



## wwPDB EM Validation Summary Report ⓘ

Nov 19, 2022 – 09:49 am GMT

PDB ID : 4V91  
EMDB ID : EMD-2599  
Title : Kluyveromyces lactis 80S ribosome in complex with CrPV-IRES  
Authors : Fernandez, I.S.; Bai, X.; Scheres, S.H.W.; Ramakrishnan, V.  
Deposited on : 2014-03-21  
Resolution : 3.70 Å (reported)  
Based on initial model : 3B31

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.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

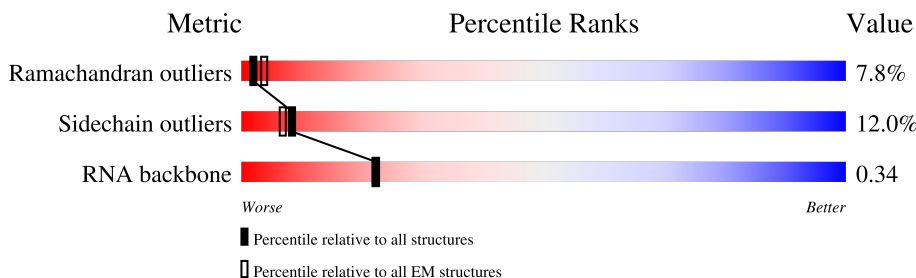
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.70 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	1	3397	14% (red), 44% (green), 34% (yellow), 16% (orange), 6% (grey)
2	3	121	7% (red), 51% (green), 35% (yellow), 14% (orange)
3	4	158	51% (green), 31% (yellow), 18% (orange)
4	A	254	20% (red), 85% (green), 11% (yellow), 2% (orange), 2% (grey)
5	B	387	31% (red), 80% (green), 17% (yellow), 2% (orange), 2% (grey)
6	C	362	59% (red), 83% (green), 14% (yellow), 2% (orange)
7	D	297	42% (red), 84% (green), 13% (yellow), 2% (orange)
8	E	176	63% (red), 76% (green), 11% (yellow), 2% (orange), 11% (grey)

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Mol	Chain	Length	Quality of chain
9	F	244	54% 78% 13% 9%
10	G	256	52% 77% 12% 9%
11	H	191	61% 84% 15%
12	I	221	38% 81% 11% 5%
13	J	174	38% 79% 13% 6%
14	L	199	58% 79% 15%
15	M	138	67% 82% 15%
16	N	204	40% 84% 14%
17	O	398	22% 22% 21% 5% 51%
18	P	184	26% 84% 12%
19	Q	186	57% 84% 12%
20	R	189	22% 79% 16%
21	S	172	68% 84% 15%
22	T	160	50% 83% 15%
23	U	121	20% 74% 8% 17%
24	V	137	23% 88% 10%
25	W	155	11% 34% 5% 61%
26	X	142	31% 70% 13% 15%
27	Y	127	53% 80% 18%
28	Z	136	54% 81% 18%
29	a	149	52% 85% 11%
30	b	59	42% 83% 10%
31	c	105	36% 73% 17% 8%
32	d	113	20% 81% 13%
33	e	130	59% 81% 15%

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Mol	Chain	Length	Quality of chain
34	f	107	
35	g	121	
36	h	120	
37	i	100	
38	j	88	
39	k	78	
40	l	51	
41	m	128	
42	n	25	
43	o	106	
44	p	92	
45	t	217	

## 2 Entry composition

There are 45 unique types of molecules in this entry. The entry contains 125665 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 25S RRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	1	3203	68514	30602	12358	22351	3203	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	3	121	2579	1152	461	845	121	0	0

- Molecule 3 is a RNA chain called 5.8S RRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	4	158	3353	1500	586	1109	158	0	0

- Molecule 4 is a protein called UL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	A	252	1914	1191	388	334	1	0	0

- Molecule 5 is a protein called UL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	B	386	3075	1950	584	533	8	0	0

- Molecule 6 is a protein called UL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	C	361	2748	1729	522	494	3	0	0

- Molecule 7 is a protein called UL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	D	296	2375	1501	414	458	2	0	0

- Molecule 8 is a protein called EL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	E	156	1239	800	222	216	1	0	0

- Molecule 9 is a protein called UL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	F	222	1784	1151	324	308	1	0	0

- Molecule 10 is a protein called EL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	G	233	1804	1151	323	327	3	0	0

- Molecule 11 is a protein called UL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	H	191	1518	963	274	277	4	0	0

- Molecule 12 is a protein called UL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	I	211	1705	1083	322	294	6	0	0

- Molecule 13 is a protein called UL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	J	169	1353	847	253	249	4	0	0

- Molecule 14 is a protein called EL13.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	L	193	Total	C	N	O	0	0
			1543	962	315	266		

- Molecule 15 is a protein called EL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	M	136	Total	C	N	O	S	0	0
			1053	675	199	177	2		

- Molecule 16 is a protein called EL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	N	203	Total	C	N	O	S	0	0
			1720	1077	361	281	1		

- Molecule 17 is a protein called UL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	197	Total	C	N	O	S	0	0
			1555	1003	289	262	1		

- Molecule 18 is a protein called UL22.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	P	183	Total	C	N	O	0	0
			1420	882	281	257		

- Molecule 19 is a protein called EL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Q	185	Total	C	N	O	S	0	0
			1441	908	290	241	2		

- Molecule 20 is a protein called EL19.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	R	188	Total	C	N	O	0	0
			1521	935	326	260		

- Molecule 21 is a protein called EL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	S	172	Total	C	N	O	S	0	0
			1445	930	267	244	4		

- Molecule 22 is a protein called EL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	T	159	Total	C	N	O	S	0	0
			1276	805	246	221	4		

- Molecule 23 is a protein called EL22.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	U	100	Total	C	N	O	0	0
			796	516	131	149		

- Molecule 24 is a protein called UL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	V	136	Total	C	N	O	S	0	0
			1003	628	189	179	7		

- Molecule 25 is a protein called EL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	W	60	Total	C	N	O	S	0	0
			500	322	98	79	1		

- Molecule 26 is a protein called UL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	X	121	Total	C	N	O	S	0	0
			964	620	169	173	2		

- Molecule 27 is a protein called UL24.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	Y	126	Total	C	N	O	0	0
			993	625	192	176		

- Molecule 28 is a protein called EL27.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
28	Z	135	1092	710	202	180	0	0

- Molecule 29 is a protein called UL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	a	148	1173	749	231	190	3	0	0

- Molecule 30 is a protein called EL29.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
30	b	58	462	289	100	73	0	0

- Molecule 31 is a protein called EL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	c	97	743	479	124	139	1	0	0

- Molecule 32 is a protein called EL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	d	109	876	556	167	152	1	0	0

- Molecule 33 is a protein called EL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	e	127	1020	647	205	167	1	0	0

- Molecule 34 is a protein called EL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	f	106	850	540	165	144	1	0	0

- Molecule 35 is a protein called EL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	g	112	Total	C	N	O	S	0	0
			880	545	179	152	4		

- Molecule 36 is a protein called UL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	h	119	Total	C	N	O	S	0	0
			969	615	186	167	1		

- Molecule 37 is a protein called EL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	i	99	Total	C	N	O	S	0	0
			771	481	156	132	2		

- Molecule 38 is a protein called EL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	j	87	Total	C	N	O	S	0	0
			681	414	148	114	5		

- Molecule 39 is a protein called EL38.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	k	77	Total	C	N	O	0	0
			612	391	115	106		

- Molecule 40 is a protein called EL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	l	50	Total	C	N	O	S	0	0
			436	272	97	65	2		

- Molecule 41 is a protein called EL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	m	52	Total	C	N	O	S	0	0
			417	259	86	67	5		

- Molecule 42 is a protein called EL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	n	25	233	142	63	27	1	0	0

- Molecule 43 is a protein called EL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	o	105	847	534	170	138	5	0	0

- Molecule 44 is a protein called EL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	p	91	694	429	138	121	6	0	0

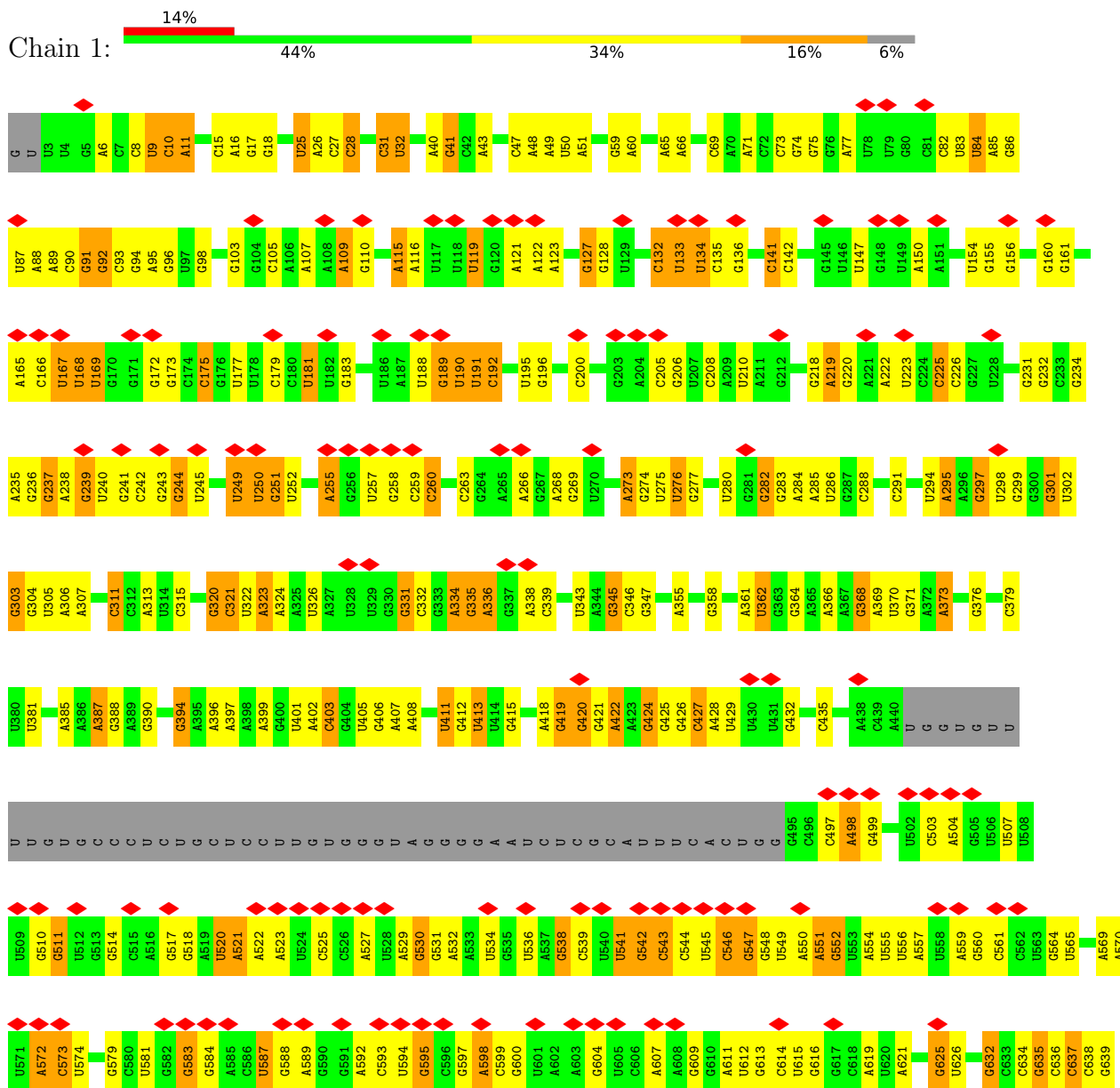
- Molecule 45 is a protein called UL1.

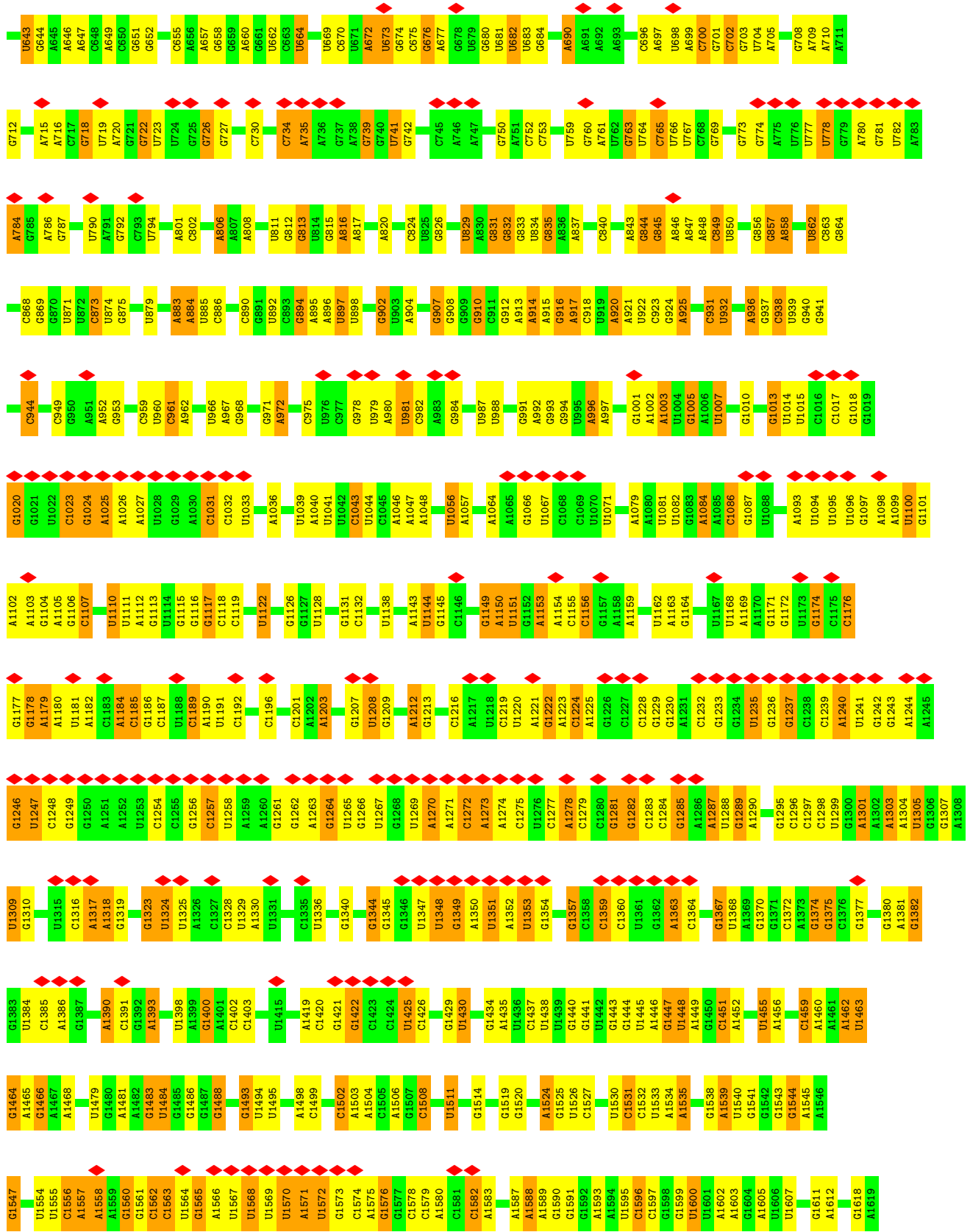
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	t	217	1718	1097	299	312	10	0	0

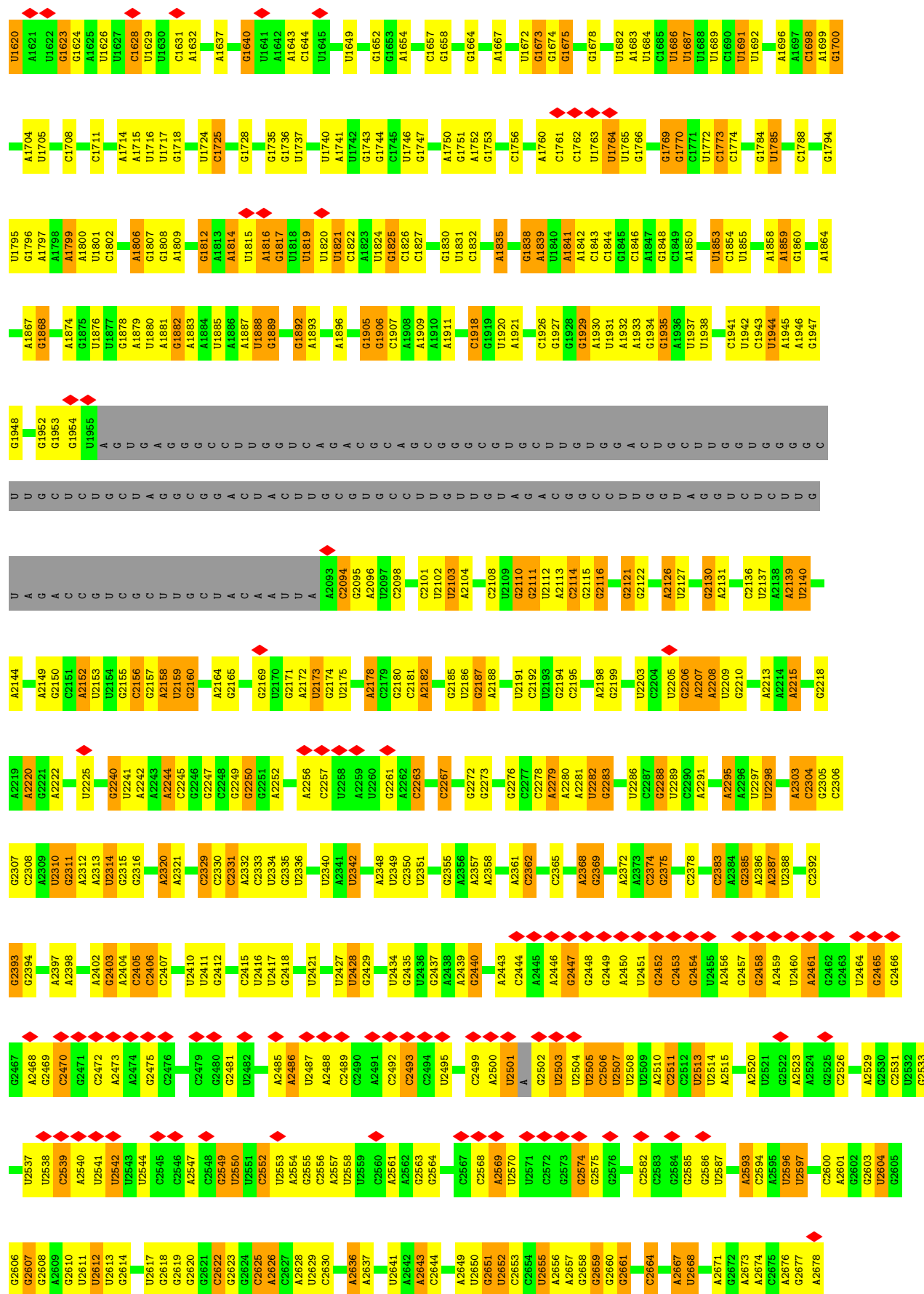
### 3 Residue-property plots [i](#)

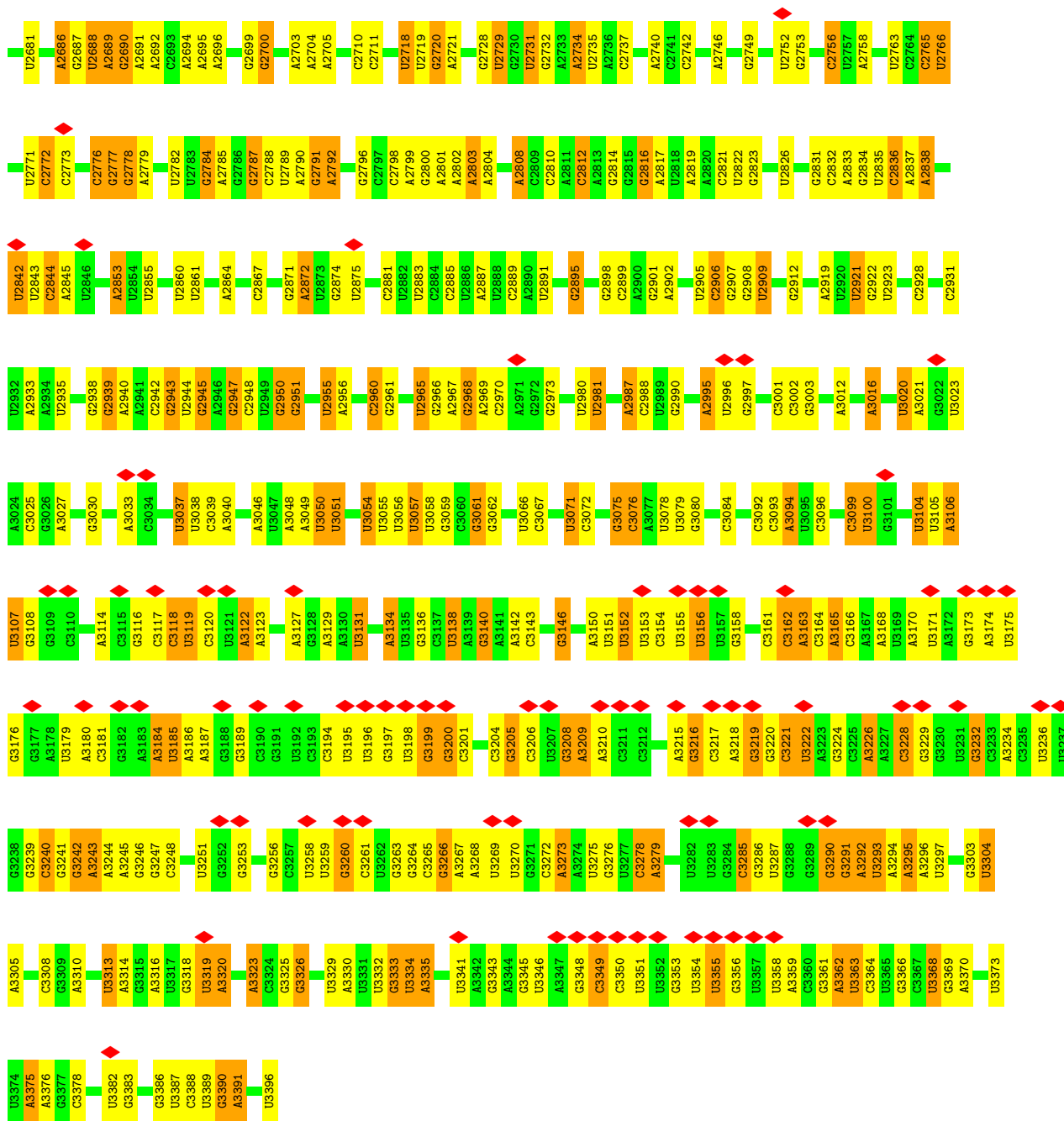
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 25S RRNA

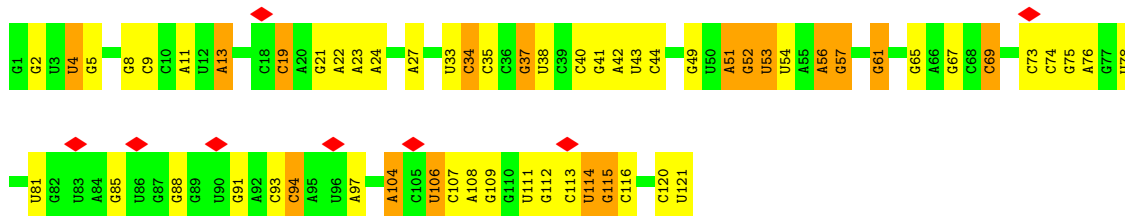




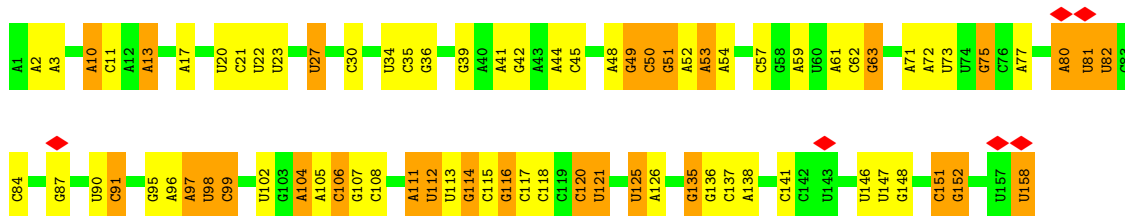




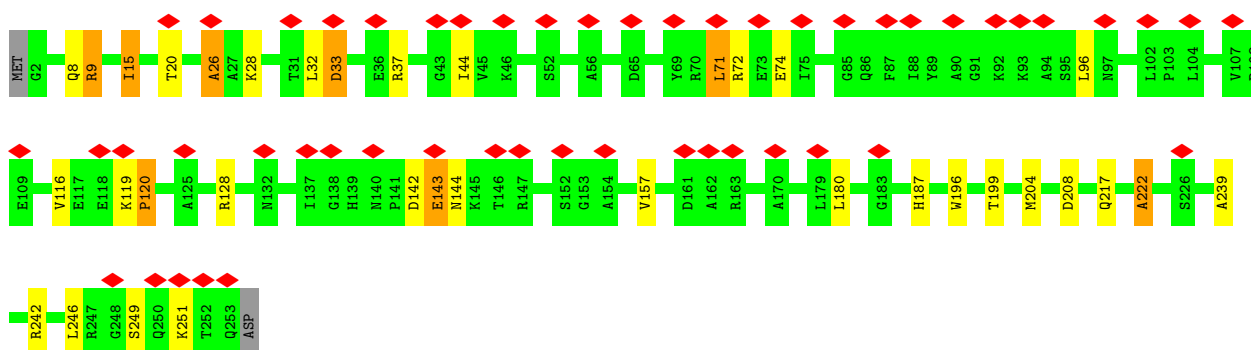
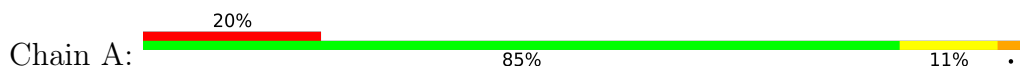
• Molecule 2: 5S rRNA



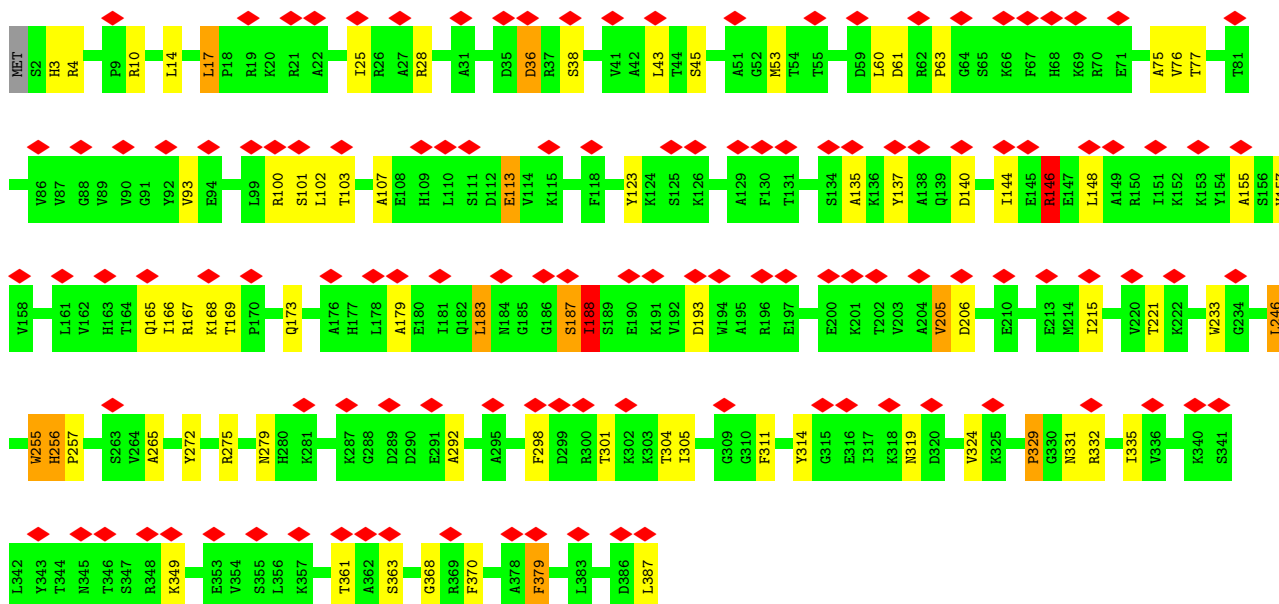
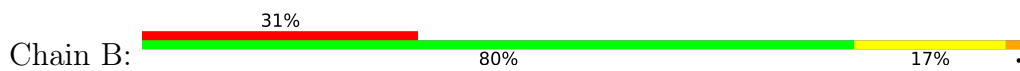
• Molecule 3: 5.8S rRNA



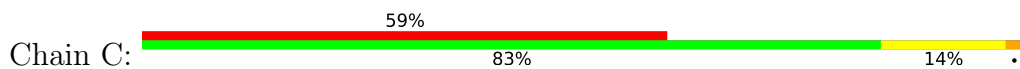
• Molecule 4: UL2



• Molecule 5: UL3

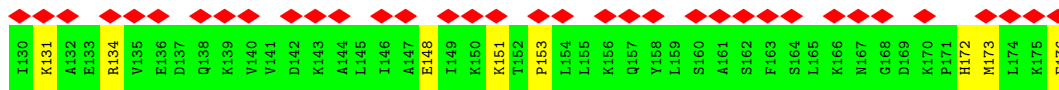


• Molecule 6: UL4

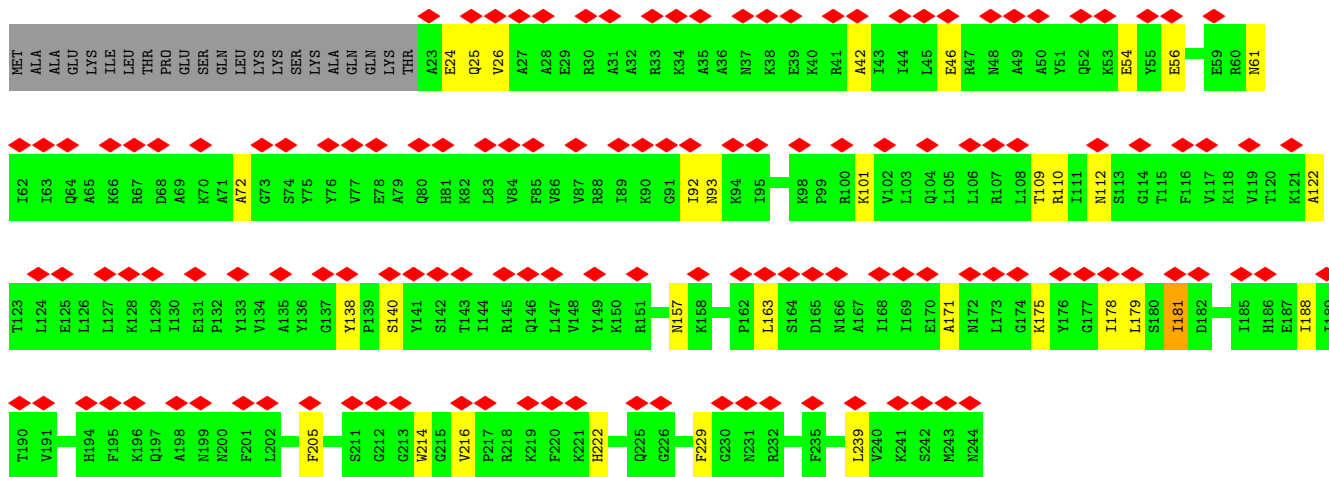
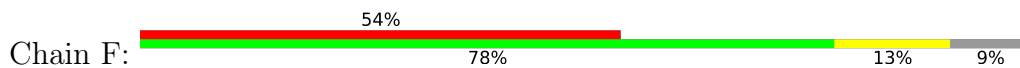




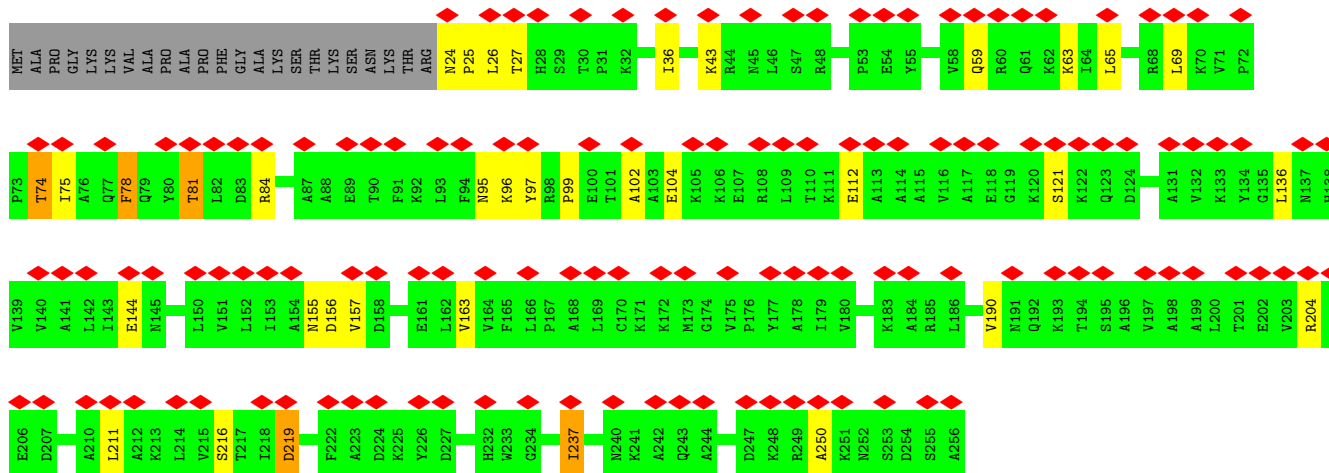
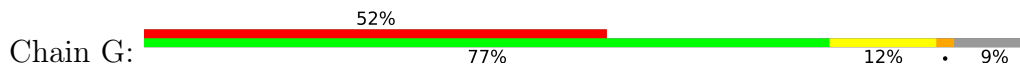




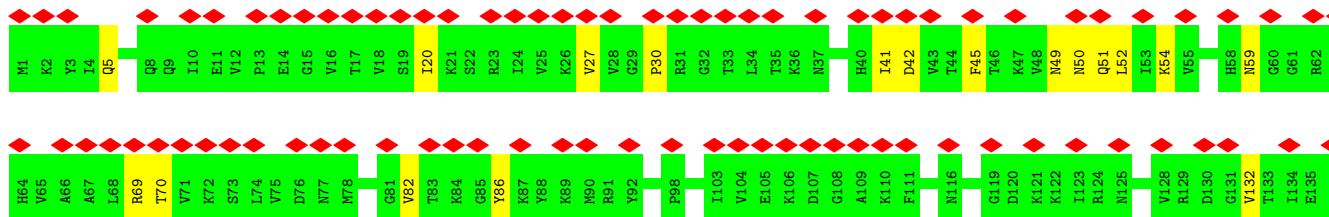
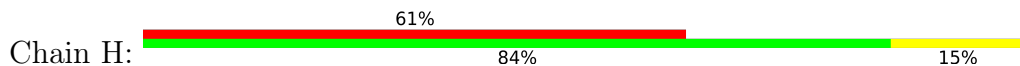
• Molecule 9: UL30

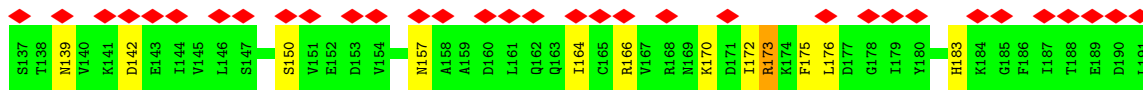


• Molecule 10: EL8



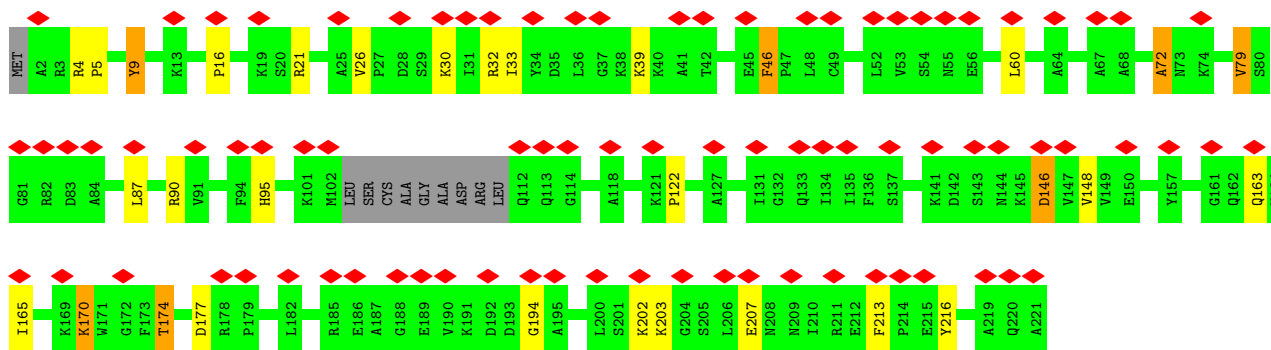
• Molecule 11: UL6





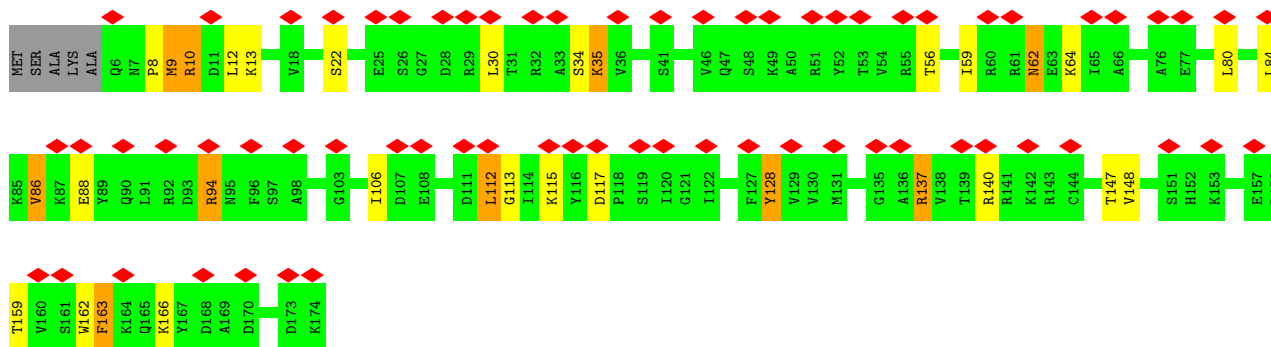
• Molecule 12: UL16

Chain I:



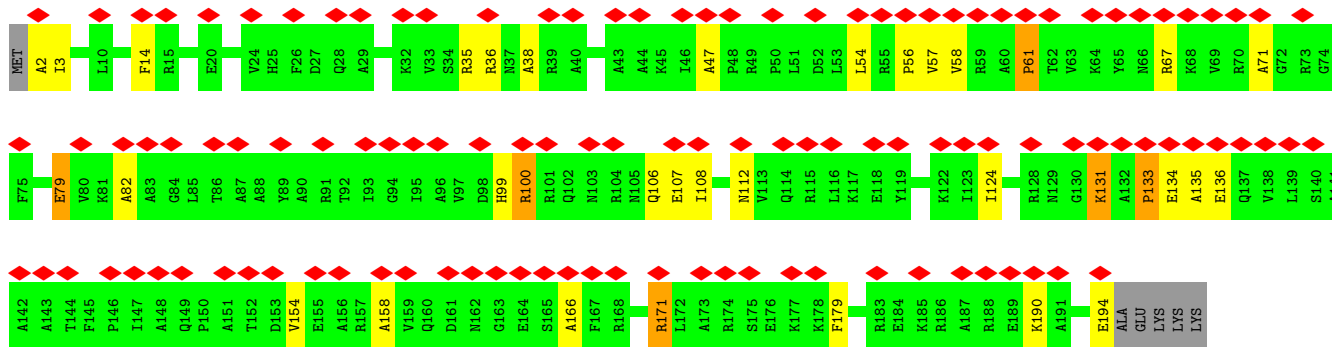
• Molecule 13: UL5

Chain J:



• Molecule 14: EL13

Chain L:



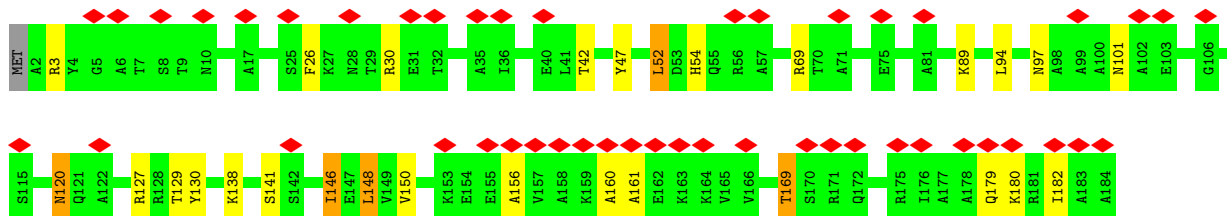
• Molecule 15: EL14



PHE  
THR  
LYS  
VAL  
ALA  
SER  
ASN  
THR  
ALA  
ALA  
GLU  
SER  
ASP  
VAL  
ALA  
LYS  
GLN  
LEU  
ALA  
LEU  
GLY  
TYR

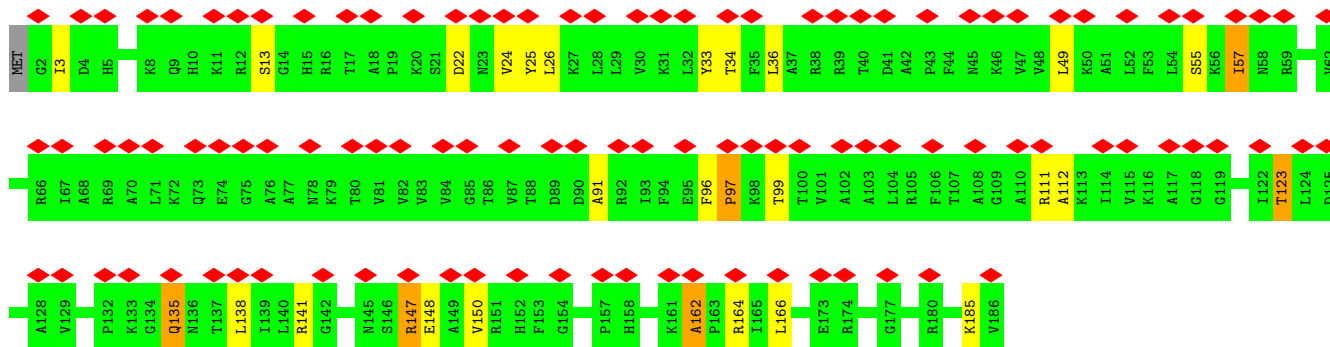
- Molecule 18: UL22

Chain P: 26% 84% 12%



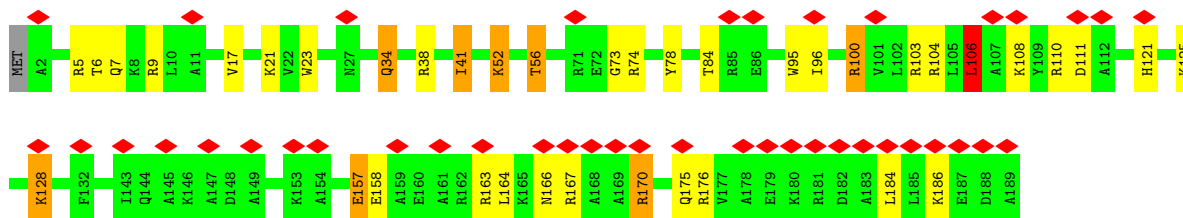
- Molecule 19: EL18

Chain Q: 57% 84% 12%



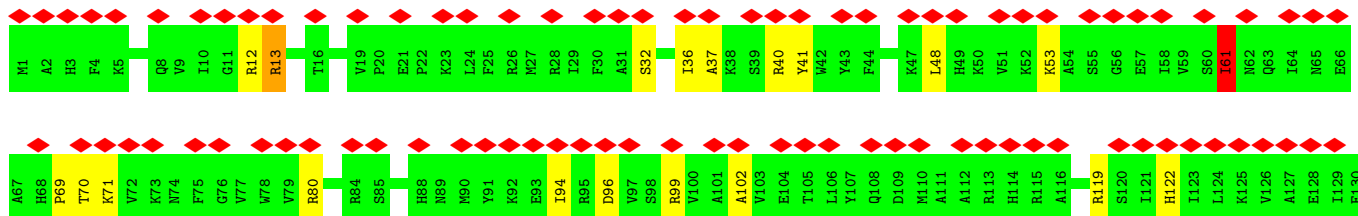
- Molecule 20: EL19

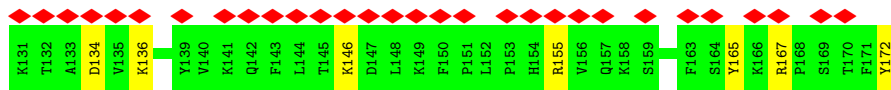
Chain R: 22% 79% 16%



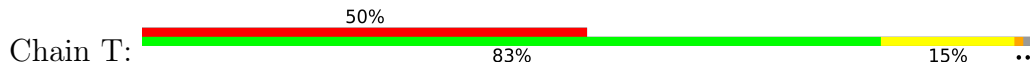
- Molecule 21: EL20

Chain S: 68% 84% 15%

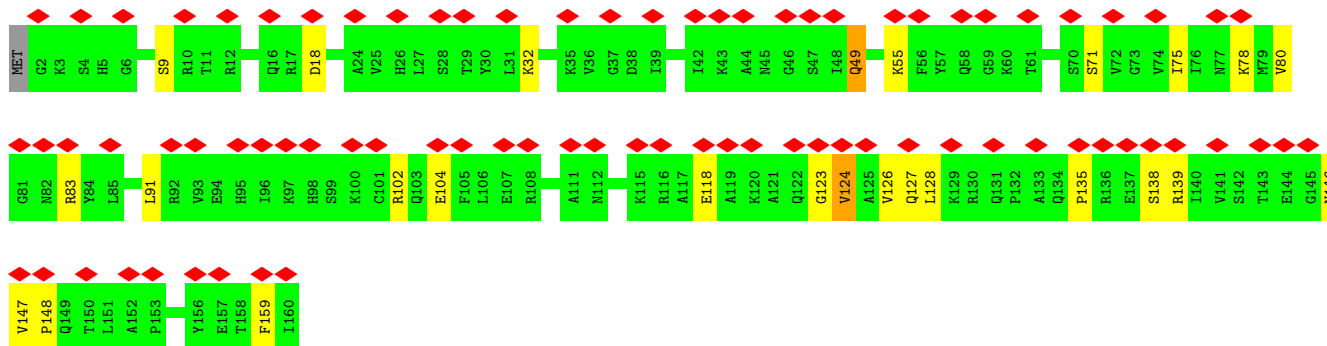




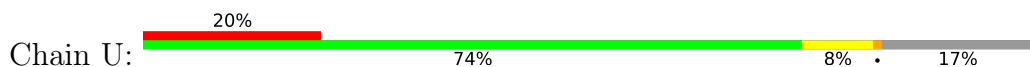
• Molecule 22: EL21



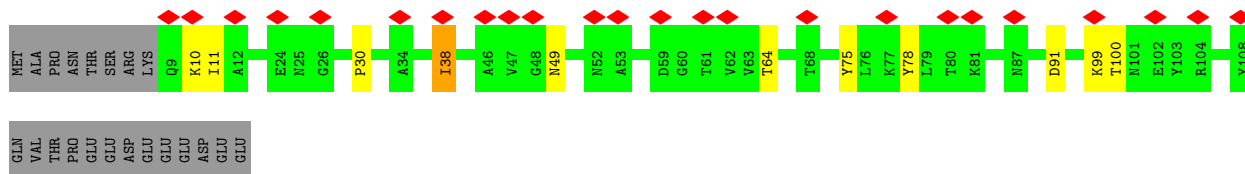
Chain T:



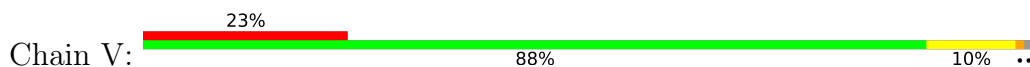
• Molecule 23: EL22



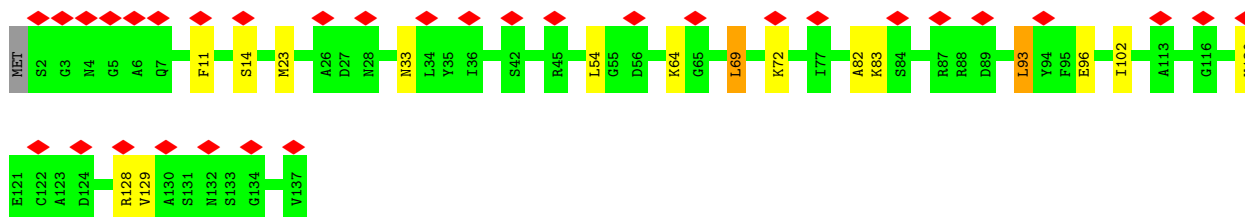
Chain U:



• Molecule 24: UL14



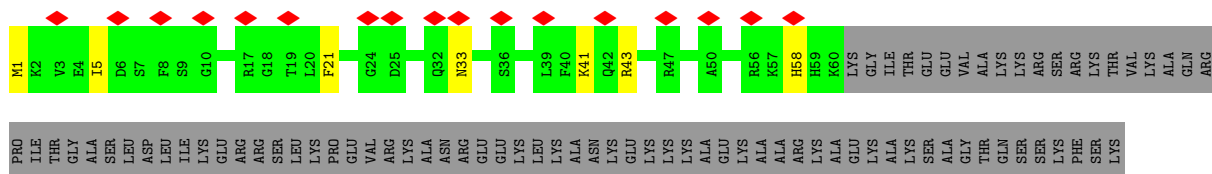
Chain V:



• Molecule 25: EL24



Chain W:



GLN  
GLN  
ALA  
LYS  
GLY  
ALA  
PHE  
GLN  
LYS  
VAL  
ALA  
ALA  
THR  
SER  
ARG

- Molecule 26: UL23

Chain X: 31% 70% 13% 15%

MET  
ALA  
PRO  
SER  
ALA  
LYS  
ALA  
THR  
ALA  
LYS  
LYS  
VAL  
VAL  
LYS  
GLY  
THR  
ASN  
GLY  
LYS  
K22  
A23  
L24  
K25  
V26  
R27  
T28  
S29  
F32  
R33  
L34  
P35  
K36  
T37  
L38  
K39  
L40  
A41  
R42  
K45  
Y46  
A47  
S48  
K49  
A50  
V51  
P52  
R53  
Y54  
N55  
R56  
L57  
D58  
S59  
Y60  
K61  
V62

I63  
E64  
Q65  
P66  
L67  
T68  
S69  
E70  
M73  
E77  
R80  
I81  
L82  
W83  
F84  
Q85  
A90  
N91  
K92  
Y93  
Q94  
I95  
K96  
K97  
A98  
L102  
Y103  
L113  
V114  
R115  
A122  
Y123  
V124  
D134  
I135  
M137  
G140  
Y141  
L142

- Molecule 27: UL24

Chain Y: 53% 80% 18%

MET  
A2  
K3  
Q4  
S5  
L6  
D7  
V8  
S9  
S10  
D11  
R12  
A15  
R16  
A22  
P23  
S24  
S25  
Q26  
R27  
R28  
V29  
L30  
L31  
S32  
A33  
P34  
L35  
S36  
K37  
E38  
L39  
R40  
A41  
Q42  
Y43  
G44  
I45  
K46  
A47  
L48  
P49  
I50  
R51  
R52  
D53  
D54  
L57  
V58  
V59  
S62  
K63  
K64  
Q65  
Q66  
E67

I70  
S71  
S72  
V73  
Y74  
K77  
V80  
Q81  
V82  
D83  
R84  
V85  
T86  
E88  
N91  
G92  
N98  
L99  
H100  
P101  
S102  
K103  
L104  
V105  
I106  
T107  
K108  
L109  
H110  
L111  
D114  
R115  
K116  
A117  
L118  
I119  
K122  
G123  
G124  
K125  
L126  
E127

- Molecule 28: EL27

Chain Z: 54% 81% 18%

MET  
A2  
K3  
F4  
L5  
K6  
A7  
G8  
R9  
V10  
A11  
V12  
V13  
V14  
R17  
G20  
K21  
K22  
V23  
V24  
I25  
V26  
K27  
P28  
H29  
G32  
S33  
K34  
S35  
A44  
G45  
I46  
E47  
R48  
Y49  
P50  
L51  
K52  
V53  
T54  
K55  
K56  
H57  
G58  
A59  
K60  
K61  
A63  
K64  
R65  
T66  
K67  
K69  
P70

F71  
I72  
N76  
Y77  
H79  
L81  
P82  
T83  
R84  
Y85  
T86  
L87  
D88  
A91  
F92  
K93  
S94  
V95  
E99  
T100  
F101  
E102  
Q103  
P104  
S105  
E108  
E109  
A110  
K111  
K112  
V113  
V114  
K115  
K116  
E119  
E120  
R121  
H122  
Q123  
A124  
G125  
K126  
M127  
Q128  
V129  
F130  
F131  
S132  
K133  
L134  
R135  
F136

- Molecule 29: UL15

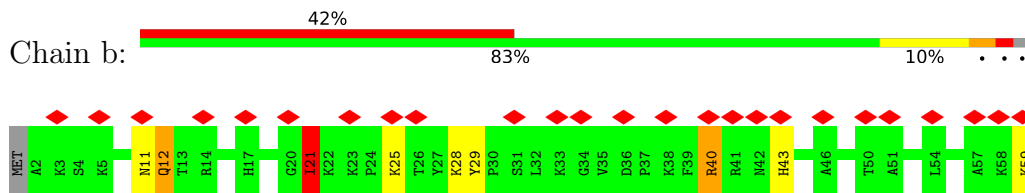
Chain a: 52% 85% 11%

MET  
P2  
S3  
R4  
F5  
T6  
K7  
T8  
R9  
K10  
H11  
R12  
G13  
H14  
R21  
I22  
G23  
K24  
G33  
M34  
A35  
G36  
G37  
H40  
H41  
R42  
I43  
M44  
M45  
D46  
Y52  
F53  
V56  
G57  
M58  
K63  
Q64  
Q65  
A66  
H67  
F68  
V72  
L73  
N74  
L75  
D76  
K77  
L78  
W79  
T80  
L81  
I82  
P83

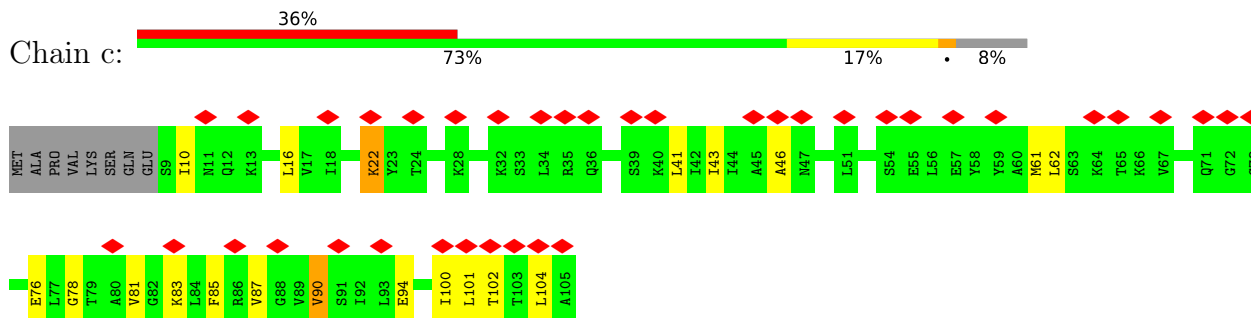
E84  
D85  
K86  
R87  
D88  
Q89  
Y90  
L91  
K92  
S93  
A94  
S95  
K96  
E97  
T98  
A99  
P100  
V101  
I102  
D103  
T104  
L105  
A106  
A107  
G108  
G109  
G110  
K111  
I112  
L113  
G114  
K115  
G116  
R117  
I118  
P119  
N120  
V121  
P122  
V123  
I124  
V125  
K126  
A127  
R128  
F129  
V130  
S131  
K132  
L133  
A134  
E135  
E136  
K137  
I138  
R139  
A140  
A141  
V144

V145  
E146  
L147  
I148  
A149

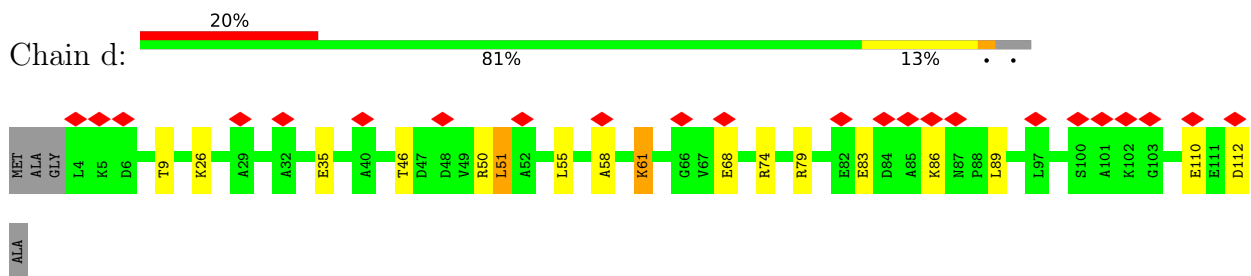
• Molecule 30: EL29



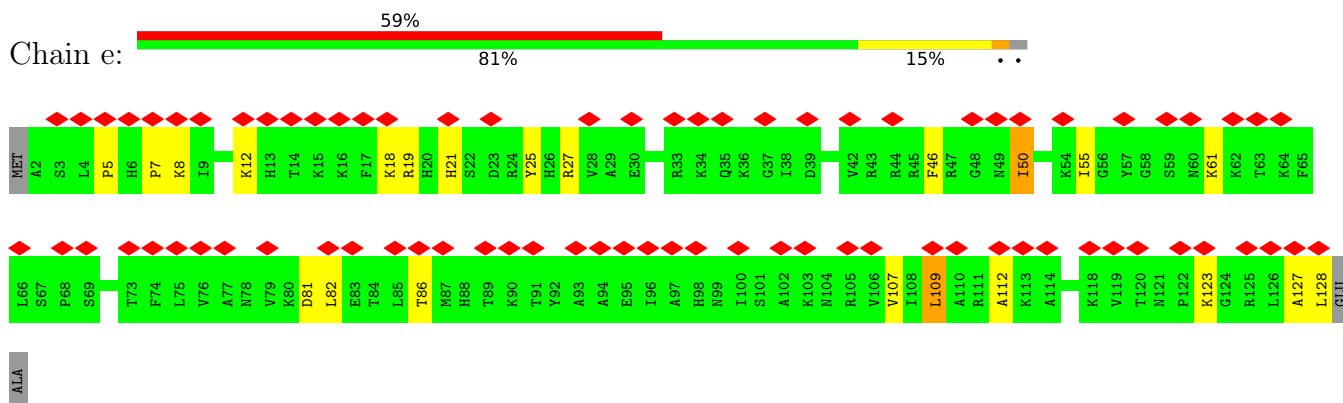
• Molecule 31: EL30



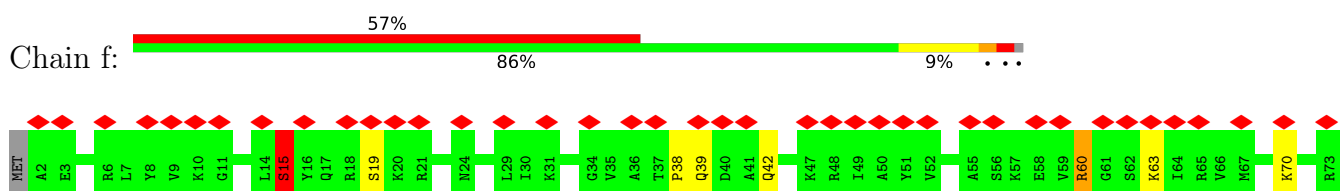
• Molecule 32: EL31



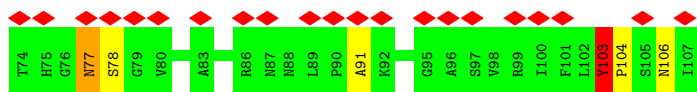
• Molecule 33: EL32



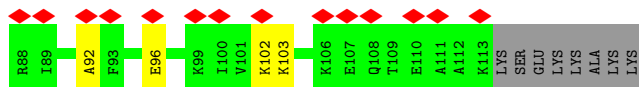
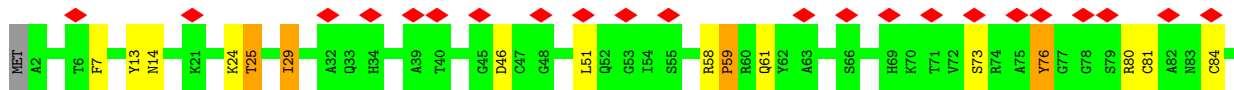
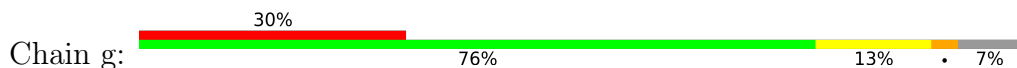
• Molecule 34: EL33



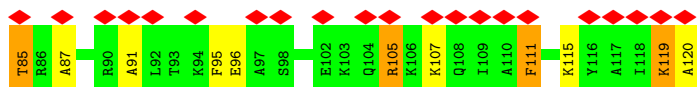
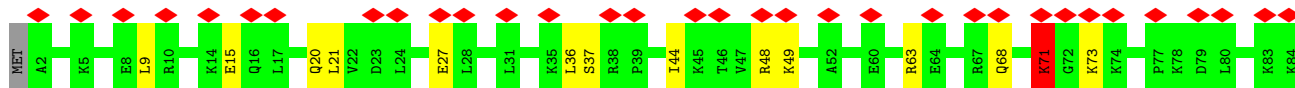
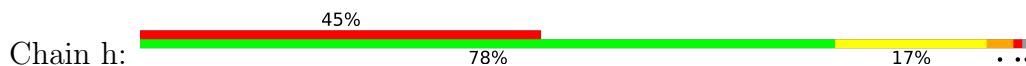




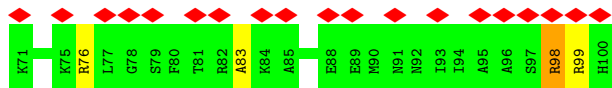
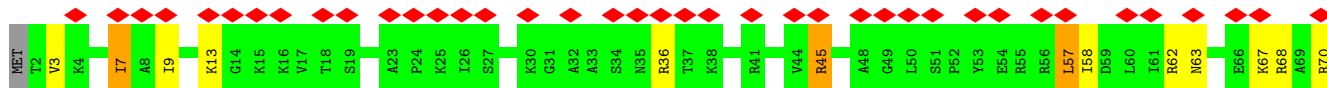
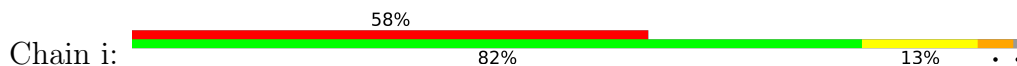
• Molecule 35: EL34



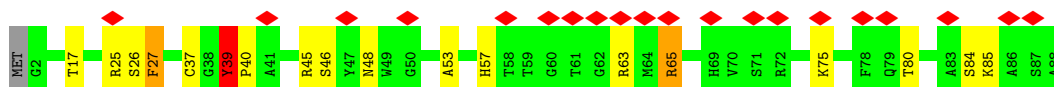
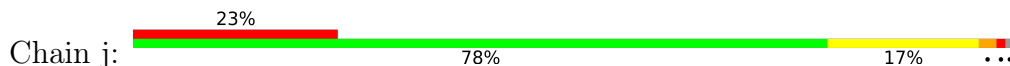
• Molecule 36: UL29



• Molecule 37: EL36

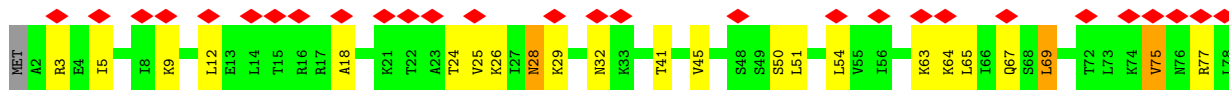


• Molecule 38: EL37

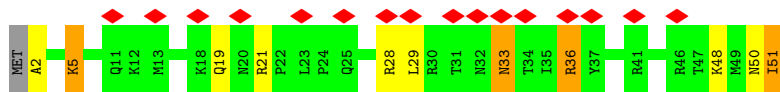
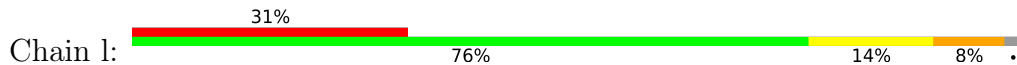


• Molecule 39: EL38

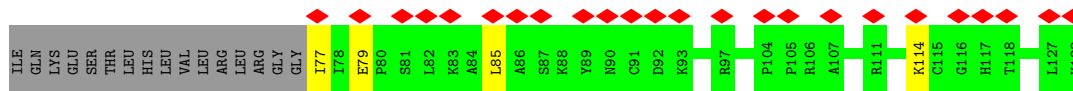
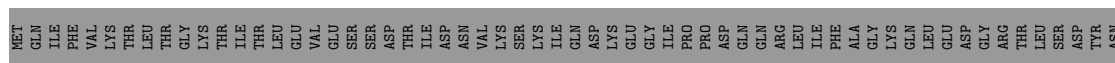




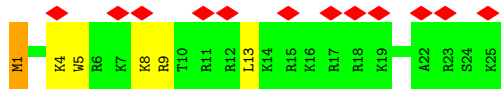
• Molecule 40: EL39



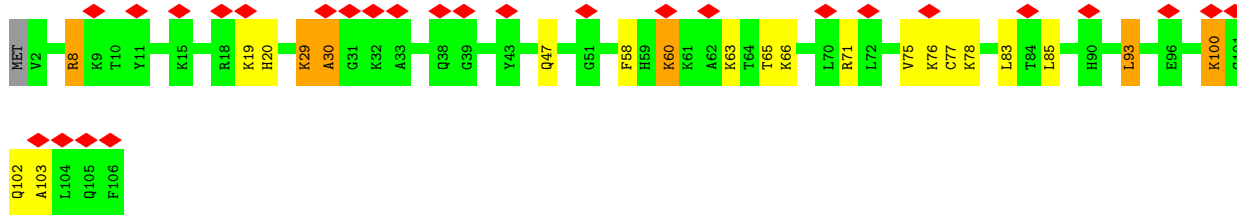
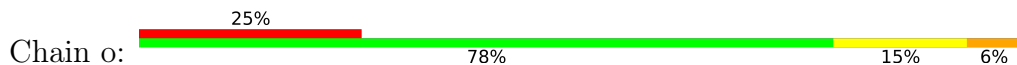
• Molecule 41: EL40



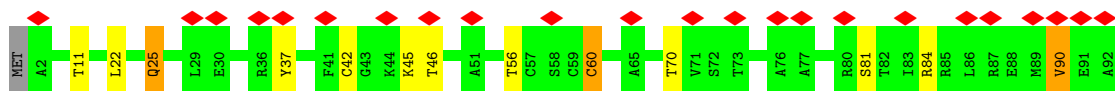
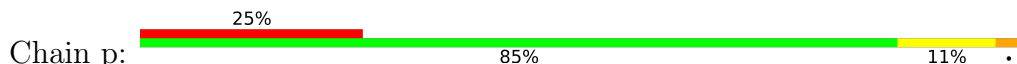
• Molecule 42: EL41



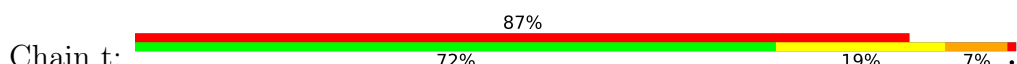
• Molecule 43: EL42



• Molecule 44: EL43



• Molecule 45: UL1



M1	S2	K3	I4	T5	S6	S7	Q8	V9	R10	E11	H12	V13	K14	E15	L16	L17	K18	Y19	S20	N21	E22	R26	N27	F28	L29	E30	T31	V32	E33	L34	Q35	V36	G37	L38	K39	M40	Y41	D42	P43	Q44	R45	D46	K47	R48	F49	S50	G51	S52	L53	K54	L55	P56	N57	C58	P59	R60	P61	M62
M63	S64	I65	C66	I67	F68	G69	D70	A71	F72	D73	V74	D75	R76	A77	K78	S79	C80	G81	V82	D83	A84	M85	S86	V87	D88	D89	L90	K91	K92	L93	N94	K95	N96	K97	K98	L99	I100	K101	S104	K105	K106	Y107	N108	A109	F110	I111	A112	S113	E114	V115	L116	I117	K118	Q119	V120	P121	R122	L123
L124	G125	P126	Q127	L128	S129	K130	A131	G132	K133	F134	P135	T136	P137	V138	S139	H140	N141	D142	Y145	G146	T149	D150	V151	R152	S153	T154	I155	K156	F157	Q158	L159	K160	K161	V162	L163	C164	L165	A166	V167	A168	V169	G170	N171	V172	E173	M174	E175	E176	D177	V178	L179	V180	N181	Q182	I183	L184	M185	
S186	V187	N188	F189	V191	S192	L193	L194	K195	K196	N197	M198	Q199	N200	V201	G202	S203	L204	V205	V206	K207	S208	S209	M210	G211	P212	A213	F214	R215	L216	Y217																												

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	18132	Depositor
Resolution determination method	Not provided	
CTF correction method	EACH PARTICLE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	1.8	Depositor
Maximum defocus (nm)	3	Depositor
Magnification	47000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	1.275	Depositor
Minimum map value	-0.841	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.050	Depositor
Recommended contour level	0.12	Depositor
Map size ( $\text{\AA}$ )	428.80002, 428.80002, 428.80002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.34, 1.34, 1.34	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	1	0.86	28/76106 (0.0%)	1.13	1805/117228 (1.5%)
2	3	0.27	0/2857	1.10	75/4387 (1.7%)
3	4	1.27	3/3723 (0.1%)	1.19	101/5740 (1.8%)
4	A	0.34	0/1881	0.90	15/2416 (0.6%)
5	B	0.38	0/3064	0.97	35/3982 (0.9%)
6	C	0.36	0/2721	0.90	19/3553 (0.5%)
7	D	0.38	0/2353	0.91	18/3055 (0.6%)
8	E	0.35	0/1233	0.88	9/1613 (0.6%)
9	F	0.35	0/1773	0.90	14/2307 (0.6%)
10	G	0.35	0/1771	0.89	16/2286 (0.7%)
11	H	0.36	0/1493	0.89	12/1935 (0.6%)
12	I	0.75	1/1690 (0.1%)	0.88	12/2182 (0.5%)
13	J	0.35	0/1339	0.92	10/1737 (0.6%)
14	L	0.82	1/1518 (0.1%)	0.98	16/1956 (0.8%)
15	M	0.32	0/1040	0.77	4/1354 (0.3%)
16	N	0.35	0/1706	0.87	12/2201 (0.5%)
17	O	2.16	23/1577 (1.5%)	4.80	87/2104 (4.1%)
18	P	0.35	0/1400	0.91	13/1815 (0.7%)
19	Q	0.33	0/1417	0.96	12/1821 (0.7%)
20	R	0.58	1/1492 (0.1%)	1.10	22/1912 (1.2%)
21	S	0.32	0/1435	0.88	10/1852 (0.5%)
22	T	0.33	0/1266	0.82	4/1641 (0.2%)
23	U	0.38	0/788	0.81	3/1027 (0.3%)
24	V	0.36	0/984	0.86	5/1267 (0.4%)
25	W	0.31	0/496	0.73	2/632 (0.3%)
26	X	0.30	0/957	0.76	5/1255 (0.4%)
27	Y	0.32	0/974	0.95	11/1251 (0.9%)
28	Z	0.38	0/1080	0.97	7/1383 (0.5%)
29	a	0.32	0/1163	0.82	8/1489 (0.5%)
30	b	0.31	0/456	0.94	4/578 (0.7%)
31	c	0.38	0/727	0.96	7/936 (0.7%)
32	d	0.32	0/867	0.81	4/1127 (0.4%)
33	e	0.32	0/1015	0.91	5/1316 (0.4%)
34	f	0.36	0/837	0.95	8/1075 (0.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
35	g	0.39	0/863	1.12	13/1108 (1.2%)
36	h	0.31	0/948	0.85	9/1211 (0.7%)
37	i	0.33	0/748	0.92	7/944 (0.7%)
38	j	0.37	0/674	0.97	8/857 (0.9%)
39	k	1.22	1/599 (0.2%)	0.93	6/769 (0.8%)
40	l	0.39	0/431	1.01	6/552 (1.1%)
41	m	0.30	0/409	0.64	0/520
42	n	0.66	0/228	1.00	1/282 (0.4%)
43	o	0.37	0/843	0.99	10/1085 (0.9%)
44	p	0.36	0/684	0.86	5/883 (0.6%)
45	t	0.48	0/1692	1.11	24/2183 (1.1%)
All	All	0.77	58/133318 (0.0%)	1.17	2479/192807 (1.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1	103	0
2	3	1	0
3	4	4	0
4	A	7	0
5	B	11	3
6	C	11	3
7	D	6	0
8	E	3	0
9	F	5	0
10	G	6	0
11	H	5	0
12	I	4	0
13	J	3	0
14	L	6	1
15	M	2	0
16	N	2	0
17	O	3	16
18	P	5	0
19	Q	4	0
20	R	13	0
21	S	5	0
22	T	6	0
24	V	3	0

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Mol	Chain	#Chirality outliers	#Planarity outliers
25	W	2	0
26	X	2	0
27	Y	4	0
28	Z	2	0
29	a	3	0
30	b	2	0
31	c	3	0
32	d	3	0
33	e	2	0
34	f	4	2
35	g	4	0
36	h	4	0
37	i	2	0
38	j	3	1
40	l	3	0
43	o	7	0
44	p	1	0
45	t	8	5
All	All	277	31

The worst 5 of 58 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	41	G	O3'-P	49.28	2.20	1.61
1	1	1708	C	O3'-P	49.19	2.20	1.61
1	1	2361	A	O3'-P	49.04	2.19	1.61
1	1	554	A	O3'-P	48.77	2.19	1.61
1	1	968	G	O3'-P	48.44	2.19	1.61

The worst 5 of 2479 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	O	72	HIS	O-C-N	-63.40	21.26	122.70
17	O	186	ALA	O-C-N	-61.98	23.52	122.70
17	O	64	PHE	O-C-N	-60.21	26.36	122.70
17	O	129	LEU	O-C-N	-56.56	32.21	122.70
17	O	153	VAL	O-C-N	-52.15	39.27	122.70

5 of 277 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	1	69	C	C2'

*Continued on next page...*

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Mol	Chain	Res	Type	Atom
1	1	92	G	C2'
1	1	95	A	C2'
1	1	109	A	C3'
1	1	167	U	C3'

5 of 31 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	B	17	LEU	Peptide
5	B	256	HIS	Peptide
5	B	36	ASP	Peptide
6	C	148	ILE	Peptide
6	C	226	GLU	Peptide

## 5.2 Too-close contacts [i](#)

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	135/254 (53%)	107 (79%)	21 (16%)	7 (5%)	2	21
5	B	240/387 (62%)	198 (82%)	25 (10%)	17 (7%)	1	15
6	C	215/362 (59%)	168 (78%)	26 (12%)	21 (10%)	0	8
7	D	164/297 (55%)	128 (78%)	25 (15%)	11 (7%)	1	16
8	E	103/176 (58%)	91 (88%)	7 (7%)	5 (5%)	2	22
9	F	136/244 (56%)	121 (89%)	10 (7%)	5 (4%)	3	28
10	G	122/256 (48%)	100 (82%)	13 (11%)	9 (7%)	1	13
11	H	106/191 (56%)	84 (79%)	18 (17%)	4 (4%)	3	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	I	119/221 (54%)	102 (86%)	12 (10%)	5 (4%)	3	25
13	J	103/174 (59%)	85 (82%)	10 (10%)	8 (8%)	1	12
14	L	103/199 (52%)	79 (77%)	14 (14%)	10 (10%)	0	8
15	M	84/138 (61%)	68 (81%)	10 (12%)	6 (7%)	1	15
16	N	114/204 (56%)	94 (82%)	11 (10%)	9 (8%)	1	12
17	O	181/398 (46%)	69 (38%)	53 (29%)	59 (33%)	0	0
18	P	106/184 (58%)	96 (91%)	7 (7%)	3 (3%)	5	33
19	Q	100/186 (54%)	81 (81%)	13 (13%)	6 (6%)	1	18
20	R	105/189 (56%)	74 (70%)	26 (25%)	5 (5%)	2	22
21	S	87/172 (51%)	63 (72%)	17 (20%)	7 (8%)	1	12
22	T	93/160 (58%)	69 (74%)	19 (20%)	5 (5%)	2	20
23	U	58/121 (48%)	50 (86%)	5 (9%)	3 (5%)	2	21
24	V	73/137 (53%)	65 (89%)	6 (8%)	2 (3%)	5	33
25	W	33/155 (21%)	29 (88%)	4 (12%)	0	100	100
26	X	76/142 (54%)	63 (83%)	8 (10%)	5 (7%)	1	16
27	Y	71/127 (56%)	50 (70%)	17 (24%)	4 (6%)	2	19
28	Z	66/136 (48%)	48 (73%)	13 (20%)	5 (8%)	1	13
29	a	75/149 (50%)	56 (75%)	13 (17%)	6 (8%)	1	12
30	b	27/59 (46%)	19 (70%)	5 (18%)	3 (11%)	0	5
31	c	56/105 (53%)	44 (79%)	8 (14%)	4 (7%)	1	15
32	d	68/113 (60%)	59 (87%)	6 (9%)	3 (4%)	2	24
33	e	82/130 (63%)	68 (83%)	8 (10%)	6 (7%)	1	14
34	f	52/107 (49%)	42 (81%)	7 (14%)	3 (6%)	1	19
35	g	65/121 (54%)	57 (88%)	6 (9%)	2 (3%)	4	32
36	h	66/120 (55%)	52 (79%)	8 (12%)	6 (9%)	1	9
37	i	47/100 (47%)	33 (70%)	10 (21%)	4 (8%)	1	10
38	j	48/88 (54%)	35 (73%)	7 (15%)	6 (12%)	0	4
39	k	43/78 (55%)	32 (74%)	9 (21%)	2 (5%)	2	23
40	l	27/51 (53%)	20 (74%)	5 (18%)	2 (7%)	1	13
41	m	26/128 (20%)	22 (85%)	3 (12%)	1 (4%)	3	27
42	n	14/25 (56%)	9 (64%)	4 (29%)	1 (7%)	1	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	o	71/106 (67%)	58 (82%)	10 (14%)	3 (4%)	3	25
44	p	59/92 (64%)	53 (90%)	4 (7%)	2 (3%)	3	30
45	t	121/217 (56%)	82 (68%)	24 (20%)	15 (12%)	0	4
All	All	3740/6999 (53%)	2923 (78%)	527 (14%)	290 (8%)	2	12

5 of 290 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	33	ASP
4	A	120	PRO
5	B	61	ASP
5	B	113	GLU
5	B	146	ARG

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	193/196 (98%)	172 (89%)	21 (11%)	6	29
5	B	320/323 (99%)	277 (87%)	43 (13%)	4	21
6	C	288/289 (100%)	261 (91%)	27 (9%)	8	35
7	D	244/245 (100%)	215 (88%)	29 (12%)	5	25
8	E	134/153 (88%)	123 (92%)	11 (8%)	11	41
9	F	186/205 (91%)	172 (92%)	14 (8%)	13	43
10	G	187/208 (90%)	170 (91%)	17 (9%)	9	36
11	H	171/171 (100%)	154 (90%)	17 (10%)	8	32
12	I	177/187 (95%)	156 (88%)	21 (12%)	5	25
13	J	147/150 (98%)	123 (84%)	24 (16%)	2	15
14	L	154/159 (97%)	140 (91%)	14 (9%)	9	36
15	M	107/109 (98%)	92 (86%)	15 (14%)	3	20
16	N	175/176 (99%)	162 (93%)	13 (7%)	13	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	O	160/324 (49%)	134 (84%)	26 (16%)	2	15
18	P	140/146 (96%)	120 (86%)	20 (14%)	3	19
19	Q	150/151 (99%)	133 (89%)	17 (11%)	6	28
20	R	153/154 (99%)	132 (86%)	21 (14%)	3	21
21	S	156/156 (100%)	143 (92%)	13 (8%)	11	40
22	T	136/137 (99%)	117 (86%)	19 (14%)	3	20
23	U	87/107 (81%)	81 (93%)	6 (7%)	15	46
24	V	104/105 (99%)	93 (89%)	11 (11%)	6	30
25	W	53/129 (41%)	48 (91%)	5 (9%)	8	35
26	X	104/118 (88%)	88 (85%)	16 (15%)	2	17
27	Y	109/110 (99%)	99 (91%)	10 (9%)	9	36
28	Z	115/116 (99%)	101 (88%)	14 (12%)	5	24
29	a	118/119 (99%)	107 (91%)	11 (9%)	9	35
30	b	46/47 (98%)	40 (87%)	6 (13%)	4	22
31	c	81/88 (92%)	70 (86%)	11 (14%)	3	21
32	d	92/97 (95%)	80 (87%)	12 (13%)	4	22
33	e	109/111 (98%)	96 (88%)	13 (12%)	5	25
34	f	90/91 (99%)	83 (92%)	7 (8%)	12	42
35	g	95/103 (92%)	84 (88%)	11 (12%)	5	27
36	h	104/105 (99%)	88 (85%)	16 (15%)	2	17
37	i	81/82 (99%)	71 (88%)	10 (12%)	4	24
38	j	70/71 (99%)	62 (89%)	8 (11%)	5	27
39	k	68/69 (99%)	50 (74%)	18 (26%)	0	3
40	l	45/46 (98%)	38 (84%)	7 (16%)	2	17
41	m	47/116 (40%)	44 (94%)	3 (6%)	17	48
42	n	23/23 (100%)	18 (78%)	5 (22%)	1	7
43	o	90/91 (99%)	75 (83%)	15 (17%)	2	14
44	p	71/72 (99%)	61 (86%)	10 (14%)	3	20
45	t	198/198 (100%)	161 (81%)	37 (19%)	1	10
All	All	5378/5853 (92%)	4734 (88%)	644 (12%)	8	25

5 of 644 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
31	c	41	LEU
40	l	51	ILE
32	d	55	LEU
31	c	22	LYS
36	h	44	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 67 such sidechains are listed below:

Mol	Chain	Res	Type
40	l	4	GLN
40	l	50	ASN
45	t	199	GLN
12	I	163	GLN
12	I	100	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	2683/3397 (78%)	1145 (42%)	379 (14%)
2	3	97/121 (80%)	31 (31%)	10 (10%)
3	4	135/158 (85%)	52 (38%)	14 (10%)
All	All	2915/3676 (79%)	1228 (42%)	403 (13%)

5 of 1228 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	6	A
1	1	9	U
1	1	10	C
1	1	11	A
1	1	15	C

5 of 403 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	2206	G
1	1	2622	C
3	4	112	U
1	1	2267	C
1	1	2458	G

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	1	614
5	B	82
6	C	79
7	D	72
4	A	67
10	G	65
45	t	53
12	I	52
14	L	51
16	N	51
19	Q	48
9	F	48
20	R	46
11	H	46
21	S	46
18	P	43
29	a	41
28	Z	38
13	J	35
24	V	34

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Mol	Chain	Number of breaks
22	T	34
34	f	31
37	i	30
27	Y	30
36	h	30
15	M	28
8	E	27
35	g	27
33	e	26
2	3	26
3	4	26
17	O	25
23	U	24
31	c	24
32	d	23
38	j	22
26	X	22
39	k	20
43	o	17
30	b	17
44	p	17
25	W	16
41	m	14
40	l	12
42	n	6

The worst 5 of 2185 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	R	171:ASP	C	172:ARG	N	8.98
1	t	52:SER	C	53:LEU	N	8.07
1	1	2511:C	O3'	2512:C	P	7.92
1	R	170:ARG	C	171:ASP	N	7.88
1	1	2468:A	O3'	2469:G	P	6.79

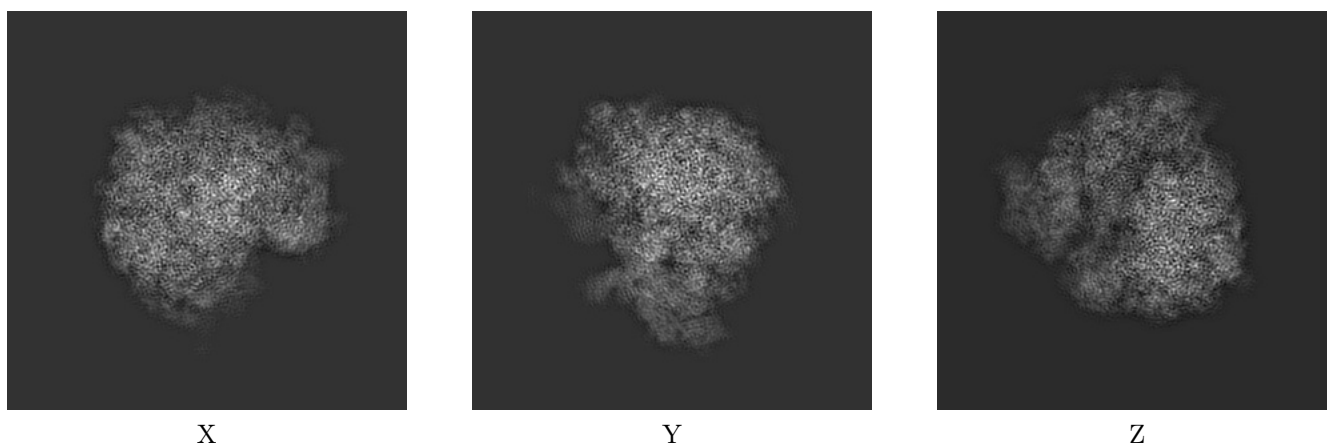
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2599. 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](#)

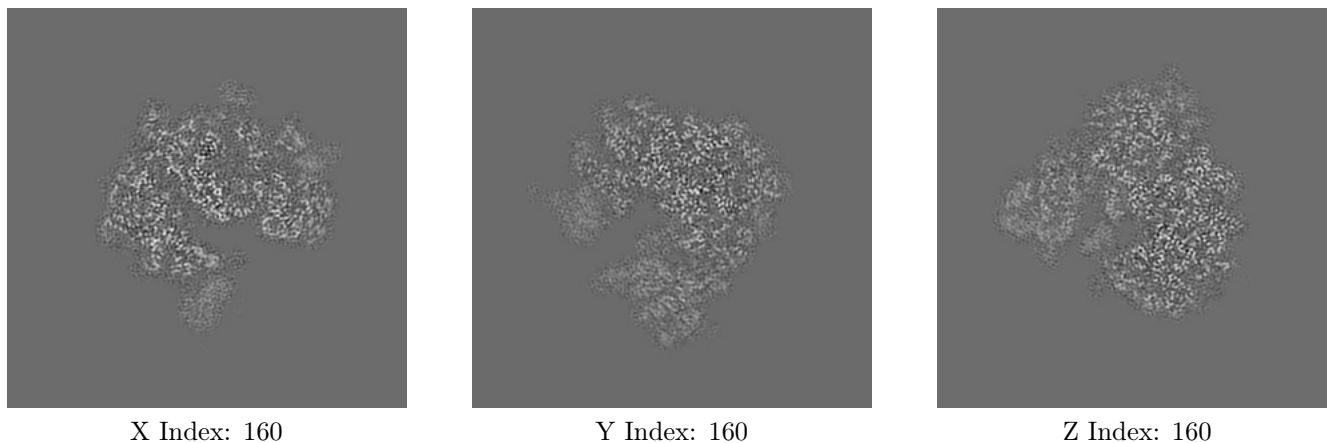
#### 6.1.1 Primary map



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

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

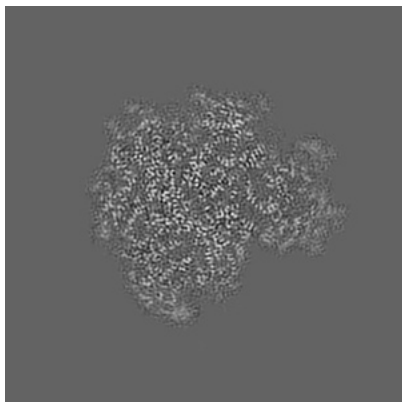
#### 6.2.1 Primary map



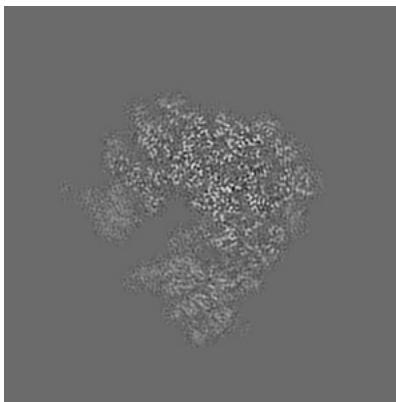
The images above show central slices of the map in three orthogonal directions.

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

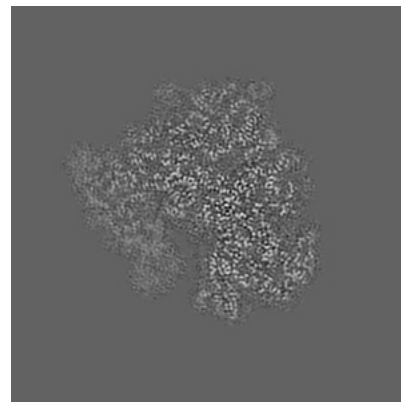
### 6.3.1 Primary map



X Index: 184



Y Index: 160



Z Index: 180

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

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

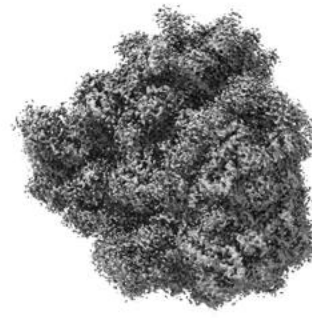
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.



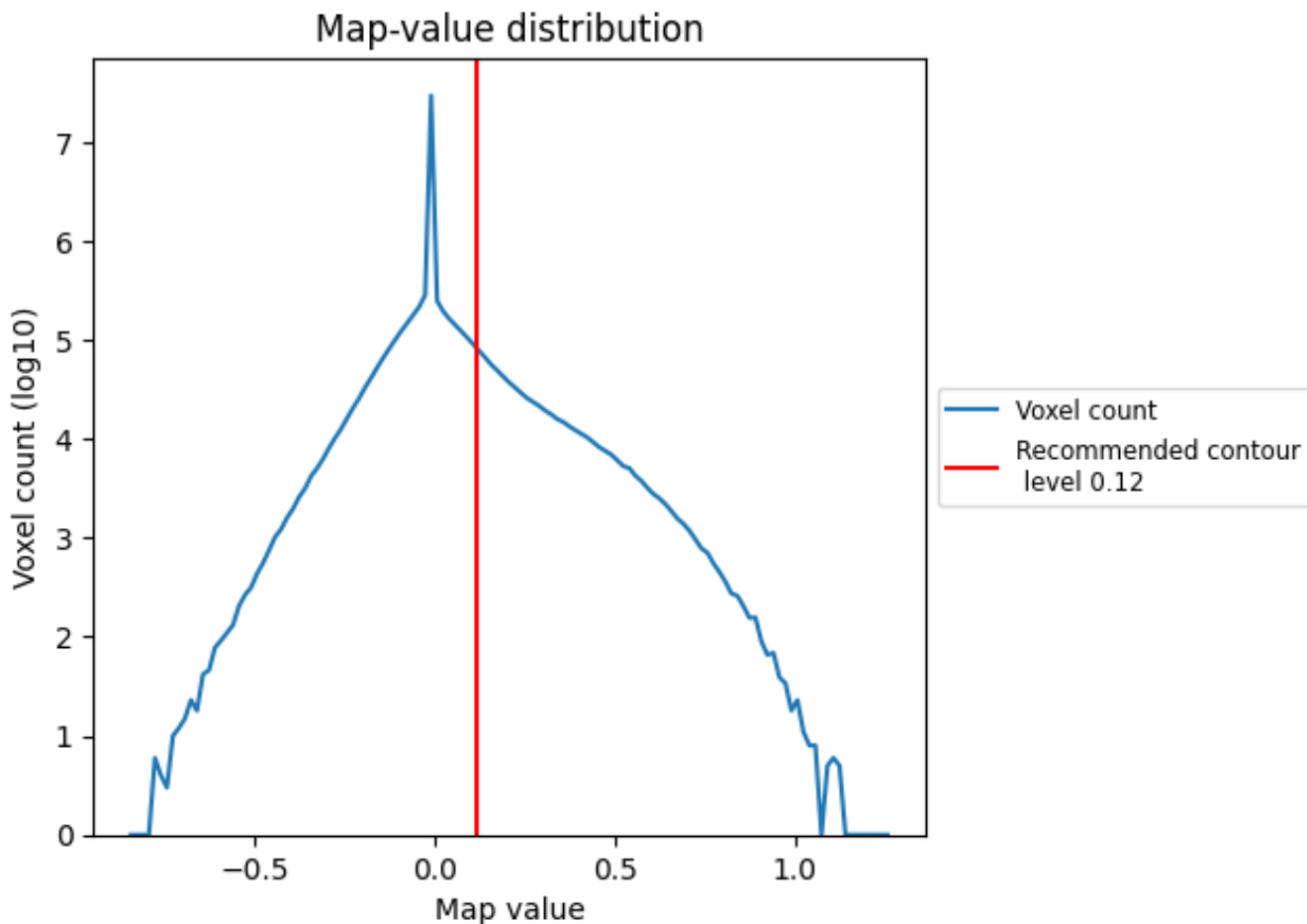
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

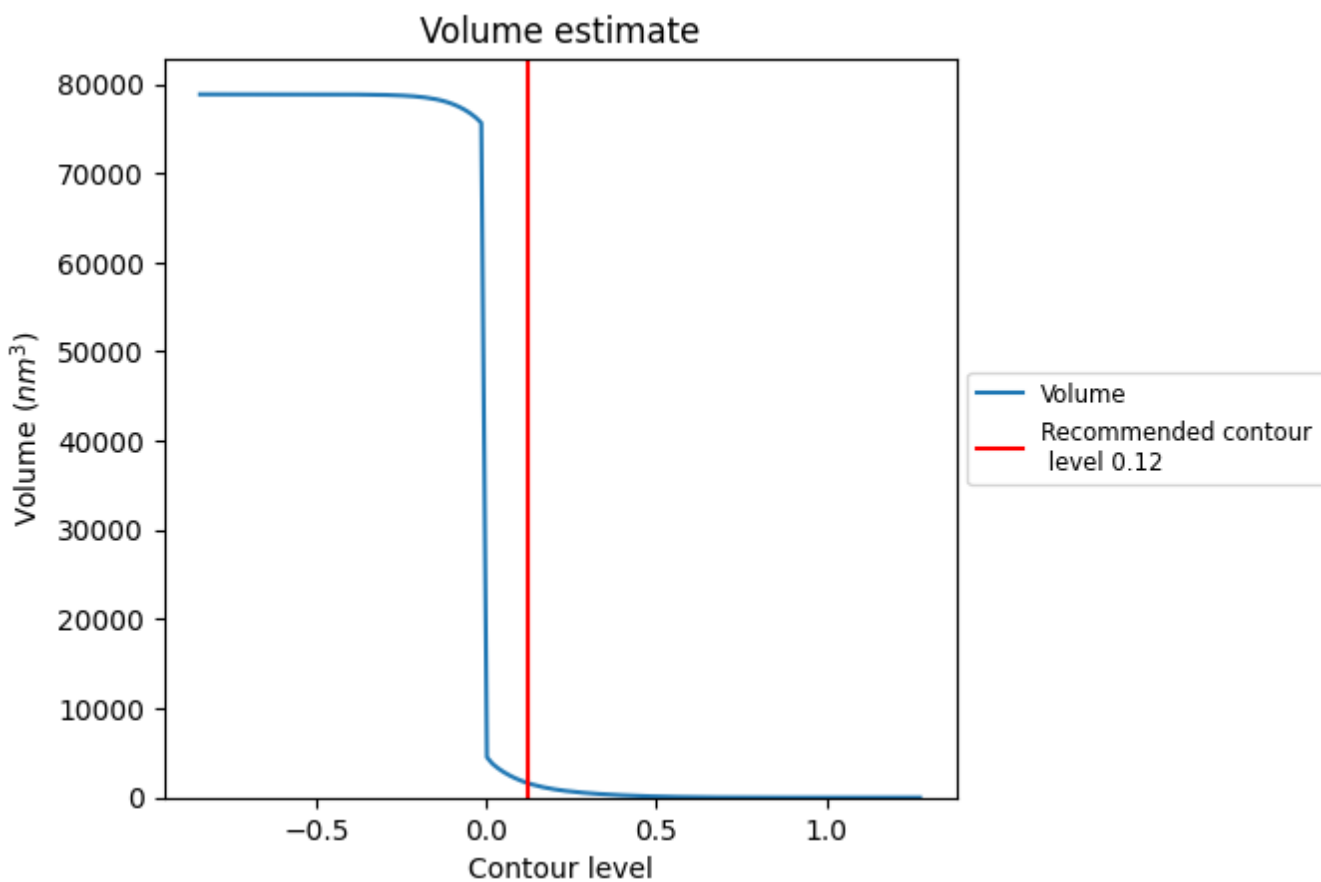
This section contains the results of statistical analysis of the map.

### 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.

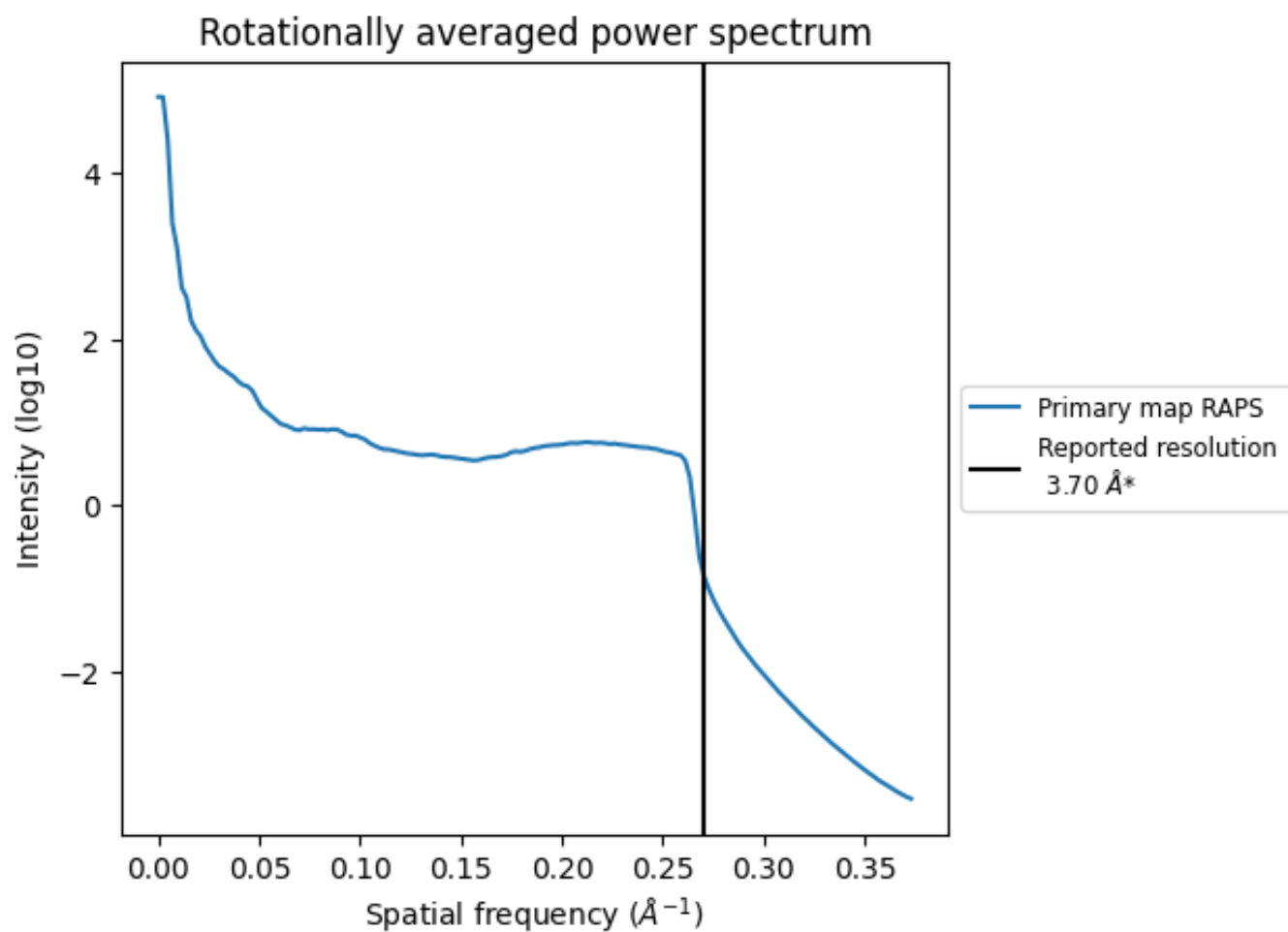
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1648 nm<sup>3</sup>; this corresponds to an approximate mass of 1489 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.270 \text{\AA}^{-1}$

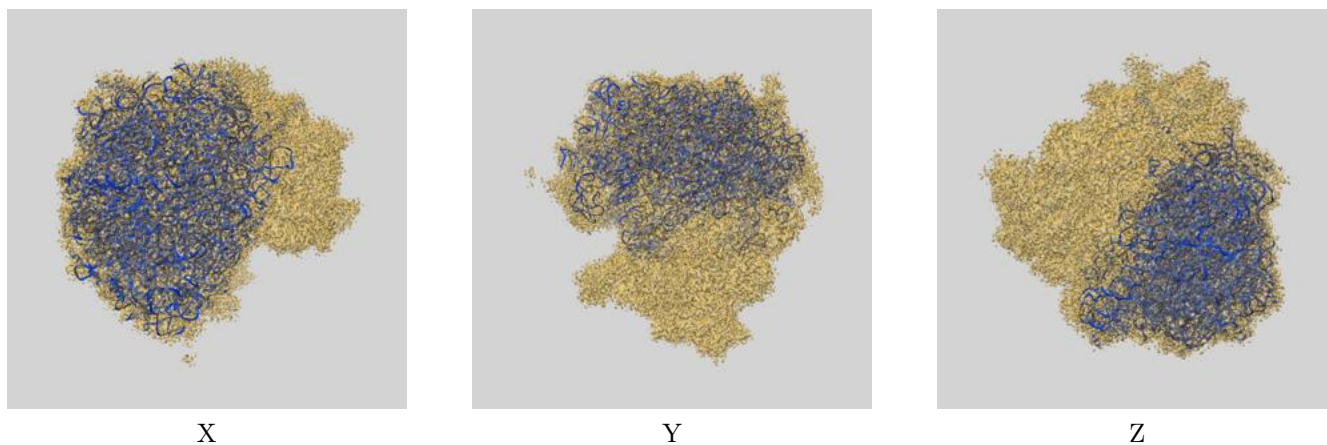
## 8 Fourier-Shell correlation

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

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

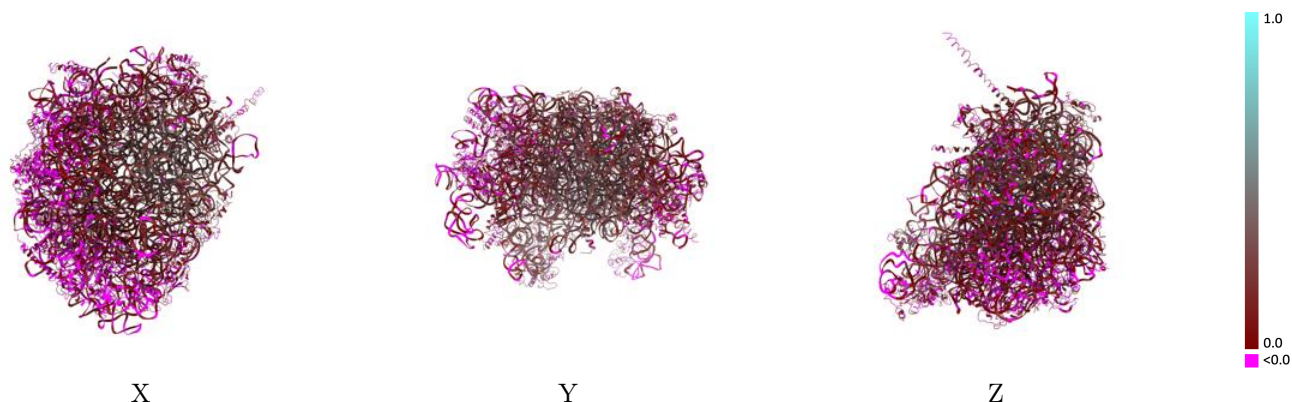
This section contains information regarding the fit between EMDB map EMD-2599 and PDB model 4V91. Per-residue inclusion information can be found in section 3 on page 12.

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



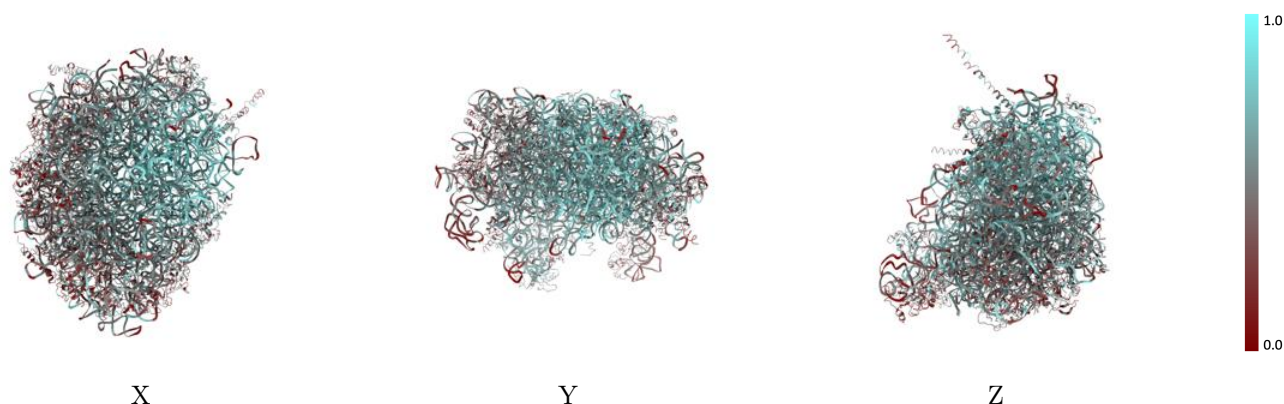
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



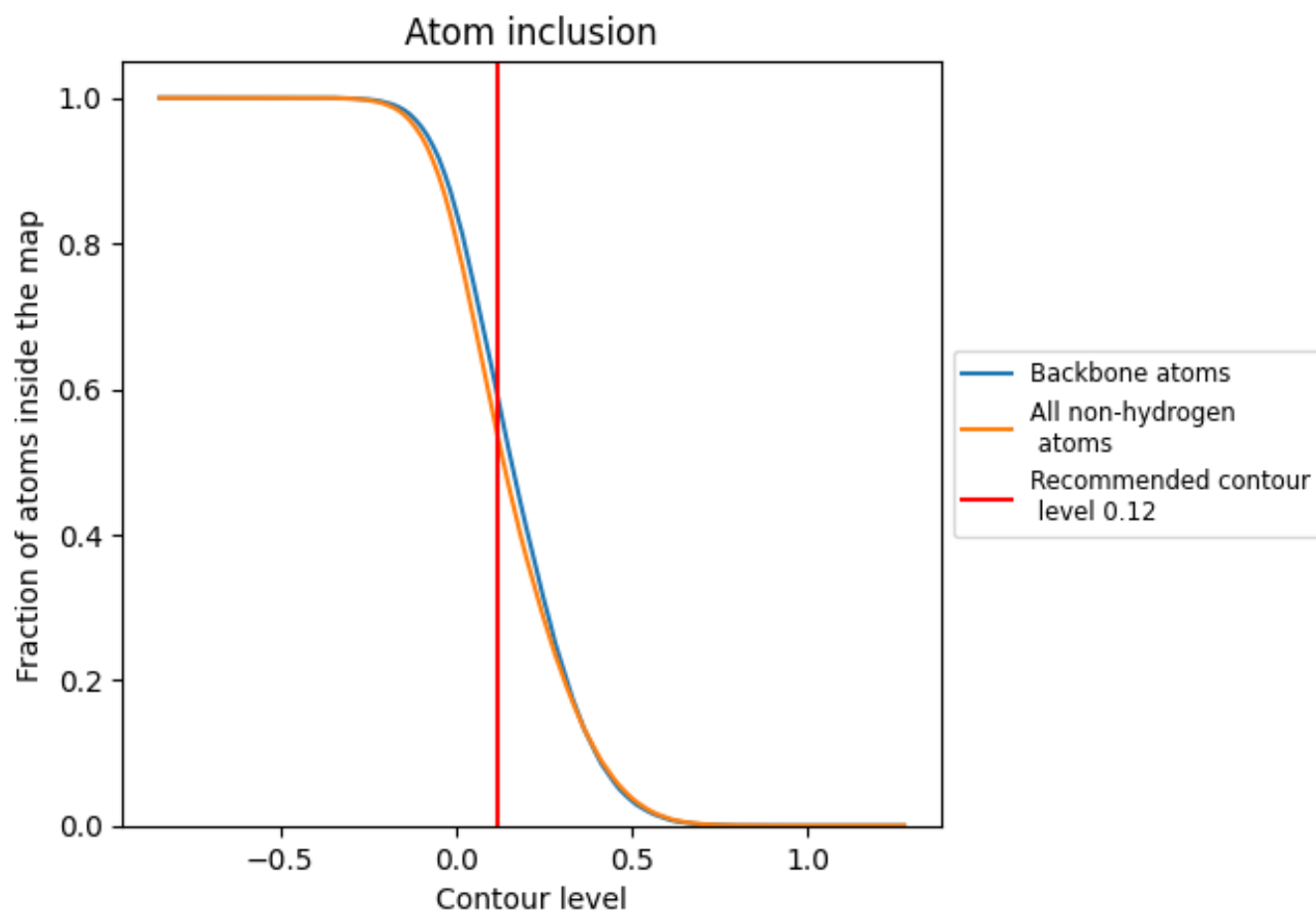
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.12).

## 9.4 Atom inclusion [i](#)









































































At the recommended contour level, 59% of all backbone atoms, 53% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5335	 0.1340
1	 0.5927	 0.1600
3	 0.5979	 0.1370
4	 0.5950	 0.1370
A	 0.5944	 0.2230
B	 0.5264	 0.1570
C	 0.3675	 0.0180
D	 0.4589	 0.1080
E	 0.2869	 -0.0390
F	 0.3605	 0.0040
G	 0.3871	 0.0320
H	 0.3658	 0.0180
I	 0.4837	 0.1280
J	 0.5125	 0.1870
L	 0.3726	 0.0280
M	 0.3109	 -0.0470
N	 0.4643	 0.1000
O	 0.4379	 0.0820
P	 0.5647	 0.1900
Q	 0.3857	 0.0350
R	 0.5888	 0.2100
S	 0.3267	 -0.0120
T	 0.4315	 0.0910
U	 0.5754	 0.2370
V	 0.5587	 0.2220
W	 0.5248	 0.1610
X	 0.5053	 0.1530
Y	 0.4079	 0.0450
Z	 0.3996	 0.0490
a	 0.4054	 0.0640
b	 0.4381	 0.1040
c	 0.4501	 0.1090
d	 0.6471	 0.2700
e	 0.3702	 0.0600
f	 0.3654	 0.0310



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Chain	Atom inclusion	Q-score
g	 0.5452	 0.1720
h	 0.4380	 0.0830
i	 0.3852	 0.0410
j	 0.5878	 0.2040
k	 0.5008	 0.1560
l	 0.5398	 0.2220
m	 0.4367	 0.0880
n	 0.4623	 0.1890
o	 0.5278	 0.1710
p	 0.5800	 0.2120
t	 0.2019	 0.0280