Full wwPDB EM Validation Report ⓘ

Nov 6, 2022 – 06:34 PM EST

PDB ID	:	6C4I
EMDB ID	:	EMD-7341
Title	:	Conformation of methylated GGQ in the peptidyl transferase center during translation termination
Authors	:	Zeng, F.; Jin, H.
Deposited on	:	2018-01-12
Resolution	:	3.24 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

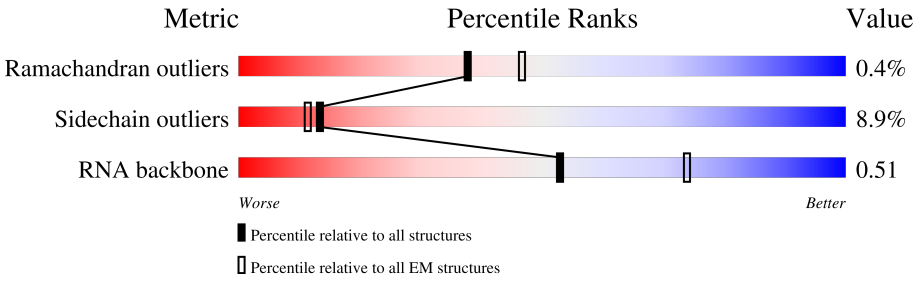
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (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 3.24 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 >=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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2904	14% 79% 20%
2	B	120	28% 85% 15%
3	C	273	8% 93% 7%
4	D	209	13% 94% 6%
5	E	201	38% 93% 7%
6	F	177	86% 89% 11%
7	G	177	59% 93% 6%
8	H	149	93% 89% 11%

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Mol	Chain	Length	Quality of chain
9	I	165	79% 70% 8% 21%
10	J	142	95% 85% 11% 5%
11	K	142	7% 93% 7%
12	L	123	15% 92% 8%
13	M	144	22% 92% 8%
14	N	136	10% 93% 7%
15	O	127	7% 88% 6% 6%
16	P	117	55% 93% 6%
17	Q	115	20% 90% 9%
18	R	118	5% 92% 7%
19	S	103	19% 94% 6%
20	T	110	13% 96%
21	U	100	31% 88% 6% 6%
22	V	104	43% 89% 10%
23	W	94	24% 96%
24	X	85	9% 84% 6% 11%
25	Y	78	22% 97%
26	Z	63	49% 95%
27	0	59	8% 92% 7%
28	1	70	89% 89% 6% 6%
29	2	57	14% 96%
30	3	52	27% 94% 6%
31	4	46	7% 96%
32	5	65	8% 91% 8%
33	6	38	11% 95% 5%

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Mol	Chain	Length	Quality of chain
34	a	1534	49% 81% 19%
35	b	241	92% 88% 5% 7%
36	c	233	84% 85% 11%
37	d	206	96% 94% 6%
38	e	167	77% 86% 8% 7%
39	f	135	55% 69% 8% 23%
40	g	179	81% 77% 7% 15%
41	h	130	83% 94% 5%
42	i	130	95% 89% 8%
43	j	103	96% 81% 15%
44	k	129	50% 84% 6% 9%
45	l	124	51% 85% 14%
46	m	118	92% 92% 7%
47	n	101	98% 90% 9%
48	o	89	49% 83% 16%
49	p	82	90% 93% 7%
50	q	84	76% 86% 10% 5%
51	r	66	70% 97%
52	s	92	90% 84% 7% 10%
53	t	87	84% 90% 9%
54	u	71	85% 87% 11%
55	v	384	77% 88% 6% 6%
56	w	57	42% 77% 19%
57	x	77	42% 74% 26%
57	y	77	99% 77% 23%

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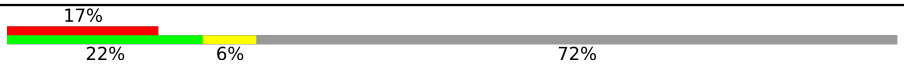
Mol	Chain	Length	Quality of chain
58	z	18	

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 151446 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	2904	62356	27825	11472	20155	2904	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	887	A	U	conflict	GB 687670942

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	120	2569	1144	468	837	120	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	271	2082	1288	423	364	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	209	1565	979	288	294	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	201	1552	974	283	290	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	175	Total	C	N	O	S	0	0
			1313	826	241	244	2		

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 9 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	130	Total	C	N	O	S	0	0
			980	620	174	182	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	135	Total	C	N	O	S	0	0
			984	622	171	185	6		

- Molecule 11 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 12 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 13 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 14 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 15 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	119	Total	C	N	O	S	0	0
			951	588	195	163	5		

- Molecule 16 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	P	116	Total	C	N	O	0	0
			892	552	178	162		

- Molecule 17 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 18 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	R	117	Total	C	N	O	0	0
			947	604	192	151		

- Molecule 19 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 20 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 21 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	94	Total	C	N	O	S	0	0
			746	470	140	134	2		

- Molecule 22 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	V	103	Total	C	N	O	0	0
			788	498	148	142		

- Molecule 23 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	76	Total	C	N	O	S	0	0
			582	360	117	104	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	0	58	Total	C	N	O	S	0	0
			448	281	87	78	2		

- Molecule 28 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	1	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

- Molecule 29 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	2	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 30 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	3	52	Total	C	N	O	0	0
			426	275	78	73		

- Molecule 31 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	4	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 32 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	5	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 33 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	6	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 34 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	a	1534	Total	C	N	O	P	0	0
			32929	14693	6041	10661	1534		

- Molecule 35 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	b	225	Total	C	N	O	S	0	0
			1760	1113	316	323	8		

- Molecule 36 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	c	208	Total	C	N	O	S	0	0
			1636	1036	307	290	3		

- Molecule 37 is a protein called 30S ribosomal protein S4.

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

- Molecule 38 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	e	156	Total	C	N	O	S	0	0
			1152	717	217	212	6		

- Molecule 39 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	f	104	Total	C	N	O	S	0	0
			848	536	153	152	7		

- Molecule 40 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	g	152	Total	C	N	O	S	0	0
			1191	741	230	216	4		

- Molecule 41 is a protein called 30S ribosomal protein S8.

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

- Molecule 42 is a protein called 30S ribosomal protein S9.

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

- Molecule 43 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	j	99	Total	C	N	O	S	0	0
			790	495	151	143	1		

- Molecule 44 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	k	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 45 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	l	123	Total	C	N	O	S	0	0
			957	591	196	165	5		

- Molecule 46 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	m	116	Total	C	N	O	S	0	0
			900	558	181	158	3		

- Molecule 47 is a protein called 30S ribosomal protein S14.

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

- Molecule 48 is a protein called 30S ribosomal protein S15.

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

- Molecule 49 is a protein called 30S ribosomal protein S16.

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

- Molecule 50 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	q	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 51 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	r	66	Total	C	N	O	S	0	0
			544	344	102	97	1		

- Molecule 52 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	s	83	Total	C	N	O	S	0	0
			663	424	126	111	2		

- Molecule 53 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	t	86	Total	C	N	O	S	0	0
			669	414	138	114	3		

- Molecule 54 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	u	70	Total	C	N	O	S	0	0
			589	366	125	97	1		

- Molecule 55 is a protein called Peptide chain release factor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	v	362	Total	C	N	O	S	0	0
			2869	1765	504	590	10		

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
v	-18	ALA	-	expression tag	UNP P07012
v	-17	HIS	-	expression tag	UNP P07012
v	-16	HIS	-	expression tag	UNP P07012
v	-15	HIS	-	expression tag	UNP P07012
v	-14	HIS	-	expression tag	UNP P07012
v	-13	HIS	-	expression tag	UNP P07012
v	-12	HIS	-	expression tag	UNP P07012
v	-11	SER	-	expression tag	UNP P07012
v	-10	ALA	-	expression tag	UNP P07012
v	-9	ALA	-	expression tag	UNP P07012
v	-8	LEU	-	expression tag	UNP P07012
v	-7	GLU	-	expression tag	UNP P07012
v	-6	VAL	-	expression tag	UNP P07012
v	-5	LEU	-	expression tag	UNP P07012
v	-4	PHE	-	expression tag	UNP P07012
v	-3	GLN	-	expression tag	UNP P07012
v	-2	GLY	-	expression tag	UNP P07012
v	-1	PRO	-	expression tag	UNP P07012
v	0	GLY	-	expression tag	UNP P07012

- Molecule 56 is a protein called Alternative ribosome-rescue factor A.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	w	46	Total	C	N	O	S	0	0
			377	234	77	64	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
w	-1	GLY	-	expression tag	UNP P36675
w	0	SER	-	expression tag	UNP P36675

- Molecule 57 is a RNA chain called E-site or P-site tRNA fMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	x	77	Total	C	N	O	P	0	0
			1643	732	297	537	77		

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Mol	Chain	Residues	Atoms					AltConf	Trace
57	y	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		

- Molecule 58 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	z	5	Total	C	N	O	P	0	0
			109	49	22	33	5		

- Molecule 59 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
59	A	230	Total	Mg	0
			230	230	
59	B	5	Total	Mg	0
			5	5	
59	C	1	Total	Mg	0
			1	1	
59	D	1	Total	Mg	0
			1	1	
59	O	2	Total	Mg	0
			2	2	
59	2	1	Total	Mg	0
			1	1	
59	a	71	Total	Mg	0
			71	71	
59	d	1	Total	Mg	0
			1	1	
59	n	1	Total	Mg	0
			1	1	
59	x	4	Total	Mg	0
			4	4	

- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
60	1	1	Total	Zn	0
			1	1	
60	6	1	Total	Zn	0
			1	1	

- Molecule 61 is water.

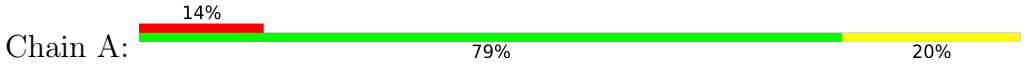
Mol	Chain	Residues	Atoms		AltConf
61	C	2	Total	O	0
			2	2	

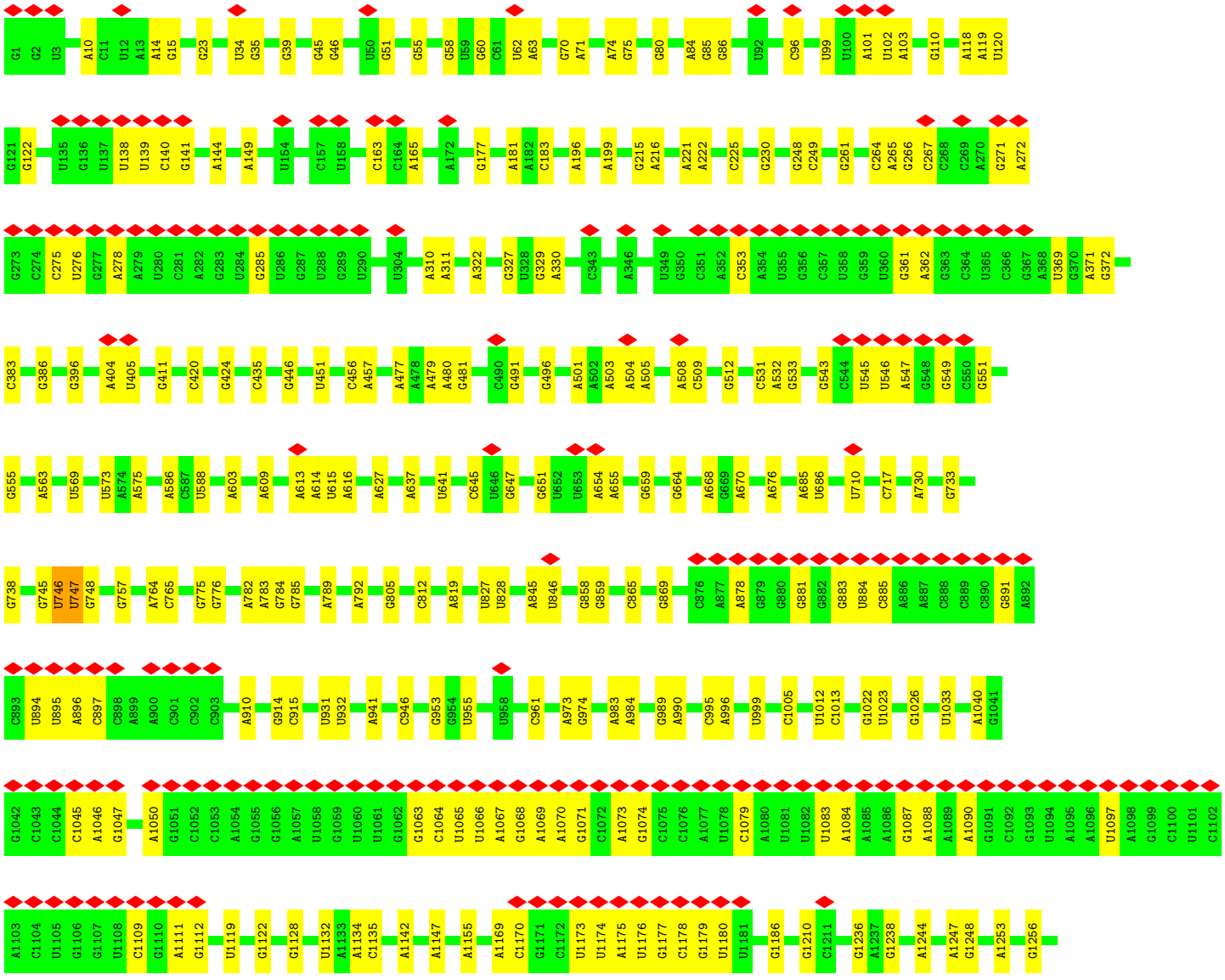
3 Residue-property plots (i)

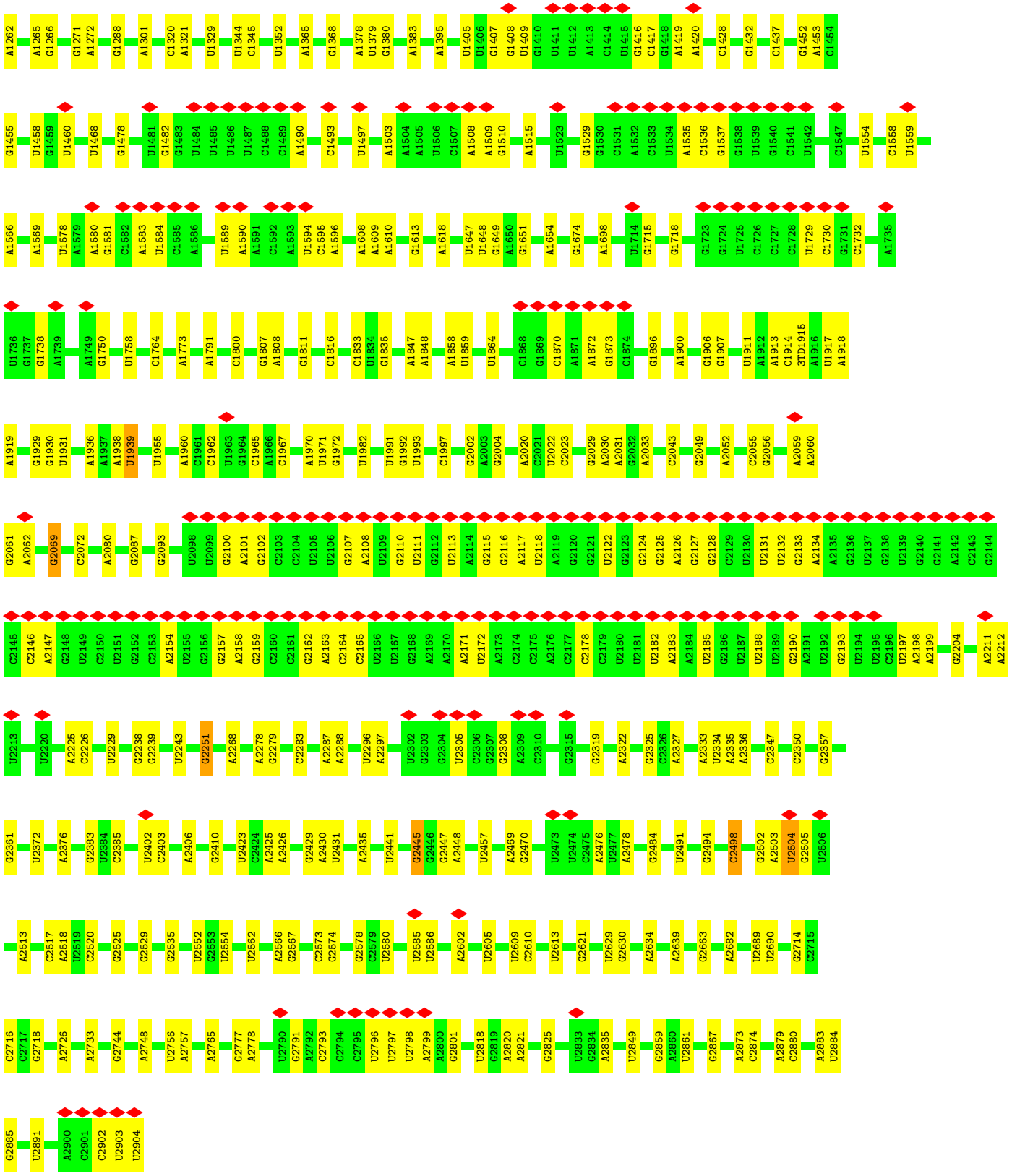
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: 23S rRNA

Chain A:

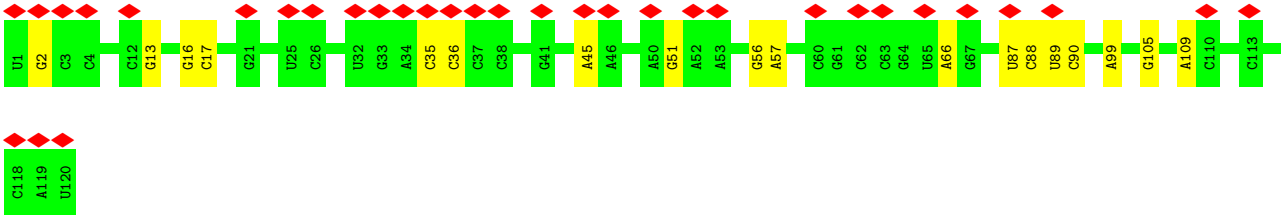






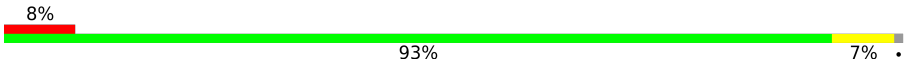
- Molecule 2: 5S rRNA

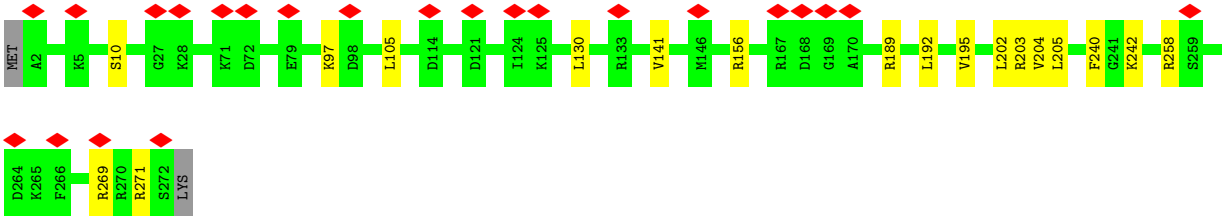
Chain B:



• Molecule 3: 50S ribosomal protein L2

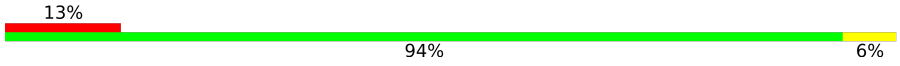
Chain C:

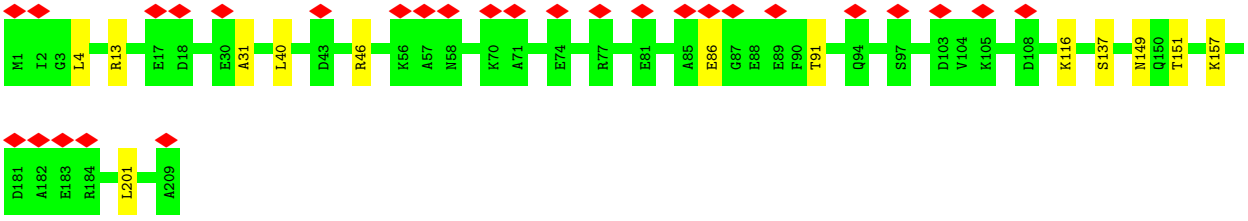




• Molecule 4: 50S ribosomal protein L3

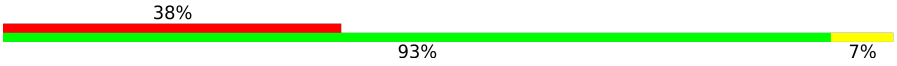
Chain D:

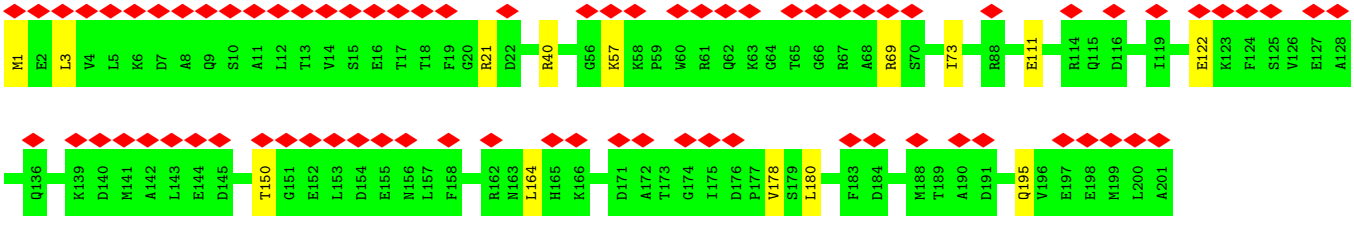




• Molecule 5: 50S ribosomal protein L4

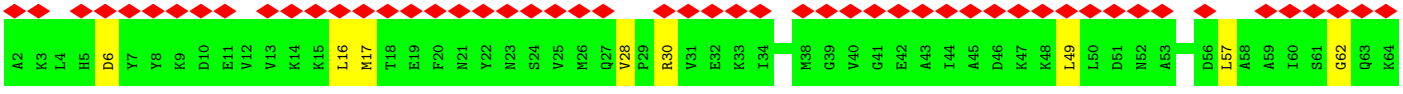
Chain E:

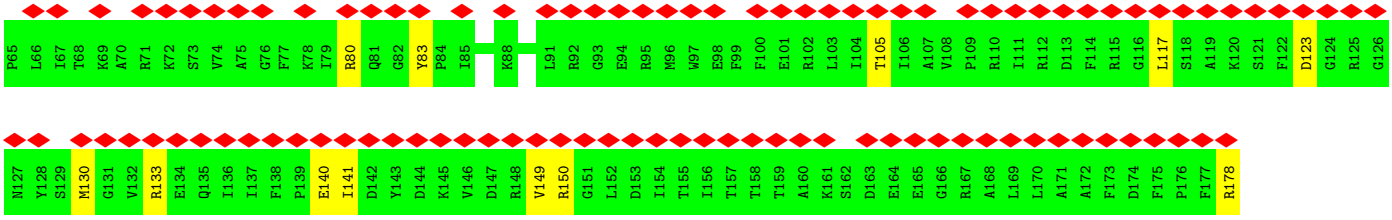




• Molecule 6: 50S ribosomal protein L5

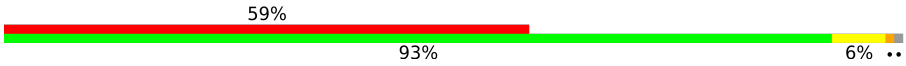
Chain F:

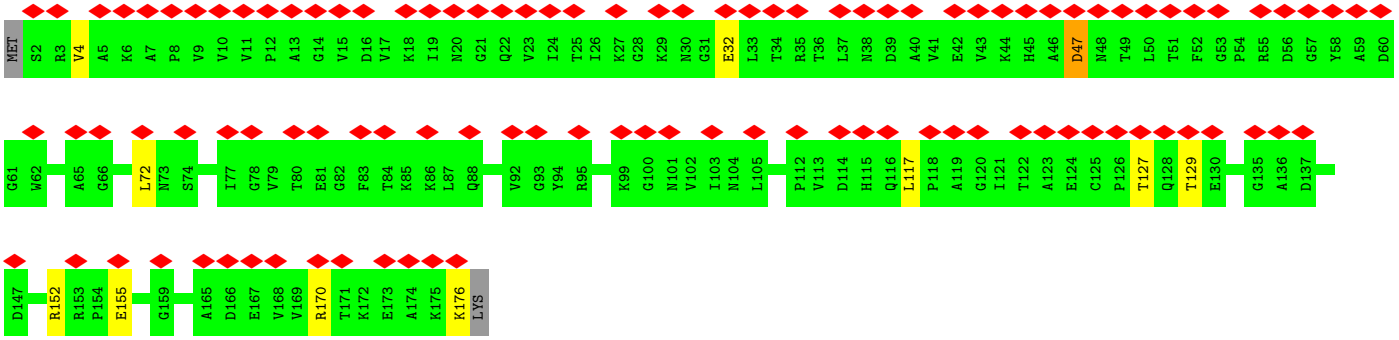




• Molecule 7: 50S ribosomal protein L6

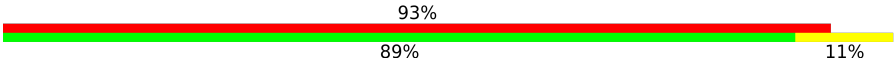
Chain G:

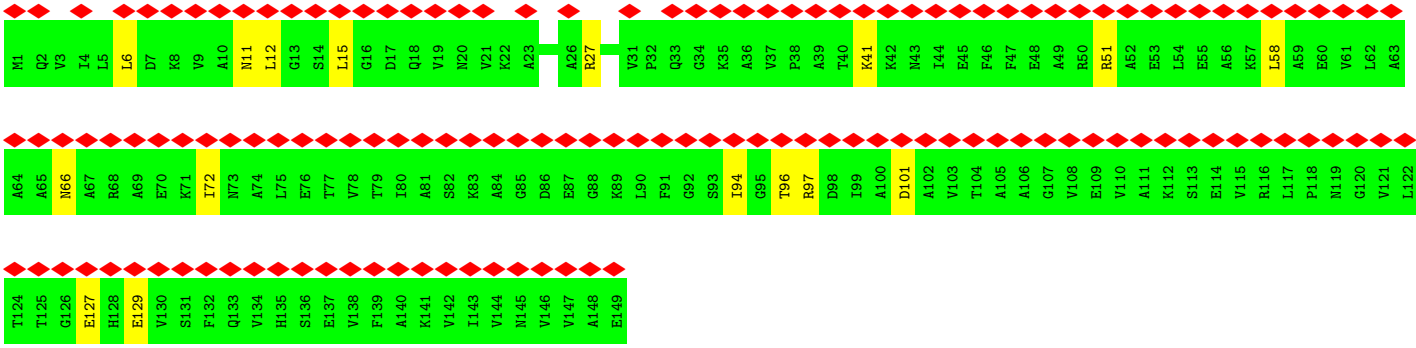




• Molecule 8: 50S ribosomal protein L9

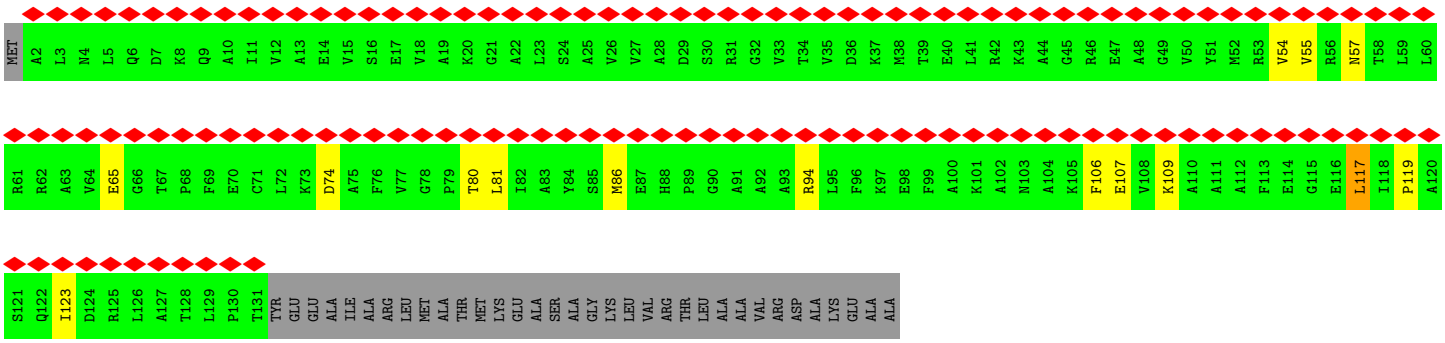
Chain H:





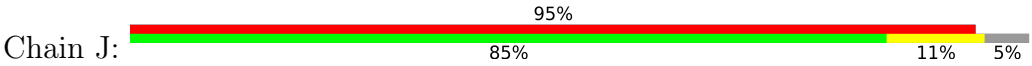
• Molecule 9: 50S ribosomal protein L10

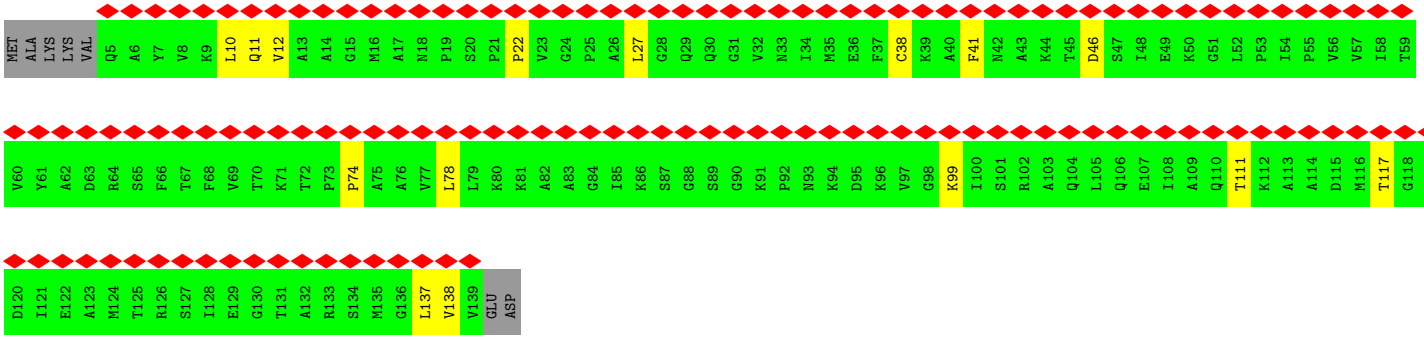
Chain I:



• Molecule 10: 50S ribosomal protein L11

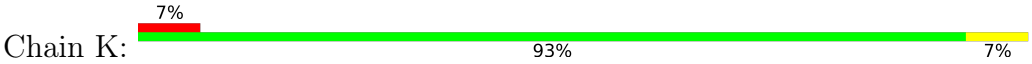
Chain J:

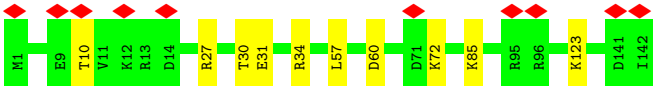




• Molecule 11: 50S ribosomal protein L13

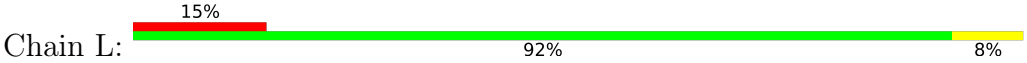
Chain K:

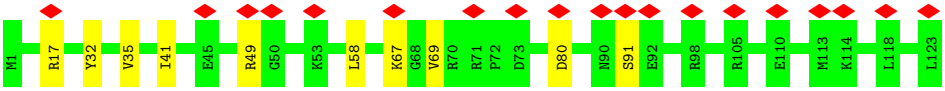




• Molecule 12: 50S ribosomal protein L14

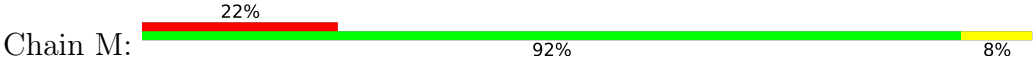
Chain L:

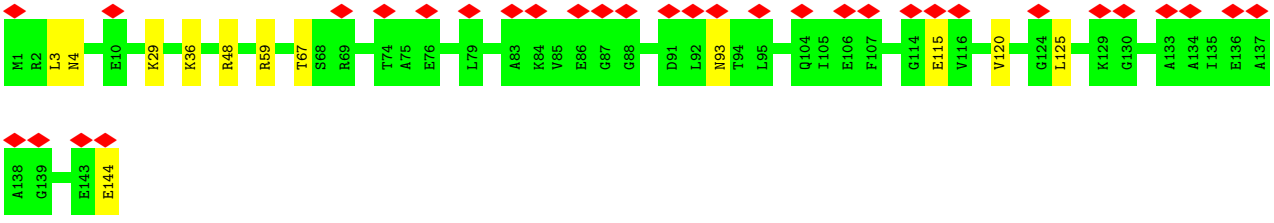




• Molecule 13: 50S ribosomal protein L15

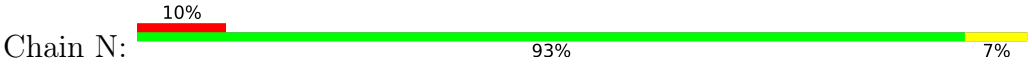
Chain M:

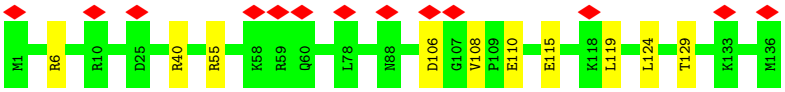




• Molecule 14: 50S ribosomal protein L16

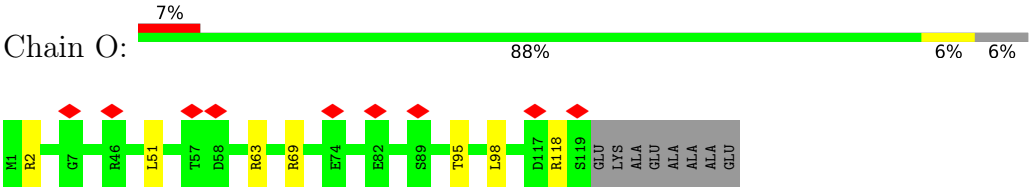
Chain N:





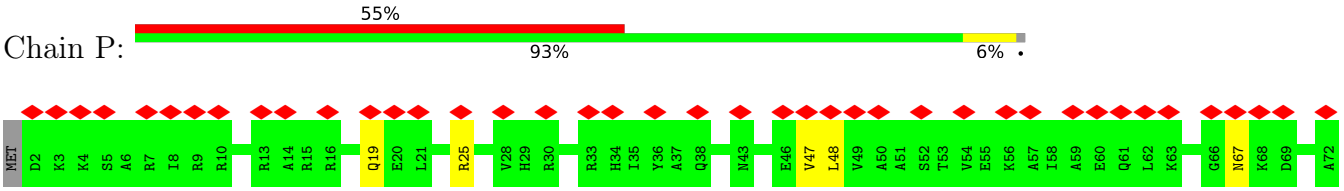
• Molecule 15: 50S ribosomal protein L17

Chain O:



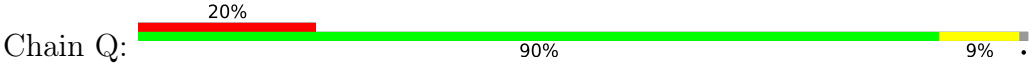
• Molecule 16: 50S ribosomal protein L18

Chain P:



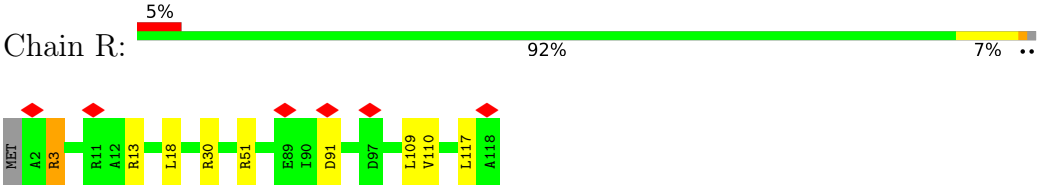
• Molecule 17: 50S ribosomal protein L19

Chain Q:



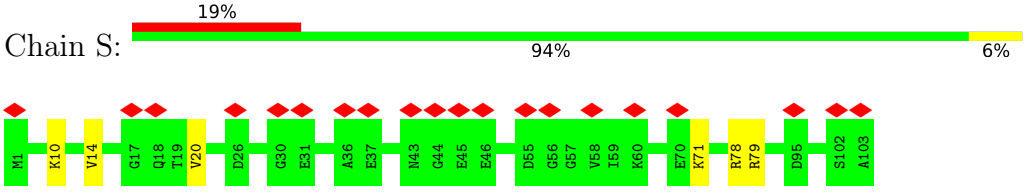
• Molecule 18: 50S ribosomal protein L20

Chain R:



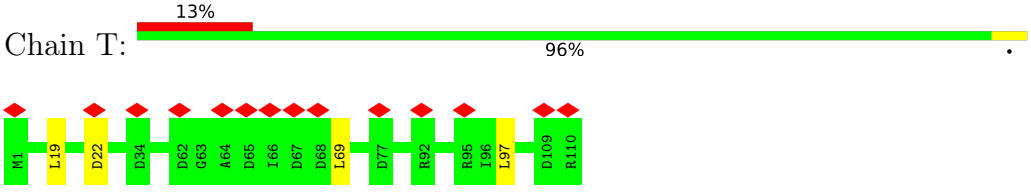
• Molecule 19: 50S ribosomal protein L21

Chain S:



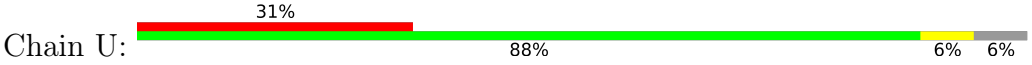
• Molecule 20: 50S ribosomal protein L22

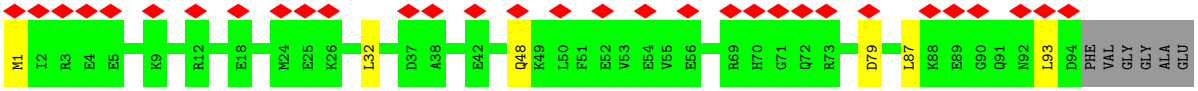
Chain T:



• Molecule 21: 50S ribosomal protein L23

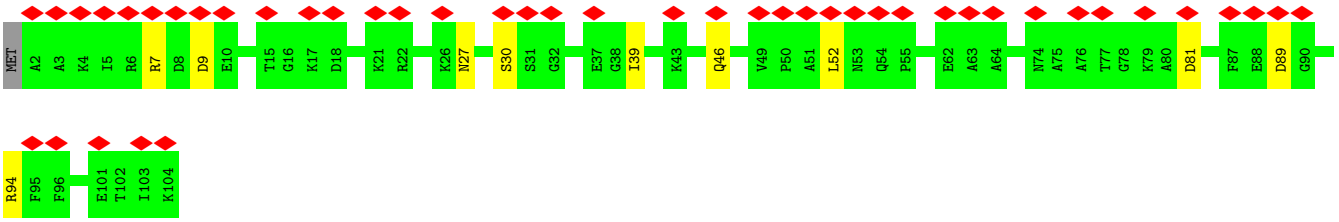
Chain U:





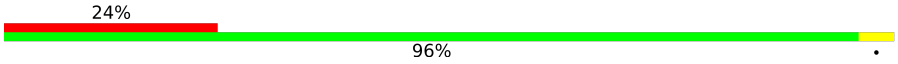
• Molecule 22: 50S ribosomal protein L24

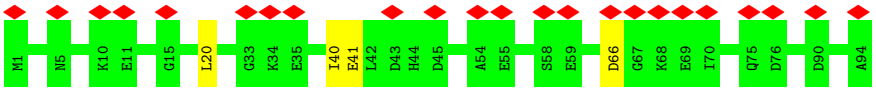
Chain V:



• Molecule 23: 50S ribosomal protein L25

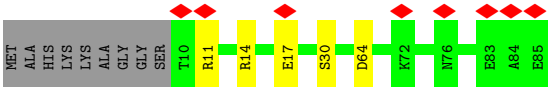
Chain W:





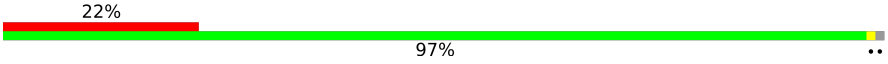
• Molecule 24: 50S ribosomal protein L27

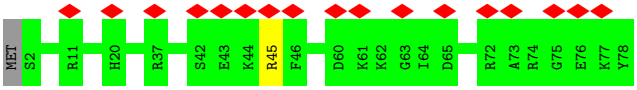
Chain X:



• Molecule 25: 50S ribosomal protein L28

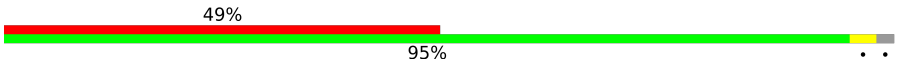
Chain Y:

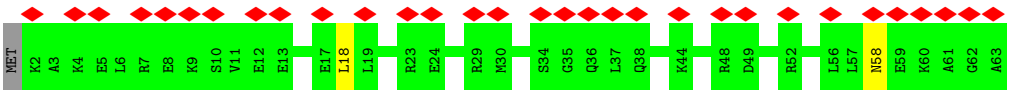




• Molecule 26: 50S ribosomal protein L29

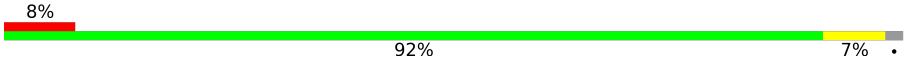
Chain Z:

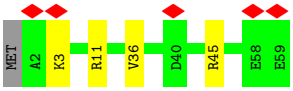




• Molecule 27: 50S ribosomal protein L30

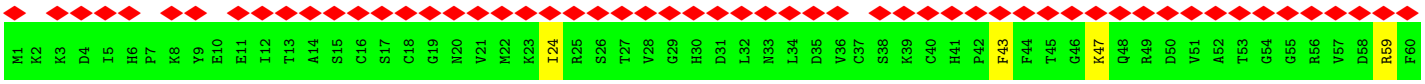
Chain 0:

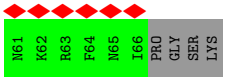




• Molecule 28: 50S ribosomal protein L31

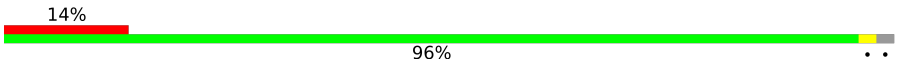
Chain 1:

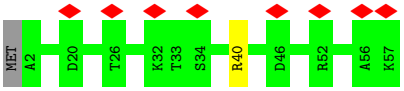




• Molecule 29: 50S ribosomal protein L32

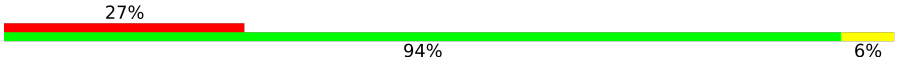
Chain 2:

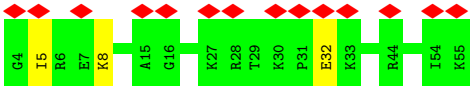




• Molecule 30: 50S ribosomal protein L33

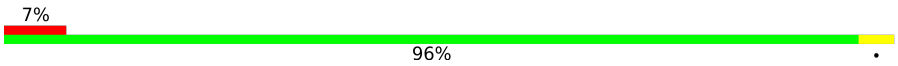
Chain 3:

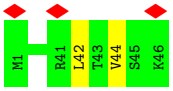




• Molecule 31: 50S ribosomal protein L34

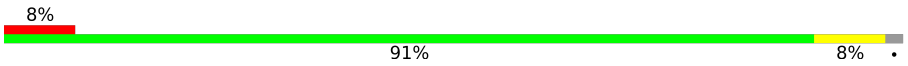
Chain 4:

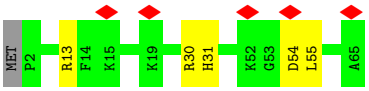




• Molecule 32: 50S ribosomal protein L35

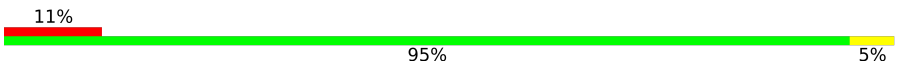
Chain 5:

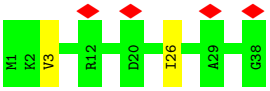




• Molecule 33: 50S ribosomal protein L36

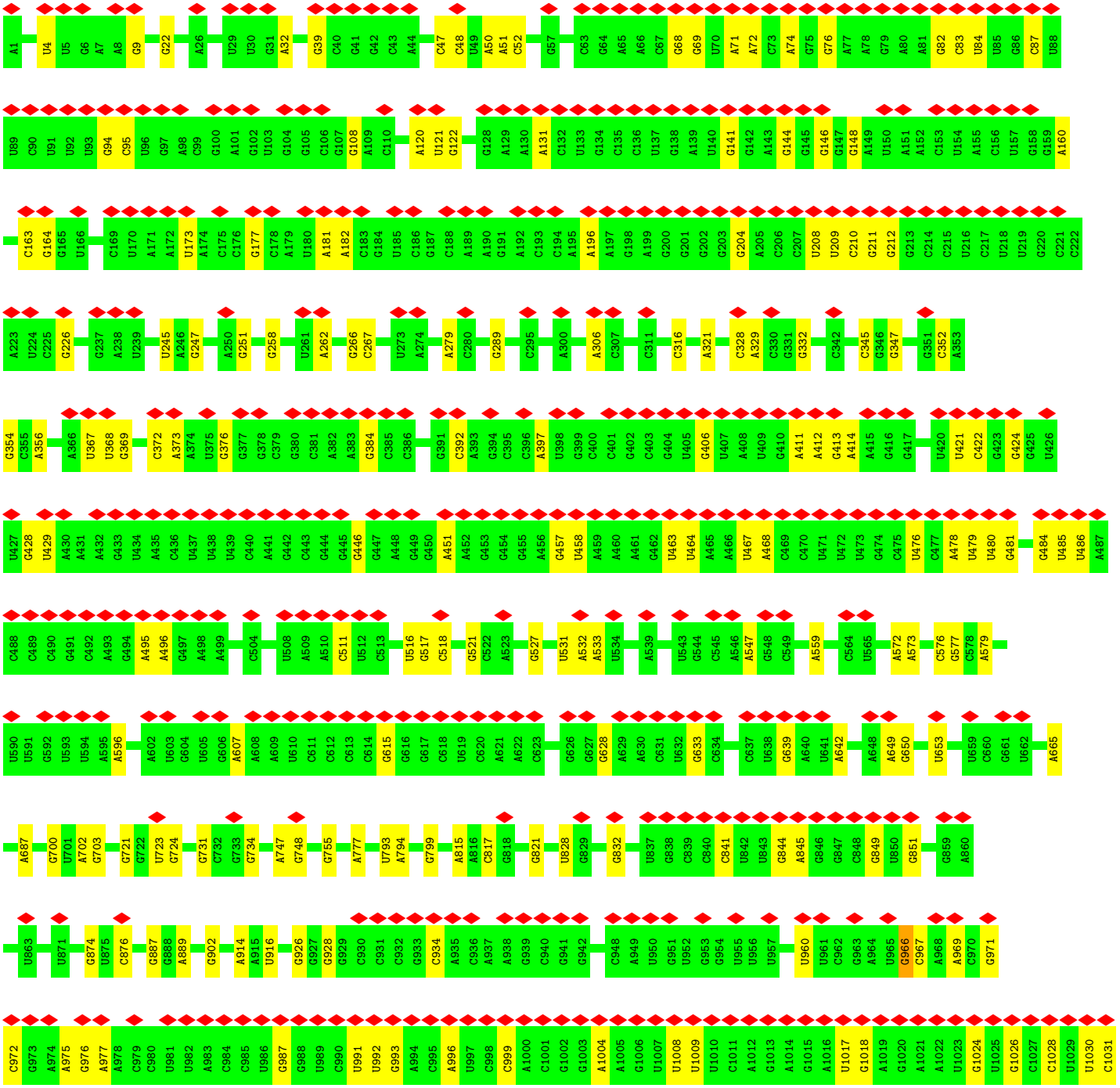
Chain 6:

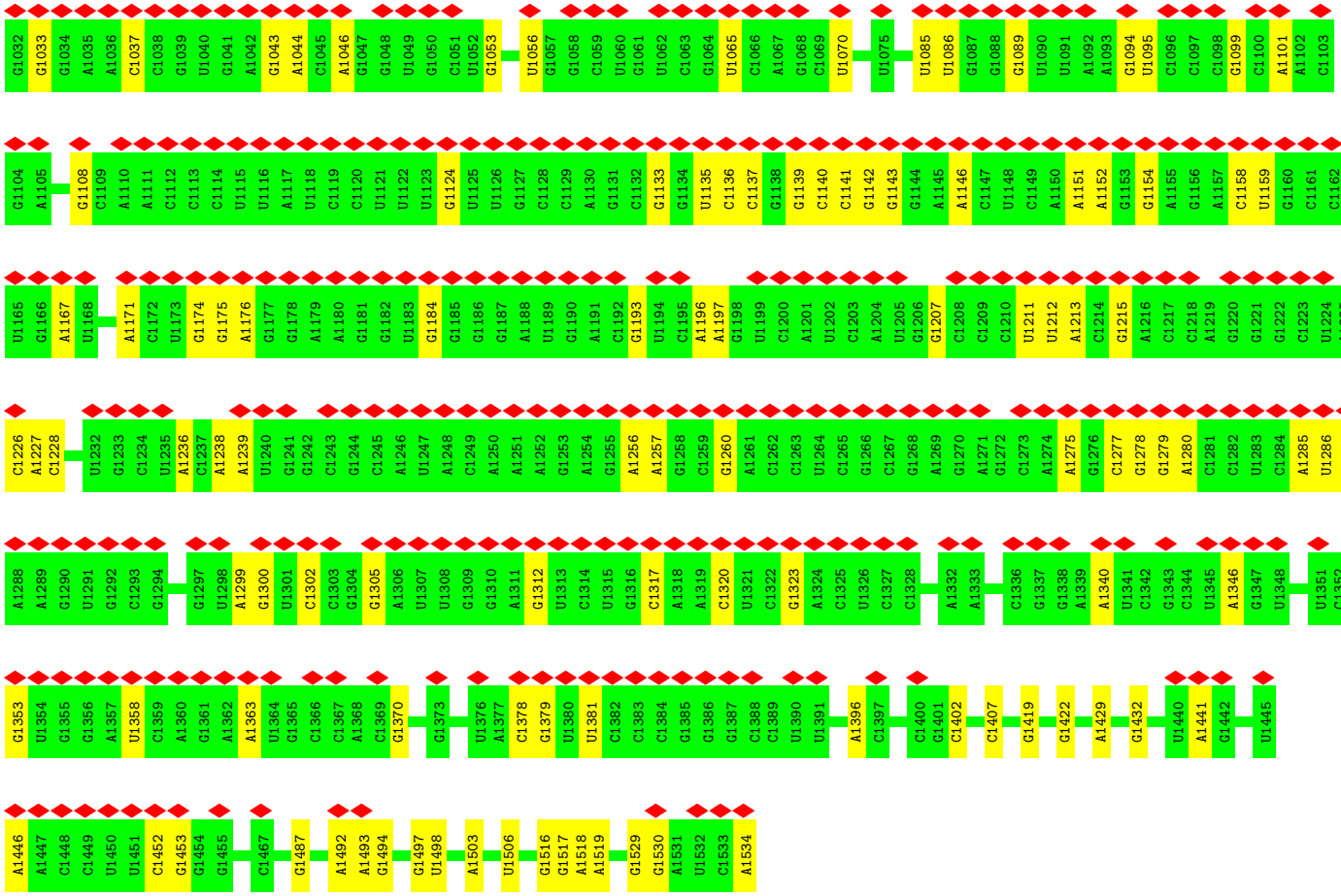




• Molecule 34: 16S rRNA

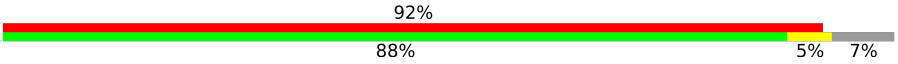
Chain a:

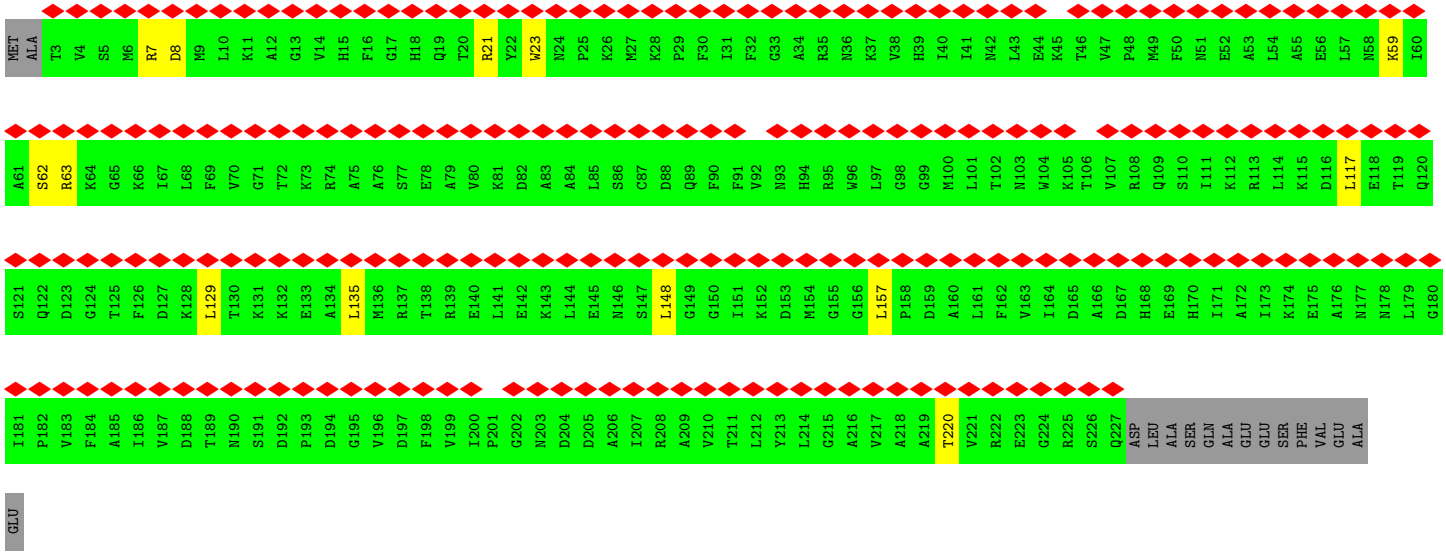




- Molecule 35: 30S ribosomal protein S2

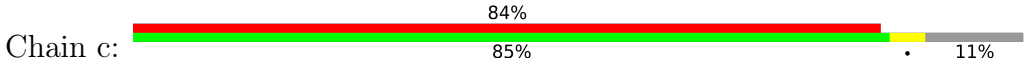
Chain b:

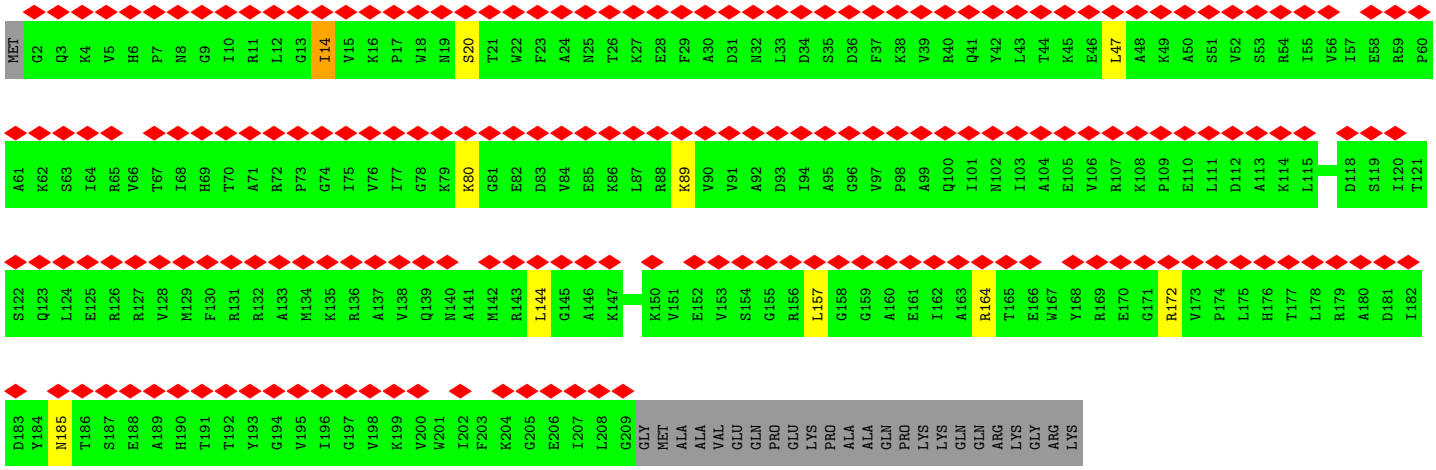




- Molecule 36: 30S ribosomal protein S3

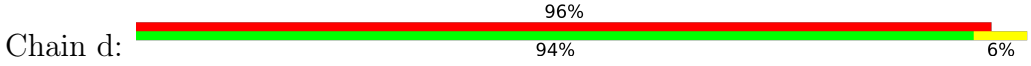
Chain c:

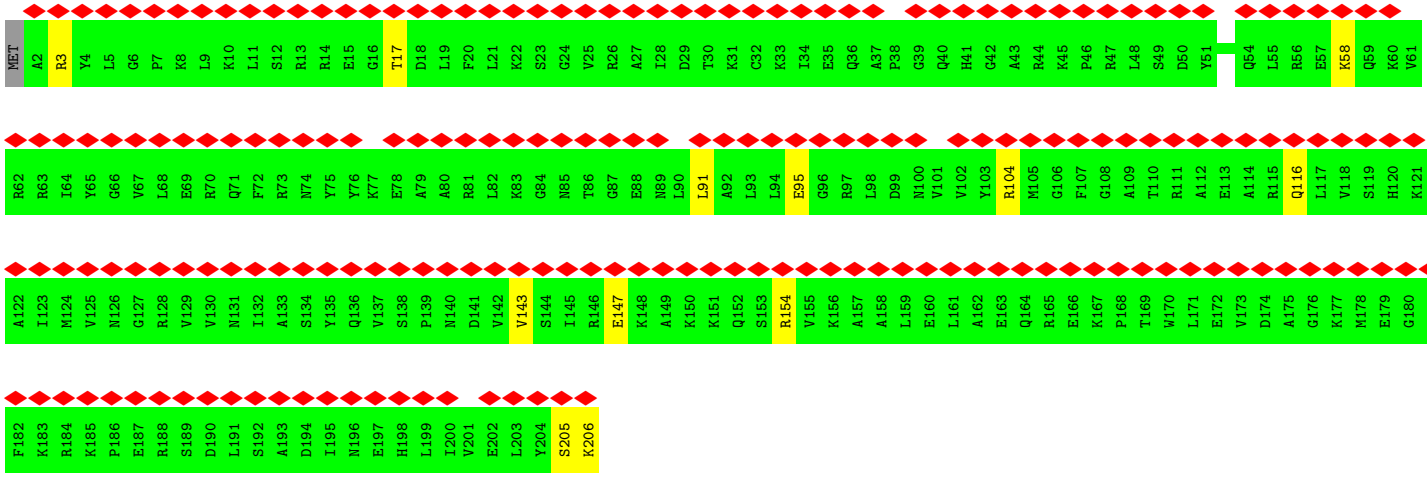




• Molecule 37: 30S ribosomal protein S4

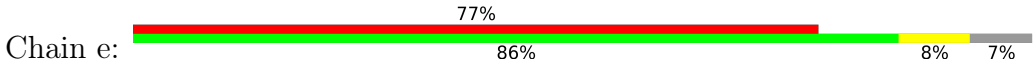
Chain d:

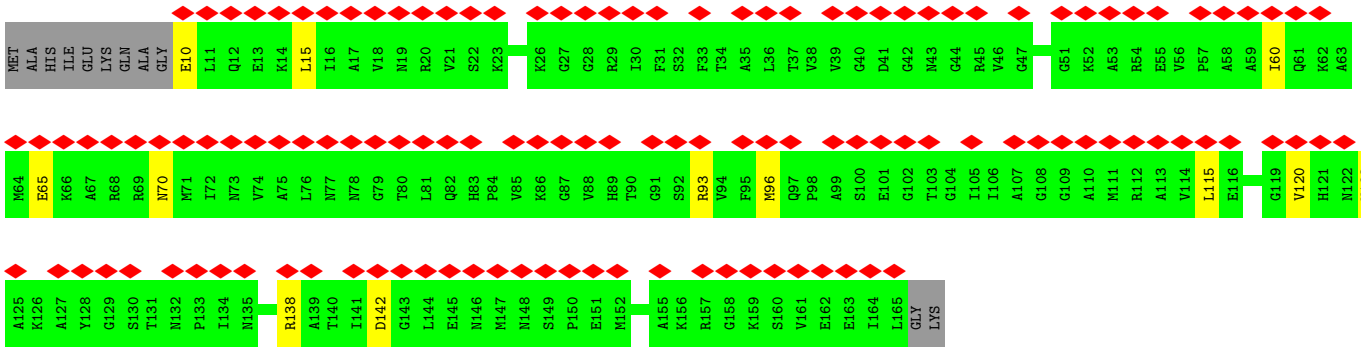




• Molecule 38: 30S ribosomal protein S5

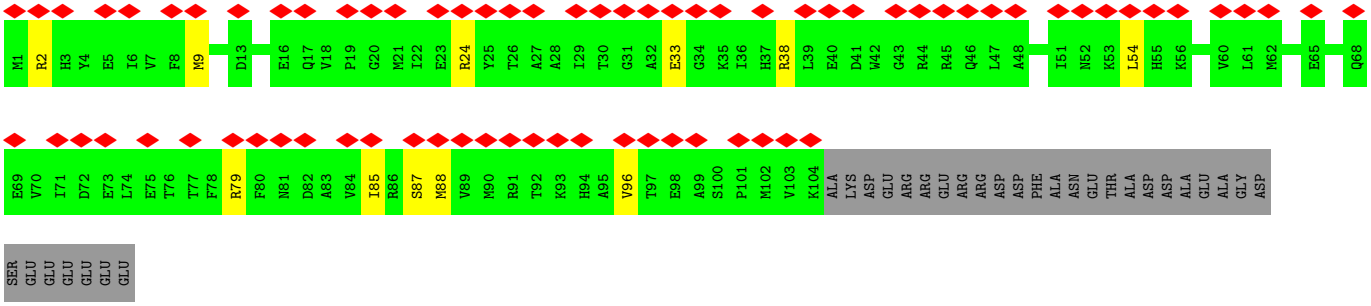
Chain e:





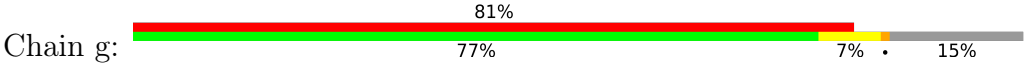
• Molecule 39: 30S ribosomal protein S6

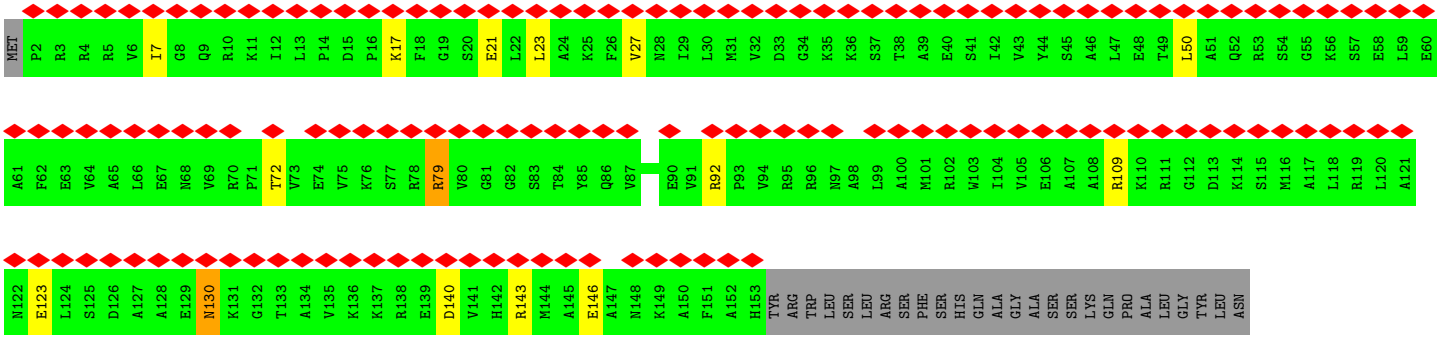
Chain f:



• Molecule 40: 30S ribosomal protein S7

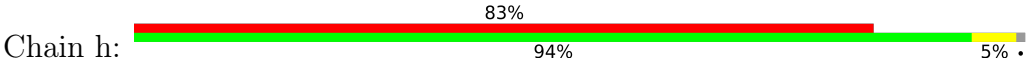
Chain g:

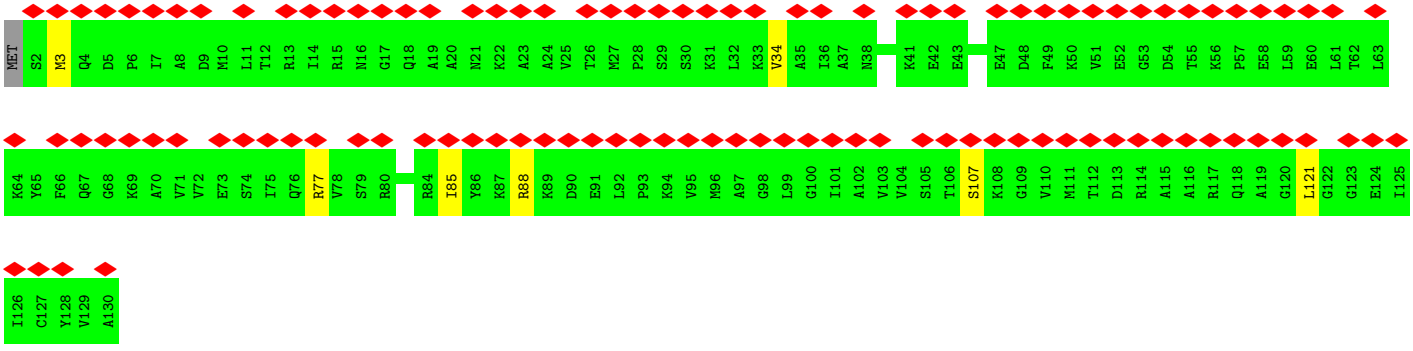




• Molecule 41: 30S ribosomal protein S8

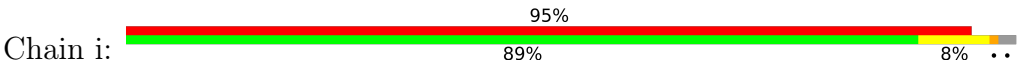
Chain h:

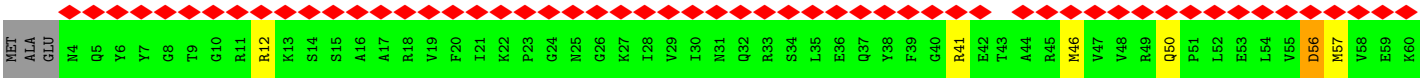


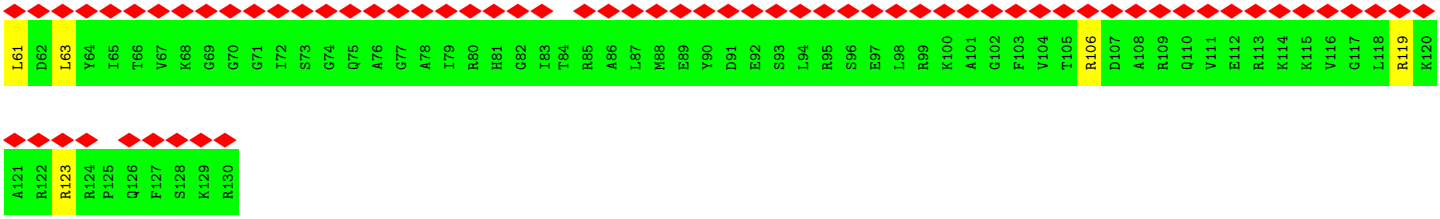


• Molecule 42: 30S ribosomal protein S9

Chain i:

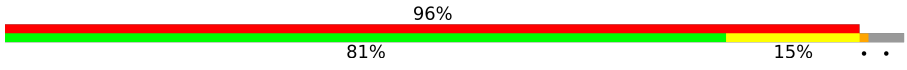






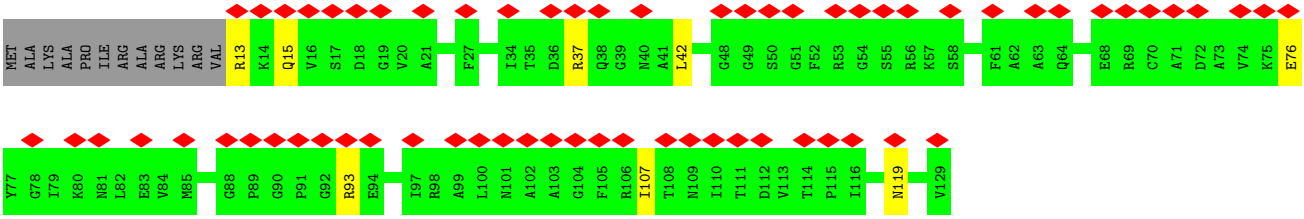
• Molecule 43: 30S ribosomal protein S10

Chain j:



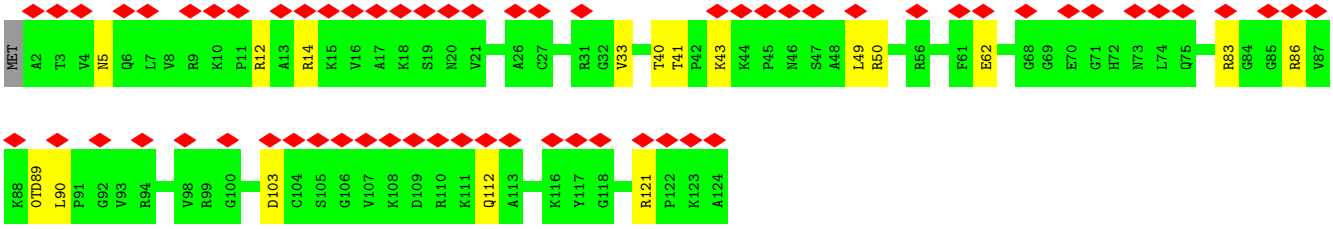
• Molecule 44: 30S ribosomal protein S11

Chain k:



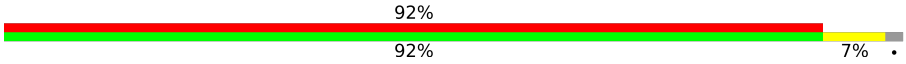
• Molecule 45: 30S ribosomal protein S12

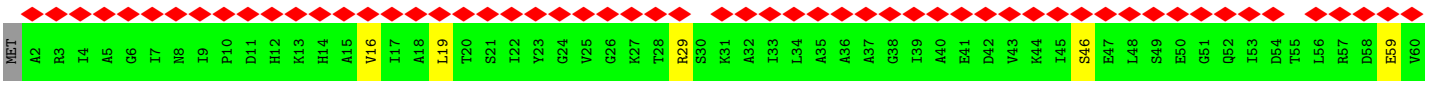
Chain l:

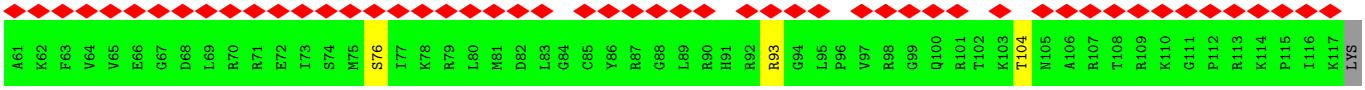


• Molecule 46: 30S ribosomal protein S13

Chain m:

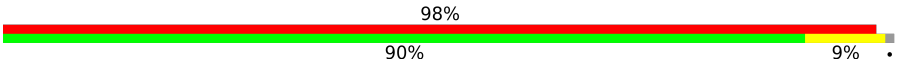


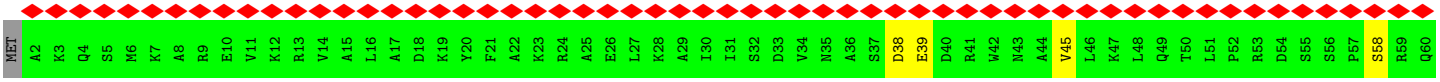


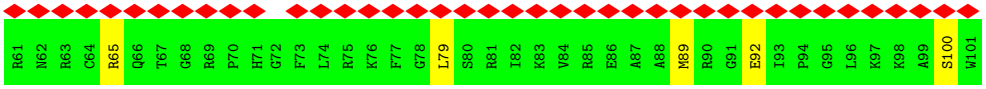


• Molecule 47: 30S ribosomal protein S14

Chain n:

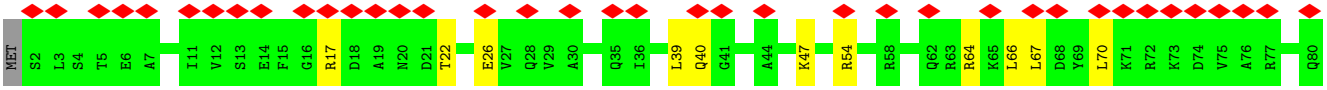






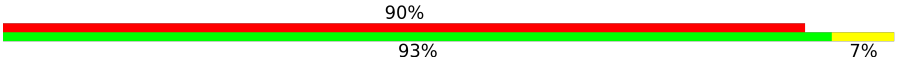
• Molecule 48: 30S ribosomal protein S15

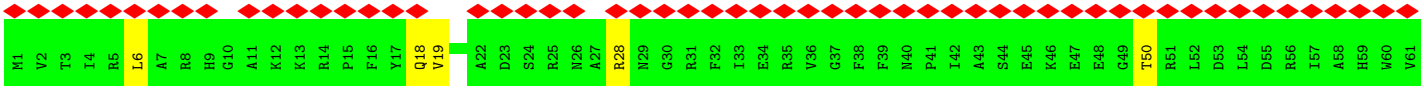
Chain o:

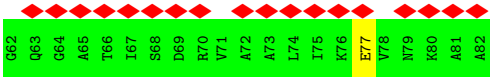


• Molecule 49: 30S ribosomal protein S16

Chain p:

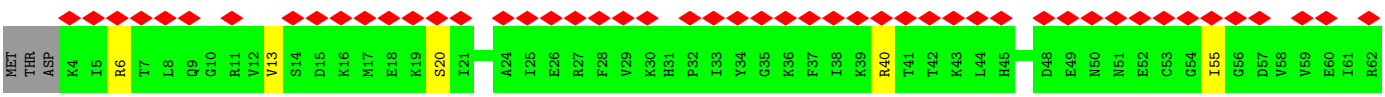


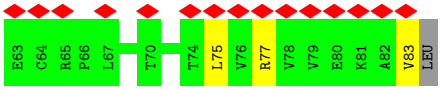




• Molecule 50: 30S ribosomal protein S17

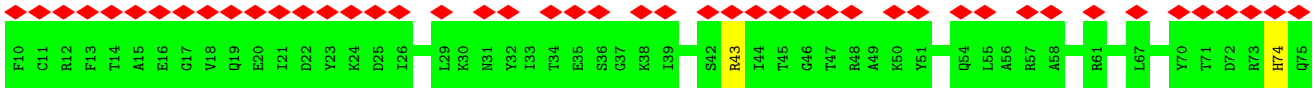
Chain q:





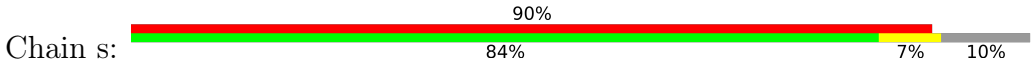
• Molecule 51: 30S ribosomal protein S18

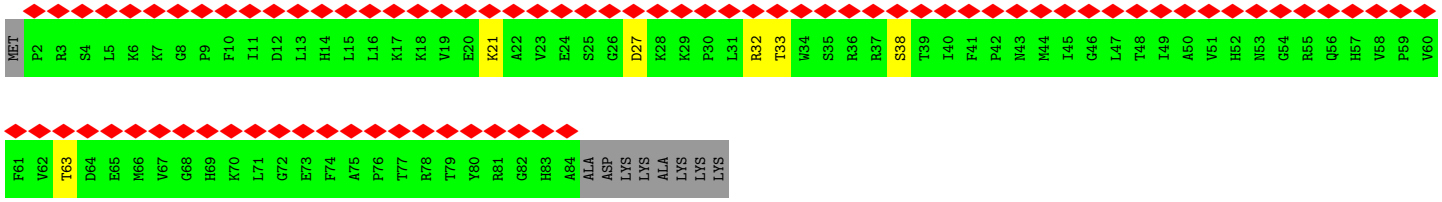
Chain r:



• Molecule 52: 30S ribosomal protein S19

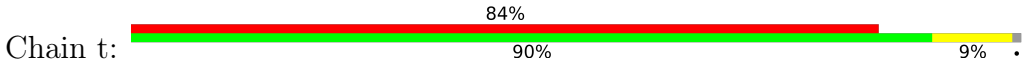
Chain s:

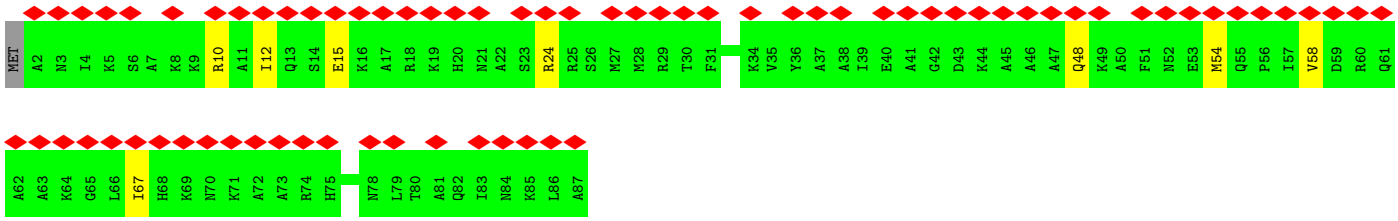




• Molecule 53: 30S ribosomal protein S20

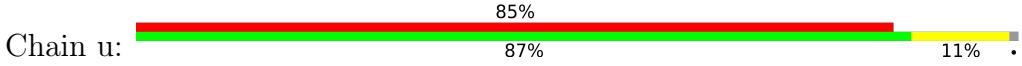
Chain t:

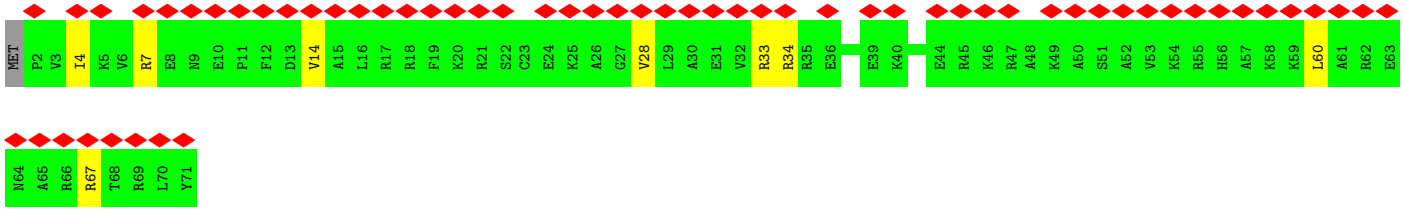




• Molecule 54: 30S ribosomal protein S21

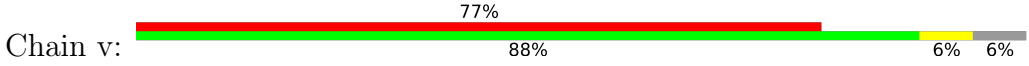
Chain u:

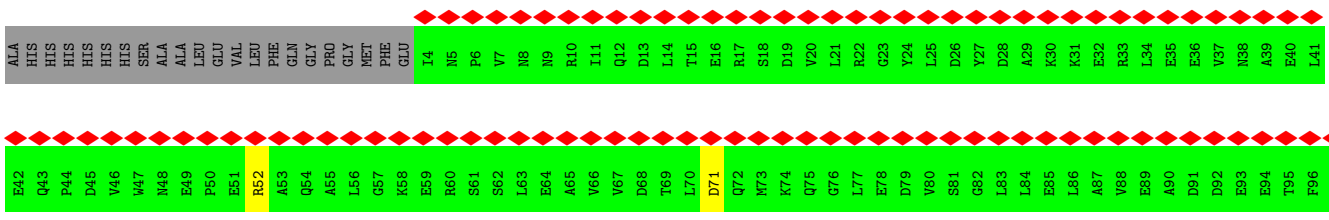


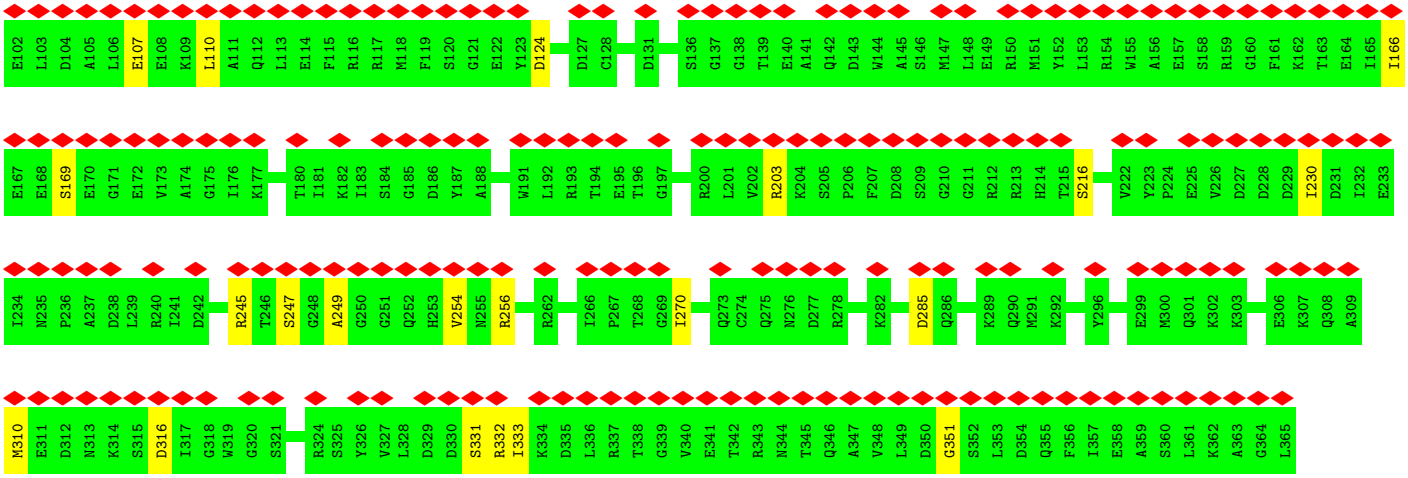


• Molecule 55: Peptide chain release factor 2

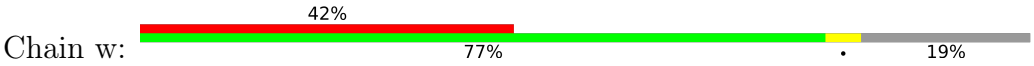
Chain v:

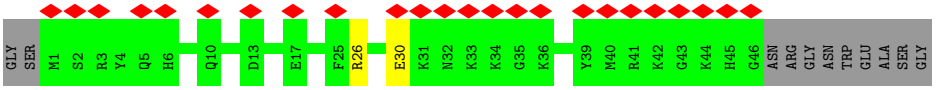




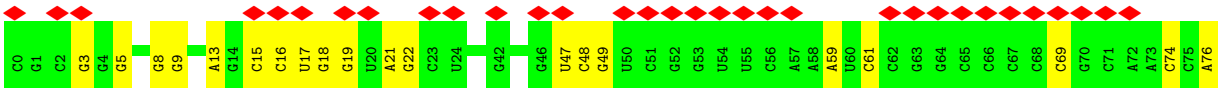


• Molecule 56: Alternative ribosome-rescue factor A

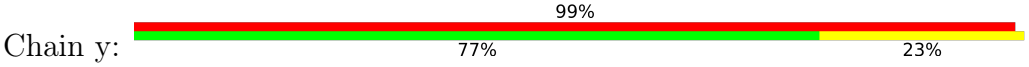


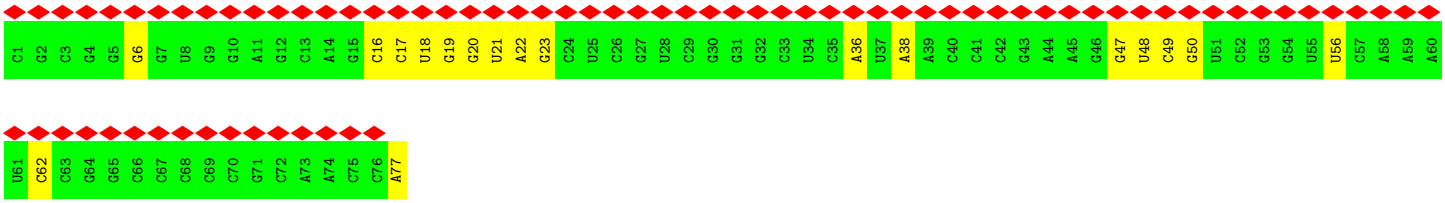


• Molecule 57: E-site or P-site tRNA fMet



• Molecule 57: E-site or P-site tRNA fMet





• Molecule 58: mRNA

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	143372	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL 3200FS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	83822	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.448	Depositor
Minimum map value	-0.283	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	460.80002, 460.80002, 460.80002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2, 1.2, 1.2	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MEQ, 2MA, 4OC, MG, G7M, UR3, 2MG, ZN, 5MC, 5MU, MA6, 6MZ, OMU, 0TD, OMG, OMC, 1MG, PSU, 3TD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.28	0/69308	0.66	0/108121
2	B	0.23	0/2872	0.66	0/4478
3	C	0.37	0/2121	0.69	0/2852
4	D	0.38	0/1586	0.62	0/2134
5	E	0.38	0/1571	0.69	0/2113
6	F	0.39	0/1434	0.69	0/1926
7	G	0.37	0/1333	0.64	0/1805
8	H	0.39	0/1122	0.64	0/1515
9	I	0.44	0/993	0.72	0/1340
10	J	0.42	0/998	0.68	0/1348
11	K	0.40	0/1152	0.68	0/1551
12	L	0.36	0/955	0.68	0/1279
13	M	0.36	0/1062	0.71	0/1413
14	N	0.41	0/1093	0.71	0/1460
15	O	0.39	0/964	0.74	0/1289
16	P	0.36	0/902	0.70	0/1209
17	Q	0.36	0/929	0.66	0/1242
18	R	0.46	0/960	0.74	0/1278
19	S	0.39	0/829	0.61	0/1107
20	T	0.37	0/864	0.71	0/1156
21	U	0.34	0/752	0.63	0/1005
22	V	0.37	0/796	0.62	0/1062
23	W	0.37	0/766	0.59	0/1025
24	X	0.35	0/589	0.63	0/779
25	Y	0.37	0/635	0.62	0/848
26	Z	0.33	0/502	0.68	0/667
27	0	0.33	0/452	0.64	0/605
28	1	0.40	0/531	0.61	0/709
29	2	0.35	0/450	0.66	0/599
30	3	0.38	0/433	0.60	0/576
31	4	0.42	0/380	0.76	0/498

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
32	5	0.36	0/513	0.68	0/676
33	6	0.33	0/303	0.68	0/397
34	a	0.22	0/36590	0.65	0/57074
35	b	0.39	0/1791	0.67	0/2413
36	c	0.38	0/1663	0.65	0/2241
37	d	0.38	0/1665	0.69	0/2227
38	e	0.37	0/1165	0.70	0/1568
39	f	0.38	0/867	0.67	0/1171
40	g	0.39	0/1206	0.76	0/1617
41	h	0.38	0/989	0.68	0/1326
42	i	0.38	0/1034	0.70	0/1375
43	j	0.36	0/800	0.73	0/1082
44	k	0.36	0/893	0.66	0/1205
45	l	0.36	0/960	0.70	0/1286
46	m	0.36	0/909	0.72	0/1215
47	n	0.36	0/817	0.70	0/1088
48	o	0.39	0/722	0.75	0/964
49	p	0.38	0/659	0.66	0/884
50	q	0.38	0/657	0.64	0/881
51	r	0.38	0/553	0.65	0/743
52	s	0.38	0/680	0.60	0/915
53	t	0.37	0/675	0.69	0/895
54	u	0.38	0/597	0.77	0/792
55	v	0.38	0/2898	0.67	0/3904
56	w	0.43	0/383	0.58	0/504
57	x	0.23	0/1835	0.65	0/2859
57	y	0.22	0/1832	0.65	0/2855
58	z	0.20	0/122	0.62	0/188
All	All	0.30	0/163112	0.66	0/243334

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
3	C	269/273 (98%)	257 (96%)	11 (4%)	1 (0%)	34 68
4	D	207/209 (99%)	200 (97%)	5 (2%)	2 (1%)	15 50
5	E	199/201 (99%)	193 (97%)	6 (3%)	0	100 100
6	F	175/177 (99%)	165 (94%)	9 (5%)	1 (1%)	25 61
7	G	173/177 (98%)	164 (95%)	8 (5%)	1 (1%)	25 61
8	H	147/149 (99%)	134 (91%)	13 (9%)	0	100 100
9	I	128/165 (78%)	103 (80%)	21 (16%)	4 (3%)	4 24
10	J	133/142 (94%)	119 (90%)	12 (9%)	2 (2%)	10 41
11	K	140/142 (99%)	137 (98%)	3 (2%)	0	100 100
12	L	121/123 (98%)	115 (95%)	6 (5%)	0	100 100
13	M	142/144 (99%)	134 (94%)	7 (5%)	1 (1%)	22 58
14	N	134/136 (98%)	131 (98%)	3 (2%)	0	100 100
15	O	117/127 (92%)	106 (91%)	11 (9%)	0	100 100
16	P	114/117 (97%)	107 (94%)	7 (6%)	0	100 100
17	Q	112/115 (97%)	108 (96%)	4 (4%)	0	100 100
18	R	115/118 (98%)	111 (96%)	3 (3%)	1 (1%)	17 52
19	S	101/103 (98%)	99 (98%)	2 (2%)	0	100 100
20	T	108/110 (98%)	106 (98%)	2 (2%)	0	100 100
21	U	92/100 (92%)	92 (100%)	0	0	100 100
22	V	101/104 (97%)	95 (94%)	5 (5%)	1 (1%)	15 50
23	W	92/94 (98%)	90 (98%)	2 (2%)	0	100 100
24	X	74/85 (87%)	69 (93%)	5 (7%)	0	100 100
25	Y	75/78 (96%)	73 (97%)	2 (3%)	0	100 100
26	Z	60/63 (95%)	59 (98%)	1 (2%)	0	100 100
27	0	56/59 (95%)	52 (93%)	3 (5%)	1 (2%)	8 38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	1	64/70 (91%)	61 (95%)	3 (5%)	0	100	100
29	2	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
30	3	50/52 (96%)	50 (100%)	0	0	100	100
31	4	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
32	5	62/65 (95%)	57 (92%)	5 (8%)	0	100	100
33	6	36/38 (95%)	36 (100%)	0	0	100	100
35	b	223/241 (92%)	213 (96%)	10 (4%)	0	100	100
36	c	206/233 (88%)	194 (94%)	10 (5%)	2 (1%)	15	50
37	d	203/206 (98%)	197 (97%)	6 (3%)	0	100	100
38	e	154/167 (92%)	145 (94%)	9 (6%)	0	100	100
39	f	102/135 (76%)	99 (97%)	2 (2%)	1 (1%)	15	50
40	g	150/179 (84%)	145 (97%)	3 (2%)	2 (1%)	12	44
41	h	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
42	i	125/130 (96%)	118 (94%)	5 (4%)	2 (2%)	9	40
43	j	97/103 (94%)	93 (96%)	3 (3%)	1 (1%)	15	50
44	k	115/129 (89%)	106 (92%)	8 (7%)	1 (1%)	17	52
45	l	120/124 (97%)	115 (96%)	5 (4%)	0	100	100
46	m	114/118 (97%)	109 (96%)	5 (4%)	0	100	100
47	n	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
48	o	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
49	p	80/82 (98%)	78 (98%)	2 (2%)	0	100	100
50	q	78/84 (93%)	74 (95%)	4 (5%)	0	100	100
51	r	64/66 (97%)	63 (98%)	1 (2%)	0	100	100
52	s	81/92 (88%)	79 (98%)	2 (2%)	0	100	100
53	t	84/87 (97%)	84 (100%)	0	0	100	100
54	u	68/71 (96%)	67 (98%)	1 (2%)	0	100	100
55	v	359/384 (94%)	346 (96%)	11 (3%)	2 (1%)	25	61
56	w	44/57 (77%)	40 (91%)	4 (9%)	0	100	100
All	All	6273/6647 (94%)	5984 (95%)	263 (4%)	26 (0%)	38	68

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
18	R	3	ARG
42	i	56	ASP
43	j	57	VAL
4	D	149	ASN
6	F	62	GLY
9	I	117	LEU
13	M	36	LYS
39	f	96	VAL
22	V	7	ARG
40	g	130	ASN
3	C	240	PHE
27	0	3	LYS
36	c	80	LYS
7	G	47	ASP
9	I	106	PHE
40	g	79	ARG
55	v	249	ALA
4	D	31	ALA
10	J	12	VAL
10	J	22	PRO
44	k	119	ASN
36	c	14	ILE
9	I	119	PRO
55	v	351	GLY
9	I	55	VAL
42	i	50	GLN

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
3	C	216/218 (99%)	199 (92%)	17 (8%)	12 40
4	D	164/164 (100%)	153 (93%)	11 (7%)	16 47
5	E	165/165 (100%)	151 (92%)	14 (8%)	10 36
6	F	148/148 (100%)	129 (87%)	19 (13%)	4 19
7	G	136/138 (99%)	125 (92%)	11 (8%)	11 39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	H	114/114 (100%)	98 (86%)	16 (14%)	3 15
9	I	99/123 (80%)	87 (88%)	12 (12%)	5 21
10	J	104/110 (94%)	91 (88%)	13 (12%)	4 20
11	K	116/116 (100%)	106 (91%)	10 (9%)	10 36
12	L	104/104 (100%)	94 (90%)	10 (10%)	8 30
13	M	103/103 (100%)	92 (89%)	11 (11%)	6 26
14	N	109/109 (100%)	99 (91%)	10 (9%)	9 32
15	O	99/103 (96%)	92 (93%)	7 (7%)	14 45
16	P	86/87 (99%)	79 (92%)	7 (8%)	11 39
17	Q	99/100 (99%)	89 (90%)	10 (10%)	7 28
18	R	89/90 (99%)	80 (90%)	9 (10%)	7 28
19	S	84/84 (100%)	78 (93%)	6 (7%)	14 45
20	T	93/93 (100%)	89 (96%)	4 (4%)	29 62
21	U	81/84 (96%)	75 (93%)	6 (7%)	13 43
22	V	84/85 (99%)	75 (89%)	9 (11%)	6 26
23	W	78/78 (100%)	74 (95%)	4 (5%)	24 57
24	X	58/63 (92%)	53 (91%)	5 (9%)	10 36
25	Y	67/68 (98%)	66 (98%)	1 (2%)	65 83
26	Z	54/55 (98%)	52 (96%)	2 (4%)	34 66
27	0	48/49 (98%)	45 (94%)	3 (6%)	18 50
28	1	59/62 (95%)	55 (93%)	4 (7%)	16 46
29	2	47/48 (98%)	46 (98%)	1 (2%)	53 77
30	3	47/47 (100%)	44 (94%)	3 (6%)	17 50
31	4	38/38 (100%)	36 (95%)	2 (5%)	22 56
32	5	51/52 (98%)	46 (90%)	5 (10%)	8 29
33	6	34/34 (100%)	32 (94%)	2 (6%)	19 52
35	b	187/199 (94%)	174 (93%)	13 (7%)	15 46
36	c	171/190 (90%)	162 (95%)	9 (5%)	22 56
37	d	172/173 (99%)	160 (93%)	12 (7%)	15 46
38	e	119/126 (94%)	106 (89%)	13 (11%)	6 25
39	f	91/116 (78%)	81 (89%)	10 (11%)	6 25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
40	g	125/147 (85%)	110 (88%)	15 (12%)	5 21
41	h	104/105 (99%)	97 (93%)	7 (7%)	16 47
42	i	105/107 (98%)	95 (90%)	10 (10%)	8 30
43	j	86/90 (96%)	70 (81%)	16 (19%)	1 7
44	k	90/99 (91%)	83 (92%)	7 (8%)	12 41
45	l	102/103 (99%)	86 (84%)	16 (16%)	2 11
46	m	94/96 (98%)	86 (92%)	8 (8%)	10 36
47	n	83/84 (99%)	74 (89%)	9 (11%)	6 25
48	o	76/77 (99%)	62 (82%)	14 (18%)	1 7
49	p	65/65 (100%)	59 (91%)	6 (9%)	9 32
50	q	74/78 (95%)	66 (89%)	8 (11%)	6 25
51	r	57/57 (100%)	55 (96%)	2 (4%)	36 67
52	s	72/79 (91%)	66 (92%)	6 (8%)	11 38
53	t	65/66 (98%)	57 (88%)	8 (12%)	4 20
54	u	60/61 (98%)	52 (87%)	8 (13%)	4 17
55	v	307/324 (95%)	286 (93%)	21 (7%)	16 46
56	w	39/46 (85%)	37 (95%)	2 (5%)	24 57
All	All	5218/5420 (96%)	4754 (91%)	464 (9%)	13 34

All (464) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	10	SER
3	C	97	LYS
3	C	105	LEU
3	C	130	LEU
3	C	141	VAL
3	C	156	ARG
3	C	189	ARG
3	C	192	LEU
3	C	195	VAL
3	C	202	LEU
3	C	203	ARG
3	C	204	VAL
3	C	205	LEU
3	C	242	LYS

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Mol	Chain	Res	Type
3	C	258	ARG
3	C	269	ARG
3	C	271	ARG
4	D	4	LEU
4	D	13	ARG
4	D	40	LEU
4	D	46	ARG
4	D	86	GLU
4	D	91	THR
4	D	116	LYS
4	D	137	SER
4	D	151	THR
4	D	157	LYS
4	D	201	LEU
5	E	1	MET
5	E	3	LEU
5	E	21	ARG
5	E	40	ARG
5	E	57	LYS
5	E	69	ARG
5	E	73	ILE
5	E	111	GLU
5	E	122	GLU
5	E	150	THR
5	E	164	LEU
5	E	178	VAL
5	E	180	LEU
5	E	195	GLN
6	F	6	ASP
6	F	16	LEU
6	F	17	MET
6	F	28	VAL
6	F	30	ARG
6	F	49	LEU
6	F	57	LEU
6	F	80	ARG
6	F	83	TYR
6	F	105	THR
6	F	117	LEU
6	F	123	ASP
6	F	130	MET
6	F	133	ARG

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Mol	Chain	Res	Type
6	F	140	GLU
6	F	141	ILE
6	F	149	VAL
6	F	150	ARG
6	F	178	ARG
7	G	4	VAL
7	G	32	GLU
7	G	47	ASP
7	G	72	LEU
7	G	117	LEU
7	G	127	THR
7	G	129	THR
7	G	152	ARG
7	G	155	GLU
7	G	170	ARG
7	G	176	LYS
8	H	6	LEU
8	H	11	ASN
8	H	12	LEU
8	H	15	LEU
8	H	27	ARG
8	H	41	LYS
8	H	51	ARG
8	H	58	LEU
8	H	66	ASN
8	H	72	ILE
8	H	94	ILE
8	H	96	THR
8	H	97	ARG
8	H	101	ASP
8	H	127	GLU
8	H	129	GLU
9	I	54	VAL
9	I	57	ASN
9	I	65	GLU
9	I	74	ASP
9	I	80	THR
9	I	81	LEU
9	I	86	MET
9	I	94	ARG
9	I	107	GLU
9	I	109	LYS

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Mol	Chain	Res	Type
9	I	117	LEU
9	I	123	ILE
10	J	10	LEU
10	J	11	GLN
10	J	27	LEU
10	J	38	CYS
10	J	41	PHE
10	J	46	ASP
10	J	74	PRO
10	J	78	LEU
10	J	99	LYS
10	J	111	THR
10	J	117	THR
10	J	137	LEU
10	J	138	VAL
11	K	10	THR
11	K	27	ARG
11	K	30	THR
11	K	31	GLU
11	K	34	ARG
11	K	57	LEU
11	K	60	ASP
11	K	72	LYS
11	K	85	LYS
11	K	123	LYS
12	L	17	ARG
12	L	32	TYR
12	L	35	VAL
12	L	41	ILE
12	L	49	ARG
12	L	58	LEU
12	L	67	LYS
12	L	69	VAL
12	L	80	ASP
12	L	91	SER
13	M	3	LEU
13	M	4	ASN
13	M	29	LYS
13	M	48	ARG
13	M	59	ARG
13	M	67	THR
13	M	93	ASN

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Mol	Chain	Res	Type
13	M	115	GLU
13	M	120	VAL
13	M	125	LEU
13	M	144	GLU
14	N	6	ARG
14	N	40	ARG
14	N	55	ARG
14	N	106	ASP
14	N	108	VAL
14	N	110	GLU
14	N	115	GLU
14	N	119	LEU
14	N	124	LEU
14	N	129	THR
15	O	2	ARG
15	O	51	LEU
15	O	63	ARG
15	O	69	ARG
15	O	95	THR
15	O	98	LEU
15	O	118	ARG
16	P	19	GLN
16	P	25	ARG
16	P	47	VAL
16	P	48	LEU
16	P	67	ASN
16	P	83	LEU
16	P	94	ARG
17	Q	16	ASP
17	Q	19	SER
17	Q	26	VAL
17	Q	57	SER
17	Q	63	LYS
17	Q	80	VAL
17	Q	81	VAL
17	Q	89	ARG
17	Q	104	THR
17	Q	114	LEU
18	R	3	ARG
18	R	13	ARG
18	R	18	LEU
18	R	30	ARG

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Mol	Chain	Res	Type
18	R	51	ARG
18	R	91	ASP
18	R	109	LEU
18	R	110	VAL
18	R	117	LEU
19	S	10	LYS
19	S	14	VAL
19	S	20	VAL
19	S	71	LYS
19	S	78	ARG
19	S	79	ARG
20	T	19	LEU
20	T	22	ASP
20	T	69	LEU
20	T	97	LEU
21	U	1	MET
21	U	32	LEU
21	U	48	GLN
21	U	79	ASP
21	U	87	LEU
21	U	93	LEU
22	V	9	ASP
22	V	27	ASN
22	V	30	SER
22	V	39	ILE
22	V	46	GLN
22	V	52	LEU
22	V	81	ASP
22	V	89	ASP
22	V	94	ARG
23	W	20	LEU
23	W	40	ILE
23	W	41	GLU
23	W	66	ASP
24	X	11	ARG
24	X	14	ARG
24	X	17	GLU
24	X	30	SER
24	X	64	ASP
25	Y	45	ARG
26	Z	18	LEU
26	Z	58	ASN

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Mol	Chain	Res	Type
27	0	11	ARG
27	0	36	VAL
27	0	45	ARG
28	1	24	ILE
28	1	43	PHE
28	1	47	LYS
28	1	59	ARG
29	2	40	ARG
30	3	5	ILE
30	3	8	LYS
30	3	32	GLU
31	4	42	LEU
31	4	44	VAL
32	5	13	ARG
32	5	30	ARG
32	5	31	HIS
32	5	54	ASP
32	5	55	LEU
33	6	3	VAL
33	6	26	ILE
35	b	7	ARG
35	b	8	ASP
35	b	21	ARG
35	b	23	TRP
35	b	59	LYS
35	b	62	SER
35	b	63	ARG
35	b	117	LEU
35	b	129	LEU
35	b	135	LEU
35	b	148	LEU
35	b	157	LEU
35	b	220	THR
36	c	14	ILE
36	c	20	SER
36	c	47	LEU
36	c	89	LYS
36	c	144	LEU
36	c	157	LEU
36	c	164	ARG
36	c	172	ARG
36	c	185	ASN

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Mol	Chain	Res	Type
37	d	3	ARG
37	d	17	THR
37	d	58	LYS
37	d	91	LEU
37	d	95	GLU
37	d	104	ARG
37	d	116	GLN
37	d	143	VAL
37	d	147	GLU
37	d	154	ARG
37	d	205	SER
37	d	206	LYS
38	e	10	GLU
38	e	15	LEU
38	e	60	ILE
38	e	65	GLU
38	e	70	ASN
38	e	93	ARG
38	e	96	MET
38	e	115	LEU
38	e	120	VAL
38	e	123	VAL
38	e	124	LEU
38	e	138	ARG
38	e	142	ASP
39	f	2	ARG
39	f	9	MET
39	f	24	ARG
39	f	33	GLU
39	f	38	ARG
39	f	54	LEU
39	f	79	ARG
39	f	85	ILE
39	f	87	SER
39	f	88	MET
40	g	7	ILE
40	g	17	LYS
40	g	21	GLU
40	g	23	LEU
40	g	27	VAL
40	g	50	LEU
40	g	72	THR

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Mol	Chain	Res	Type
40	g	79	ARG
40	g	92	ARG
40	g	109	ARG
40	g	123	GLU
40	g	130	ASN
40	g	140	ASP
40	g	143	ARG
40	g	146	GLU
41	h	3	MET
41	h	34	VAL
41	h	77	ARG
41	h	85	ILE
41	h	88	ARG
41	h	107	SER
41	h	121	LEU
42	i	12	ARG
42	i	41	ARG
42	i	46	MET
42	i	56	ASP
42	i	57	MET
42	i	61	LEU
42	i	63	LEU
42	i	106	ARG
42	i	119	ARG
42	i	123	ARG
43	j	5	ARG
43	j	6	ILE
43	j	7	ARG
43	j	16	ARG
43	j	17	LEU
43	j	19	ASP
43	j	24	GLU
43	j	25	ILE
43	j	27	GLU
43	j	37	ARG
43	j	42	LEU
43	j	48	ARG
43	j	57	VAL
43	j	60	ASP
43	j	76	ILE
43	j	87	LEU
44	k	13	ARG

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Mol	Chain	Res	Type
44	k	15	GLN
44	k	37	ARG
44	k	42	LEU
44	k	76	GLU
44	k	93	ARG
44	k	107	ILE
45	l	5	ASN
45	l	12	ARG
45	l	14	ARG
45	l	33	VAL
45	l	40	THR
45	l	41	THR
45	l	43	LYS
45	l	49	LEU
45	l	50	ARG
45	l	62	GLU
45	l	83	ARG
45	l	86	ARG
45	l	90	LEU
45	l	103	ASP
45	l	112	GLN
45	l	121	ARG
46	m	16	VAL
46	m	19	LEU
46	m	29	ARG
46	m	46	SER
46	m	59	GLU
46	m	76	SER
46	m	93	ARG
46	m	104	THR
47	n	38	ASP
47	n	39	GLU
47	n	45	VAL
47	n	58	SER
47	n	65	ARG
47	n	79	LEU
47	n	89	MET
47	n	92	GLU
47	n	100	SER
48	o	17	ARG
48	o	22	THR
48	o	26	GLU

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Mol	Chain	Res	Type
48	o	39	LEU
48	o	40	GLN
48	o	47	LYS
48	o	54	ARG
48	o	64	ARG
48	o	66	LEU
48	o	67	LEU
48	o	70	LEU
48	o	84	ARG
48	o	87	LEU
48	o	88	ARG
49	p	6	LEU
49	p	18	GLN
49	p	19	VAL
49	p	28	ARG
49	p	50	THR
49	p	77	GLU
50	q	6	ARG
50	q	13	VAL
50	q	20	SER
50	q	40	ARG
50	q	55	ILE
50	q	75	LEU
50	q	77	ARG
50	q	83	VAL
51	r	43	ARG
51	r	74	HIS
52	s	21	LYS
52	s	27	ASP
52	s	32	ARG
52	s	33	THR
52	s	38	SER
52	s	63	THR
53	t	10	ARG
53	t	12	ILE
53	t	15	GLU
53	t	24	ARG
53	t	48	GLN
53	t	54	MET
53	t	58	VAL
53	t	67	ILE
54	u	4	ILE

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Mol	Chain	Res	Type
54	u	7	ARG
54	u	14	VAL
54	u	28	VAL
54	u	33	ARG
54	u	34	ARG
54	u	60	LEU
54	u	67	ARG
55	v	52	ARG
55	v	71	ASP
55	v	107	GLU
55	v	110	LEU
55	v	124	ASP
55	v	166	ILE
55	v	169	SER
55	v	203	ARG
55	v	216	SER
55	v	230	ILE
55	v	245	ARG
55	v	247	SER
55	v	254	VAL
55	v	256	ARG
55	v	270	ILE
55	v	285	ASP
55	v	310	MET
55	v	316	ASP
55	v	331	SER
55	v	332	ARG
55	v	333	ILE
56	w	26	ARG
56	w	30	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	86	ASN
13	M	99	ASN
16	P	98	GLN
21	U	59	ASN
24	X	12	ASN
24	X	76	ASN
36	c	3	GLN
37	d	40	GLN

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Mol	Chain	Res	Type
37	d	131	ASN
41	h	4	GLN
43	j	35	GLN
44	k	109	ASN
50	q	51	ASN
52	s	52	HIS
52	s	69	HIS
55	v	253	HIS
56	w	14	ASN
56	w	32	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2899/2904 (99%)	552 (19%)	75 (2%)
2	B	119/120 (99%)	17 (14%)	1 (0%)
34	a	1528/1534 (99%)	288 (18%)	0
57	x	76/77 (98%)	20 (26%)	0
57	y	76/77 (98%)	18 (23%)	0
58	z	4/18 (22%)	1 (25%)	0
All	All	4702/4730 (99%)	896 (19%)	76 (1%)

All (896) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	10	A
1	A	14	A
1	A	15	G
1	A	23	G
1	A	34	U
1	A	35	G
1	A	39	G
1	A	45	G
1	A	46	G
1	A	51	G
1	A	55	G
1	A	58	G
1	A	60	G
1	A	62	U
1	A	63	A
1	A	71	A

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Mol	Chain	Res	Type
1	A	74	A
1	A	75	G
1	A	80	G
1	A	84	A
1	A	85	G
1	A	86	G
1	A	96	C
1	A	99	U
1	A	101	A
1	A	102	U
1	A	103	A
1	A	110	G
1	A	118	A
1	A	119	A
1	A	120	U
1	A	122	G
1	A	139	U
1	A	140	C
1	A	141	G
1	A	144	A
1	A	149	A
1	A	163	C
1	A	165	A
1	A	181	A
1	A	196	A
1	A	199	A
1	A	215	G
1	A	216	A
1	A	221	A
1	A	222	A
1	A	225	C
1	A	230	G
1	A	248	G
1	A	249	C
1	A	261	G
1	A	264	C
1	A	265	A
1	A	266	G
1	A	267	C
1	A	272	A
1	A	275	C
1	A	276	U

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Mol	Chain	Res	Type
1	A	278	A
1	A	285	G
1	A	311	A
1	A	322	A
1	A	327	G
1	A	329	G
1	A	330	A
1	A	353	C
1	A	361	G
1	A	362	A
1	A	371	A
1	A	372	G
1	A	383	C
1	A	386	G
1	A	396	G
1	A	404	A
1	A	405	U
1	A	411	G
1	A	420	C
1	A	424	G
1	A	435	C
1	A	451	U
1	A	456	C
1	A	457	A
1	A	477	A
1	A	480	A
1	A	481	G
1	A	491	G
1	A	496	G
1	A	501	A
1	A	503	A
1	A	504	A
1	A	505	A
1	A	508	A
1	A	509	C
1	A	531	C
1	A	532	A
1	A	533	G
1	A	543	G
1	A	545	U
1	A	546	U
1	A	547	A

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Mol	Chain	Res	Type
1	A	549	G
1	A	551	G
1	A	563	A
1	A	569	U
1	A	573	U
1	A	575	A
1	A	586	A
1	A	588	U
1	A	603	A
1	A	609	A
1	A	613	A
1	A	614	A
1	A	615	U
1	A	616	A
1	A	627	A
1	A	637	A
1	A	645	C
1	A	647	G
1	A	651	G
1	A	654	A
1	A	655	A
1	A	659	G
1	A	664	G
1	A	668	A
1	A	670	A
1	A	676	A
1	A	686	U
1	A	710	U
1	A	717	C
1	A	730	A
1	A	738	G
1	A	746	PSU
1	A	747	5MU
1	A	757	G
1	A	764	A
1	A	765	C
1	A	775	G
1	A	776	G
1	A	782	A
1	A	783	A
1	A	784	G
1	A	785	G

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Mol	Chain	Res	Type
1	A	789	A
1	A	792	A
1	A	805	G
1	A	812	C
1	A	819	A
1	A	827	U
1	A	828	U
1	A	845	A
1	A	846	U
1	A	858	G
1	A	859	G
1	A	869	G
1	A	878	A
1	A	881	G
1	A	884	U
1	A	885	C
1	A	891	G
1	A	895	U
1	A	896	A
1	A	897	C
1	A	910	A
1	A	914	G
1	A	915	C
1	A	931	U
1	A	932	U
1	A	941	A
1	A	946	C
1	A	953	G
1	A	961	C
1	A	973	A
1	A	974	G
1	A	983	A
1	A	989	G
1	A	990	A
1	A	995	C
1	A	996	A
1	A	999	U
1	A	1005	C
1	A	1012	U
1	A	1013	C
1	A	1022	G
1	A	1023	U

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Mol	Chain	Res	Type
1	A	1026	G
1	A	1033	U
1	A	1040	A
1	A	1045	C
1	A	1046	A
1	A	1047	G
1	A	1050	A
1	A	1063	G
1	A	1064	C
1	A	1065	U
1	A	1066	U
1	A	1067	A
1	A	1068	G
1	A	1069	A
1	A	1070	A
1	A	1071	G
1	A	1073	A
1	A	1074	G
1	A	1079	C
1	A	1083	U
1	A	1084	A
1	A	1087	G
1	A	1088	A
1	A	1090	A
1	A	1097	U
1	A	1111	A
1	A	1112	G
1	A	1119	U
1	A	1122	G
1	A	1132	U
1	A	1134	A
1	A	1135	C
1	A	1142	A
1	A	1155	A
1	A	1169	A
1	A	1170	C
1	A	1173	U
1	A	1174	U
1	A	1175	A
1	A	1176	U
1	A	1177	G
1	A	1178	C

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Mol	Chain	Res	Type
1	A	1179	G
1	A	1180	U
1	A	1186	G
1	A	1210	G
1	A	1236	G
1	A	1238	G
1	A	1244	A
1	A	1247	A
1	A	1248	G
1	A	1253	A
1	A	1256	G
1	A	1262	A
1	A	1265	A
1	A	1266	G
1	A	1271	G
1	A	1272	A
1	A	1301	A
1	A	1321	A
1	A	1329	U
1	A	1345	C
1	A	1352	U
1	A	1365	A
1	A	1368	G
1	A	1378	A
1	A	1379	U
1	A	1380	G
1	A	1383	A
1	A	1395	A
1	A	1405	U
1	A	1407	G
1	A	1408	G
1	A	1409	U
1	A	1416	G
1	A	1417	C
1	A	1419	A
1	A	1420	A
1	A	1428	C
1	A	1437	C
1	A	1452	G
1	A	1453	A
1	A	1455	G
1	A	1458	U

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Mol	Chain	Res	Type
1	A	1460	U
1	A	1468	U
1	A	1478	G
1	A	1482	G
1	A	1490	A
1	A	1493	C
1	A	1497	U
1	A	1503	A
1	A	1508	A
1	A	1509	A
1	A	1510	G
1	A	1515	A
1	A	1529	G
1	A	1535	A
1	A	1536	C
1	A	1537	G
1	A	1554	U
1	A	1558	C
1	A	1559	U
1	A	1566	A
1	A	1569	A
1	A	1578	U
1	A	1580	A
1	A	1581	G
1	A	1583	A
1	A	1584	U
1	A	1589	U
1	A	1590	A
1	A	1594	U
1	A	1595	C
1	A	1596	A
1	A	1608	A
1	A	1609	A
1	A	1610	A
1	A	1613	G
1	A	1647	U
1	A	1648	U
1	A	1649	G
1	A	1651	G
1	A	1654	A
1	A	1674	G
1	A	1698	A

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Mol	Chain	Res	Type
1	A	1715	G
1	A	1718	G
1	A	1729	U
1	A	1730	C
1	A	1732	C
1	A	1738	G
1	A	1750	G
1	A	1758	U
1	A	1764	C
1	A	1773	A
1	A	1791	A
1	A	1800	C
1	A	1807	G
1	A	1808	A
1	A	1811	G
1	A	1816	C
1	A	1833	C
1	A	1847	A
1	A	1848	A
1	A	1858	A
1	A	1859	U
1	A	1864	U
1	A	1870	C
1	A	1872	A
1	A	1873	G
1	A	1896	G
1	A	1900	A
1	A	1906	G
1	A	1907	G
1	A	1913	A
1	A	1914	C
1	A	1919	A
1	A	1929	G
1	A	1930	G
1	A	1931	U
1	A	1936	A
1	A	1938	A
1	A	1939	5MU
1	A	1955	U
1	A	1960	A
1	A	1965	C
1	A	1967	C

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Mol	Chain	Res	Type
1	A	1970	A
1	A	1971	U
1	A	1972	G
1	A	1982	U
1	A	1991	U
1	A	1992	G
1	A	1993	U
1	A	1997	C
1	A	2002	G
1	A	2004	G
1	A	2020	A
1	A	2022	U
1	A	2023	C
1	A	2029	G
1	A	2031	A
1	A	2033	A
1	A	2043	C
1	A	2049	G
1	A	2052	A
1	A	2055	C
1	A	2056	G
1	A	2059	A
1	A	2060	A
1	A	2061	G
1	A	2062	A
1	A	2069	G7M
1	A	2072	C
1	A	2080	A
1	A	2087	G
1	A	2093	G
1	A	2100	G
1	A	2101	A
1	A	2102	G
1	A	2107	G
1	A	2108	A
1	A	2110	G
1	A	2111	U
1	A	2113	U
1	A	2115	G
1	A	2116	G
1	A	2117	A
1	A	2118	U

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Mol	Chain	Res	Type
1	A	2122	U
1	A	2124	G
1	A	2125	G
1	A	2126	A
1	A	2127	G
1	A	2128	G
1	A	2131	U
1	A	2132	U
1	A	2133	G
1	A	2134	A
1	A	2146	C
1	A	2147	A
1	A	2154	A
1	A	2157	G
1	A	2158	A
1	A	2159	G
1	A	2162	G
1	A	2163	A
1	A	2164	C
1	A	2165	C
1	A	2171	A
1	A	2172	U
1	A	2178	C
1	A	2182	U
1	A	2183	A
1	A	2185	U
1	A	2188	U
1	A	2190	G
1	A	2193	G
1	A	2198	A
1	A	2199	A
1	A	2204	G
1	A	2211	A
1	A	2212	A
1	A	2225	A
1	A	2226	C
1	A	2229	U
1	A	2238	G
1	A	2239	G
1	A	2243	U
1	A	2251	OMG
1	A	2268	A

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Mol	Chain	Res	Type
1	A	2278	A
1	A	2279	G
1	A	2283	C
1	A	2287	A
1	A	2288	A
1	A	2297	A
1	A	2305	U
1	A	2308	G
1	A	2319	G
1	A	2322	A
1	A	2325	G
1	A	2327	A
1	A	2333	A
1	A	2334	U
1	A	2335	A
1	A	2336	A
1	A	2347	C
1	A	2350	C
1	A	2357	G
1	A	2361	G
1	A	2372	U
1	A	2376	A
1	A	2383	G
1	A	2385	C
1	A	2402	U
1	A	2403	C
1	A	2406	A
1	A	2410	G
1	A	2423	U
1	A	2425	A
1	A	2426	A
1	A	2429	G
1	A	2430	A
1	A	2431	U
1	A	2435	A
1	A	2441	U
1	A	2445	2MG
1	A	2447	G
1	A	2448	A
1	A	2469	A
1	A	2470	G
1	A	2476	A

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Mol	Chain	Res	Type
1	A	2478	A
1	A	2484	G
1	A	2491	U
1	A	2494	G
1	A	2498	OMC
1	A	2502	G
1	A	2504	PSU
1	A	2505	G
1	A	2513	A
1	A	2518	A
1	A	2520	C
1	A	2525	G
1	A	2529	G
1	A	2535	G
1	A	2554	U
1	A	2562	U
1	A	2566	A
1	A	2567	G
1	A	2573	C
1	A	2574	G
1	A	2578	G
1	A	2585	U
1	A	2586	U
1	A	2602	A
1	A	2609	U
1	A	2610	C
1	A	2613	U
1	A	2621	G
1	A	2629	U
1	A	2630	G
1	A	2634	A
1	A	2639	A
1	A	2663	G
1	A	2682	A
1	A	2689	U
1	A	2690	U
1	A	2714	G
1	A	2716	C
1	A	2718	G
1	A	2726	A
1	A	2733	A
1	A	2744	G

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Mol	Chain	Res	Type
1	A	2748	A
1	A	2757	A
1	A	2765	A
1	A	2777	G
1	A	2778	A
1	A	2791	G
1	A	2793	C
1	A	2796	U
1	A	2797	U
1	A	2798	U
1	A	2799	A
1	A	2801	G
1	A	2818	U
1	A	2820	A
1	A	2821	A
1	A	2825	G
1	A	2835	A
1	A	2849	U
1	A	2859	G
1	A	2861	U
1	A	2867	G
1	A	2873	A
1	A	2874	C
1	A	2879	A
1	A	2880	C
1	A	2883	A
1	A	2884	U
1	A	2885	G
1	A	2891	U
1	A	2902	C
1	A	2903	U
1	A	2904	U
2	B	2	G
2	B	13	G
2	B	16	G
2	B	17	C
2	B	35	C
2	B	36	C
2	B	45	A
2	B	51	G
2	B	56	G
2	B	57	A

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Mol	Chain	Res	Type
2	B	66	A
2	B	88	C
2	B	89	U
2	B	90	C
2	B	99	A
2	B	105	G
2	B	109	A
34	a	4	U
34	a	9	G
34	a	22	G
34	a	32	A
34	a	39	G
34	a	47	C
34	a	48	C
34	a	50	A
34	a	51	A
34	a	52	C
34	a	68	G
34	a	69	G
34	a	71	A
34	a	72	A
34	a	74	A
34	a	76	G
34	a	82	G
34	a	83	C
34	a	84	U
34	a	87	C
34	a	94	G
34	a	95	C
34	a	108	G
34	a	120	A
34	a	121	U
34	a	122	G
34	a	131	A
34	a	141	G
34	a	144	G
34	a	146	G
34	a	148	G
34	a	160	A
34	a	163	C
34	a	164	G
34	a	173	U

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Mol	Chain	Res	Type
34	a	177	G
34	a	181	A
34	a	182	A
34	a	196	A
34	a	204	G
34	a	208	U
34	a	209	U
34	a	210	C
34	a	211	G
34	a	212	G
34	a	226	G
34	a	245	U
34	a	247	G
34	a	251	G
34	a	258	G
34	a	262	A
34	a	266	G
34	a	267	C
34	a	279	A
34	a	289	G
34	a	306	A
34	a	316	C
34	a	321	A
34	a	328	C
34	a	329	A
34	a	332	G
34	a	345	C
34	a	347	G
34	a	352	C
34	a	354	G
34	a	356	A
34	a	367	U
34	a	368	U
34	a	369	G
34	a	372	C
34	a	373	A
34	a	376	G
34	a	384	G
34	a	392	C
34	a	397	A
34	a	406	G
34	a	411	A

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Mol	Chain	Res	Type
34	a	412	A
34	a	413	G
34	a	414	A
34	a	421	U
34	a	422	C
34	a	424	G
34	a	428	G
34	a	429	U
34	a	446	G
34	a	451	A
34	a	457	G
34	a	458	U
34	a	463	U
34	a	464	U
34	a	467	U
34	a	468	A
34	a	476	U
34	a	478	A
34	a	479	U
34	a	480	U
34	a	481	G
34	a	484	G
34	a	485	U
34	a	486	U
34	a	495	A
34	a	496	A
34	a	511	C
34	a	517	G
34	a	518	C
34	a	521	G
34	a	531	U
34	a	532	A
34	a	533	A
34	a	547	A
34	a	559	A
34	a	572	A
34	a	573	A
34	a	576	C
34	a	577	G
34	a	579	A
34	a	596	A
34	a	607	A

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Mol	Chain	Res	Type
34	a	615	G
34	a	628	G
34	a	633	G
34	a	639	G
34	a	642	A
34	a	649	A
34	a	650	G
34	a	653	U
34	a	665	A
34	a	687	A
34	a	700	G
34	a	702	A
34	a	703	G
34	a	721	G
34	a	723	U
34	a	724	G
34	a	731	G
34	a	734	G
34	a	747	A
34	a	748	G
34	a	755	G
34	a	777	A
34	a	793	U
34	a	794	A
34	a	799	G
34	a	815	A
34	a	817	C
34	a	821	G
34	a	828	U
34	a	832	G
34	a	841	C
34	a	844	G
34	a	845	A
34	a	849	G
34	a	851	G
34	a	874	G
34	a	876	C
34	a	887	G
34	a	889	A
34	a	902	G
34	a	914	A
34	a	916	U

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Mol	Chain	Res	Type
34	a	926	G
34	a	928	G
34	a	934	C
34	a	960	U
34	a	966	2MG
34	a	969	A
34	a	971	G
34	a	972	C
34	a	975	A
34	a	976	G
34	a	977	A
34	a	987	G
34	a	991	U
34	a	992	U
34	a	993	G
34	a	996	A
34	a	999	C
34	a	1004	A
34	a	1008	U
34	a	1009	U
34	a	1017	U
34	a	1018	G
34	a	1024	G
34	a	1026	G
34	a	1028	C
34	a	1030	U
34	a	1031	C
34	a	1033	G
34	a	1037	C
34	a	1043	G
34	a	1044	A
34	a	1046	A
34	a	1053	G
34	a	1056	U
34	a	1065	U
34	a	1070	U
34	a	1085	U
34	a	1086	U
34	a	1089	G
34	a	1094	G
34	a	1095	U
34	a	1099	G

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Mol	Chain	Res	Type
34	a	1101	A
34	a	1108	G
34	a	1124	G
34	a	1133	G
34	a	1135	U
34	a	1136	C
34	a	1137	C
34	a	1139	G
34	a	1140	C
34	a	1141	C
34	a	1142	G
34	a	1143	G
34	a	1146	A
34	a	1151	A
34	a	1152	A
34	a	1154	G
34	a	1158	C
34	a	1159	U
34	a	1167	A
34	a	1171	A
34	a	1174	G
34	a	1175	G
34	a	1176	A
34	a	1184	G
34	a	1193	G
34	a	1196	A
34	a	1197	A
34	a	1211	U
34	a	1212	U
34	a	1213	A
34	a	1215	G
34	a	1226	C
34	a	1227	A
34	a	1228	C
34	a	1236	A
34	a	1238	A
34	a	1239	A
34	a	1256	A
34	a	1257	A
34	a	1260	G
34	a	1275	A
34	a	1277	C

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Mol	Chain	Res	Type
34	a	1278	G
34	a	1279	G
34	a	1280	A
34	a	1285	A
34	a	1286	U
34	a	1287	A
34	a	1299	A
34	a	1300	G
34	a	1302	C
34	a	1305	G
34	a	1312	G
34	a	1317	C
34	a	1320	C
34	a	1323	G
34	a	1340	A
34	a	1346	A
34	a	1353	G
34	a	1358	U
34	a	1363	A
34	a	1370	G
34	a	1378	C
34	a	1379	G
34	a	1381	U
34	a	1396	A
34	a	1419	G
34	a	1422	G
34	a	1429	A
34	a	1432	G
34	a	1441	A
34	a	1446	A
34	a	1452	C
34	a	1453	G
34	a	1487	G
34	a	1492	A
34	a	1493	A
34	a	1494	G
34	a	1497	G
34	a	1503	A
34	a	1506	U
34	a	1517	G
34	a	1529	G
34	a	1530	G

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Mol	Chain	Res	Type
34	a	1534	A
57	x	3	G
57	x	5	G
57	x	8	G
57	x	9	G
57	x	13	A
57	x	15	C
57	x	16	C
57	x	17	U
57	x	18	G
57	x	19	G
57	x	21	A
57	x	22	G
57	x	47	U
57	x	48	C
57	x	49	G
57	x	59	A
57	x	61	C
57	x	69	C
57	x	74	C
57	x	76	A
57	y	6	G
57	y	16	C
57	y	17	C
57	y	18	U
57	y	19	G
57	y	20	G
57	y	21	U
57	y	22	A
57	y	23	G
57	y	36	A
57	y	38	A
57	y	47	G
57	y	48	U
57	y	49	C
57	y	50	G
57	y	56	U
57	y	62	C
57	y	77	A
58	z	15	A

All (76) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	62	U
1	A	70	G
1	A	71	A
1	A	101	A
1	A	138	U
1	A	140	C
1	A	177	G
1	A	181	A
1	A	183	C
1	A	199	A
1	A	221	A
1	A	271	G
1	A	310	A
1	A	369	U
1	A	404	A
1	A	446	G
1	A	479	A
1	A	503	A
1	A	512	G
1	A	545	U
1	A	546	U
1	A	555	G
1	A	641	U
1	A	685	A
1	A	733	G
1	A	748	G
1	A	764	A
1	A	784	G
1	A	865	C
1	A	883	G
1	A	884	U
1	A	894	U
1	A	896	A
1	A	974	G
1	A	984	A
1	A	1064	C
1	A	1067	A
1	A	1069	A
1	A	1070	A
1	A	1109	C
1	A	1128	G
1	A	1147	A
1	A	1173	U

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Mol	Chain	Res	Type
1	A	1174	U
1	A	1288	G
1	A	1320	C
1	A	1344	U
1	A	1378	A
1	A	1379	U
1	A	1395	A
1	A	1420	A
1	A	1432	G
1	A	1509	A
1	A	1584	U
1	A	1608	A
1	A	1647	U
1	A	1847	A
1	A	1900	A
1	A	1918	A
1	A	2062	A
1	A	2146	C
1	A	2162	G
1	A	2197	U
1	A	2198	A
1	A	2211	A
1	A	2225	A
1	A	2296	U
1	A	2425	A
1	A	2517	C
1	A	2585	U
1	A	2756	U
1	A	2797	U
1	A	2798	U
1	A	2849	U
1	A	2873	A
2	B	87	U

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

35 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	PSU	A	2605	1	18,21,22	1.45	3 (16%)	22,30,33	1.99	4 (18%)
1	6MZ	A	1618	1	18,25,26	0.92	1 (5%)	16,36,39	1.68	3 (18%)
34	2MG	a	1516	34	18,26,27	1.00	1 (5%)	16,38,41	1.18	2 (12%)
34	2MG	a	966	34	18,26,27	0.97	1 (5%)	16,38,41	1.19	3 (18%)
1	2MA	A	2503	59,1	17,25,26	0.97	0	17,37,40	1.22	3 (17%)
1	PSU	A	1911	1	18,21,22	1.37	2 (11%)	22,30,33	1.86	4 (18%)
1	1MG	A	745	1	18,26,27	0.81	0	19,39,42	1.14	3 (15%)
1	3TD	A	1915	1	18,22,23	2.16	4 (22%)	22,32,35	8.49	5 (22%)
1	PSU	A	2580	1	18,21,22	1.50	3 (16%)	22,30,33	2.05	5 (22%)
34	4OC	a	1402	34	20,23,24	0.85	1 (5%)	26,32,35	1.32	3 (11%)
34	PSU	a	516	34,59	18,21,22	1.37	2 (11%)	22,30,33	2.07	4 (18%)
1	OMG	A	2251	57,1	18,26,27	1.08	1 (5%)	19,38,41	1.04	2 (10%)
34	2MG	a	1207	34	18,26,27	1.00	1 (5%)	16,38,41	1.14	2 (12%)
34	UR3	a	1498	34	19,22,23	1.17	1 (5%)	26,32,35	1.64	2 (7%)
55	MEQ	v	252	55	8,9,10	0.45	0	5,10,12	0.39	0
1	OMC	A	2498	59,1	19,22,23	0.87	0	26,31,34	1.03	2 (7%)
1	5MU	A	1939	59,1	19,22,23	1.52	6 (31%)	28,32,35	2.34	8 (28%)
1	PSU	A	2504	1	18,21,22	1.45	3 (16%)	22,30,33	1.88	4 (18%)
34	G7M	a	527	34	20,26,27	2.72	4 (20%)	17,39,42	1.06	1 (5%)
1	G7M	A	2069	1	20,26,27	1.53	1 (5%)	17,39,42	2.36	4 (23%)
45	0TD	l	89	45	7,9,10	6.77	5 (71%)	6,11,13	4.35	4 (66%)
1	5MU	A	747	1	19,22,23	1.47	6 (31%)	28,32,35	2.15	7 (25%)
1	5MC	A	1962	1	18,22,23	0.96	2 (11%)	26,32,35	1.35	4 (15%)
34	5MC	a	1407	34	18,22,23	0.93	1 (5%)	26,32,35	1.27	4 (15%)
1	OMU	A	2552	1	19,22,23	1.27	2 (10%)	26,31,34	1.90	6 (23%)
1	6MZ	A	2030	1	18,25,26	0.99	1 (5%)	16,36,39	2.05	4 (25%)
1	PSU	A	955	1	18,21,22	1.49	3 (16%)	22,30,33	2.20	3 (13%)
1	PSU	A	2457	1	18,21,22	1.49	3 (16%)	22,30,33	2.00	5 (22%)
34	MA6	a	1519	34	19,26,27	1.20	3 (15%)	18,38,41	1.69	4 (22%)
34	5MC	a	967	34	18,22,23	1.07	1 (5%)	26,32,35	1.32	5 (19%)
1	PSU	A	1917	1	18,21,22	1.38	3 (16%)	22,30,33	2.02	4 (18%)
34	MA6	a	1518	34	19,26,27	1.17	2 (10%)	18,38,41	1.77	4 (22%)
1	PSU	A	746	59,1	18,21,22	1.38	2 (11%)	22,30,33	1.95	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	2MG	A	1835	1	18,26,27	1.05	1 (5%)	16,38,41	1.10	2 (12%)
1	2MG	A	2445	1	18,26,27	1.22	1 (5%)	16,38,41	1.06	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	A	2605	1	-	0/7/25/26	0/2/2/2
1	6MZ	A	1618	1	-	4/5/27/28	0/3/3/3
34	2MG	a	1516	34	-	0/5/27/28	0/3/3/3
34	2MG	a	966	34	-	0/5/27/28	0/3/3/3
1	2MA	A	2503	59,1	-	1/3/25/26	0/3/3/3
1	PSU	A	1911	1	-	0/7/25/26	0/2/2/2
1	1MG	A	745	1	-	0/3/25/26	0/3/3/3
1	3TD	A	1915	1	-	2/7/25/26	0/2/2/2
1	PSU	A	2580	1	-	0/7/25/26	0/2/2/2
34	4OC	a	1402	34	-	1/9/29/30	0/2/2/2
34	PSU	a	516	34,59	-	0/7/25/26	0/2/2/2
1	OMG	A	2251	57,1	-	0/5/27/28	0/3/3/3
34	2MG	a	1207	34	-	0/5/27/28	0/3/3/3
34	UR3	a	1498	34	-	0/7/25/26	0/2/2/2
55	MEQ	v	252	55	-	2/8/9/11	-
1	OMC	A	2498	59,1	-	2/9/27/28	0/2/2/2
1	5MU	A	1939	59,1	-	2/7/25/26	0/2/2/2
1	PSU	A	2504	1	-	2/7/25/26	0/2/2/2
34	G7M	a	527	34	-	1/3/25/26	0/3/3/3
1	G7M	A	2069	1	-	2/3/25/26	0/3/3/3
45	0TD	l	89	45	-	3/7/12/14	-
1	5MU	A	747	1	-	0/7/25/26	0/2/2/2
1	5MC	A	1962	1	-	0/7/25/26	0/2/2/2
34	5MC	a	1407	34	-	0/7/25/26	0/2/2/2
1	OMU	A	2552	1	-	0/9/27/28	0/2/2/2
1	6MZ	A	2030	1	-	2/5/27/28	0/3/3/3
1	PSU	A	955	1	-	0/7/25/26	0/2/2/2
1	PSU	A	2457	1	-	0/7/25/26	0/2/2/2
34	MA6	a	1519	34	-	5/7/29/30	0/3/3/3
34	5MC	a	967	34	-	0/7/25/26	0/2/2/2
1	PSU	A	1917	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	MA6	a	1518	34	-	2/7/29/30	0/3/3/3
1	PSU	A	746	59,1	-	4/7/25/26	0/2/2/2
1	2MG	A	1835	1	-	0/5/27/28	0/3/3/3
1	2MG	A	2445	1	-	2/5/27/28	0/3/3/3

All (71) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	l	89	0TD	CB-SB	-17.03	1.64	1.82
34	a	527	G7M	C8-N9	7.74	1.47	1.33
34	a	527	G7M	C8-N7	7.08	1.46	1.33
1	A	1915	3TD	C6-C5	-6.82	1.27	1.35
1	A	2069	G7M	C2'-C1'	-5.51	1.45	1.53
34	a	527	G7M	C5-C4	4.54	1.48	1.39
1	A	2504	PSU	C6-C5	4.45	1.40	1.35
1	A	1911	PSU	C6-C5	4.00	1.40	1.35
34	a	516	PSU	C6-C5	3.90	1.39	1.35
1	A	955	PSU	C6-C5	3.88	1.39	1.35
1	A	2605	PSU	C6-C5	3.74	1.39	1.35
1	A	2457	PSU	C6-C5	3.60	1.39	1.35
1	A	2580	PSU	C6-C5	3.43	1.39	1.35
1	A	1915	3TD	C2-N3	3.40	1.46	1.38
1	A	1915	3TD	C6-N1	-3.39	1.30	1.36
1	A	1917	PSU	C6-C5	3.38	1.39	1.35
1	A	746	PSU	C6-C5	3.32	1.39	1.35
34	a	967	5MC	C6-C5	3.26	1.40	1.34
45	l	89	0TD	CA-N	-3.20	1.37	1.47
1	A	2580	PSU	C4-N3	-3.11	1.33	1.38
1	A	747	5MU	C6-C5	3.09	1.39	1.34
1	A	2030	6MZ	C2'-C1'	-3.04	1.49	1.53
1	A	2605	PSU	C4-N3	-3.00	1.33	1.38
1	A	1939	5MU	C6-C5	2.88	1.39	1.34
1	A	1939	5MU	C4-C5	2.81	1.49	1.44
1	A	2445	2MG	C6-N1	-2.80	1.33	1.37
1	A	2457	PSU	C4-N3	-2.76	1.33	1.38
1	A	747	5MU	C4-N3	-2.75	1.33	1.38
1	A	2552	OMU	C4-N3	-2.74	1.33	1.38
45	l	89	0TD	CB-CG	-2.72	1.47	1.52
34	a	1498	UR3	C2-N1	2.72	1.42	1.38
34	a	1519	MA6	C5-C4	2.71	1.48	1.40
1	A	1939	5MU	C4-N3	-2.70	1.33	1.38
1	A	746	PSU	C4-N3	-2.69	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	955	PSU	C4-N3	-2.66	1.33	1.38
45	l	89	0TD	OD2-CG	-2.63	1.21	1.30
1	A	2251	OMG	C6-N1	-2.63	1.34	1.37
1	A	1917	PSU	C4-N3	-2.59	1.34	1.38
34	a	1407	5MC	C6-C5	2.57	1.38	1.34
1	A	1618	6MZ	C2'-C1'	-2.53	1.49	1.53
45	l	89	0TD	CSB-SB	-2.52	1.74	1.79
1	A	1915	3TD	C4-N3	2.48	1.45	1.40
1	A	2552	OMU	C2-N1	2.48	1.42	1.38
34	a	1518	MA6	C5-C4	2.44	1.47	1.40
34	a	1516	2MG	C6-N1	-2.43	1.34	1.37
1	A	1962	5MC	C6-C5	2.43	1.38	1.34
1	A	1835	2MG	C6-N1	-2.41	1.34	1.37
34	a	516	PSU	C4-N3	-2.40	1.34	1.38
1	A	2580	PSU	C2-N3	-2.34	1.33	1.37
1	A	1939	5MU	C6-N1	-2.34	1.34	1.38
1	A	1911	PSU	C4-N3	-2.33	1.34	1.38
1	A	1939	5MU	C2-N3	-2.33	1.33	1.38
1	A	747	5MU	C2-N1	2.32	1.42	1.38
1	A	2504	PSU	C4-N3	-2.31	1.34	1.38
1	A	747	5MU	C4-C5	2.26	1.48	1.44
34	a	1518	MA6	C6-N1	2.22	1.36	1.33
34	a	1402	4OC	C6-C5	2.21	1.40	1.35
1	A	747	5MU	C2-N3	-2.17	1.34	1.38
34	a	527	G7M	O4'-C1'	2.17	1.44	1.41
34	a	1519	MA6	C6-N1	2.12	1.36	1.33
1	A	1962	5MC	C6-N1	-2.12	1.34	1.38
1	A	747	5MU	C6-N1	-2.11	1.34	1.38
1	A	955	PSU	C2'-C1'	-2.10	1.51	1.53
34	a	1519	MA6	O4'-C1'	2.09	1.44	1.41
1	A	1939	5MU	C2-N1	2.09	1.41	1.38
1	A	2504	PSU	C4-C5	2.09	1.50	1.44
1	A	2605	PSU	C2-N3	-2.08	1.33	1.37
1	A	2457	PSU	C2-N3	-2.07	1.34	1.37
34	a	966	2MG	O4'-C1'	2.01	1.43	1.41
34	a	1207	2MG	O4'-C1'	2.00	1.43	1.41
1	A	1917	PSU	C4-C5	2.00	1.49	1.44

All (125) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1915	3TD	C5-C6-N1	27.68	163.57	122.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1915	3TD	C6-C5-C4	-26.34	100.00	118.22
1	A	1915	3TD	C6-N1-C2	-8.96	97.10	121.68
45	l	89	0TD	CB-CA-N	-7.50	93.11	109.10
1	A	955	PSU	N1-C2-N3	6.86	122.91	115.13
34	a	1498	UR3	C4-N3-C2	-6.31	118.62	124.56
45	l	89	0TD	CSB-SB-CB	6.18	113.61	102.44
34	a	516	PSU	N1-C2-N3	6.14	122.09	115.13
1	A	2457	PSU	N1-C2-N3	6.07	122.01	115.13
1	A	2580	PSU	N1-C2-N3	6.05	121.98	115.13
1	A	1917	PSU	N1-C2-N3	5.97	121.89	115.13
1	A	1939	5MU	C4-N3-C2	-5.96	119.64	127.35
1	A	746	PSU	N1-C2-N3	5.89	121.80	115.13
1	A	2605	PSU	N1-C2-N3	5.83	121.73	115.13
1	A	2504	PSU	N1-C2-N3	5.81	121.71	115.13
1	A	1939	5MU	N3-C2-N1	5.63	122.36	114.89
1	A	1911	PSU	N1-C2-N3	5.49	121.35	115.13
1	A	747	5MU	N3-C2-N1	5.48	122.17	114.89
1	A	747	5MU	C4-N3-C2	-5.15	120.68	127.35
1	A	2030	6MZ	C3'-C2'-C1'	-5.11	93.29	100.98
1	A	1618	6MZ	O3'-C3'-C4'	5.05	125.66	111.05
1	A	2552	OMU	N3-C2-N1	5.02	121.55	114.89
1	A	2069	G7M	O2'-C2'-C3'	4.95	127.85	111.82
1	A	2552	OMU	C4-N3-C2	-4.90	120.12	126.58
1	A	2069	G7M	O2'-C2'-C1'	4.87	128.85	110.85
1	A	1939	5MU	C5-C4-N3	4.86	119.46	115.31
1	A	1915	3TD	N1-C2-N3	4.78	119.91	116.14
1	A	1939	5MU	C5-C6-N1	-4.68	118.53	123.34
1	A	955	PSU	C4-N3-C2	-4.59	119.72	126.34
1	A	2069	G7M	C3'-C2'-C1'	-4.59	94.07	100.98
34	a	1518	MA6	N1-C6-N6	4.56	121.86	117.06
1	A	955	PSU	O2-C2-N1	-4.28	118.08	122.79
1	A	2605	PSU	C4-N3-C2	-4.22	120.26	126.34
1	A	747	5MU	C5-C4-N3	4.21	118.90	115.31
1	A	746	PSU	C4-N3-C2	-4.13	120.38	126.34
1	A	1917	PSU	C4-N3-C2	-4.08	120.45	126.34
1	A	2457	PSU	C4-N3-C2	-4.03	120.53	126.34
34	a	516	PSU	C4-N3-C2	-3.91	120.71	126.34
1	A	2580	PSU	C4-N3-C2	-3.85	120.79	126.34
1	A	1911	PSU	C4-N3-C2	-3.82	120.84	126.34
1	A	2030	6MZ	O3'-C3'-C4'	3.72	121.79	111.05
34	a	1518	MA6	N3-C2-N1	-3.71	122.88	128.68
34	a	1519	MA6	C4-C5-N7	-3.66	105.59	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	a	516	PSU	O2-C2-N1	-3.61	118.82	122.79
1	A	747	5MU	C5-C6-N1	-3.53	119.71	123.34
1	A	2552	OMU	C5-C4-N3	3.50	120.08	114.84
1	A	1939	5MU	O4-C4-C5	-3.50	120.85	124.90
1	A	2504	PSU	C4-N3-C2	-3.50	121.30	126.34
1	A	1917	PSU	O2-C2-N1	-3.37	119.08	122.79
1	A	2030	6MZ	O3'-C3'-C2'	3.34	122.64	111.82
1	A	747	5MU	O4-C4-C5	-3.32	121.05	124.90
34	a	1519	MA6	C10-N6-C6	-3.32	109.47	119.51
1	A	1915	3TD	C3'-C2'-C1'	3.28	105.46	101.64
34	a	516	PSU	C3'-C2'-C1'	3.24	105.41	101.64
34	a	967	5MC	O2-C2-N3	-3.20	117.13	122.33
34	a	1402	4OC	O2-C2-N3	-3.14	117.22	122.33
34	a	1407	5MC	C5-C4-N3	-3.13	118.29	121.67
1	A	1618	6MZ	C2-N1-C6	3.13	119.28	116.59
1	A	1962	5MC	CM5-C5-C6	-3.13	118.67	122.85
45	l	89	0TD	OD2-CG-CB	3.11	119.87	113.15
1	A	746	PSU	O2-C2-N1	-3.08	119.40	122.79
1	A	2457	PSU	O2-C2-N1	-3.05	119.44	122.79
45	l	89	0TD	OD1-CG-CB	-3.04	116.08	122.44
1	A	2030	6MZ	C2-N1-C6	3.01	119.17	116.59
1	A	2580	PSU	C3'-C2'-C1'	3.01	105.14	101.64
1	A	1911	PSU	O2-C2-N1	-3.00	119.49	122.79
34	a	527	G7M	CN7-N7-C8	-2.99	111.02	125.43
1	A	1962	5MC	C5-C4-N3	-2.97	118.47	121.67
1	A	1917	PSU	C3'-C2'-C1'	2.95	105.08	101.64
1	A	2069	G7M	C2'-C3'-C4'	-2.94	96.93	102.64
34	a	1518	MA6	C4-C5-N7	-2.93	106.34	109.40
1	A	2504	PSU	O2-C2-N1	-2.93	119.56	122.79
34	a	1519	MA6	N3-C2-N1	-2.90	124.15	128.68
34	a	1519	MA6	C10-N6-C9	-2.88	106.83	116.12
1	A	2552	OMU	O4-C4-C5	-2.82	120.19	125.16
34	a	1407	5MC	O2-C2-N3	-2.80	117.78	122.33
1	A	1911	PSU	C6-C5-C4	-2.79	116.25	118.20
34	a	967	5MC	C5-C4-N3	-2.78	118.67	121.67
1	A	2605	PSU	O2-C2-N1	-2.77	119.74	122.79
1	A	1962	5MC	O2-C2-N3	-2.77	117.83	122.33
1	A	1962	5MC	C5-C6-N1	-2.69	120.57	123.34
1	A	2605	PSU	C6-C5-C4	-2.66	116.34	118.20
1	A	2503	2MA	C8-N7-C5	2.66	108.05	102.99
1	A	1835	2MG	C5-C6-N1	2.64	118.61	113.95
34	a	1402	4OC	O4'-C1'-N1	2.60	114.30	108.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	a	1407	5MC	C5-C6-N1	-2.58	120.69	123.34
34	a	1516	2MG	C5-C6-N1	2.57	118.48	113.95
34	a	1402	4OC	C6-C5-C4	2.49	120.01	116.96
34	a	1207	2MG	C5-C6-N1	2.48	118.33	113.95
1	A	2504	PSU	C6-C5-C4	-2.45	116.48	118.20
1	A	745	1MG	C5-C6-N1	2.42	117.55	113.90
1	A	2552	OMU	O2-C2-N3	-2.42	116.99	121.50
1	A	2503	2MA	C5-C6-N1	2.41	118.17	114.02
34	a	1207	2MG	C8-N7-C5	2.38	107.53	102.99
1	A	1939	5MU	O2-C2-N1	-2.37	119.64	122.79
34	a	966	2MG	C5-C6-N1	2.37	118.13	113.95
34	a	966	2MG	C3'-C2'-C1'	2.36	104.54	100.98
1	A	2498	OMC	O4'-C1'-N1	2.34	113.72	108.36
1	A	747	5MU	O2-C2-N1	-2.34	119.68	122.79
34	a	1516	2MG	C8-N7-C5	2.30	107.37	102.99
1	A	2251	OMG	C5-C6-N1	2.30	118.01	113.95
34	a	1518	MA6	C10-N6-C9	-2.30	108.72	116.12
1	A	2498	OMC	O2-C2-N3	-2.26	118.66	122.33
1	A	2503	2MA	C3'-C2'-C1'	2.26	104.37	100.98
1	A	747	5MU	O4'-C1'-N1	2.24	113.48	108.36
1	A	745	1MG	C8-N7-C5	2.22	107.21	102.99
1	A	2580	PSU	O2-C2-N3	-2.21	117.64	121.82
1	A	1835	2MG	C8-N7-C5	2.20	107.19	102.99
34	a	966	2MG	C8-N7-C5	2.19	107.17	102.99
1	A	2580	PSU	O2-C2-N1	-2.19	120.38	122.79
34	a	967	5MC	O4'-C1'-N1	2.18	113.34	108.36
1	A	1939	5MU	C5M-C5-C6	-2.16	119.96	122.85
1	A	1939	5MU	C5M-C5-C4	2.15	121.14	118.77
1	A	2251	OMG	C8-N7-C5	2.15	107.08	102.99
1	A	746	PSU	C5-C6-N1	-2.14	118.90	122.11
34	a	967	5MC	CM5-C5-C6	-2.13	120.00	122.85
1	A	2445	2MG	C5-C6-N1	2.13	117.72	113.95
1	A	2552	OMU	C6-N1-C2	-2.13	118.26	120.99
34	a	1407	5MC	CM5-C5-C6	-2.10	120.04	122.85
34	a	967	5MC	C5-C6-N1	-2.10	121.18	123.34
1	A	2457	PSU	C3'-C2'-C1'	2.08	104.06	101.64
1	A	745	1MG	O6-C6-C5	-2.07	120.52	124.19
1	A	2457	PSU	C5-C6-N1	-2.03	119.07	122.11
34	a	1498	UR3	O4-C4-C5	-2.02	118.31	124.37
1	A	1618	6MZ	C3'-C2'-C1'	-2.01	97.95	100.98

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	746	PSU	C2'-C1'-C5-C6
1	A	1618	6MZ	N1-C6-N6-C9
1	A	1618	6MZ	O4'-C4'-C5'-O5'
1	A	1618	6MZ	C3'-C4'-C5'-O5'
1	A	1915	3TD	O4'-C1'-C5-C4
1	A	1915	3TD	O4'-C1'-C5-C6
1	A	2445	2MG	C3'-C4'-C5'-O5'
34	a	1518	MA6	C5-C6-N6-C9
34	a	1519	MA6	O4'-C4'-C5'-O5'
34	a	1519	MA6	C5-C6-N6-C10
34	a	1519	MA6	N1-C6-N6-C10
55	v	252	MEQ	N-CA-CB-CG
34	a	1519	MA6	C3'-C4'-C5'-O5'
1	A	2445	2MG	O4'-C4'-C5'-O5'
1	A	2498	OMC	C3'-C4'-C5'-O5'
1	A	2498	OMC	O4'-C4'-C5'-O5'
55	v	252	MEQ	C-CA-CB-CG
1	A	1939	5MU	O4'-C4'-C5'-O5'
1	A	1618	6MZ	C5-C6-N6-C9
1	A	2030	6MZ	O4'-C4'-C5'-O5'
1	A	2069	G7M	O4'-C4'-C5'-O5'
45	l	89	0TD	CG-CB-SB-CSB
1	A	746	PSU	O4'-C4'-C5'-O5'
34	a	1518	MA6	O4'-C4'-C5'-O5'
45	l	89	0TD	SB-CB-CG-OD1
1	A	2069	G7M	C4'-C5'-O5'-P
1	A	2504	PSU	O4'-C4'-C5'-O5'
34	a	527	G7M	C4'-C5'-O5'-P
1	A	1939	5MU	C3'-C4'-C5'-O5'
34	a	1519	MA6	C4'-C5'-O5'-P
45	l	89	0TD	SB-CB-CG-OD2
1	A	746	PSU	C3'-C4'-C5'-O5'
1	A	2030	6MZ	C3'-C4'-C5'-O5'
1	A	2504	PSU	C3'-C4'-C5'-O5'
34	a	1402	4OC	O4'-C4'-C5'-O5'
1	A	746	PSU	O4'-C1'-C5-C6
1	A	2503	2MA	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 319 ligands modelled in this entry, 319 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

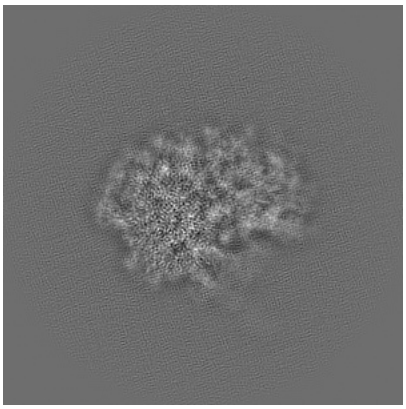
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-7341. These allow visual inspection of the internal detail of the map and identification of artifacts.

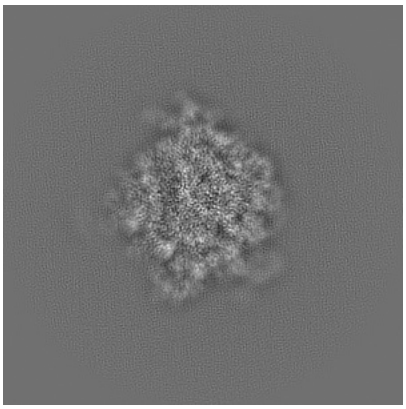
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

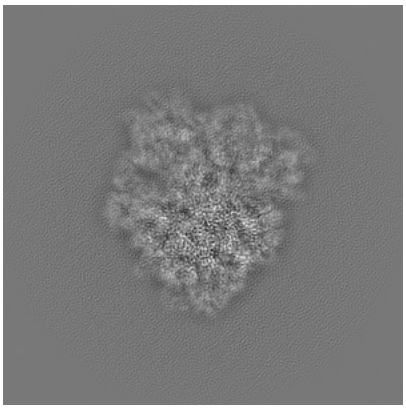
6.1.1 Primary map



X

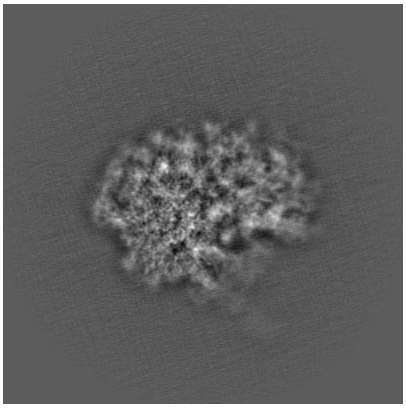


Y

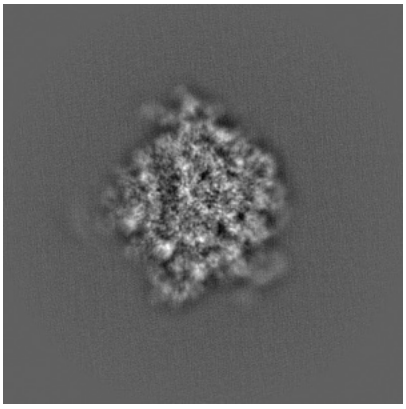


Z

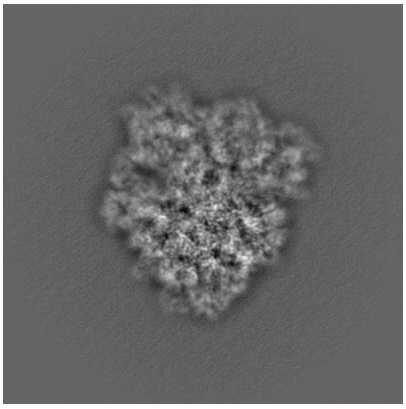
6.1.2 Raw map



X



Y

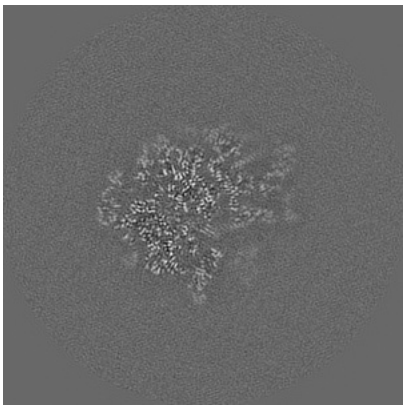


Z

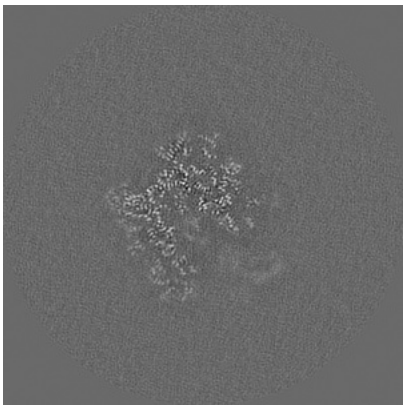
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

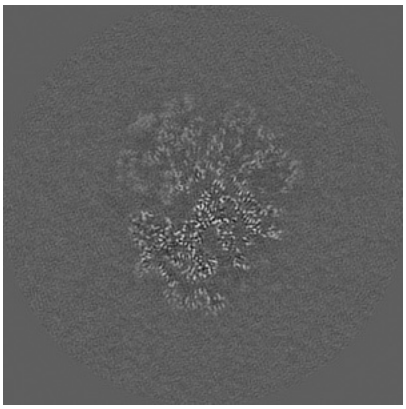
6.2.1 Primary map



X Index: 192

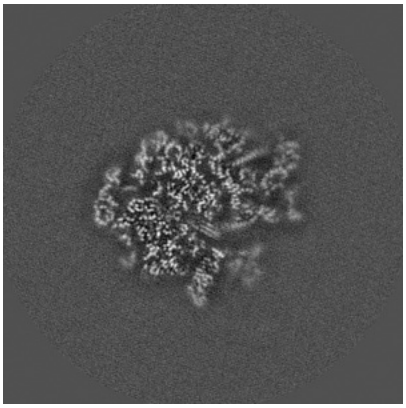


Y Index: 192

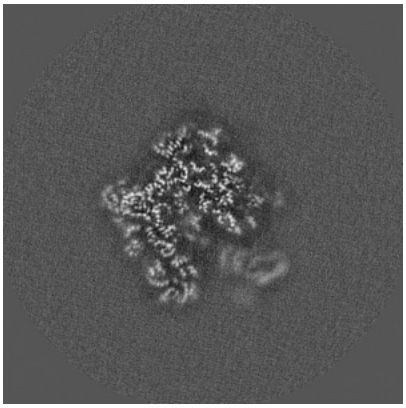


Z Index: 192

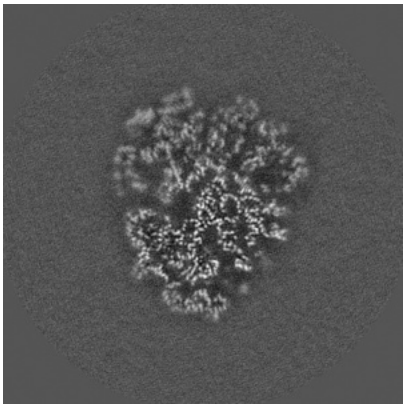
6.2.2 Raw map



X Index: 192



Y Index: 192

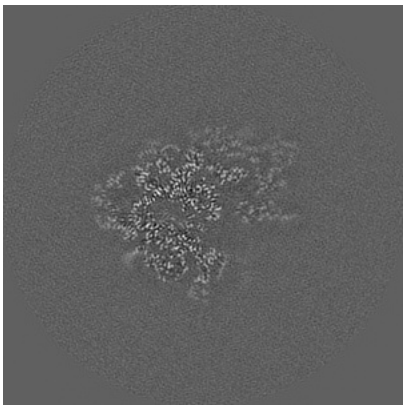


Z Index: 192

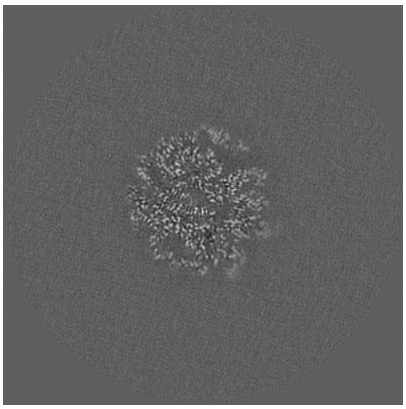
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

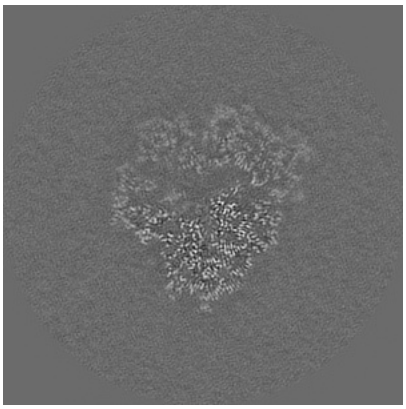
6.3.1 Primary map



X Index: 198

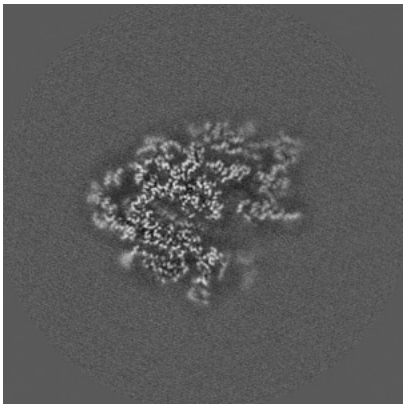


Y Index: 158

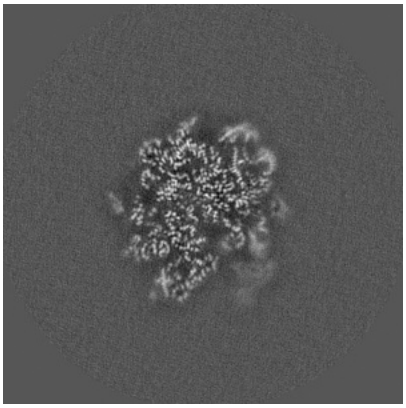


Z Index: 176

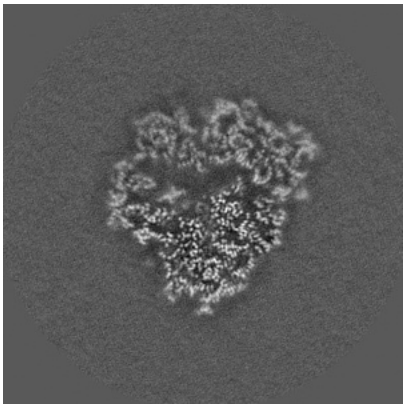
6.3.2 Raw map



X Index: 198



Y Index: 177

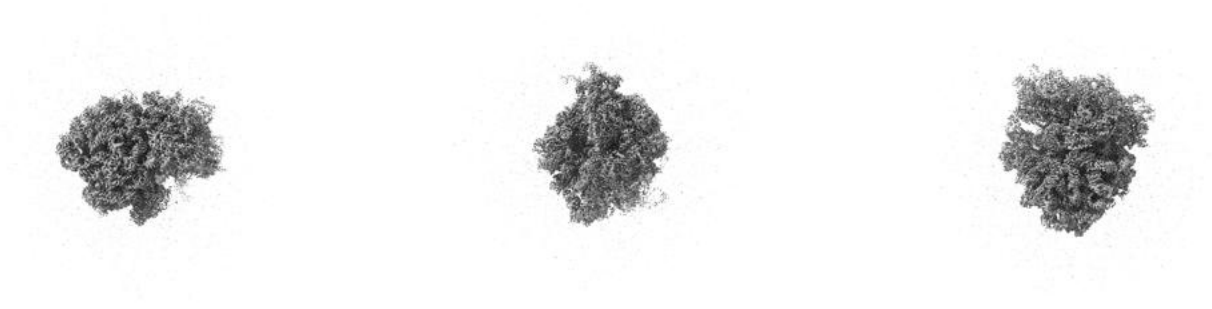


Z Index: 176

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

6.4 Orthogonal surface views (i)

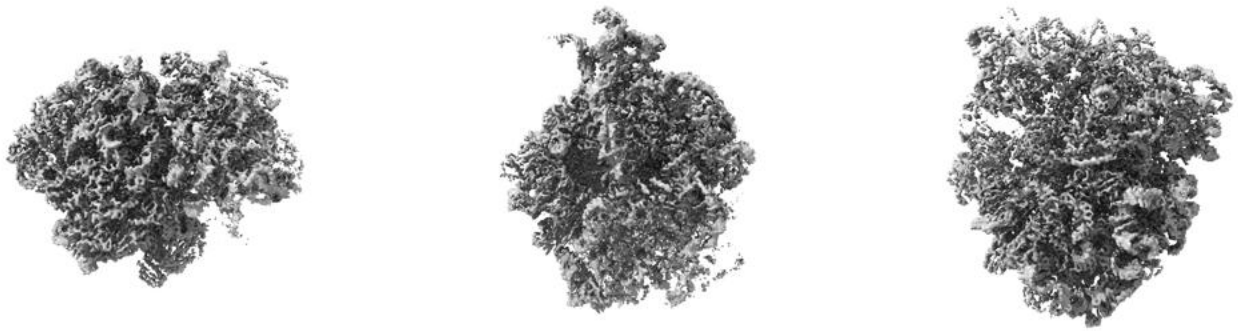
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

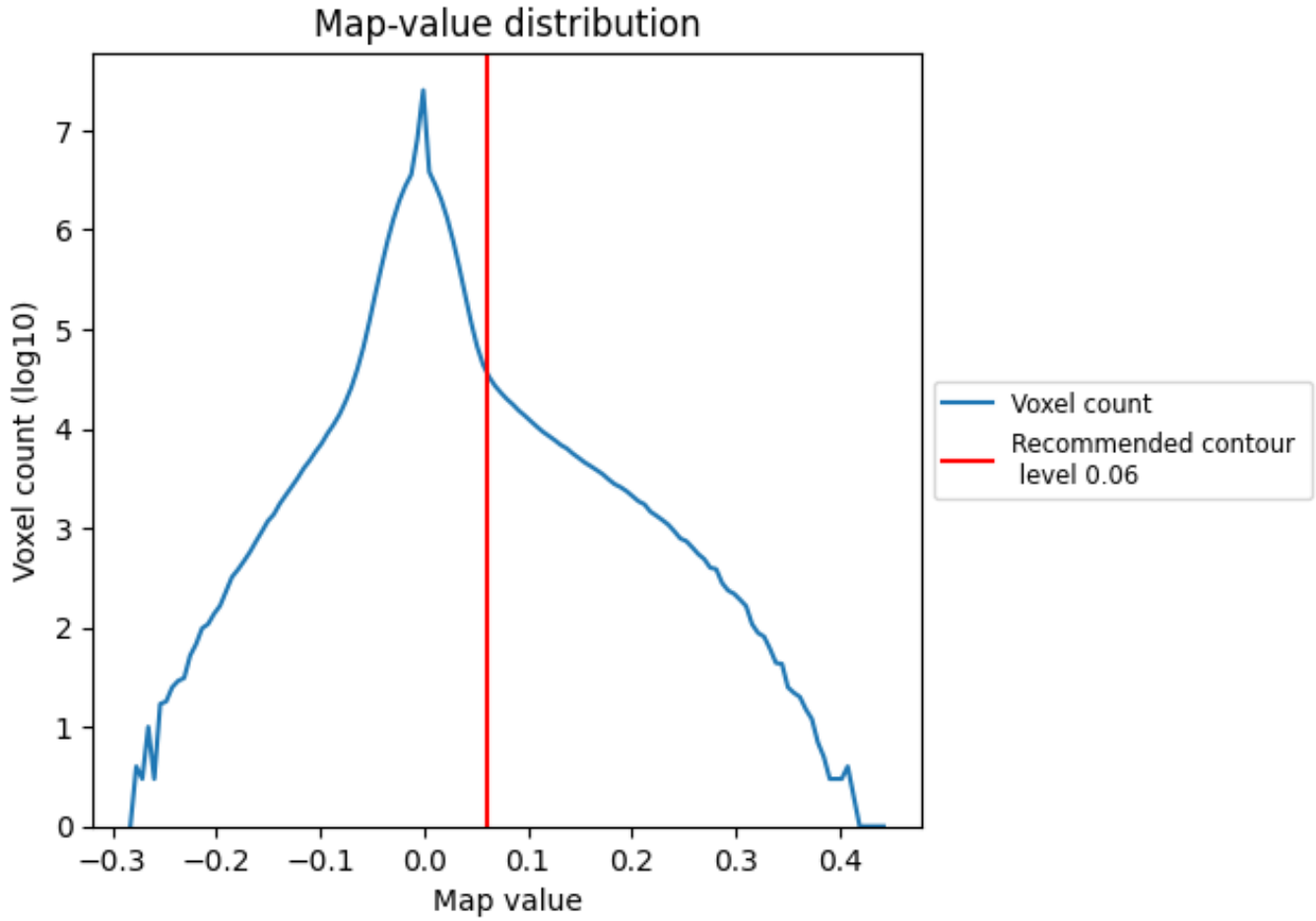
6.5 Mask visualisation (i)

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

7 Map analysis

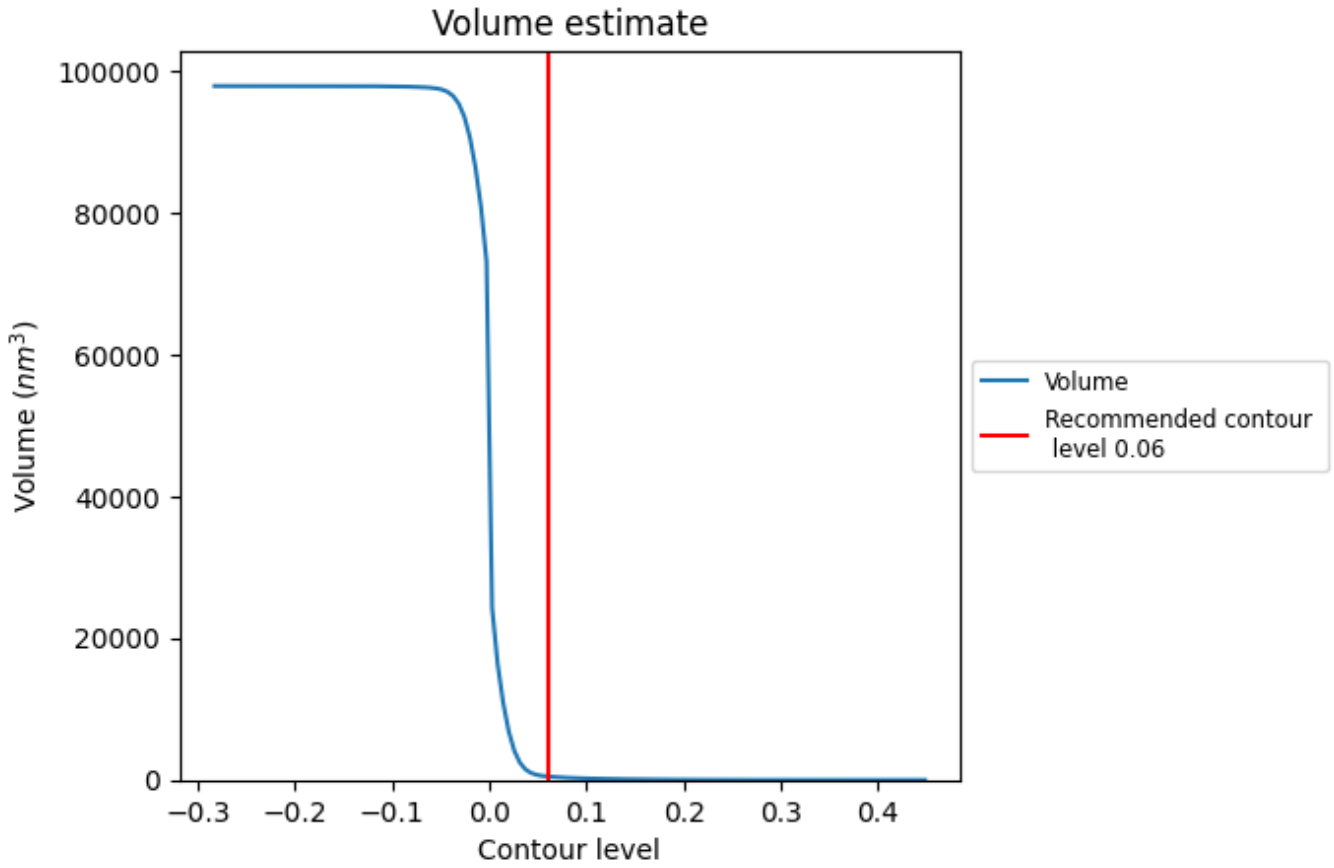
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

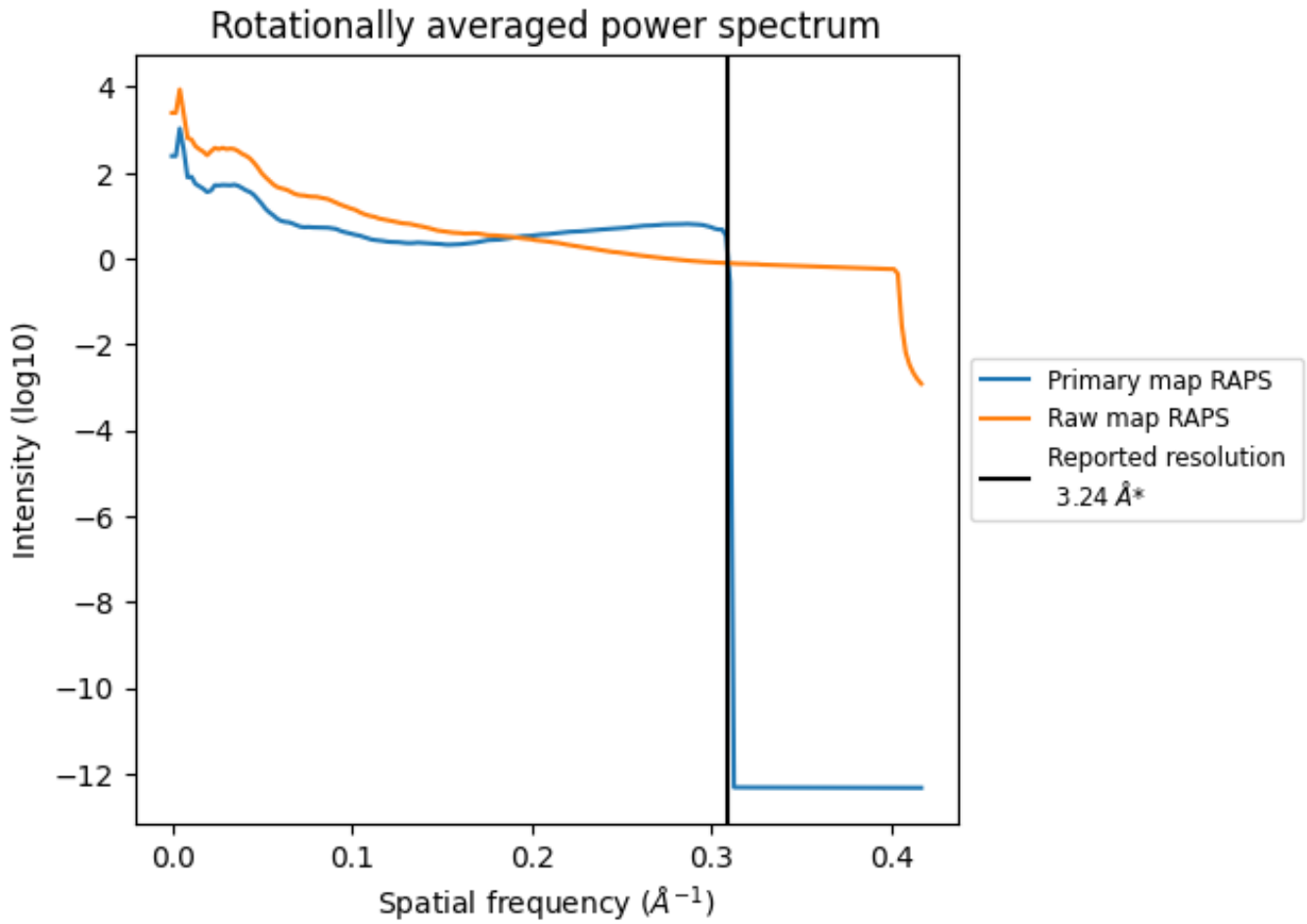
7.2 Volume estimate



The volume at the recommended contour level is 487 nm^3; this corresponds to an approximate mass of 440 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)

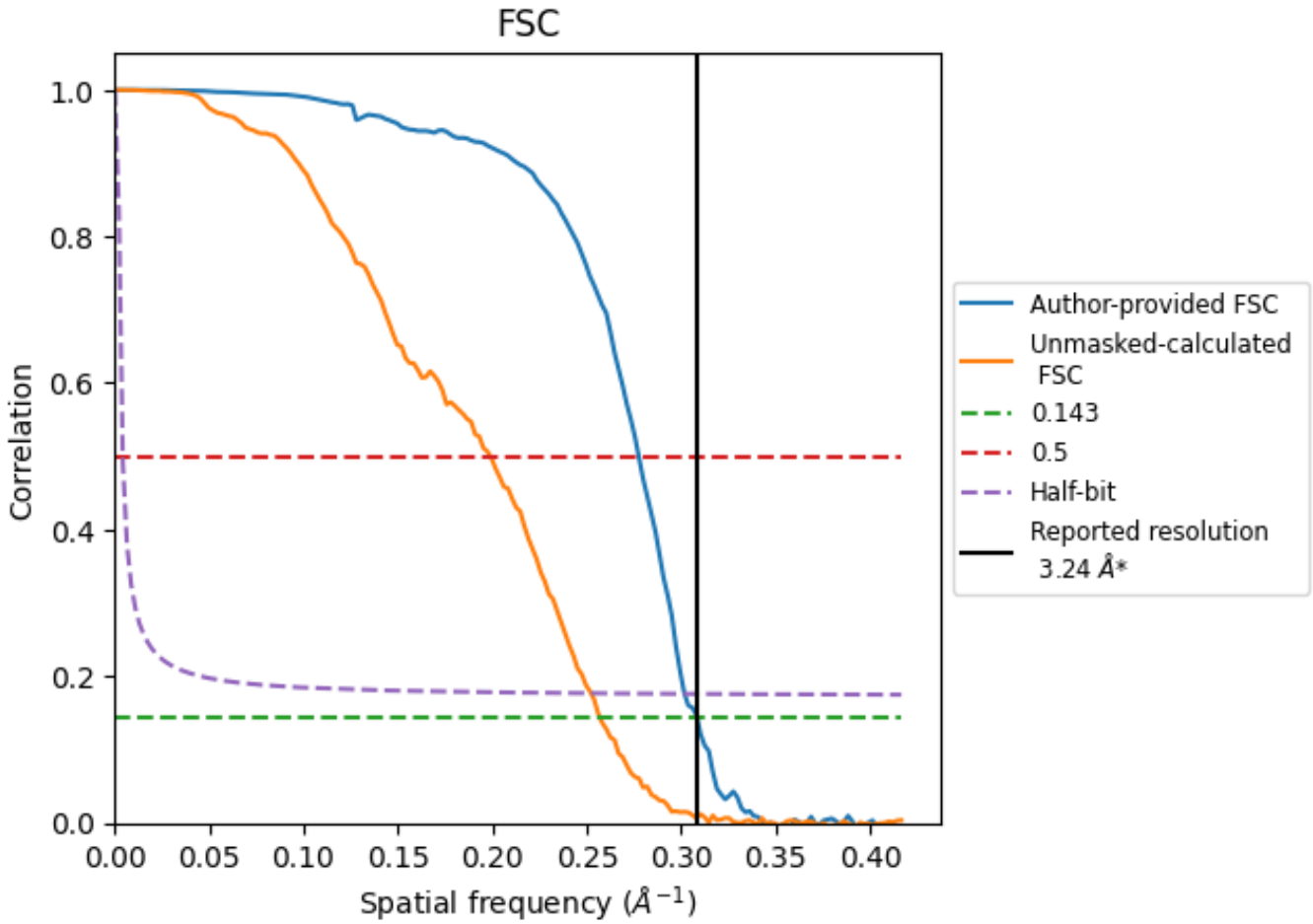


*Reported resolution corresponds to spatial frequency of 0.309 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.309 Å^{-1}

8.2 Resolution estimates (i)

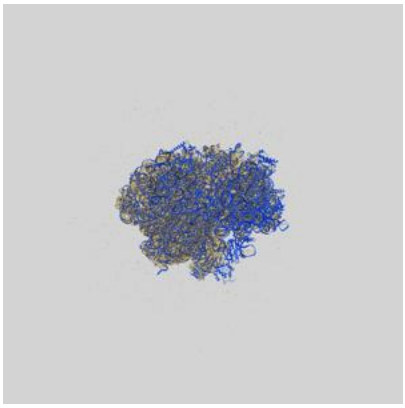
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.24	-	-
Author-provided FSC curve	3.24	3.60	3.31
Unmasked-calculated*	3.89	5.03	3.96

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.89 differs from the reported value 3.24 by more than 10 %

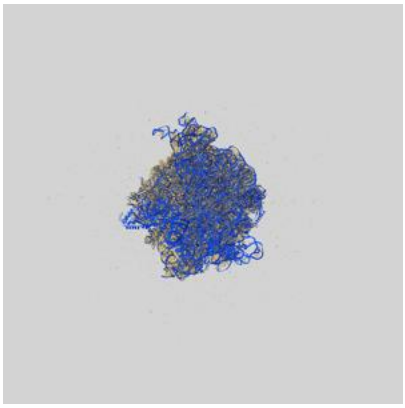
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-7341 and PDB model 6C4I. Per-residue inclusion information can be found in section 3 on page 17.

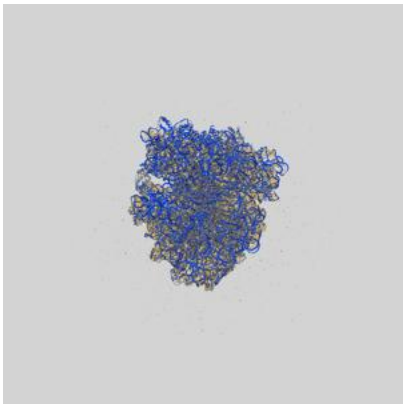
9.1 Map-model overlay



X



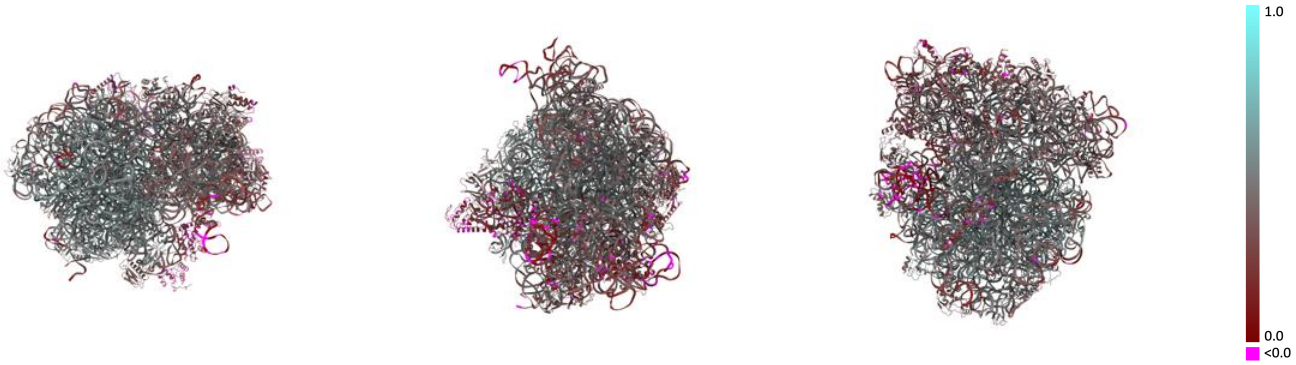
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.06 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.

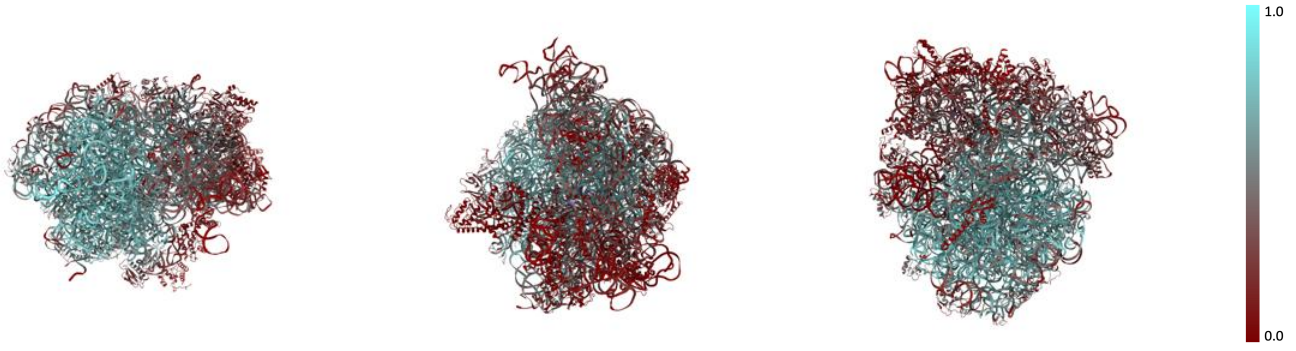
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according 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.

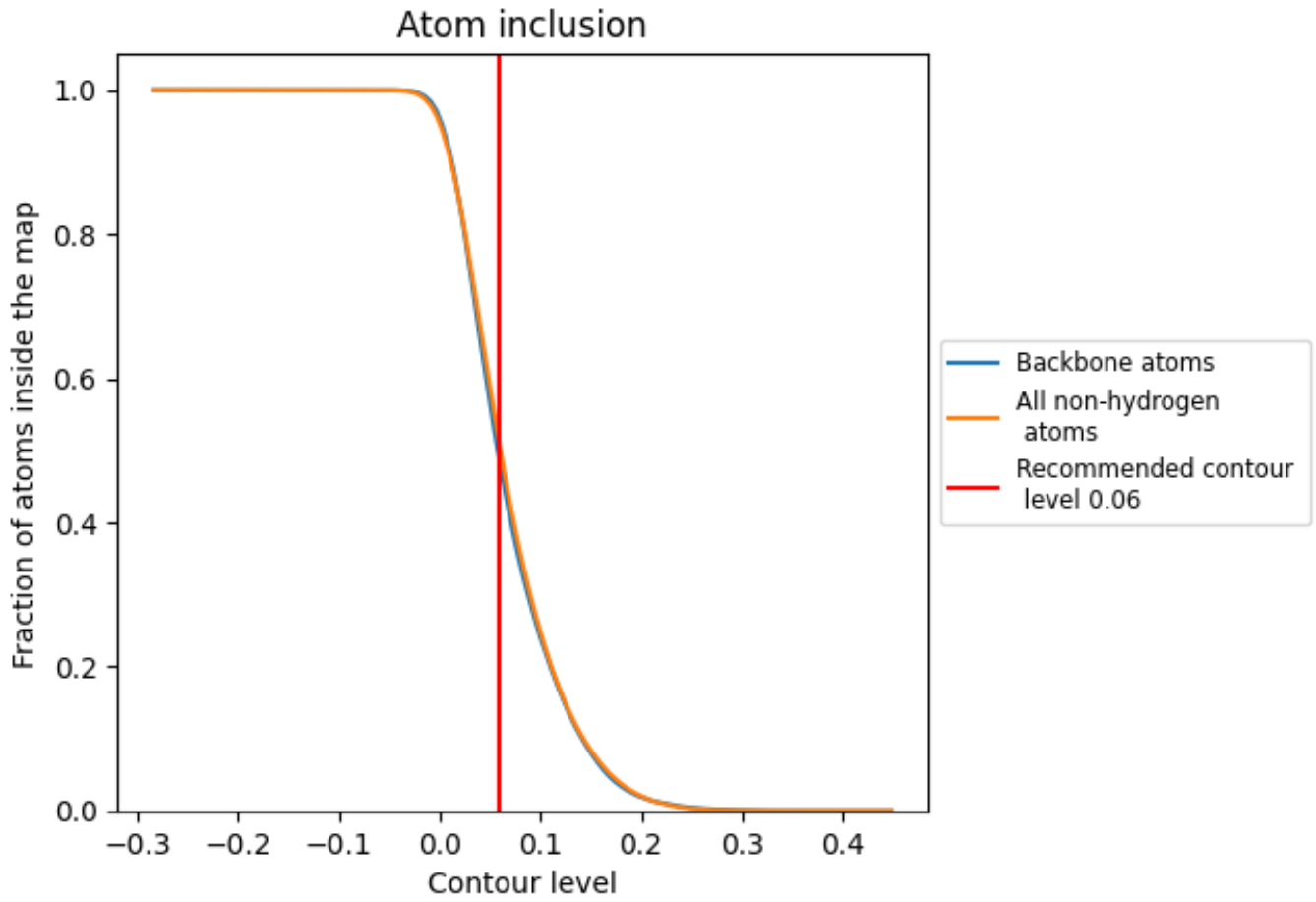
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.06).

9.4 Atom inclusion (i)



At the recommended contour level, 48% of all backbone atoms, 50% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5037	0.4320
0	0.6284	0.4970
1	0.0957	0.2600
2	0.6434	0.5010
3	0.5144	0.4540
4	0.6845	0.5350
5	0.6741	0.5390
6	0.6314	0.5260
A	0.6859	0.4760
B	0.5221	0.4180
C	0.6599	0.5220
D	0.6160	0.5120
E	0.4704	0.4500
F	0.2170	0.3670
G	0.3543	0.3980
H	0.1086	0.2400
I	0.0000	0.0840
J	0.0031	0.0930
K	0.6555	0.5060
L	0.5972	0.5110
M	0.5752	0.4820
N	0.6286	0.5110
O	0.6525	0.5200
P	0.3743	0.4260
Q	0.5732	0.4910
R	0.6872	0.5210
S	0.5872	0.4950
T	0.6160	0.5060
U	0.4863	0.4570
V	0.4201	0.4400
W	0.5542	0.4630
X	0.6237	0.5130
Y	0.5840	0.4980
Z	0.4192	0.4260
a	0.4224	0.4130

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Chain	Atom inclusion	Q-score
b	0.1018	0.2890
c	0.1421	0.3450
d	0.1094	0.3380
e	0.2469	0.3960
f	0.3011	0.3780
g	0.1672	0.3090
h	0.2604	0.4010
i	0.0950	0.3210
j	0.0562	0.2800
k	0.3810	0.4260
l	0.3738	0.4500
m	0.1509	0.3300
n	0.1032	0.3430
o	0.3942	0.4060
p	0.2313	0.3920
q	0.2547	0.3990
r	0.2868	0.3540
s	0.1236	0.3480
t	0.2691	0.3820
u	0.1753	0.3240
v	0.1905	0.3170
w	0.3924	0.4690
x	0.4232	0.3990
y	0.0287	0.1220
z	0.3670	0.4340