



wwPDB EM Validation Summary Report ⓘ

Jun 24, 2026 – 04:53 AM EDT

PDB ID : 9O2X / pdb_00009o2x
EMDB ID : EMD-70050
Title : Structure of WT E.coli ribosome 70S subunit with complexed with mRNA, P-site fMet-NH-tRNA^{fMet} and A-site (S)-betahydroxyBocK charged NH-tRNA^{Pyl}
Authors : Majumdar, C.; Kent, A.; Hamlish, N.; Zhu, C.; Cate, J.
Deposited on : 2025-04-04
Resolution : 2.29 Å (reported)
Based on initial model : 8EMM

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

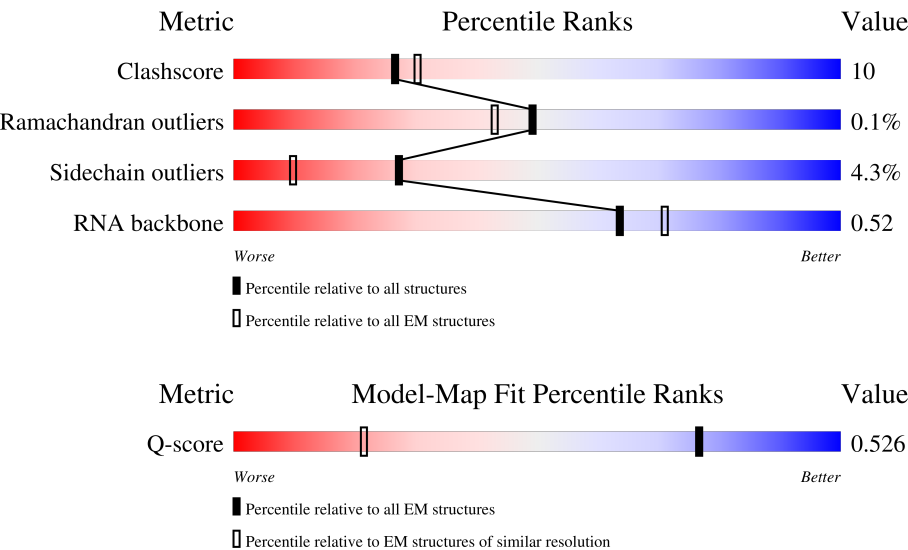
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 2.29 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.



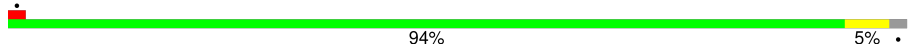
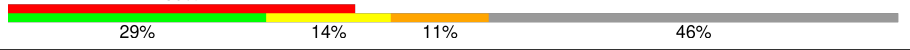
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	3699 (1.79 - 2.79)

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	

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Mol	Chain	Length	Quality of chain
3	2	65	
4	3	38	
5	B	241	
6	C	233	
7	D	206	
8	E	167	
9	F	135	
10	G	179	
11	H	130	
12	I	130	
13	J	103	
14	K	129	
15	L	124	
16	M	118	
17	N	101	
18	O	89	
19	P	82	
20	Q	84	
21	R	75	
22	S	92	
23	T	87	
24	U	71	
25	X	28	
26	Z	77	
27	b	120	

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Mol	Chain	Length	Quality of chain
28	c	273	
29	d	209	
30	e	201	
31	f	179	
32	g	177	
33	h	149	
34	i	142	
35	j	123	
36	k	144	
37	l	136	
38	m	127	
39	n	117	
40	o	115	
41	p	118	
42	q	103	
43	r	110	
44	s	100	
45	t	104	
46	u	94	
47	v	85	
48	w	78	
49	x	63	
50	y	59	
51	z	57	
52	A	1542	

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Mol	Chain	Length	Quality of chain
53	a	2904	9% 57% 34% 5%
54	4	70	83% 53% 30% 14%
55	Y	71	72% 18% 41% 41%

2 Entry composition

There are 64 unique types of molecules in this entry. The entry contains 145519 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 30S ribosomal protein S2.

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

- Molecule 6 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 7 is a protein called Small ribosomal subunit protein uS4.

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

- Molecule 8 is a protein called Small ribosomal subunit protein uS5.

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

- Molecule 9 is a protein called Small ribosomal subunit protein bS6.

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

- Molecule 10 is a protein called Small ribosomal subunit protein uS7.

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

- Molecule 11 is a protein called Small ribosomal subunit protein uS8.

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

- Molecule 12 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 13 is a protein called Small ribosomal subunit protein uS10.

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

- Molecule 14 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	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 15 is a protein called Small ribosomal subunit protein uS12.

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

- Molecule 16 is a protein called Small ribosomal subunit protein uS13.

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

- Molecule 17 is a protein called Small ribosomal subunit protein uS14.

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

- Molecule 18 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 19 is a protein called Small ribosomal subunit protein bS16.

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

- Molecule 20 is a protein called Small ribosomal subunit protein uS17.

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

- Molecule 21 is a protein called Small ribosomal subunit protein bS18.

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

- Molecule 22 is a protein called Small ribosomal subunit protein uS19.

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

- Molecule 23 is a protein called Small ribosomal subunit protein bS20.

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

- Molecule 24 is a protein called Small ribosomal subunit protein bS21.

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

- Molecule 25 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	X	15	Total	C	N	O	P	0	0
			322	145	61	101	15		

- Molecule 26 is a RNA chain called P-site tRNA fMet.

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

- Molecule 27 is a RNA chain called 5S rRNA.

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

- Molecule 28 is a protein called 50S ribosomal protein L2.

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

- Molecule 29 is a protein called 50S ribosomal protein L3.

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

- Molecule 30 is a protein called Large ribosomal subunit protein uL4.

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

- Molecule 31 is a protein called Large ribosomal subunit protein uL5.

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

- Molecule 32 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	173	Total	C	N	O	S	0	0
			1295	814	237	242	2		

- Molecule 33 is a protein called Large ribosomal subunit protein bL9.

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

- Molecule 34 is a protein called Large ribosomal subunit protein uL13.

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

- Molecule 35 is a protein called Large ribosomal subunit protein uL14.

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

- Molecule 36 is a protein called Large ribosomal subunit protein uL15.

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

- Molecule 37 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	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
l	138	MS6	MET	conflict	UNP P0ADY7

- Molecule 38 is a protein called Large ribosomal subunit protein bL17.

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

- Molecule 39 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 40 is a protein called Large ribosomal subunit protein bL19.

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

- Molecule 41 is a protein called 50S ribosomal protein L20.

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

- Molecule 42 is a protein called Large ribosomal subunit protein bL21.

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

- Molecule 43 is a protein called Large ribosomal subunit protein uL22.

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

- Molecule 44 is a protein called 50S ribosomal protein L23.

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

- Molecule 45 is a protein called 50S ribosomal protein L24.

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

- Molecule 46 is a protein called Large ribosomal subunit protein bL25.

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

- Molecule 47 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	v	77	Total	C	N	O	S	0	0
			582	360	115	106	1		

- Molecule 48 is a protein called 50S ribosomal protein L28.

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

- Molecule 49 is a protein called Large ribosomal subunit protein uL29.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L32.

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

- Molecule 52 is a RNA chain called 16S rRNA.

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

- Molecule 53 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	a	2753	Total	C	N	O	P	0	0
			59130	26384	10897	19096	2753		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
54	4	60	Total	C	N	O	S	0	0
			480	299	90	85	6		

- Molecule 55 is a RNA chain called A-site tRNA^{Pyl}.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	Y	71	Total	C	N	O	P	0	0
			1518	675	276	496	71		

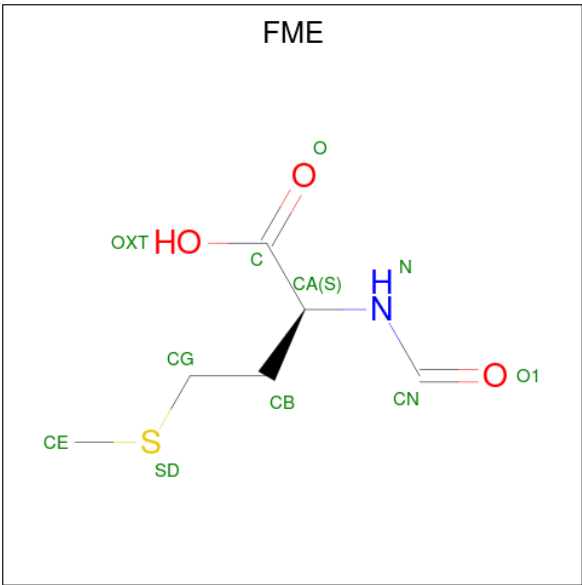
- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
56	3	1	Total	Zn	0
			1	1	
56	4	1	Total	Zn	0
			1	1	

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
57	C	1	Total	Mg	0
			1	1	
57	N	1	Total	Mg	0
			1	1	
57	Q	1	Total	Mg	0
			1	1	
57	Z	1	Total	Mg	0
			1	1	
57	b	5	Total	Mg	0
			5	5	
57	d	1	Total	Mg	0
			1	1	
57	z	1	Total	Mg	0
			1	1	
57	A	90	Total	Mg	0
			90	90	
57	a	219	Total	Mg	0
			219	219	

- Molecule 58 is N-FORMYLMETHIONINE (CCD ID: FME) (formula: C₆H₁₁NO₃S).

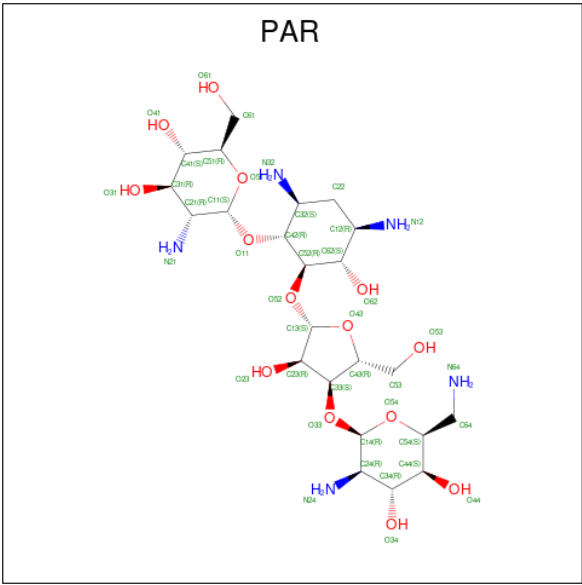


Mol	Chain	Residues	Atoms					AltConf
58	Z	1	Total	C	N	O	S	0
			10	6	1	2	1	

- Molecule 59 is POTASSIUM ION (CCD ID: K) (formula: K).

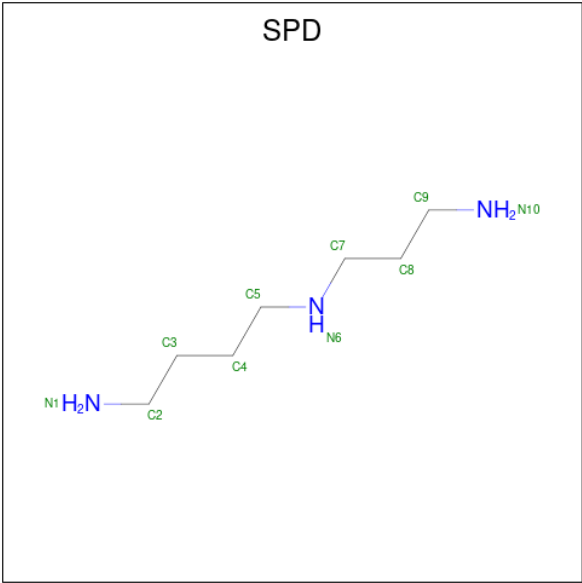
Mol	Chain	Residues	Atoms		AltConf
59	c	1	Total	K	0
			1	1	
59	a	9	Total	K	0
			9	9	

- Molecule 60 is PAROMOMYCIN (CCD ID: PAR) (formula: C₂₃H₄₅N₅O₁₄).



Mol	Chain	Residues	Atoms				AltConf
60	A	1	Total	C	N	O	0
			42	23	5	14	

- Molecule 61 is SPERMIDINE (CCD ID: SPD) (formula: C₇H₁₉N₃).



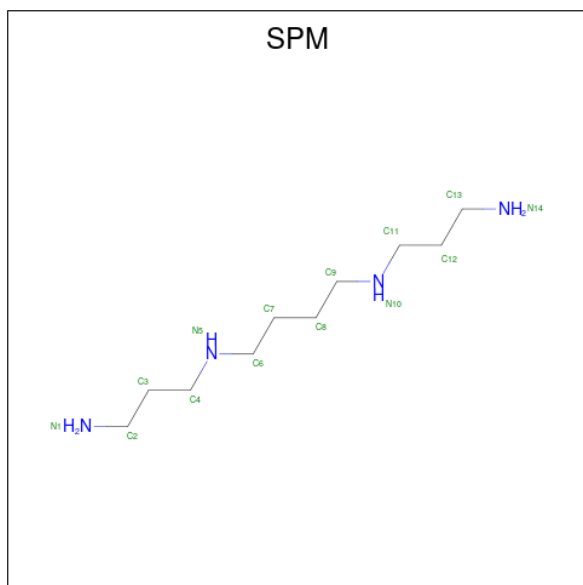
Mol	Chain	Residues	Atoms			AltConf
61	A	1	Total	C	N	0
			10	7	3	
61	a	1	Total	C	N	0
			10	7	3	
61	a	1	Total	C	N	0
			10	7	3	
61	a	1	Total	C	N	0
			10	7	3	
61	a	1	Total	C	N	0
			10	7	3	
61	a	1	Total	C	N	0
			10	7	3	
61	a	1	Total	C	N	0
			10	7	3	
61	a	1	Total	C	N	0
			10	7	3	

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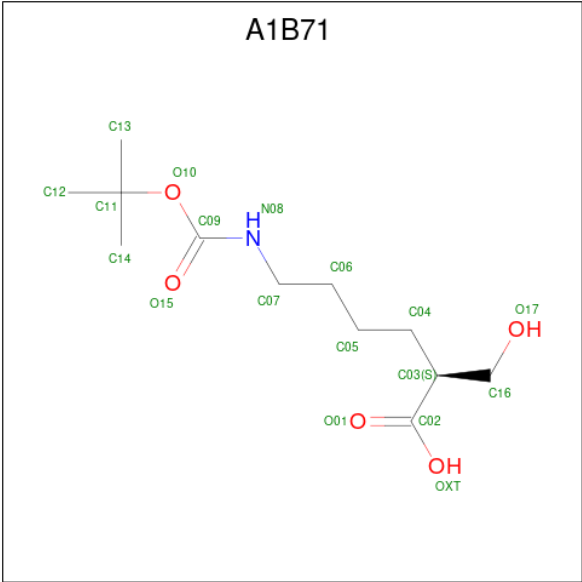
Mol	Chain	Residues	Atoms			AltConf
61	a	1	Total	C	N	0
			10	7	3	
61	a	1	Total	C	N	0
			10	7	3	
61	a	1	Total	C	N	0
			10	7	3	

- Molecule 62 is SPERMINE (CCD ID: SPM) (formula: $C_{10}H_{26}N_4$).



Mol	Chain	Residues	Atoms			AltConf
62	a	1	Total	C	N	0
			14	10	4	

- Molecule 63 is (2S)-6-[(tert-butoxycarbonyl)amino]-2-(hydroxymethyl)hexanoic acid (CCD ID: A1B71) (formula: $C_{12}H_{23}NO_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
63	Y	1	Total	C	N	O	0
			17	12	1	4	

- Molecule 64 is water.

Mol	Chain	Residues	Atoms		AltConf
64	0	2	Total	O	0
			2	2	
64	1	15	Total	O	0
			15	15	
64	2	19	Total	O	0
			19	19	
64	3	4	Total	O	0
			4	4	
64	Z	4	Total	O	0
			4	4	
64	b	41	Total	O	0
			41	41	
64	c	84	Total	O	0
			84	84	
64	d	36	Total	O	0
			36	36	
64	e	29	Total	O	0
			29	29	
64	h	1	Total	O	0
			1	1	
64	i	13	Total	O	0
			13	13	

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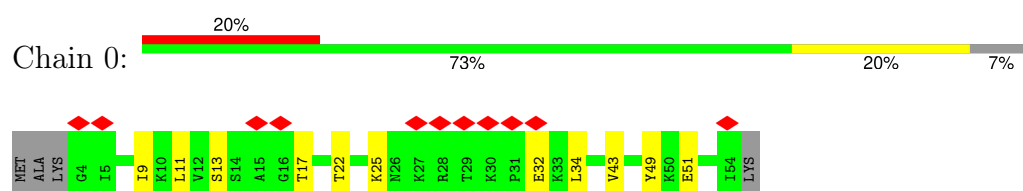
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Mol	Chain	Residues	Atoms		AltConf
64	j	14	Total 14	O 14	0
64	k	34	Total 34	O 34	0
64	l	25	Total 25	O 25	0
64	m	23	Total 23	O 23	0
64	o	13	Total 13	O 13	0
64	p	24	Total 24	O 24	0
64	q	13	Total 13	O 13	0
64	r	26	Total 26	O 26	0
64	s	5	Total 5	O 5	0
64	t	1	Total 1	O 1	0
64	u	3	Total 3	O 3	0
64	v	11	Total 11	O 11	0
64	w	12	Total 12	O 12	0
64	x	1	Total 1	O 1	0
64	z	24	Total 24	O 24	0
64	A	2	Total 2	O 2	0
64	a	2993	Total 2993	O 2993	0
64	Y	2	Total 2	O 2	0

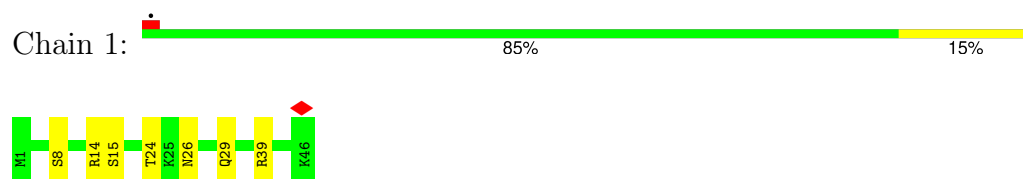
3 Residue-property plots [i](#)

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.

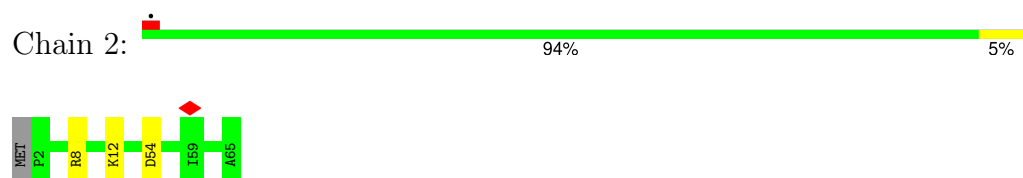
- Molecule 1: 50S ribosomal protein L33



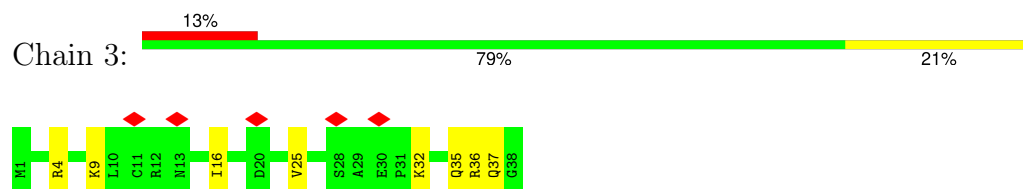
- Molecule 2: 50S ribosomal protein L34



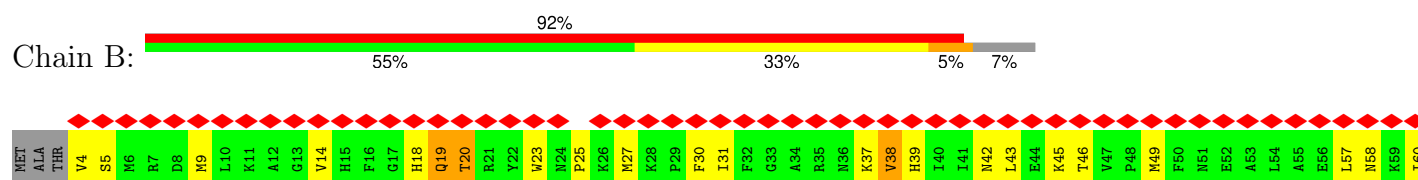
- Molecule 3: 50S ribosomal protein L35

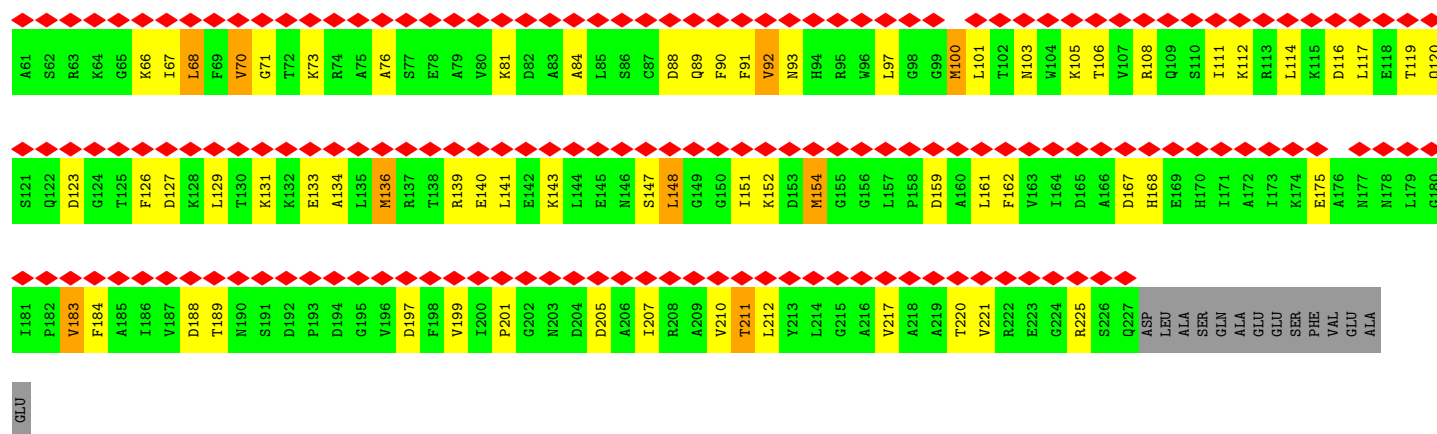


- Molecule 4: 50S ribosomal protein L36

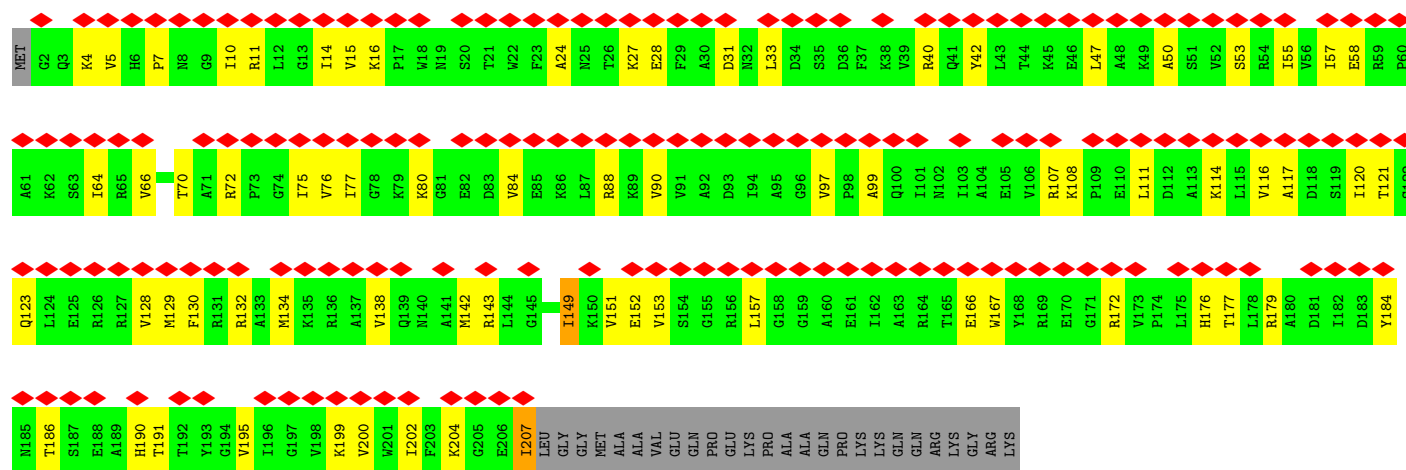


- Molecule 5: 30S ribosomal protein S2

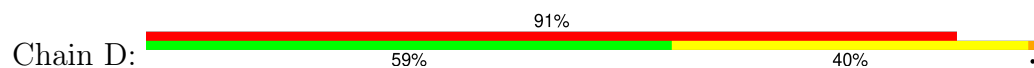




• Molecule 6: Small ribosomal subunit protein uS3

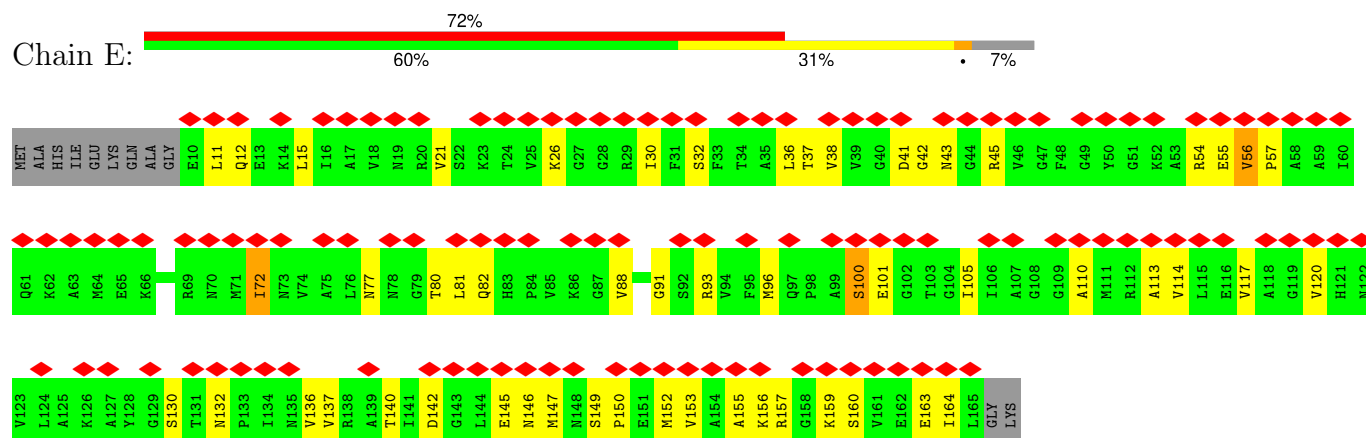


• Molecule 7: Small ribosomal subunit protein uS4



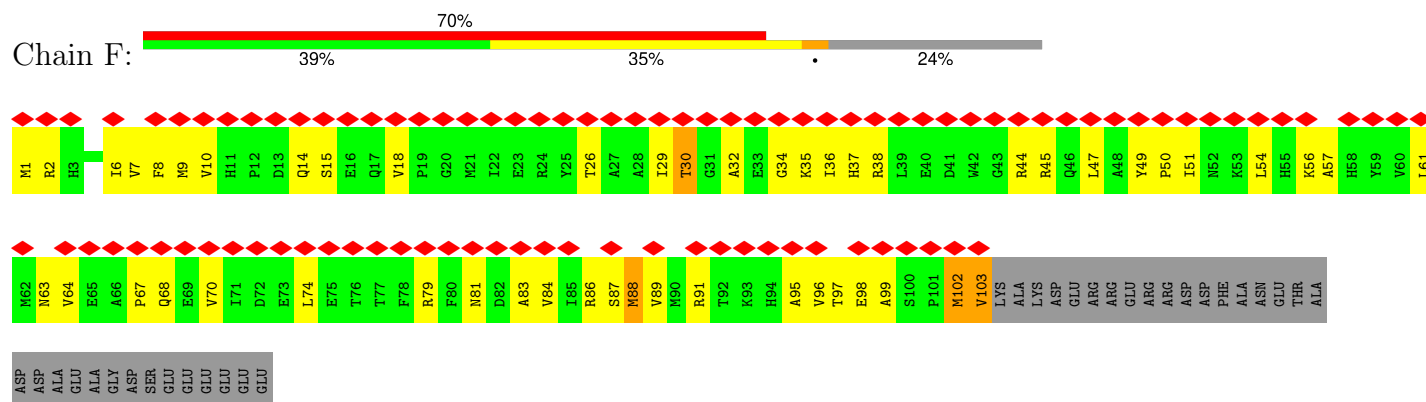
- Molecule 8: Small ribosomal subunit protein uS5

Chain E:



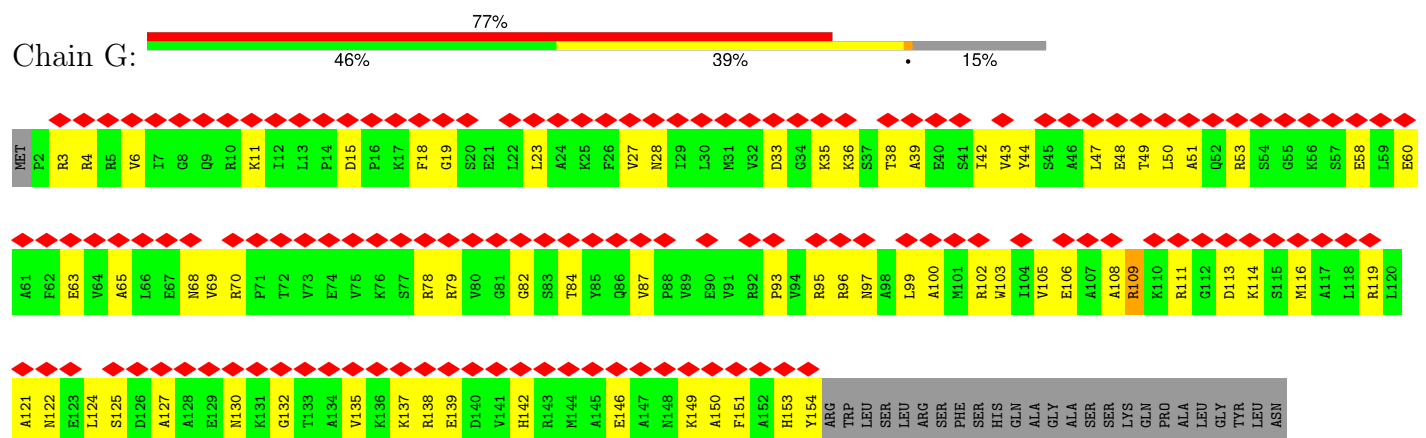
- Molecule 9: Small ribosomal subunit protein bS6

Chain F:



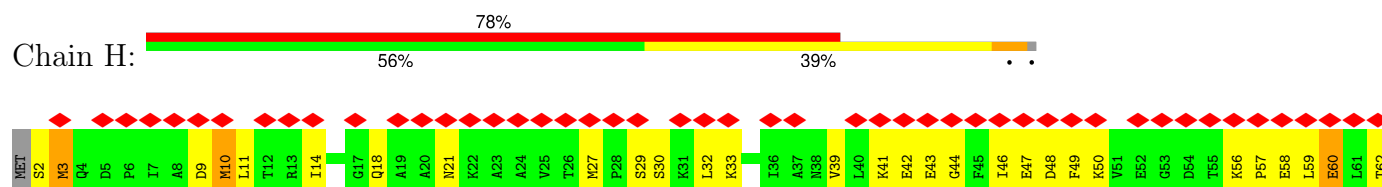
- Molecule 10: Small ribosomal subunit protein uS7

Chain G:



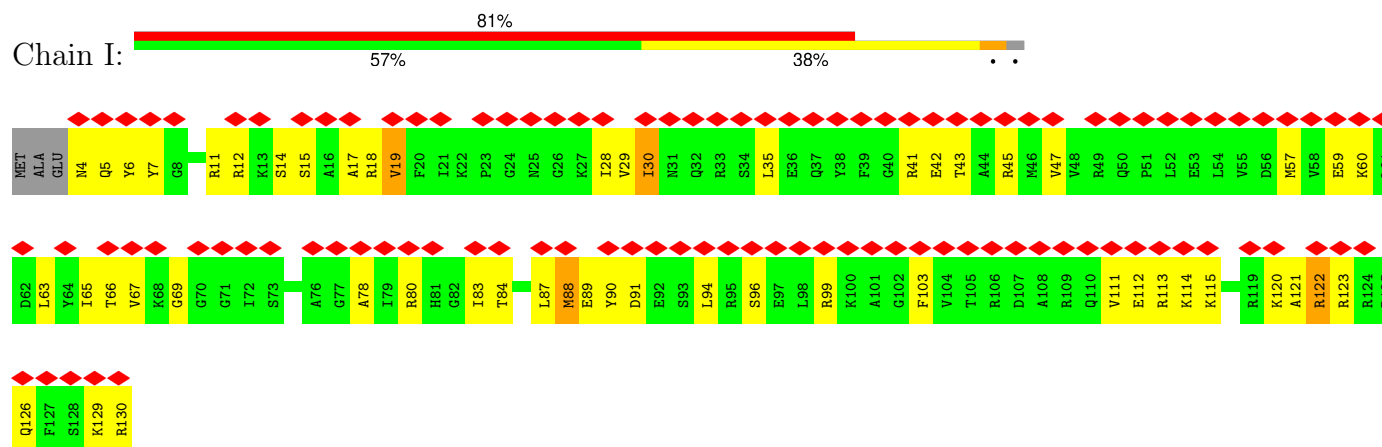
- Molecule 11: Small ribosomal subunit protein uS8

Chain H:

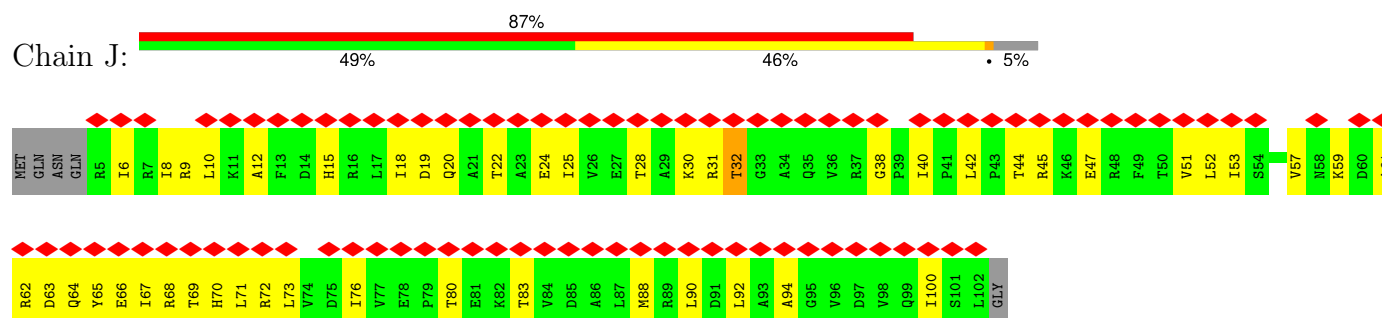




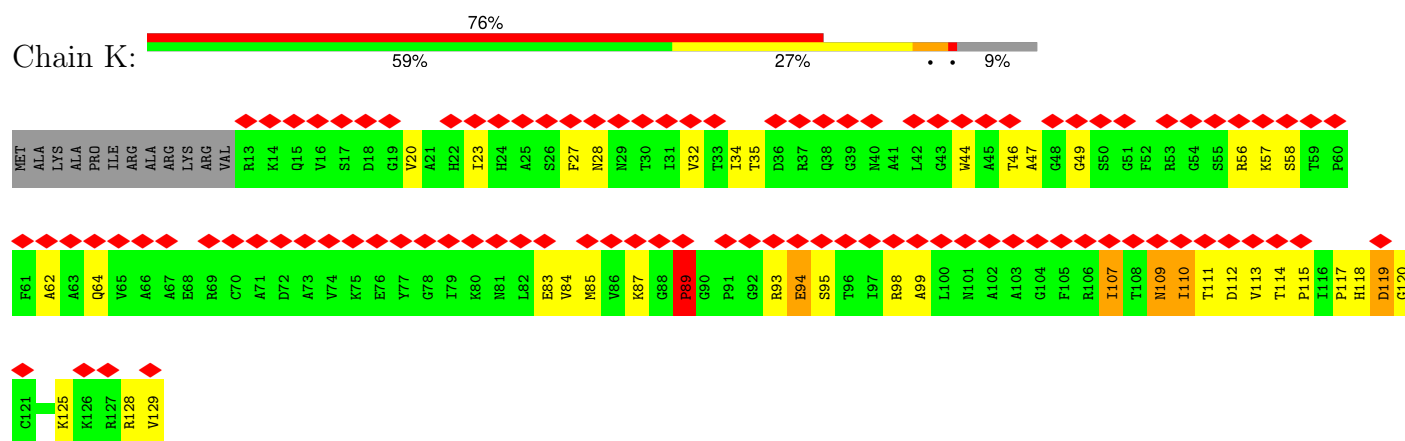
- Molecule 12: Small ribosomal subunit protein uS9



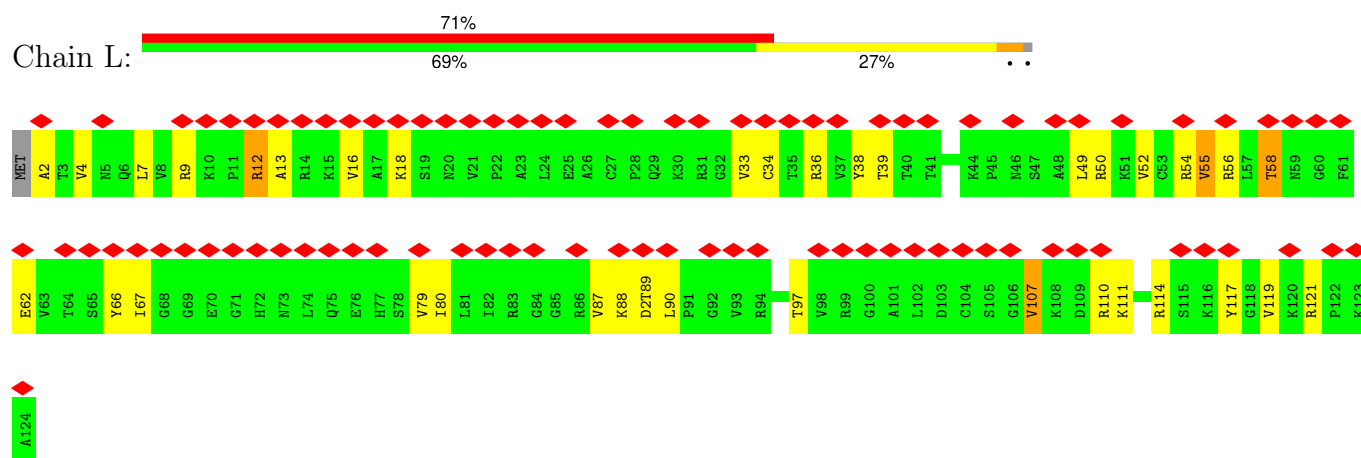
- Molecule 13: Small ribosomal subunit protein uS10



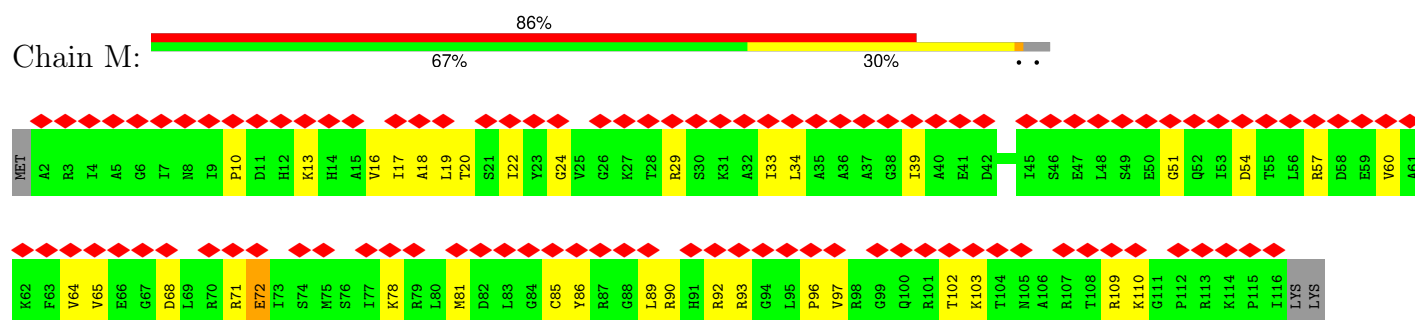
- Molecule 14: Small ribosomal subunit protein uS11



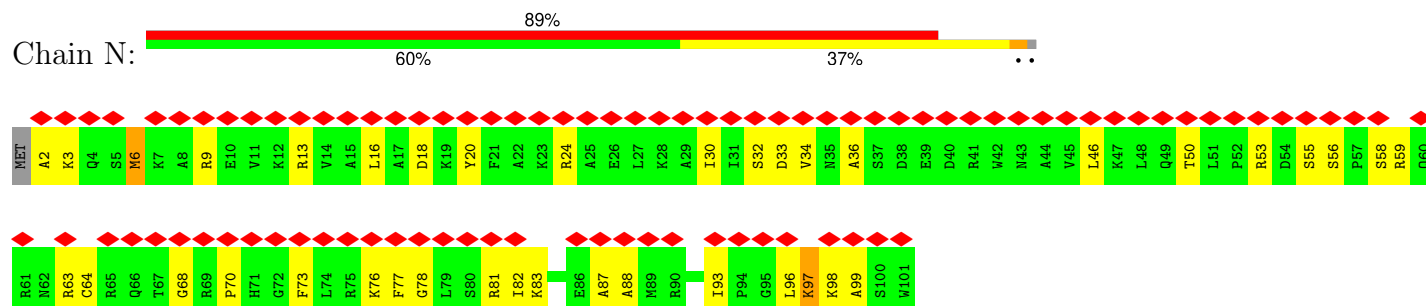
- Molecule 15: Small ribosomal subunit protein uS12



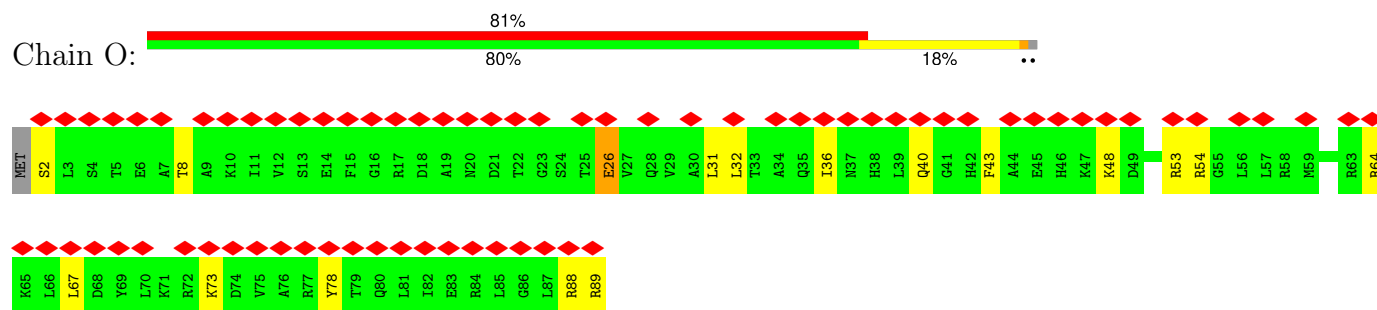
- Molecule 16: Small ribosomal subunit protein uS13



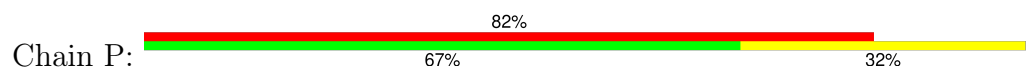
- Molecule 17: Small ribosomal subunit protein uS14

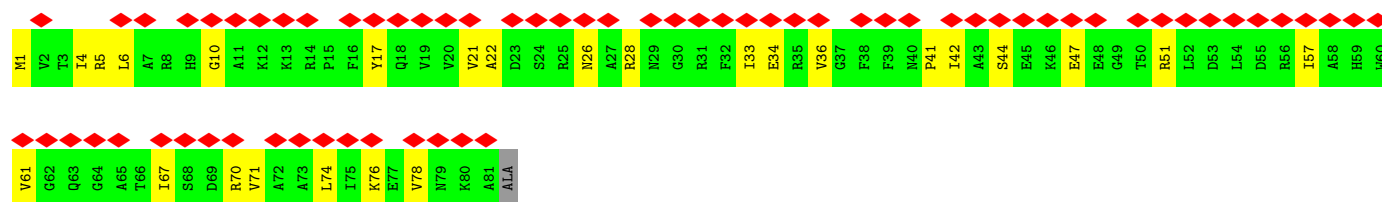


- Molecule 18: Small ribosomal subunit protein uS15

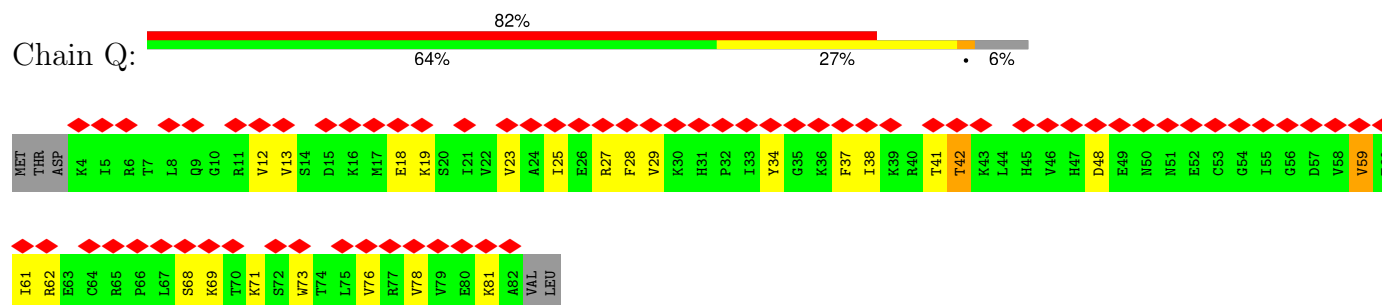


- Molecule 19: Small ribosomal subunit protein bS16

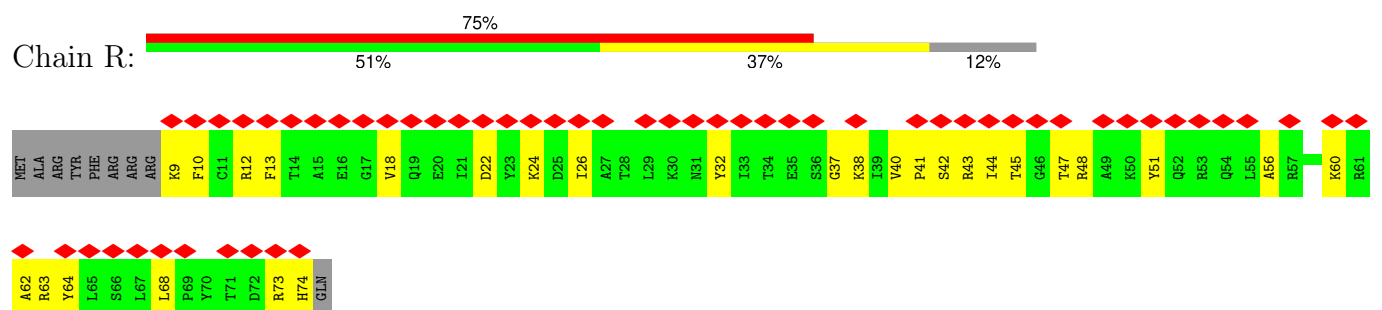




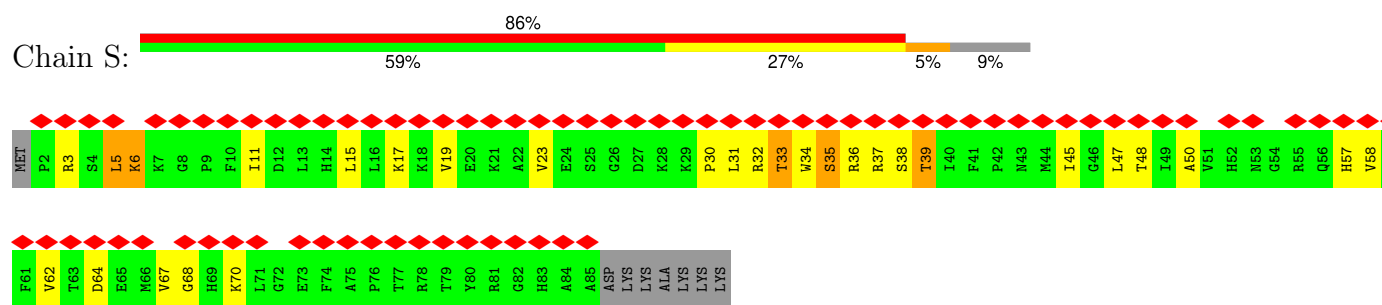
- Molecule 20: Small ribosomal subunit protein uS17



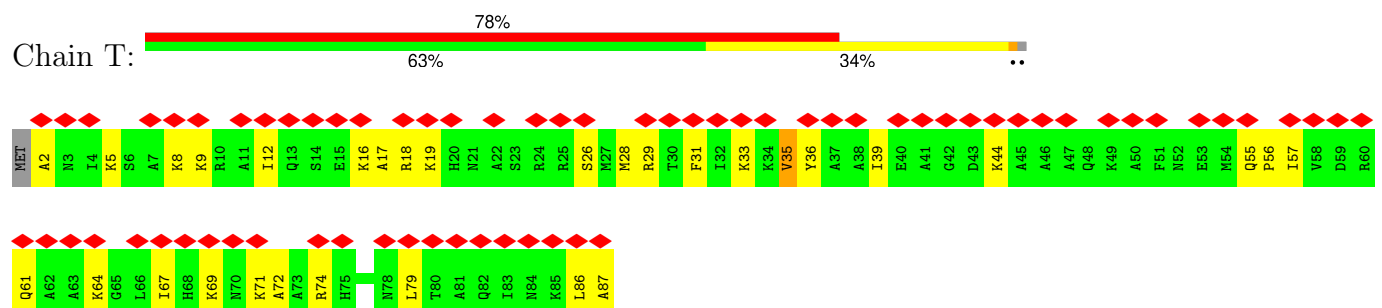
- Molecule 21: Small ribosomal subunit protein bS18



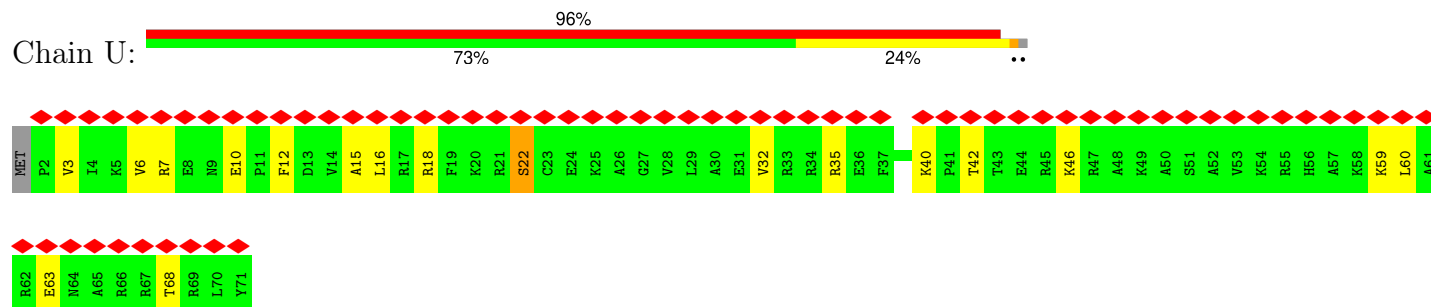
- Molecule 22: Small ribosomal subunit protein uS19



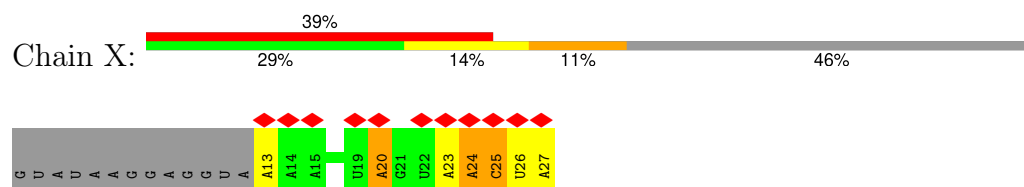
- Molecule 23: Small ribosomal subunit protein bS20



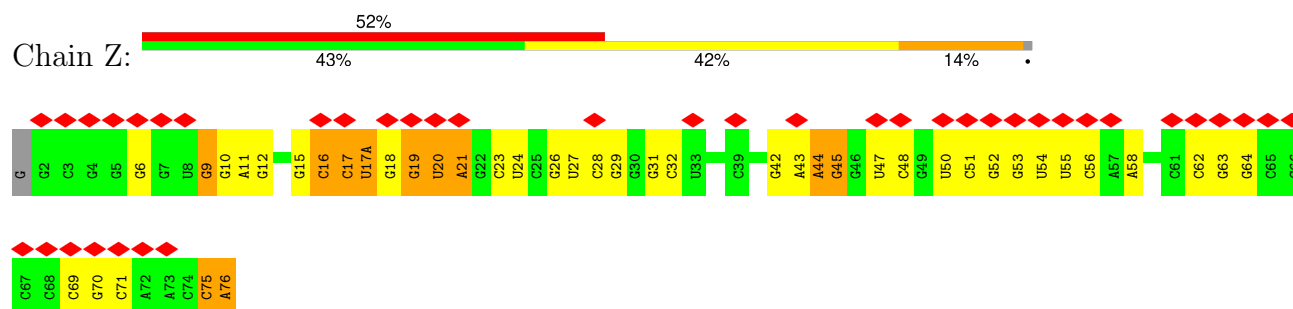
- Molecule 24: Small ribosomal subunit protein bS21



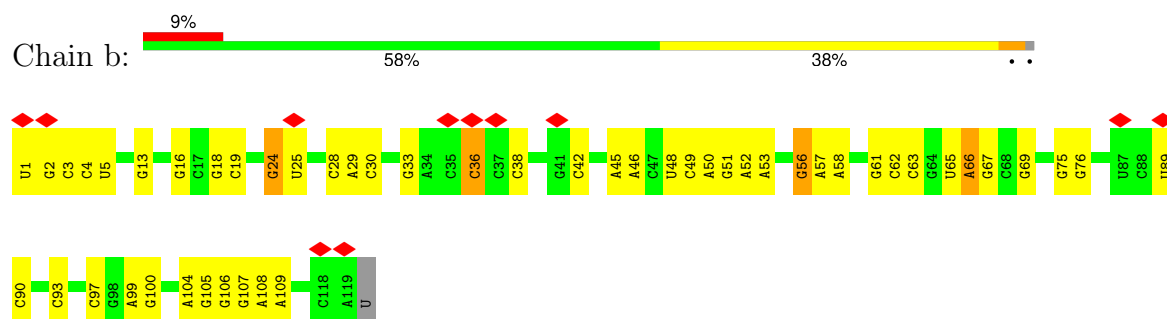
- Molecule 25: mRNA



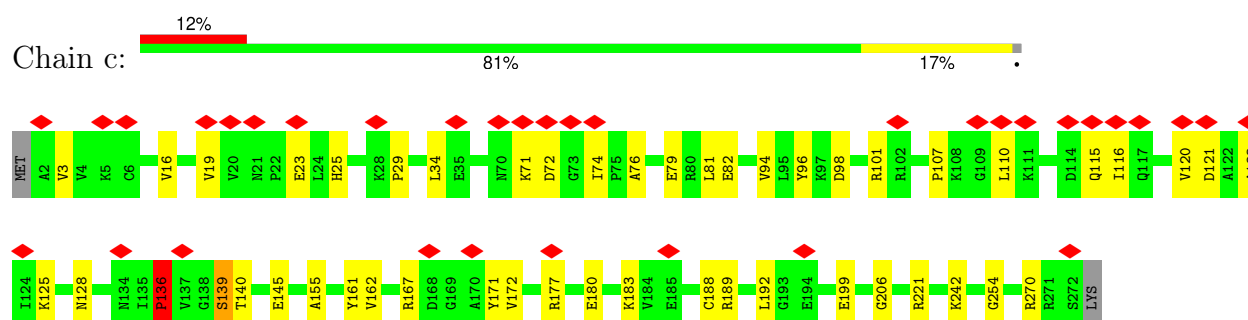
- Molecule 26: P-site tRNA fMet



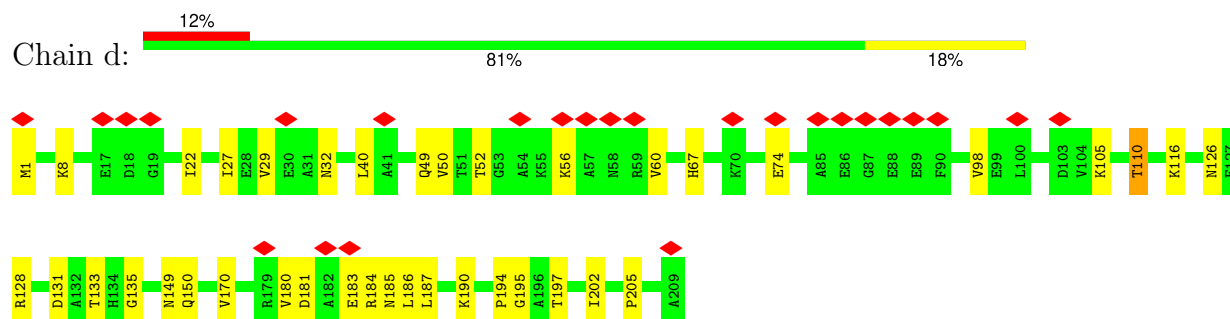
- Molecule 27: 5S rRNA



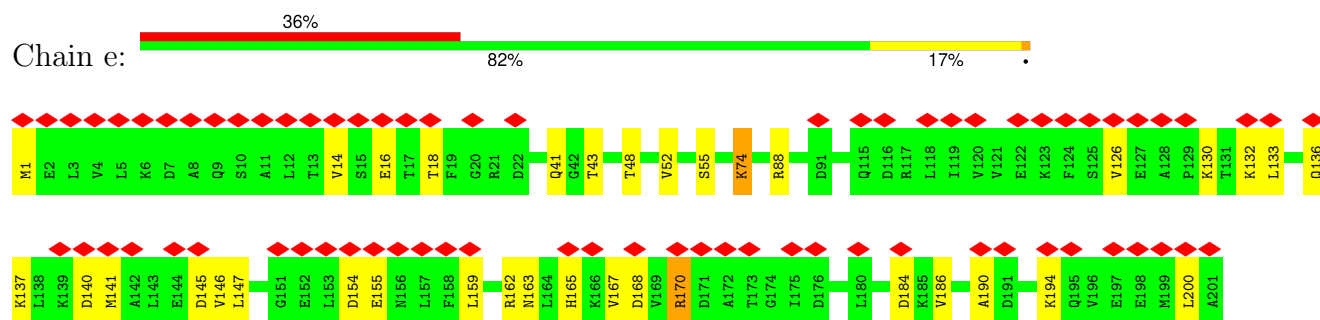
- Molecule 28: 50S ribosomal protein L2



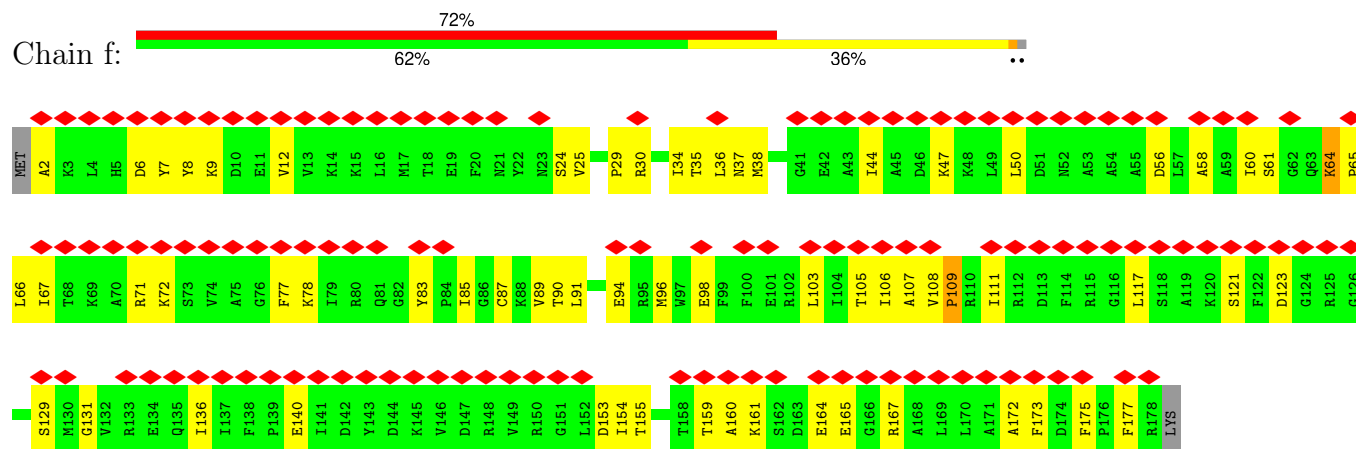
- Molecule 29: 50S ribosomal protein L3



- Molecule 30: Large ribosomal subunit protein uL4

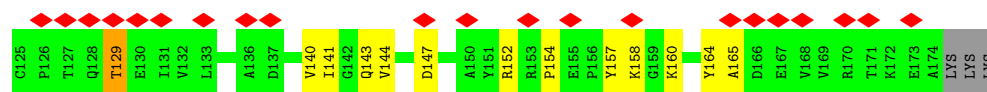


- Molecule 31: Large ribosomal subunit protein uL5

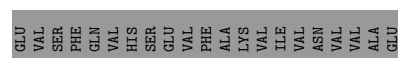


- Molecule 32: Large ribosomal subunit protein uL6

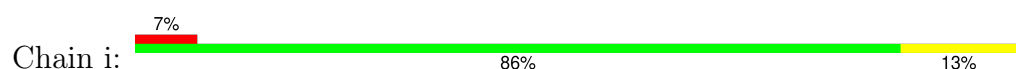




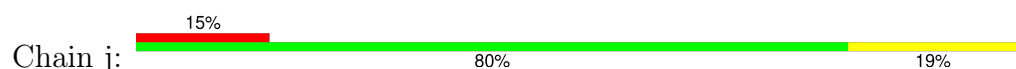
- Molecule 33: Large ribosomal subunit protein bL9



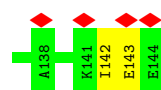
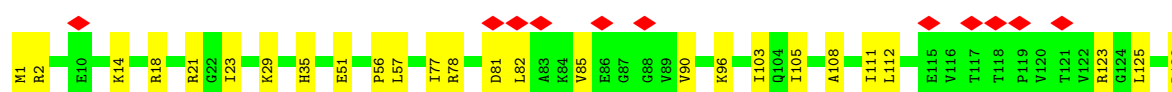
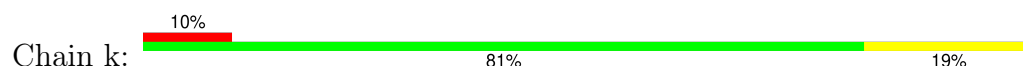
- Molecule 34: Large ribosomal subunit protein uL13



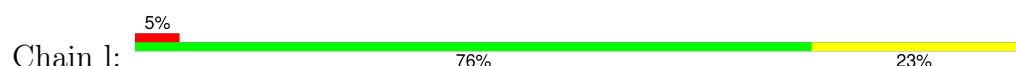
- Molecule 35: Large ribosomal subunit protein uL14

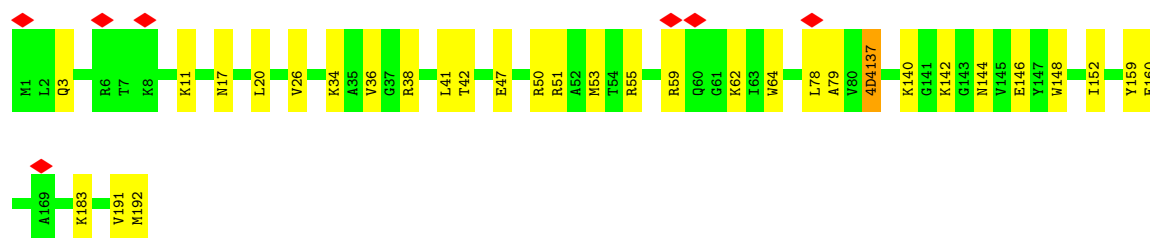


- Molecule 36: Large ribosomal subunit protein uL15

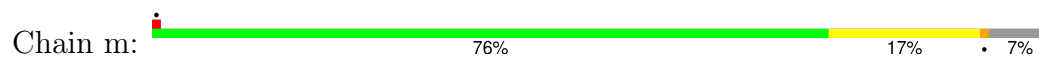


- Molecule 37: Large ribosomal subunit protein uL16

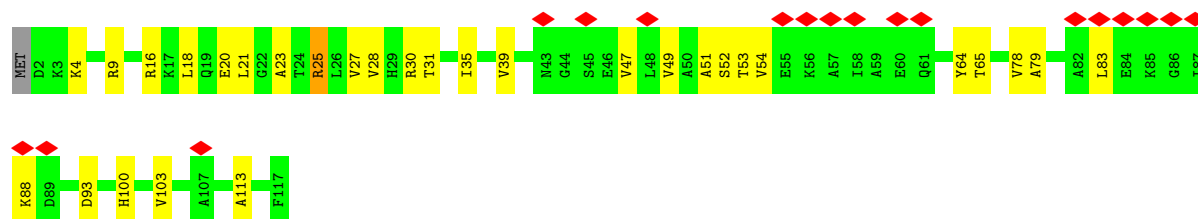




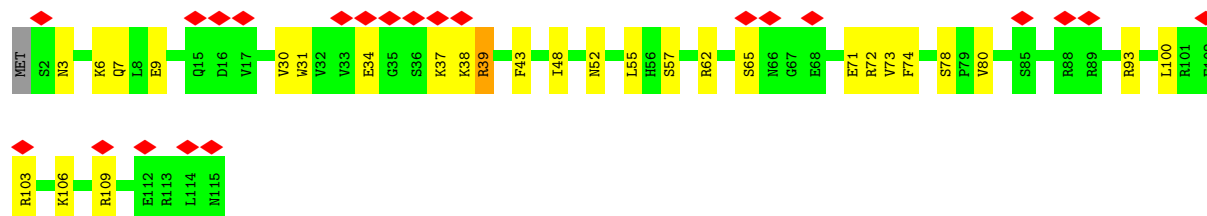
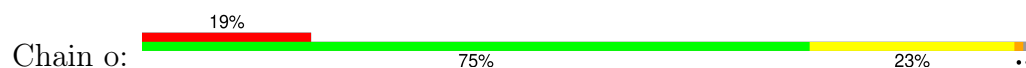
- Molecule 38: Large ribosomal subunit protein bL17



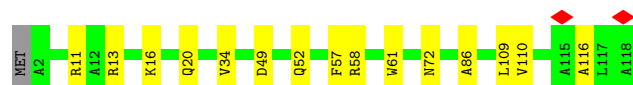
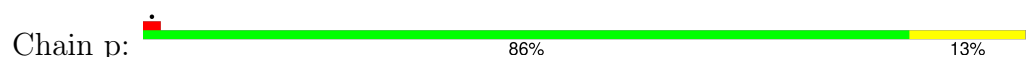
- Molecule 39: Large ribosomal subunit protein uL18



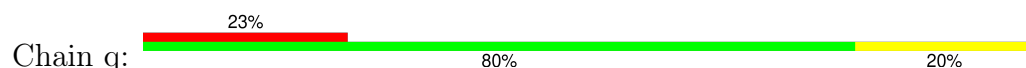
- Molecule 40: Large ribosomal subunit protein bL19

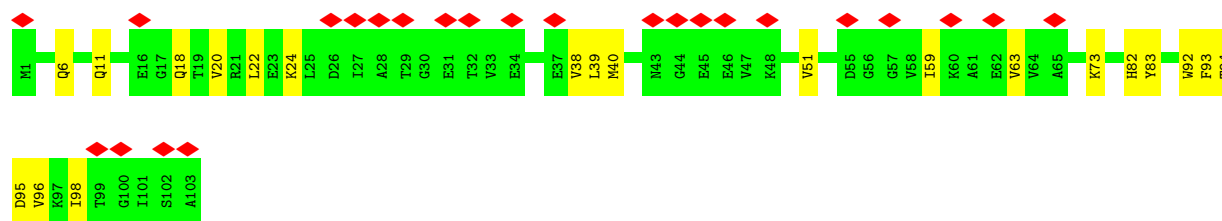


- Molecule 41: 50S ribosomal protein L20

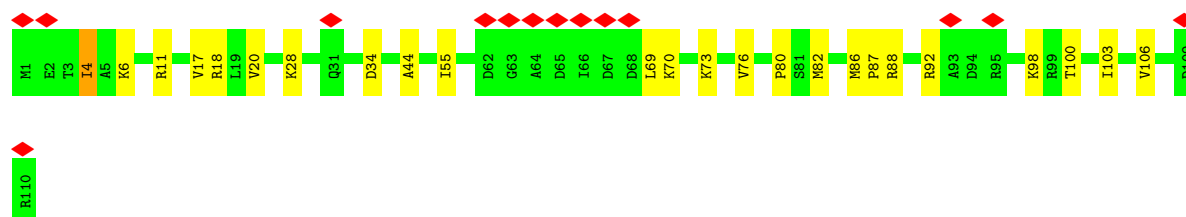
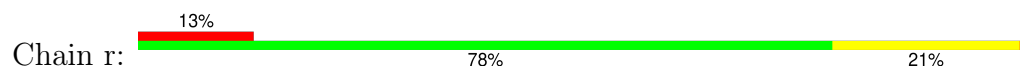


- Molecule 42: Large ribosomal subunit protein bL21

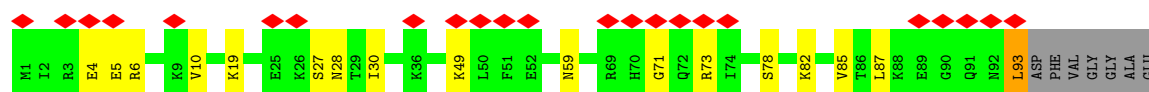
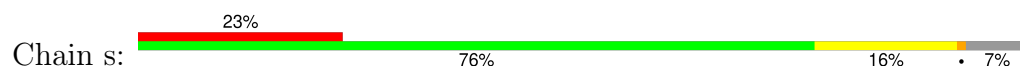




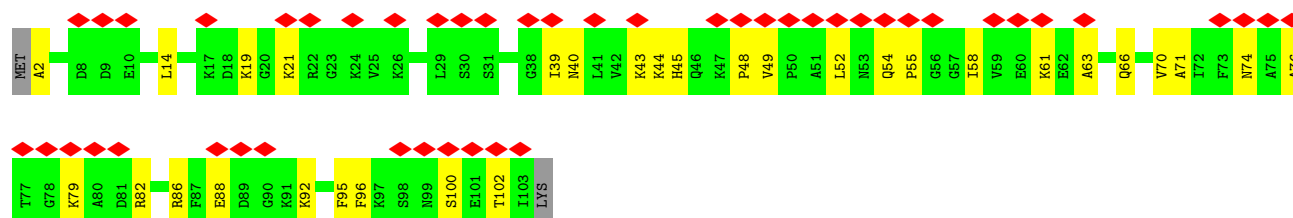
- Molecule 43: Large ribosomal subunit protein uL22



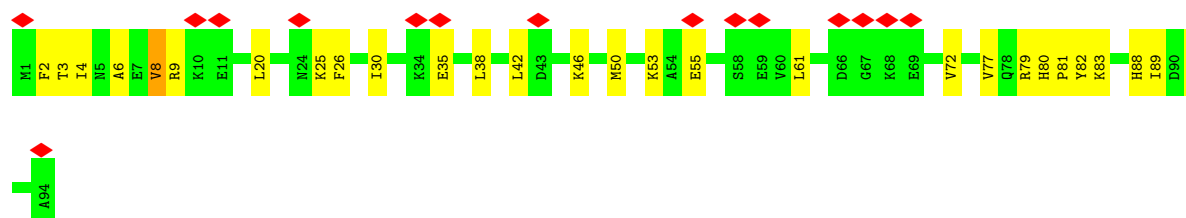
- Molecule 44: 50S ribosomal protein L23



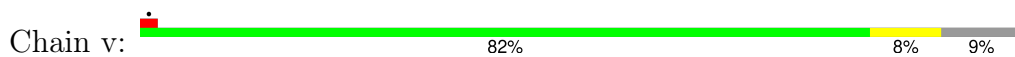
- Molecule 45: 50S ribosomal protein L24



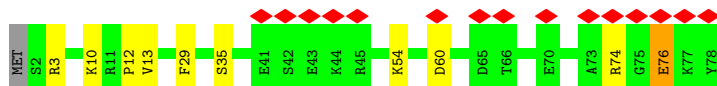
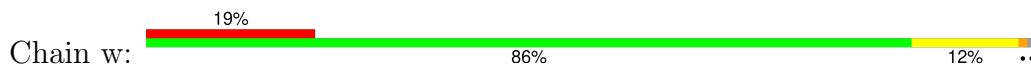
- Molecule 46: Large ribosomal subunit protein bL25



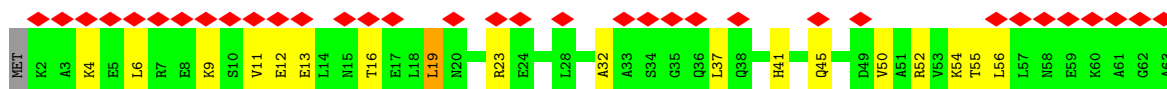
- Molecule 47: Large ribosomal subunit protein bL27



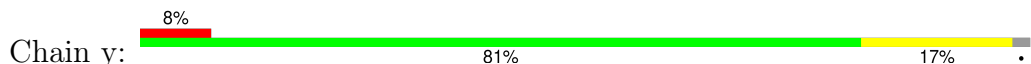
- Molecule 48: 50S ribosomal protein L28



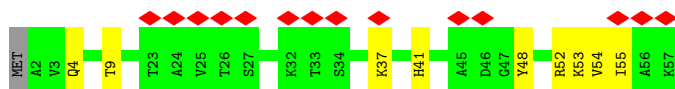
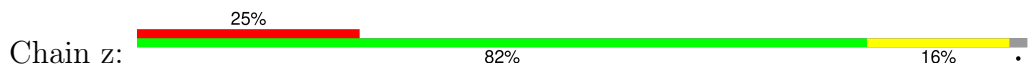
- Molecule 49: Large ribosomal subunit protein uL29



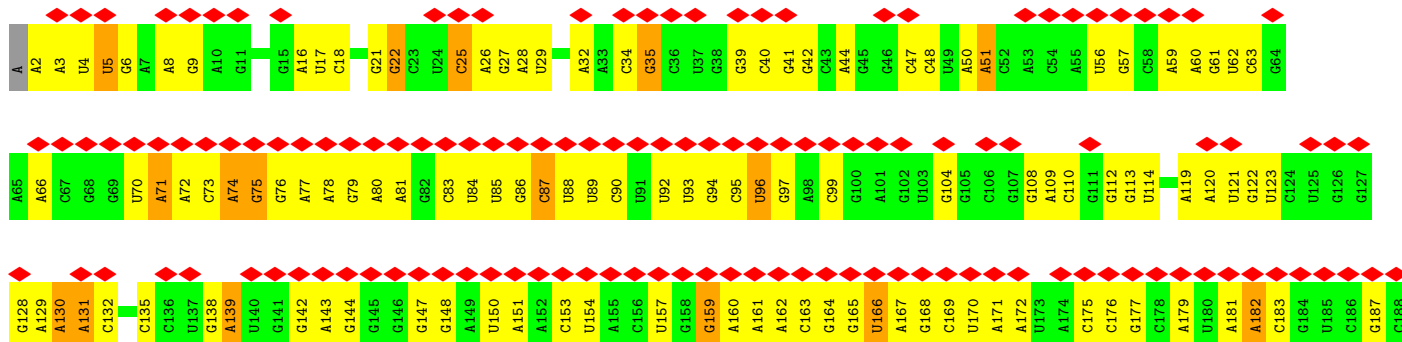
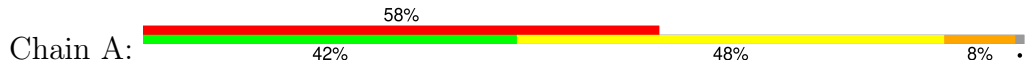
- Molecule 50: 50S ribosomal protein L30



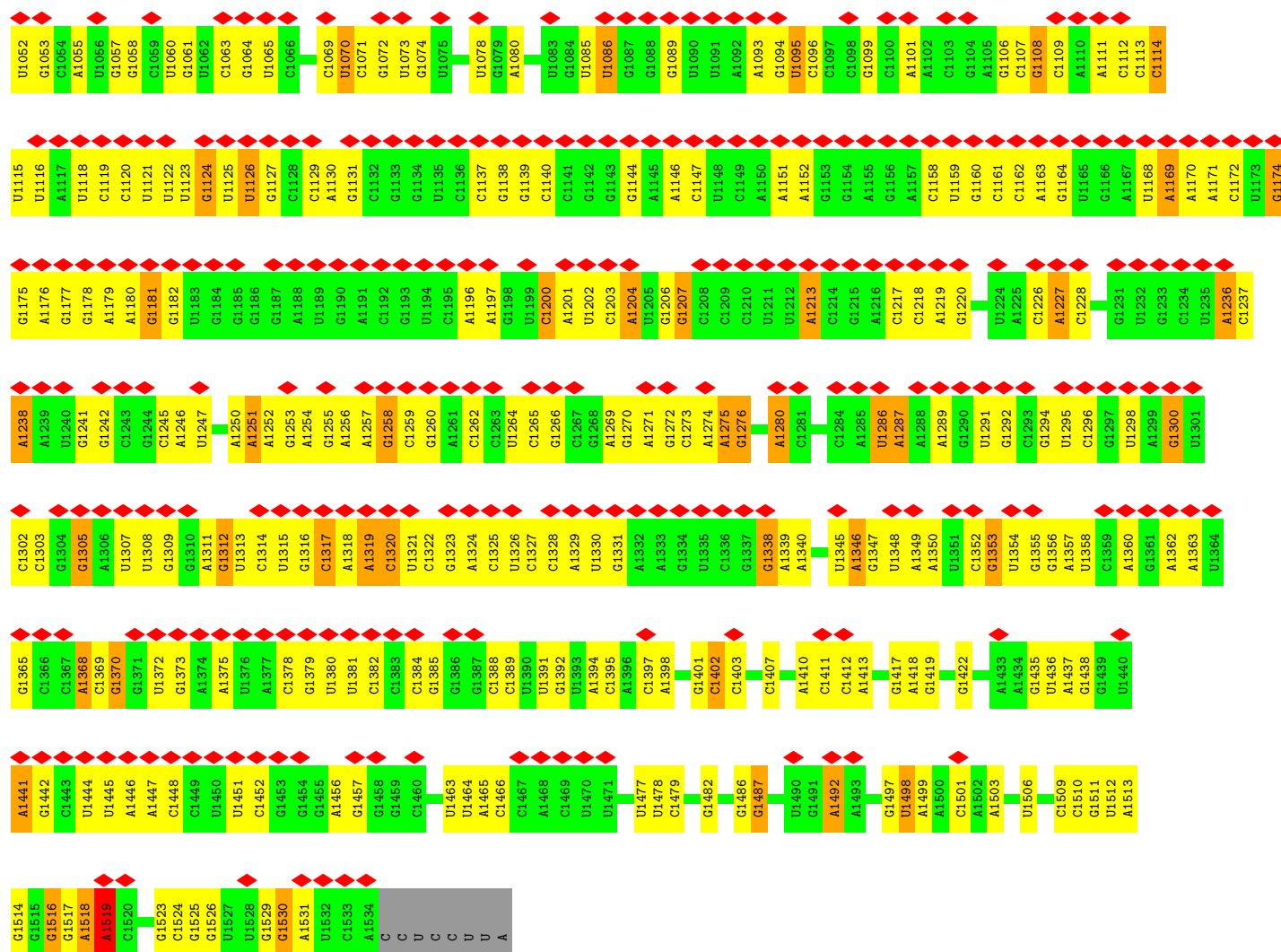
- Molecule 51: 50S ribosomal protein L32



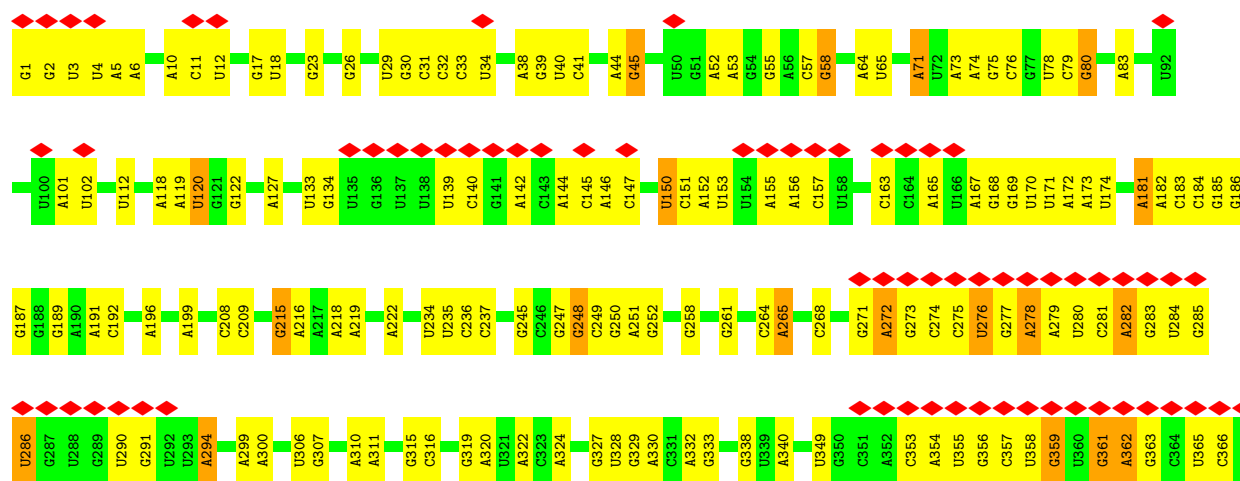
- Molecule 52: 16S rRNA







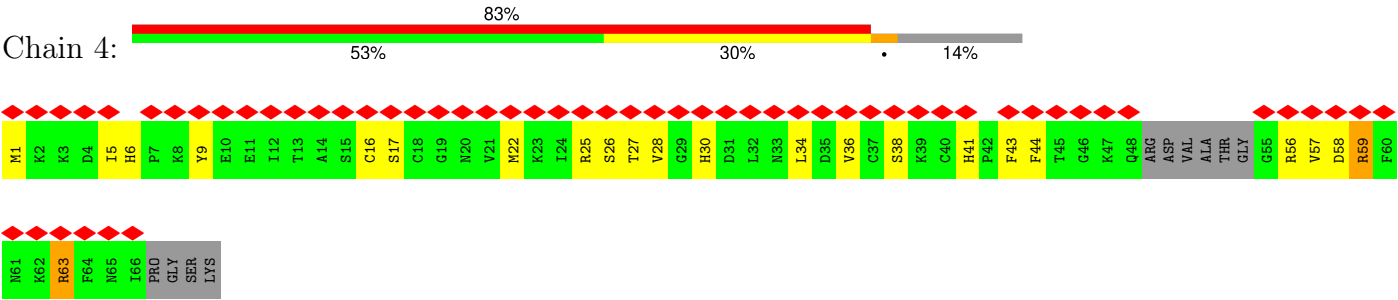
• Molecule 53: 23S rRNA



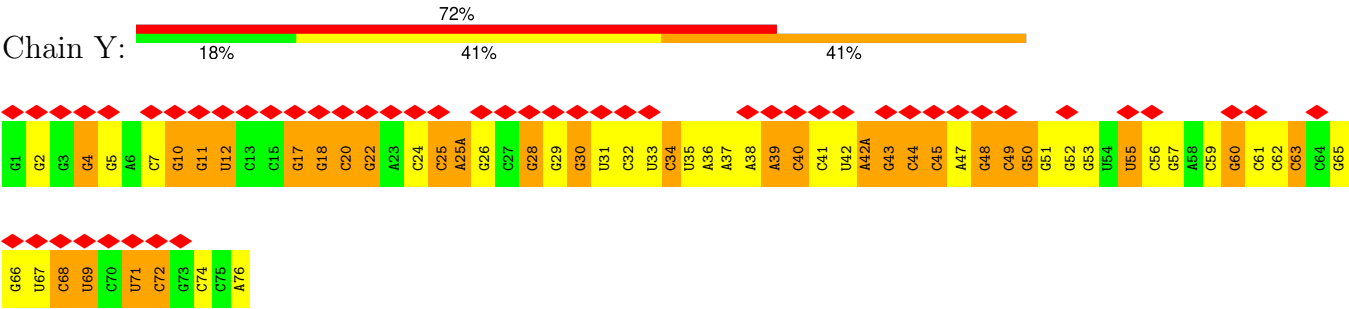




● Molecule 54: 50S ribosomal protein L31



● Molecule 55: A-site tRNA^{Pyl}



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	105571	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	5000	Depositor
Maximum defocus (nm)	15000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.192	Depositor
Minimum map value	-0.084	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0267	Depositor
Map size (Å)	422.1952, 422.1952, 422.1952	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8246, 0.8246, 0.8246	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 8AN, PAR, H2U, D2T, MS6, G7M, PSU, 5MC, 1MG, 3TD, OMG, MA6, SPM, 4OC, 5MU, MG, A1B71, MEQ, OMC, SPD, FME, K, 6MZ, OMU, 4D4, 2MA, IAS, ZN, UR3, 2MG

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	0.15	0/424	0.35	0/565
2	1	0.19	0/380	0.42	0/498
3	2	0.17	0/513	0.37	0/676
4	3	0.19	0/303	0.35	0/397
5	B	0.18	0/1784	0.42	0/2403
6	C	0.17	0/1651	0.40	0/2225
7	D	0.17	0/1665	0.38	0/2227
8	E	0.17	0/1165	0.40	0/1568
9	F	0.18	0/858	0.43	0/1160
10	G	0.17	0/1219	0.42	0/1635
11	H	0.17	0/989	0.43	0/1326
12	I	0.16	0/1034	0.38	0/1375
13	J	0.17	0/796	0.42	0/1077
14	K	0.20	0/884	0.49	1/1191 (0.1%)
15	L	0.16	0/960	0.38	0/1286
16	M	0.17	0/900	0.39	0/1204
17	N	0.16	0/817	0.38	0/1088
18	O	0.15	0/722	0.34	0/964
19	P	0.18	0/653	0.45	0/877
20	Q	0.16	0/650	0.38	0/871
21	R	0.19	0/553	0.46	0/742
22	S	0.15	0/685	0.38	0/922
23	T	0.20	0/676	0.37	0/895
24	U	0.16	0/597	0.34	0/792
25	X	0.29	0/361	0.43	0/560
26	Z	0.33	1/1788 (0.1%)	0.45	1/2786 (0.0%)
27	b	0.24	0/2850	0.33	0/4444
28	c	0.25	1/2121 (0.0%)	0.57	4/2852 (0.1%)
29	d	0.19	0/1576	0.37	0/2119
30	e	0.18	0/1571	0.38	0/2113
31	f	0.20	0/1434	0.47	1/1926 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	g	0.19	0/1315	0.48	0/1783
33	h	0.21	0/306	0.50	0/413
34	i	0.19	0/1152	0.38	0/1551
35	j	0.19	0/955	0.37	0/1279
36	k	0.20	0/1062	0.40	0/1413
37	l	0.21	0/1073	0.40	0/1433
38	m	0.20	0/958	0.43	0/1281
39	n	0.16	0/902	0.40	0/1209
40	o	0.19	0/929	0.40	0/1242
41	p	0.18	0/960	0.36	0/1278
42	q	0.20	0/829	0.51	0/1107
43	r	0.19	0/864	0.37	0/1156
44	s	0.17	0/744	0.38	0/994
45	t	0.19	0/787	0.48	0/1051
46	u	0.19	0/766	0.39	0/1025
47	v	0.17	0/589	0.39	0/780
48	w	0.16	0/635	0.37	0/848
49	x	0.19	0/502	0.38	0/667
50	y	0.18	0/453	0.38	0/605
51	z	0.15	0/450	0.33	0/599
52	A	0.26	1/36236 (0.0%)	0.34	0/56520
53	a	0.26	1/65651 (0.0%)	0.35	0/102413
54	4	0.17	0/488	0.39	0/649
55	Y	0.33	0/1665	0.62	0/2581
All	All	0.24	4/152850 (0.0%)	0.37	7/228641 (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
32	g	0	2
37	l	0	1
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	Z	75	C	C2'-C1'	8.69	1.66	1.53
28	c	136	PRO	CG-CD	-8.02	1.23	1.50
53	a	2069	G7M	O3'-P	5.40	1.61	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	A	527	G7M	O3'-P	5.20	1.61	1.56

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	c	136	PRO	N-CD-CG	-14.21	81.89	103.20
28	c	136	PRO	CA-CB-CG	-13.13	79.56	104.50
26	Z	75	C	C1'-C2'-O2'	7.70	119.96	108.40
28	c	136	PRO	CA-N-CD	-6.71	102.61	112.00
28	c	136	PRO	N-CA-CB	-6.00	97.97	103.31

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
32	g	46	ALA	Peptide
32	g	47	ASP	Peptide
37	l	137	4D4	Mainchain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	417	0	451	7	0
2	1	377	0	418	5	0
3	2	504	0	572	3	0
4	3	302	0	340	6	0
5	B	1753	0	1780	61	0
6	C	1624	0	1696	52	0
7	D	1643	0	1707	67	0
8	E	1152	0	1196	39	0
9	F	839	0	833	42	0
10	G	1203	0	1254	52	0
11	H	979	0	1031	39	0
12	I	1022	0	1070	45	0
13	J	786	0	828	48	0
14	K	877	0	882	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	L	957	0	1017	28	0
16	M	891	0	952	26	0
17	N	805	0	844	36	0
18	O	714	0	734	14	0
19	P	643	0	661	22	0
20	Q	641	0	682	16	0
21	R	544	0	565	23	0
22	S	668	0	693	24	0
23	T	670	0	719	21	0
24	U	589	0	629	17	0
25	X	322	0	162	5	0
26	Z	1623	0	825	28	0
27	b	2549	0	1291	33	0
28	c	2082	0	2154	33	0
29	d	1566	0	1618	22	0
30	e	1552	0	1619	21	0
31	f	1410	0	1444	41	0
32	g	1295	0	1332	41	0
33	h	303	0	327	6	0
34	i	1129	0	1162	12	0
35	j	946	0	1023	17	0
36	k	1053	0	1129	17	0
37	l	1075	0	1146	22	0
38	m	945	0	989	14	0
39	n	892	0	923	21	0
40	o	917	0	962	22	0
41	p	947	0	1019	12	0
42	q	816	0	839	13	0
43	r	857	0	922	19	0
44	s	738	0	807	10	0
45	t	779	0	831	21	0
46	u	753	0	780	21	0
47	v	582	0	593	5	0
48	w	625	0	652	5	0
49	x	501	0	531	11	0
50	y	449	0	488	6	0
51	z	444	0	458	7	0
52	A	32612	0	16432	647	0
53	a	59130	0	29763	677	0
54	4	480	0	478	21	0
55	Y	1518	0	776	45	0
56	3	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	4	1	0	0	0	0
57	A	90	0	0	0	0
57	C	1	0	0	0	0
57	N	1	0	0	0	0
57	Q	1	0	0	0	0
57	Z	1	0	0	0	0
57	a	219	0	0	0	0
57	b	5	0	0	0	0
57	d	1	0	0	0	0
57	z	1	0	0	0	0
58	Z	10	0	10	0	0
59	a	9	0	0	0	0
59	c	1	0	0	0	0
60	A	42	0	45	1	0
61	A	10	0	19	0	0
61	a	130	0	247	16	0
62	a	14	0	26	3	0
63	Y	17	0	0	0	0
64	0	2	0	0	0	0
64	1	15	0	0	1	0
64	2	19	0	0	0	0
64	3	4	0	0	0	0
64	A	2	0	0	0	0
64	Y	2	0	0	0	0
64	Z	4	0	0	1	0
64	a	2993	0	0	61	0
64	b	41	0	0	2	0
64	c	84	0	0	1	0
64	d	36	0	0	0	0
64	e	29	0	0	0	0
64	h	1	0	0	0	0
64	i	13	0	0	1	0
64	j	14	0	0	0	0
64	k	34	0	0	2	0
64	l	25	0	0	0	0
64	m	23	0	0	1	0
64	o	13	0	0	1	0
64	p	24	0	0	3	0
64	q	13	0	0	0	0
64	r	26	0	0	1	0
64	s	5	0	0	0	0
64	t	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
64	u	3	0	0	0	0
64	v	11	0	0	0	0
64	w	12	0	0	0	0
64	x	1	0	0	0	0
64	z	24	0	0	0	0
All	All	145519	0	95376	2328	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

The worst 5 of 2328 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:R:9:LYS:HG3	21:R:10:PHE:H	1.17	1.04
11:H:2:SER:N	52:A:823:C:HO2'	1.67	0.93
52:A:1086:U:H3	52:A:1099:G:H22	1.14	0.91
55:Y:52:G:N2	55:Y:62:C:O2	2.05	0.90
26:Z:76:8AN:O2P	64:Z:201:HOH:O	1.91	0.88

There are no symmetry-related clashes.

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%)	60 (97%)	2 (3%)	0	100	100
4	3	36/38 (95%)	36 (100%)	0	0	100	100
5	B	222/241 (92%)	204 (92%)	18 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	C	204/233 (88%)	193 (95%)	11 (5%)	0	100	100
7	D	203/206 (98%)	196 (97%)	7 (3%)	0	100	100
8	E	154/167 (92%)	147 (96%)	7 (4%)	0	100	100
9	F	101/135 (75%)	91 (90%)	10 (10%)	0	100	100
10	G	151/179 (84%)	138 (91%)	13 (9%)	0	100	100
11	H	127/130 (98%)	123 (97%)	4 (3%)	0	100	100
12	I	125/130 (96%)	117 (94%)	8 (6%)	0	100	100
13	J	96/103 (93%)	93 (97%)	2 (2%)	1 (1%)	12	15
14	K	113/129 (88%)	109 (96%)	4 (4%)	0	100	100
15	L	120/124 (97%)	113 (94%)	7 (6%)	0	100	100
16	M	113/118 (96%)	104 (92%)	9 (8%)	0	100	100
17	N	98/101 (97%)	93 (95%)	5 (5%)	0	100	100
18	O	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
19	P	79/82 (96%)	72 (91%)	7 (9%)	0	100	100
20	Q	77/84 (92%)	75 (97%)	2 (3%)	0	100	100
21	R	64/75 (85%)	57 (89%)	7 (11%)	0	100	100
22	S	82/92 (89%)	78 (95%)	4 (5%)	0	100	100
23	T	84/87 (97%)	82 (98%)	2 (2%)	0	100	100
24	U	68/71 (96%)	68 (100%)	0	0	100	100
28	c	269/273 (98%)	262 (97%)	7 (3%)	0	100	100
29	d	206/209 (99%)	197 (96%)	8 (4%)	1 (0%)	24	31
30	e	199/201 (99%)	192 (96%)	7 (4%)	0	100	100
31	f	175/179 (98%)	162 (93%)	13 (7%)	0	100	100
32	g	171/177 (97%)	146 (85%)	24 (14%)	1 (1%)	21	27
33	h	39/149 (26%)	34 (87%)	5 (13%)	0	100	100
34	i	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
35	j	121/123 (98%)	118 (98%)	3 (2%)	0	100	100
36	k	142/144 (99%)	137 (96%)	5 (4%)	0	100	100
37	l	132/136 (97%)	126 (96%)	6 (4%)	0	100	100
38	m	116/127 (91%)	110 (95%)	6 (5%)	0	100	100
39	n	114/117 (97%)	111 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	o	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
41	p	115/118 (98%)	115 (100%)	0	0	100	100
42	q	101/103 (98%)	96 (95%)	5 (5%)	0	100	100
43	r	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
44	s	91/100 (91%)	86 (94%)	5 (6%)	0	100	100
45	t	100/104 (96%)	91 (91%)	9 (9%)	0	100	100
46	u	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
47	v	75/85 (88%)	73 (97%)	2 (3%)	0	100	100
48	w	75/78 (96%)	75 (100%)	0	0	100	100
49	x	60/63 (95%)	58 (97%)	2 (3%)	0	100	100
50	y	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
51	z	54/57 (95%)	54 (100%)	0	0	100	100
54	4	56/70 (80%)	53 (95%)	3 (5%)	0	100	100
All	All	5477/5913 (93%)	5222 (95%)	252 (5%)	3 (0%)	49	60

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	J	57	VAL
32	g	47	ASP
29	d	149	ASN

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%)	35 (92%)	3 (8%)	11	15
3	2	51/52 (98%)	51 (100%)	0	100	100
4	3	34/34 (100%)	33 (97%)	1 (3%)	37	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	B	186/199 (94%)	168 (90%)	18 (10%)	8	10
6	C	170/190 (90%)	159 (94%)	11 (6%)	15	22
7	D	172/173 (99%)	167 (97%)	5 (3%)	37	55
8	E	119/126 (94%)	115 (97%)	4 (3%)	32	49
9	F	90/116 (78%)	81 (90%)	9 (10%)	7	9
10	G	126/147 (86%)	122 (97%)	4 (3%)	34	51
11	H	104/105 (99%)	98 (94%)	6 (6%)	18	26
12	I	105/107 (98%)	96 (91%)	9 (9%)	10	13
13	J	86/90 (96%)	80 (93%)	6 (7%)	14	19
14	K	89/98 (91%)	81 (91%)	8 (9%)	9	12
15	L	102/103 (99%)	95 (93%)	7 (7%)	14	20
16	M	93/96 (97%)	90 (97%)	3 (3%)	34	51
17	N	83/84 (99%)	79 (95%)	4 (5%)	23	35
18	O	76/77 (99%)	74 (97%)	2 (3%)	40	59
19	P	65/65 (100%)	63 (97%)	2 (3%)	35	52
20	Q	73/78 (94%)	67 (92%)	6 (8%)	10	14
21	R	57/65 (88%)	54 (95%)	3 (5%)	20	30
22	S	72/79 (91%)	65 (90%)	7 (10%)	8	10
23	T	65/66 (98%)	62 (95%)	3 (5%)	24	36
24	U	60/61 (98%)	57 (95%)	3 (5%)	22	33
28	c	216/218 (99%)	212 (98%)	4 (2%)	50	69
29	d	163/163 (100%)	157 (96%)	6 (4%)	30	45
30	e	165/165 (100%)	161 (98%)	4 (2%)	43	62
31	f	148/150 (99%)	139 (94%)	9 (6%)	17	24
32	g	134/138 (97%)	126 (94%)	8 (6%)	17	25
33	h	32/114 (28%)	30 (94%)	2 (6%)	16	23
34	i	116/116 (100%)	113 (97%)	3 (3%)	40	59
35	j	104/104 (100%)	101 (97%)	3 (3%)	37	55
36	k	103/103 (100%)	99 (96%)	4 (4%)	28	43
37	l	107/107 (100%)	105 (98%)	2 (2%)	50	69
38	m	98/103 (95%)	96 (98%)	2 (2%)	48	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	n	86/87 (99%)	83 (96%)	3 (4%)	32	48
40	o	99/100 (99%)	96 (97%)	3 (3%)	36	53
41	p	89/90 (99%)	89 (100%)	0	100	100
42	q	84/84 (100%)	82 (98%)	2 (2%)	43	62
43	r	93/93 (100%)	92 (99%)	1 (1%)	65	81
44	s	80/84 (95%)	77 (96%)	3 (4%)	29	44
45	t	83/85 (98%)	80 (96%)	3 (4%)	31	47
46	u	78/78 (100%)	76 (97%)	2 (3%)	40	59
47	v	58/63 (92%)	58 (100%)	0	100	100
48	w	67/68 (98%)	64 (96%)	3 (4%)	24	37
49	x	54/55 (98%)	52 (96%)	2 (4%)	30	45
50	y	48/49 (98%)	48 (100%)	0	100	100
51	z	47/48 (98%)	47 (100%)	0	100	100
54	4	55/62 (89%)	53 (96%)	2 (4%)	31	47
All	All	4569/4825 (95%)	4374 (96%)	195 (4%)	27	39

5 of 195 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
22	S	39	THR
31	f	72	LYS
23	T	35	VAL
29	d	105	LYS
32	g	76	VAL

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

Mol	Chain	Res	Type
35	j	29	HIS
48	w	36	HIS
35	j	88	ASN
40	o	41	GLN
49	x	39	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
25	X	14/28 (50%)	4 (28%)	1 (7%)
26	Z	74/77 (96%)	23 (31%)	1 (1%)
27	b	118/120 (98%)	12 (10%)	0
52	A	1516/1542 (98%)	270 (17%)	5 (0%)
53	a	2749/2904 (94%)	334 (12%)	0
55	Y	66/71 (92%)	37 (56%)	8 (12%)
All	All	4537/4742 (95%)	680 (14%)	15 (0%)

5 of 680 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
25	X	20	A
25	X	24	A
25	X	25	C
25	X	27	A
26	Z	6	G

5 of 15 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
55	Y	10	G
55	Y	48	G
55	Y	17	G
55	Y	71	U
55	Y	43	G

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

42 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
53	2MG	a	1835	53	23,26,27	1.26	4 (17%)	33,38,41	2.20	6 (18%)
53	6MZ	a	1618	53	22,25,26	1.51	5 (22%)	29,36,39	2.16	10 (34%)
52	2MG	A	1207	52	23,26,27	1.30	4 (17%)	33,38,41	2.27	9 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
52	2MG	A	1516	52	23,26,27	1.22	3 (13%)	33,38,41	2.20	8 (24%)
53	PSU	a	2457	53	18,21,22	1.36	3 (16%)	21,30,33	2.09	3 (14%)
53	PSU	a	746	53,57	18,21,22	1.37	3 (16%)	21,30,33	1.95	4 (19%)
29	MEQ	d	150	29	8,9,10	0.50	0	5,10,12	0.27	0
53	6MZ	a	2030	53	22,25,26	1.45	5 (22%)	29,36,39	2.37	11 (37%)
52	UR3	A	1498	52	19,22,23	0.99	1 (5%)	26,32,35	1.75	4 (15%)
52	4OC	A	1402	52	20,23,24	0.75	0	25,32,35	0.91	1 (4%)
53	3TD	a	1915	53	19,22,23	1.63	5 (26%)	23,32,35	2.07	4 (17%)
53	G7M	a	2069	53	23,26,27	1.51	3 (13%)	34,39,42	1.74	5 (14%)
53	H2U	a	2449	53	18,21,22	1.07	2 (11%)	19,30,33	1.00	2 (10%)
26	8AN	Z	76	58,57,26	21,24,25	0.90	1 (4%)	26,35,38	0.61	0
52	PSU	A	516	57,52	18,21,22	1.36	2 (11%)	21,30,33	2.06	4 (19%)
15	D2T	L	89	15	8,9,10	2.53	3 (37%)	6,11,13	1.54	1 (16%)
53	5MU	a	747	53	19,22,23	1.37	5 (26%)	27,32,35	2.10	9 (33%)
53	PSU	a	2605	53	18,21,22	1.39	3 (16%)	21,30,33	2.02	5 (23%)
53	OMG	a	2251	53,26,59	23,26,27	1.20	3 (13%)	32,38,41	2.04	6 (18%)
52	G7M	A	527	52	23,26,27	1.55	3 (13%)	34,39,42	1.73	5 (14%)
53	OMU	a	2552	53,57	19,22,23	1.23	3 (15%)	25,31,34	1.85	5 (20%)
53	PSU	a	2504	53,59	18,21,22	1.37	2 (11%)	21,30,33	2.02	3 (14%)
52	MA6	A	1519	52	23,26,27	1.54	5 (21%)	33,38,41	2.10	10 (30%)
53	5MU	a	1939	53	19,22,23	1.39	5 (26%)	27,32,35	2.16	6 (22%)
53	PSU	a	1911	53	18,21,22	1.31	2 (11%)	21,30,33	2.08	3 (14%)
53	5MC	a	1962	53	19,22,23	1.54	3 (15%)	26,32,35	1.18	2 (7%)
52	5MC	A	1407	52	19,22,23	1.67	3 (15%)	26,32,35	1.17	3 (11%)
14	IAS	K	119	14	6,7,8	1.42	1 (16%)	3,8,10	1.30	1 (33%)
52	MA6	A	1518	52	23,26,27	1.52	4 (17%)	33,38,41	2.10	10 (30%)
53	2MA	a	2503	53,57,59	22,25,26	1.49	4 (18%)	32,37,40	2.33	8 (25%)
52	2MG	A	966	52	23,26,27	1.24	4 (17%)	33,38,41	2.20	7 (21%)
52	5MC	A	967	52	19,22,23	1.54	3 (15%)	26,32,35	1.11	2 (7%)
55	8AN	Y	76	53,55,63	21,24,25	1.61	4 (19%)	26,35,38	2.26	7 (26%)
53	PSU	a	955	53	18,21,22	1.34	2 (11%)	21,30,33	2.09	4 (19%)
37	MS6	l	138	37	5,7,8	0.22	0	2,7,9	0.12	0
53	PSU	a	1917	53	18,21,22	1.34	2 (11%)	21,30,33	2.15	5 (23%)
53	1MG	a	745	53	23,26,27	1.19	3 (13%)	33,39,42	1.75	5 (15%)
53	PSU	a	2604	53	18,21,22	1.37	3 (16%)	21,30,33	1.99	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
53	OMC	a	2498	53,57	19,22,23	0.78	0	25,31,34	0.86	1 (4%)
53	PSU	a	2580	53	18,21,22	1.43	3 (16%)	21,30,33	2.01	4 (19%)
37	4D4	l	137	37	9,11,12	2.04	2 (22%)	7,13,15	0.89	0
53	2MG	a	2445	53	23,26,27	1.26	4 (17%)	33,38,41	2.17	7 (21%)

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
53	2MG	a	1835	53	-	0/9/27/28	0/3/3/3
53	6MZ	a	1618	53	-	0/9/27/28	0/3/3/3
52	2MG	A	1207	52	-	1/9/27/28	0/3/3/3
52	2MG	A	1516	52	-	0/9/27/28	0/3/3/3
53	PSU	a	2457	53	-	0/7/25/26	0/2/2/2
53	PSU	a	746	53,57	-	2/7/25/26	0/2/2/2
29	MEQ	d	150	29	-	2/8/9/11	-
53	6MZ	a	2030	53	-	2/9/27/28	0/3/3/3
52	UR3	A	1498	52	-	0/7/25/26	0/2/2/2
52	4OC	A	1402	52	-	0/9/29/30	0/2/2/2
53	3TD	a	1915	53	-	0/7/25/26	0/2/2/2
53	G7M	a	2069	53	-	0/7/25/26	0/3/3/3
53	H2U	a	2449	53	-	0/7/38/39	0/2/2/2
26	8AN	Z	76	58,57,26	-	3/7/25/26	0/3/3/3
52	PSU	A	516	57,52	-	0/7/25/26	0/2/2/2
15	D2T	L	89	15	-	4/7/12/14	-
53	5MU	a	747	53	-	0/7/25/26	0/2/2/2
53	PSU	a	2605	53	-	0/7/25/26	0/2/2/2
53	OMG	a	2251	53,26,59	-	0/9/27/28	0/3/3/3
52	G7M	A	527	52	-	1/7/25/26	0/3/3/3
53	OMU	a	2552	53,57	-	0/9/27/28	0/2/2/2
53	PSU	a	2504	53,59	-	0/7/25/26	0/2/2/2
52	MA6	A	1519	52	-	2/11/29/30	0/3/3/3
53	5MU	a	1939	53	-	0/7/25/26	0/2/2/2
53	PSU	a	1911	53	-	0/7/25/26	0/2/2/2
53	5MC	a	1962	53	-	1/7/25/26	0/2/2/2
52	5MC	A	1407	52	-	0/7/25/26	0/2/2/2
14	IAS	K	119	14	-	2/7/7/8	-
52	MA6	A	1518	52	-	0/11/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	2MA	a	2503	53,57,59	-	1/7/25/26	0/3/3/3
52	2MG	A	966	52	-	0/9/27/28	0/3/3/3
52	5MC	A	967	52	-	0/7/25/26	0/2/2/2
55	8AN	Y	76	53,55,63	-	1/7/25/26	0/3/3/3
53	PSU	a	955	53	-	0/7/25/26	0/2/2/2
37	MS6	l	138	37	-	0/4/6/8	-
53	PSU	a	1917	53	-	0/7/25/26	0/2/2/2
53	1MG	a	745	53	-	0/7/25/26	0/3/3/3
53	PSU	a	2604	53	-	0/7/25/26	0/2/2/2
53	OMC	a	2498	53,57	-	1/9/27/28	0/2/2/2
53	PSU	a	2580	53	-	0/7/25/26	0/2/2/2
37	4D4	l	137	37	-	0/11/12/14	-
53	2MG	a	2445	53	-	1/9/27/28	0/3/3/3

The worst 5 of 120 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	A	1407	5MC	C5-C4	5.96	1.48	1.44
52	A	967	5MC	C5-C4	5.45	1.48	1.44
53	a	1962	5MC	C5-C4	5.42	1.48	1.44
15	L	89	D2T	CB-CA	5.22	1.56	1.54
53	a	2069	G7M	C5-N7	-4.86	1.33	1.39

The worst 5 of 195 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	a	2503	2MA	C5-C4-N3	-7.97	118.78	127.18
53	a	1915	3TD	N1-C2-N3	7.92	121.89	116.13
52	A	1207	2MG	C2-N3-C4	7.35	121.19	112.00
53	a	2445	2MG	C2-N3-C4	7.32	121.16	112.00
52	A	966	2MG	C2-N3-C4	7.32	121.16	112.00

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	L	89	D2T	CA-CB-CG-OD1
15	L	89	D2T	CA-CB-CG-OD2
26	Z	76	8AN	O4'-C4'-C5'-O5'
52	A	1207	2MG	N3-C2-N2-CM2
26	Z	76	8AN	C3'-C4'-C5'-O5'

There are no ring outliers.

16 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	A	1207	2MG	2	0
52	A	1516	2MG	1	0
29	d	150	MEQ	1	0
53	a	2030	6MZ	2	0
52	A	1498	UR3	1	0
52	A	1402	4OC	2	0
53	a	1915	3TD	1	0
26	Z	76	8AN	5	0
52	A	516	PSU	1	0
52	A	1519	MA6	1	0
53	a	1939	5MU	1	0
14	K	119	IAS	1	0
52	A	1518	MA6	1	0
52	A	967	5MC	1	0
53	a	1917	PSU	2	0
53	a	745	1MG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 350 ligands modelled in this entry, 332 are monoatomic - leaving 18 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	$\# Z > 2$
61	SPD	a	3213	-	9,9,9	0.33	0	8,8,8	0.69	0
61	SPD	a	3214	-	9,9,9	0.33	0	8,8,8	0.78	0
61	SPD	a	3217	-	9,9,9	0.34	0	8,8,8	0.55	0
61	SPD	a	3215	-	9,9,9	0.29	0	8,8,8	0.81	0
61	SPD	a	3221	-	9,9,9	0.34	0	8,8,8	0.85	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
61	SPD	a	3209	-	9,9,9	0.33	0	8,8,8	0.77	0
60	PAR	A	1601	-	44,45,45	0.53	0	63,67,67	0.93	3 (4%)
63	A1B71	Y	101	55	16,16,17	0.90	0	16,20,22	2.14	3 (18%)
61	SPD	A	1691	-	9,9,9	0.33	0	8,8,8	0.78	0
61	SPD	a	3211	-	9,9,9	0.34	0	8,8,8	0.90	0
61	SPD	a	3216	-	9,9,9	0.34	0	8,8,8	0.72	0
61	SPD	a	3212	-	9,9,9	0.35	0	8,8,8	0.79	0
61	SPD	a	3208	-	9,9,9	0.34	0	8,8,8	0.63	0
62	SPM	a	3220	-	13,13,13	0.35	0	12,12,12	0.74	0
61	SPD	a	3218	-	9,9,9	0.34	0	8,8,8	0.73	0
61	SPD	a	3219	-	9,9,9	0.35	0	8,8,8	0.66	0
58	FME	Z	101	26	8,9,10	0.99	0	8,9,11	1.10	1 (12%)
61	SPD	a	3210	-	9,9,9	0.34	0	8,8,8	0.64	0

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
61	SPD	a	3213	-	-	4/7/7/7	-
61	SPD	a	3214	-	-	3/7/7/7	-
61	SPD	a	3217	-	-	4/7/7/7	-
61	SPD	a	3215	-	-	4/7/7/7	-
61	SPD	a	3221	-	-	3/7/7/7	-
61	SPD	a	3209	-	-	3/7/7/7	-
60	PAR	A	1601	-	-	3/18/94/94	0/4/4/4
63	A1B71	Y	101	55	-	1/17/17/19	-
61	SPD	A	1691	-	-	5/7/7/7	-
61	SPD	a	3211	-	-	4/7/7/7	-
61	SPD	a	3216	-	-	4/7/7/7	-
61	SPD	a	3212	-	-	1/7/7/7	-
61	SPD	a	3208	-	-	5/7/7/7	-
62	SPM	a	3220	-	-	4/11/11/11	-
61	SPD	a	3218	-	-	2/7/7/7	-
61	SPD	a	3219	-	-	3/7/7/7	-
58	FME	Z	101	26	-	3/7/9/11	-
61	SPD	a	3210	-	-	2/7/7/7	-

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
63	Y	101	A1B71	O10-C09-N08	5.71	118.11	110.00
63	Y	101	A1B71	O15-C09-N08	-3.98	118.94	124.93
63	Y	101	A1B71	O01-C02-C03	-3.51	117.21	125.24
60	A	1601	PAR	C22-C12-C62	-2.37	106.54	110.08
60	A	1601	PAR	C13-O52-C52	-2.25	112.64	117.98

There are no chirality outliers.

5 of 58 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	Z	101	FME	N-CA-CB-CG
58	Z	101	FME	C-CA-CB-CG
60	A	1601	PAR	C44-C54-C64-N64
60	A	1601	PAR	O54-C54-C64-N64
61	a	3212	SPD	C2-C3-C4-C5

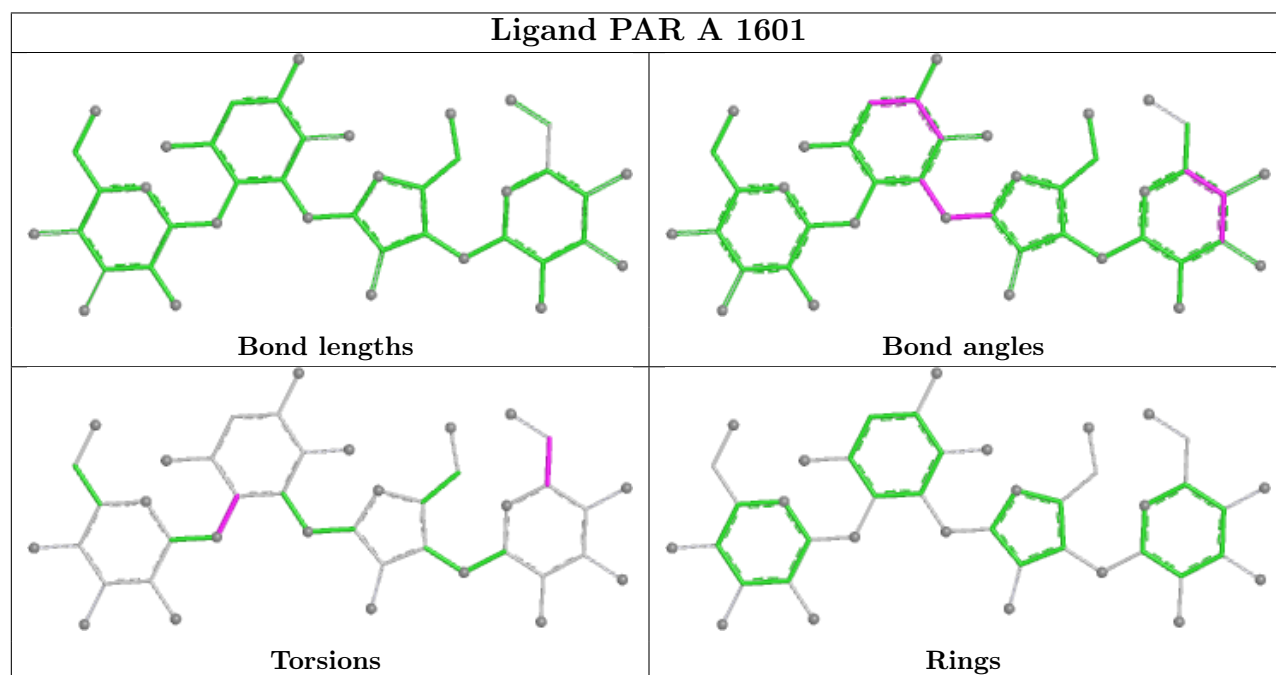
There are no ring outliers.

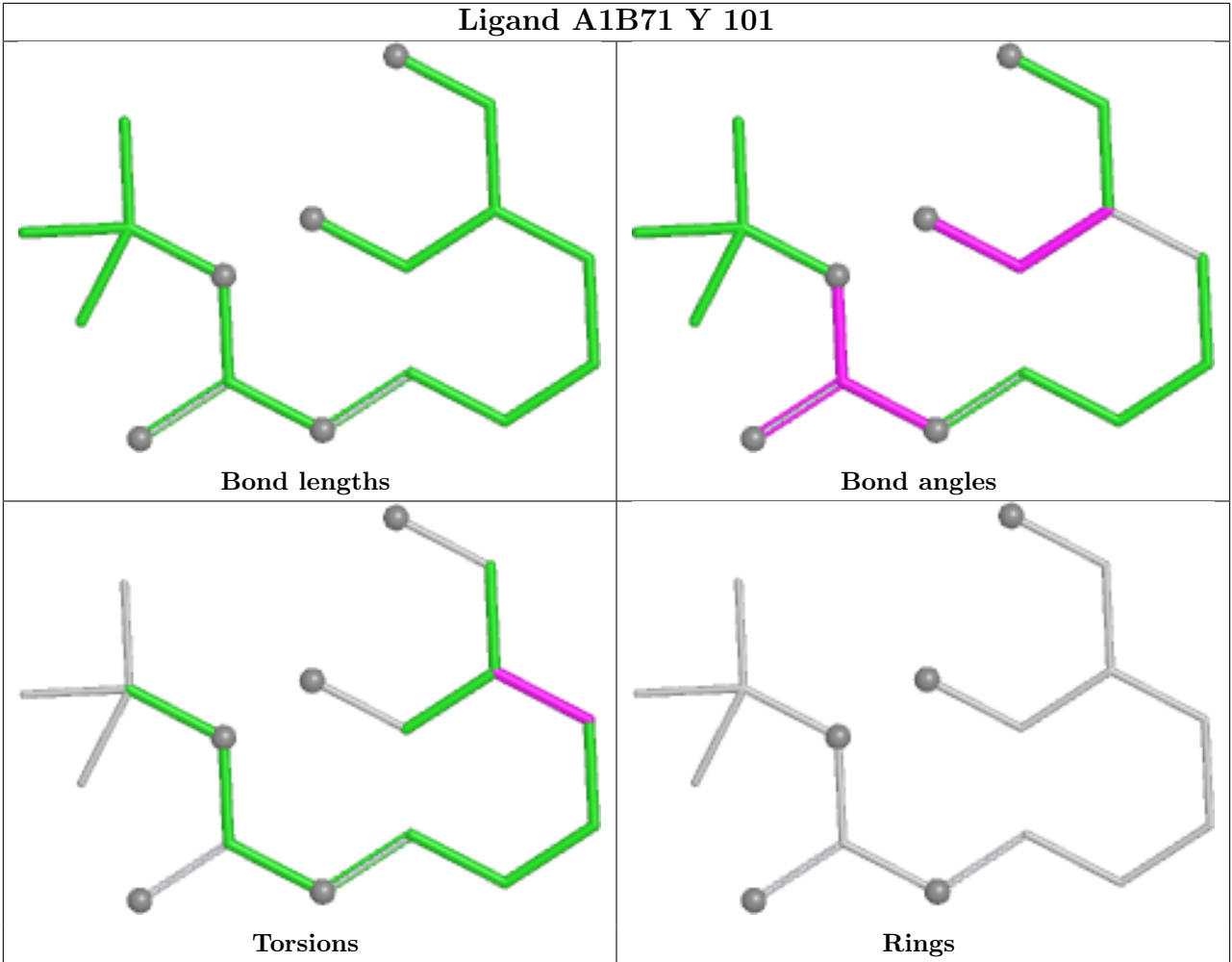
12 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
61	a	3213	SPD	1	0
61	a	3214	SPD	2	0
61	a	3217	SPD	3	0
61	a	3215	SPD	1	0
61	a	3221	SPD	1	0
61	a	3209	SPD	1	0
60	A	1601	PAR	1	0
61	a	3216	SPD	2	0
61	a	3212	SPD	1	0
61	a	3208	SPD	2	0
62	a	3220	SPM	3	0
61	a	3218	SPD	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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
55	Y	5

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Y	15:C	O3'	17:G	P	5.81
1	Y	45:C	O3'	47:A	P	5.36
1	Y	13:C	O3'	15:C	P	5.22

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Y	66:G	O3'	67:U	P	4.34
1	Y	7:C	O3'	10:G	P	3.06

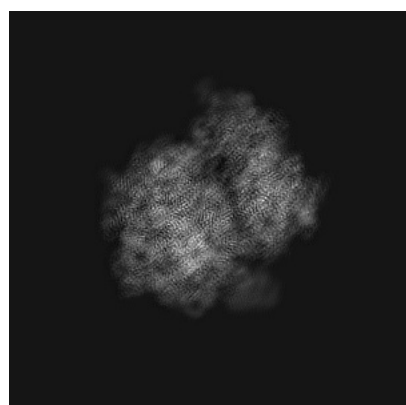
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-70050. These allow visual inspection of the internal detail of the map and identification of artifacts.

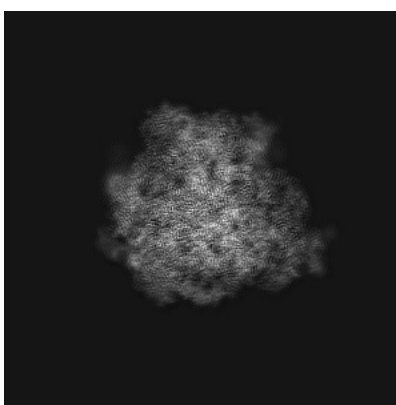
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

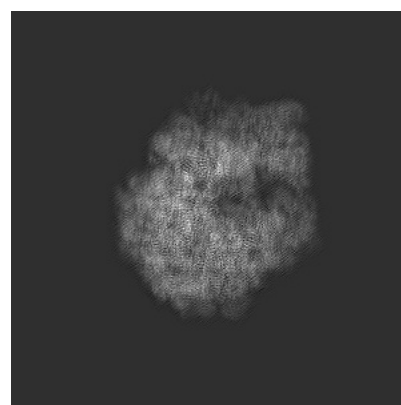
6.1.1 Primary map



X



Y

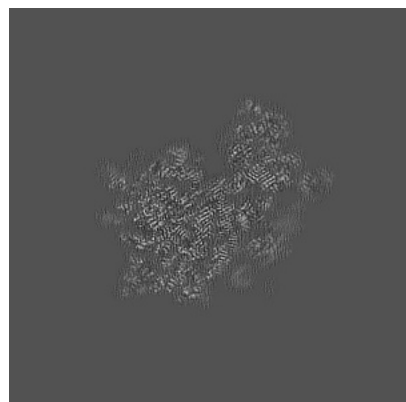


Z

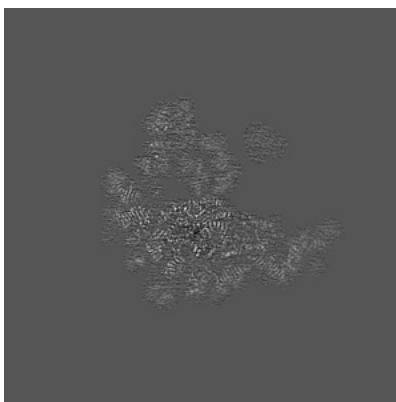
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

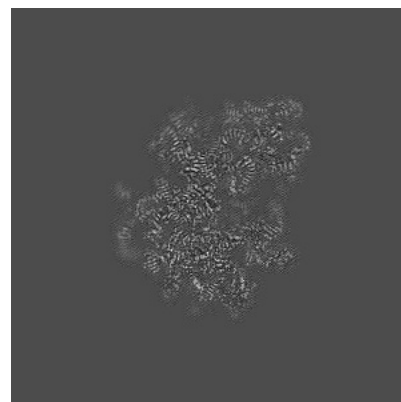
6.2.1 Primary map



X Index: 256



Y Index: 256

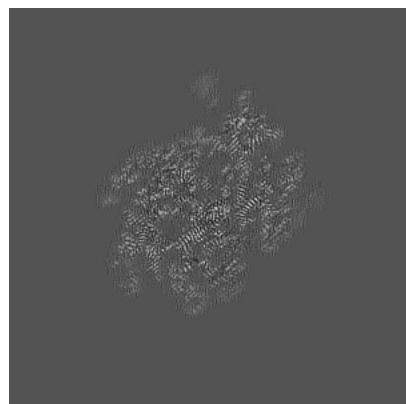


Z Index: 256

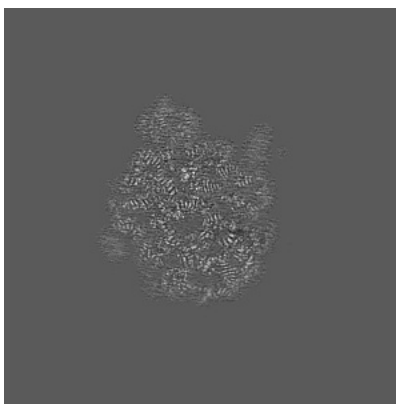
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

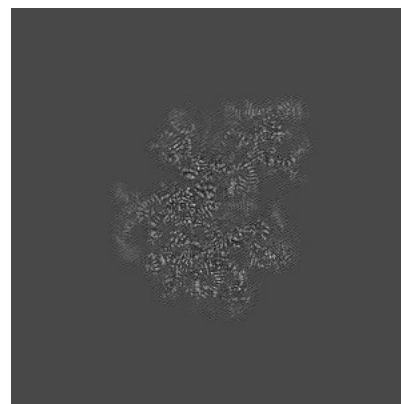
6.3.1 Primary map



X Index: 226



Y Index: 219

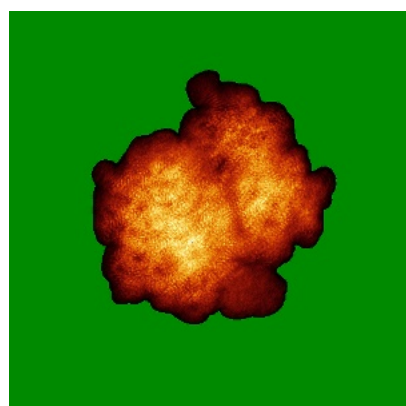


Z Index: 252

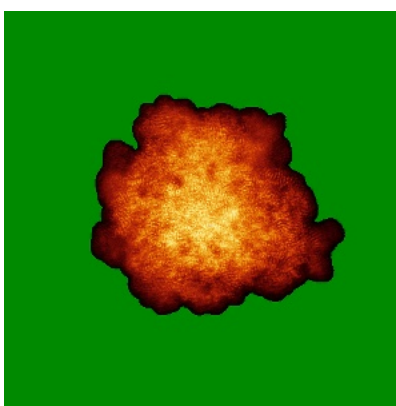
The images above show the largest variance slices of the map in three orthogonal directions.

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

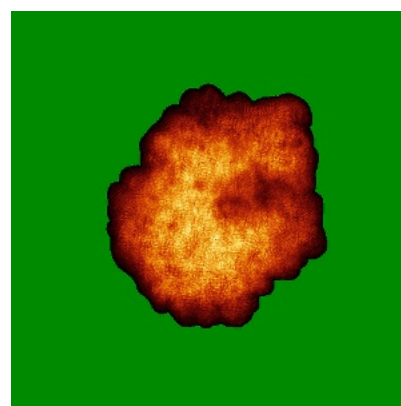
6.4.1 Primary map



X



Y

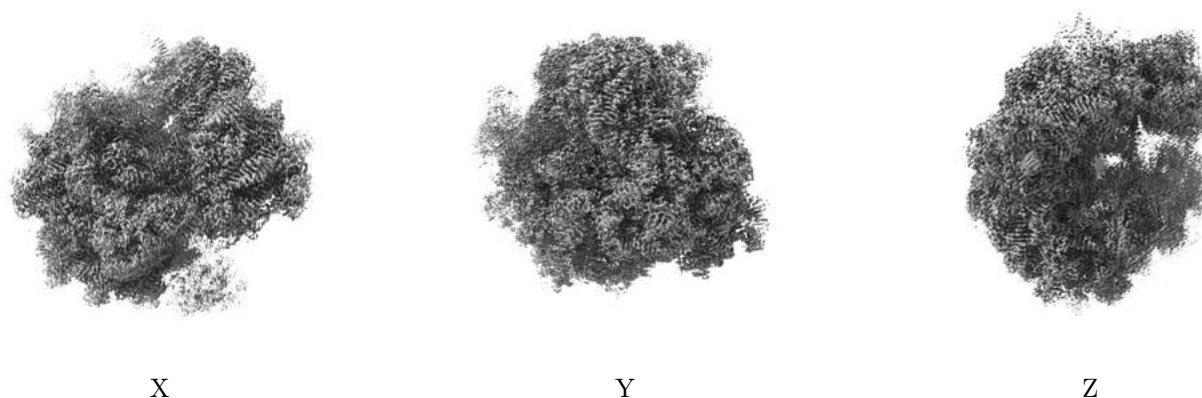


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0267. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

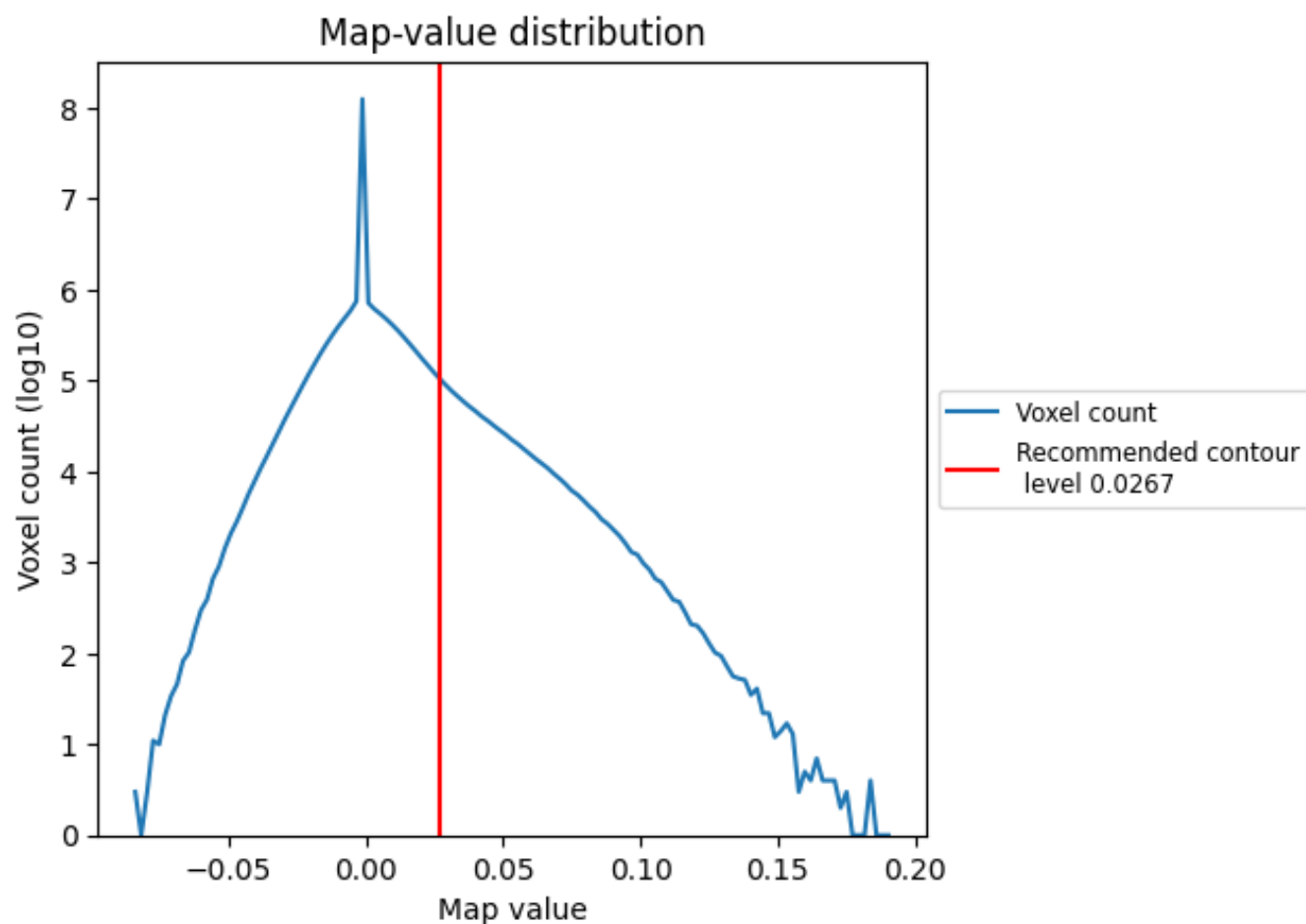
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

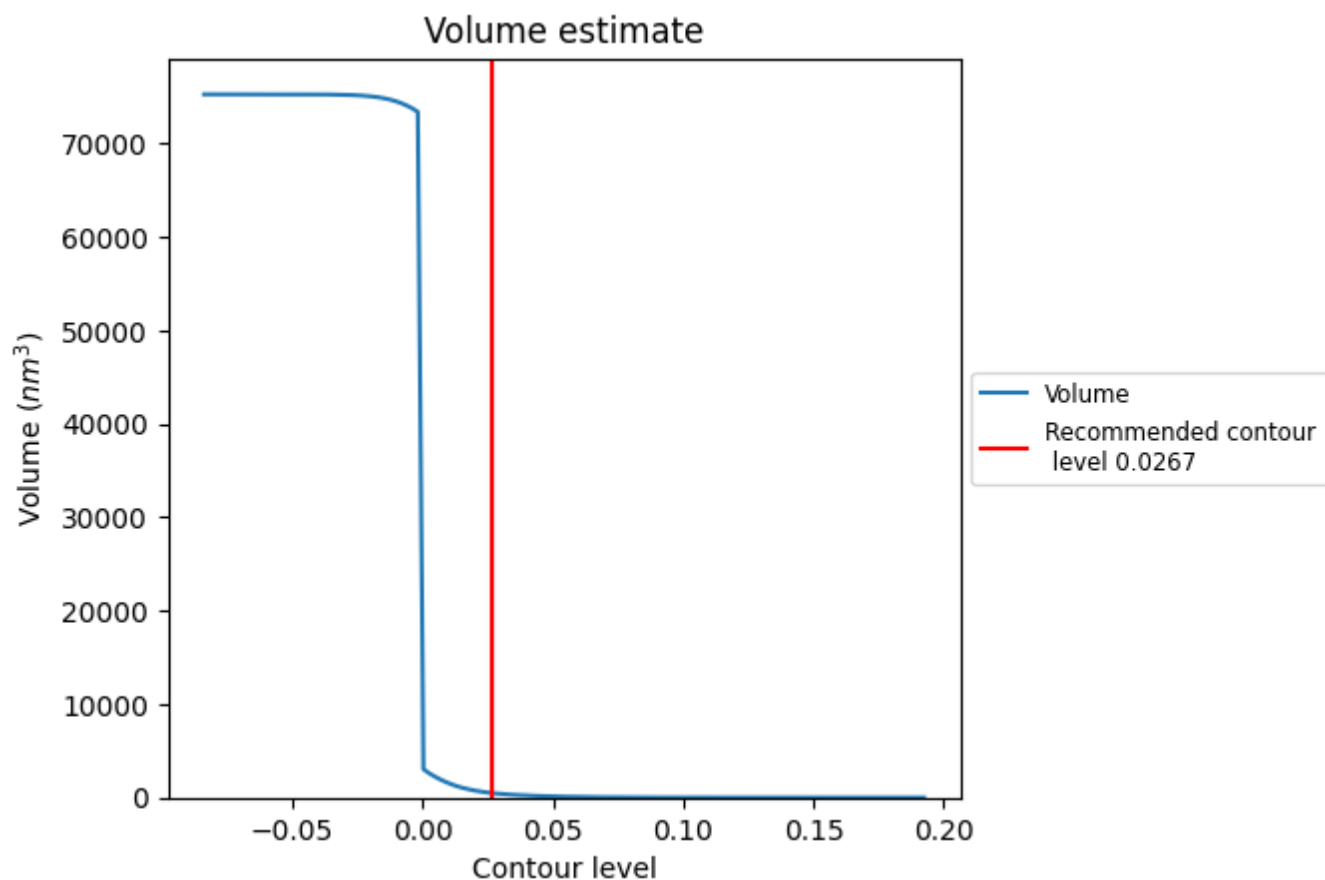
This section contains the results of statistical analysis of the map.

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.

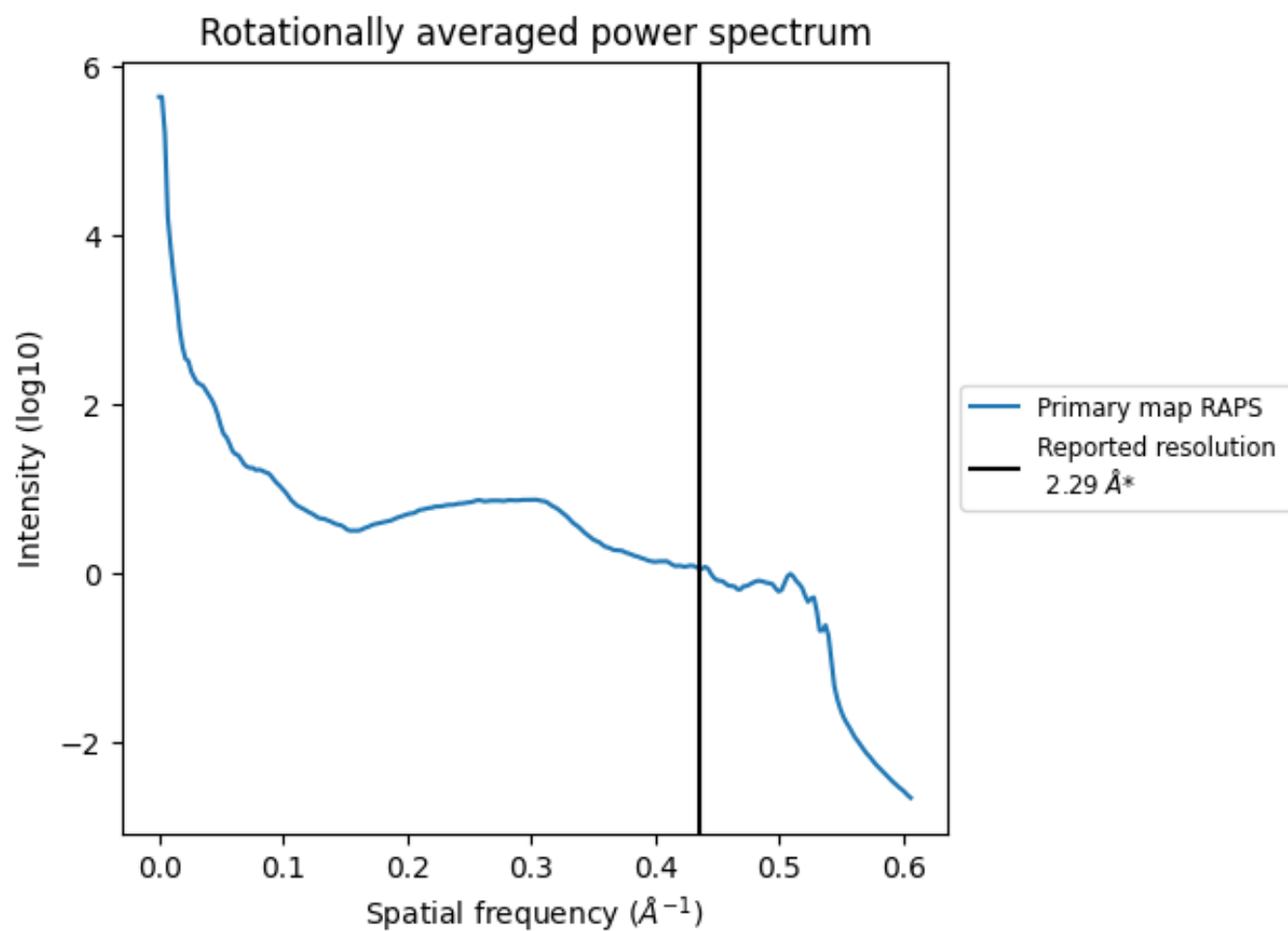
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 480 nm^3 ; this corresponds to an approximate mass of 434 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 ⓘ

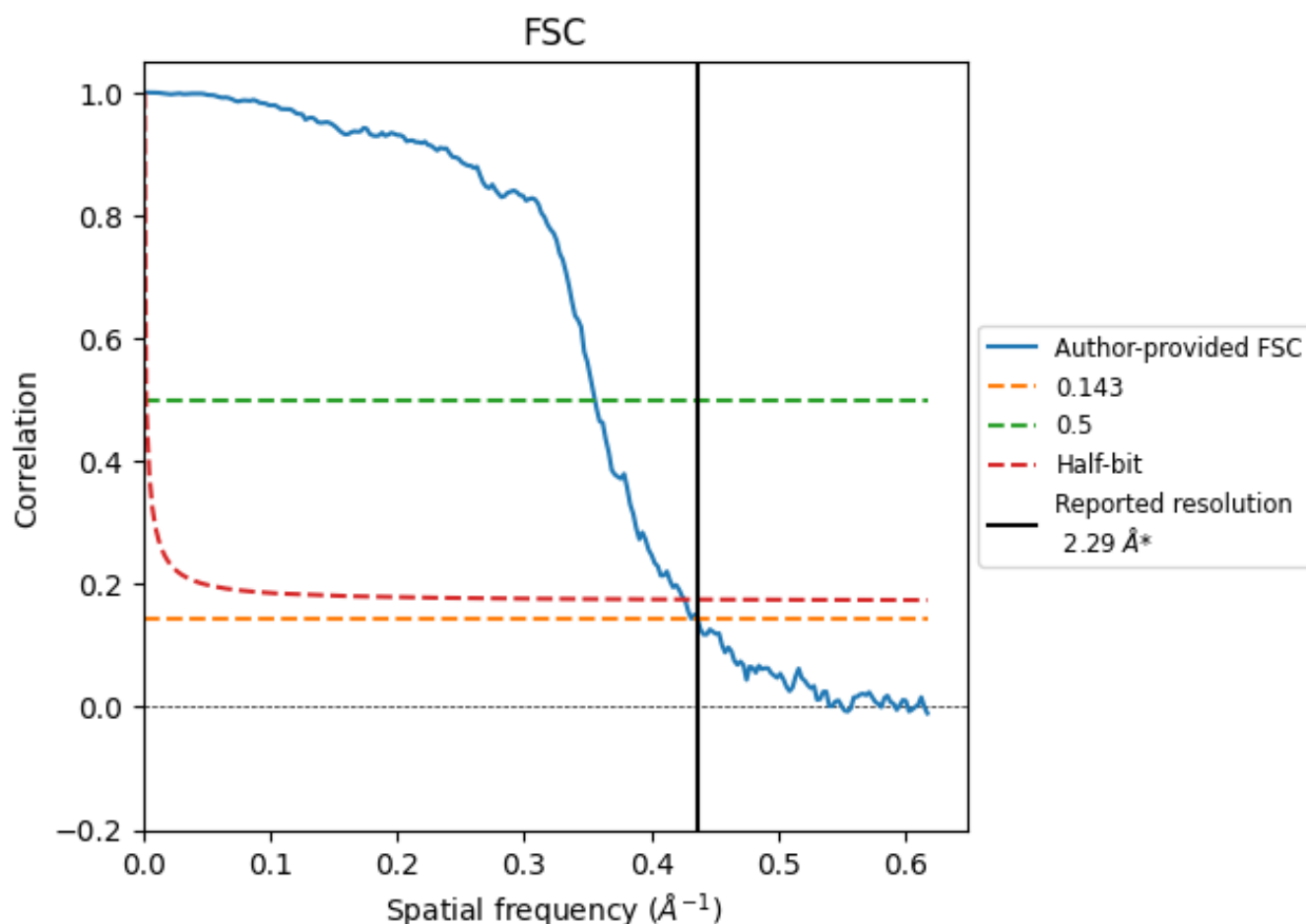


*Reported resolution corresponds to spatial frequency of 0.437 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.437 Å⁻¹

8.2 Resolution estimates [i](#)

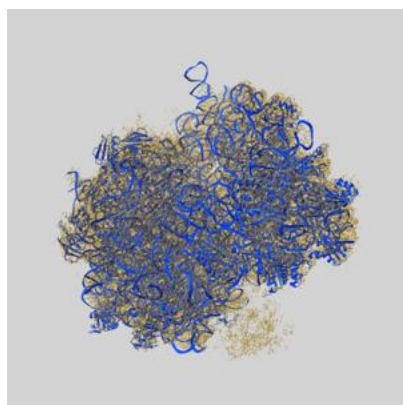
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.29	-	-
Author-provided FSC curve	2.29	2.81	2.35
Unmasked-calculated*	-	-	-

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

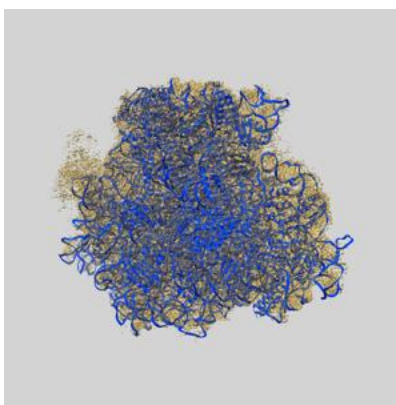
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-70050 and PDB model 9O2X. Per-residue inclusion information can be found in [section 3](#) on [page 20](#).

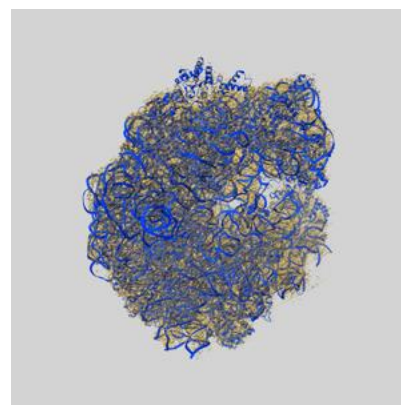
9.1 Map-model overlay [i](#)



X



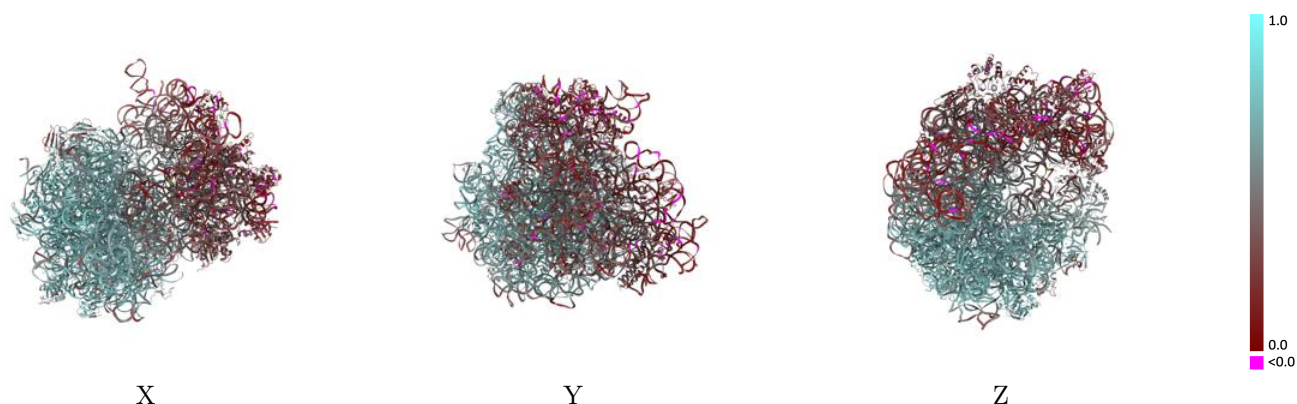
Y



Z

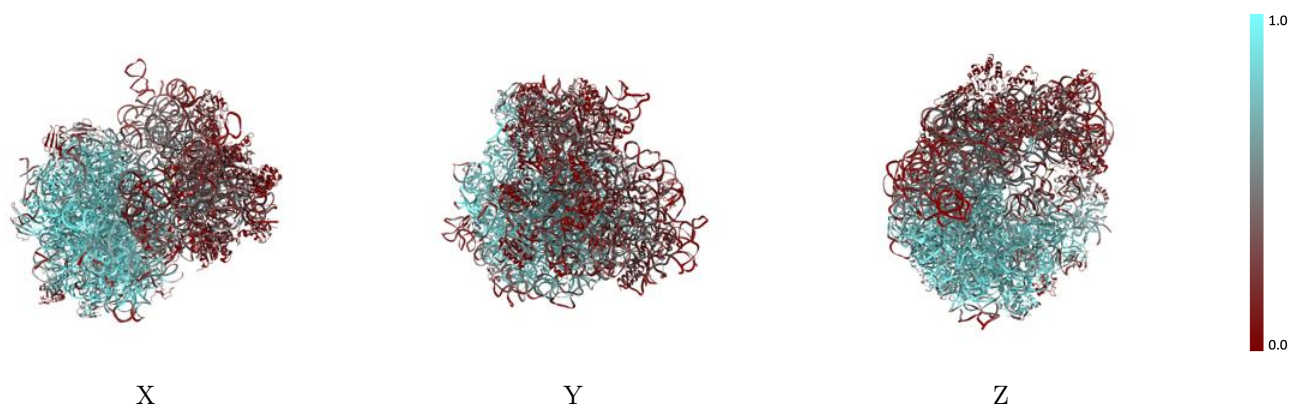
The images above show the 3D surface view of the map at the recommended contour level 0.0267 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



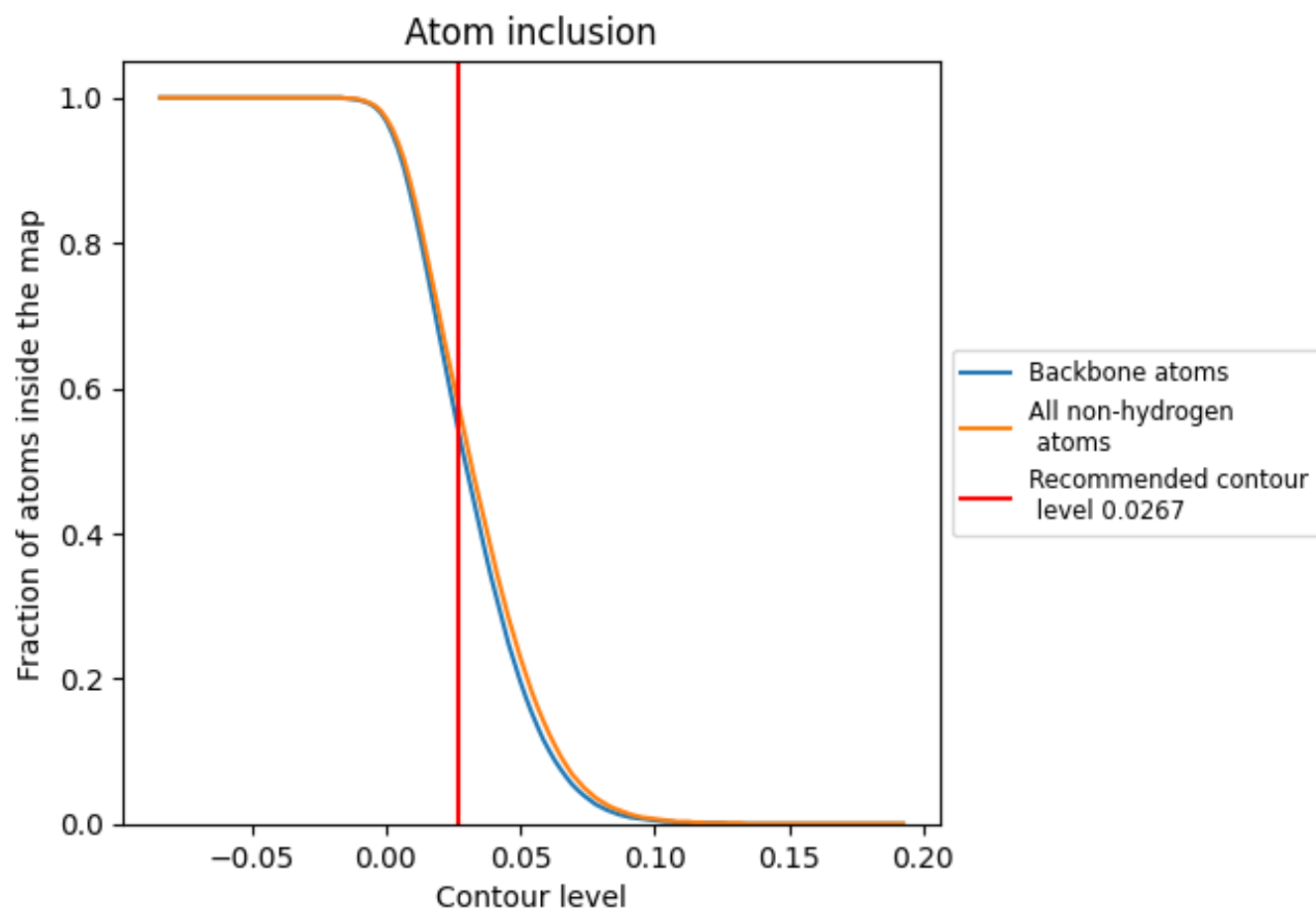
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0267).

9.4 Atom inclusion [i](#)



At the recommended contour level, 55% of all backbone atoms, 58% 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 (0.0267) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5800	 0.5260
0	 0.6500	 0.6560
1	 0.8700	 0.7330
2	 0.8840	 0.7360
3	 0.7440	 0.6770
4	 0.0980	 0.3010
A	 0.3590	 0.3330
B	 0.0670	 0.2580
C	 0.2120	 0.2870
D	 0.1570	 0.2580
E	 0.2570	 0.3380
F	 0.1300	 0.3690
G	 0.1550	 0.3020
H	 0.2460	 0.3240
I	 0.2040	 0.2660
J	 0.1510	 0.1960
K	 0.2170	 0.3620
L	 0.2870	 0.4270
M	 0.1770	 0.3160
N	 0.2050	 0.2140
O	 0.2170	 0.3790
P	 0.2500	 0.2640
Q	 0.2010	 0.3360
R	 0.2030	 0.3350
S	 0.1400	 0.2350
T	 0.2370	 0.3800
U	 0.0450	 0.2690
X	 0.2670	 0.3190
Y	 0.3110	 0.3820
Z	 0.3840	 0.4460
a	 0.8040	 0.6590
b	 0.7260	 0.6020
c	 0.7330	 0.6710
d	 0.7710	 0.7010
e	 0.5800	 0.6610



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Chain	Atom inclusion	Q-score
f	 0.3090	 0.4540
g	 0.3030	 0.4810
h	 0.2100	 0.5190
i	 0.8140	 0.7100
j	 0.6660	 0.6520
k	 0.7290	 0.6890
l	 0.8120	 0.7050
m	 0.8510	 0.7210
n	 0.6790	 0.6250
o	 0.6330	 0.6520
p	 0.8790	 0.7390
q	 0.7060	 0.6810
r	 0.7490	 0.6940
s	 0.5720	 0.6480
t	 0.4620	 0.6110
u	 0.6560	 0.6320
v	 0.8570	 0.7240
w	 0.7140	 0.6800
x	 0.4170	 0.5750
y	 0.7800	 0.6910
z	 0.7110	 0.7030