



wwPDB EM Validation Summary Report ⓘ

Nov 3, 2024 – 09:17 pm GMT

PDB ID : 7QGU
EMDB ID : EMD-13959
Title : Structure of the B. subtilis disome - stalled 70S ribosome
Authors : Kratzat, H.; Buschauer, R.; Berninghausen, O.; Beckmann, R.
Deposited on : 2021-12-10
Resolution : 4.75 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

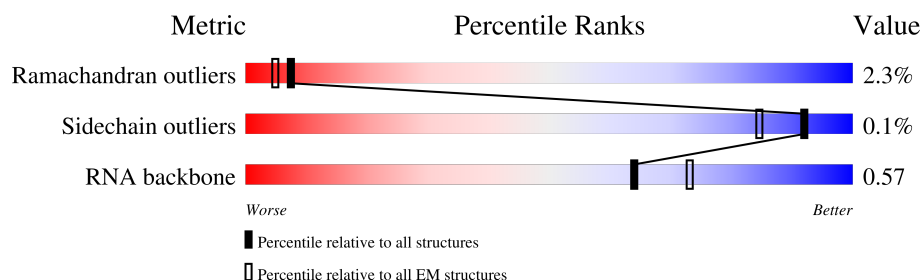
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.75 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	A	2928	
2	B	119	
3	C	277	
4	D	208	
5	E	207	
6	F	179	
7	G	179	
8	H	166	

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Mol	Chain	Length	Quality of chain
9	I	141	
10	J	145	
11	K	122	
12	L	146	
13	M	144	
14	N	120	
15	O	120	
16	P	115	
17	Q	119	
18	R	102	
19	S	113	
20	T	95	
21	U	103	
22	V	94	
23	X	149	
24	Y	62	
25	Z	66	
26	a	59	
27	b	59	
28	c	49	
29	d	44	
30	e	66	
31	f	37	
32	W	1555	
33	g	246	

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Mol	Chain	Length	Quality of chain
34	h	218	
35	i	200	
36	j	166	
37	k	95	
38	l	156	
39	m	132	
40	n	130	
41	o	102	
42	p	131	
43	q	138	
44	r	121	
45	s	61	
46	t	89	
47	u	90	
48	v	87	
49	w	79	
50	x	92	
51	y	88	
52	z	77	
53	2	95	
54	3	66	

2 Entry composition

There are 54 unique types of molecules in this entry. The entry contains 135606 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2923	Total	C	N	O	P	0	0
			62767	28002	11589	20253	2923		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1558	C	G	conflict	GB 1864548803

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	112	Total	C	N	O	P	0	0
			2395	1068	435	780	112		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	275	Total	C	N	O	S	0	0
			2111	1312	416	377	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	207	Total	C	N	O	S	0	0
			1575	988	290	292	5		

- Molecule 5 is a protein called 50S ribosomal protein L4.

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

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	178	Total	C	N	O	S	0	0
			1404	893	245	259	7		

- Molecule 7 is a protein called Ribosomal protein L6.

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

- Molecule 8 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	123	Total	C	N	O	S	0	0
			955	602	163	189	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	154	THR	ALA	variant	UNP A0A063X7V1

- Molecule 9 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	133	Total	C	N	O	S	0	0
			981	617	173	185	6		

- Molecule 10 is a protein called 50S ribosomal protein L13.

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

- Molecule 11 is a protein called 50S ribosomal protein L14.

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

- Molecule 12 is a protein called 50S ribosomal protein L15.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	138	Total	C	N	O	S	0	0
			1097	703	208	181	5		

- Molecule 14 is a protein called 50S ribosomal protein L17.

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

- Molecule 15 is a protein called 50S ribosomal protein L18.

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

- Molecule 16 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	P	114	Total	C	N	O	0	0
			936	595	184	157		

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

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

- Molecule 18 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	R	101	Total	C	N	O	0	0
			786	501	139	146		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	93	Total	C	N	O	S	0	0
			752	472	137	139	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	100	Total	C	N	O	S	0	0
			754	473	141	137	3		

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	V	82	Total	C	N	O		
			630	390	123	117	0	0

- Molecule 23 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	X	149	Total	C	N	O		
			733	435	149	149	0	0

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

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

- Molecule 25 is a protein called 50S ribosomal protein L29.

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	54	Total	C	N	O	S	0	0
			426	262	86	71	7		

- Molecule 28 is a protein called 50S ribosomal protein L33.

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

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

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

- Molecule 30 is a protein called 50S ribosomal protein L35.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	36	Total	C	N	O	S	0	0
			288	181	59	44	4		

- Molecule 32 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	W	1544	Total	C	N	O	P	0	0
			33115	14768	6067	10736	1544		

- Molecule 33 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	g	224	Total	C	N	O	0	0
			896	448	224	224		

- Molecule 34 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	h	210	Total	C	N	O	0	0
			840	420	210	210		

- Molecule 35 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	i	199	Total	C	N	O	0	0
			797	398	199	200		

- Molecule 36 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	j	165	Total	C	N	O	0	0
			661	330	165	166		

- Molecule 37 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	k	95	Total	C	N	O	0	0
			381	190	95	96		

- Molecule 38 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	l	153	Total	C	N	O	0	0
			613	306	153	154		

- Molecule 39 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	m	131	Total	C	N	O	0	0
			525	262	131	132		

- Molecule 40 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	n	130	Total	C	N	O	0	0
			521	260	130	131		

- Molecule 41 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	o	102	Total	C	N	O	0	0
			409	204	102	103		

- Molecule 42 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	p	118	Total	C	N	O	0	0
			472	236	118	118		

- Molecule 43 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	q	137	Total	C	N	O	0	0
			549	274	137	138		

- Molecule 44 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	r	119	Total	C	N	O	0	0
			476	238	119	119		

- Molecule 45 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	s	60	Total	C	N	O	0	0
			241	120	60	61		

- Molecule 46 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	t	88	Total	C	N	O	0	0
			353	176	88	89		

- Molecule 47 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	u	89	Total	C	N	O	0	0
			357	178	89	90		

- Molecule 48 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	v	86	Total	C	N	O	0	0
			345	172	86	87		

- Molecule 49 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	w	71	Total	C	N	O	0	0
			285	142	71	72		

- Molecule 50 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms				AltConf	Trace
50	x	84	Total	C	N	O	0	0
			336	168	84	84		

- Molecule 51 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	y	86	Total	C	N	O	0	0
			345	172	86	87		

- Molecule 52 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	z	77	Total	C	N	O	P	0	0
			1643	731	290	545	77		

- Molecule 53 is a protein called YqzJ.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	2	24	Total	C	N	O	S	0	0
			107	64	28	14	1		

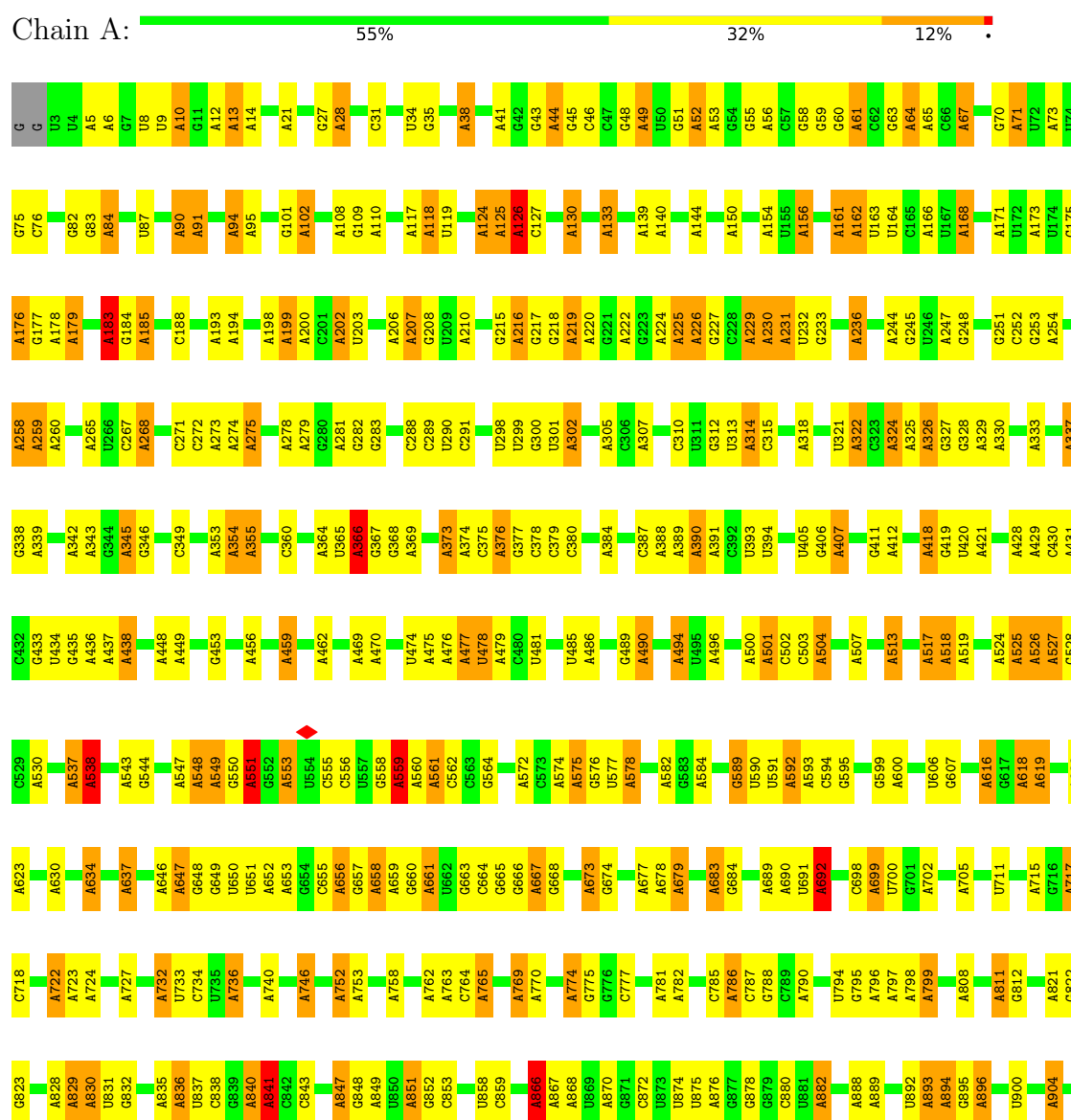
- Molecule 54 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	3	45	Total	C	N	O	S	0	0
			366	227	66	71	2		

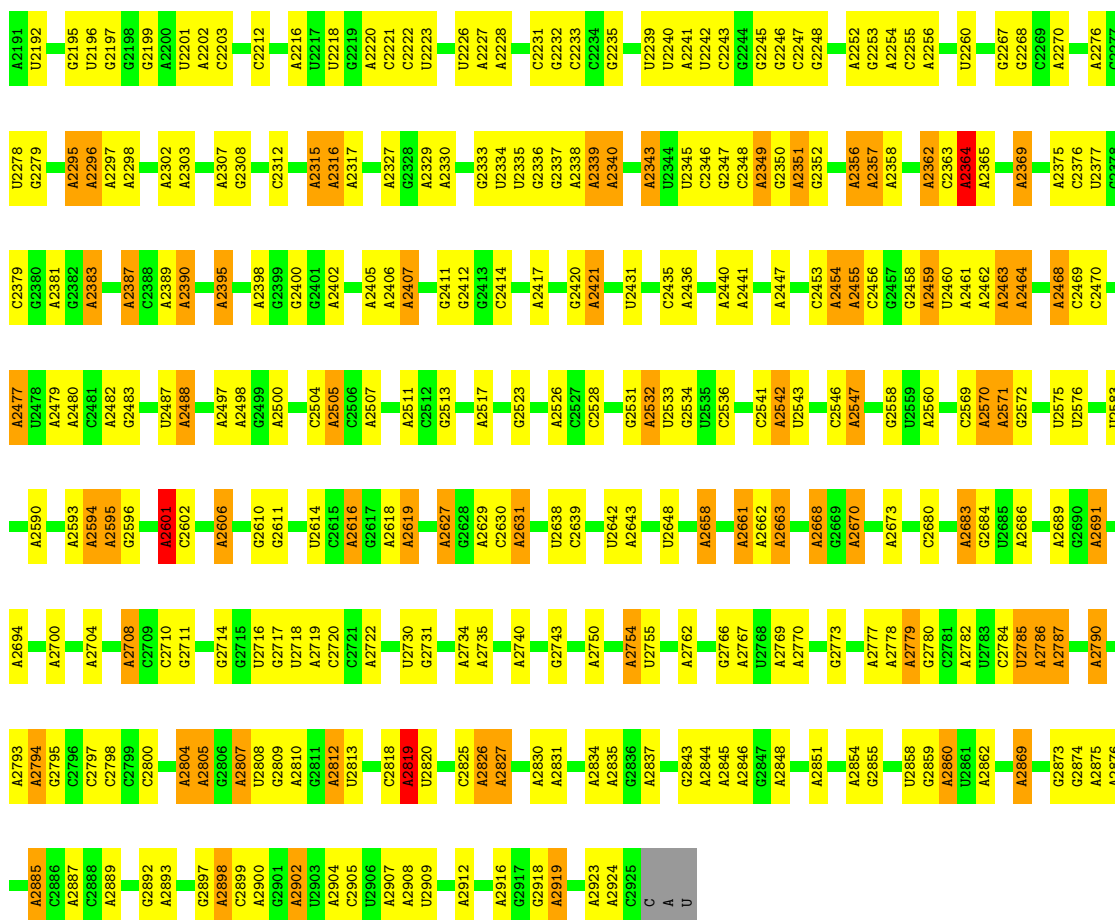
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 23S rRNA

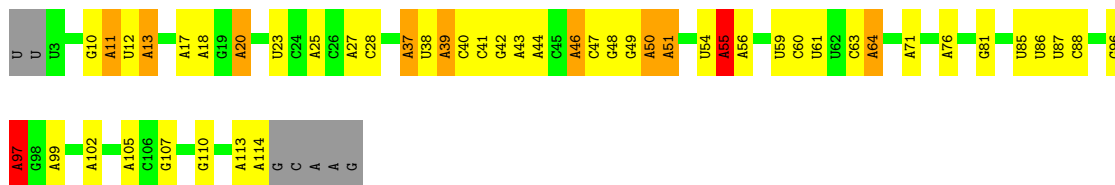






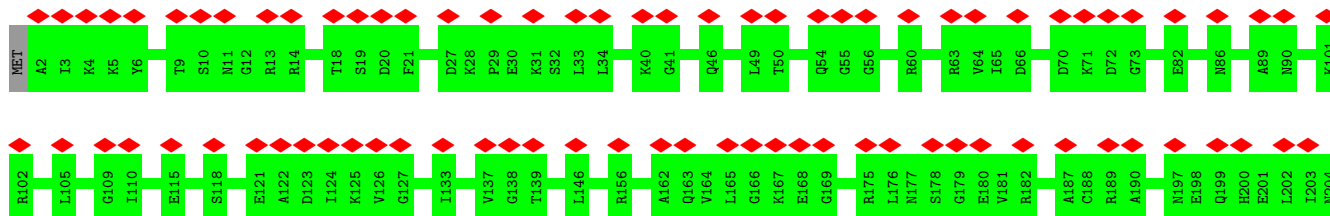
• Molecule 2: 5S rRNA

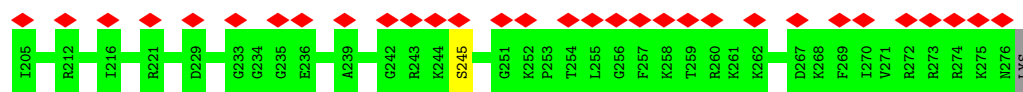
Chain B: 53% 32% 8% 6%



• Molecule 3: 50S ribosomal protein L2

Chain C: 40% 99%

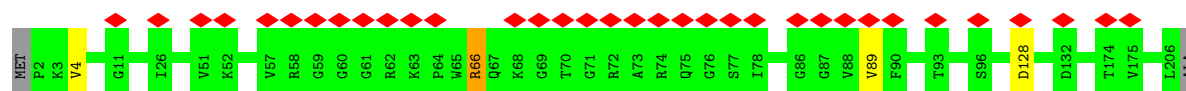




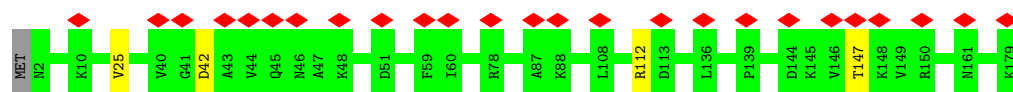
- Molecule 4: 50S ribosomal protein L3



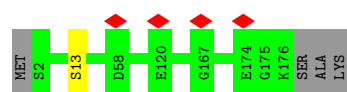
- Molecule 5: 50S ribosomal protein L4



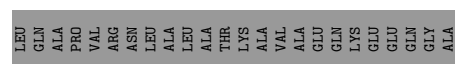
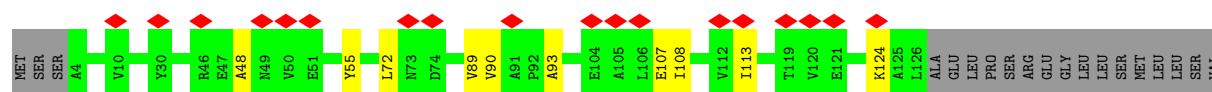
- Molecule 6: 50S ribosomal protein L5



- Molecule 7: Ribosomal protein L6

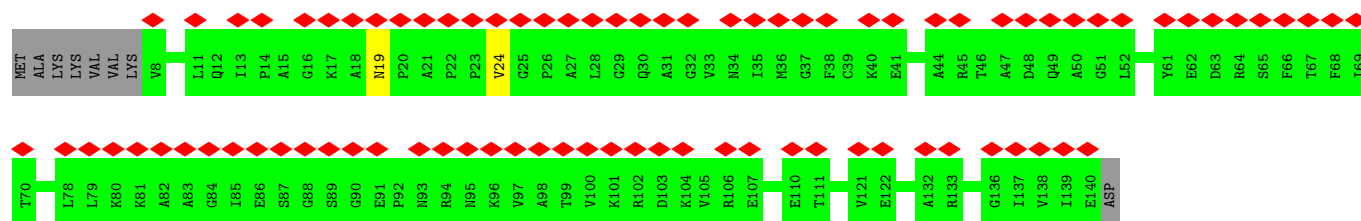


- Molecule 8: 50S ribosomal protein L10

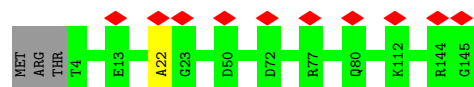


- Molecule 9: 50S ribosomal protein L11

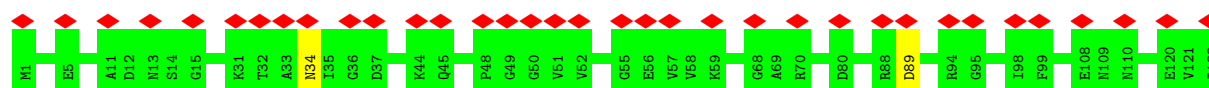




- Molecule 10: 50S ribosomal protein L13



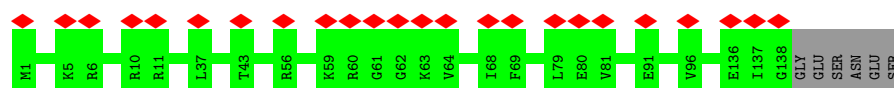
- Molecule 11: 50S ribosomal protein L14



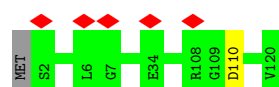
- Molecule 12: 50S ribosomal protein L15



- Molecule 13: 50S ribosomal protein L16



- Molecule 14: 50S ribosomal protein L17

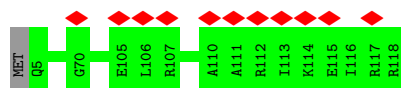


- Molecule 15: 50S ribosomal protein L18

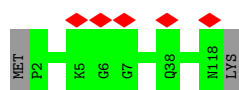




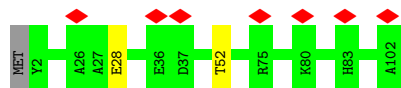
- Molecule 16: 50S ribosomal protein L19



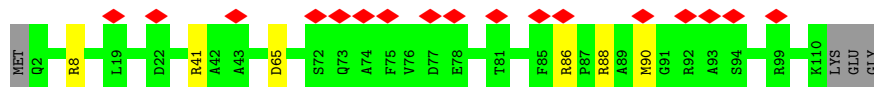
- Molecule 17: 50S ribosomal protein L20



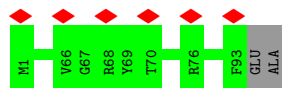
- Molecule 18: 50S ribosomal protein L21



- Molecule 19: 50S ribosomal protein L22



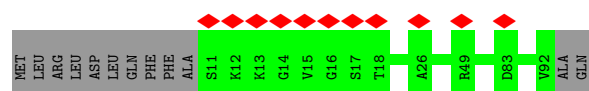
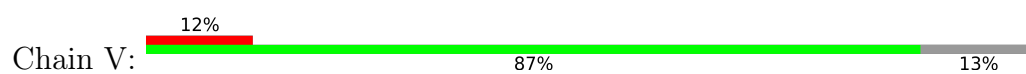
- Molecule 20: 50S ribosomal protein L23



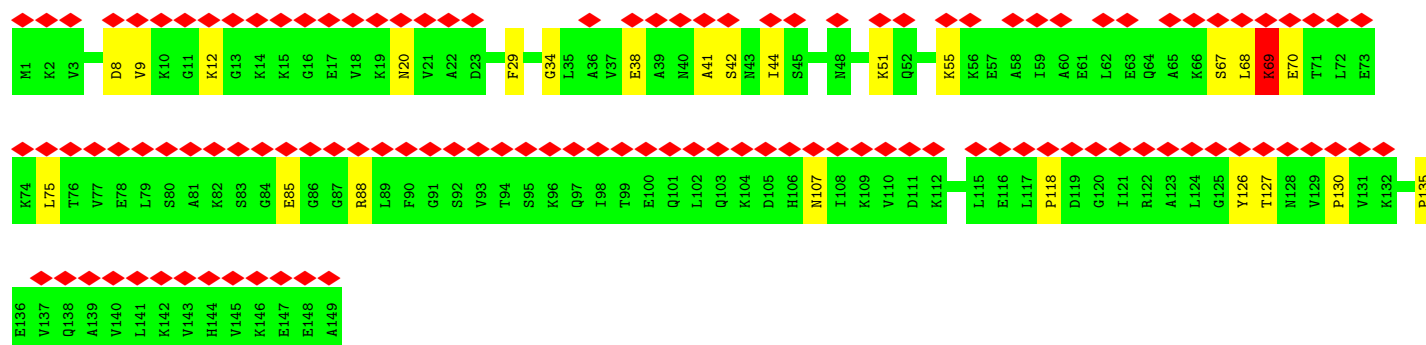
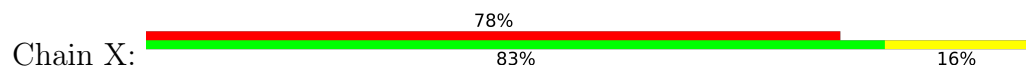
- Molecule 21: 50S ribosomal protein L24



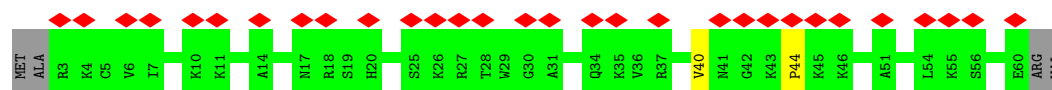
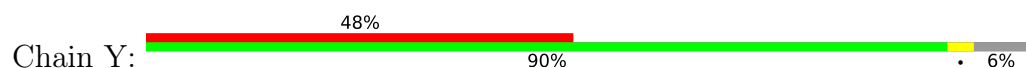
- Molecule 22: 50S ribosomal protein L27



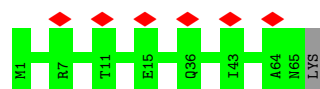
• Molecule 23: 50S ribosomal protein L9



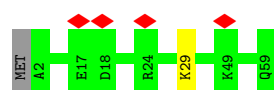
• Molecule 24: 50S ribosomal protein L28



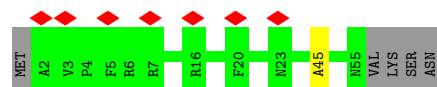
• Molecule 25: 50S ribosomal protein L29



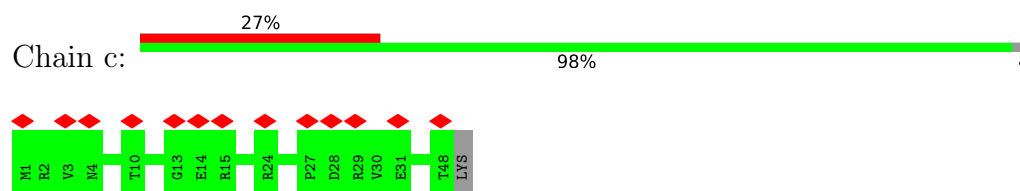
• Molecule 26: 50S ribosomal protein L30



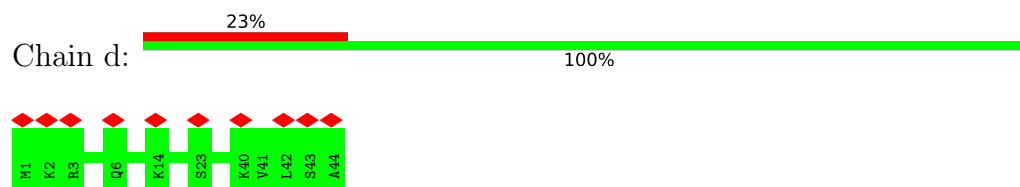
• Molecule 27: 50S ribosomal protein L32



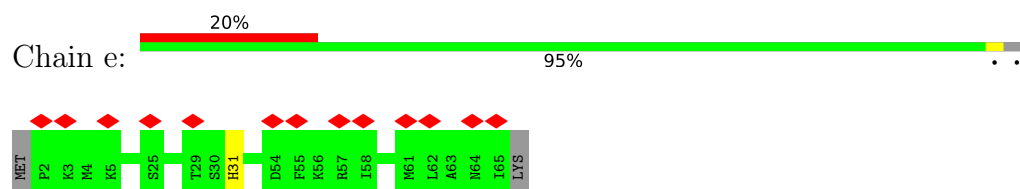
- Molecule 28: 50S ribosomal protein L33



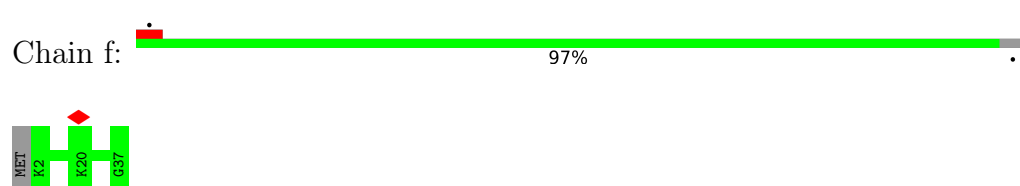
- Molecule 29: 50S ribosomal protein L34



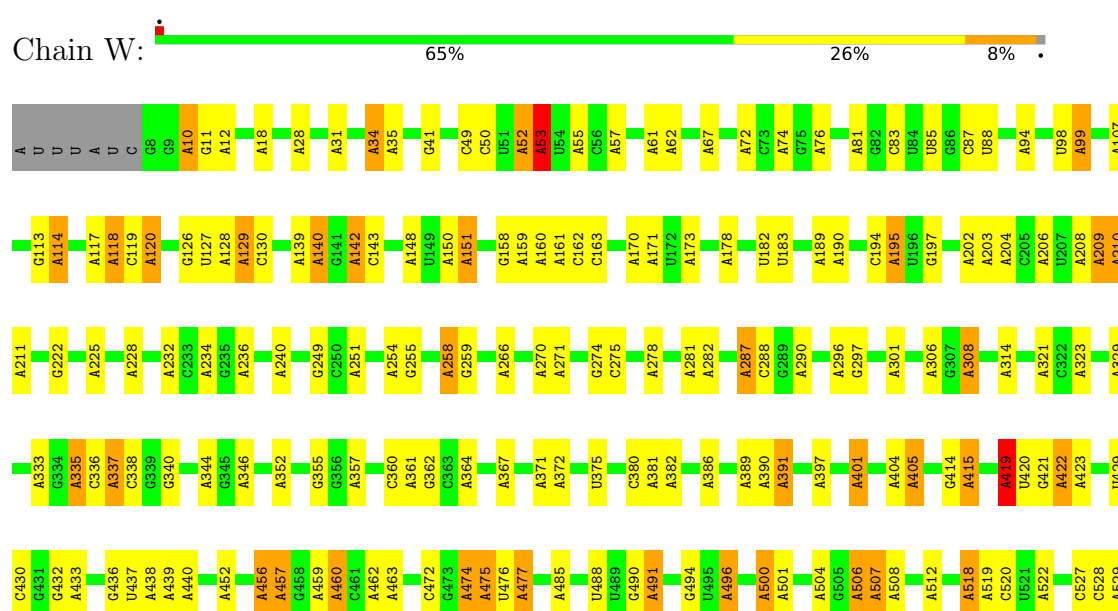
- Molecule 30: 50S ribosomal protein L35

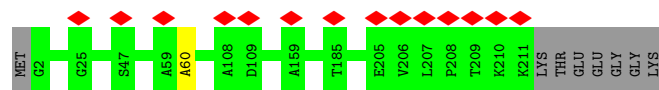


- Molecule 31: 50S ribosomal protein L36

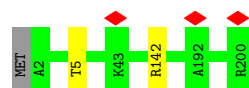


- Molecule 32: 16S rRNA

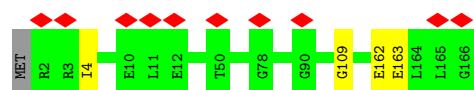




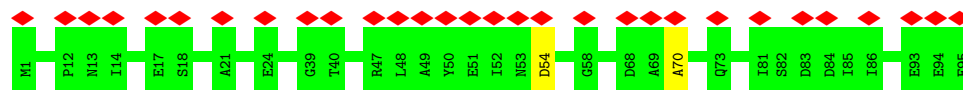
- Molecule 35: 30S ribosomal protein S4



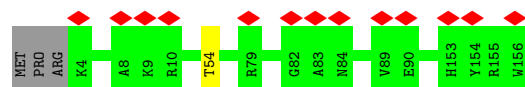
- Molecule 36: 30S ribosomal protein S5



- Molecule 37: 30S ribosomal protein S6



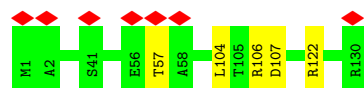
- Molecule 38: 30S ribosomal protein S7



- Molecule 39: 30S ribosomal protein S8



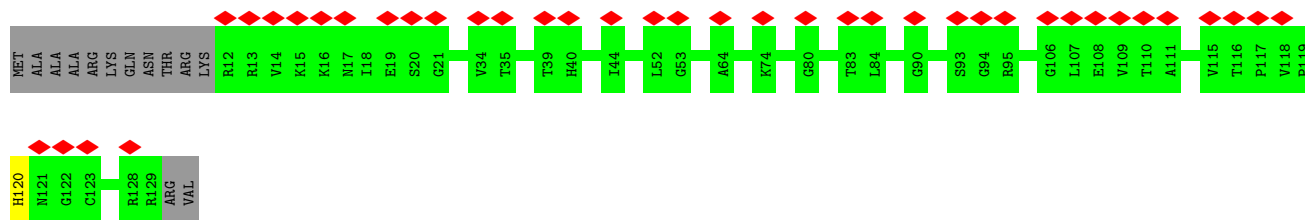
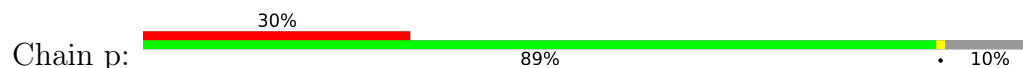
- Molecule 40: 30S ribosomal protein S9



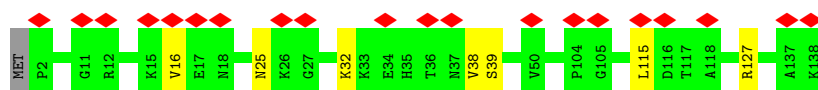
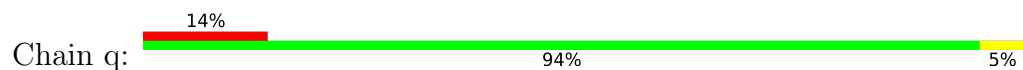
- Molecule 41: 30S ribosomal protein S10



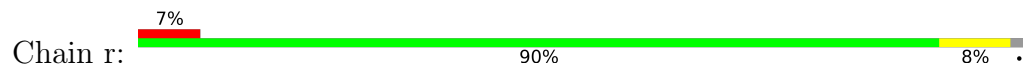
- Molecule 42: 30S ribosomal protein S11



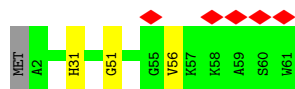
- Molecule 43: 30S ribosomal protein S12



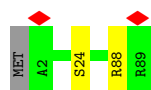
- Molecule 44: 30S ribosomal protein S13



- Molecule 45: 30S ribosomal protein S14 type Z

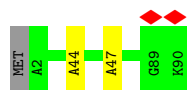


- Molecule 46: 30S ribosomal protein S15



- Molecule 47: 30S ribosomal protein S16

Chain u:  97%




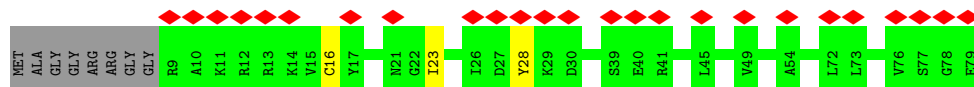
- Molecule 48: 30S ribosomal protein S17

Chain v:  11% 99%




- Molecule 49: 30S ribosomal protein S18

Chain w:  32% 86% 10%



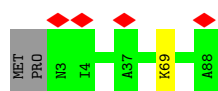
- Molecule 50: 30S ribosomal protein S19

Chain x:  89% 9%



- Molecule 51: 30S ribosomal protein S20

Chain y:  5% 97%



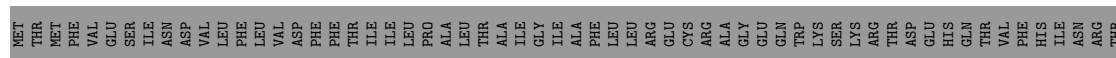
- Molecule 52: P-site tRNA

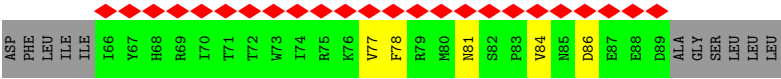
Chain z:  5% 71% 22% 5%



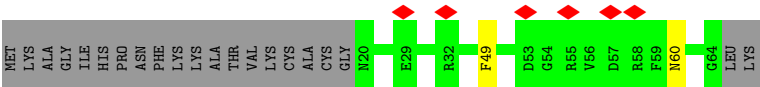
- Molecule 53: YqzJ

Chain 2:  25% 20% 5% 75%





● Molecule 54: 50S ribosomal protein L31



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	12739	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	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	1.709	Depositor
Minimum map value	-0.823	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.090	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	650.4, 650.4, 650.4	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.084, 1.084, 1.084	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	A	1.37	1874/70307 (2.7%)	2.92	7344/109687 (6.7%)
2	B	1.30	64/2678 (2.4%)	2.78	247/4174 (5.9%)
3	C	0.27	0/2148	0.48	0/2881
4	D	0.28	0/1597	0.47	0/2140
5	E	0.27	0/1580	0.50	0/2132
6	F	0.29	0/1423	0.50	0/1910
7	G	0.24	0/1360	0.43	0/1832
8	H	0.26	0/963	0.49	0/1298
9	I	0.26	0/995	0.48	0/1346
10	J	0.26	0/1146	0.49	0/1542
11	K	0.28	0/927	0.47	0/1245
12	L	0.23	0/1093	0.44	0/1457
13	M	0.21	0/1120	0.38	0/1496
14	N	0.26	0/960	0.50	0/1284
15	O	0.30	0/921	0.54	1/1236 (0.1%)
16	P	0.24	0/949	0.44	0/1269
17	Q	0.27	0/952	0.45	0/1266
18	R	0.28	0/797	0.53	0/1070
19	S	0.34	0/851	0.59	0/1146
20	T	0.30	0/759	0.47	0/1011
21	U	0.27	0/764	0.52	0/1022
22	V	0.30	0/638	0.50	0/847
23	X	0.64	1/732 (0.1%)	1.01	5/1016 (0.5%)
24	Y	0.30	0/448	0.58	0/596
25	Z	0.24	0/531	0.48	0/707
26	a	0.24	0/457	0.44	0/613
27	b	0.23	0/433	0.48	0/574
28	c	0.26	0/406	0.44	0/540
29	d	0.21	0/370	0.44	0/483
30	e	0.23	0/519	0.48	0/680
31	f	0.20	0/291	0.37	0/383
32	W	1.36	968/37074 (2.6%)	2.90	3819/57834 (6.6%)
33	g	0.32	0/895	0.40	0/1117
34	h	0.29	0/839	0.38	0/1047

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
35	i	0.26	0/796	0.41	0/992
36	j	0.26	0/660	0.46	0/822
37	k	0.31	0/380	0.41	0/472
38	l	0.27	0/612	0.39	0/762
39	m	0.24	0/524	0.43	0/652
40	n	0.26	0/520	0.51	0/647
41	o	0.28	0/408	0.39	0/507
42	p	0.22	0/471	0.42	0/587
43	q	0.24	0/548	0.50	0/682
44	r	0.31	0/475	0.52	0/592
45	s	0.21	0/240	0.49	0/297
46	t	0.27	0/352	0.42	0/437
47	u	0.27	0/356	0.41	0/442
48	v	0.27	0/344	0.43	0/427
49	w	0.31	0/284	0.43	0/352
50	x	0.33	0/335	0.46	0/417
51	y	0.26	0/344	0.40	0/427
52	z	1.04	30/1834 (1.6%)	2.18	104/2858 (3.6%)
53	2	0.50	0/106	1.02	0/122
54	3	0.29	0/373	0.45	0/497
All	All	1.19	2937/147885 (2.0%)	2.58	11520/221872 (5.2%)

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	79
2	B	0	2
5	E	0	1
19	S	0	2
23	X	0	2
32	W	0	33
52	z	0	2
All	All	0	121

The worst 5 of 2937 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	W	508	A	C8-N7	8.39	1.37	1.31
1	A	1188	A	C8-N7	8.37	1.37	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	526	A	C8-N7	8.21	1.37	1.31
1	A	2916	A	C8-N7	8.17	1.37	1.31
1	A	504	A	C8-N7	8.14	1.37	1.31

The worst 5 of 11520 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1691	A	C2-N3-C4	20.51	120.85	110.60
1	A	1134	A	C2-N3-C4	20.48	120.84	110.60
32	W	1308	A	C2-N3-C4	20.41	120.80	110.60
1	A	226	A	C2-N3-C4	20.26	120.73	110.60
1	A	732	A	C2-N3-C4	20.18	120.69	110.60

There are no chirality outliers.

5 of 121 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	126	A	Sidechain
1	A	168	A	Sidechain
1	A	52	A	Sidechain
1	A	64	A	Sidechain
1	A	67	A	Sidechain

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	C	273/277 (99%)	264 (97%)	8 (3%)	1 (0%)	30 68

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	205/208 (99%)	189 (92%)	11 (5%)	5 (2%)	5	27
5	E	203/207 (98%)	185 (91%)	15 (7%)	3 (2%)	8	39
6	F	176/179 (98%)	154 (88%)	18 (10%)	4 (2%)	5	28
7	G	173/179 (97%)	164 (95%)	8 (5%)	1 (1%)	22	59
8	H	121/166 (73%)	97 (80%)	14 (12%)	10 (8%)	0	10
9	I	131/141 (93%)	122 (93%)	7 (5%)	2 (2%)	8	39
10	J	140/145 (97%)	130 (93%)	9 (6%)	1 (1%)	19	56
11	K	120/122 (98%)	112 (93%)	6 (5%)	2 (2%)	7	36
12	L	144/146 (99%)	132 (92%)	10 (7%)	2 (1%)	9	40
13	M	136/144 (94%)	129 (95%)	7 (5%)	0	100	100
14	N	117/120 (98%)	109 (93%)	7 (6%)	1 (1%)	14	50
15	O	118/120 (98%)	106 (90%)	7 (6%)	5 (4%)	2	17
16	P	112/115 (97%)	100 (89%)	12 (11%)	0	100	100
17	Q	115/119 (97%)	112 (97%)	3 (3%)	0	100	100
18	R	99/102 (97%)	82 (83%)	15 (15%)	2 (2%)	6	31
19	S	107/113 (95%)	96 (90%)	8 (8%)	3 (3%)	4	24
20	T	91/95 (96%)	86 (94%)	5 (6%)	0	100	100
21	U	98/103 (95%)	87 (89%)	8 (8%)	3 (3%)	3	22
22	V	80/94 (85%)	77 (96%)	3 (4%)	0	100	100
23	X	147/149 (99%)	83 (56%)	42 (29%)	22 (15%)	0	3
24	Y	56/62 (90%)	53 (95%)	1 (2%)	2 (4%)	3	20
25	Z	63/66 (96%)	60 (95%)	3 (5%)	0	100	100
26	a	56/59 (95%)	54 (96%)	1 (2%)	1 (2%)	7	34
27	b	52/59 (88%)	47 (90%)	4 (8%)	1 (2%)	6	32
28	c	46/49 (94%)	44 (96%)	2 (4%)	0	100	100
29	d	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
30	e	62/66 (94%)	56 (90%)	5 (8%)	1 (2%)	8	37
31	f	34/37 (92%)	33 (97%)	1 (3%)	0	100	100
33	g	222/246 (90%)	204 (92%)	13 (6%)	5 (2%)	5	28
34	h	208/218 (95%)	193 (93%)	14 (7%)	1 (0%)	25	64
35	i	197/200 (98%)	191 (97%)	4 (2%)	2 (1%)	13	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	j	163/166 (98%)	150 (92%)	9 (6%)	4 (2%)	4	26
37	k	93/95 (98%)	88 (95%)	3 (3%)	2 (2%)	5	29
38	l	151/156 (97%)	144 (95%)	6 (4%)	1 (1%)	19	56
39	m	129/132 (98%)	123 (95%)	5 (4%)	1 (1%)	16	53
40	n	128/130 (98%)	113 (88%)	10 (8%)	5 (4%)	2	19
41	o	100/102 (98%)	88 (88%)	8 (8%)	4 (4%)	2	18
42	p	116/131 (88%)	106 (91%)	9 (8%)	1 (1%)	14	50
43	q	135/138 (98%)	119 (88%)	9 (7%)	7 (5%)	1	15
44	r	117/121 (97%)	94 (80%)	13 (11%)	10 (8%)	0	9
45	s	58/61 (95%)	51 (88%)	4 (7%)	3 (5%)	1	15
46	t	86/89 (97%)	82 (95%)	2 (2%)	2 (2%)	5	28
47	u	87/90 (97%)	82 (94%)	3 (3%)	2 (2%)	5	28
48	v	84/87 (97%)	78 (93%)	6 (7%)	0	100	100
49	w	69/79 (87%)	64 (93%)	2 (3%)	3 (4%)	2	17
50	x	82/92 (89%)	75 (92%)	5 (6%)	2 (2%)	5	27
51	y	84/88 (96%)	77 (92%)	6 (7%)	1 (1%)	11	44
53	2	22/95 (23%)	17 (77%)	2 (9%)	3 (14%)	0	4
54	3	43/66 (65%)	37 (86%)	4 (9%)	2 (5%)	2	17
All	All	5691/6068 (94%)	5180 (91%)	378 (7%)	133 (2%)	7	28

5 of 133 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	93	ALA
9	I	19	ASN
15	O	26	ALA
21	U	87	ASP
23	X	29	PHE

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	
3	C	223/225 (99%)	223 (100%)	0	100	100
4	D	168/169 (99%)	168 (100%)	0	100	100
5	E	169/170 (99%)	168 (99%)	1 (1%)	84	88
6	F	153/154 (99%)	153 (100%)	0	100	100
7	G	148/151 (98%)	148 (100%)	0	100	100
8	H	105/139 (76%)	105 (100%)	0	100	100
9	I	103/110 (94%)	103 (100%)	0	100	100
10	J	120/123 (98%)	120 (100%)	0	100	100
11	K	101/101 (100%)	101 (100%)	0	100	100
12	L	110/110 (100%)	110 (100%)	0	100	100
13	M	111/116 (96%)	111 (100%)	0	100	100
14	N	99/100 (99%)	99 (100%)	0	100	100
15	O	93/93 (100%)	93 (100%)	0	100	100
16	P	99/100 (99%)	99 (100%)	0	100	100
17	Q	96/98 (98%)	96 (100%)	0	100	100
18	R	83/84 (99%)	83 (100%)	0	100	100
19	S	90/93 (97%)	89 (99%)	1 (1%)	70	80
20	T	84/85 (99%)	84 (100%)	0	100	100
21	U	84/87 (97%)	84 (100%)	0	100	100
22	V	64/74 (86%)	64 (100%)	0	100	100
24	Y	47/50 (94%)	47 (100%)	0	100	100
25	Z	56/57 (98%)	56 (100%)	0	100	100
26	a	52/53 (98%)	52 (100%)	0	100	100
27	b	48/53 (91%)	48 (100%)	0	100	100
28	c	46/47 (98%)	46 (100%)	0	100	100
29	d	39/39 (100%)	39 (100%)	0	100	100
30	e	54/56 (96%)	54 (100%)	0	100	100
31	f	34/35 (97%)	34 (100%)	0	100	100
53	2	6/87 (7%)	4 (67%)	2 (33%)	0	2
54	3	39/55 (71%)	39 (100%)	0	100	100
All	All	2724/2914 (94%)	2720 (100%)	4 (0%)	92	95

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	E	66	ARG
19	S	90	MET
53	2	81	ASN
53	2	86	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
22	V	37	GLN
29	d	9	ASN
24	Y	23	ASN
26	a	40	ASN
30	e	35	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2922/2928 (99%)	828 (28%)	85 (2%)
2	B	111/119 (93%)	32 (28%)	4 (3%)
32	W	1543/1555 (99%)	235 (15%)	17 (1%)
52	z	76/77 (98%)	15 (19%)	0
All	All	4652/4679 (99%)	1110 (23%)	106 (2%)

5 of 1110 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	8	U
1	A	9	U
1	A	10	A
1	A	13	A
1	A	27	G

5 of 106 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1965	A
1	A	2351	A
32	W	873	U
1	A	2139	G

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Mol	Chain	Res	Type
1	A	2254	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.

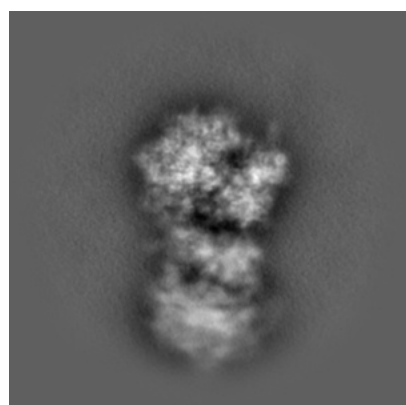
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13959. These allow visual inspection of the internal detail of the map and identification of artifacts.

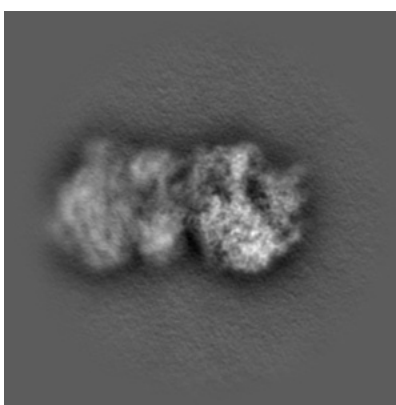
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

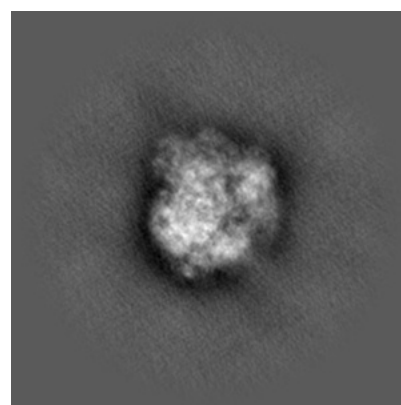
6.1.1 Primary map



X



Y

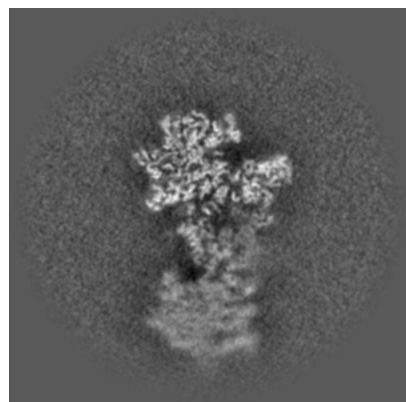


Z

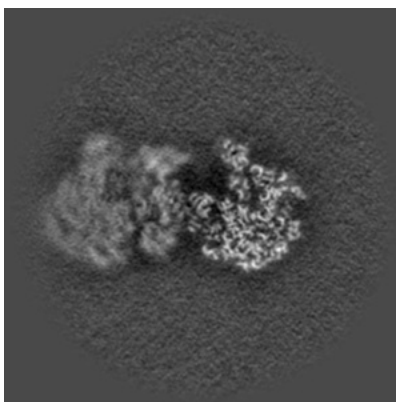
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

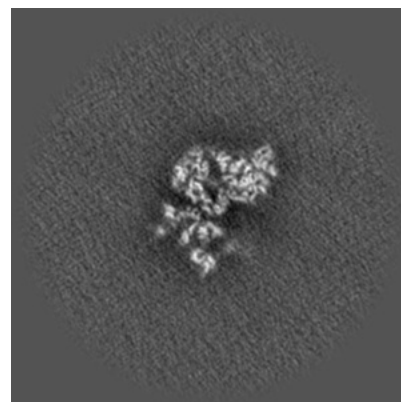
6.2.1 Primary map



X Index: 300



Y Index: 300

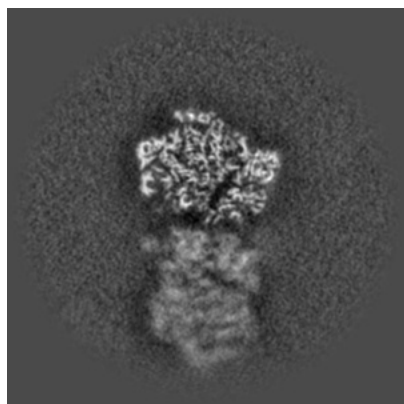


Z Index: 300

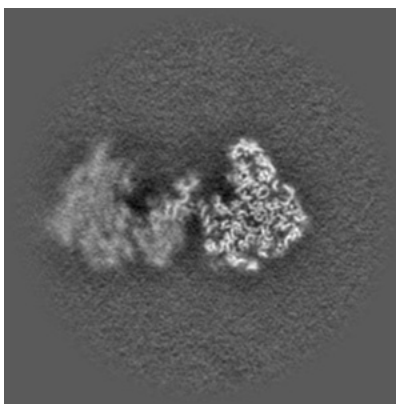
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

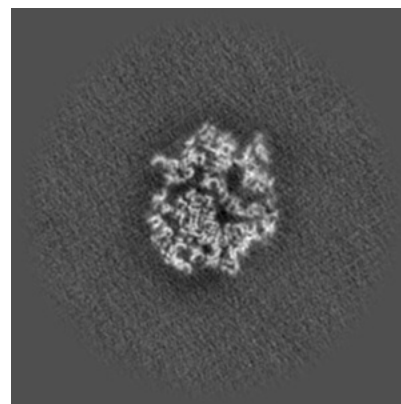
6.3.1 Primary map



X Index: 267



Y Index: 275

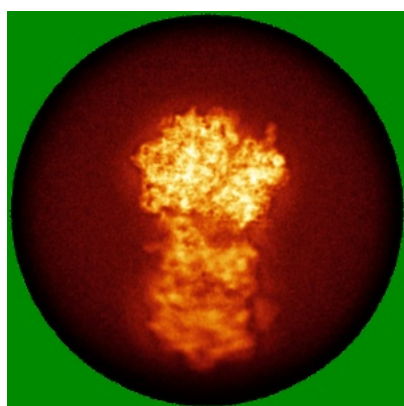


Z Index: 349

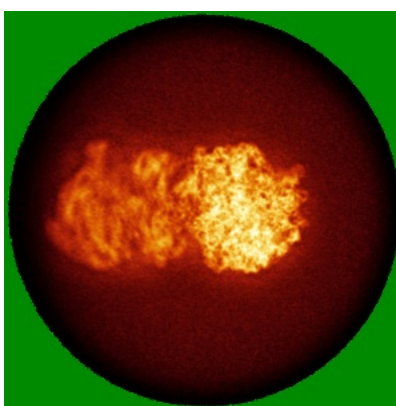
The images above show the largest variance slices of the map in three orthogonal directions.

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

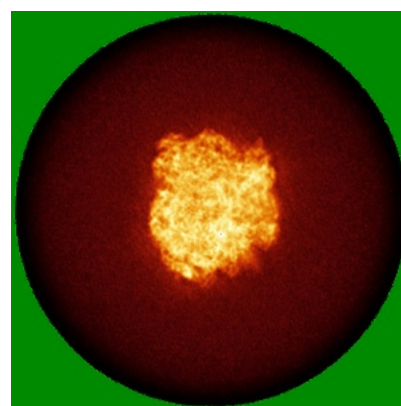
6.4.1 Primary map



X



Y

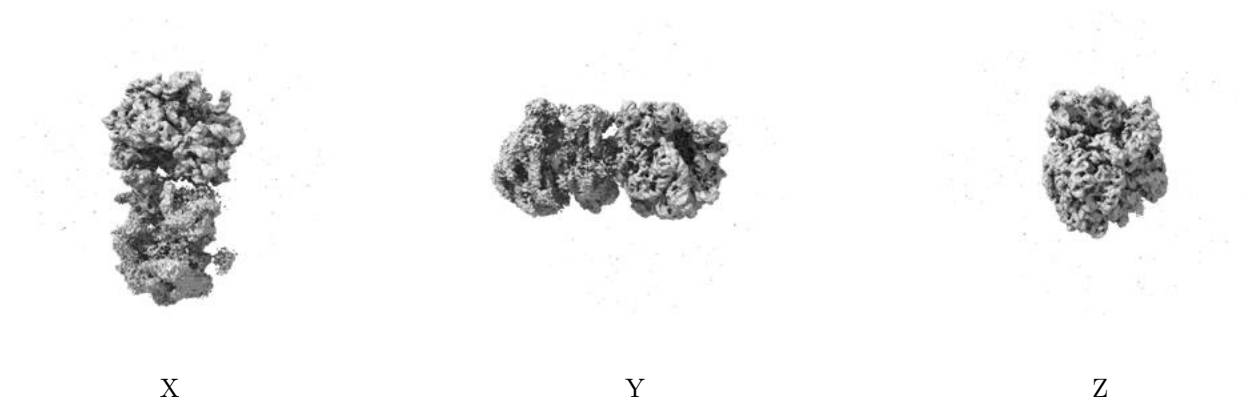


Z

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

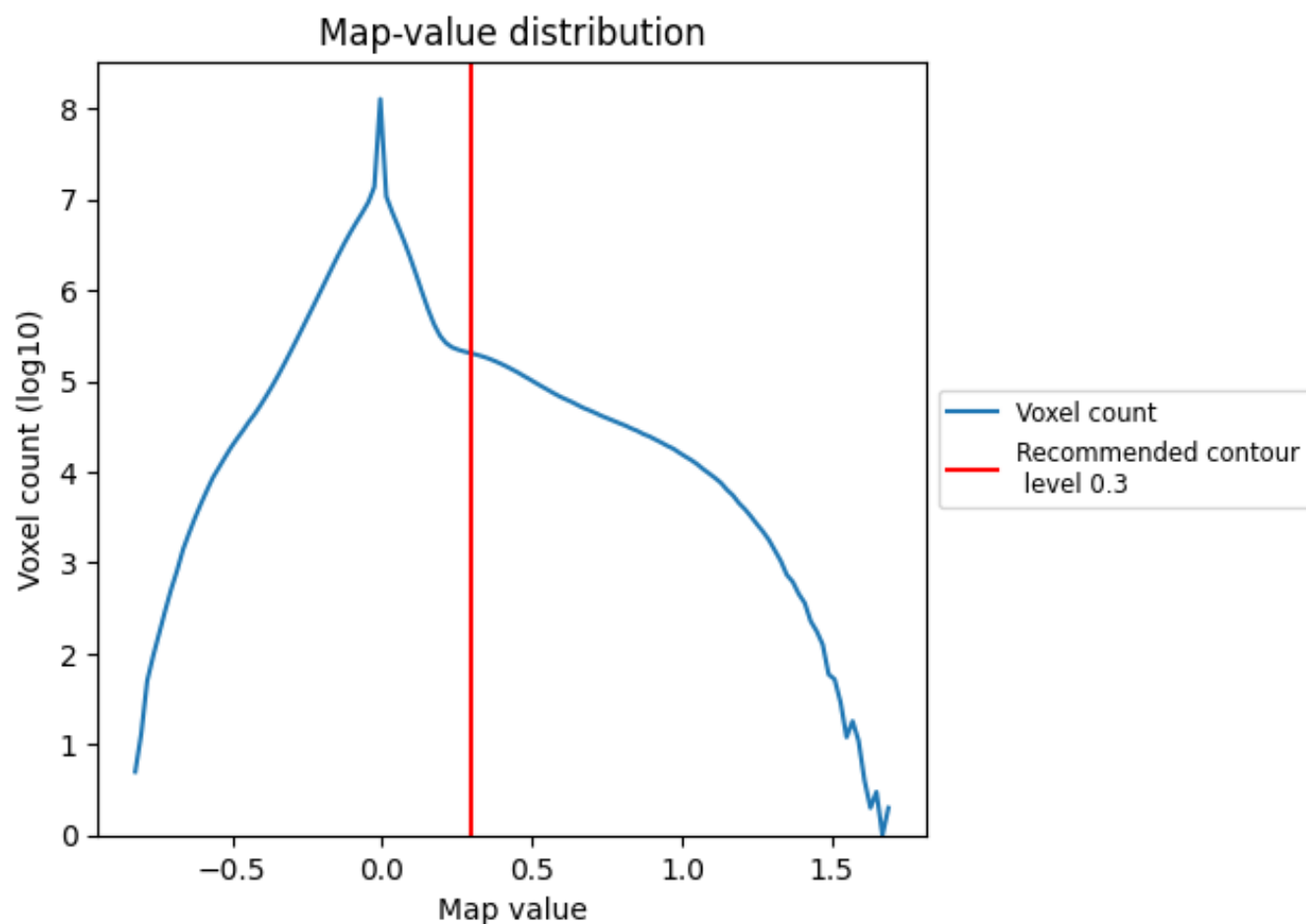
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

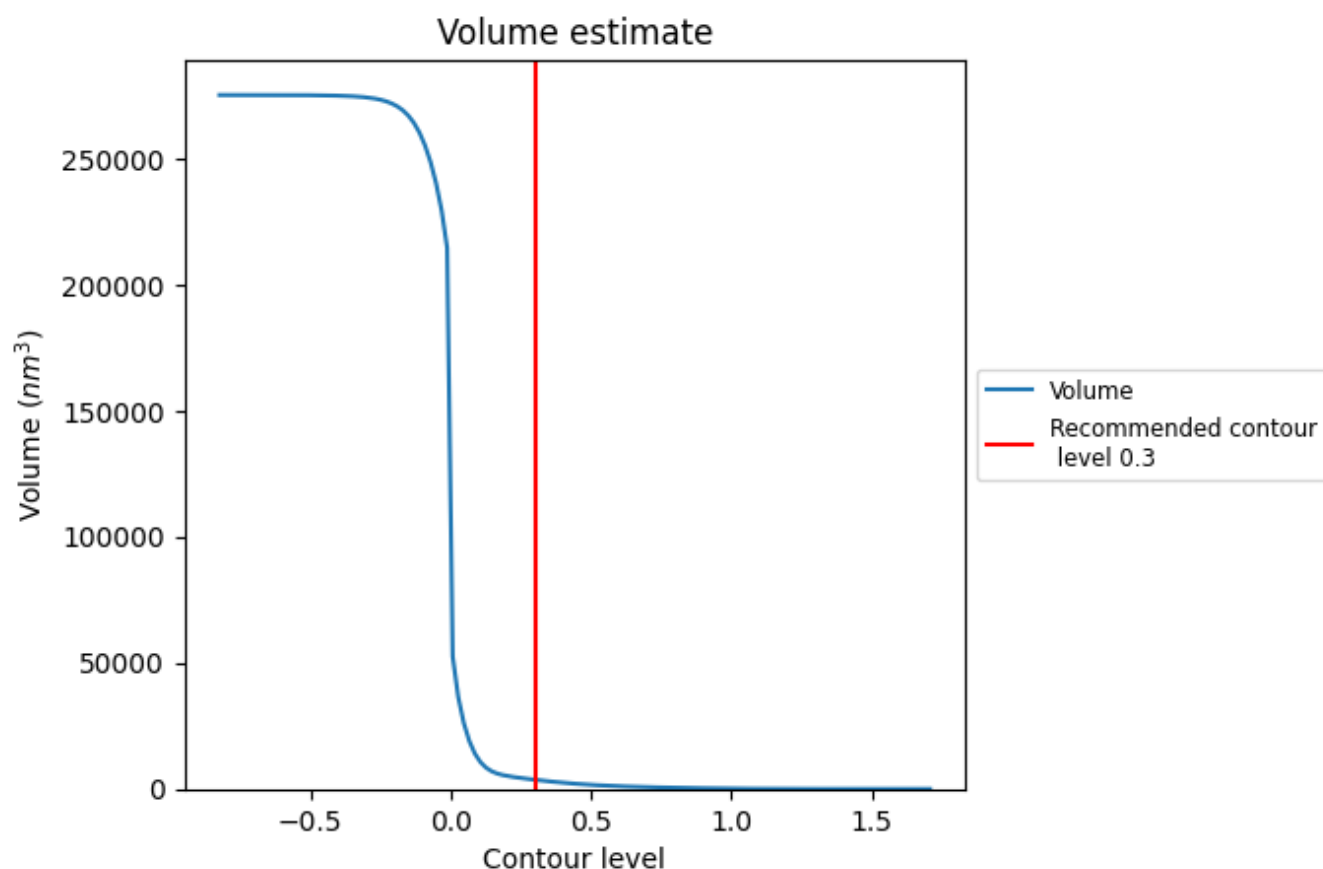
This section contains the results of statistical analysis of the map.

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.

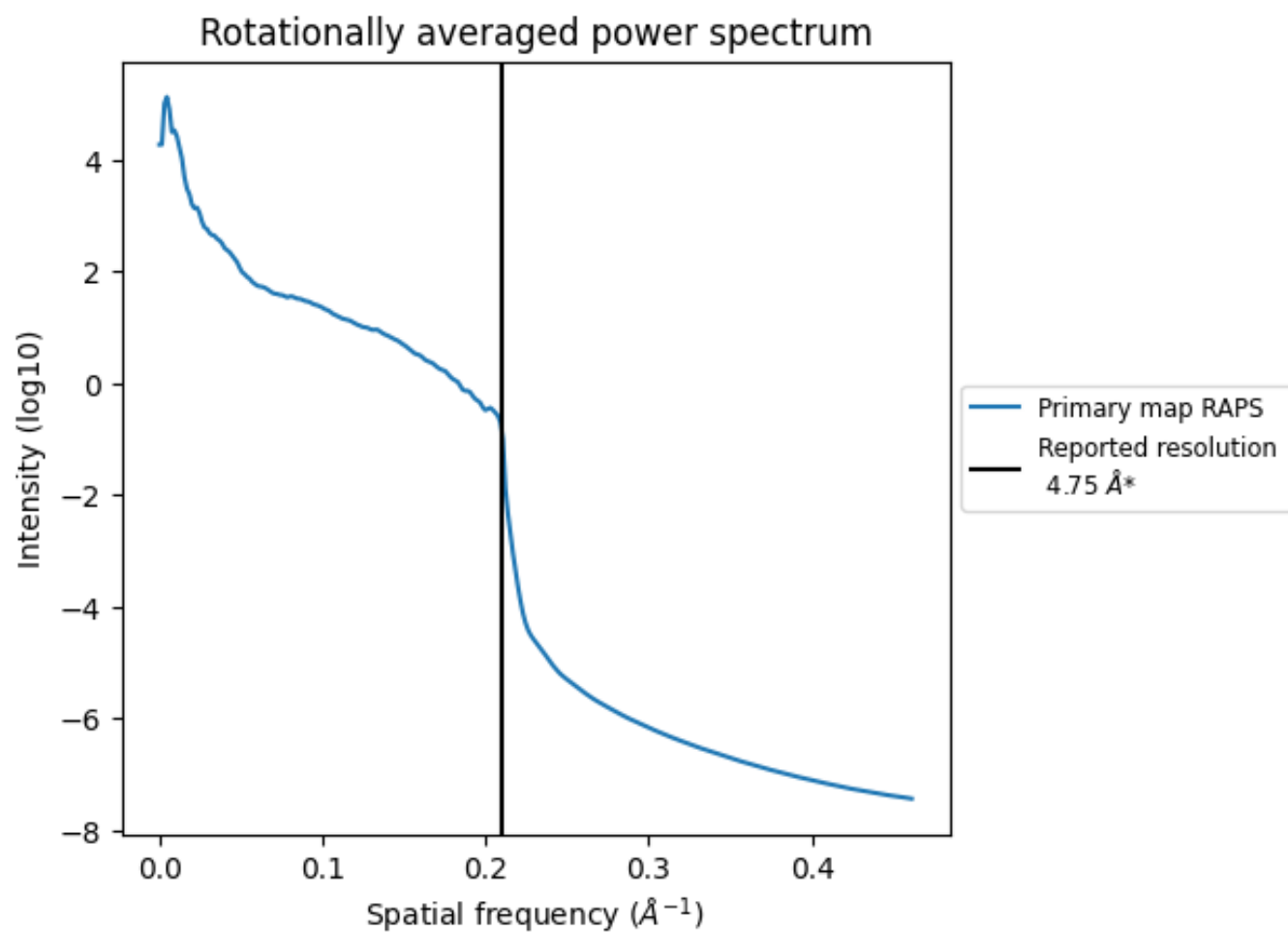
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3652 nm^3 ; this corresponds to an approximate mass of 3299 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 0.211 Å⁻¹

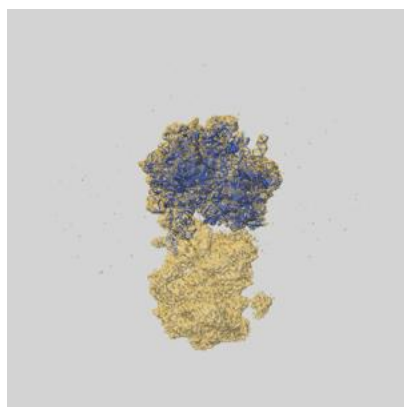
8 Fourier-Shell correlation

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

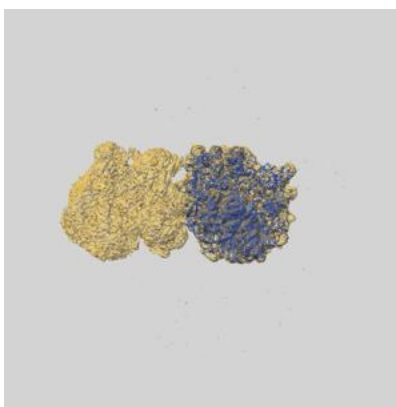
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-13959 and PDB model 7QGU. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

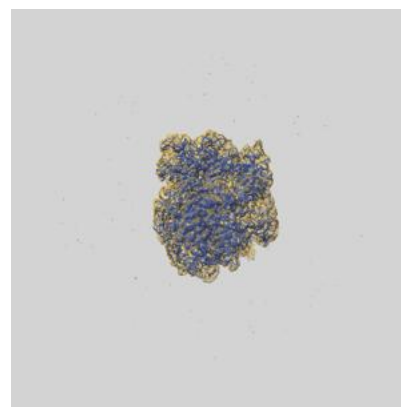
9.1 Map-model overlay [i](#)



X



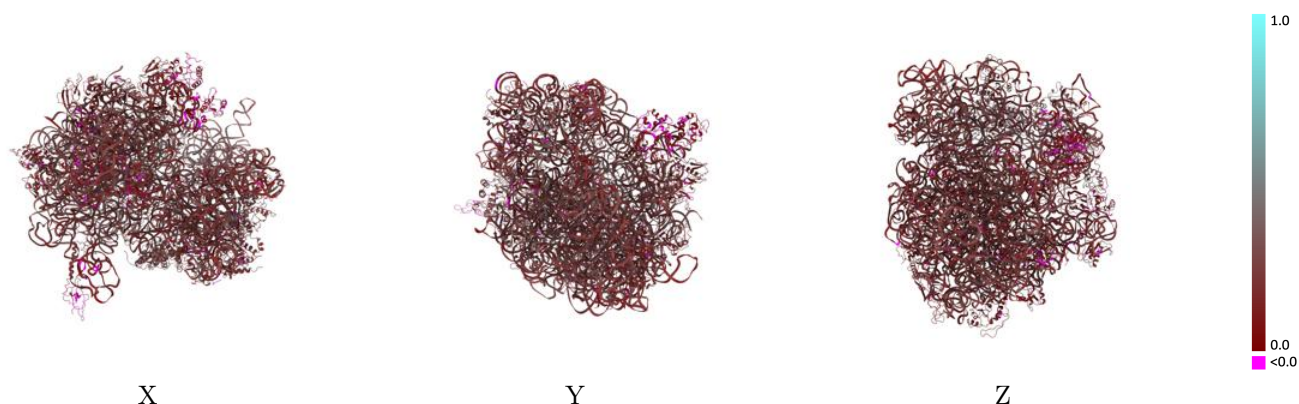
Y



Z

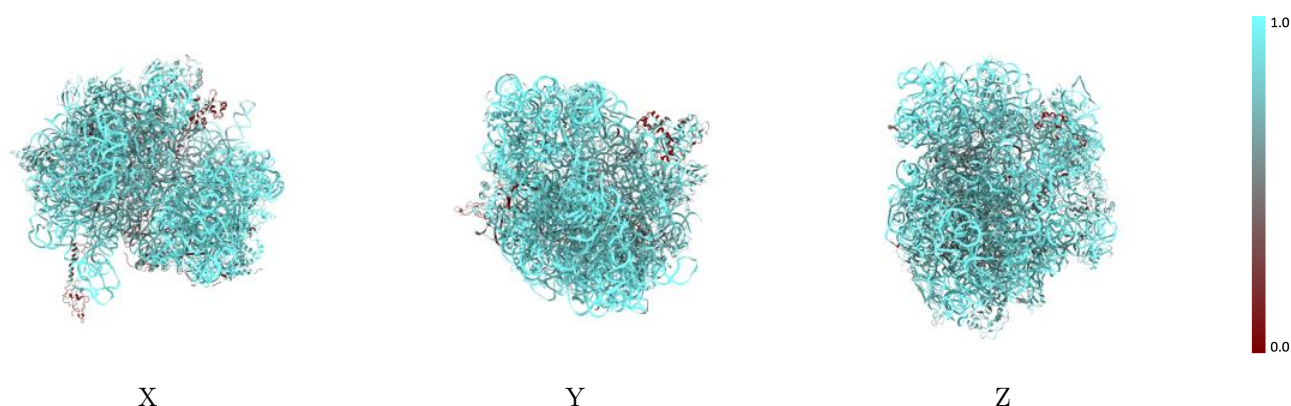
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



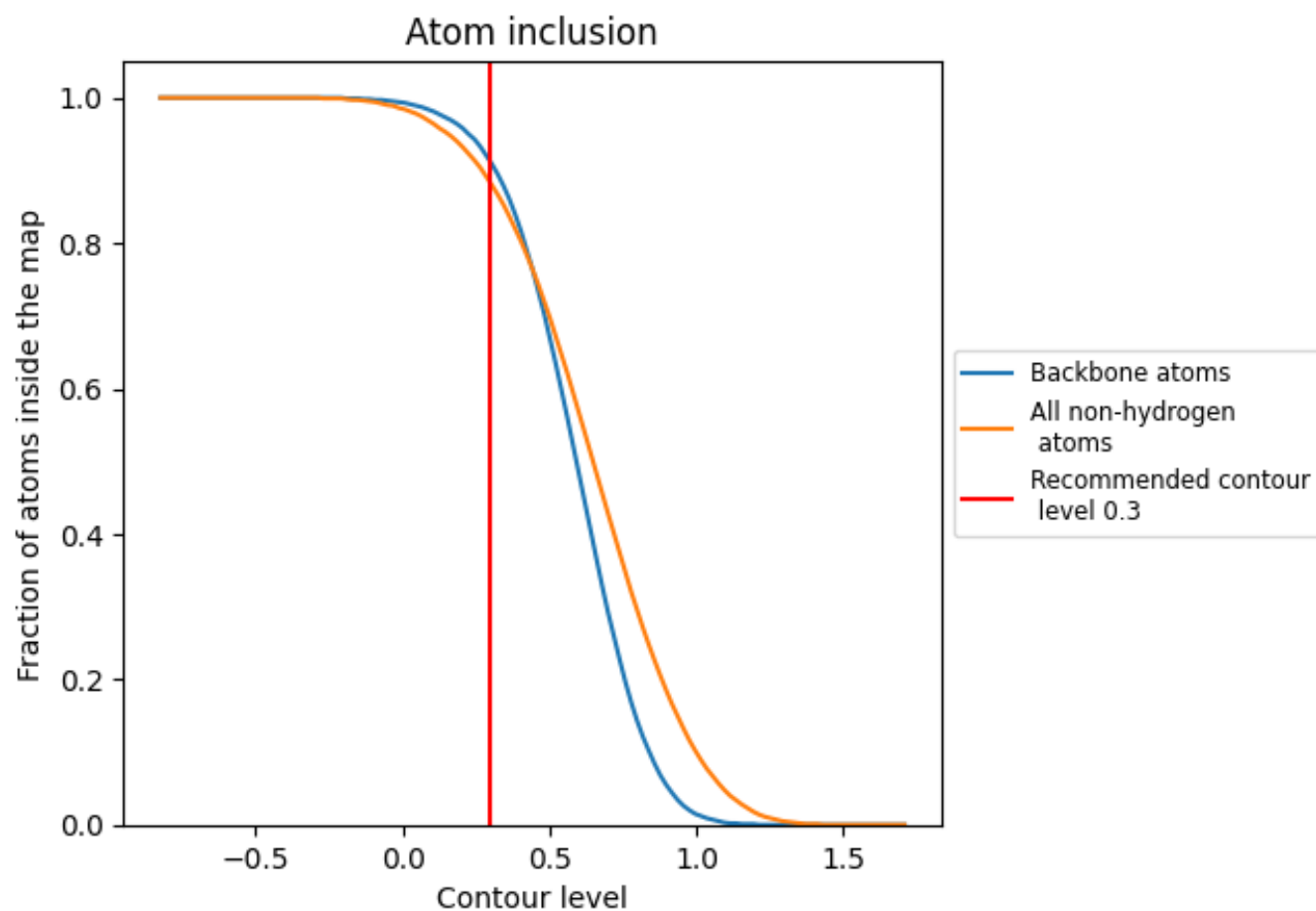
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 88% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8830	 0.2250
2	 0.0380	 0.1920
3	 0.7720	 0.1350
A	 0.9460	 0.2410
B	 0.9770	 0.2340
C	 0.4580	 0.1710
D	 0.7070	 0.1810
E	 0.6430	 0.1760
F	 0.6920	 0.1480
G	 0.8030	 0.1800
H	 0.7230	 0.0760
I	 0.3210	 0.0580
J	 0.7190	 0.1850
K	 0.5130	 0.1810
L	 0.6860	 0.1560
M	 0.6150	 0.1930
N	 0.7360	 0.1580
O	 0.8300	 0.1530
P	 0.6890	 0.1770
Q	 0.7420	 0.1400
R	 0.7680	 0.1870
S	 0.6120	 0.1770
T	 0.7160	 0.1760
U	 0.7340	 0.1640
V	 0.7110	 0.1570
W	 0.9520	 0.2320
X	 0.2320	 0.0990
Y	 0.4280	 0.1200
Z	 0.7020	 0.1510
a	 0.7660	 0.1420
b	 0.6800	 0.1730
c	 0.6180	 0.1400
d	 0.5590	 0.1310
e	 0.6110	 0.1430
f	 0.7380	 0.1730



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Chain	Atom inclusion	Q-score
g	 0.8040	 0.2740
h	 0.9000	 0.2780
i	 0.9650	 0.2740
j	 0.9210	 0.2940
k	 0.6270	 0.2930
l	 0.8790	 0.2850
m	 0.9790	 0.2960
n	 0.9170	 0.2620
o	 0.9270	 0.2700
p	 0.5930	 0.2830
q	 0.8110	 0.2800
r	 0.9120	 0.2550
s	 0.9090	 0.2540
t	 0.9520	 0.2970
u	 0.9610	 0.2840
v	 0.8440	 0.2900
w	 0.5510	 0.2780
x	 0.9520	 0.2850
y	 0.9270	 0.2630
z	 0.8210	 0.2190