%)	87 (76%)	20 (18%)	7 (6%)	1	17
17	O	121/123 (98%)	92 (76%)	23 (19%)	6 (5%)	2	20
18	P	112/114 (98%)	95 (85%)	14 (12%)	3 (3%)	5	31
19	Q	98/100 (98%)	79 (81%)	14 (14%)	5 (5%)	2	19
20	R	86/88 (98%)	77 (90%)	9 (10%)	0	100	100
21	S	80/82 (98%)	66 (82%)	12 (15%)	2 (2%)	5	32
22	T	78/80 (98%)	63 (81%)	13 (17%)	2 (3%)	5	31
23	U	63/65 (97%)	51 (81%)	8 (13%)	4 (6%)	1	17
24	V	77/79 (98%)	63 (82%)	13 (17%)	1 (1%)	12	48
25	W	83/85 (98%)	66 (80%)	16 (19%)	1 (1%)	13	50
26	X	63/65 (97%)	47 (75%)	12 (19%)	4 (6%)	1	17
All	All	5523/5767 (96%)	4533 (82%)	805 (15%)	185 (3%)	6	26

5 of 185 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	02	20	SER
2	02	136	GLU
2	02	137	ASN
3	03	398	SER
3	03	625	GLU

### 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	01	194/197 (98%)	192 (99%)	2 (1%)	76	86
2	02	194/197 (98%)	189 (97%)	5 (3%)	46	66
3	03	1098/1155 (95%)	1081 (98%)	17 (2%)	65	80
4	04	1103/1141 (97%)	1088 (99%)	15 (1%)	67	80
5	05	49/49 (100%)	49 (100%)	0	100	100
6	B	6/7 (86%)	6 (100%)	0	100	100
7	E	180/180 (100%)	173 (96%)	7 (4%)	32	56
8	F	170/170 (100%)	167 (98%)	3 (2%)	59	77
9	G	172/172 (100%)	165 (96%)	7 (4%)	30	55
10	H	119/119 (100%)	117 (98%)	2 (2%)	60	78
11	I	87/87 (100%)	87 (100%)	0	100	100
12	J	124/124 (100%)	122 (98%)	2 (2%)	62	79
13	K	104/104 (100%)	101 (97%)	3 (3%)	42	64
14	L	105/105 (100%)	102 (97%)	3 (3%)	42	64
15	M	86/86 (100%)	84 (98%)	2 (2%)	50	70
16	N	89/89 (100%)	87 (98%)	2 (2%)	52	71
17	O	103/103 (100%)	101 (98%)	2 (2%)	57	75
18	P	92/92 (100%)	92 (100%)	0	100	100
19	Q	83/83 (100%)	82 (99%)	1 (1%)	71	83
20	R	76/76 (100%)	75 (99%)	1 (1%)	69	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	S	65/65 (100%)	62 (95%)	3 (5%)	27	52
22	T	74/74 (100%)	74 (100%)	0	100	100
23	U	56/56 (100%)	55 (98%)	1 (2%)	59	77
24	V	70/70 (100%)	70 (100%)	0	100	100
25	W	65/65 (100%)	60 (92%)	5 (8%)	13	37
26	X	55/55 (100%)	51 (93%)	4 (7%)	14	39
All	All	4619/4721 (98%)	4532 (98%)	87 (2%)	59	75

5 of 87 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	H	145	ASN
17	O	88	ASP
12	J	78	ARG
14	L	122	ARG
21	S	25	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 99 such sidechains are listed below:

Mol	Chain	Res	Type
8	F	40	GLN
12	J	27	ASN
8	F	184	ASN
9	G	163	GLN
14	L	30	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1441/1539 (93%)	164 (11%)	2 (0%)

5 of 164 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	31	G
1	A	32	A
1	A	39	G

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Mol	Chain	Res	Type
1	A	40	C

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	69	G
1	A	343	U

#### 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](#)

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
6	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	10:GLU	C	107:UNK	N	53.99
1	B	179:UNK	C	191:UNK	N	19.24

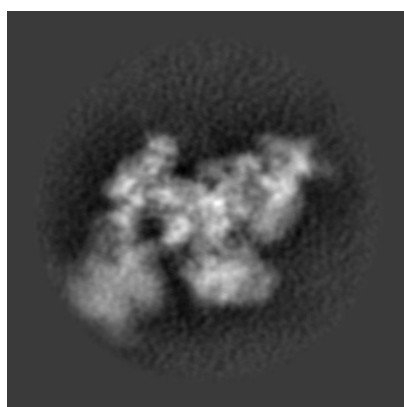
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7015. These allow visual inspection of the internal detail of the map and identification of artifacts.

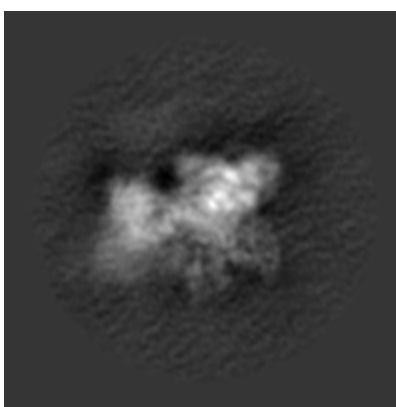
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

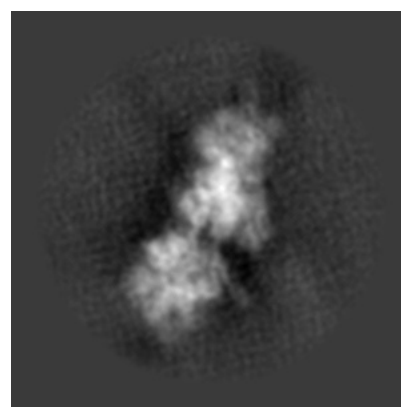
#### 6.1.1 Primary map



X



Y

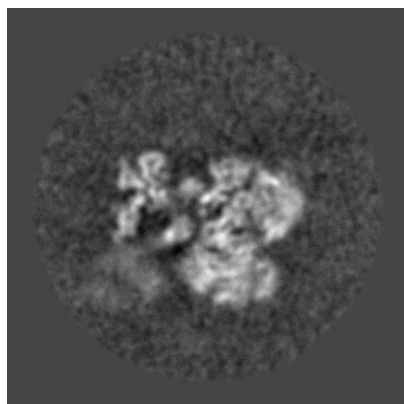


Z

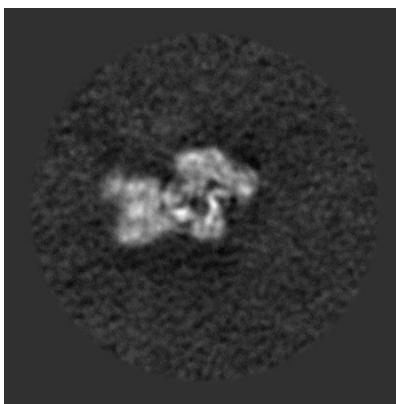
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

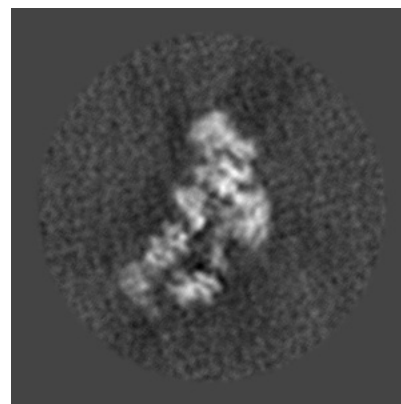
#### 6.2.1 Primary map



X Index: 140



Y Index: 140

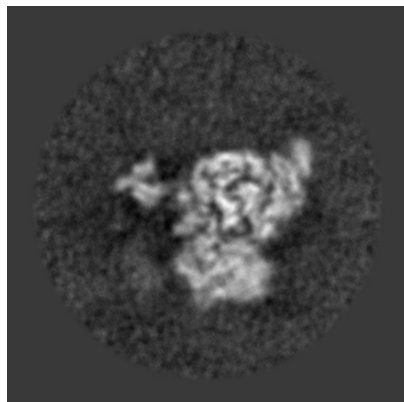


Z Index: 140

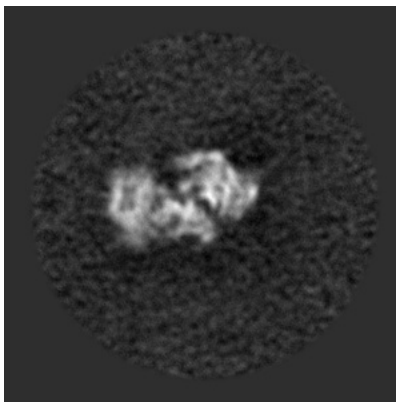
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [\(i\)](#)

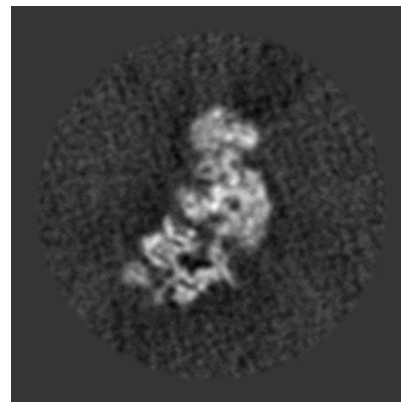
### 6.3.1 Primary map



X Index: 149



Y Index: 150

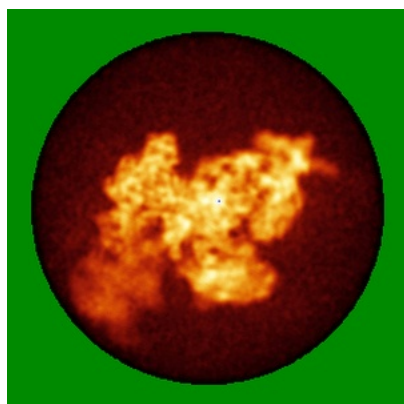


Z Index: 146

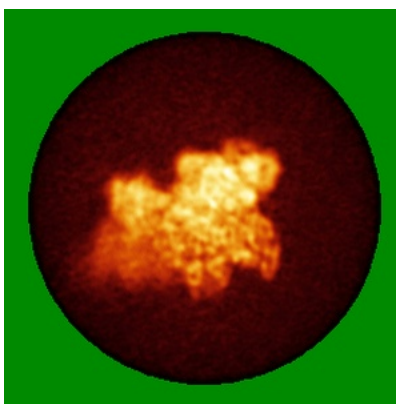
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [\(i\)](#)

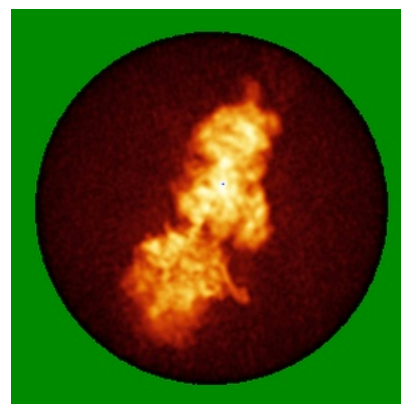
### 6.4.1 Primary map



X



Y

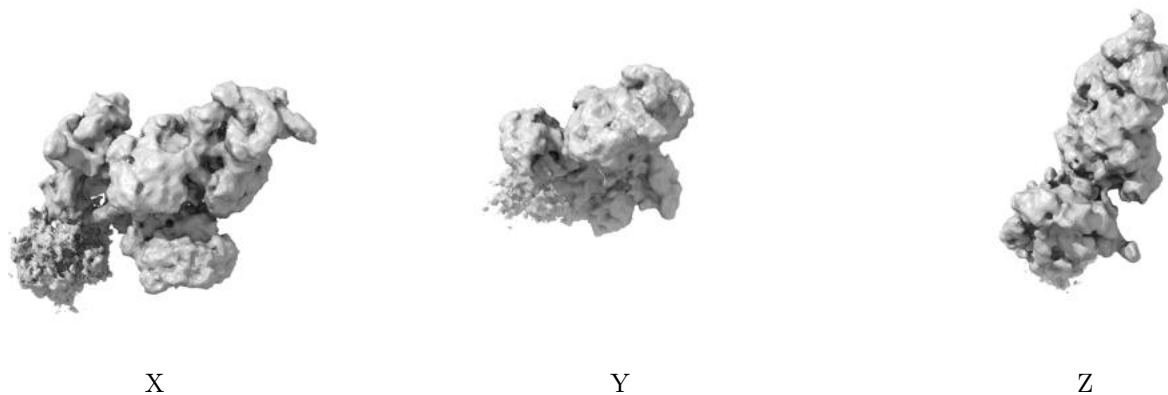


Z

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



The images above show the 3D surface view of the map at the recommended contour level 2.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

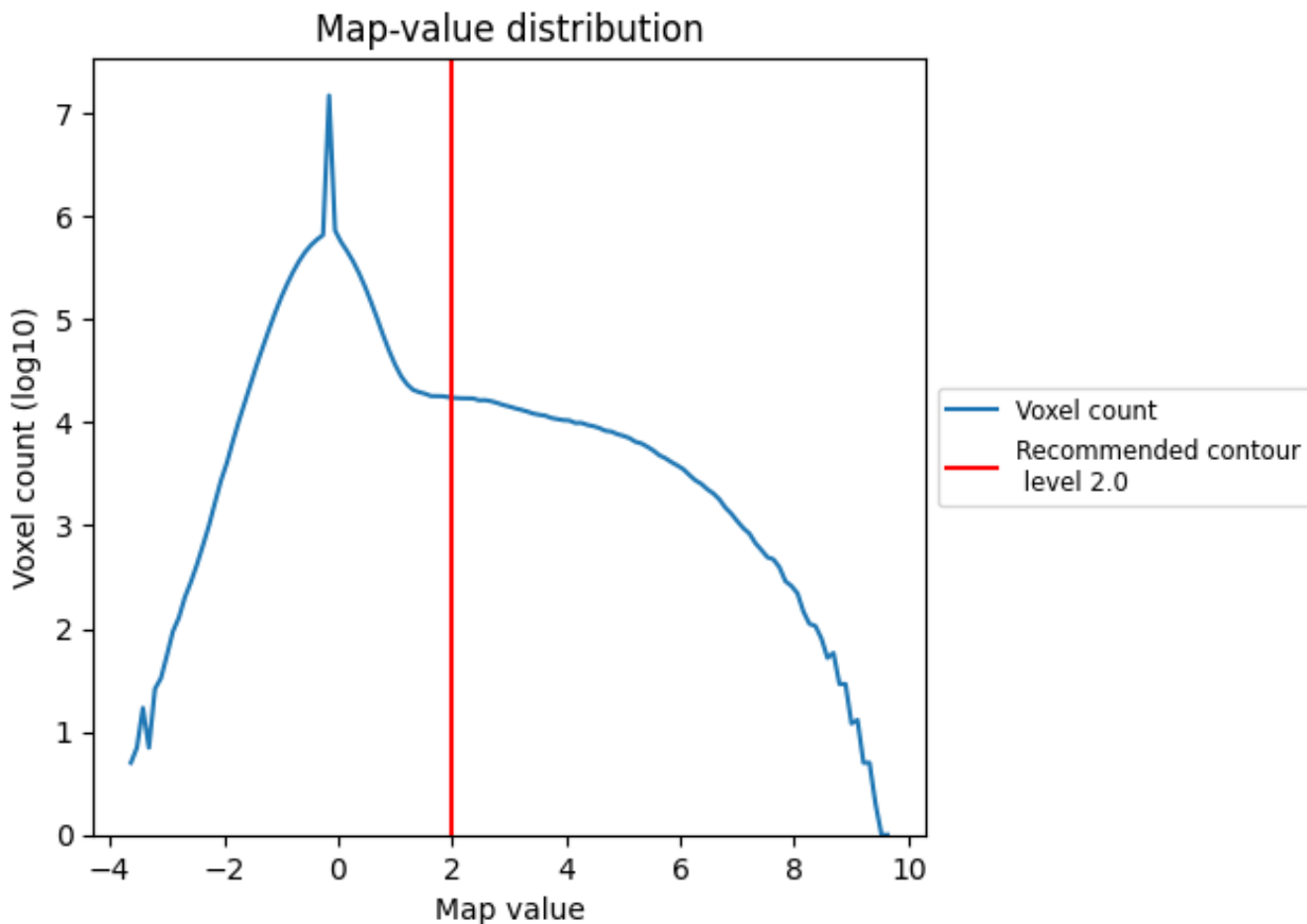
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

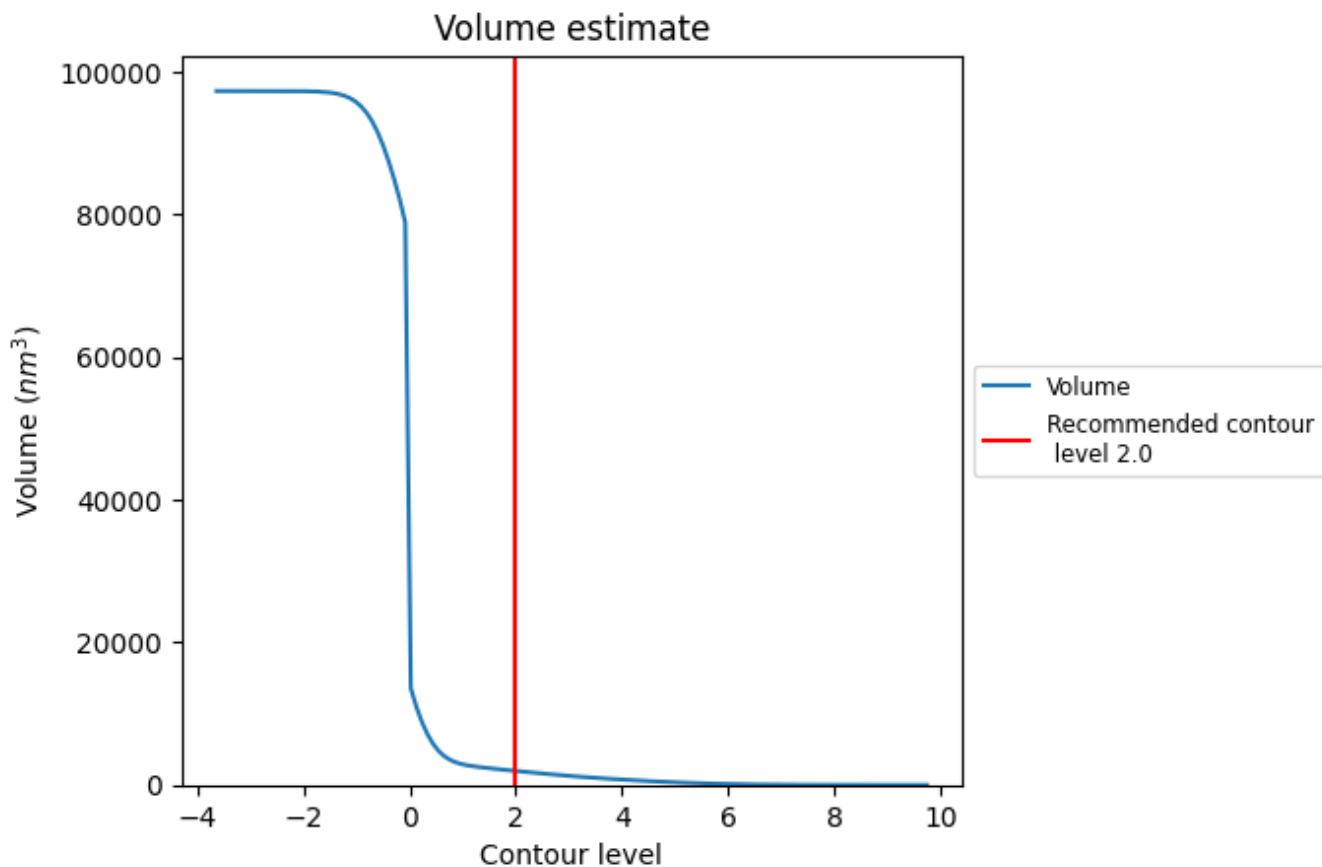
This section contains the results of statistical analysis of the map.

### 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.

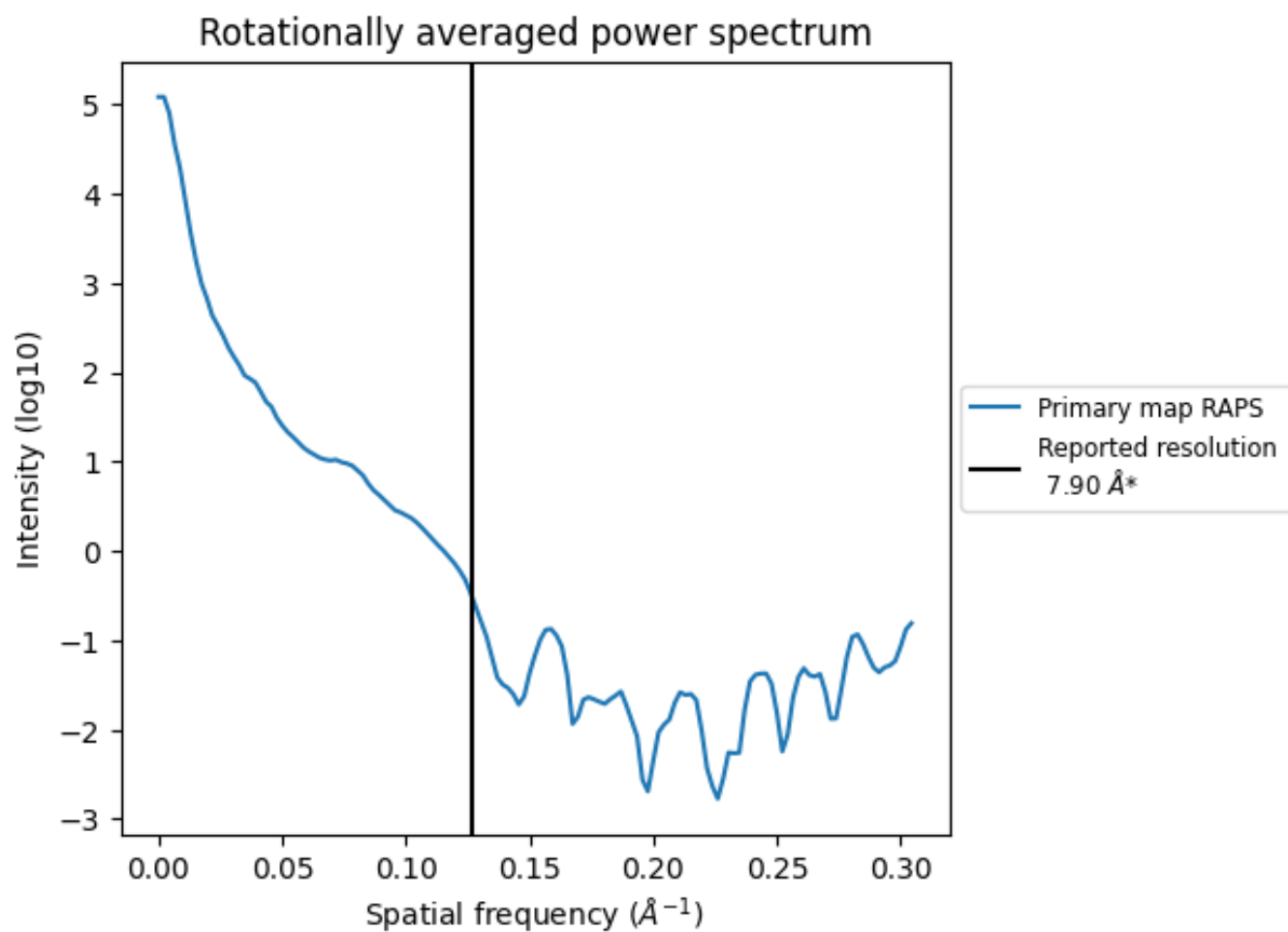
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1962 nm<sup>3</sup>; this corresponds to an approximate mass of 1773 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 0.127 Å<sup>-1</sup>

## 8 Fourier-Shell correlation

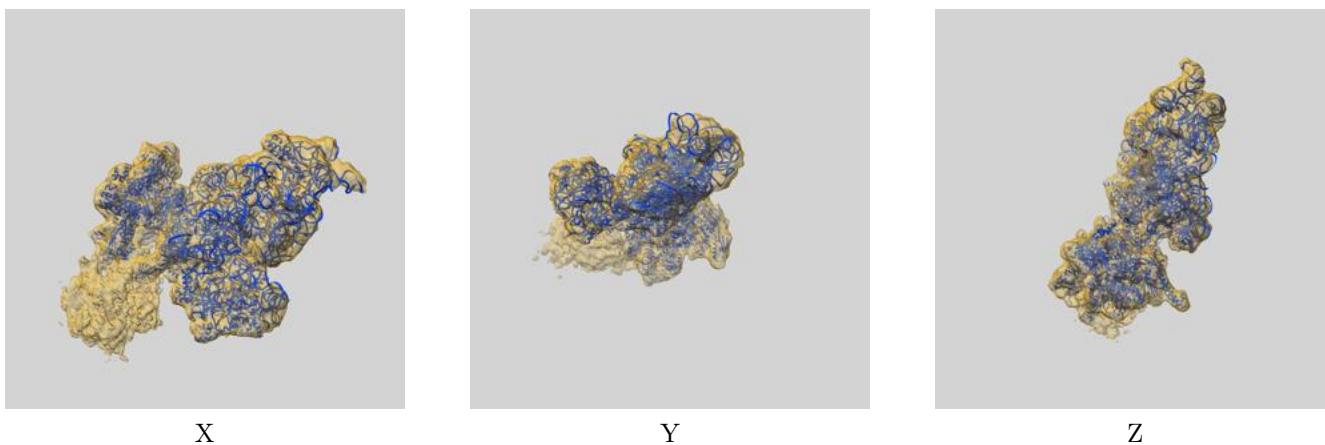
This section was not generated. No FSC curve or half-maps provided.



## 9 Map-model fit [i](#)

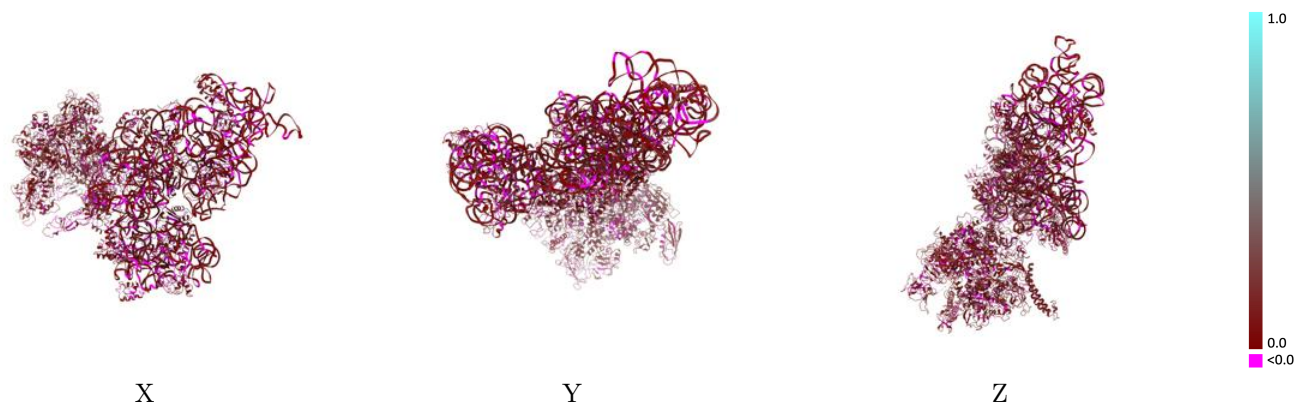
This section contains information regarding the fit between EMDB map EMD-7015 and PDB model 6AWC. Per-residue inclusion information can be found in section [3](#) on page [8](#).

### 9.1 Map-model overlay [i](#)



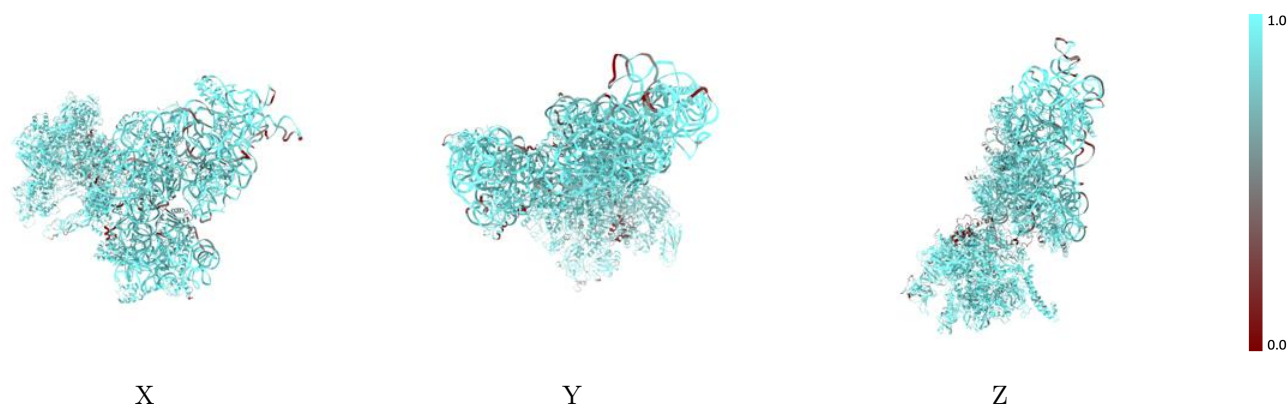
The images above show the 3D surface view of the map at the recommended contour level 2.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [\(i\)](#)



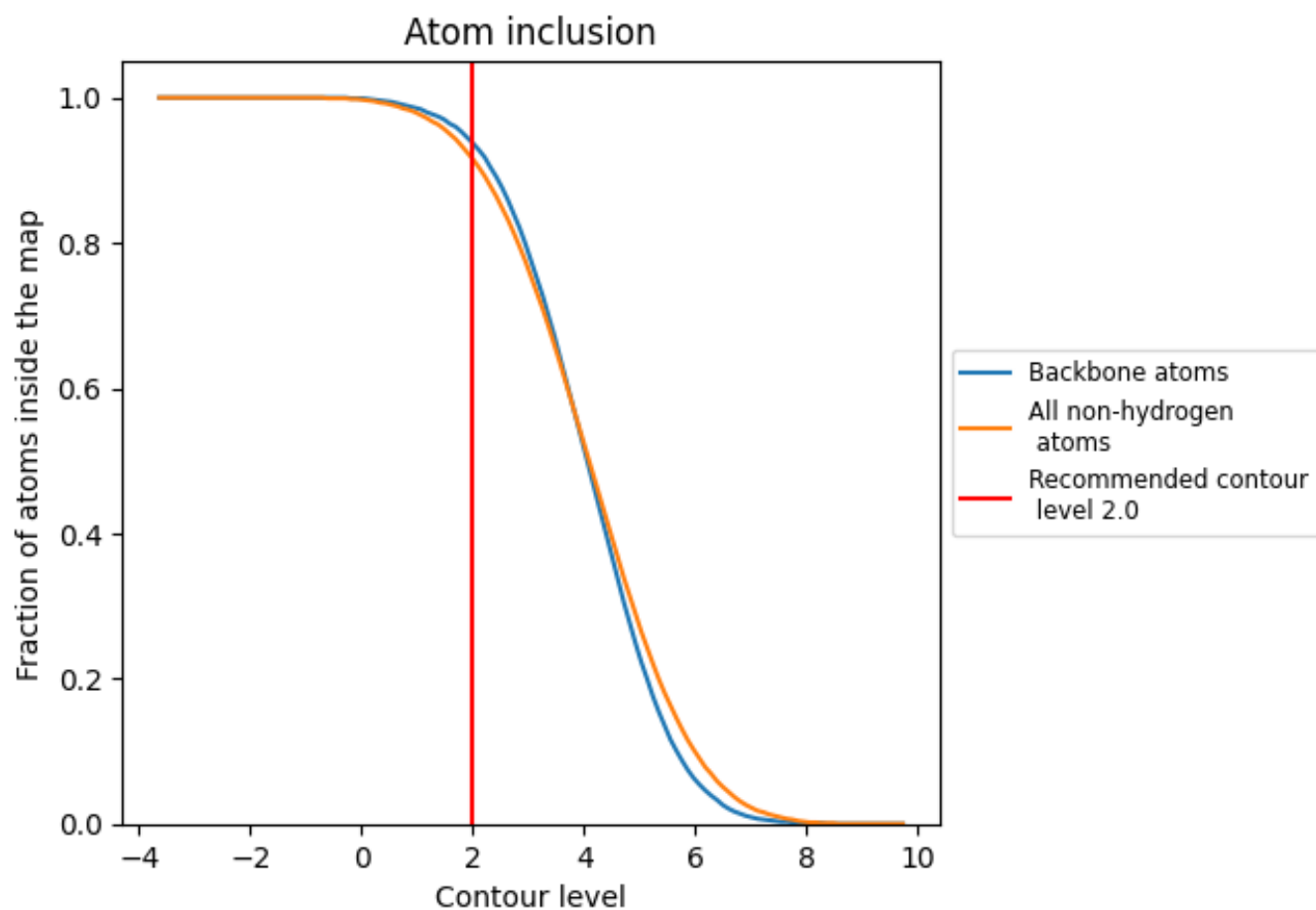
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 [\(i\)](#)



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 (2.0).

























































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 92% 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 (2.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9160	 0.0950
01	 0.9410	 0.1410
02	 0.9460	 0.1200
03	 0.9060	 0.1110
04	 0.9140	 0.1210
05	 0.2890	 0.0470
A	 0.9260	 0.0890
B	 0.8900	 0.0700
E	 0.9680	 0.1250
F	 0.8560	 0.0970
G	 0.9270	 0.0660
H	 0.9180	 0.1200
I	 0.8470	 0.1130
J	 0.8500	 0.0660
K	 0.9290	 0.0960
L	 0.8980	 0.0530
M	 0.8910	 0.0440
N	 0.9720	 0.0530
O	 0.8790	 0.0640
P	 0.9270	 0.0590
Q	 0.9700	 0.0330
R	 0.9350	 0.0940
S	 0.9430	 0.0640
T	 0.9590	 0.0860
U	 0.9110	 0.0610
V	 0.9320	 0.0380
W	 0.9680	 0.0750
X	 0.8820	 0.1080

