



wwPDB EM Validation Summary Report ⓘ

Oct 28, 2024 – 09:32 pm GMT

PDB ID : 7AS9
EMDB ID : EMD-11890
Title : Bacillus subtilis ribosome-associated quality control complex state A. Ribosomal 50S subunit with peptidyl tRNA in the A/P position and RqcH.
Authors : Crowe-McAuliffe, C.; Wilson, D.N.
Deposited on : 2020-10-27
Resolution : 3.50 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 ⓘ symbol.

The types of validation reports are described at

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

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

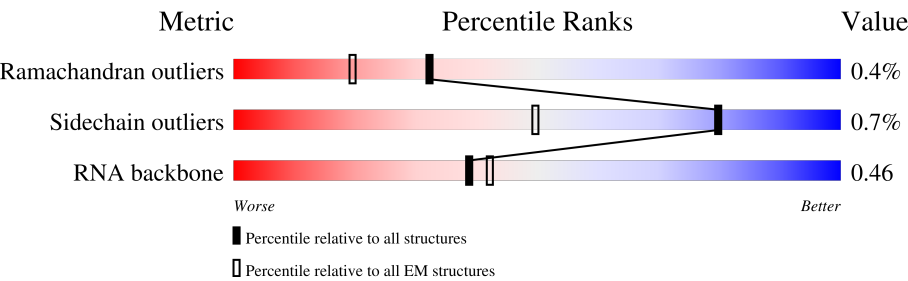
EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.50 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)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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 $\leq 5\%$. 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	0	597	<div><div>26%</div><div><div></div><div>86%</div><div></div><div>10%</div></div><div></div></div>
2	2	76	<div><div></div><div><div></div><div>68%</div><div></div><div>30%</div></div><div></div></div>
3	A	2926	<div><div></div><div><div></div><div>66%</div><div></div><div>29%</div></div><div></div></div>
4	B	119	<div><div></div><div><div></div><div>61%</div><div></div><div>32%</div></div><div></div></div>
5	E	277	<div><div></div><div><div></div><div>97%</div><div></div><div></div></div><div></div></div>
6	F	209	<div><div>8%</div><div><div></div><div>99%</div><div></div><div></div></div><div></div></div>
7	G	207	<div><div>5%</div><div><div></div><div>98%</div><div></div><div></div></div><div></div></div>
8	H	179	<div><div>10%</div><div><div></div><div>86%</div><div></div><div>5% 8%</div></div><div></div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	I	179	
10	K	141	
11	L	166	
12	N	145	
13	O	122	
14	P	146	
15	Q	144	
16	R	120	
17	S	120	
18	T	115	
19	U	119	
20	V	102	
21	W	113	
22	X	95	
23	Y	103	
24	a	94	
25	b	62	
26	c	66	
27	d	59	
28	f	59	
29	g	49	
30	h	44	
31	i	66	
32	j	37	

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 93137 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Rqc2 homolog RqcH.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	535	Total	C	N	O	S	0	0
			3987	2517	712	748	10		

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	571	GLY	-	expression tag	UNP O34693
0	572	SER	-	expression tag	UNP O34693
0	573	GLY	-	expression tag	UNP O34693
0	574	GLY	-	expression tag	UNP O34693
0	575	ASP	-	expression tag	UNP O34693
0	576	TYR	-	expression tag	UNP O34693
0	577	LYS	-	expression tag	UNP O34693
0	578	ASP	-	expression tag	UNP O34693
0	579	HIS	-	expression tag	UNP O34693
0	580	ASP	-	expression tag	UNP O34693
0	581	GLY	-	expression tag	UNP O34693
0	582	ASP	-	expression tag	UNP O34693
0	583	TYR	-	expression tag	UNP O34693
0	584	LYS	-	expression tag	UNP O34693
0	585	ASP	-	expression tag	UNP O34693
0	586	HIS	-	expression tag	UNP O34693
0	587	ASP	-	expression tag	UNP O34693
0	588	ILE	-	expression tag	UNP O34693
0	589	ASP	-	expression tag	UNP O34693
0	590	TYR	-	expression tag	UNP O34693
0	591	LYS	-	expression tag	UNP O34693
0	592	ASP	-	expression tag	UNP O34693
0	593	ASP	-	expression tag	UNP O34693
0	594	ASP	-	expression tag	UNP O34693
0	595	ASP	-	expression tag	UNP O34693
0	596	LYS	-	expression tag	UNP O34693
0	597	GLY	-	expression tag	UNP O34693

- Molecule 2 is a RNA chain called tRNA-Ala-1-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	75	Total	C	N	O	P	0	0
			1603	713	288	527	75		

- Molecule 3 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	2812	Total	C	N	O	P	0	0
			60389	26942	11160	19477	2810		

- Molecule 4 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	112	Total	C	N	O	P	0	0
			2392	1068	435	778	111		

- Molecule 5 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	272	Total	C	N	O	S	0	0
			2083	1296	408	373	6		

- Molecule 6 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	206	Total	C	N	O	S	0	0
			1569	985	289	290	5		

- Molecule 7 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	205	Total	C	N	O	S	0	0
			1561	980	289	290	2		

- Molecule 8 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	164	Total	C	N	O	S	0	0
			1284	813	228	236	7		

- Molecule 9 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	175	Total	C	N	O	S	0	0
			1342	835	248	257	2		

- Molecule 10 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	132	Total	C	N	O	S	0	0
			974	612	172	184	6		

- Molecule 11 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	113	Total	C	N	O	S	0	0
			886	559	152	174	1		

- Molecule 12 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	N	142	Total	C	N	O	S	0	0
			1123	710	206	202	5		

- Molecule 13 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	122	Total	C	N	O	S	0	0
			920	571	173	172	4		

- Molecule 14 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	146	Total	C	N	O	S	0	0
			1081	671	207	201	2		

- Molecule 15 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Q	135	Total	C	N	O	S	0	0
			1076	690	205	176	5		

- Molecule 16 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	R	119	Total	C	N	O	S	0	0
			953	583	186	180	4		

- Molecule 17 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	120	Total	C	N	O	S	0	0
			912	564	176	171	1		

- Molecule 18 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	115	Total	C	N	O	S	0	0
			944	600	185	158	1		

- Molecule 19 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	117	Total	C	N	O	S	0	0
			940	591	189	156	4		

- Molecule 20 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	V	100	Total	C	N	O	0	0
			781	498	138	145		

- Molecule 21 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	109	Total	C	N	O	S	0	0
			842	525	164	150	3		

- Molecule 22 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	90	Total	C	N	O	S	0	0
			725	452	134	136	3		

- Molecule 23 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Y	101	Total	C	N	O	S	0	0
			762	478	142	138	4		

- Molecule 24 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	a	75	Total	C	N	O		0	0
			585	363	114	108			

- Molecule 25 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	b	58	Total	C	N	O	S	0	0
			444	275	92	75	2		

- Molecule 26 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	c	65	Total	C	N	O	S	0	0
			530	328	102	98	2		

- Molecule 27 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	d	58	Total	C	N	O	S	0	0
			455	281	89	84	1		

- Molecule 28 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	f	53	Total	C	N	O	S	0	0
			418	258	84	69	7		

- Molecule 29 is a protein called 50S ribosomal protein L33 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	g	48	Total	C	N	O	S	0	0
			401	244	80	73	4		

- Molecule 30 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	h	44	Total	C	N	O	S	0	0
			367	222	89	54	2		

- Molecule 31 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	i	64	Total	C	N	O	S	0	0
			512	321	107	82	2		

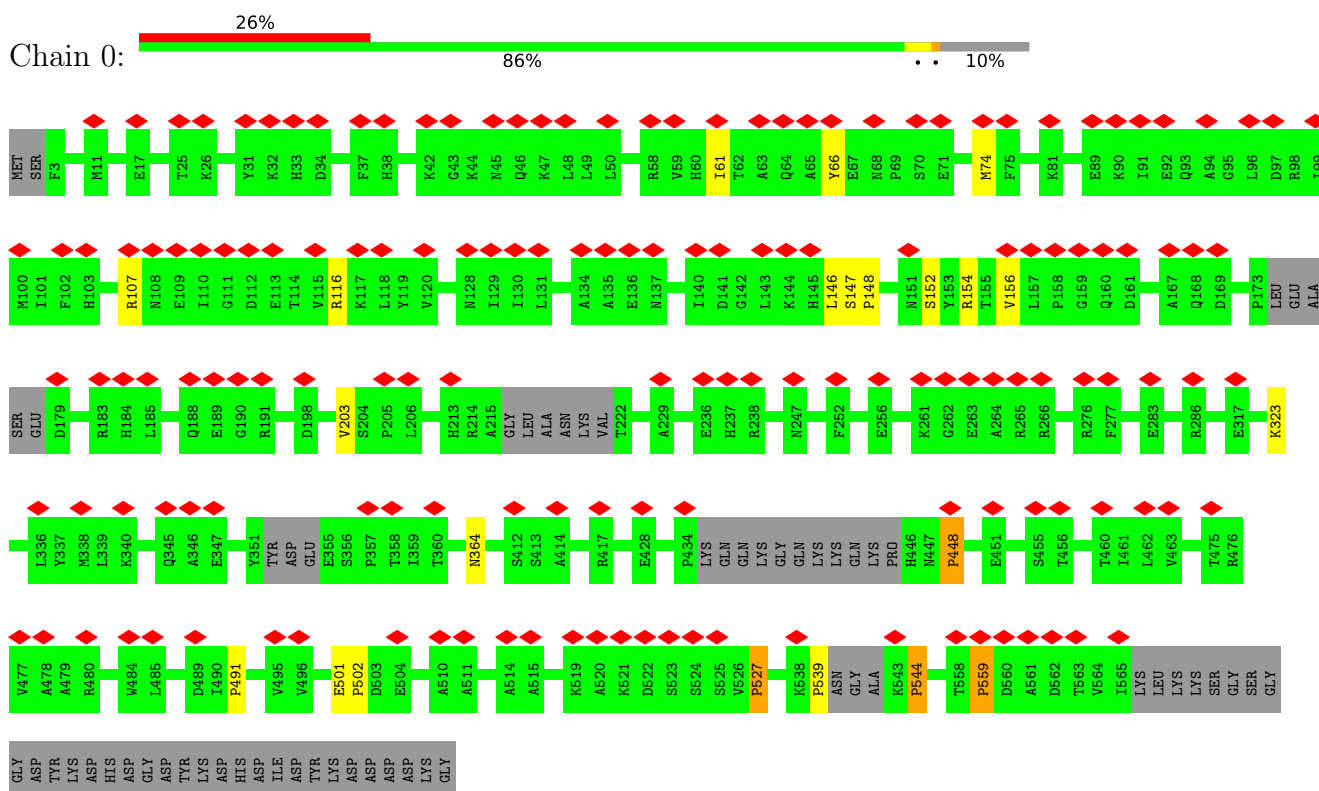
- Molecule 32 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	j	37	Total	C	N	O	S	0	0
			296	186	60	45	5		

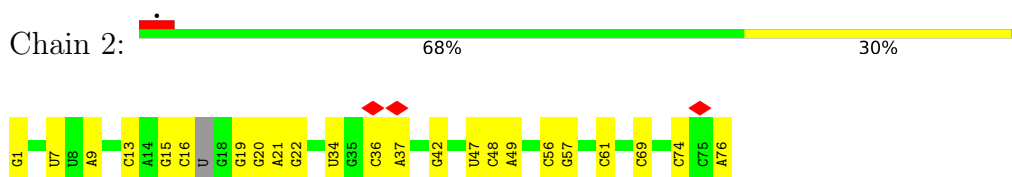
3 Residue-property plots [i](#)

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: Rqc2 homolog RqcH

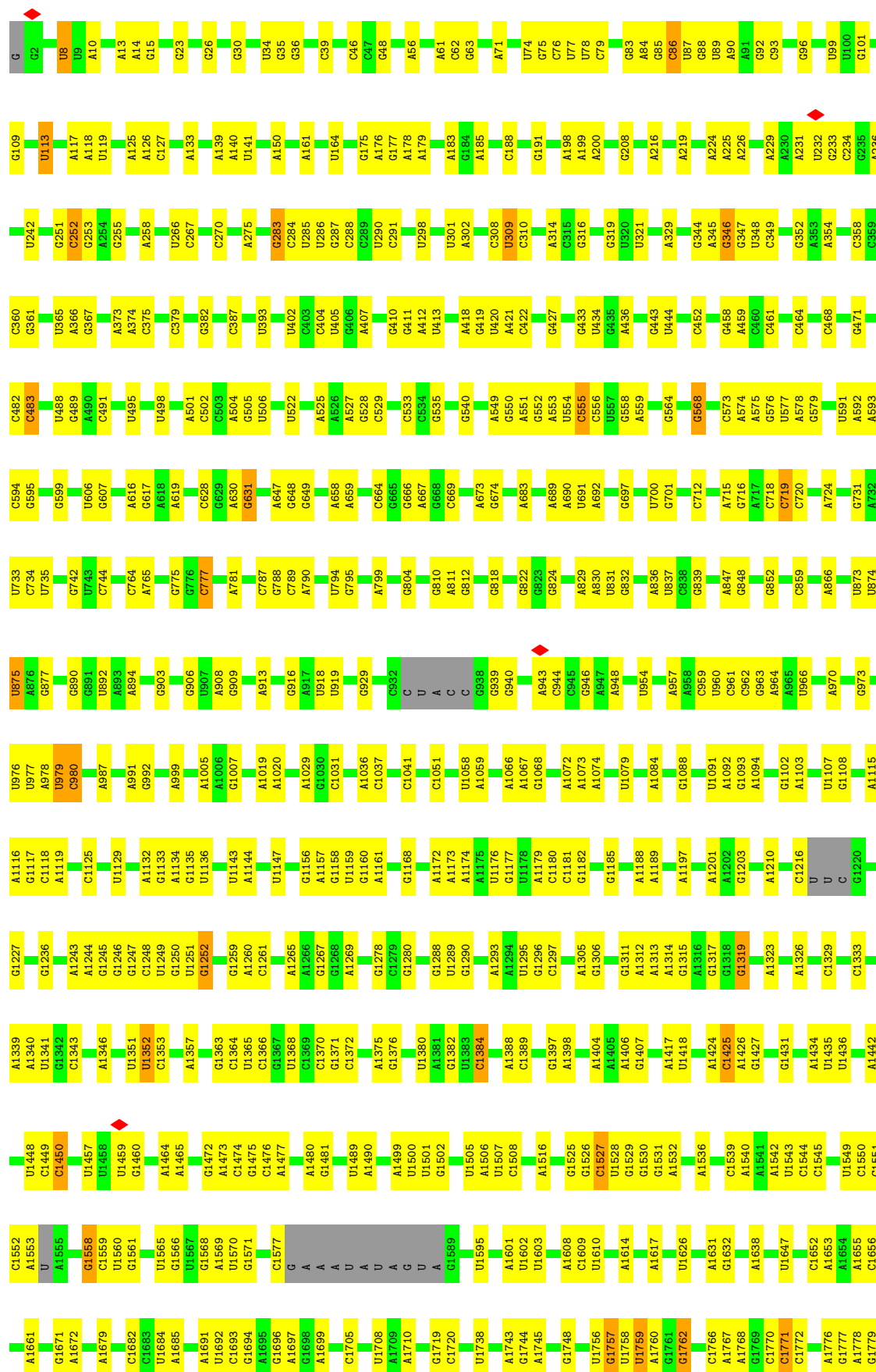


- Molecule 2: tRNA-Ala-1-1



- Molecule 3: 23S rRNA

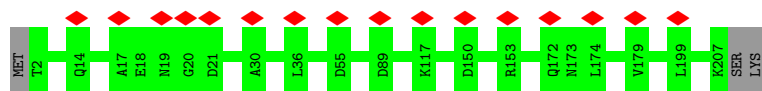




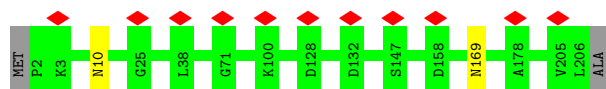




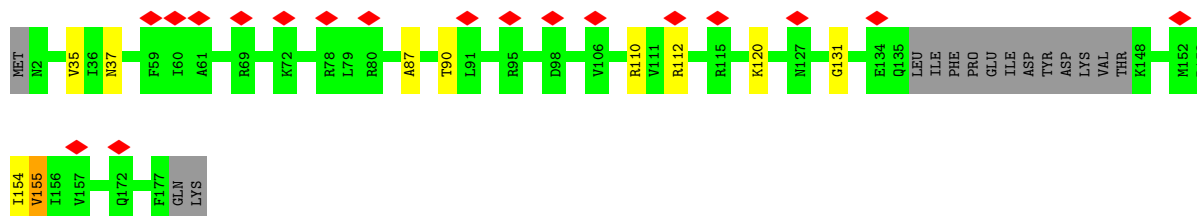
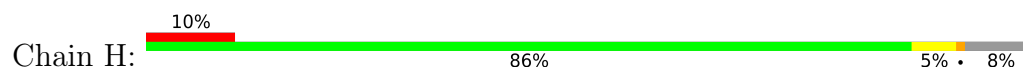
- Molecule 6: 50S ribosomal protein L3



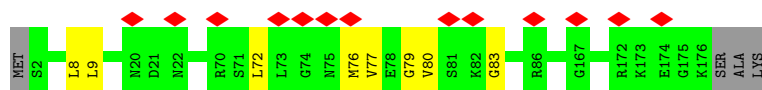
- Molecule 7: 50S ribosomal protein L4



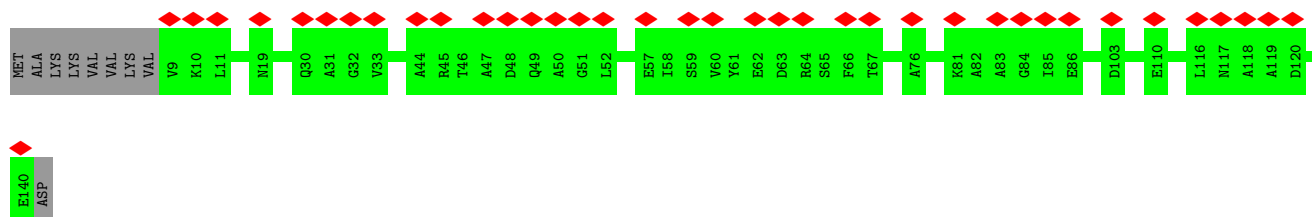
- Molecule 8: 50S ribosomal protein L5



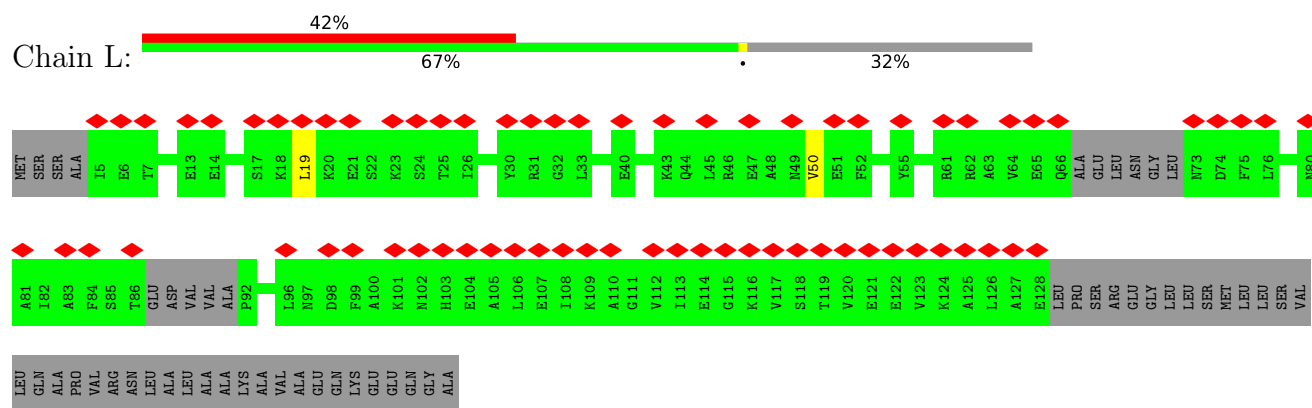
- Molecule 9: 50S ribosomal protein L6



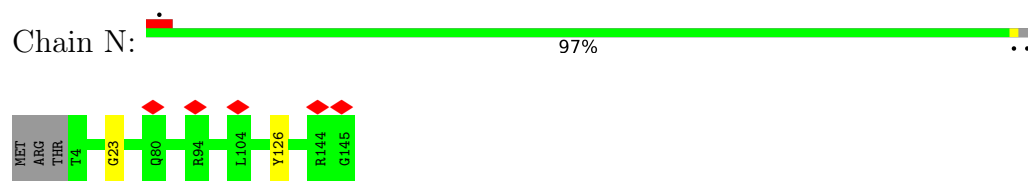
- Molecule 10: 50S ribosomal protein L11



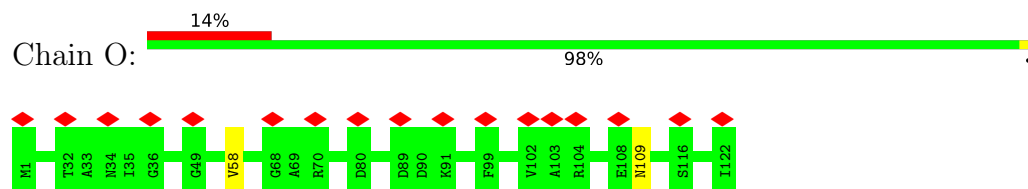
- Molecule 11: 50S ribosomal protein L10



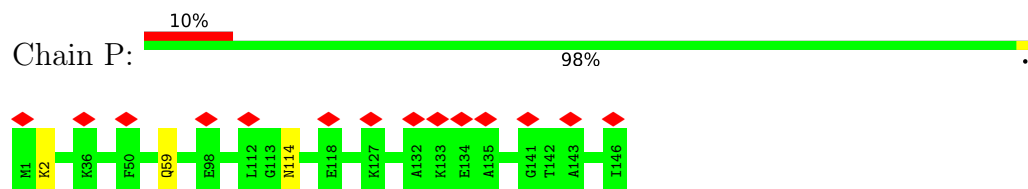
- Molecule 12: 50S ribosomal protein L13



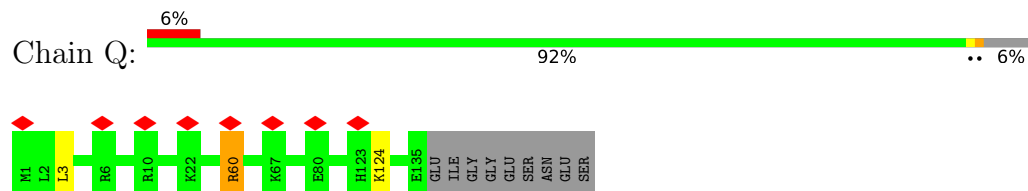
- Molecule 13: 50S ribosomal protein L14



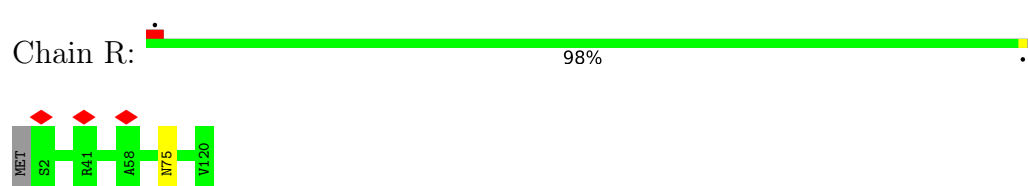
- Molecule 14: 50S ribosomal protein L15



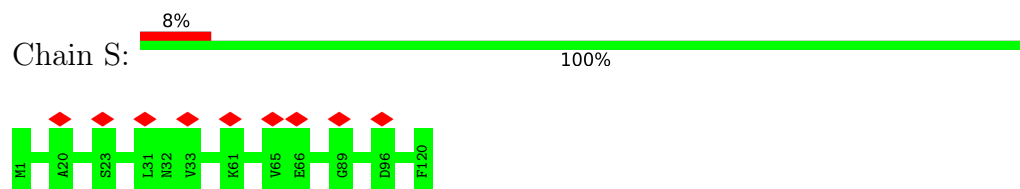
- Molecule 15: 50S ribosomal protein L16



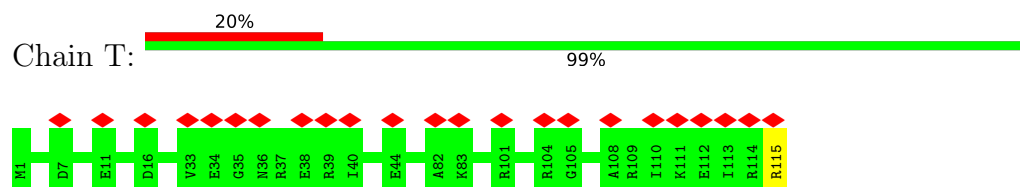
- Molecule 16: 50S ribosomal protein L17



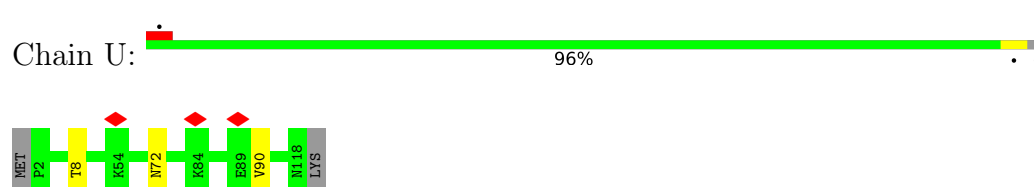
• Molecule 17: 50S ribosomal protein L18



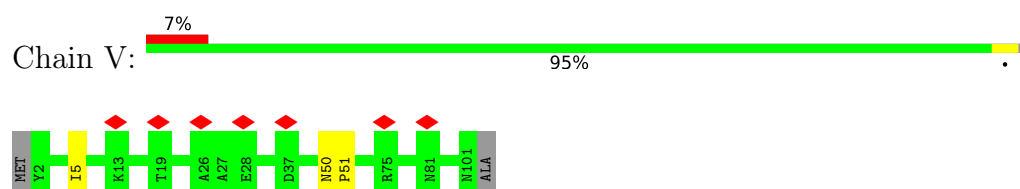
• Molecule 18: 50S ribosomal protein L19



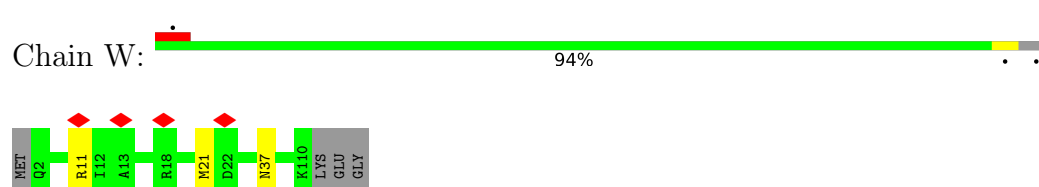
• Molecule 19: 50S ribosomal protein L20



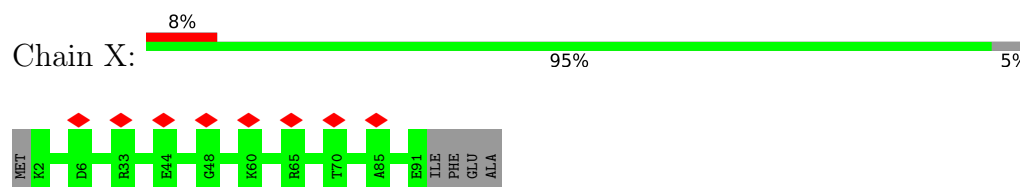
• Molecule 20: 50S ribosomal protein L21



• Molecule 21: 50S ribosomal protein L22

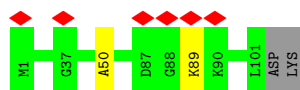


• Molecule 22: 50S ribosomal protein L23

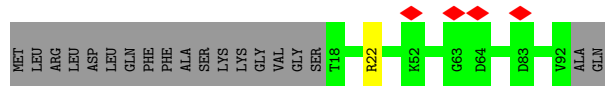
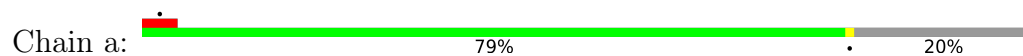


• Molecule 23: 50S ribosomal protein L24

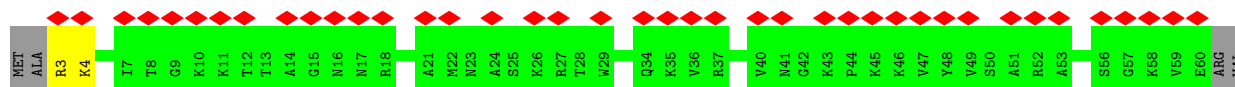
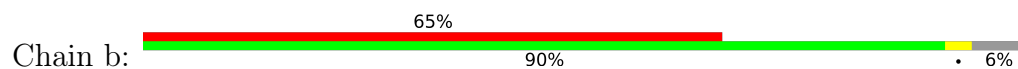




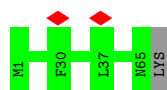
- Molecule 24: 50S ribosomal protein L27



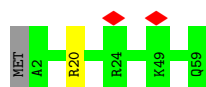
- Molecule 25: 50S ribosomal protein L28



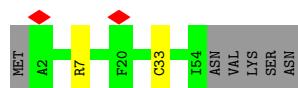
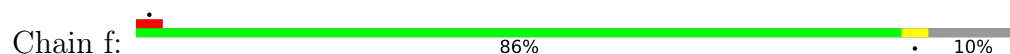
- Molecule 26: 50S ribosomal protein L29



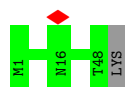
- Molecule 27: 50S ribosomal protein L30



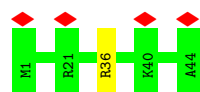
- Molecule 28: 50S ribosomal protein L32



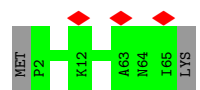
- Molecule 29: 50S ribosomal protein L33 1



- Molecule 30: 50S ribosomal protein L34



- Molecule 31: 50S ribosomal protein L35



- Molecule 32: 50S ribosomal protein L36



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	10703	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 ($e^-/\text{\AA}^2$)	29	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.032	Depositor
Minimum map value	-0.012	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.007	Depositor
Map size (\AA)	344.4, 344.4, 344.4	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.82, 0.82, 0.82	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	0	0.34	0/4052	0.69	8/5477 (0.1%)
2	2	0.64	1/1790 (0.1%)	1.08	0/2788
3	A	0.78	1/67640 (0.0%)	1.13	150/105516 (0.1%)
4	B	0.66	0/2675	1.13	4/4170 (0.1%)
5	E	0.42	0/2120	0.66	0/2845
6	F	0.43	0/1591	0.63	0/2132
7	G	0.44	0/1580	0.62	0/2132
8	H	0.45	1/1299 (0.1%)	0.79	2/1740 (0.1%)
9	I	0.49	2/1360 (0.1%)	0.95	4/1832 (0.2%)
10	K	0.33	0/988	0.58	0/1336
11	L	0.32	0/892	0.61	1/1196 (0.1%)
12	N	0.46	0/1146	0.66	0/1542
13	O	0.40	0/927	0.74	0/1245
14	P	0.41	0/1093	0.68	0/1457
15	Q	0.45	0/1099	0.70	0/1468
16	R	0.43	0/960	0.68	0/1284
17	S	0.36	0/921	0.69	0/1236
18	T	0.41	0/957	0.75	1/1279 (0.1%)
19	U	0.49	0/952	0.70	0/1266
20	V	0.45	0/792	0.69	0/1063
21	W	0.42	0/851	0.69	0/1146
22	X	0.40	0/731	0.67	0/974
23	Y	0.41	0/772	0.69	1/1032 (0.1%)
24	a	0.45	0/593	0.75	0/789
25	b	0.35	0/448	0.78	0/596
26	c	0.39	0/531	0.70	0/707
27	d	0.38	0/457	0.68	1/613 (0.2%)
28	f	0.43	0/425	0.69	0/563
29	g	0.43	0/406	0.65	0/540
30	h	0.48	0/370	0.67	0/483
31	i	0.44	0/519	0.74	0/680
32	j	0.52	0/299	0.72	0/393
All	All	0.69	5/101236 (0.0%)	1.04	172/151520 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	0	6
8	H	0	4
9	I	0	3
11	L	0	1
12	N	0	2
13	O	0	2
14	P	0	2
15	Q	0	3
19	U	0	1
20	V	0	2
21	W	0	1
25	b	0	1
30	h	0	1
All	All	0	29

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1	G	OP3-P	-10.62	1.48	1.61
9	I	77	VAL	CB-CG1	-5.80	1.40	1.52
8	H	155	VAL	C-N	5.40	1.46	1.34
9	I	80	VAL	CB-CG2	-5.31	1.41	1.52
3	A	568	G	N7-C5	-5.16	1.36	1.39

The worst 5 of 172 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	72	LEU	CA-CB-CG	18.50	157.86	115.30
8	H	35	VAL	CG1-CB-CG2	-9.47	95.75	110.90
3	A	2019	C	N3-C2-O2	-9.45	115.28	121.90
3	A	2237	C	N3-C2-O2	-8.92	115.66	121.90
3	A	2019	C	N1-C2-O2	8.53	124.02	118.90

There are no chirality outliers.

5 of 29 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	146	LEU	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	0	152	SER	Peptide
1	0	156	VAL	Peptide
1	0	61	ILE	Peptide
1	0	66	TYR	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	
1	0	523/597 (88%)	439 (84%)	78 (15%)	6 (1%)	12	45
5	E	270/277 (98%)	245 (91%)	23 (8%)	2 (1%)	19	53
6	F	204/209 (98%)	181 (89%)	23 (11%)	0	100	100
7	G	203/207 (98%)	176 (87%)	27 (13%)	0	100	100
8	H	160/179 (89%)	128 (80%)	29 (18%)	3 (2%)	6	34
9	I	173/179 (97%)	137 (79%)	36 (21%)	0	100	100
10	K	130/141 (92%)	115 (88%)	15 (12%)	0	100	100
11	L	107/166 (64%)	103 (96%)	4 (4%)	0	100	100
12	N	140/145 (97%)	130 (93%)	10 (7%)	0	100	100
13	O	120/122 (98%)	99 (82%)	21 (18%)	0	100	100
14	P	144/146 (99%)	122 (85%)	22 (15%)	0	100	100
15	Q	133/144 (92%)	120 (90%)	13 (10%)	0	100	100
16	R	117/120 (98%)	102 (87%)	15 (13%)	0	100	100
17	S	118/120 (98%)	105 (89%)	13 (11%)	0	100	100
18	T	113/115 (98%)	98 (87%)	15 (13%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	U	115/119 (97%)	104 (90%)	10 (9%)	1 (1%)	14	49
20	V	98/102 (96%)	80 (82%)	17 (17%)	1 (1%)	13	46
21	W	107/113 (95%)	89 (83%)	18 (17%)	0	100	100
22	X	88/95 (93%)	80 (91%)	8 (9%)	0	100	100
23	Y	99/103 (96%)	84 (85%)	15 (15%)	0	100	100
24	a	73/94 (78%)	65 (89%)	8 (11%)	0	100	100
25	b	56/62 (90%)	42 (75%)	14 (25%)	0	100	100
26	c	63/66 (96%)	57 (90%)	6 (10%)	0	100	100
27	d	56/59 (95%)	49 (88%)	7 (12%)	0	100	100
28	f	51/59 (86%)	46 (90%)	5 (10%)	0	100	100
29	g	46/49 (94%)	36 (78%)	10 (22%)	0	100	100
30	h	42/44 (96%)	39 (93%)	3 (7%)	0	100	100
31	i	62/66 (94%)	56 (90%)	6 (10%)	0	100	100
32	j	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
All	All	3646/3935 (93%)	3158 (87%)	475 (13%)	13 (0%)	32	64

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0	448	PRO
1	0	544	PRO
1	0	559	PRO
5	E	156	ARG
8	H	37	ASN

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	371/527 (70%)	365 (98%)	6 (2%)	58	76
5	E	220/225 (98%)	220 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	167/170 (98%)	167 (100%)	0	100	100
7	G	169/170 (99%)	167 (99%)	2 (1%)	67	82
8	H	139/154 (90%)	137 (99%)	2 (1%)	62	79
9	I	148/151 (98%)	147 (99%)	1 (1%)	81	89
10	K	102/110 (93%)	102 (100%)	0	100	100
11	L	98/138 (71%)	98 (100%)	0	100	100
12	N	120/123 (98%)	120 (100%)	0	100	100
13	O	101/101 (100%)	101 (100%)	0	100	100
14	P	110/110 (100%)	109 (99%)	1 (1%)	75	86
15	Q	109/116 (94%)	108 (99%)	1 (1%)	75	86
16	R	99/100 (99%)	98 (99%)	1 (1%)	73	84
17	S	93/93 (100%)	93 (100%)	0	100	100
18	T	100/100 (100%)	100 (100%)	0	100	100
19	U	96/98 (98%)	95 (99%)	1 (1%)	73	84
20	V	83/84 (99%)	83 (100%)	0	100	100
21	W	90/93 (97%)	88 (98%)	2 (2%)	47	70
22	X	81/85 (95%)	81 (100%)	0	100	100
23	Y	85/87 (98%)	84 (99%)	1 (1%)	67	82
24	a	59/74 (80%)	58 (98%)	1 (2%)	56	75
25	b	47/50 (94%)	46 (98%)	1 (2%)	48	71
26	c	56/57 (98%)	56 (100%)	0	100	100
27	d	52/53 (98%)	52 (100%)	0	100	100
28	f	47/53 (89%)	45 (96%)	2 (4%)	25	54
29	g	46/47 (98%)	46 (100%)	0	100	100
30	h	39/39 (100%)	39 (100%)	0	100	100
31	i	54/56 (96%)	54 (100%)	0	100	100
32	j	35/35 (100%)	35 (100%)	0	100	100
All	All	3016/3299 (91%)	2994 (99%)	22 (1%)	80	89

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
19	U	72	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
23	Y	89	LYS
21	W	37	ASN
24	a	22	ARG
7	G	10	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
13	O	45	GLN
21	W	37	ASN
31	i	35	ASN
30	h	26	ASN
9	I	129	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	2	74/76 (97%)	22 (29%)	1 (1%)
3	A	2805/2926 (95%)	814 (29%)	65 (2%)
4	B	111/119 (93%)	38 (34%)	3 (2%)
All	All	2990/3121 (95%)	874 (29%)	69 (2%)

5 of 874 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	2	7	U
2	2	9	A
2	2	13	C
2	2	15	G
2	2	16	C

5 of 69 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	A	2454	A
3	A	2631	A
3	A	2904	A
3	A	1250	G
3	A	1243	A

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

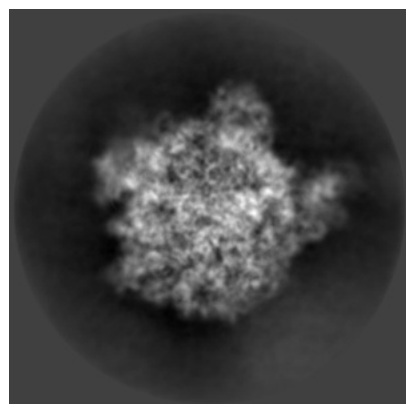
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11890. These allow visual inspection of the internal detail of the map and identification of artifacts.

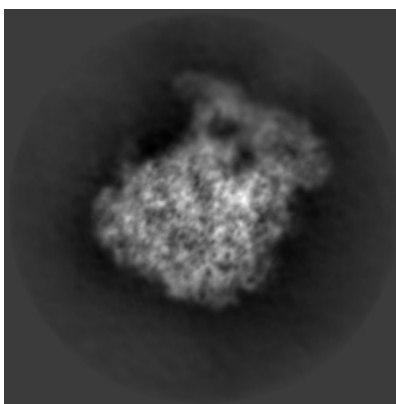
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

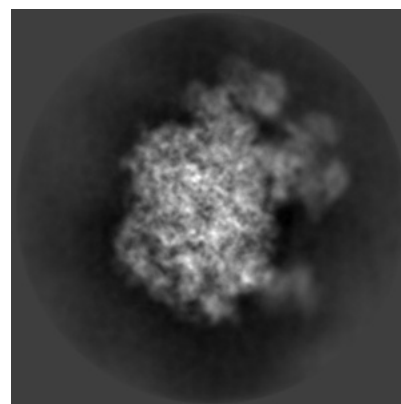
6.1.1 Primary map



X

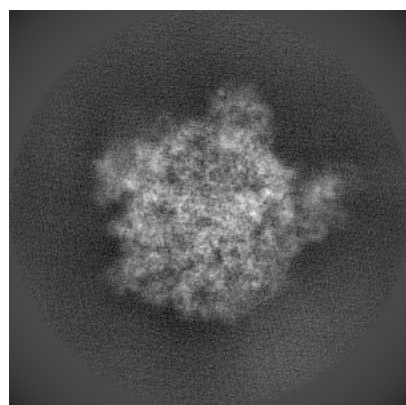


Y

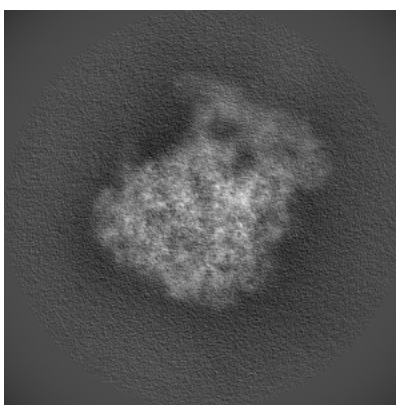


Z

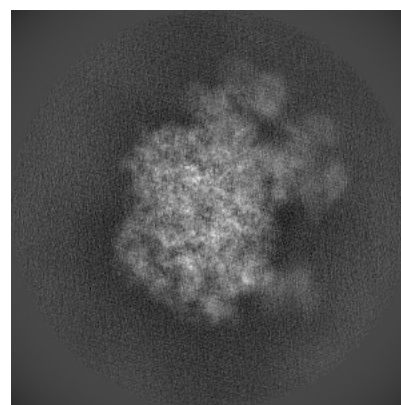
6.1.2 Raw map



X



Y

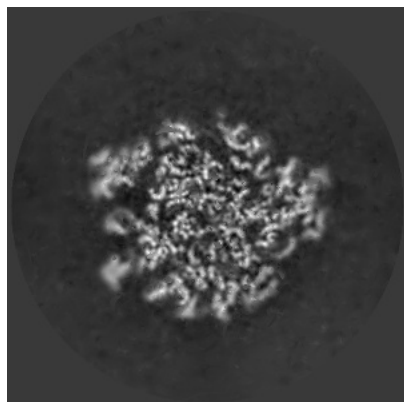


Z

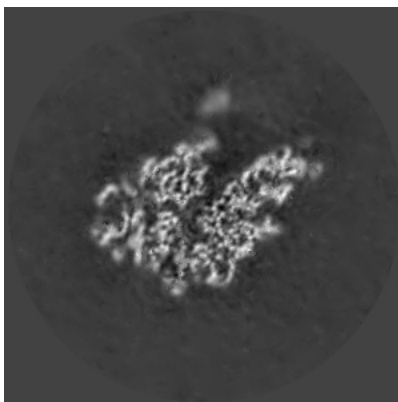
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

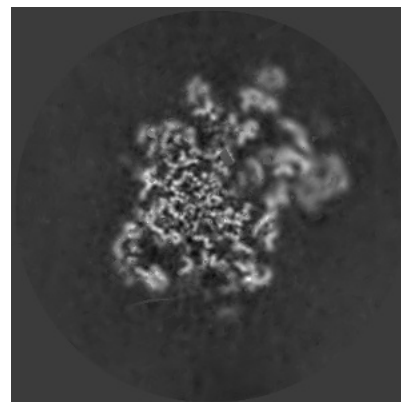
6.2.1 Primary map



X Index: 210

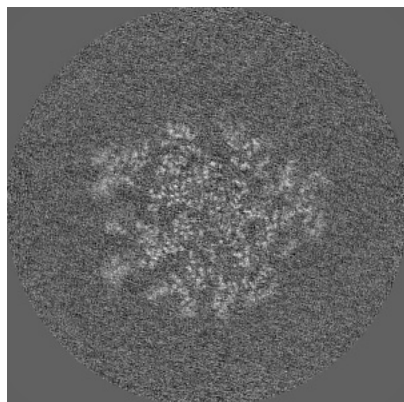


Y Index: 210

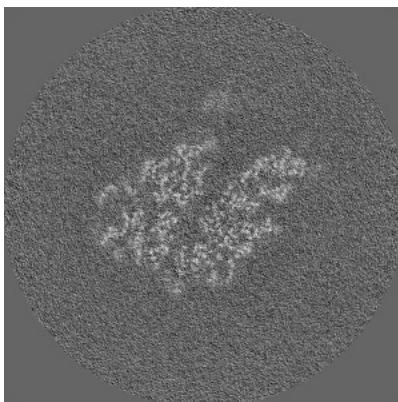


Z Index: 210

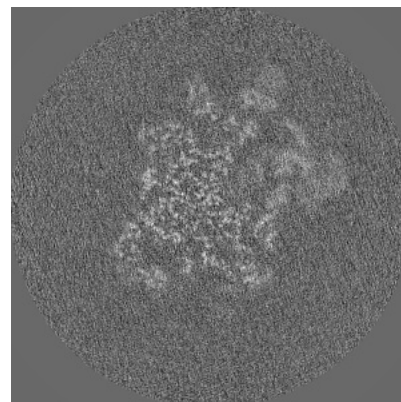
6.2.2 Raw map



X Index: 210



Y Index: 210

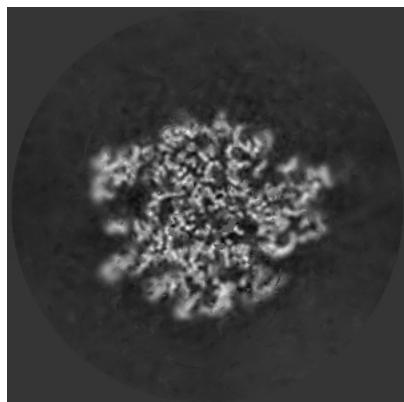


Z Index: 210

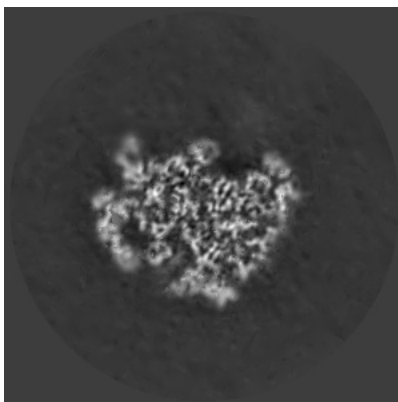
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

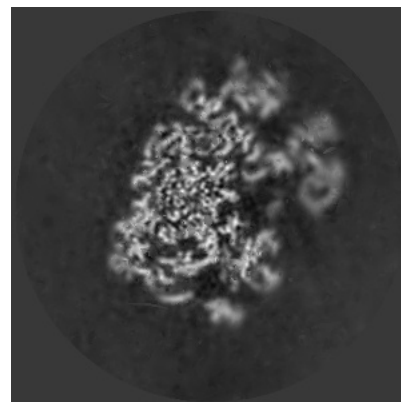
6.3.1 Primary map



X Index: 215

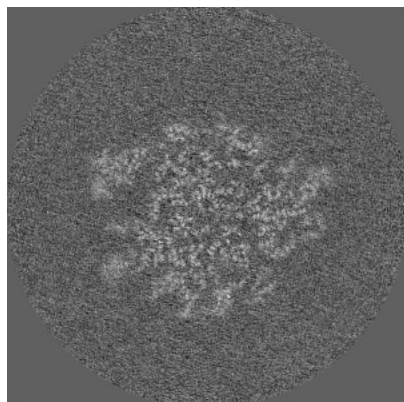


Y Index: 185

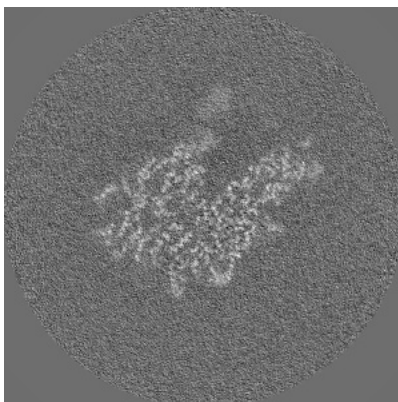


Z Index: 222

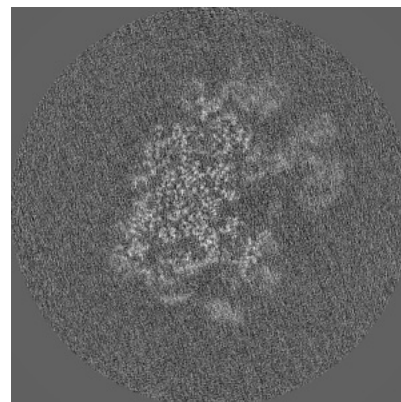
6.3.2 Raw map



X Index: 213



Y Index: 213

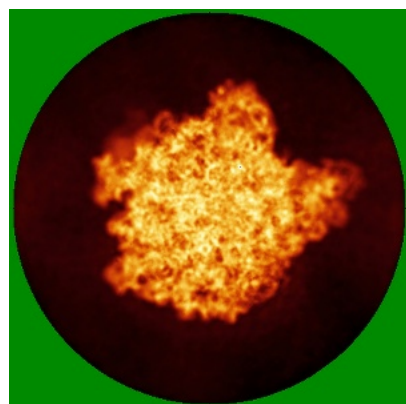


Z Index: 222

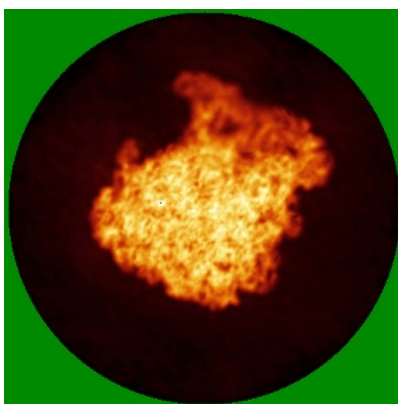
The images above show the largest variance slices of the map in three orthogonal directions.

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

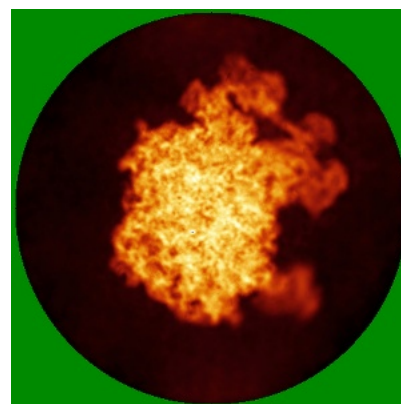
6.4.1 Primary map



X

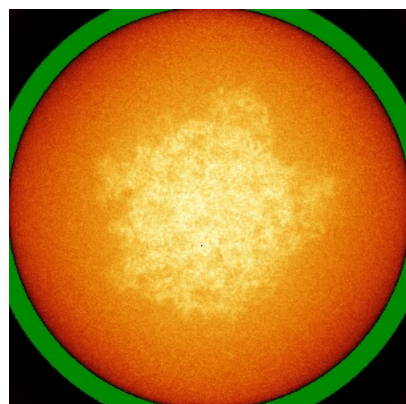


Y

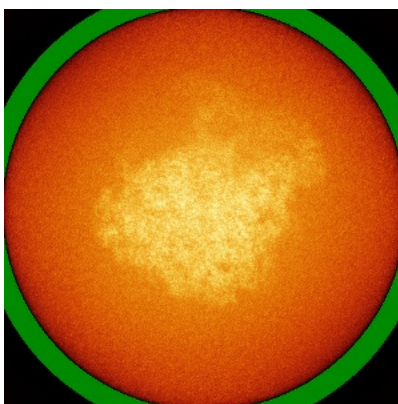


Z

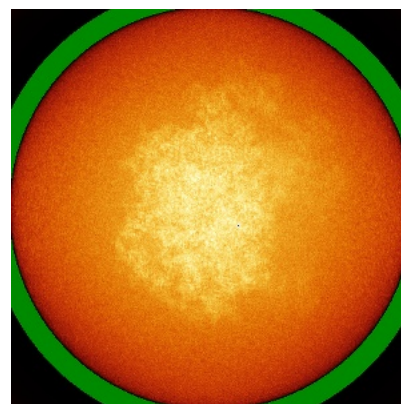
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

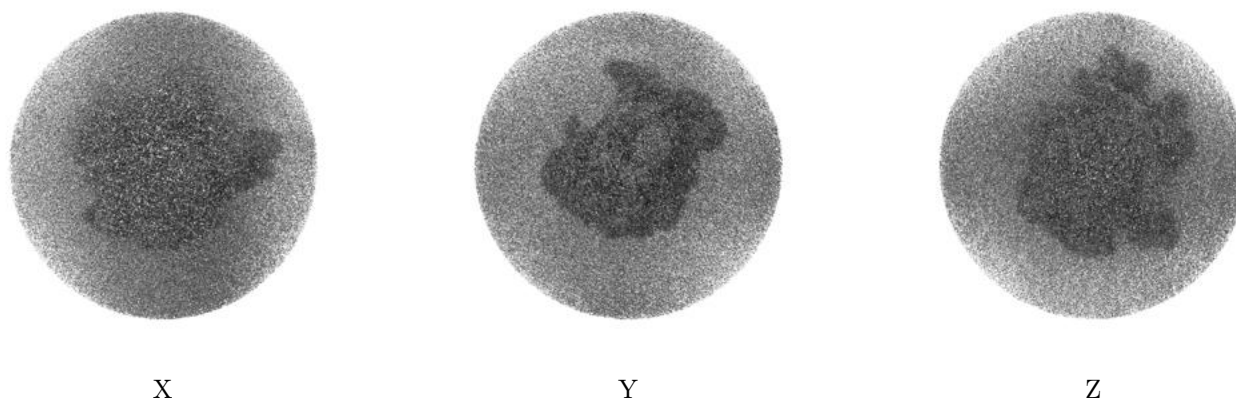
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.007. 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



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.

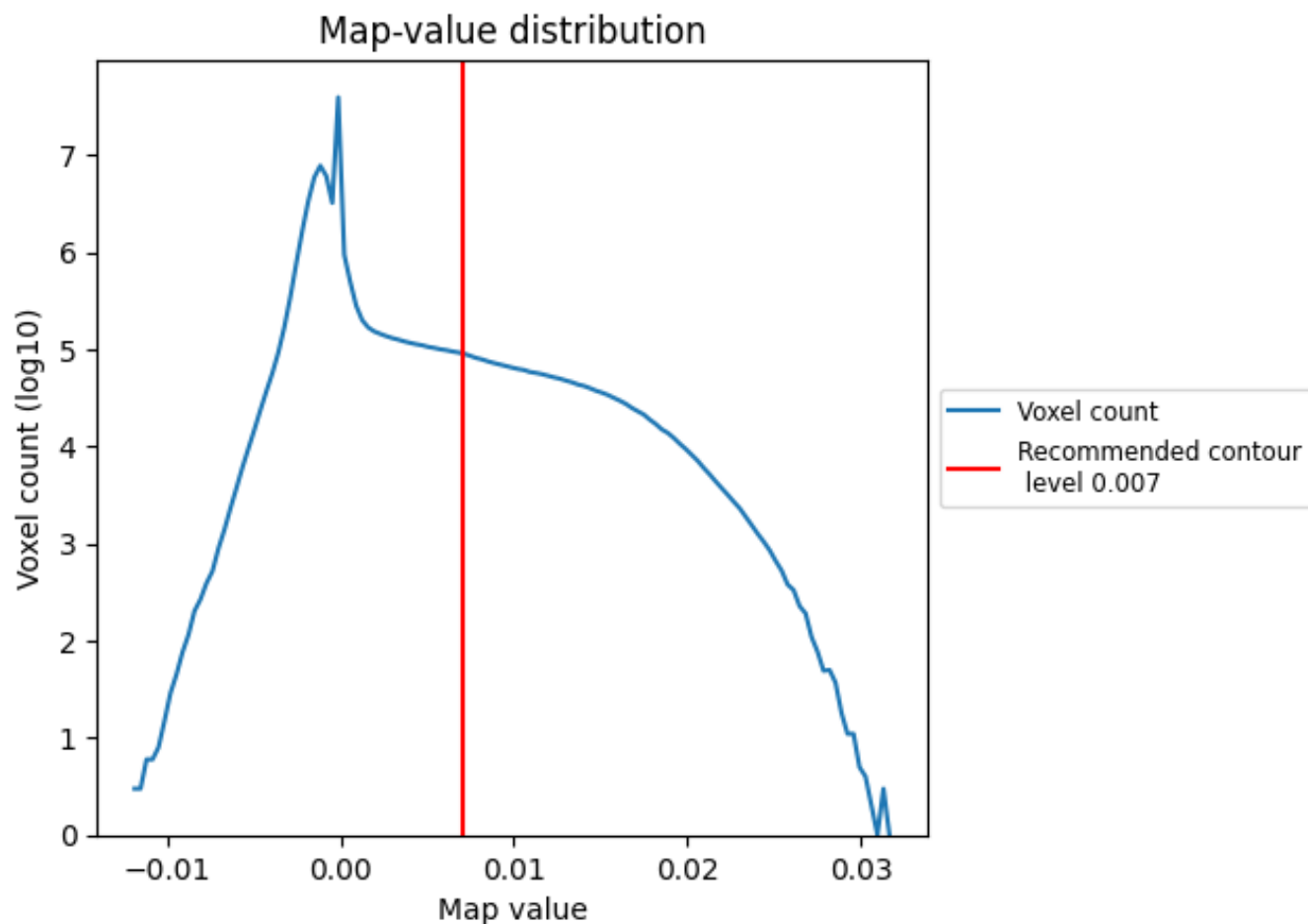
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

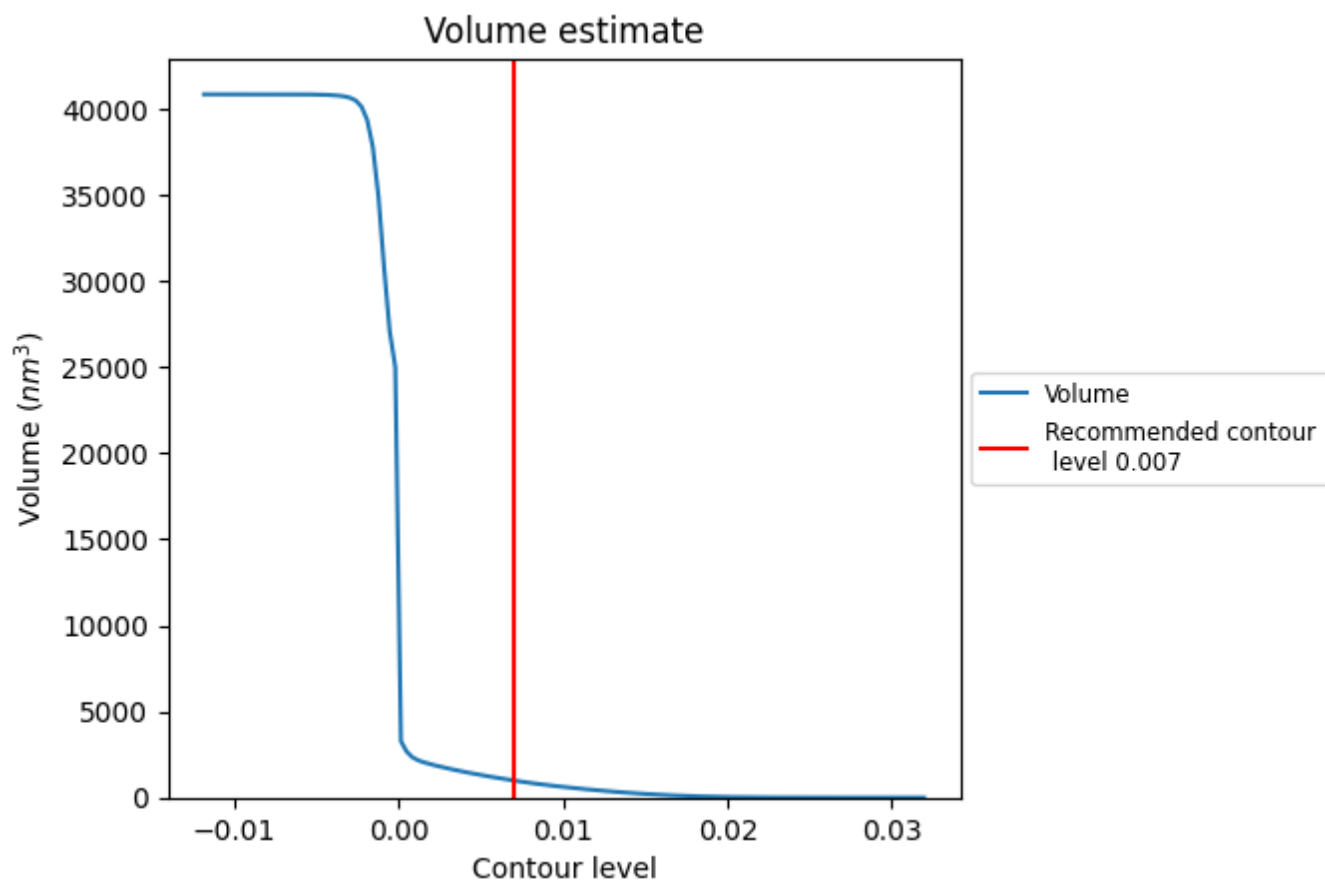
This section contains the results of statistical analysis of the map.

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.

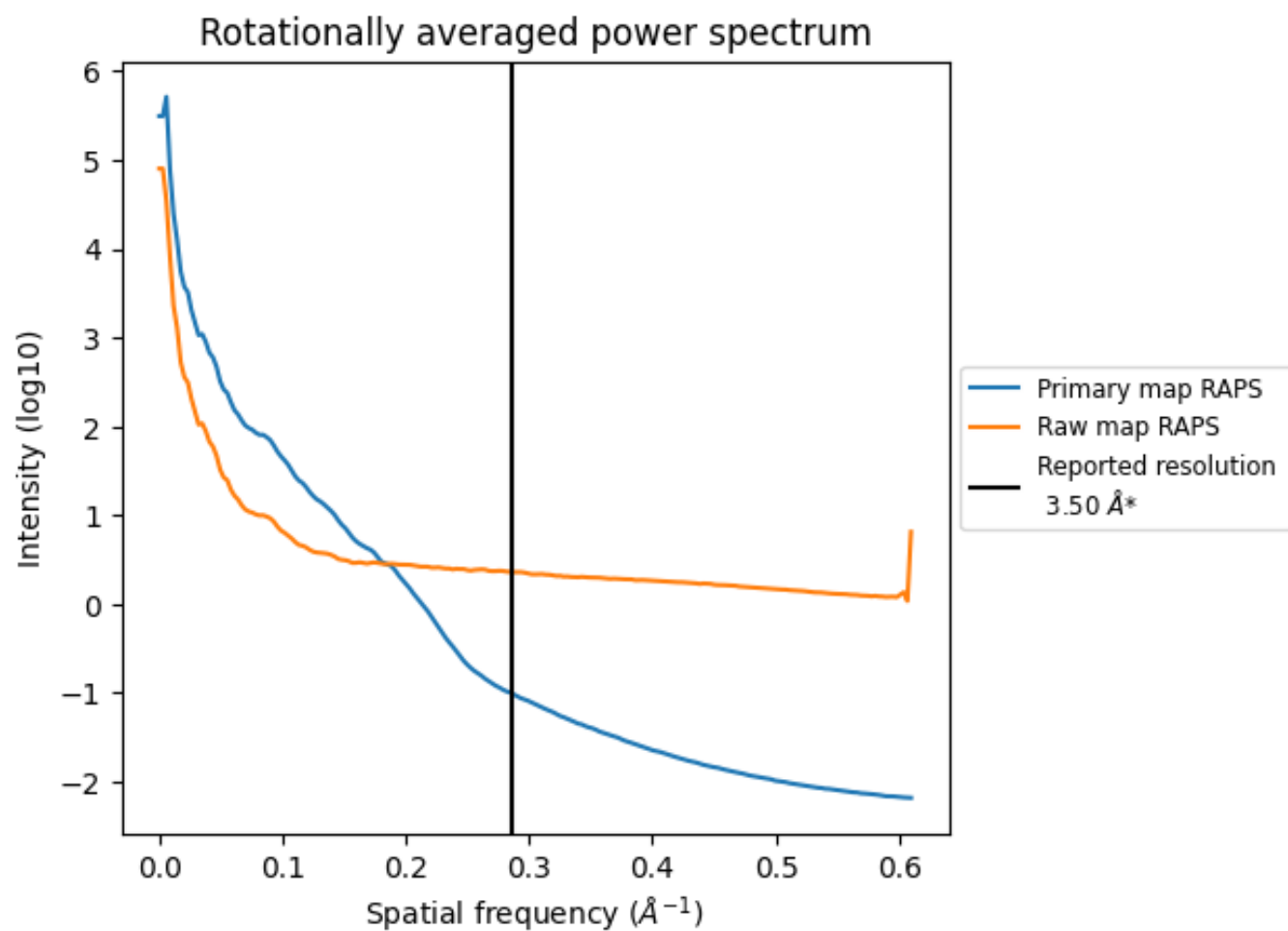
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 990 nm³; this corresponds to an approximate mass of 894 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 ⓘ

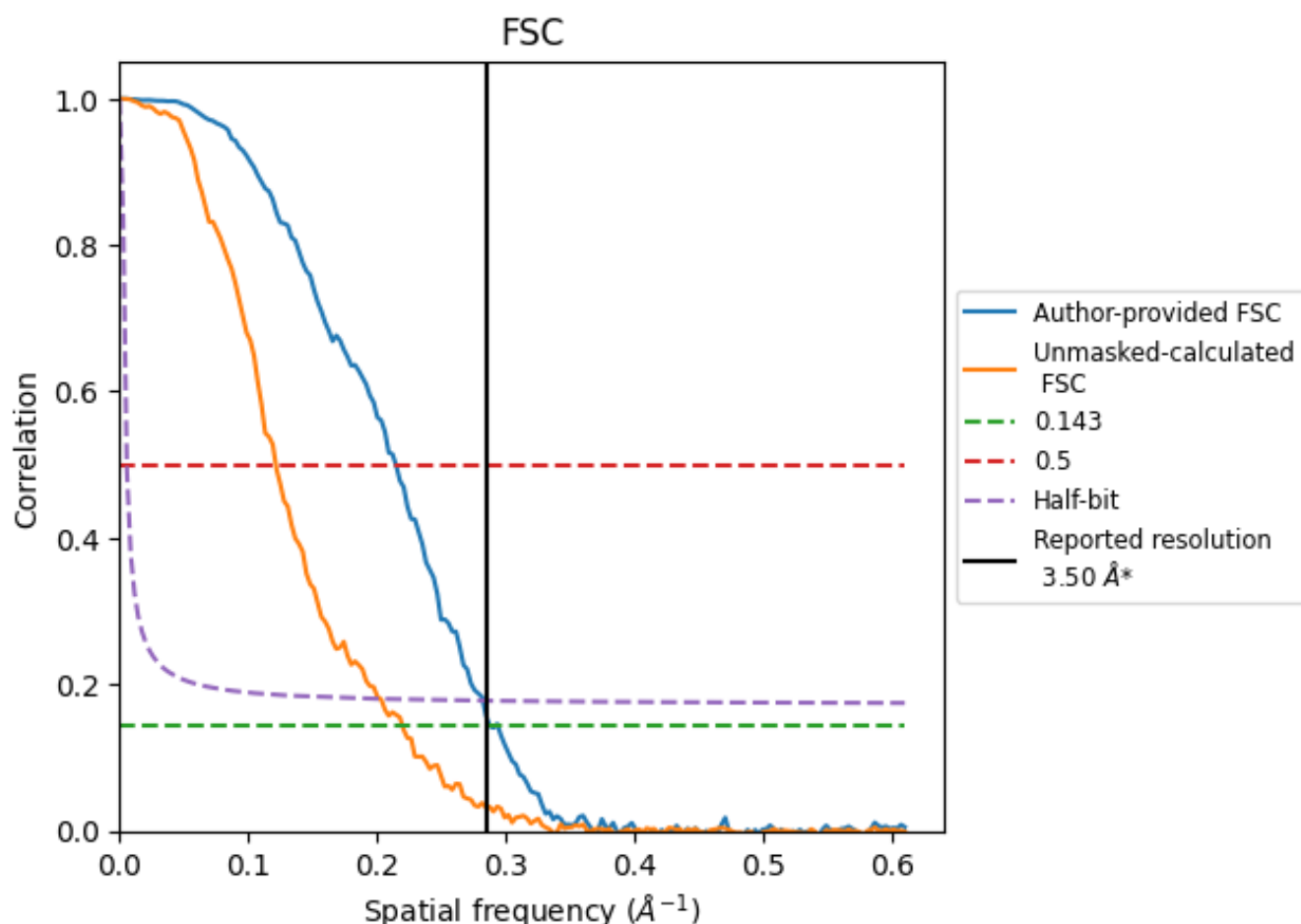


*Reported resolution corresponds to spatial frequency of 0.286 \AA^{-1}

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 0.286 \AA^{-1}

8.2 Resolution estimates [i](#)

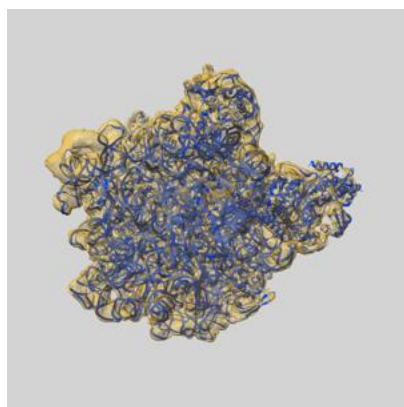
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.48	4.66	3.54
Unmasked-calculated*	4.55	8.24	4.94

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.55 differs from the reported value 3.5 by more than 10 %

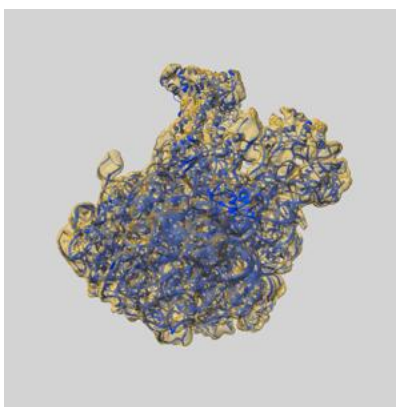
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11890 and PDB model 7AS9. Per-residue inclusion information can be found in section [3](#) on page [10](#).

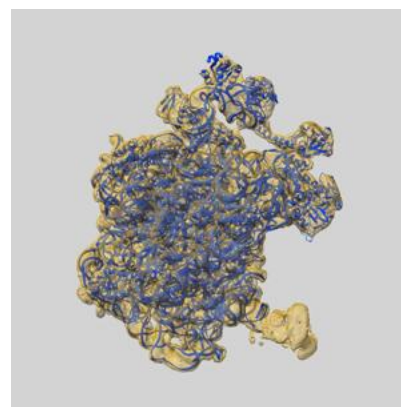
9.1 Map-model overlay [i](#)



X



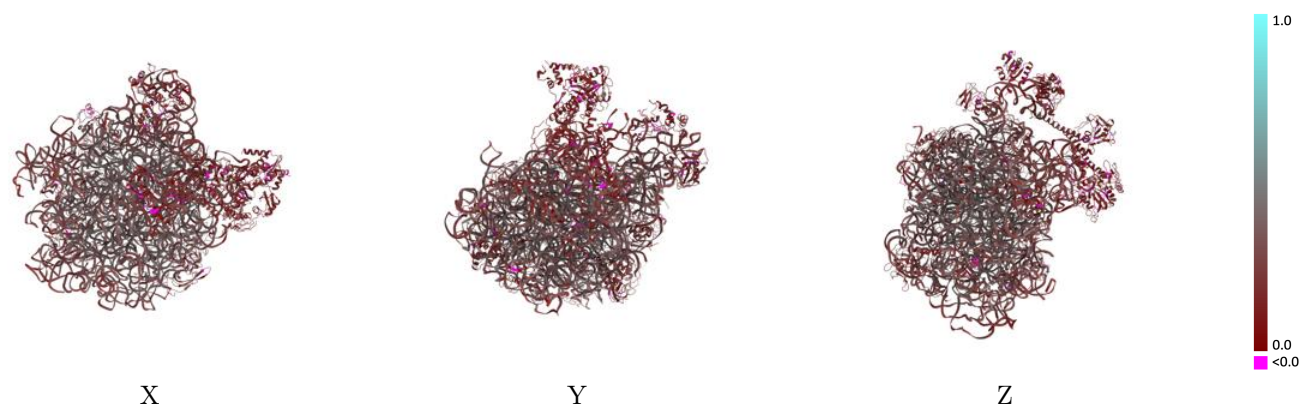
Y



Z

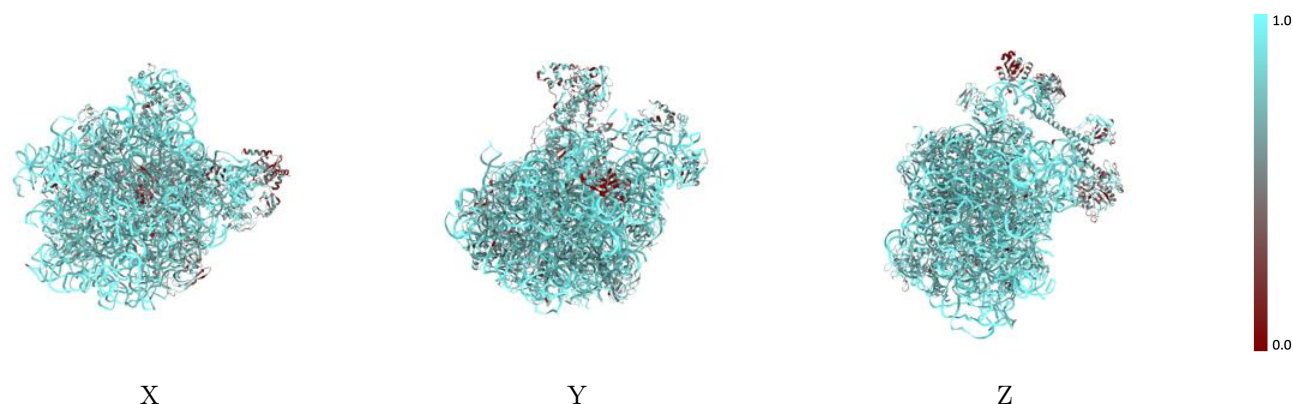
The images above show the 3D surface view of the map at the recommended contour level 0.007 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



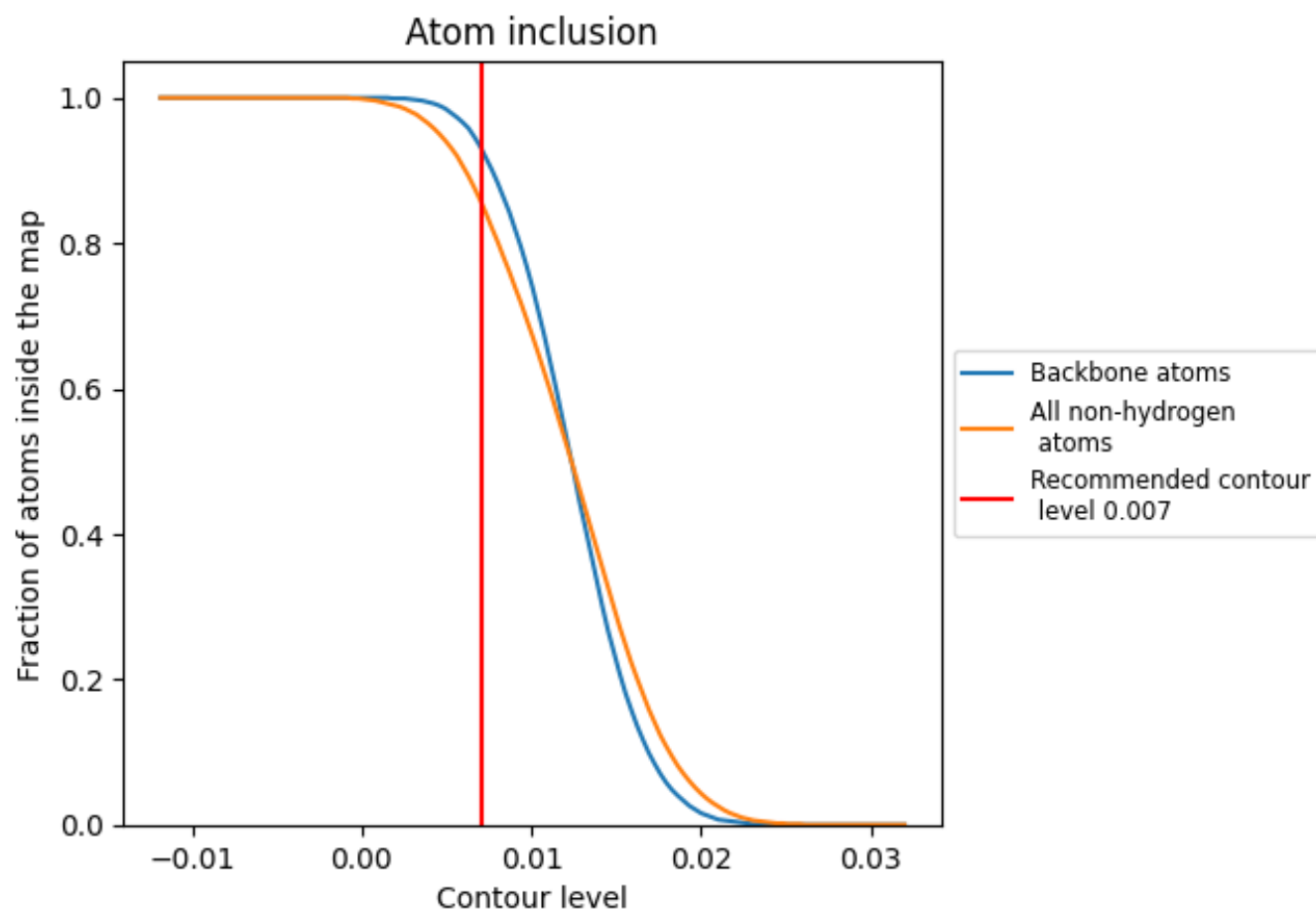
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.007).



































































9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8580	 0.3000
0	 0.5820	 0.1600
2	 0.8500	 0.2330
A	 0.9460	 0.3290
B	 0.9630	 0.2840
E	 0.7590	 0.2980
F	 0.6640	 0.2830
G	 0.6970	 0.2730
H	 0.6790	 0.1650
I	 0.7280	 0.1940
K	 0.5450	 0.1620
L	 0.2930	 0.1650
N	 0.7420	 0.2910
O	 0.6300	 0.2690
P	 0.6870	 0.2870
Q	 0.6930	 0.2730
R	 0.7090	 0.2540
S	 0.7060	 0.1930
T	 0.5920	 0.2520
U	 0.7460	 0.2940
V	 0.7060	 0.2790
W	 0.7290	 0.3070
X	 0.6720	 0.2840
Y	 0.7140	 0.2330
a	 0.7500	 0.3100
b	 0.2760	 0.2300
c	 0.6650	 0.2000
d	 0.7330	 0.2600
f	 0.7480	 0.3210
g	 0.7440	 0.2510
h	 0.6990	 0.3550
i	 0.7030	 0.3580
j	 0.6930	 0.2950

