



Full wwPDB EM Validation Report ⓘ

Feb 10, 2025 – 07:17 PM EST

PDB ID : 8FTO
EMDB ID : EMD-29449
Title : E. coli 70S ribosome with an improved MS2 tag inserted in H98
Authors : Nissley, A.J.; Cate, J.H.D.
Deposited on : 2023-01-12
Resolution : 1.85 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:

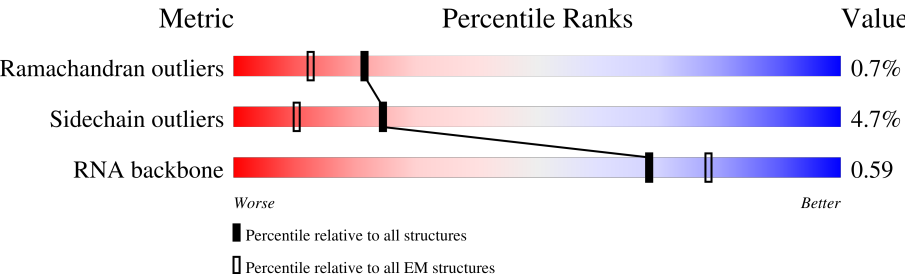
EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

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 1.85 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	0	55	
2	1	46	
3	2	65	
4	3	38	
5	4	70	
6	A	1542	
7	B	241	
8	C	233	

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Mol	Chain	Length	Quality of chain
9	D	206	
10	E	167	
11	F	135	
12	G	179	
13	H	130	
14	I	130	
15	J	103	
16	K	129	
17	L	124	
18	M	118	
19	N	101	
20	O	89	
21	P	82	
22	Q	84	
23	R	75	
24	S	92	
25	T	87	
26	U	71	
27	X	27	
28	Z	76	
29	a	2937	
30	b	120	
31	c	273	
32	d	209	
33	e	201	

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Mol	Chain	Length	Quality of chain
34	f	179	
35	g	177	
36	h	149	
37	i	142	
38	j	123	
39	k	144	
40	l	136	
41	m	127	
42	n	117	
43	o	115	
44	p	118	
45	q	103	
46	r	110	
47	s	100	
48	t	104	
49	u	94	
50	v	85	
51	w	78	
52	x	63	
53	y	59	
54	z	57	

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 146561 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
1	0	51	Total	C	N	O	0	0
			417	269	76	72		

- Molecule 2 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 3 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 4 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 5 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	60	Total	C	N	O	S	0	0
			480	299	90	85	6		

- Molecule 6 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	1519	Total	C	N	O	P	0	0
			32612	14552	5986	10555	1519		

- Molecule 7 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	224	Total	C	N	O	S	0	0
			1753	1109	315	321	8		

- Molecule 8 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 9 is a protein called 30S ribosomal protein S4.

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

- Molecule 10 is a protein called 30S ribosomal protein S5.

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

- Molecule 11 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	103	Total	C	N	O	S	0	0
			839	530	151	151	7		

- Molecule 12 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	G	153	Total	C	N	O	S	0	0
			1203	750	231	218	4		

- Molecule 13 is a protein called 30S ribosomal protein S8.

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

- Molecule 14 is a protein called 30S ribosomal protein S9.

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

- Molecule 15 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	J	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 16 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	K	117	Total	C	N	O	S	0	0
			877	540	173	161	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	119	IAS	ASN	conflict	UNP A0A0H3PWX2

- Molecule 17 is a protein called 30S ribosomal protein S12.

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

- Molecule 18 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	M	115	Total	C	N	O	S	0	0
			891	552	179	157	3		

- Molecule 19 is a protein called 30S ribosomal protein S14.

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

- Molecule 20 is a protein called 30S ribosomal protein S15.

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

- Molecule 21 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	P	81	Total	C	N	O	S	0	0
			643	403	127	112	1		

- Molecule 22 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Q	79	Total	C	N	O	S	0	0
			641	406	120	112	3		

- Molecule 23 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	R	66	Total	C	N	O	S	0	0
			544	345	102	96	1		

- Molecule 24 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	S	84	Total	C	N	O	S	0	0
			668	427	127	112	2		

- Molecule 25 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	T	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 26 is a protein called 30S ribosomal protein S21.

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

- Molecule 27 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	X	9	Total	C	N	O	P	0	0
			189	85	31	64	9		

- Molecule 28 is a RNA chain called P-site tRNA-fMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Z	76	Total	C	N	O	P	0	0
			1623	723	295	529	76		

- Molecule 29 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	a	2767	Total	C	N	O	P	0	0
			59422	26515	10942	19198	2767		

- Molecule 30 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	b	119	Total	C	N	O	P	0	0
			2549	1135	466	829	119		

- Molecule 31 is a protein called 50S ribosomal protein L2.

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

- Molecule 32 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	d	209	Total	C	N	O	S	0	0
			1566	980	288	294	4		

- Molecule 33 is a protein called 50S ribosomal protein L4.

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

- Molecule 34 is a protein called 50S ribosomal protein L5.

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

- Molecule 35 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	g	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 36 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	h	41	Total	C	N	O	S	0	0
			303	194	54	54	1		

- Molecule 37 is a protein called 50S ribosomal protein L13.

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

- Molecule 38 is a protein called 50S ribosomal protein L14.

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

- Molecule 39 is a protein called 50S ribosomal protein L15.

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

- Molecule 40 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	l	136	Total	C	N	O	S	0	0
			1075	686	205	177	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	82	MV6	MET	conflict	UNP A0A0H3EMH6

- Molecule 41 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	m	118	Total	C	N	O	S	0	0
			945	585	194	161	5		

- Molecule 42 is a protein called 50S ribosomal protein L18.

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

- Molecule 43 is a protein called 50S ribosomal protein L19.

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

- Molecule 44 is a protein called 50S ribosomal protein L20.

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

- Molecule 45 is a protein called Ribosomal protein L21.

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

- Molecule 46 is a protein called 50S ribosomal protein L22.

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

- Molecule 47 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	s	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 48 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	t	102	Total	C	N	O	S	0	0
			779	492	146	141			

- Molecule 49 is a protein called 50S ribosomal protein L25.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	v	76	Total	C	N	O	S	0	0
			576	357	114	104	1		

- Molecule 51 is a protein called 50S ribosomal protein L28.

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

- Molecule 52 is a protein called 50S ribosomal protein L29.

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

- Molecule 53 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	y	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

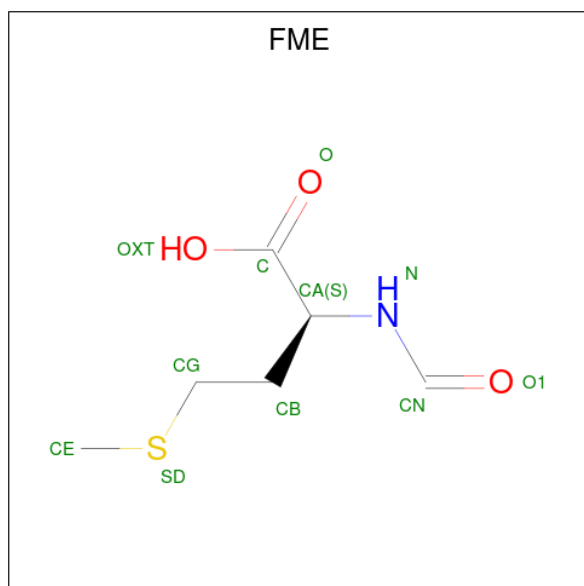
- Molecule 54 is a protein called 50S ribosomal protein L32.

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

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
55	A	81	Total	Mg	0
			81	81	
55	a	195	Total	Mg	0
			195	195	
55	b	5	Total	Mg	0
			5	5	
55	c	1	Total	Mg	0
			1	1	
55	d	1	Total	Mg	0
			1	1	
55	z	1	Total	Mg	0
			1	1	

- Molecule 56 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: C₆H₁₁NO₃S).



Mol	Chain	Residues	Atoms					AltConf
56	a	1	Total	C	N	O	S	0
			10	6	1	2	1	

- Molecule 57 is water.

Mol	Chain	Residues	Atoms		AltConf
57	0	7	Total 7	O 7	0
57	1	24	Total 24	O 24	0
57	2	19	Total 19	O 19	0
57	3	2	Total 2	O 2	0
57	A	1650	Total 1650	O 1650	0
57	B	1	Total 1	O 1	0
57	C	39	Total 39	O 39	0
57	D	3	Total 3	O 3	0
57	E	12	Total 12	O 12	0
57	G	4	Total 4	O 4	0
57	H	29	Total 29	O 29	0
57	I	20	Total 20	O 20	0
57	J	14	Total 14	O 14	0
57	K	12	Total 12	O 12	0
57	L	18	Total 18	O 18	0
57	M	12	Total 12	O 12	0
57	N	27	Total 27	O 27	0
57	O	11	Total 11	O 11	0
57	P	8	Total 8	O 8	0
57	Q	4	Total 4	O 4	0
57	R	2	Total 2	O 2	0
57	S	10	Total 10	O 10	0

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Mol	Chain	Residues	Atoms		AltConf
57	T	2	Total 2	O 2	0
57	U	4	Total 4	O 4	0
57	X	6	Total 6	O 6	0
57	Z	21	Total 21	O 21	0
57	a	3559	Total 3559	O 3559	0
57	b	93	Total 93	O 93	0
57	c	90	Total 90	O 90	0
57	d	40	Total 40	O 40	0
57	e	44	Total 44	O 44	0
57	f	9	Total 9	O 9	0
57	h	3	Total 3	O 3	0
57	i	16	Total 16	O 16	0
57	j	14	Total 14	O 14	0
57	k	42	Total 42	O 42	0
57	l	27	Total 27	O 27	0
57	m	26	Total 26	O 26	0
57	n	23	Total 23	O 23	0
57	o	12	Total 12	O 12	0
57	p	28	Total 28	O 28	0
57	q	20	Total 20	O 20	0
57	r	21	Total 21	O 21	0

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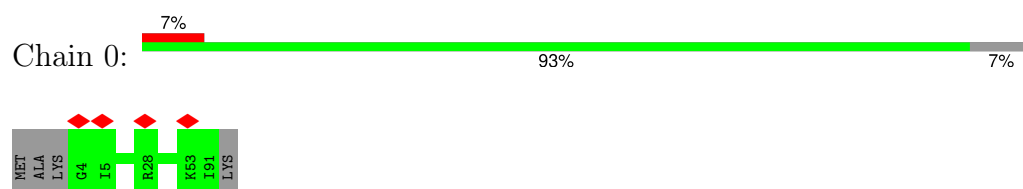
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Mol	Chain	Residues	Atoms		AltConf
57	s	12	Total 12	O 12	0
57	t	2	Total 2	O 2	0
57	u	4	Total 4	O 4	0
57	v	15	Total 15	O 15	0
57	w	18	Total 18	O 18	0
57	x	2	Total 2	O 2	0
57	y	5	Total 5	O 5	0
57	z	28	Total 28	O 28	0

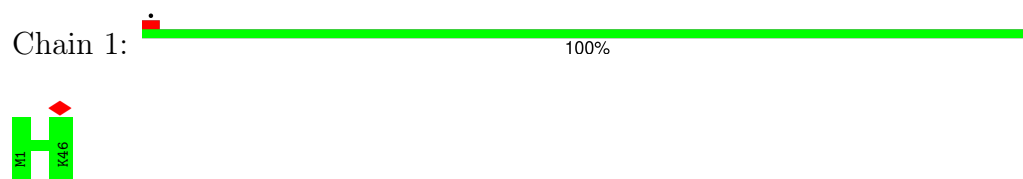
3 Residue-property plots [i](#)

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

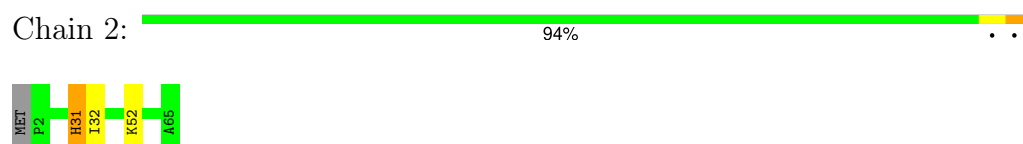
- Molecule 1: 50S ribosomal protein L33



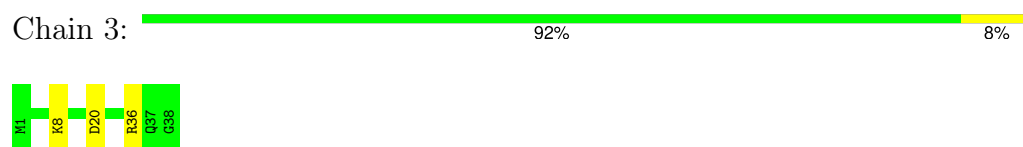
- Molecule 2: 50S ribosomal protein L34



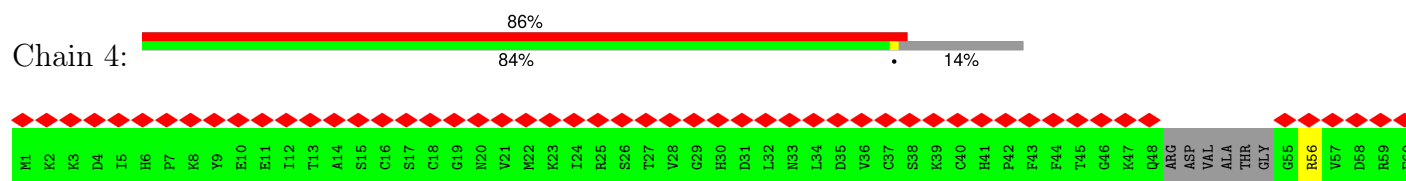
- Molecule 3: 50S ribosomal protein L35

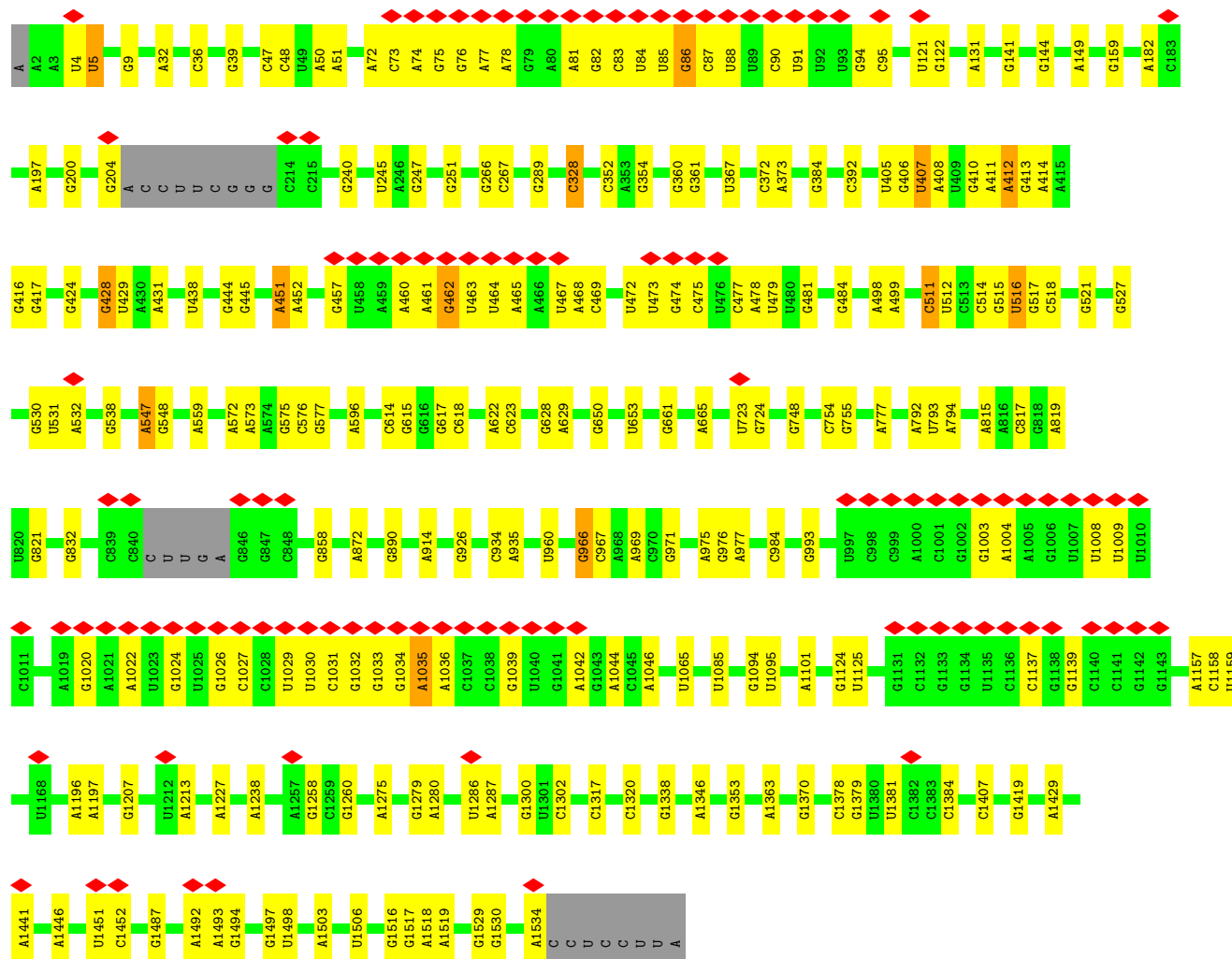


- Molecule 4: 50S ribosomal protein L36

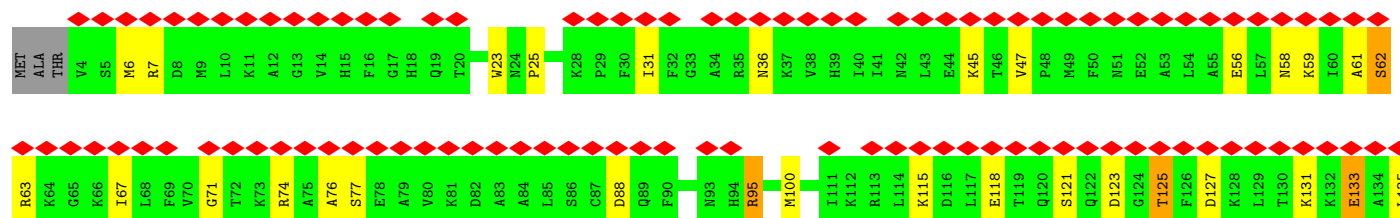
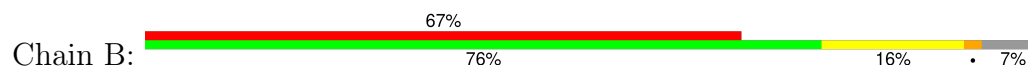


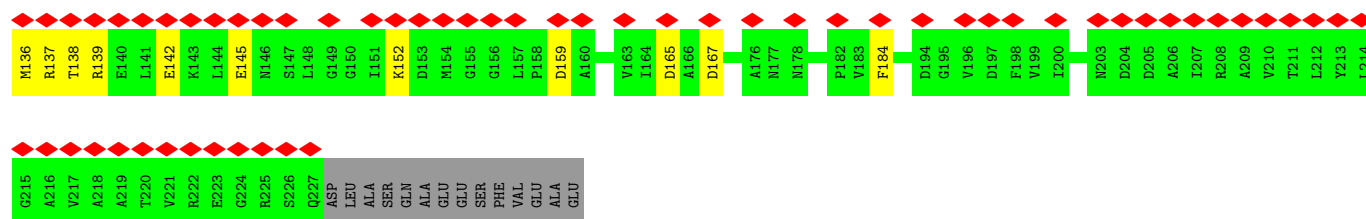
- Molecule 5: 50S ribosomal protein L31



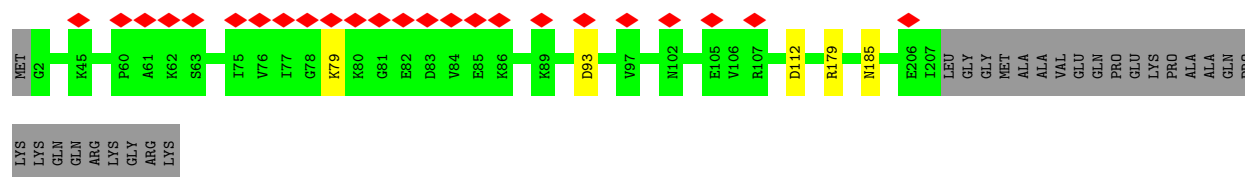
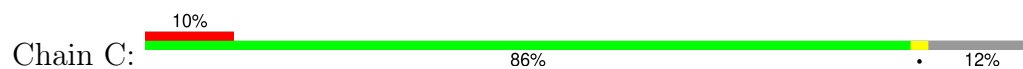


- Molecule 7: 30S ribosomal protein S2

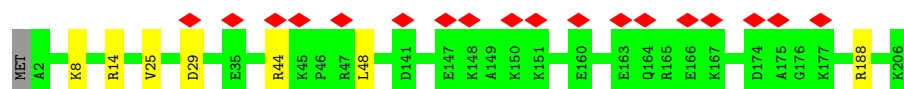




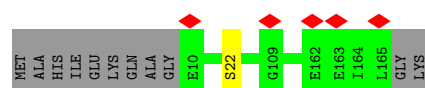
• Molecule 8: 30S ribosomal protein S3



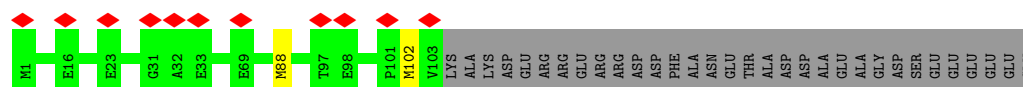
• Molecule 9: 30S ribosomal protein S4



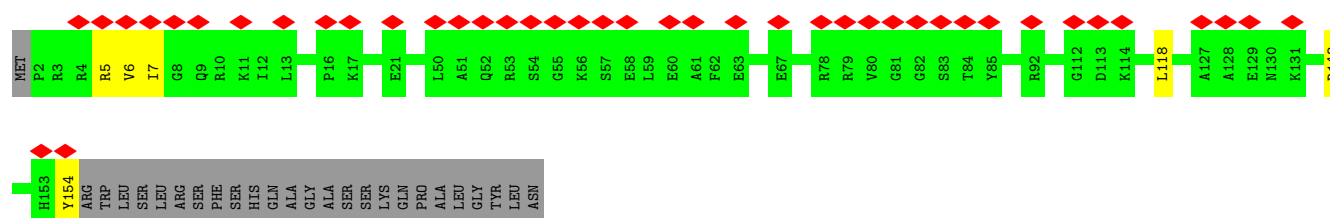
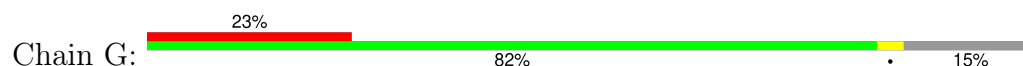
• Molecule 10: 30S ribosomal protein S5



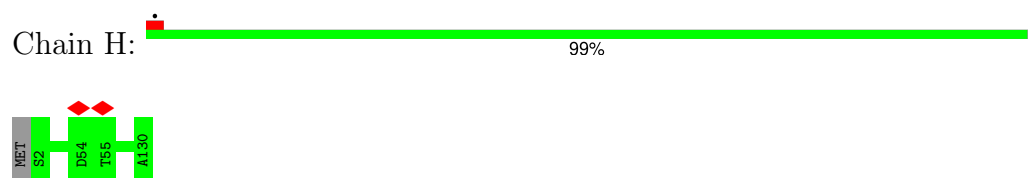
• Molecule 11: 30S ribosomal protein S6



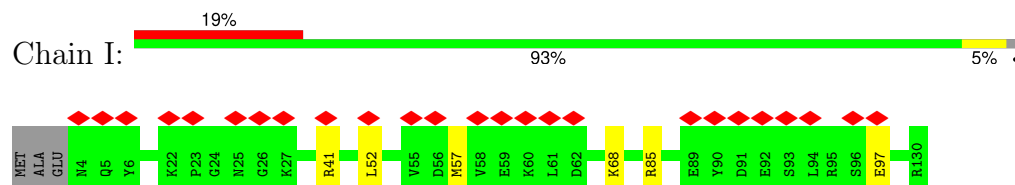
• Molecule 12: 30S ribosomal protein S7



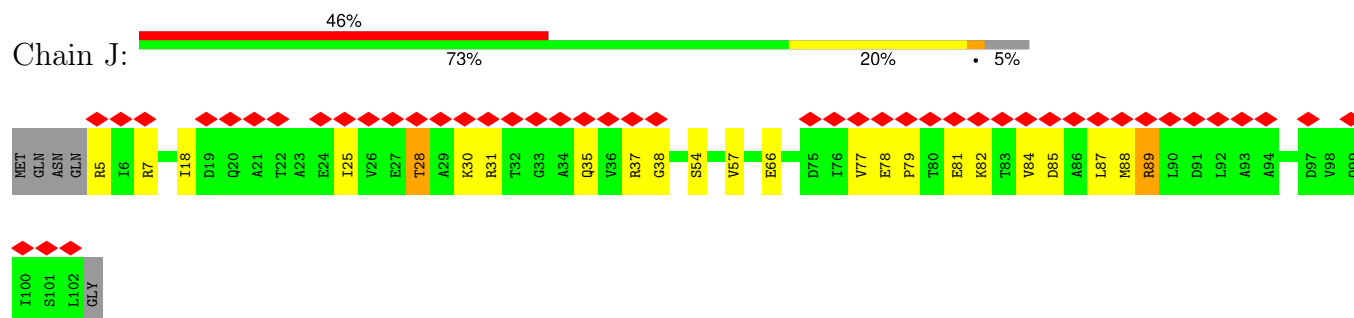
- Molecule 13: 30S ribosomal protein S8



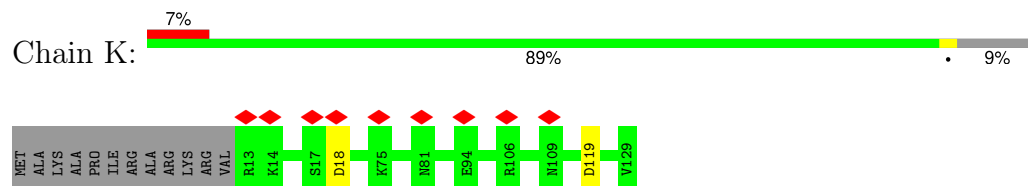
- Molecule 14: 30S ribosomal protein S9



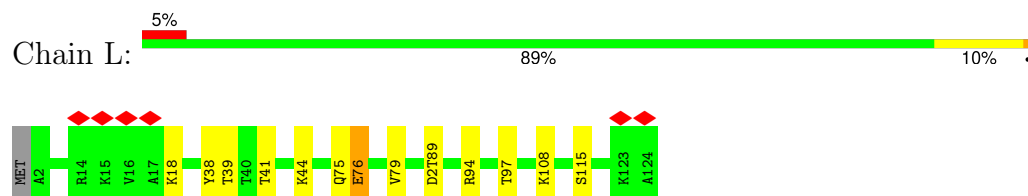
- Molecule 15: 30S ribosomal protein S10



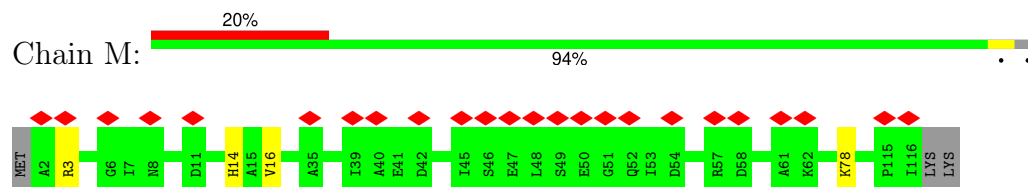
- Molecule 16: 30S ribosomal protein S11



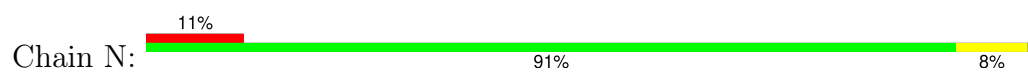
- Molecule 17: 30S ribosomal protein S12



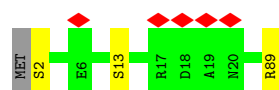
- Molecule 18: 30S ribosomal protein S13



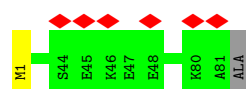
- Molecule 19: 30S ribosomal protein S14



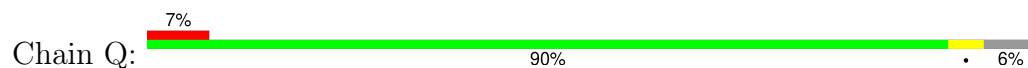
- Molecule 20: 30S ribosomal protein S15



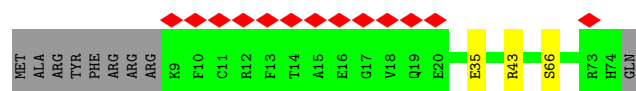
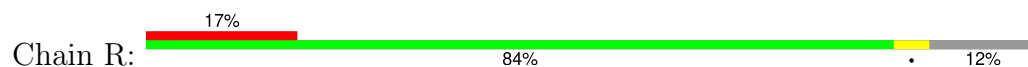
- Molecule 21: 30S ribosomal protein S16



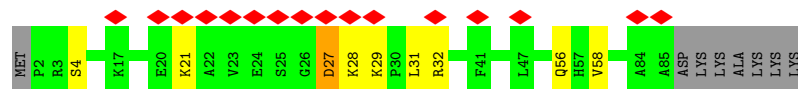
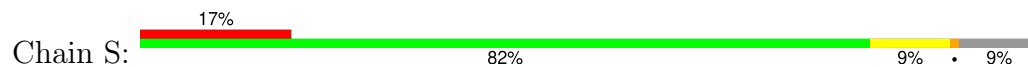
- Molecule 22: 30S ribosomal protein S17



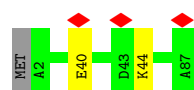
- Molecule 23: 30S ribosomal protein S18



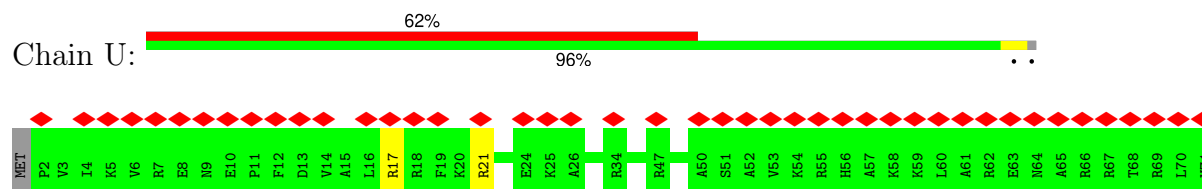
- Molecule 24: 30S ribosomal protein S19



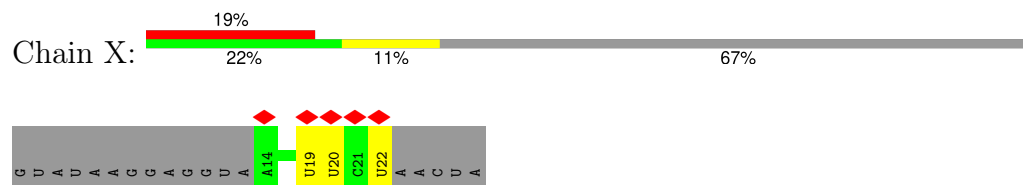
- Molecule 25: 30S ribosomal protein S20



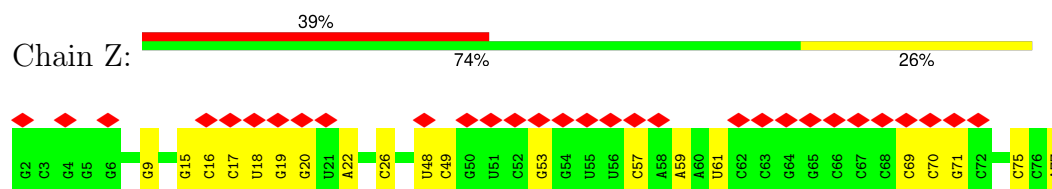
- Molecule 26: 30S ribosomal protein S21



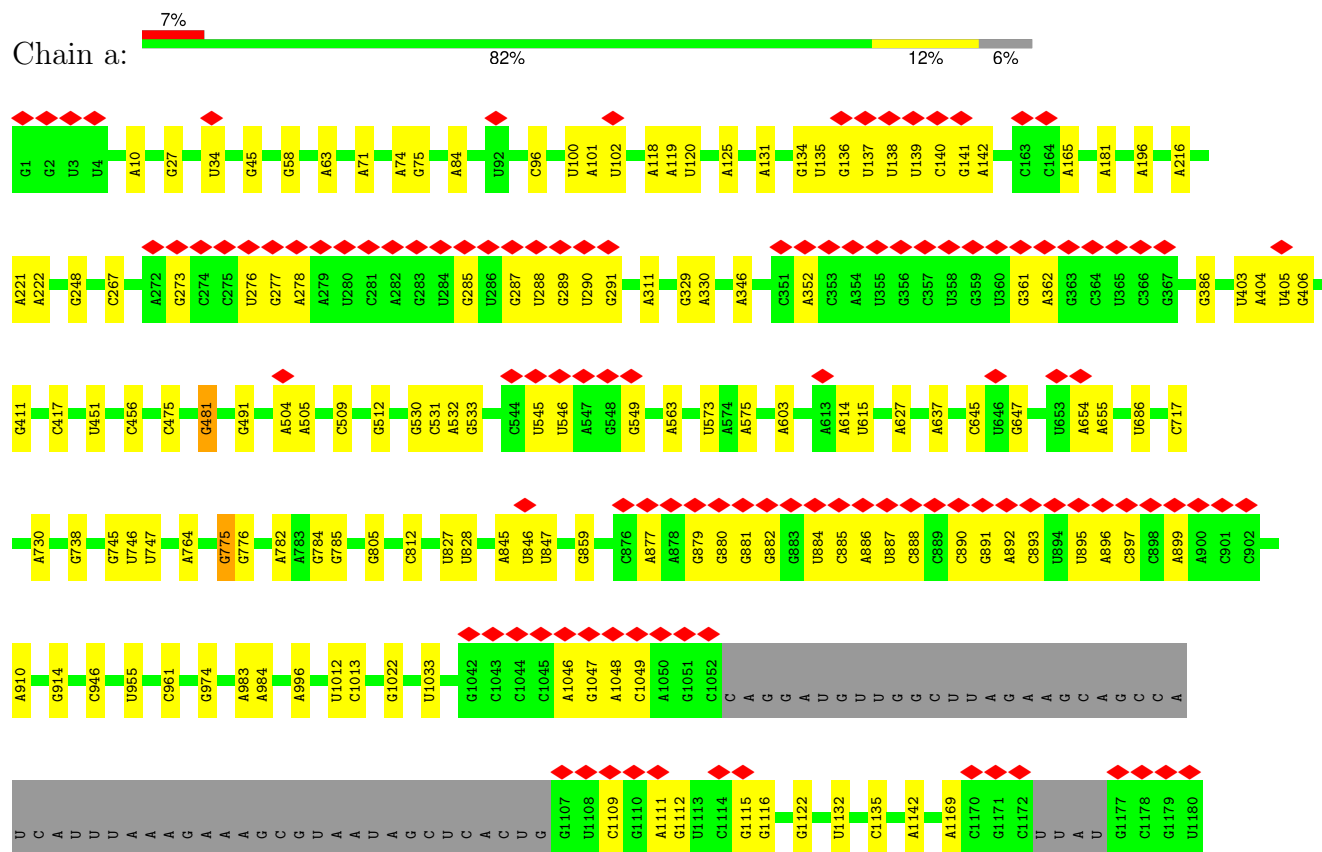
- Molecule 27: mRNA

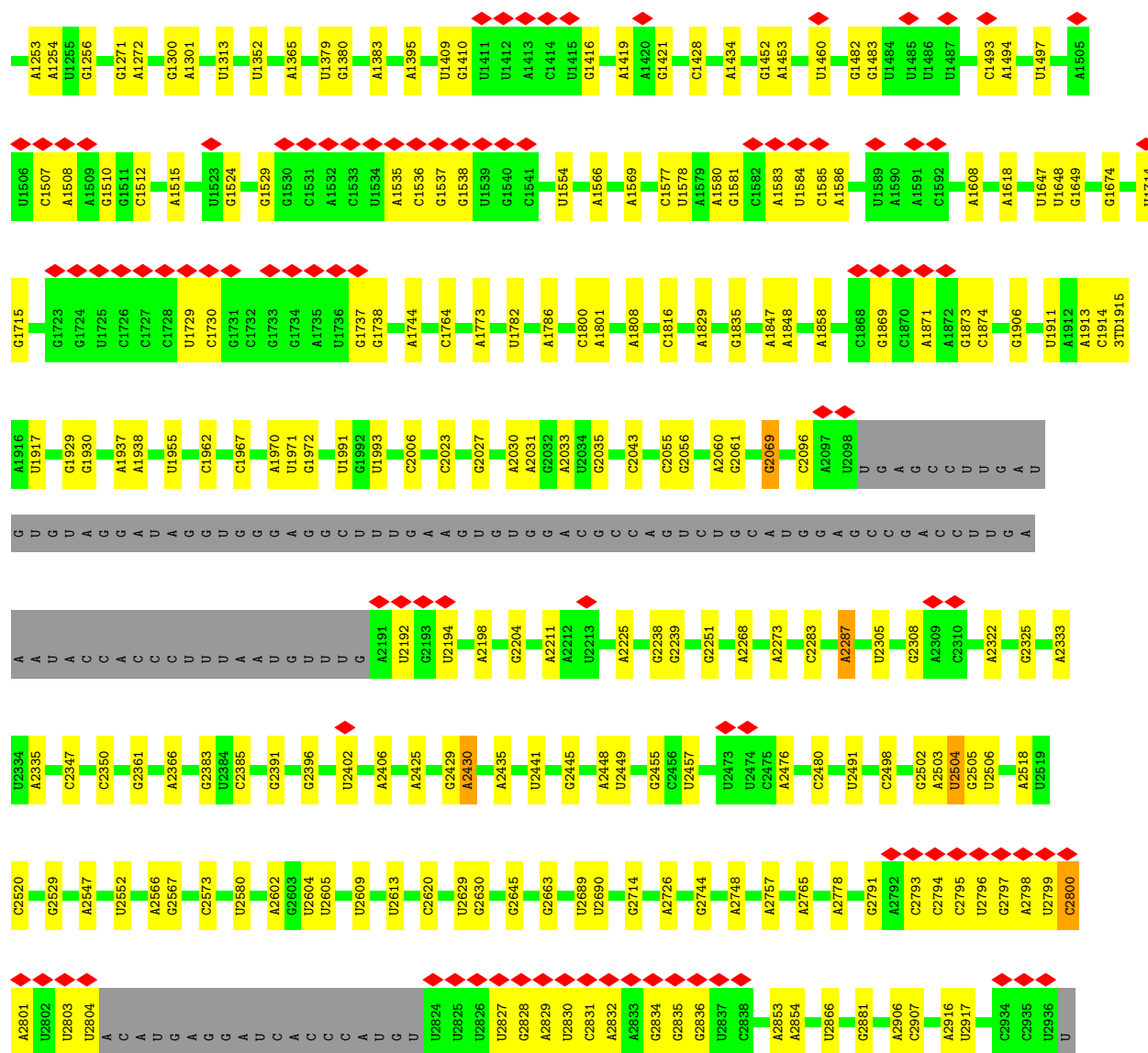


- Molecule 28: P-site tRNA-fMet

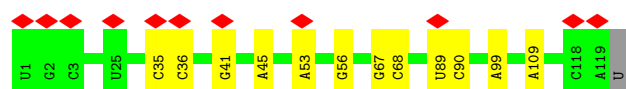
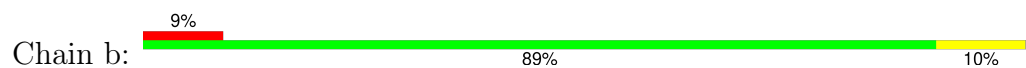


- Molecule 29: 23S rRNA





• Molecule 30: 5S rRNA

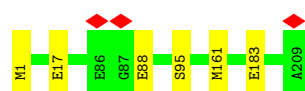


• Molecule 31: 50S ribosomal protein L2



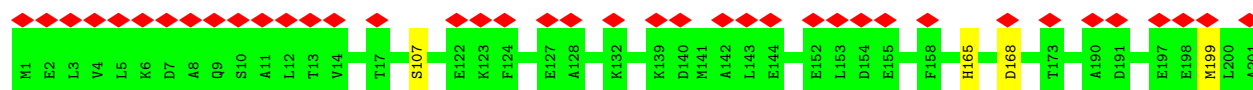
• Molecule 32: 50S ribosomal protein L3

Chain d:  97%




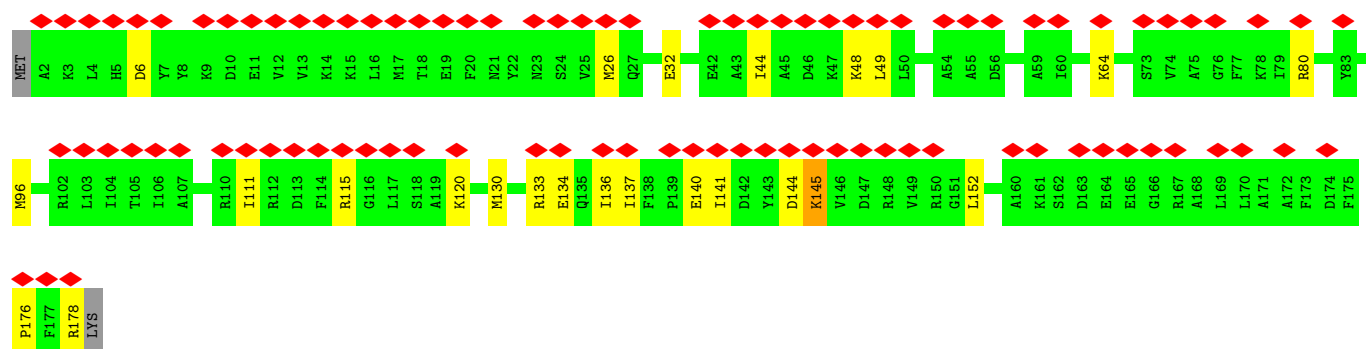
- Molecule 33: 50S ribosomal protein L4

Chain e:  19% 98%




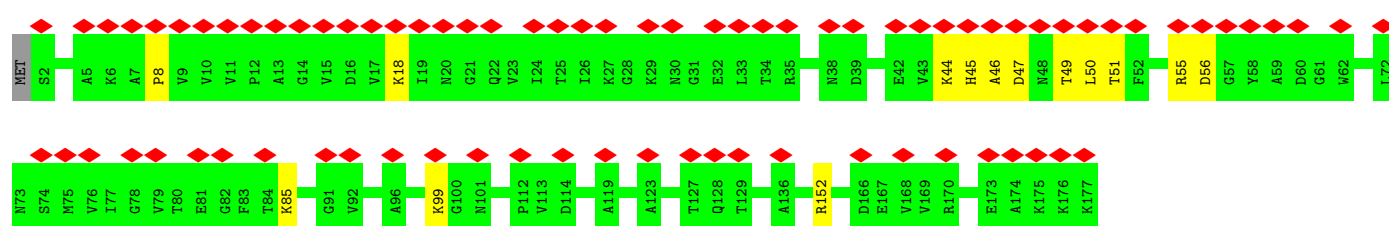
- Molecule 34: 50S ribosomal protein L5

Chain f:  51% 85% 13%



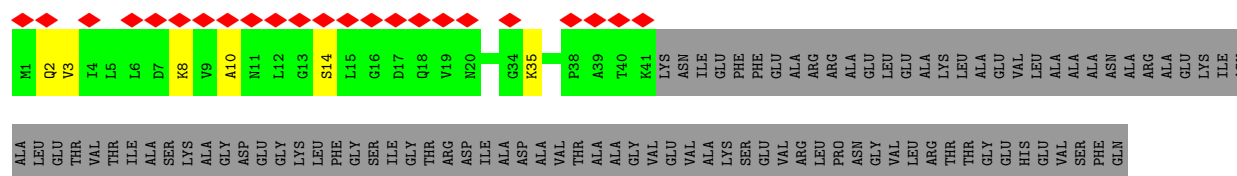
- Molecule 35: 50S ribosomal protein L6

Chain g:  45% 92% 8%



- Molecule 36: 50S ribosomal protein L9

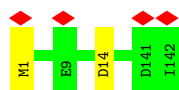
Chain h:  15% 23% 72%



VAL
HIS
SER
GLU
VAL
PHE
ALA
LYS
TLE
VAL
ASN
VAL
ALA
GLU

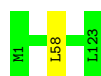
- Molecule 37: 50S ribosomal protein L13

Chain i:  99%



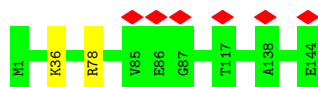
- Molecule 38: 50S ribosomal protein L14

Chain j:  99%



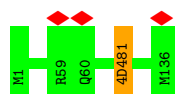
- Molecule 39: 50S ribosomal protein L15

Chain k:  99%



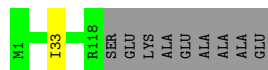
- Molecule 40: 50S ribosomal protein L16

Chain l:  99%




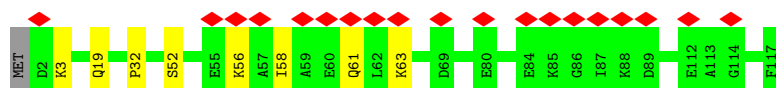
- Molecule 41: 50S ribosomal protein L17

Chain m:  92% 7%



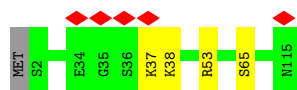
- Molecule 42: 50S ribosomal protein L18

Chain n:  16% 92% 7%



- Molecule 43: 50S ribosomal protein L19

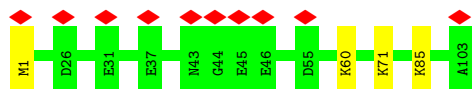
Chain o:  96%



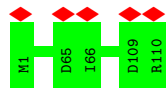
- Molecule 44: 50S ribosomal protein L20



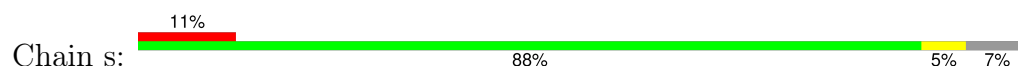
- Molecule 45: Ribosomal protein L21



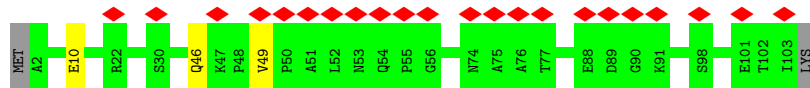
- Molecule 46: 50S ribosomal protein L22



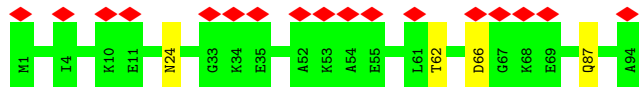
- Molecule 47: 50S ribosomal protein L23




- Molecule 48: 50S ribosomal protein L24

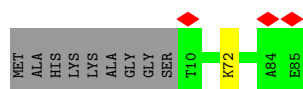


- Molecule 49: 50S ribosomal protein L25



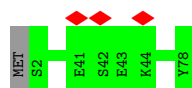
- Molecule 50: 50S ribosomal protein L27

Chain v:  88% 11%



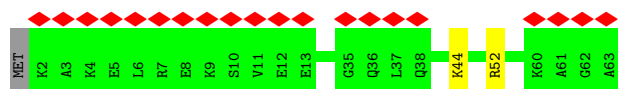
- Molecule 51: 50S ribosomal protein L28

Chain w:  99%



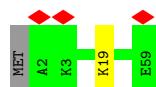
- Molecule 52: 50S ribosomal protein L29

Chain x:  32% 95%




- Molecule 53: 50S ribosomal protein L30

Chain y:  5% 97%



- Molecule 54: 50S ribosomal protein L32

Chain z:  91% 7%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	601617	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	11.389	Depositor
Minimum map value	-3.990	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.269	Depositor
Recommended contour level	0.933	Depositor
Map size (\AA)	369.5104, 369.5104, 369.5104	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.8248, 0.8248, 0.8248	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 5MU, 4D4, D2T, MA6, OMU, 5MC, FME, OMC, 3TD, 4OC, MV6, 6MZ, 2MG, H2U, G7M, UR3, 1MG, IAS, 8AN, 2MA, MEQ, OMG, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	0	0.31	0/424	0.55	0/565
2	1	0.32	0/380	0.72	0/498
3	2	0.30	0/513	0.59	0/676
4	3	0.30	0/303	0.62	0/397
5	4	0.29	0/488	0.54	0/649
6	A	0.91	1/36236 (0.0%)	0.88	24/56520 (0.0%)
7	B	0.60	0/1784	0.93	1/2403 (0.0%)
8	C	0.36	0/1651	0.56	0/2225
9	D	0.39	0/1665	0.58	0/2227
10	E	0.40	0/1165	0.59	0/1568
11	F	0.37	0/858	0.55	0/1160
12	G	0.36	0/1219	0.63	0/1635
13	H	0.39	0/989	0.56	0/1326
14	I	0.50	0/1034	0.78	0/1375
15	J	0.65	0/796	0.94	1/1077 (0.1%)
16	K	0.34	0/884	0.58	0/1191
17	L	0.41	0/960	0.72	0/1286
18	M	0.34	0/900	0.59	0/1204
19	N	0.46	0/817	0.72	0/1088
20	O	0.37	0/722	0.58	0/964
21	P	0.40	0/653	0.64	0/877
22	Q	0.39	0/650	0.59	0/871
23	R	0.41	0/553	0.68	0/742
24	S	0.40	0/685	0.68	1/922 (0.1%)
25	T	0.36	0/676	0.56	0/895
26	U	0.32	0/597	0.57	0/792
27	X	0.48	0/210	0.79	0/324
28	Z	0.44	0/1787	0.90	0/2782
29	a	0.53	0/65975	0.91	21/102914 (0.0%)
30	b	0.45	0/2850	0.85	0/4444
31	c	0.31	0/2121	0.62	0/2852

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	d	0.32	0/1576	0.58	0/2119
33	e	0.30	0/1571	0.55	0/2113
34	f	0.43	0/1434	0.62	0/1926
35	g	0.39	0/1343	0.60	0/1816
36	h	0.56	0/306	0.65	0/413
37	i	0.31	0/1152	0.56	0/1551
38	j	0.35	0/955	0.63	0/1279
39	k	0.31	0/1062	0.64	0/1413
40	l	0.31	0/1073	0.59	0/1433
41	m	0.39	0/958	0.66	0/1281
42	n	0.32	0/902	0.59	0/1209
43	o	0.36	0/929	0.60	0/1242
44	p	0.32	0/960	0.58	0/1278
45	q	0.33	0/829	0.61	0/1107
46	r	0.29	0/864	0.58	0/1156
47	s	0.31	0/744	0.55	0/994
48	t	0.30	0/787	0.57	0/1051
49	u	0.31	0/766	0.59	1/1025 (0.1%)
50	v	0.32	0/583	0.61	0/772
51	w	0.29	0/635	0.60	0/848
52	x	0.28	0/502	0.54	0/667
53	y	0.29	0/453	0.62	0/605
54	z	0.31	0/450	0.60	0/599
All	All	0.61	1/151379 (0.0%)	0.84	49/226346 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	2	0	1
9	D	0	1
15	J	0	1
40	l	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	5	U	O3'-P	-5.49	1.54	1.61

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a	512	G	O4'-C1'-N9	10.51	116.61	108.20
6	A	499	A	C6-N1-C2	8.60	123.76	118.60
6	A	511	C	C2-N1-C1'	7.70	127.27	118.80
29	a	2881	G	O4'-C1'-N9	7.58	114.27	108.20
6	A	462	G	O4'-C1'-N9	7.35	114.08	108.20
6	A	412	A	O4'-C1'-N9	7.24	114.00	108.20
6	A	428	G	P-O3'-C3'	6.99	128.09	119.70
29	a	2800	C	C2-N1-C1'	6.83	126.31	118.80
24	S	27	ASP	CB-CA-C	-6.75	96.89	110.40
6	A	514	C	N1-C2-O2	-6.68	114.89	118.90
6	A	451	A	N1-C6-N6	-6.55	114.67	118.60
29	a	2645	G	O4'-C1'-N9	6.49	113.39	108.20
6	A	511	C	N3-C2-O2	-6.32	117.48	121.90
6	A	499	A	C5-C6-N1	-6.17	114.61	117.70
6	A	547	A	C2'-C3'-O3'	6.02	123.34	113.70
6	A	5	U	C2'-C3'-O3'	-5.88	96.57	109.50
6	A	511	C	C6-N1-C1'	-5.87	113.75	120.80
6	A	511	C	N1-C2-O2	5.86	122.41	118.90
6	A	872	A	O4'-C1'-N9	5.80	112.84	108.20
29	a	775	G	O4'-C1'-N9	5.76	112.81	108.20
29	a	984	A	O4'-C1'-N9	5.75	112.80	108.20
49	u	66	ASP	CB-CG-OD1	5.70	123.43	118.30
6	A	547	A	P-O3'-C3'	5.61	126.43	119.70
6	A	499	A	N1-C2-N3	-5.57	126.52	129.30
29	a	2800	C	C6-N1-C1'	-5.51	114.19	120.80
6	A	575	G	O4'-C1'-N9	-5.41	103.88	108.20
29	a	2391	G	O4'-C1'-N9	5.35	112.48	108.20
29	a	481	G	O4'-C1'-N9	5.31	112.45	108.20
29	a	2006	C	C6-N1-C2	-5.25	118.20	120.30
6	A	328	C	O4'-C1'-N1	5.24	112.39	108.20
6	A	1035	A	OP1-P-O3'	5.23	116.70	105.20
29	a	2430	A	O4'-C1'-N9	5.20	112.36	108.20
6	A	754	C	C2-N1-C1'	5.19	124.51	118.80
29	a	1786	A	O4'-C1'-N9	5.18	112.34	108.20
29	a	1395	A	O4'-C1'-N9	5.17	112.34	108.20
6	A	407	U	P-O3'-C3'	5.15	125.88	119.70
6	A	405	U	C5-C4-O4	5.14	128.98	125.90
29	a	2620	C	C6-N1-C2	-5.14	118.25	120.30
29	a	27	G	O4'-C1'-N9	5.12	112.30	108.20
15	J	54	SER	N-CA-CB	5.12	118.18	110.50
29	a	2287	A	O4'-C1'-N9	5.12	112.29	108.20
6	A	86	G	C3'-C2'-C1'	-5.10	97.42	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a	2455	G	N3-C4-C5	-5.09	126.05	128.60
29	a	2480	C	N1-C2-O2	-5.07	115.86	118.90
29	a	2035	G	O4'-C1'-N9	5.06	112.25	108.20
6	A	792	A	O4'-C1'-N9	5.01	112.21	108.20
7	B	139	ARG	CB-CA-C	5.01	120.42	110.40
29	a	1254	A	N1-C2-N3	-5.01	126.80	129.30
29	a	1313	U	N1-C2-O2	5.00	126.30	122.80

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	2	31	HIS	Peptide
9	D	188	ARG	Sidechain
15	J	38	GLY	Peptide
40	l	81	4D4	Mainchain

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	49/55 (89%)	49 (100%)	0	0	100	100
2	1	44/46 (96%)	44 (100%)	0	0	100	100
3	2	62/65 (95%)	58 (94%)	3 (5%)	1 (2%)	8	2
4	3	36/38 (95%)	36 (100%)	0	0	100	100
5	4	56/70 (80%)	53 (95%)	3 (5%)	0	100	100
7	B	222/241 (92%)	185 (83%)	21 (10%)	16 (7%)	1	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	C	204/233 (88%)	198 (97%)	6 (3%)	0	100	100
9	D	203/206 (98%)	199 (98%)	4 (2%)	0	100	100
10	E	154/167 (92%)	150 (97%)	4 (3%)	0	100	100
11	F	101/135 (75%)	99 (98%)	2 (2%)	0	100	100
12	G	151/179 (84%)	142 (94%)	9 (6%)	0	100	100
13	H	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
14	I	125/130 (96%)	115 (92%)	10 (8%)	0	100	100
15	J	96/103 (93%)	80 (83%)	11 (12%)	5 (5%)	1	0
16	K	113/129 (88%)	109 (96%)	4 (4%)	0	100	100
17	L	120/124 (97%)	102 (85%)	16 (13%)	2 (2%)	7	2
18	M	113/118 (96%)	110 (97%)	3 (3%)	0	100	100
19	N	98/101 (97%)	95 (97%)	0	3 (3%)	3	0
20	O	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
21	P	79/82 (96%)	76 (96%)	3 (4%)	0	100	100
22	Q	77/84 (92%)	76 (99%)	1 (1%)	0	100	100
23	R	64/75 (85%)	60 (94%)	4 (6%)	0	100	100
24	S	82/92 (89%)	80 (98%)	1 (1%)	1 (1%)	11	3
25	T	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
26	U	68/71 (96%)	68 (100%)	0	0	100	100
31	c	269/273 (98%)	263 (98%)	6 (2%)	0	100	100
32	d	206/209 (99%)	202 (98%)	4 (2%)	0	100	100
33	e	199/201 (99%)	197 (99%)	2 (1%)	0	100	100
34	f	175/179 (98%)	159 (91%)	14 (8%)	2 (1%)	12	3
35	g	174/177 (98%)	160 (92%)	10 (6%)	4 (2%)	5	1
36	h	39/149 (26%)	33 (85%)	5 (13%)	1 (3%)	4	0
37	i	140/142 (99%)	140 (100%)	0	0	100	100
38	j	121/123 (98%)	117 (97%)	4 (3%)	0	100	100
39	k	142/144 (99%)	135 (95%)	6 (4%)	1 (1%)	19	8
40	l	132/136 (97%)	128 (97%)	4 (3%)	0	100	100
41	m	116/127 (91%)	109 (94%)	7 (6%)	0	100	100
42	n	114/117 (97%)	109 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	o	112/115 (97%)	109 (97%)	3 (3%)	0	100	100
44	p	115/118 (98%)	115 (100%)	0	0	100	100
45	q	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
46	r	108/110 (98%)	108 (100%)	0	0	100	100
47	s	91/100 (91%)	86 (94%)	5 (6%)	0	100	100
48	t	100/104 (96%)	92 (92%)	8 (8%)	0	100	100
49	u	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
50	v	74/85 (87%)	73 (99%)	1 (1%)	0	100	100
51	w	75/78 (96%)	75 (100%)	0	0	100	100
52	x	60/63 (95%)	58 (97%)	2 (3%)	0	100	100
53	y	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
54	z	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
All	All	5479/5913 (93%)	5237 (96%)	206 (4%)	36 (1%)	21	8

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	B	6	MET
7	B	62	SER
7	B	63	ARG
7	B	95	ARG
15	J	28	THR
24	S	27	ASP
34	f	145	LYS
36	h	10	ALA
3	2	32	ILE
7	B	76	ALA
7	B	125	THR
7	B	131	LYS
7	B	133	GLU
7	B	165	ASP
15	J	57	VAL
17	L	38	TYR
35	g	45	HIS
7	B	25	PRO
7	B	36	ASN
7	B	61	ALA
15	J	89	ARG

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Mol	Chain	Res	Type
19	N	33	ASP
35	g	51	THR
39	k	36	LYS
7	B	77	SER
17	L	76	GLU
19	N	37	SER
7	B	58	ASN
15	J	78	GLU
15	J	79	PRO
19	N	29	ALA
35	g	46	ALA
7	B	47	VAL
35	g	8	PRO
7	B	71	GLY
34	f	176	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	46/49 (94%)	46 (100%)	0	100	100
2	1	38/38 (100%)	38 (100%)	0	100	100
3	2	51/52 (98%)	49 (96%)	2 (4%)	27	13
4	3	34/34 (100%)	31 (91%)	3 (9%)	8	1
5	4	55/62 (89%)	54 (98%)	1 (2%)	54	41
7	B	186/199 (94%)	157 (84%)	29 (16%)	2	0
8	C	170/190 (90%)	165 (97%)	5 (3%)	37	22
9	D	172/173 (99%)	166 (96%)	6 (4%)	31	16
10	E	119/126 (94%)	118 (99%)	1 (1%)	79	74
11	F	90/116 (78%)	88 (98%)	2 (2%)	47	32
12	G	126/147 (86%)	120 (95%)	6 (5%)	21	8
13	H	104/105 (99%)	104 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	I	105/107 (98%)	99 (94%)	6 (6%)	17	5
15	J	86/90 (96%)	68 (79%)	18 (21%)	1	0
16	K	89/98 (91%)	88 (99%)	1 (1%)	70	62
17	L	102/103 (99%)	91 (89%)	11 (11%)	5	1
18	M	93/96 (97%)	89 (96%)	4 (4%)	25	10
19	N	83/84 (99%)	78 (94%)	5 (6%)	16	4
20	O	76/77 (99%)	73 (96%)	3 (4%)	27	13
21	P	65/65 (100%)	64 (98%)	1 (2%)	60	50
22	Q	73/78 (94%)	70 (96%)	3 (4%)	26	11
23	R	57/65 (88%)	54 (95%)	3 (5%)	19	7
24	S	72/79 (91%)	64 (89%)	8 (11%)	5	1
25	T	65/66 (98%)	63 (97%)	2 (3%)	35	20
26	U	60/61 (98%)	58 (97%)	2 (3%)	33	18
31	c	216/218 (99%)	212 (98%)	4 (2%)	52	39
32	d	163/163 (100%)	157 (96%)	6 (4%)	29	14
33	e	165/165 (100%)	161 (98%)	4 (2%)	44	29
34	f	148/150 (99%)	125 (84%)	23 (16%)	2	0
35	g	137/138 (99%)	127 (93%)	10 (7%)	11	2
36	h	32/114 (28%)	27 (84%)	5 (16%)	2	0
37	i	116/116 (100%)	114 (98%)	2 (2%)	56	44
38	j	104/104 (100%)	103 (99%)	1 (1%)	73	67
39	k	103/103 (100%)	102 (99%)	1 (1%)	73	67
40	l	107/107 (100%)	107 (100%)	0	100	100
41	m	98/103 (95%)	97 (99%)	1 (1%)	73	67
42	n	86/87 (99%)	78 (91%)	8 (9%)	7	1
43	o	99/100 (99%)	95 (96%)	4 (4%)	27	12
44	p	89/90 (99%)	87 (98%)	2 (2%)	47	32
45	q	84/84 (100%)	80 (95%)	4 (5%)	21	8
46	r	93/93 (100%)	93 (100%)	0	100	100
47	s	80/84 (95%)	75 (94%)	5 (6%)	15	4
48	t	83/85 (98%)	80 (96%)	3 (4%)	30	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	u	78/78 (100%)	75 (96%)	3 (4%)	28	13
50	v	57/63 (90%)	56 (98%)	1 (2%)	54	41
51	w	67/68 (98%)	67 (100%)	0	100	100
52	x	54/55 (98%)	52 (96%)	2 (4%)	29	14
53	y	48/49 (98%)	47 (98%)	1 (2%)	48	34
54	z	47/48 (98%)	43 (92%)	4 (8%)	8	1
All	All	4571/4825 (95%)	4355 (95%)	216 (5%)	24	9

All (216) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	2	31	HIS
3	2	52	LYS
4	3	8	LYS
4	3	20	ASP
4	3	36	ARG
5	4	56	ARG
7	B	7	ARG
7	B	23	TRP
7	B	31	ILE
7	B	45	LYS
7	B	56	GLU
7	B	59	LYS
7	B	62	SER
7	B	67	ILE
7	B	74	ARG
7	B	88	ASP
7	B	95	ARG
7	B	100	MET
7	B	115	LYS
7	B	118	GLU
7	B	121	SER
7	B	123	ASP
7	B	125	THR
7	B	127	ASP
7	B	133	GLU
7	B	135	LEU
7	B	136	MET
7	B	137	ARG
7	B	138	THR

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Mol	Chain	Res	Type
7	B	142	GLU
7	B	145	GLU
7	B	152	LYS
7	B	159	ASP
7	B	167	ASP
7	B	184	PHE
8	C	79	LYS
8	C	93	ASP
8	C	112	ASP
8	C	179	ARG
8	C	185	ASN
9	D	8	LYS
9	D	14	ARG
9	D	25	VAL
9	D	29	ASP
9	D	44	ARG
9	D	48	LEU
10	E	22	SER
11	F	88	MET
11	F	102	MET
12	G	5	ARG
12	G	6	VAL
12	G	7	ILE
12	G	118	LEU
12	G	143	ARG
12	G	154	TYR
14	I	41	ARG
14	I	52	LEU
14	I	57	MET
14	I	68	LYS
14	I	85	ARG
14	I	97	GLU
15	J	5	ARG
15	J	7	ARG
15	J	18	ILE
15	J	25	ILE
15	J	28	THR
15	J	30	LYS
15	J	31	ARG
15	J	35	GLN
15	J	37	ARG
15	J	66	GLU

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Mol	Chain	Res	Type
15	J	77	VAL
15	J	81	GLU
15	J	82	LYS
15	J	84	VAL
15	J	85	ASP
15	J	87	LEU
15	J	88	MET
15	J	89	ARG
16	K	18	ASP
17	L	18	LYS
17	L	39	THR
17	L	41	THR
17	L	44	LYS
17	L	75	GLN
17	L	76	GLU
17	L	79	VAL
17	L	94	ARG
17	L	97	THR
17	L	108	LYS
17	L	115	SER
18	M	3	ARG
18	M	14	HIS
18	M	16	VAL
18	M	78	LYS
19	N	23	LYS
19	N	30	ILE
19	N	41	ARG
19	N	46	LEU
19	N	49	GLN
20	O	2	SER
20	O	13	SER
20	O	89	ARG
21	P	1	MET
22	Q	6	ARG
22	Q	57	ASP
22	Q	65	ARG
23	R	35	GLU
23	R	43	ARG
23	R	66	SER
24	S	4	SER
24	S	21	LYS
24	S	28	LYS

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Mol	Chain	Res	Type
24	S	29	LYS
24	S	31	LEU
24	S	32	ARG
24	S	56	GLN
24	S	58	VAL
25	T	40	GLU
25	T	44	LYS
26	U	17	ARG
26	U	21	ARG
31	c	133	ARG
31	c	182	ARG
31	c	251	GLN
31	c	269	ARG
32	d	1	MET
32	d	17	GLU
32	d	88	GLU
32	d	95	SER
32	d	161	MET
32	d	183	GLU
33	e	107	SER
33	e	165	HIS
33	e	168	ASP
33	e	199	MET
34	f	6	ASP
34	f	26	MET
34	f	32	GLU
34	f	44	ILE
34	f	48	LYS
34	f	49	LEU
34	f	64	LYS
34	f	80	ARG
34	f	96	MET
34	f	111	ILE
34	f	115	ARG
34	f	120	LYS
34	f	130	MET
34	f	133	ARG
34	f	134	GLU
34	f	136	ILE
34	f	137	ILE
34	f	140	GLU
34	f	141	ILE

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Mol	Chain	Res	Type
34	f	144	ASP
34	f	145	LYS
34	f	152	LEU
34	f	178	ARG
35	g	18	LYS
35	g	44	LYS
35	g	47	ASP
35	g	49	THR
35	g	50	LEU
35	g	55	ARG
35	g	56	ASP
35	g	85	LYS
35	g	99	LYS
35	g	152	ARG
36	h	2	GLN
36	h	3	VAL
36	h	8	LYS
36	h	14	SER
36	h	35	LYS
37	i	1	MET
37	i	14	ASP
38	j	58	LEU
39	k	78	ARG
41	m	33	ILE
42	n	3	LYS
42	n	19	GLN
42	n	32	PRO
42	n	52	SER
42	n	56	LYS
42	n	58	ILE
42	n	61	GLN
42	n	63	LYS
43	o	37	LYS
43	o	38	LYS
43	o	53	ARG
43	o	65	SER
44	p	51	ARG
44	p	112	LYS
45	q	1	MET
45	q	60	LYS
45	q	71	LYS
45	q	85	LYS

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Mol	Chain	Res	Type
47	s	3	ARG
47	s	27	SER
47	s	69	ARG
47	s	72	GLN
47	s	74	ILE
48	t	10	GLU
48	t	46	GLN
48	t	49	VAL
49	u	24	ASN
49	u	62	THR
49	u	87	GLN
50	v	72	LYS
52	x	44	LYS
52	x	52	ARG
53	y	19	LYS
54	z	23	THR
54	z	26	THR
54	z	27	SER
54	z	52	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
12	G	68	ASN
12	G	153	HIS
25	T	3	ASN
35	g	45	HIS
35	g	48	ASN
36	h	20	ASN
47	s	72	GLN
51	w	20	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
27	X	8/27 (29%)	3 (37%)	0
28	Z	73/76 (96%)	19 (26%)	0
29	a	2757/2937 (93%)	337 (12%)	0
30	b	118/120 (98%)	12 (10%)	0
6	A	1513/1542 (98%)	221 (14%)	20 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	4469/4702 (95%)	592 (13%)	20 (0%)

All (592) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	A	4	U
6	A	5	U
6	A	9	G
6	A	32	A
6	A	36	C
6	A	39	G
6	A	47	C
6	A	48	C
6	A	50	A
6	A	51	A
6	A	72	A
6	A	73	C
6	A	74	A
6	A	75	G
6	A	76	G
6	A	77	A
6	A	78	A
6	A	81	A
6	A	82	G
6	A	83	C
6	A	84	U
6	A	85	U
6	A	86	G
6	A	87	C
6	A	88	U
6	A	90	C
6	A	91	U
6	A	94	G
6	A	95	C
6	A	121	U
6	A	122	G
6	A	131	A
6	A	141	G
6	A	144	G
6	A	149	A
6	A	159	G
6	A	182	A

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Mol	Chain	Res	Type
6	A	197	A
6	A	200	G
6	A	204	G
6	A	240	G
6	A	245	U
6	A	247	G
6	A	251	G
6	A	266	G
6	A	267	C
6	A	289	G
6	A	328	C
6	A	352	C
6	A	354	G
6	A	361	G
6	A	367	U
6	A	372	C
6	A	373	A
6	A	384	G
6	A	392	C
6	A	406	G
6	A	407	U
6	A	408	A
6	A	410	G
6	A	411	A
6	A	412	A
6	A	413	G
6	A	414	A
6	A	416	G
6	A	417	G
6	A	424	G
6	A	428	G
6	A	429	U
6	A	431	A
6	A	438	U
6	A	444	G
6	A	445	G
6	A	451	A
6	A	452	A
6	A	457	G
6	A	460	A
6	A	461	A
6	A	462	G

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Mol	Chain	Res	Type
6	A	463	U
6	A	464	U
6	A	465	A
6	A	467	U
6	A	468	A
6	A	469	C
6	A	472	U
6	A	473	U
6	A	474	G
6	A	475	C
6	A	477	C
6	A	478	A
6	A	479	U
6	A	481	G
6	A	484	G
6	A	498	A
6	A	511	C
6	A	512	U
6	A	515	G
6	A	517	G
6	A	518	C
6	A	521	G
6	A	530	G
6	A	531	U
6	A	532	A
6	A	538	G
6	A	548	G
6	A	559	A
6	A	572	A
6	A	573	A
6	A	576	C
6	A	577	G
6	A	596	A
6	A	614	C
6	A	615	G
6	A	617	G
6	A	618	C
6	A	623	C
6	A	628	G
6	A	629	A
6	A	650	G
6	A	653	U

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Mol	Chain	Res	Type
6	A	661	G
6	A	665	A
6	A	723	U
6	A	724	G
6	A	748	G
6	A	755	G
6	A	777	A
6	A	793	U
6	A	794	A
6	A	815	A
6	A	817	C
6	A	819	A
6	A	821	G
6	A	832	G
6	A	890	G
6	A	914	A
6	A	926	G
6	A	934	C
6	A	935	A
6	A	960	U
6	A	966	2MG
6	A	969	A
6	A	971	G
6	A	975	A
6	A	976	G
6	A	977	A
6	A	984	C
6	A	993	G
6	A	1003	G
6	A	1004	A
6	A	1008	U
6	A	1009	U
6	A	1020	G
6	A	1022	A
6	A	1024	G
6	A	1026	G
6	A	1027	C
6	A	1029	U
6	A	1030	U
6	A	1031	C
6	A	1032	G
6	A	1033	G

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Mol	Chain	Res	Type
6	A	1034	G
6	A	1036	A
6	A	1039	G
6	A	1042	A
6	A	1044	A
6	A	1046	A
6	A	1065	U
6	A	1085	U
6	A	1094	G
6	A	1095	U
6	A	1101	A
6	A	1125	U
6	A	1137	C
6	A	1139	G
6	A	1157	A
6	A	1158	C
6	A	1159	U
6	A	1196	A
6	A	1197	A
6	A	1213	A
6	A	1227	A
6	A	1238	A
6	A	1258	G
6	A	1260	G
6	A	1275	A
6	A	1279	G
6	A	1280	A
6	A	1286	U
6	A	1287	A
6	A	1300	G
6	A	1302	C
6	A	1317	C
6	A	1320	C
6	A	1338	G
6	A	1346	A
6	A	1353	G
6	A	1363	A
6	A	1370	G
6	A	1378	C
6	A	1379	G
6	A	1381	U
6	A	1419	G

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Mol	Chain	Res	Type
6	A	1429	A
6	A	1441	A
6	A	1446	A
6	A	1451	U
6	A	1452	C
6	A	1487	G
6	A	1492	A
6	A	1493	A
6	A	1494	G
6	A	1497	G
6	A	1503	A
6	A	1506	U
6	A	1517	G
6	A	1529	G
6	A	1530	G
6	A	1534	A
27	X	19	U
27	X	20	U
27	X	22	U
28	Z	9	G
28	Z	15	G
28	Z	16	C
28	Z	17	C
28	Z	18	U
28	Z	19	G
28	Z	20	G
28	Z	22	A
28	Z	26	C
28	Z	48	U
28	Z	49	C
28	Z	53	G
28	Z	57	C
28	Z	59	A
28	Z	61	U
28	Z	69	C
28	Z	70	C
28	Z	71	G
28	Z	75	C
29	a	10	A
29	a	34	U
29	a	45	G
29	a	58	G

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Mol	Chain	Res	Type
29	a	63	A
29	a	71	A
29	a	74	A
29	a	75	G
29	a	84	A
29	a	96	C
29	a	100	U
29	a	101	A
29	a	102	U
29	a	118	A
29	a	119	A
29	a	120	U
29	a	125	A
29	a	131	A
29	a	134	G
29	a	135	U
29	a	136	G
29	a	137	U
29	a	138	U
29	a	139	U
29	a	140	C
29	a	141	G
29	a	142	A
29	a	165	A
29	a	181	A
29	a	196	A
29	a	216	A
29	a	221	A
29	a	222	A
29	a	248	G
29	a	267	C
29	a	273	G
29	a	276	U
29	a	277	G
29	a	278	A
29	a	285	G
29	a	287	G
29	a	288	U
29	a	289	G
29	a	290	U
29	a	291	G
29	a	311	A

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Mol	Chain	Res	Type
29	a	329	G
29	a	330	A
29	a	346	A
29	a	352	A
29	a	361	G
29	a	362	A
29	a	386	G
29	a	403	U
29	a	404	A
29	a	405	U
29	a	406	G
29	a	411	G
29	a	417	C
29	a	451	U
29	a	456	C
29	a	475	C
29	a	481	G
29	a	491	G
29	a	504	A
29	a	505	A
29	a	509	C
29	a	530	G
29	a	531	C
29	a	532	A
29	a	533	G
29	a	545	U
29	a	546	U
29	a	549	G
29	a	563	A
29	a	573	U
29	a	575	A
29	a	603	A
29	a	614	A
29	a	615	U
29	a	627	A
29	a	637	A
29	a	645	C
29	a	647	G
29	a	654	A
29	a	655	A
29	a	686	U
29	a	717	C

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Mol	Chain	Res	Type
29	a	730	A
29	a	738	G
29	a	747	5MU
29	a	764	A
29	a	775	G
29	a	776	G
29	a	782	A
29	a	784	G
29	a	785	G
29	a	805	G
29	a	812	C
29	a	827	U
29	a	828	U
29	a	845	A
29	a	846	U
29	a	847	U
29	a	859	G
29	a	877	A
29	a	879	G
29	a	880	G
29	a	881	G
29	a	882	G
29	a	884	U
29	a	885	C
29	a	886	A
29	a	887	U
29	a	888	C
29	a	890	C
29	a	891	G
29	a	892	A
29	a	893	C
29	a	895	U
29	a	896	A
29	a	897	C
29	a	899	A
29	a	910	A
29	a	914	G
29	a	946	C
29	a	961	C
29	a	974	G
29	a	983	A
29	a	996	A

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Mol	Chain	Res	Type
29	a	1012	U
29	a	1013	C
29	a	1022	G
29	a	1033	U
29	a	1046	A
29	a	1047	G
29	a	1048	A
29	a	1049	C
29	a	1109	C
29	a	1111	A
29	a	1112	G
29	a	1115	G
29	a	1116	G
29	a	1122	G
29	a	1132	U
29	a	1135	C
29	a	1142	A
29	a	1169	A
29	a	1253	A
29	a	1256	G
29	a	1271	G
29	a	1272	A
29	a	1300	G
29	a	1301	A
29	a	1352	U
29	a	1365	A
29	a	1379	U
29	a	1380	G
29	a	1383	A
29	a	1409	U
29	a	1410	G
29	a	1416	G
29	a	1419	A
29	a	1421	G
29	a	1428	C
29	a	1434	A
29	a	1452	G
29	a	1453	A
29	a	1460	U
29	a	1482	G
29	a	1483	G
29	a	1493	C

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Mol	Chain	Res	Type
29	a	1494	A
29	a	1497	U
29	a	1507	C
29	a	1508	A
29	a	1510	G
29	a	1512	C
29	a	1515	A
29	a	1524	G
29	a	1529	G
29	a	1535	A
29	a	1536	C
29	a	1537	G
29	a	1538	G
29	a	1554	U
29	a	1566	A
29	a	1569	A
29	a	1577	C
29	a	1578	U
29	a	1580	A
29	a	1581	G
29	a	1583	A
29	a	1584	U
29	a	1585	C
29	a	1586	A
29	a	1608	A
29	a	1647	U
29	a	1648	U
29	a	1649	G
29	a	1674	G
29	a	1714	U
29	a	1715	G
29	a	1729	U
29	a	1730	C
29	a	1737	G
29	a	1738	G
29	a	1744	A
29	a	1764	C
29	a	1773	A
29	a	1782	U
29	a	1800	C
29	a	1801	A
29	a	1808	A

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Mol	Chain	Res	Type
29	a	1816	C
29	a	1829	A
29	a	1847	A
29	a	1848	A
29	a	1858	A
29	a	1869	G
29	a	1871	A
29	a	1873	G
29	a	1874	C
29	a	1906	G
29	a	1913	A
29	a	1914	C
29	a	1929	G
29	a	1930	G
29	a	1937	A
29	a	1938	A
29	a	1955	U
29	a	1967	C
29	a	1970	A
29	a	1971	U
29	a	1972	G
29	a	1991	U
29	a	1993	U
29	a	2023	C
29	a	2027	G
29	a	2031	A
29	a	2033	A
29	a	2043	C
29	a	2055	C
29	a	2056	G
29	a	2060	A
29	a	2061	G
29	a	2069	G7M
29	a	2096	C
29	a	2192	U
29	a	2194	U
29	a	2198	A
29	a	2204	G
29	a	2211	A
29	a	2225	A
29	a	2238	G
29	a	2239	G

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Mol	Chain	Res	Type
29	a	2268	A
29	a	2273	A
29	a	2283	C
29	a	2287	A
29	a	2305	U
29	a	2308	G
29	a	2322	A
29	a	2325	G
29	a	2333	A
29	a	2335	A
29	a	2347	C
29	a	2350	C
29	a	2361	G
29	a	2366	A
29	a	2383	G
29	a	2385	C
29	a	2396	G
29	a	2402	U
29	a	2406	A
29	a	2425	A
29	a	2429	G
29	a	2430	A
29	a	2435	A
29	a	2441	U
29	a	2448	A
29	a	2476	A
29	a	2491	U
29	a	2502	G
29	a	2504	PSU
29	a	2505	G
29	a	2506	U
29	a	2518	A
29	a	2520	C
29	a	2529	G
29	a	2547	A
29	a	2566	A
29	a	2567	G
29	a	2573	C
29	a	2602	A
29	a	2609	U
29	a	2613	U
29	a	2629	U

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Mol	Chain	Res	Type
29	a	2630	G
29	a	2663	G
29	a	2689	U
29	a	2690	U
29	a	2714	G
29	a	2726	A
29	a	2744	G
29	a	2748	A
29	a	2757	A
29	a	2765	A
29	a	2778	A
29	a	2791	G
29	a	2793	C
29	a	2794	C
29	a	2795	C
29	a	2796	U
29	a	2797	G
29	a	2798	A
29	a	2799	U
29	a	2800	C
29	a	2801	A
29	a	2803	U
29	a	2804	U
29	a	2827	U
29	a	2828	G
29	a	2829	A
29	a	2830	U
29	a	2831	C
29	a	2832	A
29	a	2834	G
29	a	2835	G
29	a	2836	G
29	a	2853	A
29	a	2854	A
29	a	2866	U
29	a	2906	A
29	a	2907	C
29	a	2916	A
29	a	2917	U
30	b	35	C
30	b	36	C
30	b	41	G

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Mol	Chain	Res	Type
30	b	45	A
30	b	53	A
30	b	56	G
30	b	67	G
30	b	68	C
30	b	89	U
30	b	90	C
30	b	99	A
30	b	109	A

All (20) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	A	4	U
6	A	73	C
6	A	84	U
6	A	88	U
6	A	94	G
6	A	121	U
6	A	360	G
6	A	406	G
6	A	407	U
6	A	416	G
6	A	428	G
6	A	516	PSU
6	A	531	U
6	A	547	A
6	A	622	A
6	A	858	G
6	A	1003	G
6	A	1035	A
6	A	1124	G
6	A	1384	C

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

40 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
6	MA6	A	1518	6	19,26,27	0.87	0	18,38,41	2.10	4 (22%)
29	OMU	a	2552	29	19,22,23	1.36	3 (15%)	25,31,34	2.02	7 (28%)
6	2MG	A	1207	6	18,26,27	1.08	3 (16%)	16,38,41	0.82	0
6	5MC	A	967	6	19,22,23	0.83	1 (5%)	26,32,35	0.52	0
29	PSU	a	2580	29	18,21,22	1.06	2 (11%)	21,30,33	0.89	1 (4%)
29	PSU	a	746	29,55	18,21,22	1.41	3 (16%)	21,30,33	1.95	5 (23%)
28	8AN	Z	77	28	17,24,25	1.41	1 (5%)	13,35,38	1.24	2 (15%)
6	4OC	A	1402	6	20,23,24	0.41	0	25,32,35	0.50	0
29	PSU	a	955	29	18,21,22	1.03	1 (5%)	21,30,33	0.85	0
29	PSU	a	1917	29	18,21,22	1.01	1 (5%)	21,30,33	0.72	0
6	2MG	A	966	6	18,26,27	1.13	3 (16%)	16,38,41	0.73	0
6	5MC	A	1407	6	19,22,23	0.86	1 (5%)	26,32,35	0.58	0
29	6MZ	a	1618	29	17,25,26	0.97	1 (5%)	15,36,39	0.90	1 (6%)
6	UR3	A	1498	6	19,22,23	0.38	0	26,32,35	1.01	2 (7%)
17	D2T	L	89	17	8,9,10	3.94	3 (37%)	6,11,13	1.63	2 (33%)
16	IAS	K	119	16	6,7,8	1.40	1 (16%)	3,8,10	0.92	0
29	PSU	a	2504	29	18,21,22	1.49	4 (22%)	21,30,33	2.05	5 (23%)
29	PSU	a	2457	29	18,21,22	1.05	1 (5%)	21,30,33	0.78	0
29	PSU	a	1911	29	18,21,22	0.99	1 (5%)	21,30,33	0.73	0
29	2MG	a	2445	29	18,26,27	1.32	2 (11%)	16,38,41	1.38	2 (12%)
29	OMG	a	2251	29,28	19,26,27	1.02	2 (10%)	21,38,41	0.71	0
6	MA6	A	1519	6	19,26,27	0.96	1 (5%)	18,38,41	2.19	4 (22%)
29	PSU	a	2605	29	18,21,22	0.99	1 (5%)	21,30,33	0.84	0
29	2MA	a	2503	29,55	17,25,26	1.14	0	16,37,40	1.30	2 (12%)
29	5MU	a	1939	29	19,22,23	0.42	0	27,32,35	0.78	0
6	G7M	A	527	6	20,26,27	1.10	2 (10%)	16,39,42	0.74	0
29	5MU	a	747	29	19,22,23	0.35	0	27,32,35	0.54	0
29	H2U	a	2449	29	18,21,22	0.60	0	19,30,33	0.75	1 (5%)
29	6MZ	a	2030	29	17,25,26	0.95	1 (5%)	15,36,39	0.93	1 (6%)
29	OMC	a	2498	29,55	19,22,23	0.82	0	25,31,34	1.04	2 (8%)
6	PSU	A	516	6,55	18,21,22	0.97	1 (5%)	21,30,33	1.09	1 (4%)
29	G7M	a	2069	29	20,26,27	1.15	1 (5%)	16,39,42	0.90	1 (6%)
32	MEQ	d	150	32	8,9,10	0.46	0	5,10,12	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	5MC	a	1962	29	19,22,23	0.74	1 (5%)	26,32,35	0.52	0
29	PSU	a	2604	29	18,21,22	1.02	1 (5%)	21,30,33	0.82	0
6	2MG	A	1516	6	18,26,27	1.12	3 (16%)	16,38,41	0.87	0
29	2MG	a	1835	29	18,26,27	0.93	1 (5%)	16,38,41	1.64	6 (37%)
29	1MG	a	745	29	19,26,27	0.98	1 (5%)	18,39,42	1.61	4 (22%)
40	4D4	l	81	40	9,11,12	1.97	2 (22%)	7,13,15	1.10	1 (14%)
29	3TD	a	1915	29	19,22,23	1.63	4 (21%)	23,32,35	2.22	4 (17%)

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
6	MA6	A	1518	6	-	0/7/29/30	0/3/3/3
29	OMU	a	2552	29	-	0/9/27/28	0/2/2/2
6	2MG	A	1207	6	-	0/5/27/28	0/3/3/3
6	5MC	A	967	6	-	0/7/25/26	0/2/2/2
29	PSU	a	2580	29	-	0/7/25/26	0/2/2/2
29	PSU	a	746	29,55	-	2/7/25/26	0/2/2/2
28	8AN	Z	77	28	-	1/3/25/26	0/3/3/3
6	4OC	A	1402	6	-	0/9/29/30	0/2/2/2
29	PSU	a	955	29	-	0/7/25/26	0/2/2/2
29	PSU	a	1917	29	-	0/7/25/26	0/2/2/2
6	2MG	A	966	6	-	0/5/27/28	0/3/3/3
6	5MC	A	1407	6	-	0/7/25/26	0/2/2/2
29	6MZ	a	1618	29	-	0/5/27/28	0/3/3/3
6	UR3	A	1498	6	-	0/7/25/26	0/2/2/2
17	D2T	L	89	17	-	4/7/12/14	-
16	IAS	K	119	16	-	0/7/7/8	-
29	PSU	a	2504	29	-	1/7/25/26	0/2/2/2
29	PSU	a	2457	29	-	0/7/25/26	0/2/2/2
29	PSU	a	1911	29	-	0/7/25/26	0/2/2/2
29	2MG	a	2445	29	-	1/5/27/28	0/3/3/3
29	OMG	a	2251	29,28	-	1/5/27/28	0/3/3/3
6	MA6	A	1519	6	-	2/7/29/30	0/3/3/3
29	PSU	a	2605	29	-	0/7/25/26	0/2/2/2
29	2MA	a	2503	29,55	-	1/3/25/26	0/3/3/3
29	5MU	a	1939	29	-	1/7/25/26	0/2/2/2
6	G7M	A	527	6	-	1/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	5MU	a	747	29	-	1/7/25/26	0/2/2/2
29	H2U	a	2449	29	-	0/7/38/39	0/2/2/2
29	6MZ	a	2030	29	-	2/5/27/28	0/3/3/3
29	OMC	a	2498	29,55	-	1/9/27/28	0/2/2/2
6	PSU	A	516	6,55	-	0/7/25/26	0/2/2/2
29	G7M	a	2069	29	-	2/3/25/26	0/3/3/3
32	MEQ	d	150	32	-	2/8/9/11	-
29	5MC	a	1962	29	-	0/7/25/26	0/2/2/2
29	PSU	a	2604	29	-	0/7/25/26	0/2/2/2
6	2MG	A	1516	6	-	0/5/27/28	0/3/3/3
29	2MG	a	1835	29	-	0/5/27/28	0/3/3/3
29	1MG	a	745	29	-	0/3/25/26	0/3/3/3
40	4D4	l	81	40	-	1/11/12/14	-
29	3TD	a	1915	29	-	2/7/25/26	0/2/2/2

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	L	89	D2T	CB-CA	9.42	1.57	1.54
28	Z	77	8AN	C3'-N3'	-4.85	1.40	1.47
17	L	89	D2T	CB-CG	4.27	1.59	1.52
29	a	746	PSU	C4-N3	-3.87	1.31	1.38
40	l	81	4D4	CZ-NE	3.87	1.40	1.33
29	a	2457	PSU	C6-C5	3.71	1.39	1.35
29	a	955	PSU	C6-C5	3.64	1.39	1.35
29	a	2069	G7M	C5-C4	3.63	1.46	1.39
29	a	2605	PSU	C6-C5	3.61	1.39	1.35
29	a	2604	PSU	C6-C5	3.57	1.39	1.35
29	a	1917	PSU	C6-C5	3.57	1.39	1.35
29	a	1915	3TD	C6-C5	3.52	1.39	1.35
29	a	1911	PSU	C6-C5	3.52	1.39	1.35
17	L	89	D2T	CB-SB	3.44	1.85	1.82
6	A	516	PSU	C6-C5	3.40	1.39	1.35
29	a	2580	PSU	C6-C5	3.39	1.39	1.35
6	A	1407	5MC	C5-C4	-3.36	1.41	1.44
29	a	1915	3TD	C4-N3	-3.27	1.33	1.40
29	a	2445	2MG	C6-N1	-3.23	1.32	1.37
29	a	1915	3TD	C10-N3	3.22	1.52	1.47
6	A	967	5MC	C5-C4	-3.19	1.41	1.44
29	a	2552	OMU	C4-N3	-3.18	1.33	1.38
29	a	2504	PSU	C4-N3	-3.07	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	a	2504	PSU	C6-C5	2.99	1.38	1.35
29	a	1962	5MC	C5-C4	-2.96	1.41	1.44
29	a	2552	OMU	C2-N3	-2.88	1.32	1.38
6	A	527	G7M	C5-C4	2.87	1.44	1.39
6	A	966	2MG	C5-C6	-2.83	1.41	1.47
29	a	746	PSU	C2-N3	-2.78	1.32	1.37
40	l	81	4D4	CZ-NH2	2.78	1.42	1.32
29	a	2445	2MG	C2-N1	-2.75	1.32	1.36
6	A	1516	2MG	C5-C6	-2.68	1.42	1.47
6	A	527	G7M	C6-N1	-2.67	1.33	1.37
29	a	2251	OMG	C5-C6	-2.66	1.42	1.47
6	A	1207	2MG	C5-C6	-2.65	1.42	1.47
29	a	1835	2MG	C6-N1	-2.64	1.33	1.37
29	a	1618	6MZ	C6-C5	-2.50	1.41	1.44
29	a	2030	6MZ	C6-C5	-2.49	1.41	1.44
29	a	2504	PSU	C2-N3	-2.47	1.33	1.37
29	a	745	1MG	C2-N1	2.47	1.41	1.37
6	A	1519	MA6	C6-C5	2.45	1.48	1.44
6	A	966	2MG	C8-N7	-2.42	1.31	1.34
29	a	2580	PSU	O4'-C1'	-2.35	1.40	1.43
6	A	1516	2MG	C8-N7	-2.31	1.31	1.34
16	K	119	IAS	CB-CG	2.31	1.56	1.50
29	a	746	PSU	C6-C5	2.28	1.37	1.35
6	A	1207	2MG	C8-N7	-2.20	1.31	1.34
29	a	2552	OMU	C5-C4	-2.20	1.38	1.43
29	a	1915	3TD	C2-N1	-2.14	1.34	1.37
29	a	2504	PSU	C2'-C1'	-2.12	1.50	1.53
6	A	1516	2MG	C5-C4	-2.11	1.37	1.43
29	a	2251	OMG	C8-N7	-2.08	1.31	1.34
6	A	966	2MG	C5-C4	-2.05	1.38	1.43
6	A	1207	2MG	C5-C4	-2.02	1.38	1.43

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a	1915	3TD	N1-C2-N3	8.54	122.34	116.13
6	A	1518	MA6	C2-N1-C6	6.42	123.14	116.84
6	A	1519	MA6	C2-N1-C6	6.31	123.03	116.84
29	a	2504	PSU	N1-C2-N3	6.28	121.79	115.17
29	a	746	PSU	N1-C2-N3	5.68	121.16	115.17
29	a	2552	OMU	C4-N3-C2	-5.19	120.17	126.61
29	a	2552	OMU	N3-C2-N1	4.52	120.77	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a	2504	PSU	C4-N3-C2	-4.46	120.22	126.37
6	A	1519	MA6	N3-C2-N1	-4.33	122.79	128.67
6	A	1518	MA6	N3-C2-N1	-4.21	122.96	128.67
29	a	2552	OMU	C5-C4-N3	4.03	120.45	114.80
29	a	1915	3TD	C4-N3-C2	-3.81	120.58	124.61
6	A	1519	MA6	C4-C5-N7	-3.67	105.46	109.34
29	a	2552	OMU	C2'-C1'-N1	-3.58	107.44	114.24
29	a	745	1MG	C8-N7-C5	3.51	108.52	102.55
29	a	746	PSU	C4-N3-C2	-3.27	121.86	126.37
29	a	1835	2MG	O6-C6-C5	-3.16	118.06	124.32
29	a	2503	2MA	C4-N3-C2	-3.06	120.95	123.30
29	a	2445	2MG	C8-N7-C5	2.99	107.64	102.55
29	a	2498	OMC	C2'-C1'-N1	-2.98	108.59	114.24
6	A	1518	MA6	C4-C5-N7	-2.96	106.21	109.34
29	a	745	1MG	O6-C6-C5	-2.95	119.33	124.18
29	a	1915	3TD	C1'-C5-C4	2.86	121.94	117.61
29	a	2445	2MG	C5-C6-N1	2.82	119.45	114.07
29	a	745	1MG	O4'-C1'-N9	2.79	112.45	108.75
29	a	2552	OMU	O4-C4-C5	-2.76	120.41	125.16
29	a	2504	PSU	O2-C2-N1	-2.75	119.95	122.79
29	a	745	1MG	C5-C6-N1	2.75	117.93	113.96
29	a	2503	2MA	C8-N7-C5	2.74	107.21	102.55
29	a	2552	OMU	O2-C2-N1	-2.69	119.30	122.80
6	A	1498	UR3	C6-N1-C2	-2.67	119.62	121.80
28	Z	77	8AN	C2'-C3'-C4'	2.67	106.35	102.70
6	A	1518	MA6	N1-C6-N6	2.62	119.86	116.83
29	a	746	PSU	O2-C2-N3	-2.61	117.23	121.86
6	A	516	PSU	O3'-C3'-C2'	2.59	120.11	111.82
29	a	1618	6MZ	C2-N1-C6	2.58	118.60	116.60
29	a	1835	2MG	C4'-O4'-C1'	2.56	112.27	109.92
29	a	2580	PSU	O4'-C1'-C2'	2.53	108.65	105.15
29	a	1835	2MG	C8-N7-C5	2.52	106.84	102.55
17	L	89	D2T	OD1-CG-CB	-2.48	117.24	122.44
29	a	2030	6MZ	C2-N1-C6	2.43	118.48	116.60
29	a	746	PSU	C3'-C2'-C1'	2.43	104.55	101.69
29	a	1835	2MG	N1-C2-N2	2.37	118.98	116.56
29	a	2504	PSU	C5-C6-N1	-2.36	118.86	122.14
29	a	1835	2MG	C5-C6-N1	2.34	118.53	114.07
29	a	1835	2MG	O6-C6-N1	2.33	123.39	120.62
6	A	1498	UR3	C4-N3-C2	-2.30	122.73	124.58
29	a	2498	OMC	O2-C2-N3	-2.26	118.77	122.33
29	a	2449	H2U	O2-C2-N1	-2.25	120.40	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1519	MA6	C1'-N9-C4	-2.20	122.78	126.64
28	Z	77	8AN	C5-C6-N6	2.19	123.64	120.31
40	l	81	4D4	CG-CD-NE	-2.16	105.96	111.88
29	a	2069	G7M	N2-C2-N1	2.11	121.21	116.76
29	a	2552	OMU	C5-C6-N1	-2.09	118.45	121.84
17	L	89	D2T	OD2-CG-CB	2.08	117.64	113.15
29	a	1915	3TD	C5-C6-N1	-2.06	119.28	122.14
29	a	746	PSU	O4'-C1'-C2'	-2.03	102.34	105.15
29	a	2504	PSU	O2-C2-N3	-2.03	118.25	121.86

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	L	89	D2T	CA-CB-CG-OD1
17	L	89	D2T	CA-CB-CG-OD2
17	L	89	D2T	SB-CB-CG-OD2
28	Z	77	8AN	C4'-C5'-O5'-P
29	a	2498	OMC	C1'-C2'-O2'-CM2
29	a	1915	3TD	O4'-C4'-C5'-O5'
32	d	150	MEQ	NE2-CD-CG-CB
32	d	150	MEQ	OE1-CD-CG-CB
29	a	2030	6MZ	O4'-C4'-C5'-O5'
29	a	2030	6MZ	C3'-C4'-C5'-O5'
6	A	1519	MA6	O4'-C4'-C5'-O5'
29	a	1915	3TD	C3'-C4'-C5'-O5'
29	a	2504	PSU	O4'-C4'-C5'-O5'
29	a	1939	5MU	O4'-C4'-C5'-O5'
29	a	747	5MU	C3'-C4'-C5'-O5'
29	a	2503	2MA	C4'-C5'-O5'-P
29	a	2251	OMG	C1'-C2'-O2'-CM2
29	a	2445	2MG	C3'-C4'-C5'-O5'
29	a	746	PSU	O4'-C1'-C5-C6
6	A	527	G7M	C3'-C4'-C5'-O5'
17	L	89	D2T	CG-CB-SB-CB1
29	a	746	PSU	C2'-C1'-C5-C6
6	A	1519	MA6	C3'-C4'-C5'-O5'
40	l	81	4D4	O-C-CA-CB
29	a	2069	G7M	C4'-C5'-O5'-P
29	a	2069	G7M	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 285 ligands modelled in this entry, 284 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z > 2$
56	FME	a	4196	-	8,9,10	0.78	0	8,9,11	1.10	1 (12%)

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
56	FME	a	4196	-	-	2/7/9/11	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	a	4196	FME	O-C-CA	-2.09	119.40	124.77

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	a	4196	FME	O1-CN-N-CA
56	a	4196	FME	CB-CA-N-CN

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
28	Z	1
29	a	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Z	5:G	O3'	6:G	P	3.17
1	a	1914:C	O3'	1915:3TD	P	2.35

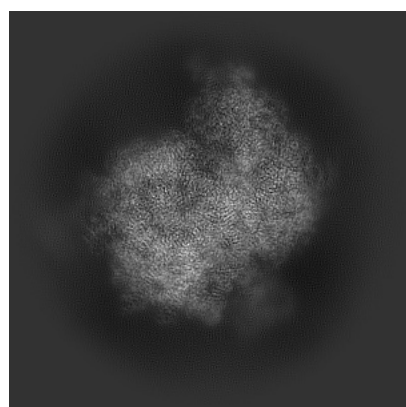
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29449. These allow visual inspection of the internal detail of the map and identification of artifacts.

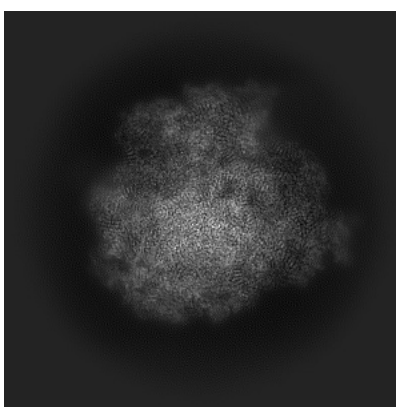
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

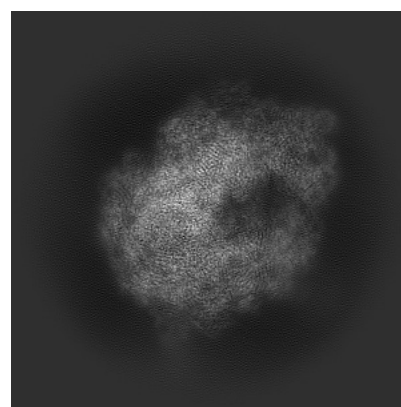
6.1.1 Primary map



X



Y

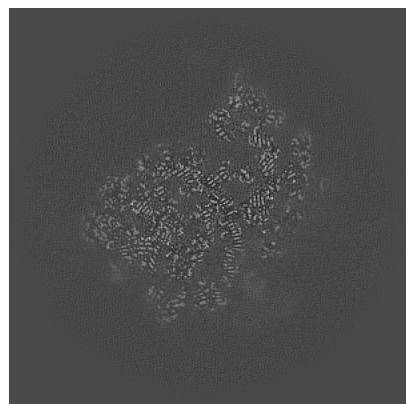


Z

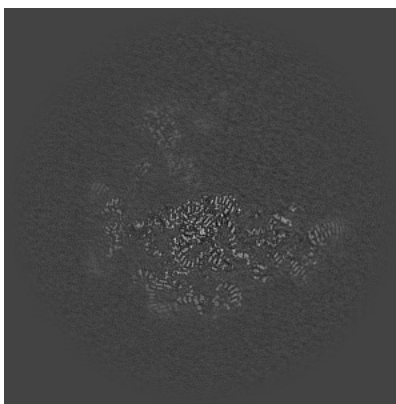
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

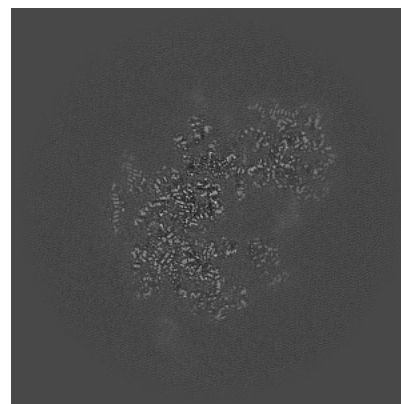
6.2.1 Primary map



X Index: 224



Y Index: 224

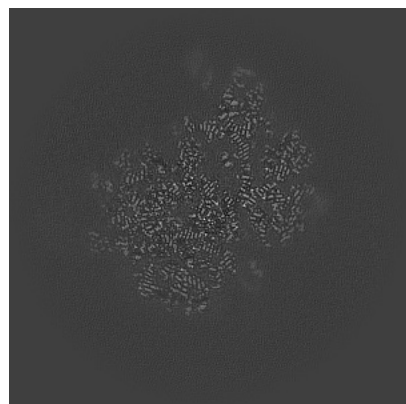


Z Index: 224

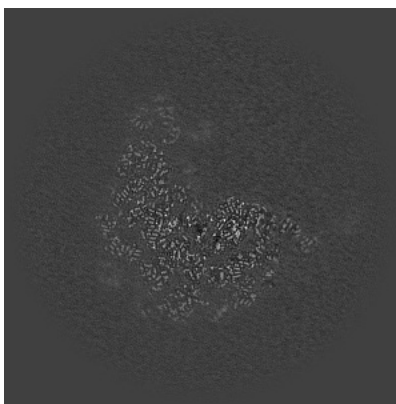
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

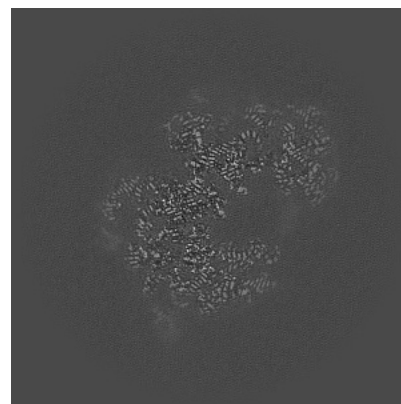
6.3.1 Primary map



X Index: 208



Y Index: 204

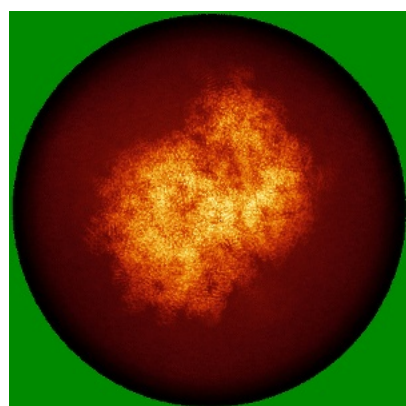


Z Index: 233

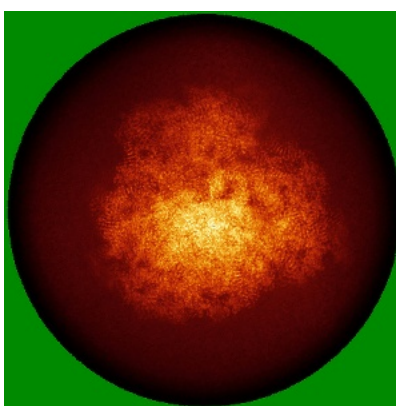
The images above show the largest variance slices of the map in three orthogonal directions.

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

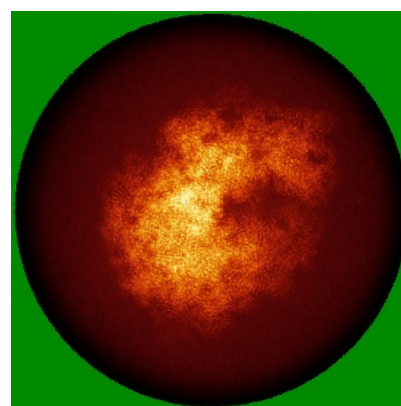
6.4.1 Primary map



X



Y

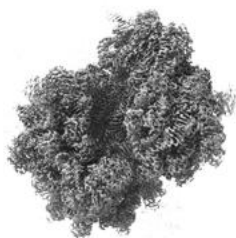


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.933. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

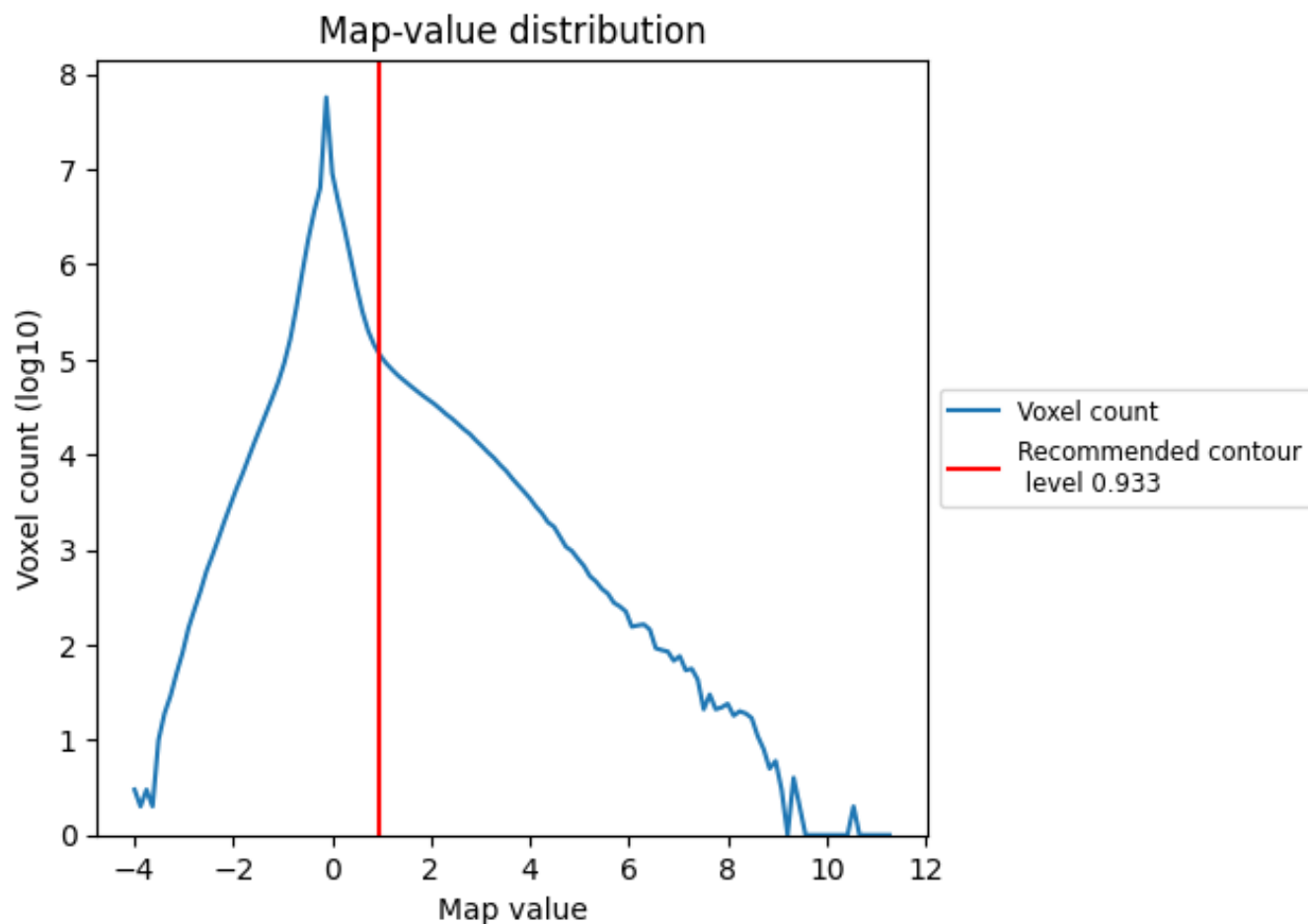
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

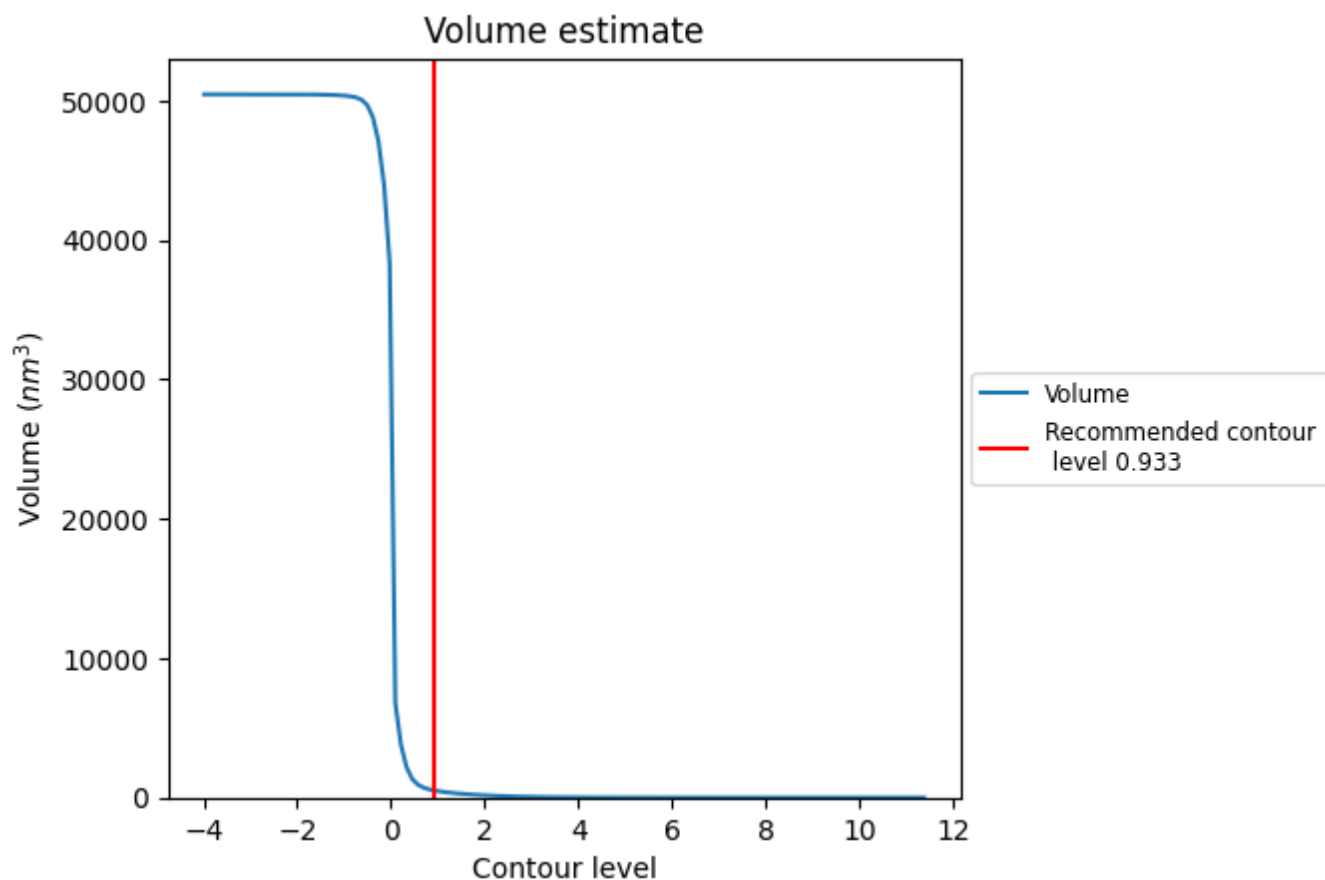
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

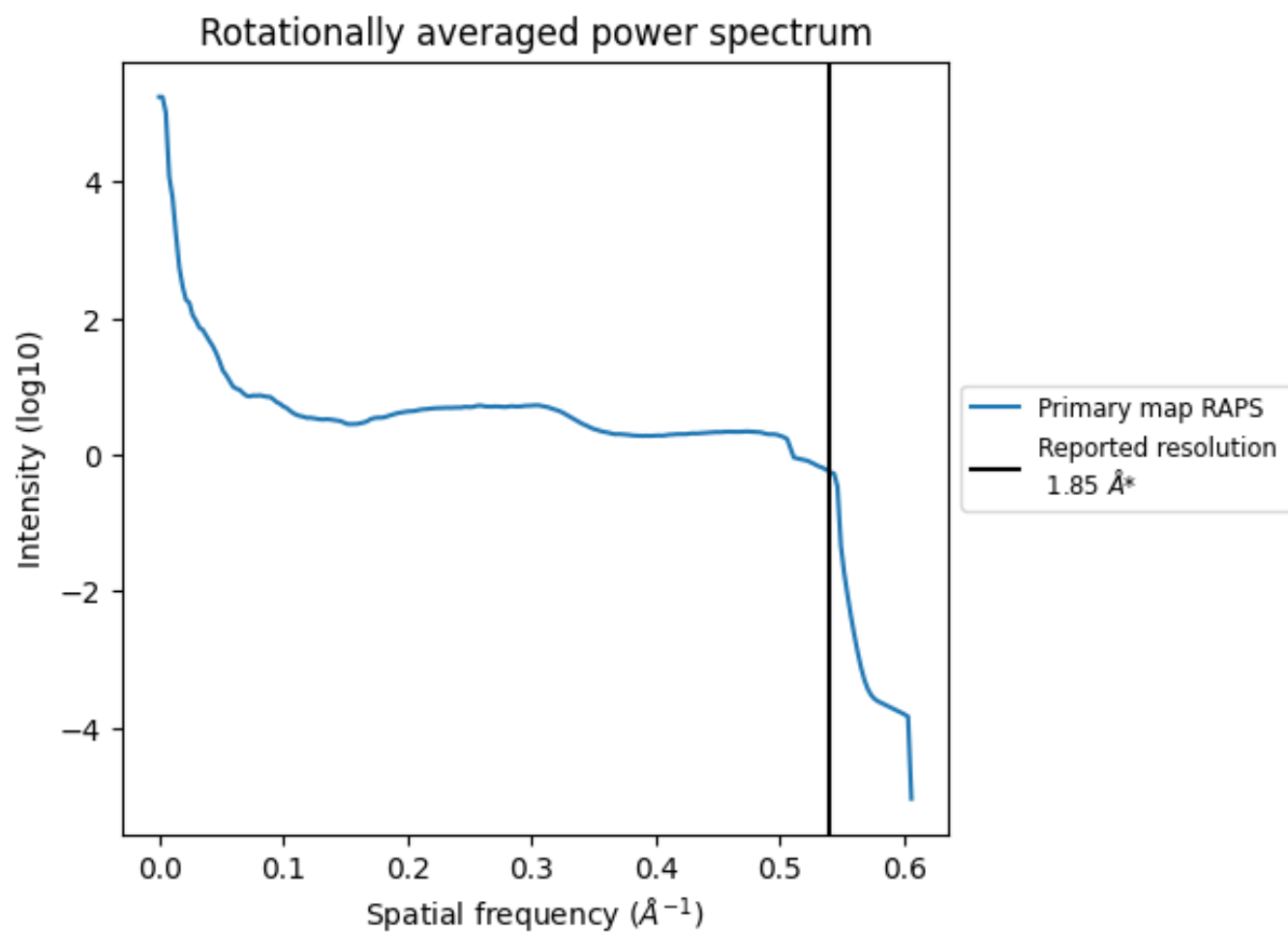
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 505 nm³; this corresponds to an approximate mass of 456 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.541 Å⁻¹

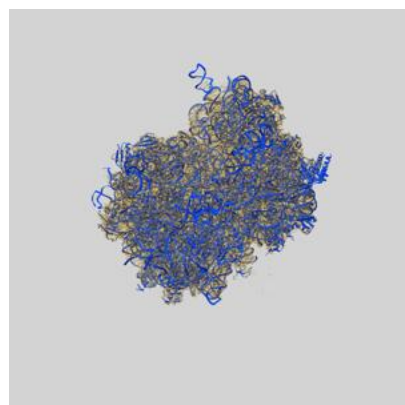
8 Fourier-Shell correlation

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

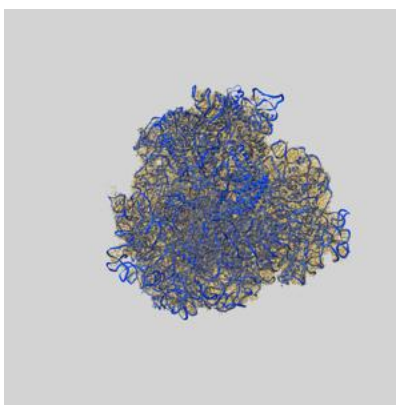
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-29449 and PDB model 8FTO. Per-residue inclusion information can be found in section 3 on page 17.

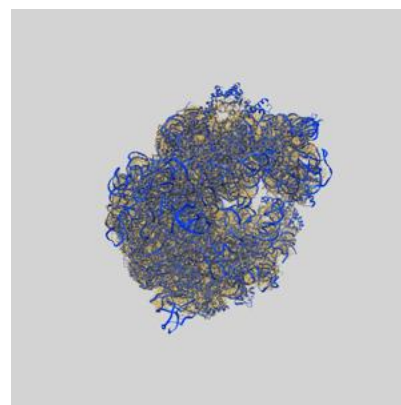
9.1 Map-model overlay [i](#)



X



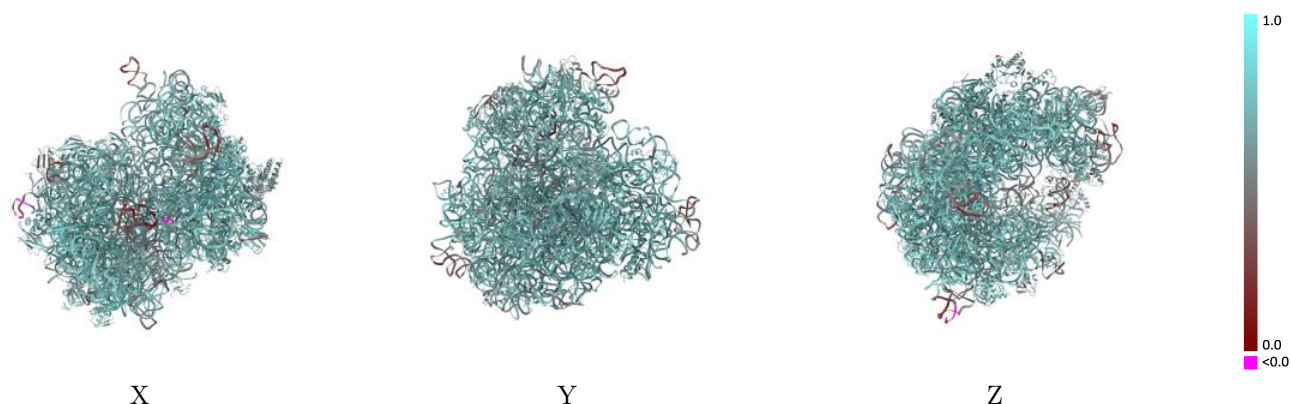
Y



Z

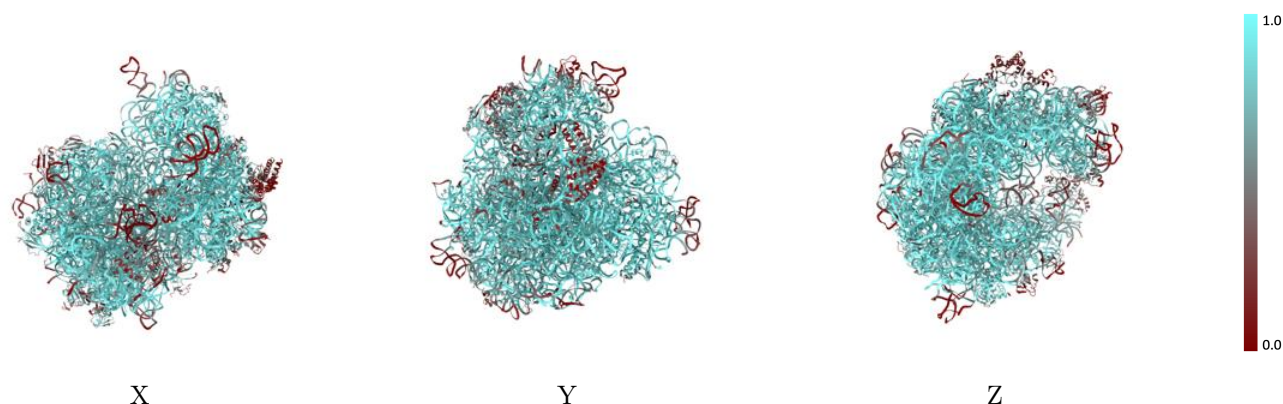
The images above show the 3D surface view of the map at the recommended contour level 0.933 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



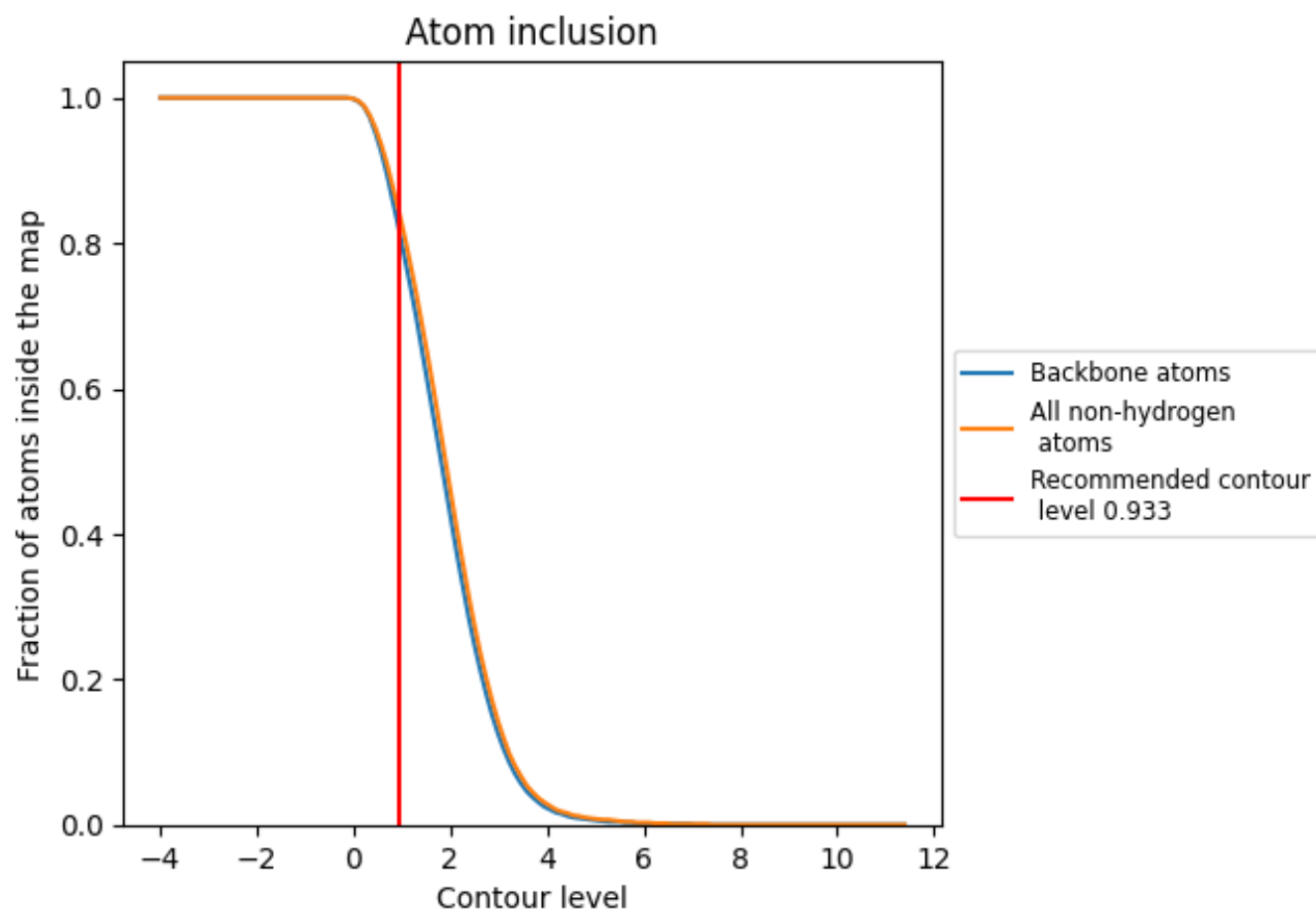
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.933).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 84% 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 (0.933) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8450	 0.7220
0	 0.8390	 0.7580
1	 0.9660	 0.8080
2	 0.9550	 0.8060
3	 0.9070	 0.7630
4	 0.0190	 0.3530
A	 0.8900	 0.7120
B	 0.2910	 0.6140
C	 0.7710	 0.7130
D	 0.8040	 0.7240
E	 0.8820	 0.7480
F	 0.7090	 0.6820
G	 0.6290	 0.6690
H	 0.8920	 0.7460
I	 0.6930	 0.7000
J	 0.5230	 0.6490
K	 0.8050	 0.7110
L	 0.8890	 0.7340
M	 0.6720	 0.6880
N	 0.8240	 0.7230
O	 0.8590	 0.7340
P	 0.8730	 0.7320
Q	 0.8060	 0.6960
R	 0.7000	 0.6570
S	 0.6860	 0.6810
T	 0.8850	 0.7340
U	 0.3830	 0.5970
X	 0.4550	 0.5630
Z	 0.5420	 0.5700
a	 0.8970	 0.7360
b	 0.7800	 0.6930
c	 0.9610	 0.7940
d	 0.9270	 0.7840
e	 0.7320	 0.7320
f	 0.3950	 0.5940



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Chain	Atom inclusion	Q-score
g	 0.4510	 0.5970
h	 0.4530	 0.6330
i	 0.9090	 0.7760
j	 0.9330	 0.7840
k	 0.8740	 0.7730
l	 0.8910	 0.7770
m	 0.9840	 0.8020
n	 0.7090	 0.7110
o	 0.8990	 0.7660
p	 0.9470	 0.7960
q	 0.7990	 0.7480
r	 0.8980	 0.7810
s	 0.7840	 0.7240
t	 0.6390	 0.6800
u	 0.7030	 0.7110
v	 0.9040	 0.7870
w	 0.8780	 0.7680
x	 0.5810	 0.6670
y	 0.8720	 0.7620
z	 0.8880	 0.7700