



## Full wwPDB EM Validation Report ⓘ

Nov 7, 2022 – 04:50 PM JST

PDB ID : 5XYI  
EMDB ID : EMD-6788  
Title : Small subunit of Trichomonas vaginalis ribosome  
Authors : Li, Z.; Guo, Q.; Zheng, L.; Ji, Y.; Xie, Y.; Lai, D.; Lun, Z.; Suo, X.; Gao, N.  
Deposited on : 2017-07-08  
Resolution : 3.35 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

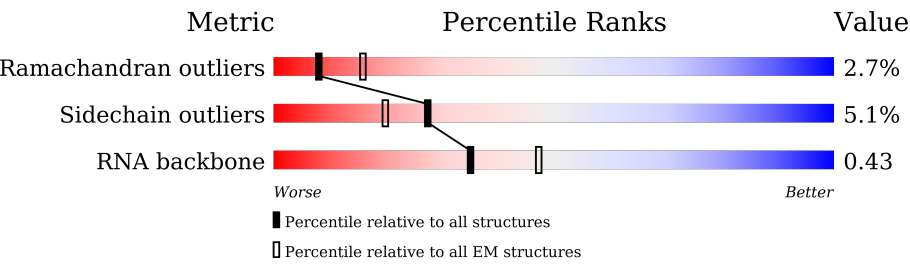
EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

# 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 3.35 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	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	2	1577	<div><div>8%</div><div>68%</div><div>26%</div><div>6%</div></div>
2	A	256	<div><div>9%</div><div>73%</div><div>6%</div><div>20%</div></div>
3	B	247	<div><div>21%</div><div>83%</div><div>5%</div><div>11%</div></div>
4	C	272	<div><div>75%</div><div>5%</div><div>20%</div></div>
5	D	216	<div><div>21%</div><div>94%</div><div>5%</div></div>
6	E	255	<div><div>31%</div><div>91%</div><div>5%</div></div>
7	F	193	<div><div>26%</div><div>90%</div><div>5%</div></div>
8	G	216	<div><div>13%</div><div>14%</div><div>86%</div></div>

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Mol	Chain	Length	Quality of chain
9	H	168	
10	I	197	
11	J	185	
12	K	141	
13	L	155	
14	M	124	
15	N	151	
16	O	159	
17	P	144	
18	Q	140	
19	R	129	
20	S	155	
21	T	148	
22	U	123	
23	V	89	
24	W	130	
25	X	144	
26	Y	140	
27	Z	115	
28	a	118	
29	b	86	
30	c	68	
31	d	57	
32	e	62	
33	g	335	

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Mol	Chain	Length	Quality of chain
34	n	25	<div><div></div><div>24%</div><div>68%</div><div>28%</div><div>.</div></div>

## 2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 65924 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 18S.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	1490	Total	C	N	O	P	0	0
			31820	14210	5694	10426	1490		

- Molecule 2 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	204	Total	C	N	O	S	0	0
			1603	1028	266	294	15		

- Molecule 3 is a protein called Ribosomal protein S3Ae, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	219	Total	C	N	O	S	0	0
			1747	1103	314	318	12		

- Molecule 4 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	217	Total	C	N	O	S	0	0
			1685	1082	299	298	6		

- Molecule 5 is a protein called Ribosomal protein S3, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	208	Total	C	N	O	S	0	0
			1655	1039	311	296	9		

- Molecule 6 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	246	Total	C	N	O	S	0	0
			1935	1236	362	329	8		

- Molecule 7 is a protein called 40s ribosomal protein S5-B, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	186	Total	C	N	O	S	0	0
			1476	915	279	273	9		

- Molecule 8 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	31	Total	C	N	O		0	0
			155	93	31	31			

- Molecule 9 is a protein called 40S ribosomal protein S7, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	163	Total	C	N	O	S	0	0
			1276	811	230	234	1		

- Molecule 10 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	166	Total	C	N	O	S	0	0
			1300	811	253	232	4		

- Molecule 11 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	162	Total	C	N	O	S	0	0
			1321	833	252	233	3		

- Molecule 12 is a protein called Plectin/S10 domain containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	90	Total	C	N	O	S	0	0
			731	472	125	128	6		

- Molecule 13 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	142	Total	C	N	O	S	0	0
			1160	742	222	193	3		

- Molecule 14 is a protein called Ribosomal protein L7Ae, putative.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	M	103	Total	C	N	O	0	0
			509	303	103	103		

- Molecule 15 is a protein called 40S ribosomal protein S13, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	150	Total	C	N	O	S	0	0
			1190	749	234	202	5		

- Molecule 16 is a protein called Ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	135	Total	C	N	O	S	0	0
			1005	615	205	182	3		

- Molecule 17 is a protein called Ribosomal protein S19, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	118	Total	C	N	O	S	0	0
			962	624	176	159	3		

- Molecule 18 is a protein called 40S ribosomal protein S16, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Q	133	Total	C	N	O	S	0	0
			1043	660	196	182	5		

- Molecule 19 is a protein called 40S ribosomal protein S17-B, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	R	118	Total	C	N	O	S	0	0
			961	603	181	171	6		

- Molecule 20 is a protein called Ribosomal protein S13p/S18e, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	135	Total	C	N	O	S	0	0
			1077	668	219	183	7		

- Molecule 21 is a protein called Ribosomal protein S19e, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	T	146	Total	C	N	O	S	0	0
			1148	725	219	200	4		

- Molecule 22 is a protein called Ribosomal protein S10p/S20e, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	U	97	Total	C	N	O	S	0	0
			777	487	150	137	3		

- Molecule 23 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	V	87	Total	C	N	O	S	0	0
			671	418	118	131	4		

- Molecule 24 is a protein called Ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	W	128	Total	C	N	O	S	0	0
			1001	637	182	175	7		

- Molecule 25 is a protein called 40S ribosomal protein S23, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	X	140	Total	C	N	O	S	0	0
			1062	670	206	182	4		

- Molecule 26 is a protein called Ribosomal protein S24e, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Y	105	Total	C	N	O	S	0	0
			792	506	144	141	1		

- Molecule 27 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Z	73	Total	C	N	O	S	0	0
			560	356	99	102	3		

- Molecule 28 is a protein called 40S ribosomal protein S26.



Mol	Chain	Residues	Atoms					AltConf	Trace
28	a	100	Total	C	N	O	S	0	0
			815	503	168	136	8		

- Molecule 29 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	b	82	Total	C	N	O	S	0	0
			632	395	114	119	4		

- Molecule 30 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	c	61	Total	C	N	O	0	0
			475	290	96	89		

- Molecule 31 is a protein called 40S ribosomal protein S29, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	d	52	Total	C	N	O	S	0	0
			438	272	95	67	4		

- Molecule 32 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	e	42	Total	C	N	O	S	0	0
			337	211	71	54	1		

- Molecule 33 is a protein called Guanine nucleotide-binding protein beta subunit, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	g	305	Total	C	N	O	S	0	0
			2380	1509	417	443	11		

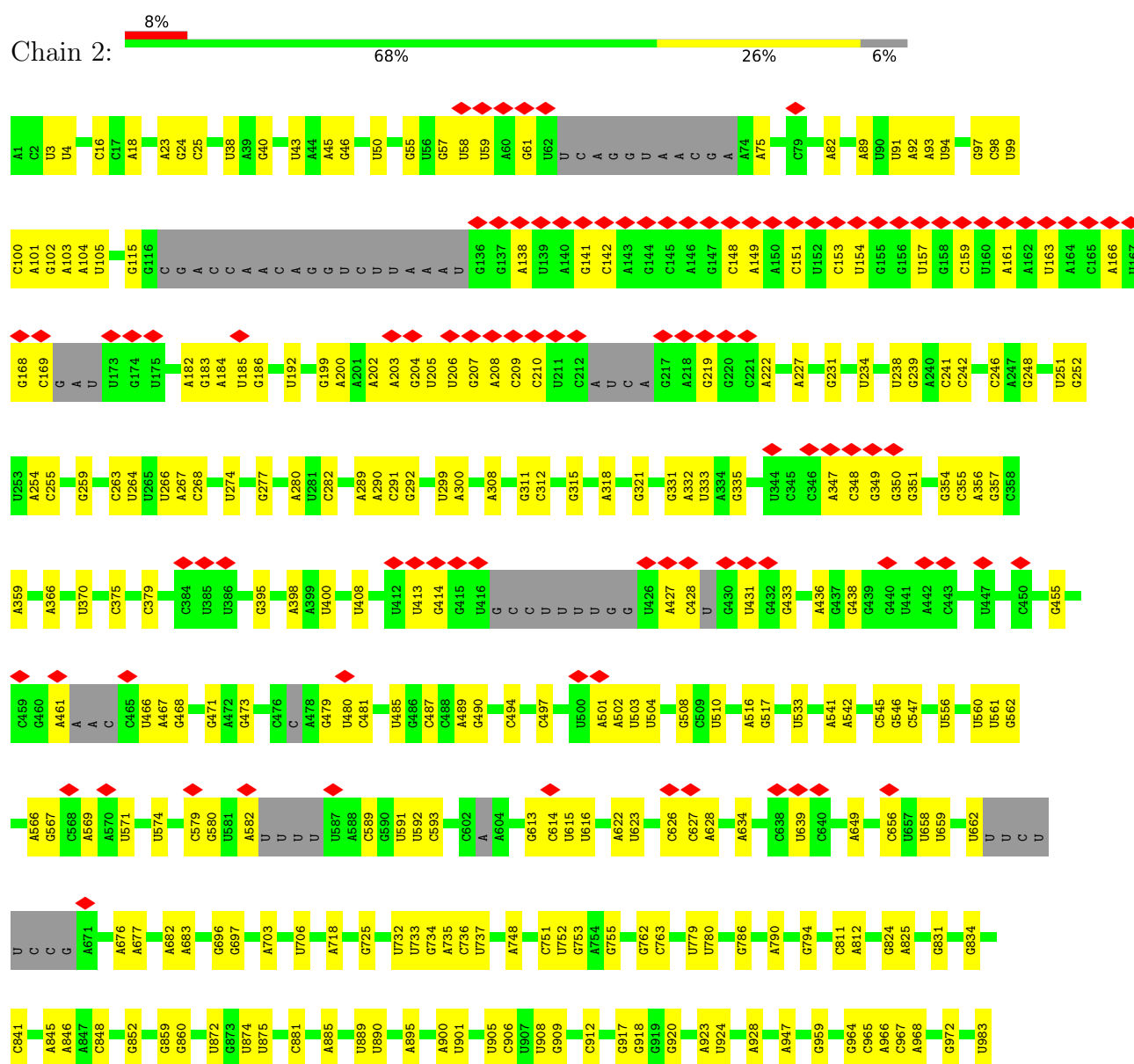
- Molecule 34 is a protein called eL41.

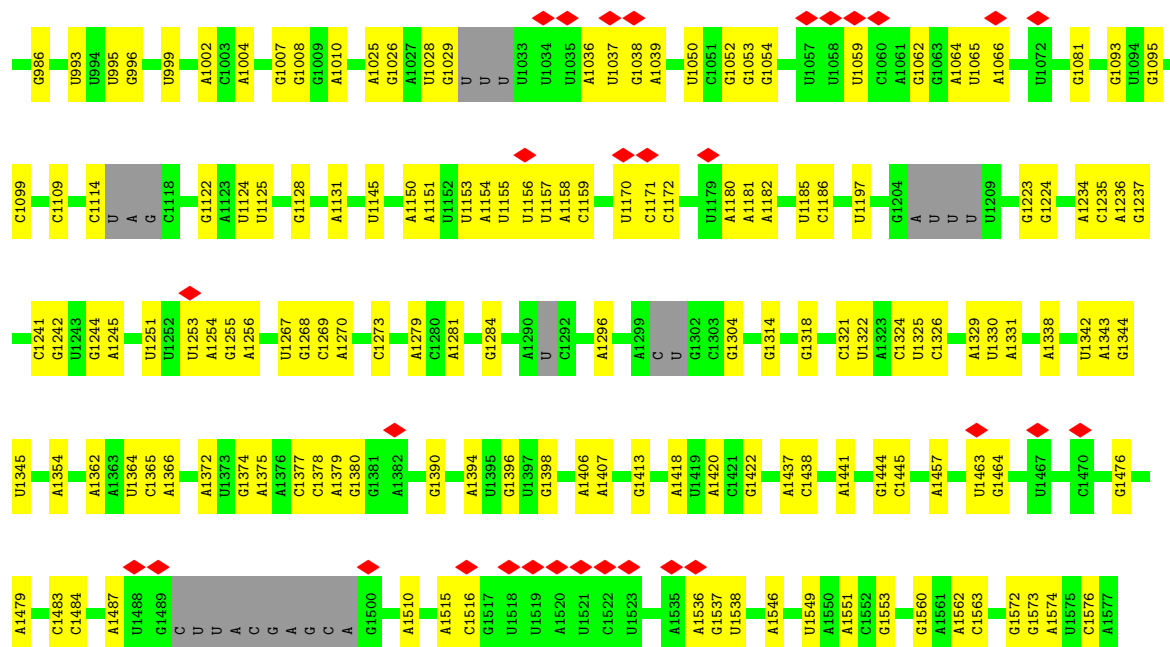
Mol	Chain	Residues	Atoms				AltConf	Trace
34	n	24	Total	C	N	O	0	0
			225	137	62	26		

### 3 Residue-property plots

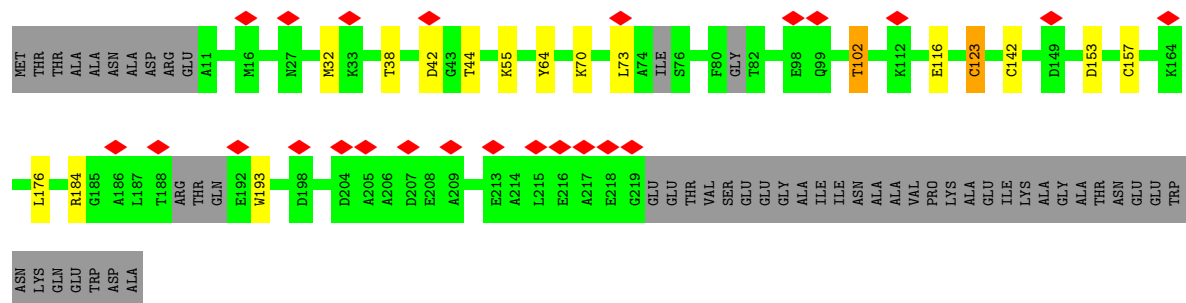
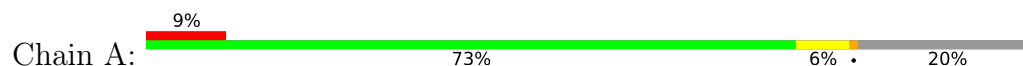
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

#### • Molecule 1: 18S

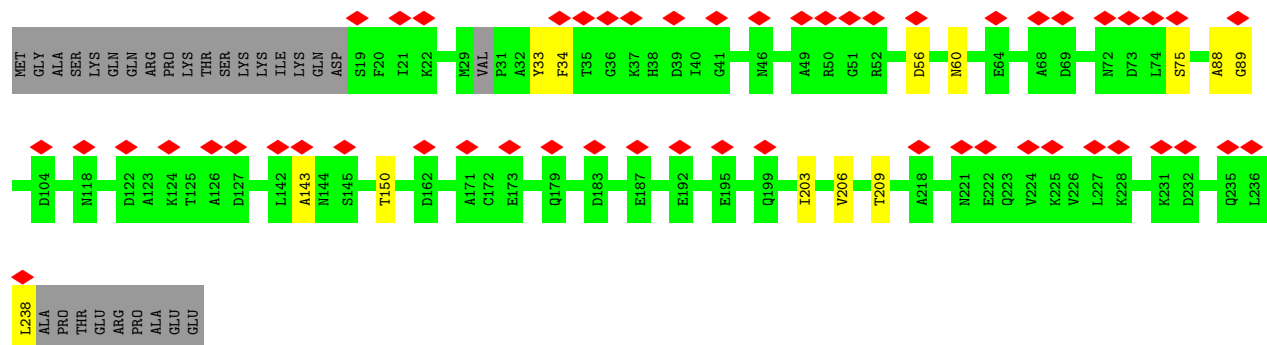
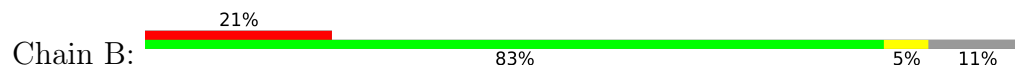





• Molecule 2: 40S ribosomal protein SA

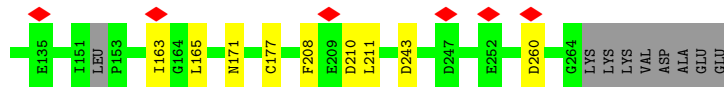
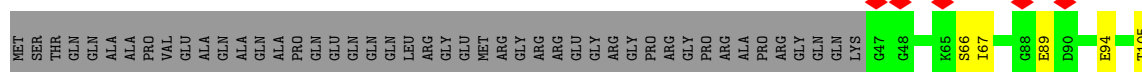


• Molecule 3: Ribosomal protein S3Ae, putative



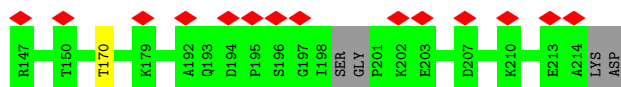
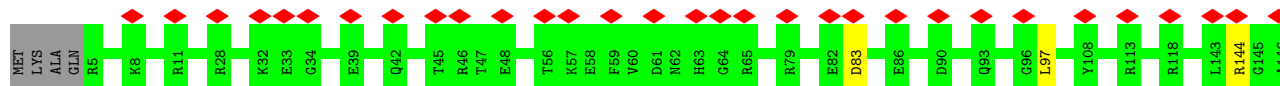
• Molecule 4: Uncharacterized protein

Chain C: 



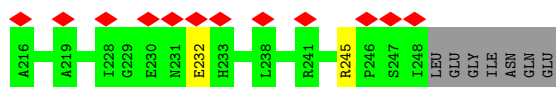
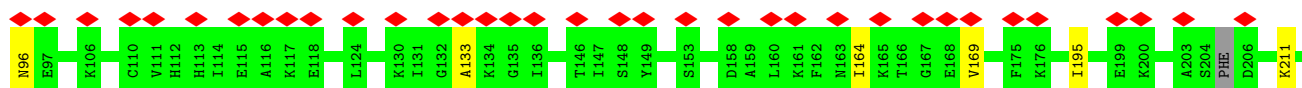
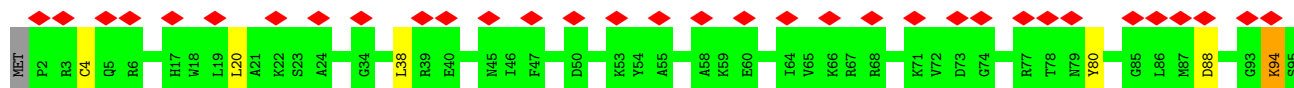
- Molecule 5: Ribosomal protein S3, putative

Chain D: 




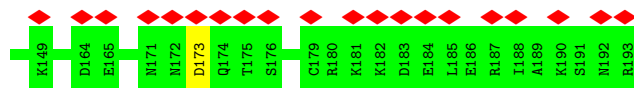
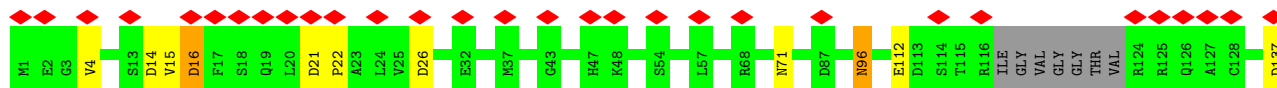
- Molecule 6: 40S ribosomal protein S4

Chain E: 



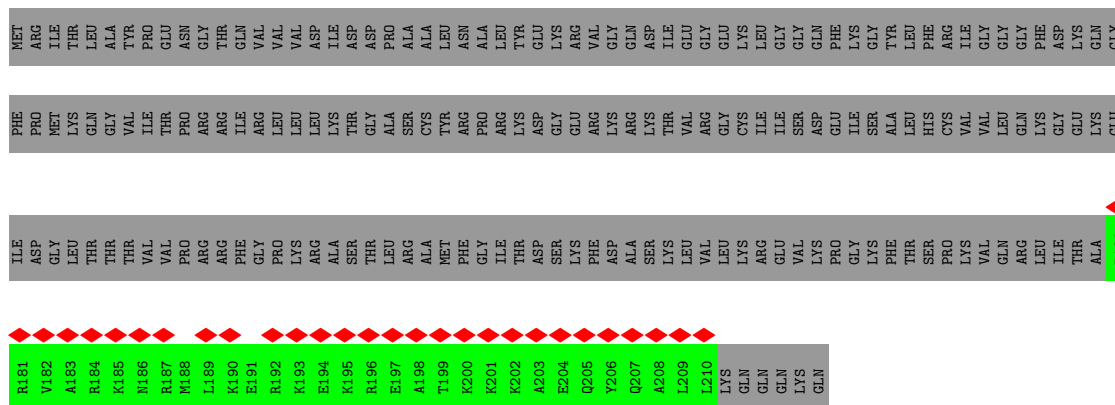
- Molecule 7: 40s ribosomal protein S5-B, putative

Chain F: 

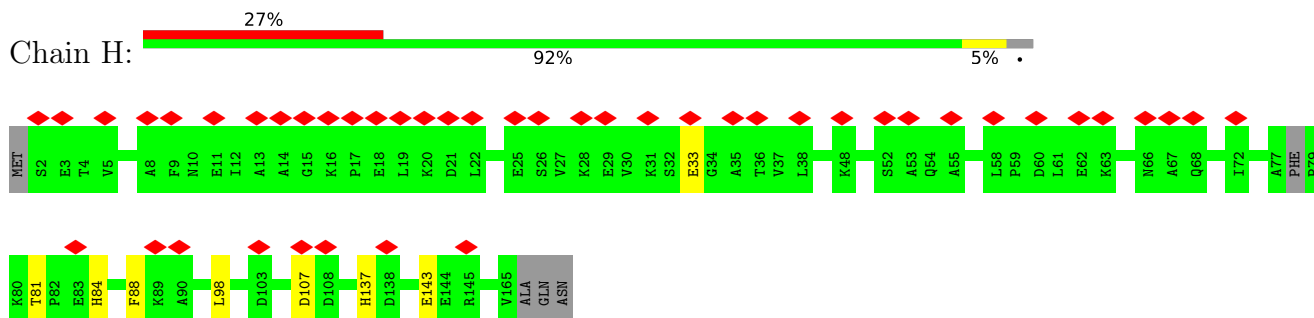


- Molecule 8: 40S ribosomal protein S6

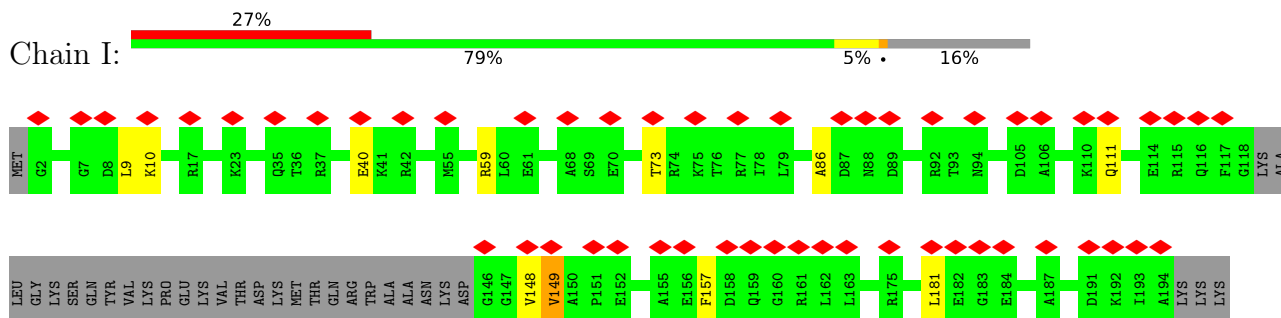
Chain G: 



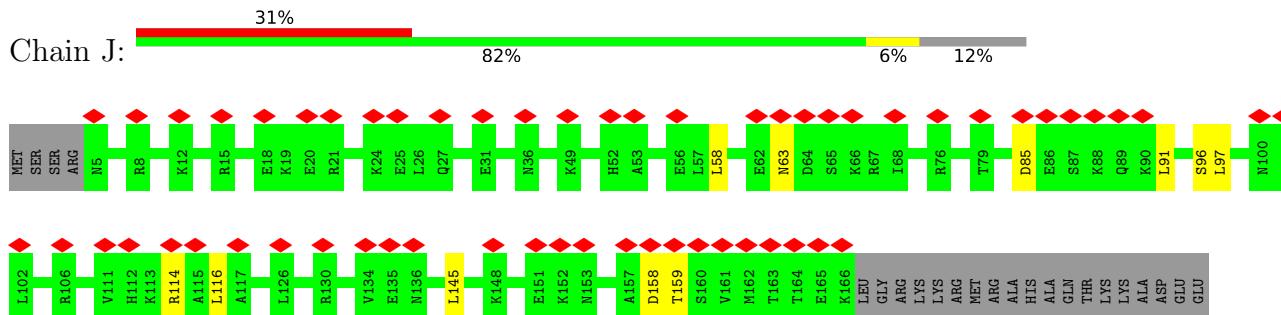
- Molecule 9: 40S ribosomal protein S7, putative



- Molecule 10: 40S ribosomal protein S8

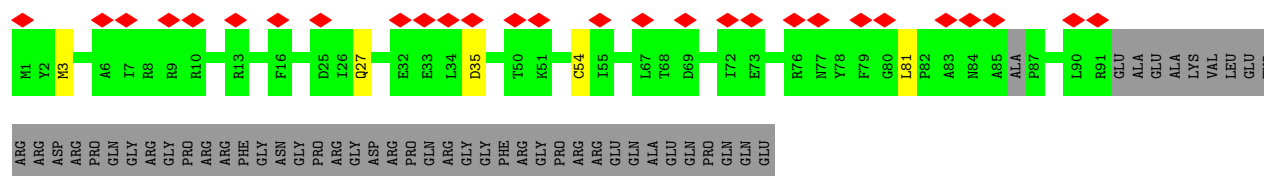


- Molecule 11: Uncharacterized protein

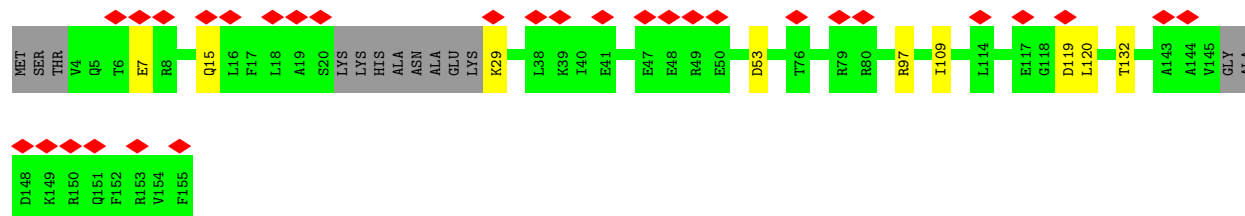
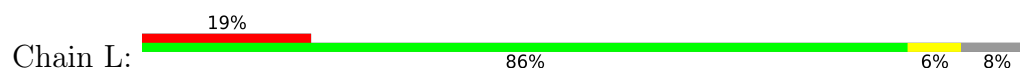


- Molecule 12: Plectin/S10 domain containing protein

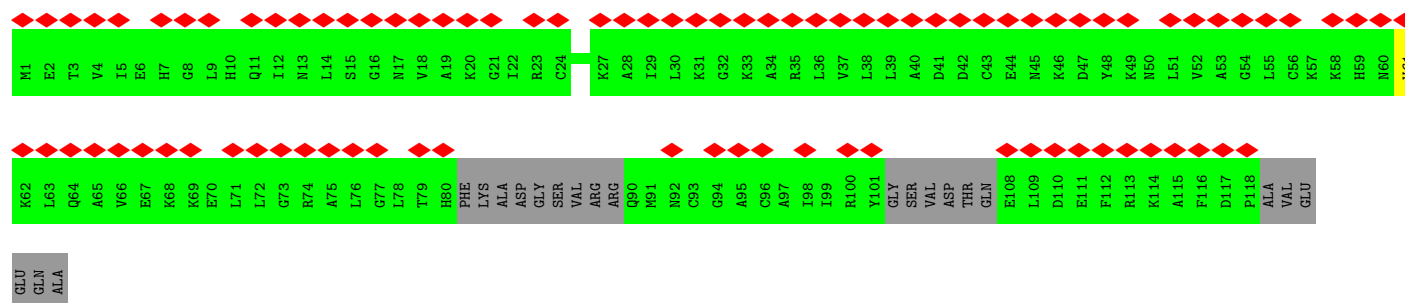
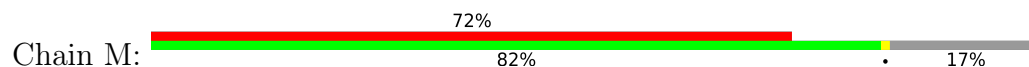




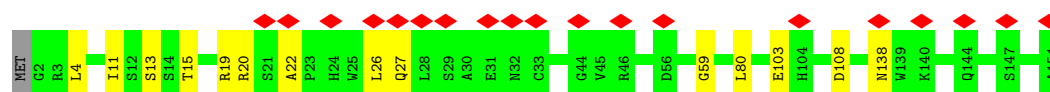
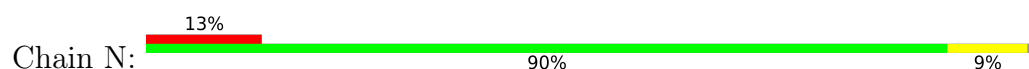
• Molecule 13: Uncharacterized protein



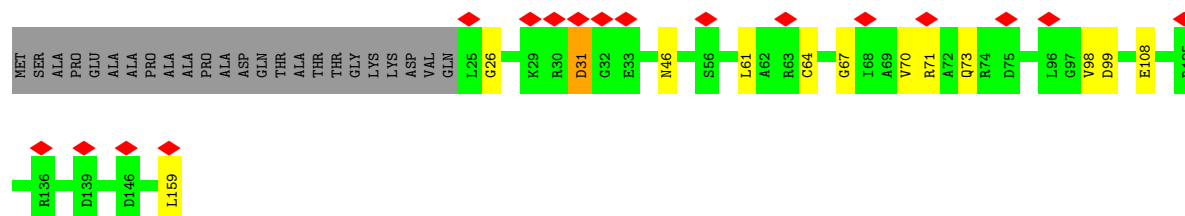
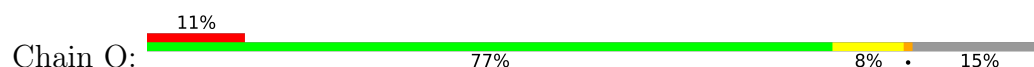
• Molecule 14: Ribosomal protein L7Ae, putative



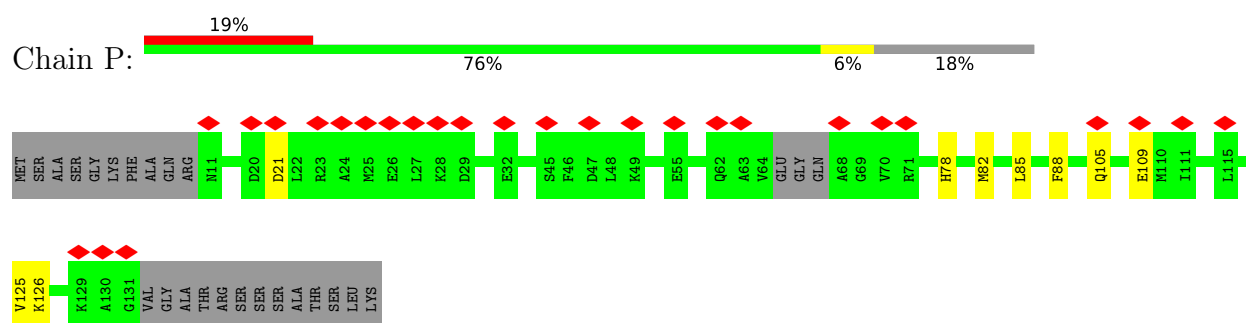
• Molecule 15: 40S ribosomal protein S13, putative



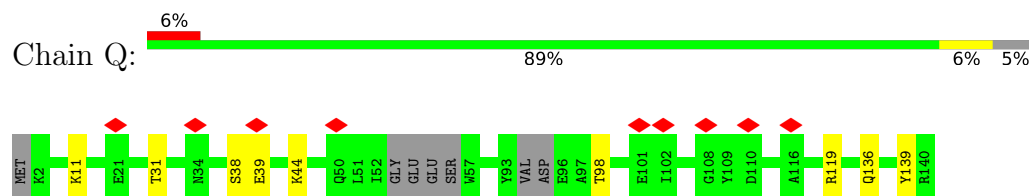
• Molecule 16: Ribosomal protein S14



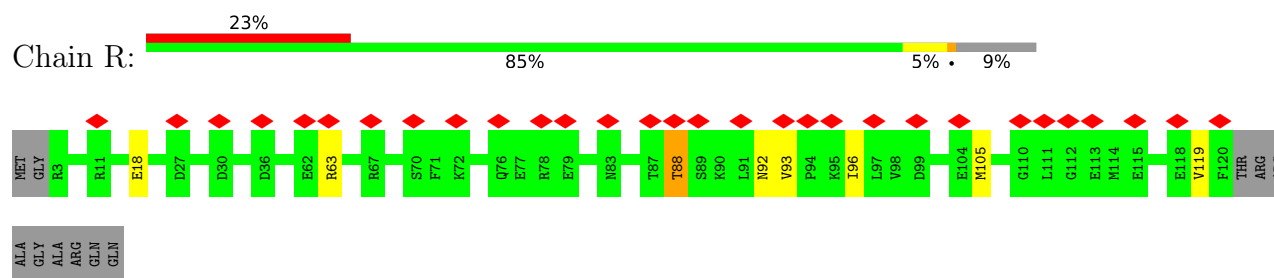
• Molecule 17: Ribosomal protein S19, putative



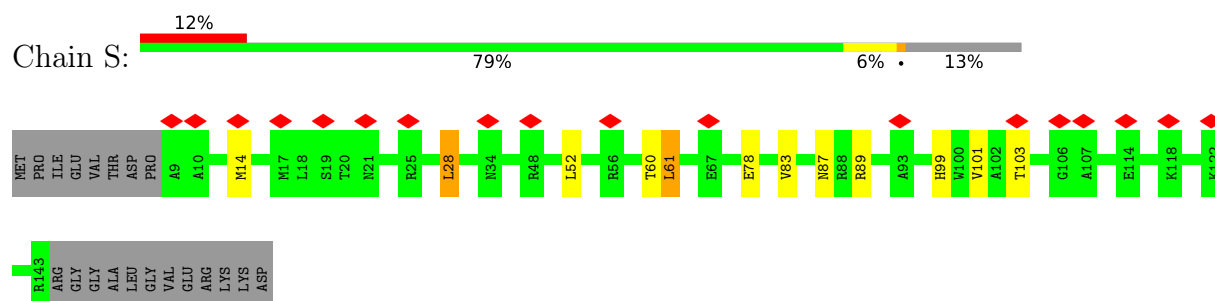
- Molecule 18: 40S ribosomal protein S16, putative



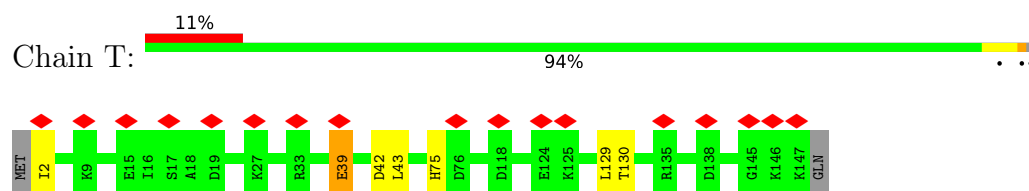
- Molecule 19: 40S ribosomal protein S17-B, putative



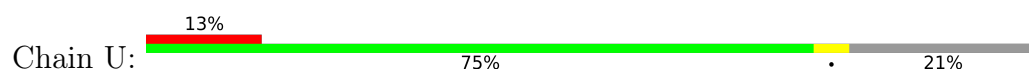
- Molecule 20: Ribosomal protein S13p/S18e, putative

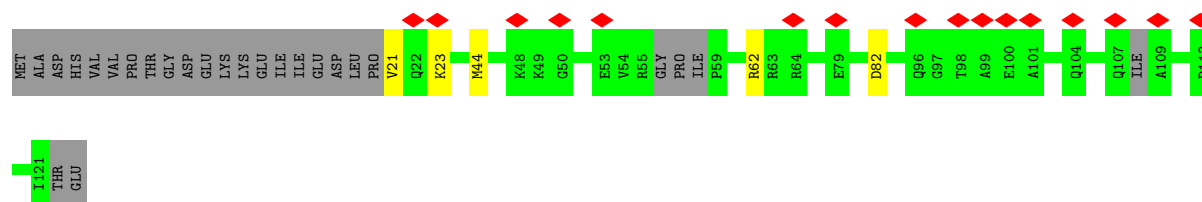


- Molecule 21: Ribosomal protein S19e, putative

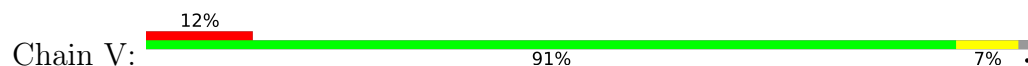


- Molecule 22: Ribosomal protein S10p/S20e, putative

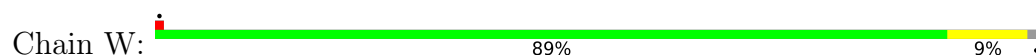




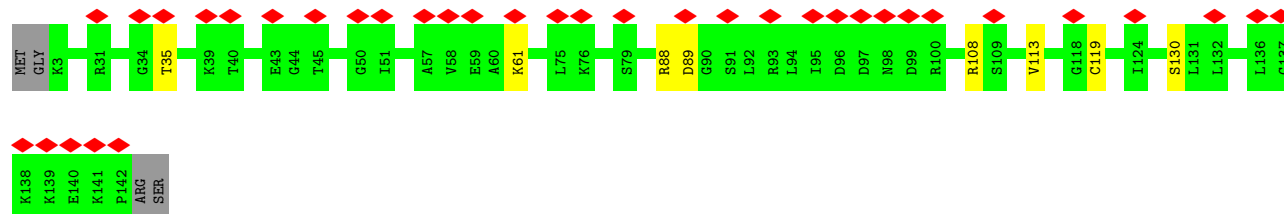
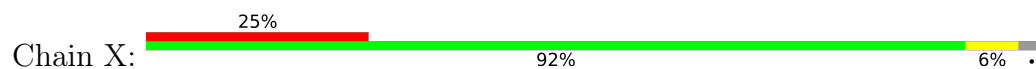
- Molecule 23: 40S ribosomal protein S21



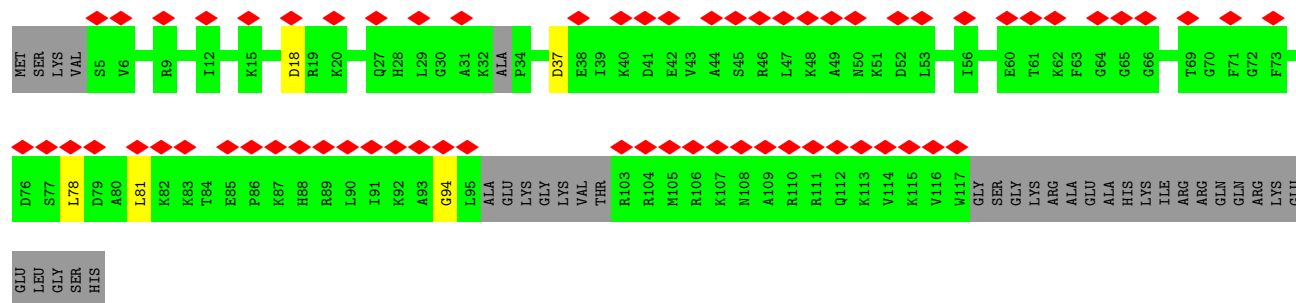
- Molecule 24: Ribosomal protein S15a



- Molecule 25: 40S ribosomal protein S23, putative



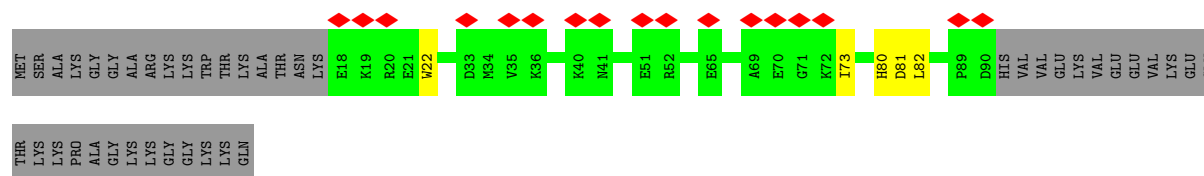
- Molecule 26: Ribosomal protein S24e, putative



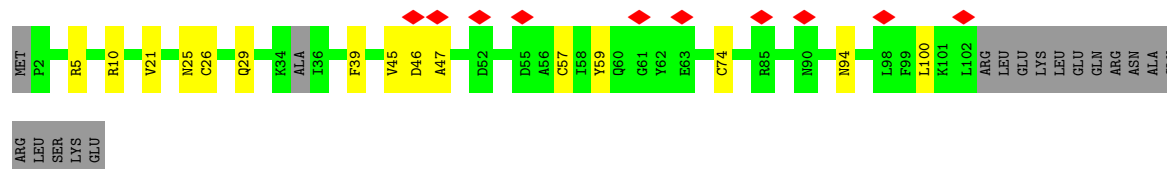
- Molecule 27: Uncharacterized protein



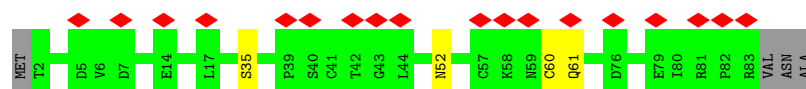
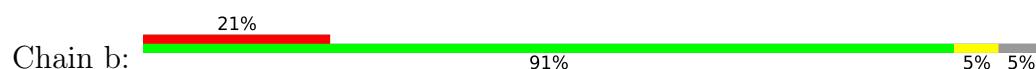




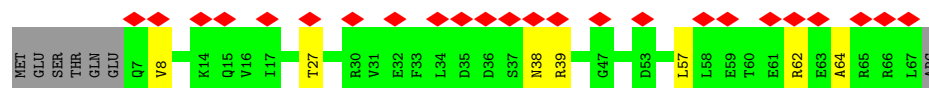
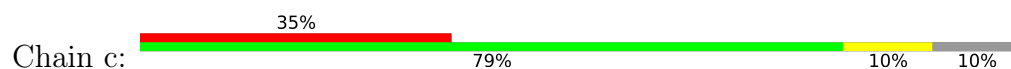
• Molecule 28: 40S ribosomal protein S26



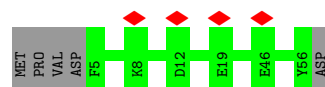
• Molecule 29: 40S ribosomal protein S27



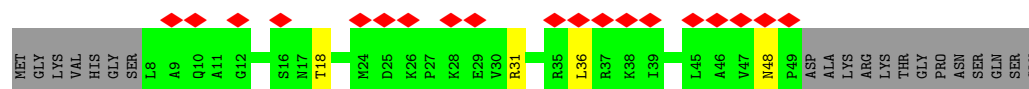
• Molecule 30: Uncharacterized protein



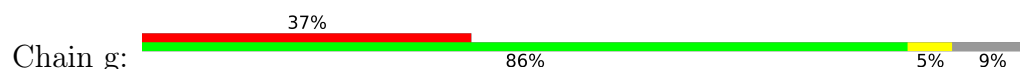
• Molecule 31: 40S ribosomal protein S29, putative

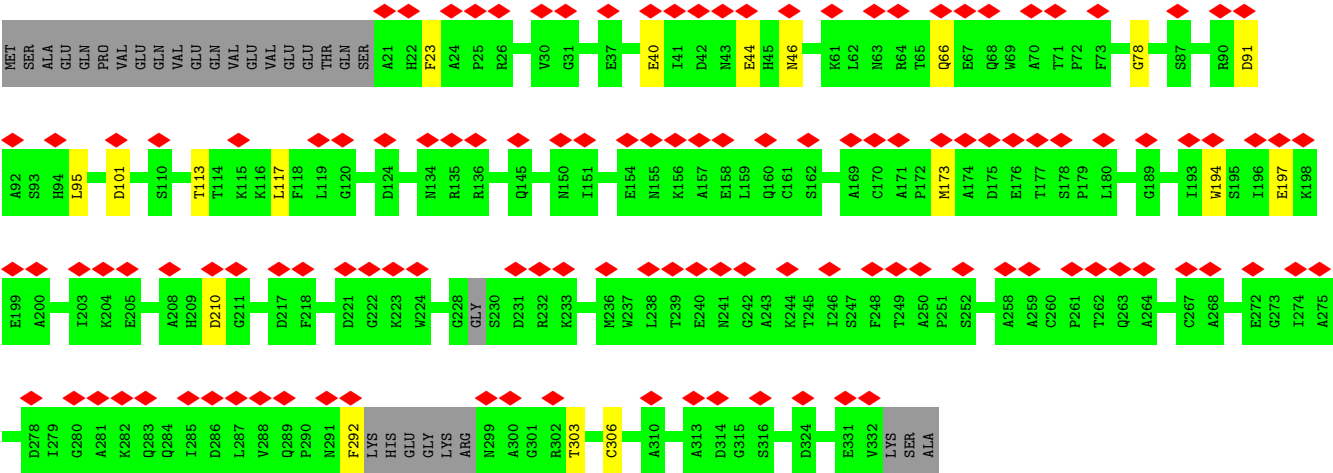


• Molecule 32: 40S ribosomal protein S30

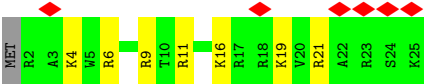


• Molecule 33: Guanine nucleotide-binding protein beta subunit, putative





• Molecule 34: eL41



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	57162	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 ( $e^-/\text{\AA}^2$ )	2	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	0.268	Depositor
Minimum map value	-0.139	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.036	Depositor
Map size ( $\text{\AA}$ )	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.32, 1.32, 1.32	Depositor

## 5 Model quality [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	2	0.22	0/35582	0.68	0/55428
2	A	0.38	0/1634	0.55	0/2210
3	B	0.35	0/1777	0.57	0/2389
4	C	0.39	0/1722	0.57	0/2318
5	D	0.36	0/1675	0.56	0/2242
6	E	0.35	0/1974	0.56	0/2657
7	F	0.38	0/1497	0.64	0/2010
8	G	0.37	0/154	0.40	0/214
9	H	0.38	0/1295	0.56	0/1746
10	I	0.40	0/1322	0.60	0/1778
11	J	0.34	0/1344	0.56	0/1808
12	K	0.43	0/749	0.60	0/1013
13	L	0.34	0/1181	0.57	0/1585
14	M	0.34	0/507	0.60	0/701
15	N	0.40	0/1213	0.62	0/1634
16	O	0.35	0/1017	0.70	0/1366
17	P	0.40	0/983	0.61	0/1320
18	Q	0.39	0/1057	0.62	0/1418
19	R	0.41	0/975	0.60	0/1305
20	S	0.42	0/1093	0.67	0/1467
21	T	0.36	0/1172	0.56	0/1576
22	U	0.37	0/785	0.62	0/1053
23	V	0.43	0/682	0.64	0/924
24	W	0.35	0/1015	0.56	0/1358
25	X	0.36	0/1076	0.61	0/1441
26	Y	0.37	0/802	0.55	0/1073
27	Z	0.36	0/570	0.55	0/770
28	a	0.40	0/829	0.69	0/1110
29	b	0.40	0/645	0.61	0/880
30	c	0.33	0/475	0.61	0/635
31	d	0.39	0/445	0.66	0/588
32	e	0.35	0/341	0.55	0/454
33	g	0.37	0/2440	0.53	0/3324
34	n	0.70	0/226	0.93	0/290

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
All	All	0.31	0/70254	0.64	0/102085

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 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	
2	A	196/256 (77%)	180 (92%)	11 (6%)	5 (3%)	5	28
3	B	215/247 (87%)	195 (91%)	11 (5%)	9 (4%)	3	19
4	C	213/272 (78%)	193 (91%)	15 (7%)	5 (2%)	6	31
5	D	204/216 (94%)	188 (92%)	15 (7%)	1 (0%)	29	63
6	E	242/255 (95%)	210 (87%)	26 (11%)	6 (2%)	5	29
7	F	182/193 (94%)	158 (87%)	16 (9%)	8 (4%)	2	18
8	G	29/216 (13%)	29 (100%)	0	0	100	100
9	H	159/168 (95%)	146 (92%)	10 (6%)	3 (2%)	8	34
10	I	162/197 (82%)	147 (91%)	10 (6%)	5 (3%)	4	25
11	J	160/185 (86%)	138 (86%)	16 (10%)	6 (4%)	3	21
12	K	86/141 (61%)	80 (93%)	6 (7%)	0	100	100
13	L	136/155 (88%)	121 (89%)	14 (10%)	1 (1%)	22	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	M	97/124 (78%)	84 (87%)	12 (12%)	1 (1%)	15	49
15	N	148/151 (98%)	128 (86%)	14 (10%)	6 (4%)	3	19
16	O	133/159 (84%)	104 (78%)	21 (16%)	8 (6%)	1	11
17	P	114/144 (79%)	102 (90%)	10 (9%)	2 (2%)	8	35
18	Q	127/140 (91%)	108 (85%)	14 (11%)	5 (4%)	3	20
19	R	116/129 (90%)	101 (87%)	11 (10%)	4 (3%)	3	23
20	S	133/155 (86%)	119 (90%)	10 (8%)	4 (3%)	4	26
21	T	144/148 (97%)	133 (92%)	9 (6%)	2 (1%)	11	40
22	U	91/123 (74%)	84 (92%)	6 (7%)	1 (1%)	14	46
23	V	85/89 (96%)	73 (86%)	9 (11%)	3 (4%)	3	23
24	W	124/130 (95%)	113 (91%)	10 (8%)	1 (1%)	19	53
25	X	138/144 (96%)	124 (90%)	10 (7%)	4 (3%)	4	26
26	Y	99/140 (71%)	84 (85%)	13 (13%)	2 (2%)	7	33
27	Z	71/115 (62%)	66 (93%)	2 (3%)	3 (4%)	3	19
28	a	96/118 (81%)	84 (88%)	6 (6%)	6 (6%)	1	10
29	b	80/86 (93%)	71 (89%)	6 (8%)	3 (4%)	3	21
30	c	59/68 (87%)	51 (86%)	3 (5%)	5 (8%)	1	5
31	d	50/57 (88%)	48 (96%)	2 (4%)	0	100	100
32	e	40/62 (64%)	38 (95%)	2 (5%)	0	100	100
33	g	299/335 (89%)	263 (88%)	30 (10%)	6 (2%)	7	33
34	n	22/25 (88%)	20 (91%)	2 (9%)	0	100	100
All	All	4250/5143 (83%)	3783 (89%)	352 (8%)	115 (3%)	8	27

All (115) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	42	ASP
3	B	88	ALA
7	F	15	VAL
7	F	26	ASP
10	I	149	VAL
11	J	63	ASN
11	J	158	ASP
11	J	159	THR
14	M	61	VAL

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Mol	Chain	Res	Type
15	N	26	LEU
15	N	27	GLN
16	O	31	ASP
16	O	70	VAL
16	O	98	VAL
16	O	99	ASP
17	P	125	VAL
18	Q	136	GLN
20	S	83	VAL
26	Y	18	ASP
27	Z	81	ASP
28	a	74	CYS
29	b	60	CYS
30	c	39	ARG
30	c	62	ARG
33	g	197	GLU
3	B	60	ASN
3	B	89	GLY
3	B	209	THR
6	E	232	GLU
7	F	16	ASP
9	H	33	GLU
10	I	40	GLU
10	I	148	VAL
11	J	96	SER
15	N	138	ASN
18	Q	139	TYR
19	R	63	ARG
20	S	61	LEU
20	S	89	ARG
25	X	130	SER
26	Y	94	GLY
28	a	46	ASP
28	a	47	ALA
30	c	64	ALA
33	g	113	THR
3	B	33	TYR
3	B	75	SER
3	B	143	ALA
4	C	66	SER
4	C	89	GLU
6	E	80	TYR

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Mol	Chain	Res	Type
9	H	137	HIS
10	I	59	ARG
13	L	53	ASP
16	O	73	GLN
20	S	28	LEU
21	T	39	GLU
21	T	75	HIS
22	U	23	LYS
23	V	4	ASP
23	V	10	ASP
25	X	61	LYS
27	Z	22	TRP
29	b	52	ASN
29	b	61	GLN
33	g	44	GLU
33	g	46	ASN
33	g	66	GLN
2	A	38	THR
2	A	123	CYS
3	B	203	ILE
4	C	163	ILE
4	C	165	LEU
4	C	260	ASP
5	D	144	ARG
6	E	94	LYS
6	E	133	ALA
6	E	245	ARG
9	H	84	HIS
10	I	86	ALA
11	J	97	LEU
11	J	145	LEU
15	N	22	ALA
16	O	71	ARG
17	P	126	LYS
18	Q	11	LYS
18	Q	38	SER
18	Q	39	GLU
19	R	88	THR
28	a	59	TYR
28	a	94	ASN
30	c	38	ASN
2	A	102	THR

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Mol	Chain	Res	Type
2	A	157	CYS
3	B	206	VAL
6	E	195	ILE
7	F	21	ASP
7	F	22	PRO
15	N	108	ASP
19	R	96	ILE
19	R	119	VAL
25	X	88	ARG
7	F	4	VAL
7	F	112	GLU
16	O	26	GLY
25	X	113	VAL
27	Z	73	ILE
28	a	45	VAL
30	c	8	VAL
33	g	78	GLY
7	F	96	ASN
15	N	59	GLY
16	O	67	GLY
24	W	95	PRO
23	V	81	VAL

### 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	
2	A	172/211 (82%)	158 (92%)	14 (8%)	11	38
3	B	192/216 (89%)	188 (98%)	4 (2%)	53	77
4	C	174/216 (81%)	165 (95%)	9 (5%)	23	55
5	D	176/182 (97%)	173 (98%)	3 (2%)	60	80
6	E	209/217 (96%)	200 (96%)	9 (4%)	29	60
7	F	161/165 (98%)	155 (96%)	6 (4%)	34	63
9	H	137/141 (97%)	132 (96%)	5 (4%)	35	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	I	131/158 (83%)	124 (95%)	7 (5%)	22	54
11	J	141/168 (84%)	136 (96%)	5 (4%)	36	66
12	K	77/116 (66%)	72 (94%)	5 (6%)	17	48
13	L	124/137 (90%)	116 (94%)	8 (6%)	17	48
14	M	1/101 (1%)	1 (100%)	0	100	100
15	N	125/126 (99%)	117 (94%)	8 (6%)	17	48
16	O	99/115 (86%)	93 (94%)	6 (6%)	18	50
17	P	105/124 (85%)	98 (93%)	7 (7%)	16	47
18	Q	108/114 (95%)	104 (96%)	4 (4%)	34	63
19	R	104/111 (94%)	99 (95%)	5 (5%)	25	57
20	S	112/128 (88%)	102 (91%)	10 (9%)	9	34
21	T	120/122 (98%)	114 (95%)	6 (5%)	24	56
22	U	87/110 (79%)	83 (95%)	4 (5%)	27	59
23	V	72/74 (97%)	69 (96%)	3 (4%)	30	60
24	W	107/109 (98%)	96 (90%)	11 (10%)	7	27
25	X	112/115 (97%)	108 (96%)	4 (4%)	35	64
26	Y	77/118 (65%)	74 (96%)	3 (4%)	32	62
27	Z	60/93 (64%)	58 (97%)	2 (3%)	38	67
28	a	91/107 (85%)	82 (90%)	9 (10%)	8	29
29	b	76/79 (96%)	75 (99%)	1 (1%)	69	84
30	c	52/59 (88%)	50 (96%)	2 (4%)	33	63
31	d	46/51 (90%)	46 (100%)	0	100	100
32	e	35/51 (69%)	31 (89%)	4 (11%)	5	22
33	g	256/282 (91%)	244 (95%)	12 (5%)	26	58
34	n	22/23 (96%)	15 (68%)	7 (32%)	0	1
All	All	3561/4139 (86%)	3378 (95%)	183 (5%)	27	55

All (183) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	32	MET
2	A	44	THR
2	A	55	LYS

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Mol	Chain	Res	Type
2	A	64	TYR
2	A	70	LYS
2	A	73	LEU
2	A	102	THR
2	A	116	GLU
2	A	123	CYS
2	A	142	CYS
2	A	153	ASP
2	A	176	LEU
2	A	184	ARG
2	A	193	TRP
3	B	34	PHE
3	B	56	ASP
3	B	150	THR
3	B	238	LEU
4	C	67	ILE
4	C	94	GLU
4	C	105	THR
4	C	171	ASN
4	C	177	CYS
4	C	208	PHE
4	C	210	ASP
4	C	211	LEU
4	C	243	ASP
5	D	83	ASP
5	D	97	LEU
5	D	170	THR
6	E	4	CYS
6	E	20	LEU
6	E	38	LEU
6	E	88	ASP
6	E	94	LYS
6	E	96	ASN
6	E	164	ILE
6	E	169	VAL
6	E	211	LYS
7	F	14	ASP
7	F	16	ASP
7	F	71	ASN
7	F	96	ASN
7	F	137	ASP
7	F	173	ASP

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Mol	Chain	Res	Type
9	H	81	THR
9	H	88	PHE
9	H	98	LEU
9	H	107	ASP
9	H	143	GLU
10	I	9	LEU
10	I	10	LYS
10	I	73	THR
10	I	111	GLN
10	I	149	VAL
10	I	157	PHE
10	I	181	LEU
11	J	58	LEU
11	J	85	ASP
11	J	91	LEU
11	J	114	ARG
11	J	116	LEU
12	K	3	MET
12	K	27	GLN
12	K	35	ASP
12	K	54	CYS
12	K	81	LEU
13	L	7	GLU
13	L	15	GLN
13	L	29	LYS
13	L	97	ARG
13	L	109	ILE
13	L	119	ASP
13	L	120	LEU
13	L	132	THR
15	N	4	LEU
15	N	11	ILE
15	N	13	SER
15	N	15	THR
15	N	19	ARG
15	N	20	ARG
15	N	80	LEU
15	N	103	GLU
16	O	31	ASP
16	O	46	ASN
16	O	61	LEU
16	O	64	CYS

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Mol	Chain	Res	Type
16	O	108	GLU
16	O	159	LEU
17	P	21	ASP
17	P	78	HIS
17	P	82	MET
17	P	85	LEU
17	P	88	PHE
17	P	105	GLN
17	P	109	GLU
18	Q	31	THR
18	Q	44	LYS
18	Q	98	THR
18	Q	119	ARG
19	R	18	GLU
19	R	88	THR
19	R	92	ASN
19	R	93	VAL
19	R	105	MET
20	S	14	MET
20	S	28	LEU
20	S	52	LEU
20	S	60	THR
20	S	61	LEU
20	S	78	GLU
20	S	87	ASN
20	S	99	HIS
20	S	101	VAL
20	S	103	THR
21	T	2	ILE
21	T	39	GLU
21	T	42	ASP
21	T	43	LEU
21	T	129	LEU
21	T	130	THR
22	U	21	VAL
22	U	44	MET
22	U	62	ARG
22	U	82	ASP
23	V	12	LEU
23	V	42	ASP
23	V	48	GLU
24	W	3	ARG

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Mol	Chain	Res	Type
24	W	7	LEU
24	W	24	GLN
24	W	31	SER
24	W	66	LEU
24	W	71	LYS
24	W	76	CYS
24	W	85	ASP
24	W	87	GLU
24	W	94	LEU
24	W	104	LEU
25	X	35	THR
25	X	89	ASP
25	X	108	ARG
25	X	119	CYS
26	Y	37	ASP
26	Y	78	LEU
26	Y	81	LEU
27	Z	80	HIS
27	Z	82	LEU
28	a	5	ARG
28	a	10	ARG
28	a	21	VAL
28	a	25	ASN
28	a	26	CYS
28	a	29	GLN
28	a	39	PHE
28	a	57	CYS
28	a	100	LEU
29	b	35	SER
30	c	27	THR
30	c	57	LEU
32	e	18	THR
32	e	31	ARG
32	e	36	LEU
32	e	48	ASN
33	g	23	PHE
33	g	40	GLU
33	g	91	ASP
33	g	95	LEU
33	g	101	ASP
33	g	117	LEU
33	g	173	MET

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Mol	Chain	Res	Type
33	g	194	TRP
33	g	210	ASP
33	g	292	PHE
33	g	303	THR
33	g	306	CYS
34	n	4	LYS
34	n	6	ARG
34	n	9	ARG
34	n	11	ARG
34	n	16	LYS
34	n	19	LYS
34	n	21	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	99	GLN
2	A	167	ASN
3	B	27	HIS
3	B	76	HIS
3	B	103	HIS
3	B	149	HIS
4	C	167	HIS
4	C	224	ASN
6	E	96	ASN
6	E	201	GLN
7	F	157	ASN
7	F	174	GLN
9	H	84	HIS
10	I	11	HIS
10	I	18	GLN
10	I	116	GLN
11	J	89	GLN
11	J	112	HIS
11	J	121	HIS
11	J	131	HIS
11	J	141	GLN
11	J	153	ASN
12	K	27	GLN
12	K	84	ASN
13	L	13	GLN
16	O	46	ASN

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Mol	Chain	Res	Type
17	P	50	HIS
17	P	91	ASN
18	Q	80	GLN
18	Q	91	GLN
20	S	79	HIS
21	T	32	ASN
21	T	70	GLN
24	W	56	HIS
24	W	98	GLN
26	Y	14	ASN
26	Y	28	HIS
27	Z	30	GLN
27	Z	78	ASN
27	Z	80	HIS
28	a	7	ASN
29	b	50	HIS
30	c	28	GLN
31	d	38	ASN
33	g	32	HIS
33	g	46	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1472/1577 (93%)	406 (27%)	47 (3%)

All (406) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	3	U
1	2	4	U
1	2	16	C
1	2	18	A
1	2	24	G
1	2	25	C
1	2	38	U
1	2	40	G
1	2	43	U
1	2	45	A
1	2	46	G
1	2	50	U

*Continued on next page...*



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Mol	Chain	Res	Type
1	2	55	G
1	2	57	G
1	2	58	U
1	2	59	U
1	2	61	G
1	2	75	A
1	2	82	A
1	2	89	A
1	2	91	U
1	2	93	A
1	2	94	U
1	2	97	G
1	2	98	C
1	2	99	U
1	2	100	C
1	2	101	A
1	2	102	G
1	2	103	A
1	2	104	A
1	2	105	U
1	2	115	G
1	2	138	A
1	2	141	G
1	2	142	C
1	2	148	C
1	2	149	A
1	2	151	C
1	2	153	C
1	2	154	U
1	2	157	U
1	2	159	C
1	2	161	A
1	2	163	U
1	2	166	A
1	2	168	G
1	2	169	C
1	2	182	A
1	2	184	A
1	2	185	U
1	2	186	G
1	2	192	U
1	2	199	G

*Continued on next page...*

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Mol	Chain	Res	Type
1	2	200	A
1	2	202	A
1	2	203	A
1	2	204	G
1	2	205	U
1	2	206	U
1	2	207	G
1	2	208	A
1	2	209	C
1	2	210	C
1	2	219	G
1	2	222	A
1	2	227	A
1	2	231	G
1	2	234	U
1	2	239	G
1	2	241	C
1	2	242	C
1	2	246	C
1	2	248	G
1	2	251	U
1	2	252	G
1	2	254	A
1	2	255	C
1	2	259	G
1	2	263	C
1	2	264	U
1	2	266	U
1	2	267	A
1	2	268	C
1	2	274	U
1	2	277	G
1	2	280	A
1	2	282	C
1	2	289	A
1	2	290	A
1	2	291	C
1	2	292	G
1	2	299	U
1	2	300	A
1	2	308	A
1	2	311	G

*Continued on next page...*

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Mol	Chain	Res	Type
1	2	312	C
1	2	315	G
1	2	318	A
1	2	321	G
1	2	331	G
1	2	332	A
1	2	333	U
1	2	335	G
1	2	347	A
1	2	349	G
1	2	350	G
1	2	351	G
1	2	354	G
1	2	355	C
1	2	356	A
1	2	357	G
1	2	359	A
1	2	366	A
1	2	370	U
1	2	375	C
1	2	379	C
1	2	395	G
1	2	398	A
1	2	400	U
1	2	408	U
1	2	413	U
1	2	414	G
1	2	427	A
1	2	428	C
1	2	431	U
1	2	433	G
1	2	436	A
1	2	438	G
1	2	455	G
1	2	461	A
1	2	466	U
1	2	467	A
1	2	468	G
1	2	471	G
1	2	473	G
1	2	479	G
1	2	480	U

*Continued on next page...*

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Mol	Chain	Res	Type
1	2	481	C
1	2	485	U
1	2	487	C
1	2	489	A
1	2	490	G
1	2	494	C
1	2	497	C
1	2	501	A
1	2	502	A
1	2	503	U
1	2	504	U
1	2	508	G
1	2	510	U
1	2	516	A
1	2	517	G
1	2	533	U
1	2	541	A
1	2	542	A
1	2	545	C
1	2	546	G
1	2	547	C
1	2	556	U
1	2	561	U
1	2	562	G
1	2	566	A
1	2	567	G
1	2	569	A
1	2	571	U
1	2	574	U
1	2	579	C
1	2	580	G
1	2	582	A
1	2	589	C
1	2	591	U
1	2	592	U
1	2	593	C
1	2	613	G
1	2	614	C
1	2	615	U
1	2	616	U
1	2	622	A
1	2	623	U

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Mol	Chain	Res	Type
1	2	626	C
1	2	627	C
1	2	628	A
1	2	634	A
1	2	639	U
1	2	649	A
1	2	656	C
1	2	658	U
1	2	659	U
1	2	662	U
1	2	676	A
1	2	677	A
1	2	682	A
1	2	683	A
1	2	696	G
1	2	697	G
1	2	703	A
1	2	706	U
1	2	718	A
1	2	725	G
1	2	732	U
1	2	733	U
1	2	734	G
1	2	735	A
1	2	736	C
1	2	737	U
1	2	748	A
1	2	751	C
1	2	752	U
1	2	753	G
1	2	755	G
1	2	762	G
1	2	763	C
1	2	779	U
1	2	780	U
1	2	786	G
1	2	790	A
1	2	794	G
1	2	811	C
1	2	812	A
1	2	824	G
1	2	825	A

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Mol	Chain	Res	Type
1	2	831	G
1	2	834	G
1	2	841	C
1	2	845	A
1	2	846	A
1	2	848	C
1	2	852	G
1	2	859	G
1	2	860	G
1	2	872	U
1	2	874	U
1	2	875	U
1	2	881	C
1	2	885	A
1	2	889	U
1	2	890	U
1	2	895	A
1	2	900	A
1	2	901	U
1	2	905	U
1	2	906	C
1	2	908	U
1	2	909	G
1	2	912	C
1	2	917	G
1	2	918	G
1	2	920	G
1	2	923	A
1	2	924	U
1	2	928	A
1	2	947	A
1	2	959	G
1	2	964	G
1	2	965	C
1	2	967	C
1	2	968	A
1	2	972	G
1	2	983	U
1	2	986	G
1	2	993	U
1	2	995	U
1	2	996	G

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Mol	Chain	Res	Type
1	2	999	U
1	2	1002	A
1	2	1004	A
1	2	1007	G
1	2	1008	G
1	2	1010	A
1	2	1025	A
1	2	1026	G
1	2	1028	U
1	2	1029	G
1	2	1036	A
1	2	1037	U
1	2	1038	G
1	2	1039	A
1	2	1050	U
1	2	1052	G
1	2	1053	G
1	2	1054	G
1	2	1059	U
1	2	1062	G
1	2	1064	A
1	2	1065	U
1	2	1066	A
1	2	1081	G
1	2	1093	G
1	2	1095	G
1	2	1099	C
1	2	1109	C
1	2	1114	C
1	2	1122	G
1	2	1124	U
1	2	1125	U
1	2	1128	G
1	2	1131	A
1	2	1145	U
1	2	1150	A
1	2	1151	A
1	2	1153	U
1	2	1154	A
1	2	1155	U
1	2	1156	U
1	2	1157	U

*Continued on next page...*

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Mol	Chain	Res	Type
1	2	1158	A
1	2	1159	C
1	2	1170	U
1	2	1171	C
1	2	1172	C
1	2	1180	A
1	2	1181	A
1	2	1182	A
1	2	1185	U
1	2	1186	C
1	2	1197	U
1	2	1223	G
1	2	1224	G
1	2	1234	A
1	2	1235	C
1	2	1236	A
1	2	1237	G
1	2	1241	C
1	2	1242	G
1	2	1244	G
1	2	1245	A
1	2	1251	U
1	2	1253	U
1	2	1254	A
1	2	1255	G
1	2	1256	A
1	2	1267	U
1	2	1268	G
1	2	1269	C
1	2	1270	A
1	2	1273	C
1	2	1279	A
1	2	1281	A
1	2	1284	G
1	2	1296	A
1	2	1304	G
1	2	1314	G
1	2	1318	G
1	2	1321	C
1	2	1322	U
1	2	1324	C
1	2	1325	U

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Mol	Chain	Res	Type
1	2	1326	C
1	2	1329	A
1	2	1330	U
1	2	1331	A
1	2	1338	A
1	2	1343	A
1	2	1344	G
1	2	1345	U
1	2	1354	A
1	2	1362	A
1	2	1364	U
1	2	1365	C
1	2	1366	A
1	2	1372	A
1	2	1374	G
1	2	1375	A
1	2	1377	C
1	2	1378	C
1	2	1379	A
1	2	1380	G
1	2	1390	G
1	2	1394	A
1	2	1396	G
1	2	1398	G
1	2	1407	A
1	2	1413	G
1	2	1418	A
1	2	1420	A
1	2	1422	G
1	2	1437	A
1	2	1438	C
1	2	1441	A
1	2	1444	G
1	2	1445	C
1	2	1457	A
1	2	1463	U
1	2	1464	G
1	2	1476	G
1	2	1479	A
1	2	1483	C
1	2	1484	C
1	2	1487	A

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Mol	Chain	Res	Type
1	2	1510	A
1	2	1516	C
1	2	1536	A
1	2	1537	G
1	2	1538	U
1	2	1546	A
1	2	1549	U
1	2	1551	A
1	2	1553	G
1	2	1560	G
1	2	1562	A
1	2	1563	C
1	2	1572	G
1	2	1573	G
1	2	1574	A
1	2	1576	C

All (47) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	23	A
1	2	24	G
1	2	57	G
1	2	92	A
1	2	94	U
1	2	97	G
1	2	98	C
1	2	101	A
1	2	102	G
1	2	103	A
1	2	183	G
1	2	203	A
1	2	208	A
1	2	238	U
1	2	251	U
1	2	299	U
1	2	311	G
1	2	331	G
1	2	348	C
1	2	427	A
1	2	466	U
1	2	480	U

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Mol	Chain	Res	Type
1	2	560	U
1	2	627	C
1	2	676	A
1	2	779	U
1	2	848	C
1	2	908	U
1	2	917	G
1	2	966	A
1	2	1026	G
1	2	1052	G
1	2	1059	U
1	2	1150	A
1	2	1153	U
1	2	1154	A
1	2	1235	C
1	2	1244	G
1	2	1254	A
1	2	1325	U
1	2	1342	U
1	2	1364	U
1	2	1374	G
1	2	1378	C
1	2	1379	A
1	2	1406	A
1	2	1515	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

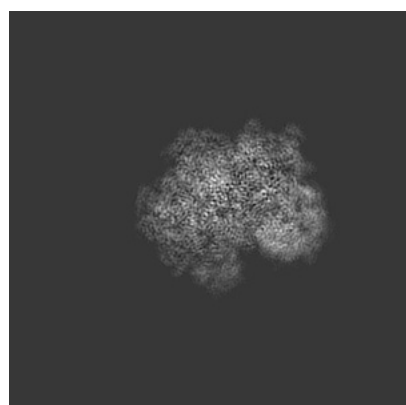
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6788. These allow visual inspection of the internal detail of the map and identification of artifacts.

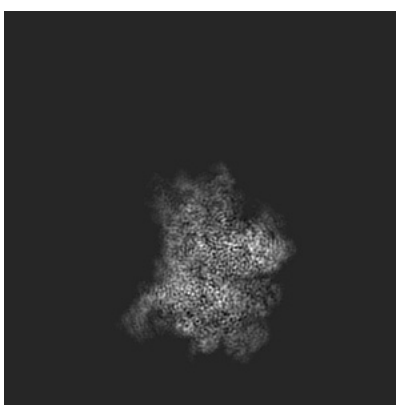
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

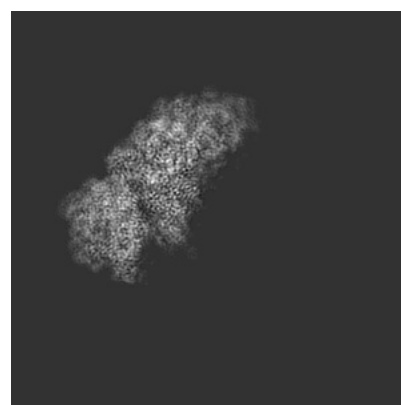
#### 6.1.1 Primary map



X



Y

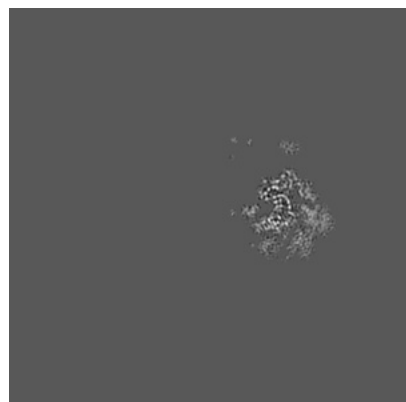


Z

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

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

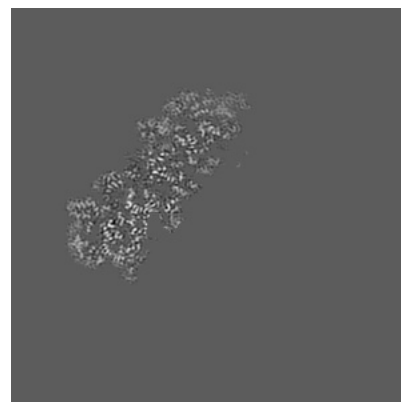
#### 6.2.1 Primary map



X Index: 160



Y Index: 160

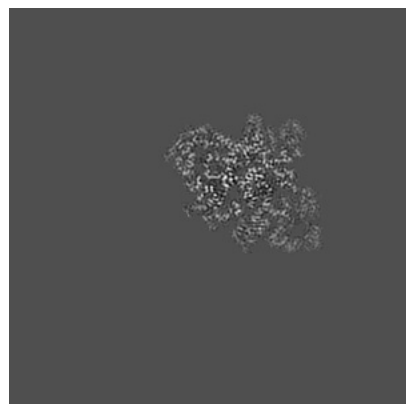


Z Index: 160

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

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

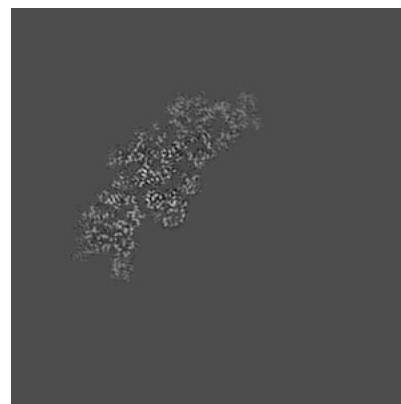
### 6.3.1 Primary map



X Index: 128



Y Index: 167



Z Index: 173

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

## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.036. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

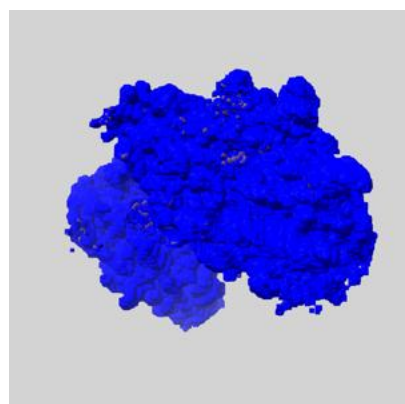
## 6.5 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

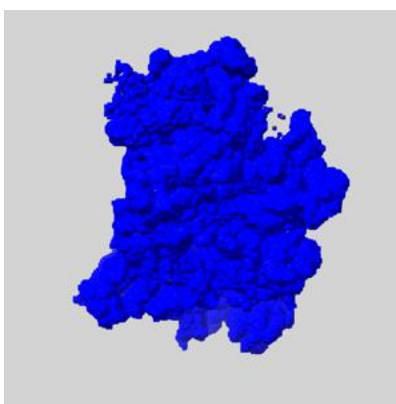
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

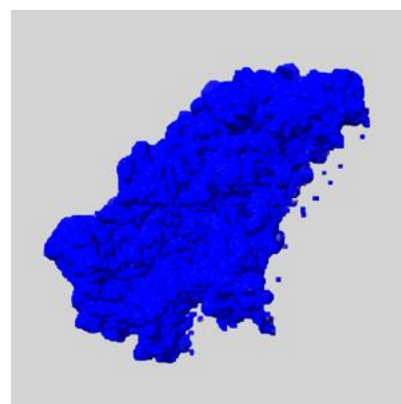
### 6.5.1 emd\_6788\_msk\_1.map [i](#)



X



Y

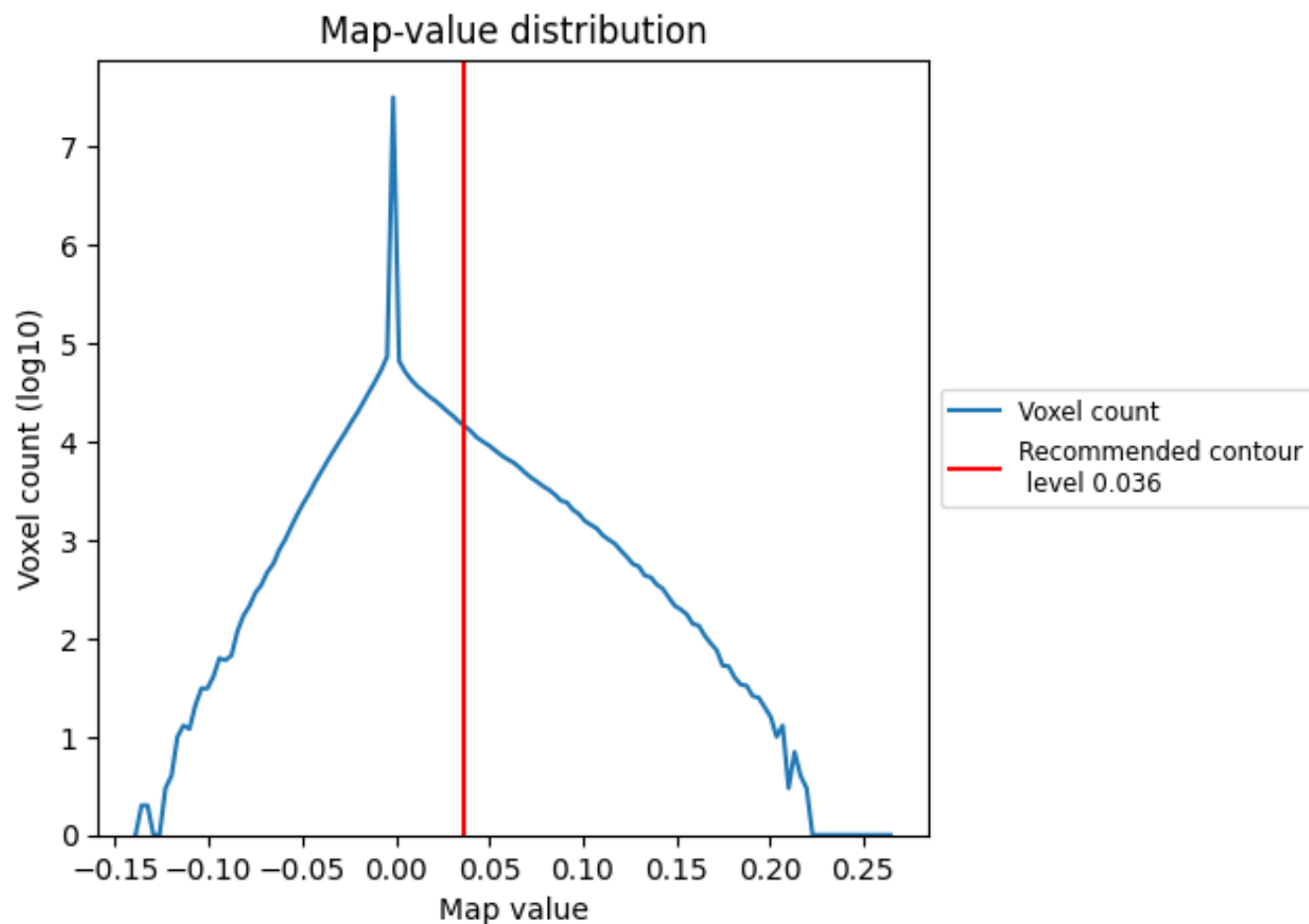


Z

## 7 Map analysis [i](#)

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

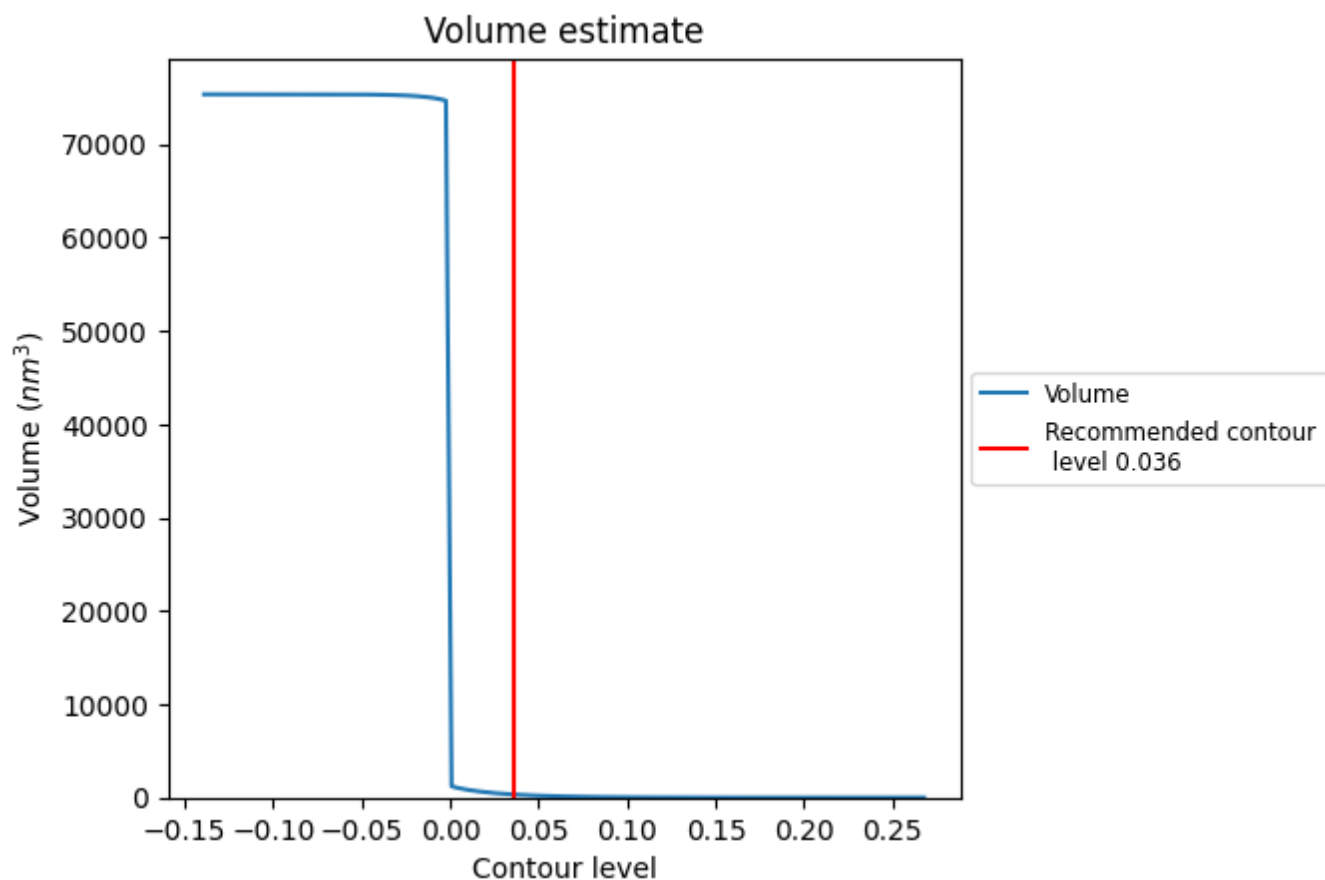
### 7.1 Map-value distribution [i](#)



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.



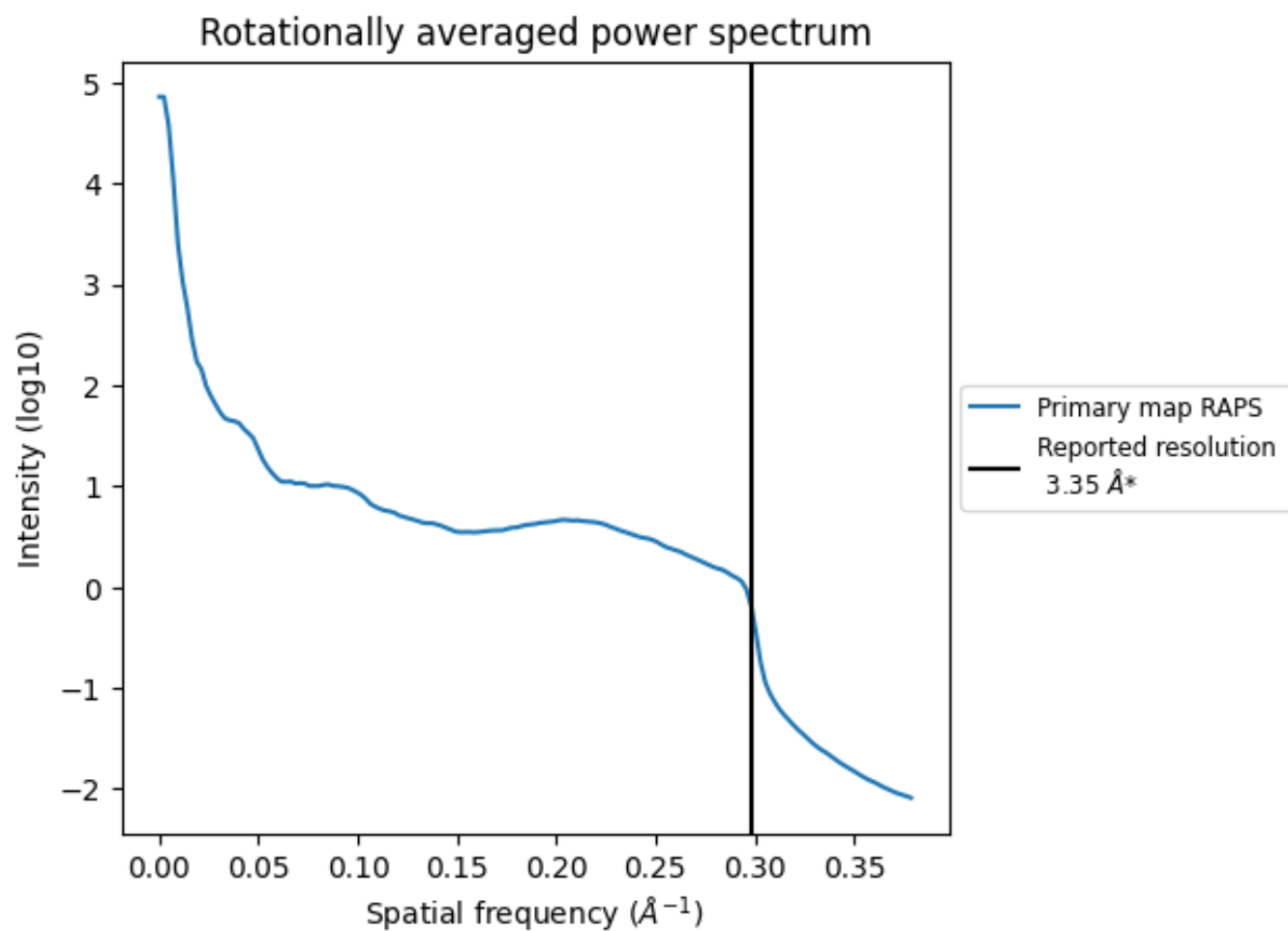
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 325  $\text{nm}^3$ ; this corresponds to an approximate mass of 294 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 ⓘ

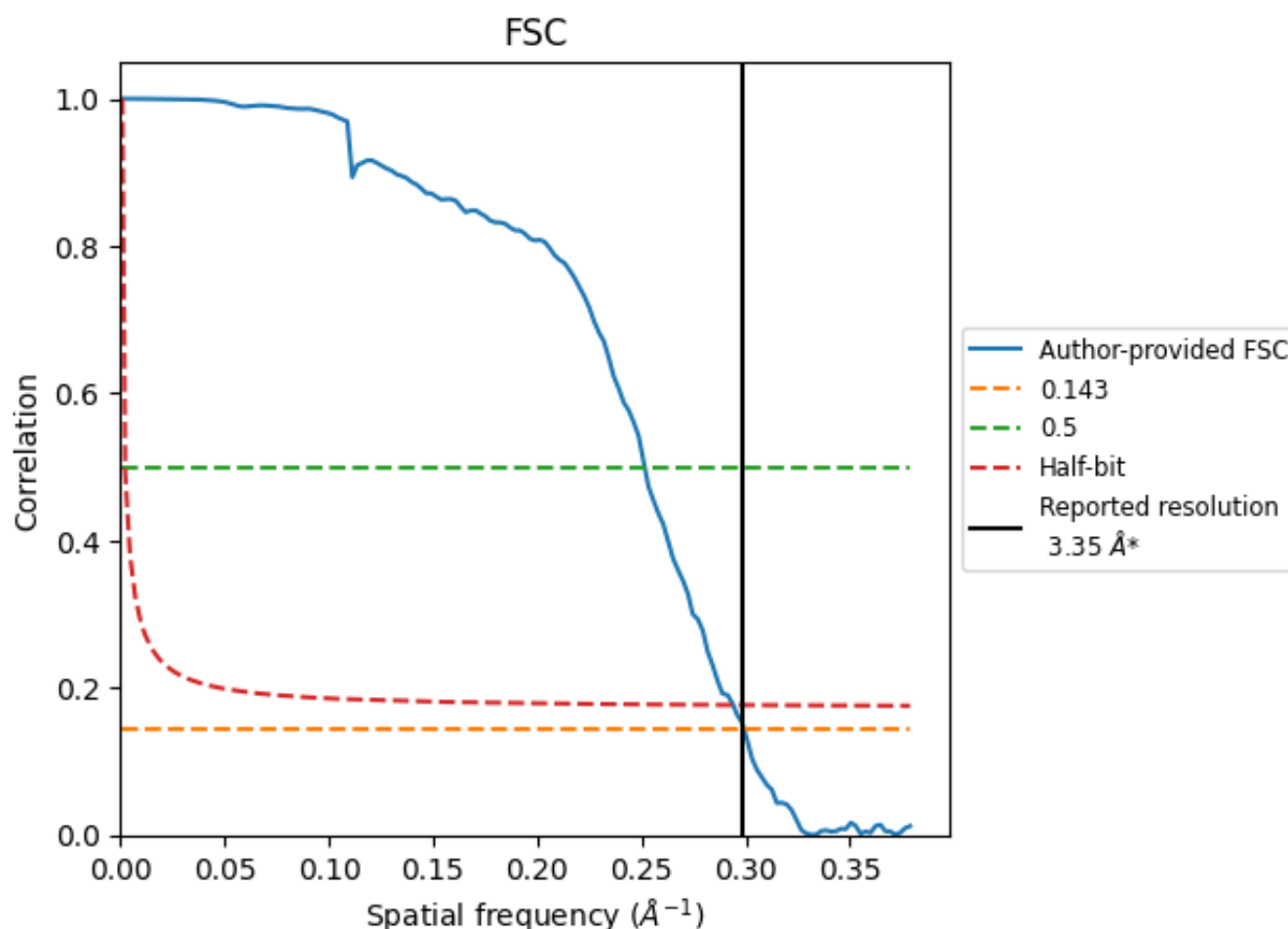


\*Reported resolution corresponds to spatial frequency of 0.299 Å<sup>-1</sup>

## 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 0.299 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

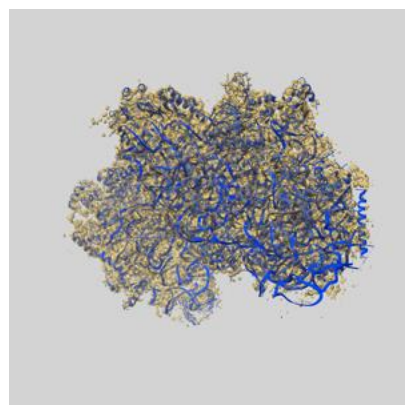
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.35	-	-
Author-provided FSC curve	3.34	3.98	3.40
Unmasked-calculated*	-	-	-

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

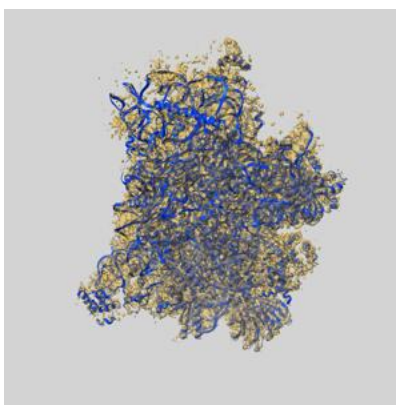
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6788 and PDB model 5XYI. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

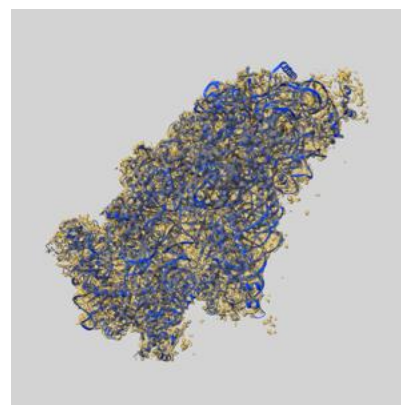
### 9.1 Map-model overlay [i](#)



X



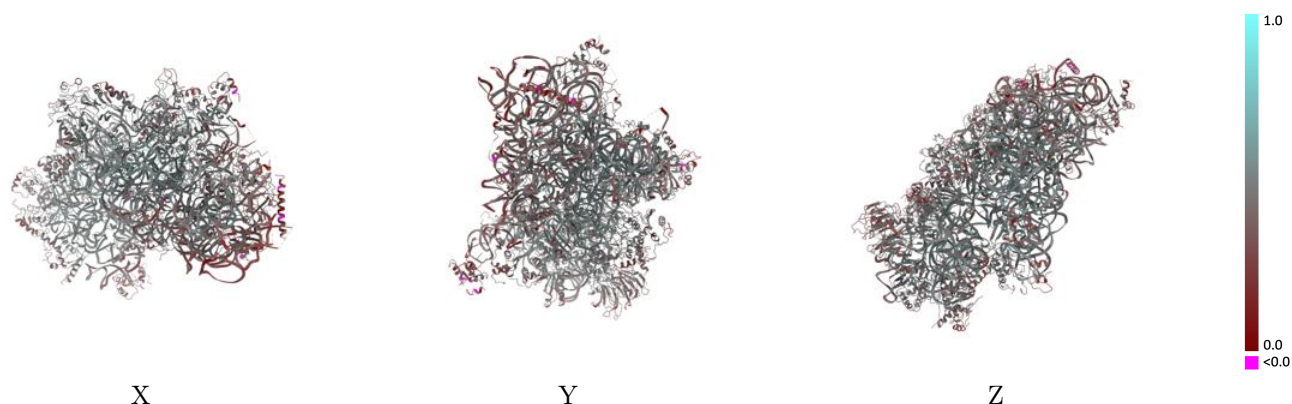
Y



Z

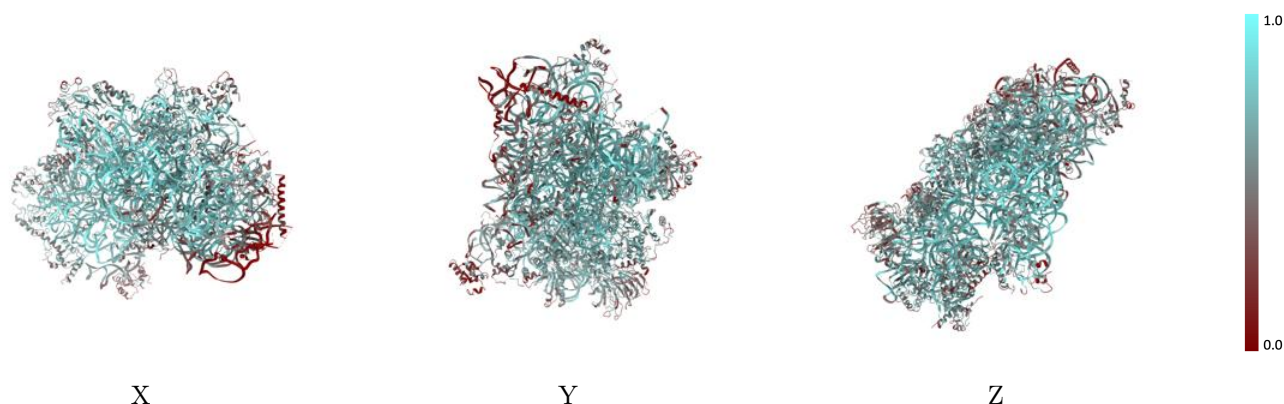
The images above show the 3D surface view of the map at the recommended contour level 0.036 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



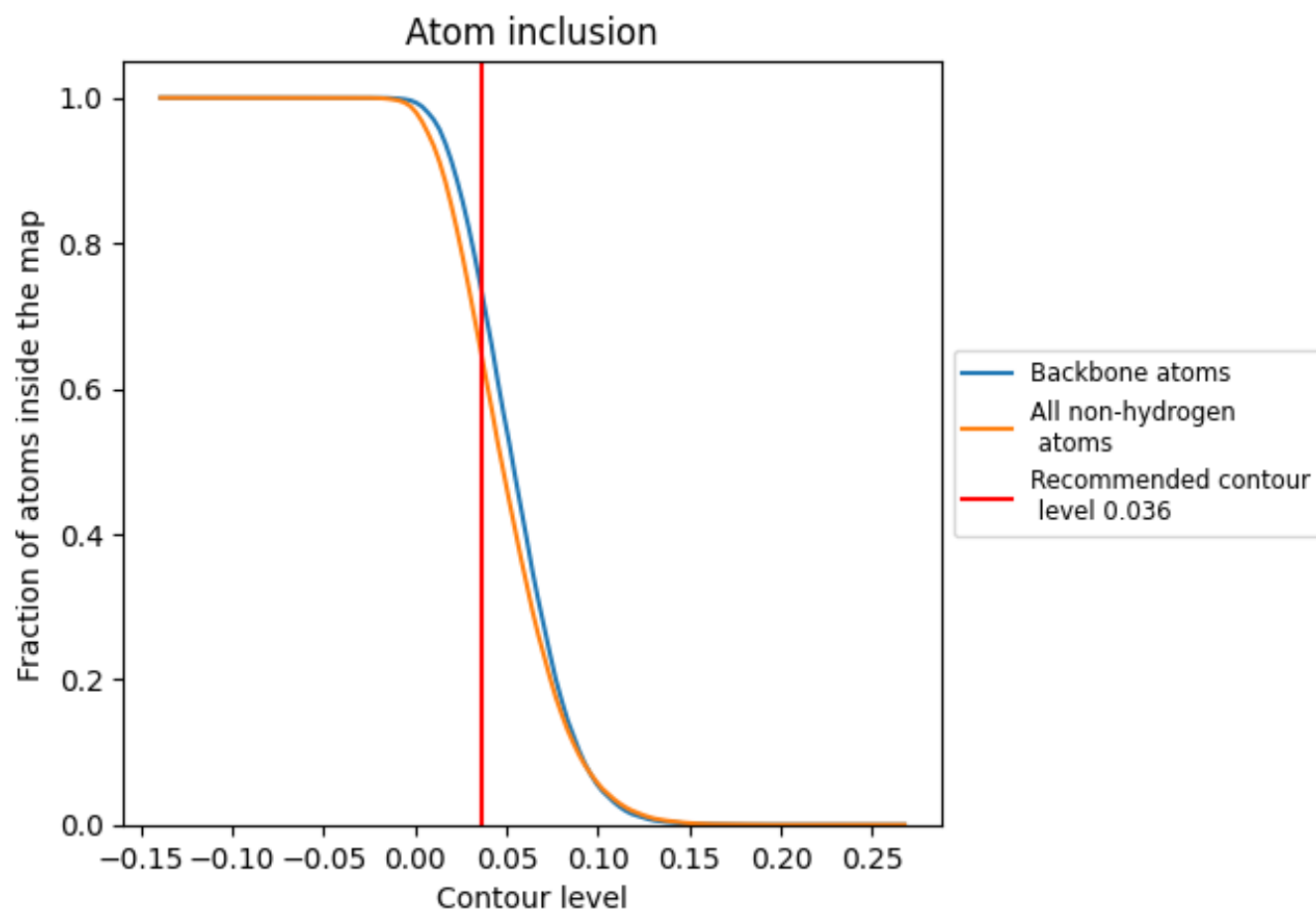
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.036).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 65% 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 (0.036) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6526	 0.4480
2	 0.7465	 0.4670
A	 0.6391	 0.4370
B	 0.5604	 0.4280
C	 0.7063	 0.4920
D	 0.5580	 0.4360
E	 0.4870	 0.4080
F	 0.5391	 0.4280
G	 0.0968	 0.2080
H	 0.5352	 0.4150
I	 0.5291	 0.4220
J	 0.5000	 0.4110
K	 0.5311	 0.4070
L	 0.5806	 0.4420
M	 0.2063	 0.2850
N	 0.6142	 0.4490
O	 0.6336	 0.4640
P	 0.5558	 0.4240
Q	 0.6597	 0.4790
R	 0.5677	 0.3970
S	 0.6137	 0.4540
T	 0.6451	 0.4630
U	 0.6082	 0.4500
V	 0.6444	 0.4520
W	 0.7239	 0.4880
X	 0.5388	 0.4380
Y	 0.3526	 0.3540
Z	 0.5209	 0.3970
a	 0.7015	 0.4960
b	 0.5595	 0.4200
c	 0.4398	 0.4370
d	 0.6860	 0.4860
e	 0.4290	 0.3820
g	 0.4664	 0.3860
n	 0.5735	 0.4270

