



Full wwPDB EM Validation Report ⓘ

Oct 13, 2024 – 09:48 am BST

PDB ID : 5L3P
EMDB ID : EMD-4001
Title : Cryo-EM structure of stringent response factor RelA bound to ErmCL-stalled ribosome complex
Authors : Arenz, S.; Wilson, D.N.
Deposited on : 2016-05-24
Resolution : 3.70 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 : 1.8.4, CSD as541be (2020)
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) : 2.39

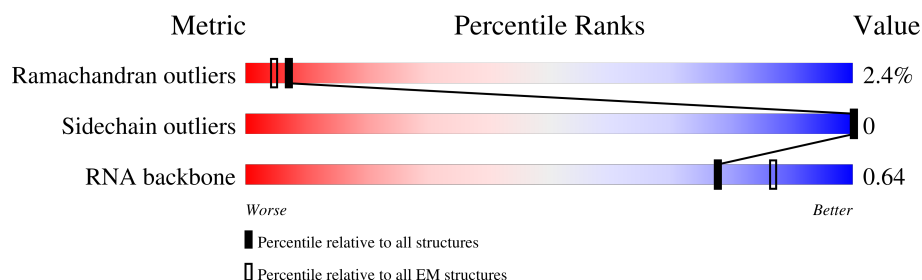
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	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	A	2903	
2	B	120	
3	D	273	
4	E	209	
5	F	201	
6	G	179	
7	H	177	
8	I	149	

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Mol	Chain	Length	Quality of chain
9	N	142	77% 99%
10	O	123	76% 95%
11	P	144	64% 95%
12	Q	136	71% 98%
13	R	127	65% 92%
14	S	117	58% 97%
15	T	115	81% 99%
16	U	118	64% 99%
17	V	103	71% 96%
18	W	110	65% 100%
19	X	100	61% 91%
20	Y	104	71% 96%
21	Z	94	67% 100%
22	0	85	54% 87%
23	1	78	68% 99%
24	2	63	65% 100%
25	3	59	71% 98%
26	4	70	47% 93%
27	5	57	56% 96%
28	6	55	67% 89%
29	7	46	52% 100%
30	8	65	72% 97%
31	9	38	55% 97%
32	a	1539	42% 88%
33	b	240	65% 89%

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Mol	Chain	Length	Quality of chain
34	c	233	
35	d	206	
36	e	167	
37	f	135	
38	g	179	
39	h	130	
40	i	130	
41	j	103	
42	k	129	
43	l	124	
44	m	118	
45	o	89	
46	p	82	
47	q	84	
48	r	75	
49	t	87	
50	u	71	
51	v	6	
52	x	77	
53	J	165	
54	K	142	
55	n	102	
56	s	92	
57	z	819	
58	y	73	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	2MG	A	1835	X	-	-	-
1	PSU	A	1911	X	-	-	-
1	3TD	A	1915	X	-	-	-
1	PSU	A	1917	X	-	-	-
1	5MU	A	1939	X	-	-	-
1	7MG	A	2069	X	-	-	-
1	OMG	A	2251	X	-	-	-
1	2MG	A	2445	X	-	-	-
1	H2U	A	2449	X	-	-	-
1	PSU	A	2457	X	-	-	-
1	OMC	A	2498	X	-	-	-
1	2MA	A	2503	X	-	-	-
1	PSU	A	2504	X	-	-	-
1	OMU	A	2552	X	-	-	-
1	PSU	A	2580	X	-	-	-
1	PSU	A	2604	X	-	-	-
1	PSU	A	2605	X	-	-	-
1	PSU	A	746	X	-	-	-
1	PSU	A	955	X	-	-	-
32	2MG	a	1207	X	-	-	-
32	4OC	a	1402	X	-	-	-
32	UR3	a	1498	X	-	-	-
32	2MG	a	1516	X	-	-	-
32	MA6	a	1518	X	-	-	-
32	MA6	a	1519	X	-	-	-
32	PSU	a	516	X	-	-	-
32	7MG	a	527	X	-	-	-
32	2MG	a	966	X	-	-	-
52	H2U	x	20	X	-	-	-
52	5MU	x	54	X	-	-	-
52	PSU	x	55	X	-	-	-
52	4SU	x	8	X	-	-	-
58	H2U	y	16	X	-	-	-
58	H2U	y	17	X	-	-	-
58	H2U	y	20	X	-	-	-
58	7MG	y	46	X	-	-	-
58	5MU	y	54	X	-	-	-
58	PSU	y	55	X	-	-	-

2 Entry composition [i](#)

There are 58 unique types of molecules in this entry. The entry contains 149606 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2890	Total	C	N	O	P	0	0
			62057	27688	11422	20057	2890		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1847	G	A	conflict	GB 802133627

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	120	Total	C	N	O	P	0	0
			2572	1145	471	836	120		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	120	A	U	conflict	GB 999944586

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 9 is a protein called 50S ribosomal protein L13.

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

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	O	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	P	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 12 is a protein called 50S ribosomal protein L16.

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

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	R	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 14 is a protein called 50S ribosomal protein L18.

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

- Molecule 15 is a protein called 50S ribosomal protein L19.

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

- Molecule 16 is a protein called 50S ribosomal protein L20.

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

- Molecule 17 is a protein called 50S ribosomal protein L21.

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

- Molecule 18 is a protein called 50S ribosomal protein L22.

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

- Molecule 19 is a protein called 50S ribosomal protein L23.

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

- Molecule 20 is a protein called 50S ribosomal protein L24.

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

- Molecule 21 is a protein called 50S ribosomal protein L25.

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

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	0	75	Total	C	N	O	S	0	0
			575	356	116	102	1		

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	1	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	2	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	3	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	4	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	5	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	6	50	Total	C	N	O	S	0	0
			409	263	75	71			

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	7	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	8	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	9	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 32 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	a	1539	Total	C	N	O	P	0	0
			33029	14738	6052	10700	1539		

- Molecule 33 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	b	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 34 is a protein called 30S ribosomal protein S3.

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

- Molecule 35 is a protein called 30S ribosomal protein S4.

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

- Molecule 36 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	e	157	Total	C	N	O	S	0	0
			1141	709	218	208	6		

- Molecule 37 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	f	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 38 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	g	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 39 is a protein called 30S ribosomal protein S8.

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

- Molecule 40 is a protein called 30S ribosomal protein S9.

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

- Molecule 41 is a protein called 30S ribosomal protein S10.

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

- Molecule 42 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	k	116	Total	C	N	O	S	0	0
			869	535	173	158	3		

- Molecule 43 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	l	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 44 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	m	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 45 is a protein called 30S ribosomal protein S15.

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

- Molecule 46 is a protein called 30S ribosomal protein S16.

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

- Molecule 47 is a protein called 30S ribosomal protein S17.

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

- Molecule 48 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	r	65	Total	C	N	O	0	0
			504	317	96	91		

- Molecule 49 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	t	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 50 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	u	65	Total	C	N	O	S	0	0
			495	307	100	87	1		

- Molecule 51 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	v	6	Total	C	N	O	P	0	0
			129	58	24	41	6		

- Molecule 52 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
52	x	77	Total	C	N	O	P	S	0	0
			1644	733	297	536	77	1		

- Molecule 53 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	J	131	Total	C	N	O	S	0	0
			988	625	175	183	5		

- Molecule 54 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	K	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 55 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	n	101	Total	C	N	O	S	0	0
			799	498	165	133	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	35	ALA	-	insertion	UNP P0AG59

- Molecule 56 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	s	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 57 is a protein called GTP pyrophosphokinase,GTP pyrophosphokinase,GTP pyrophosphokinase.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	z	545	Total	C	N	O		0	0
			2255	1165	545	545			

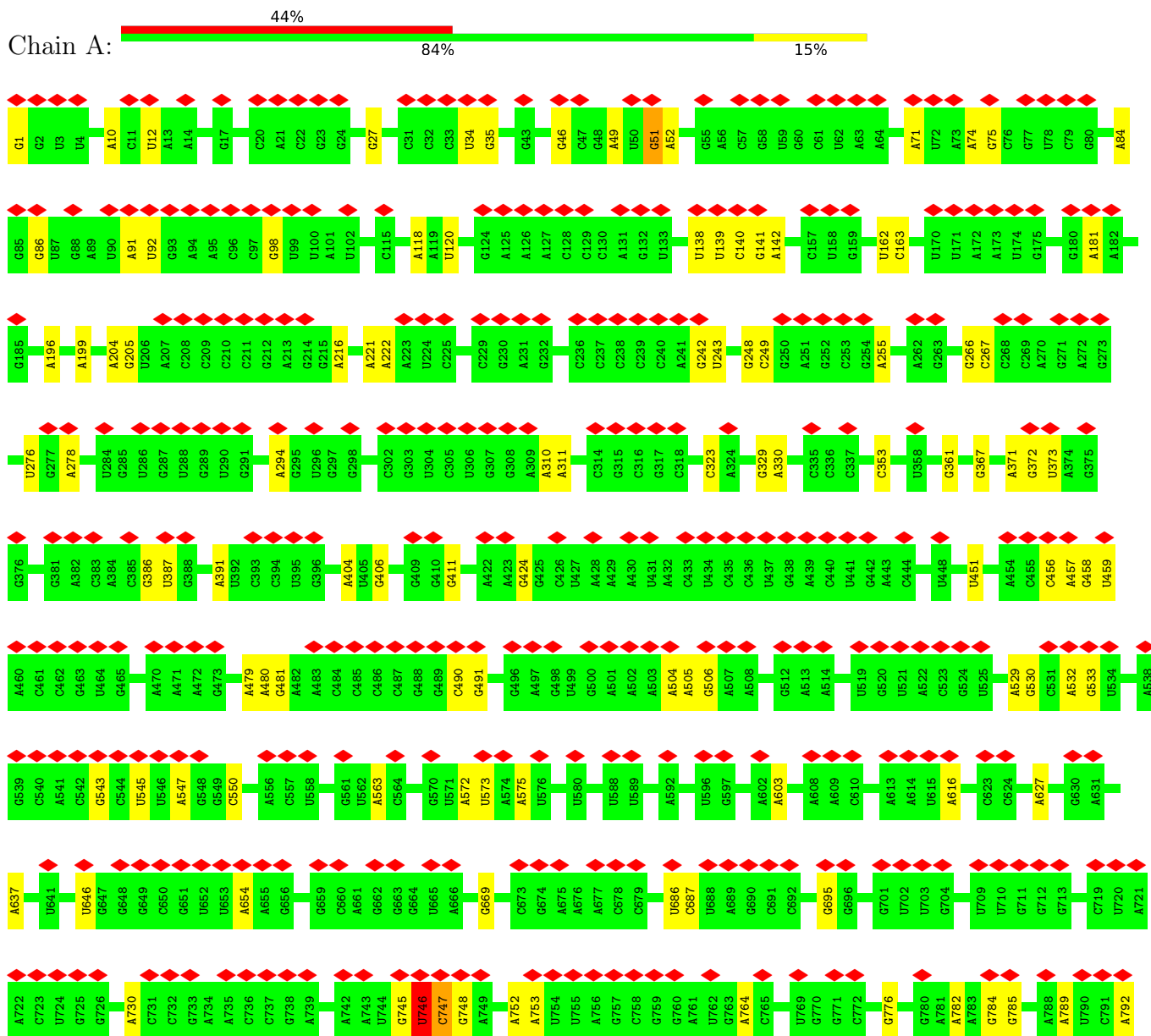
- Molecule 58 is a RNA chain called deacylated A/R-tRNA.

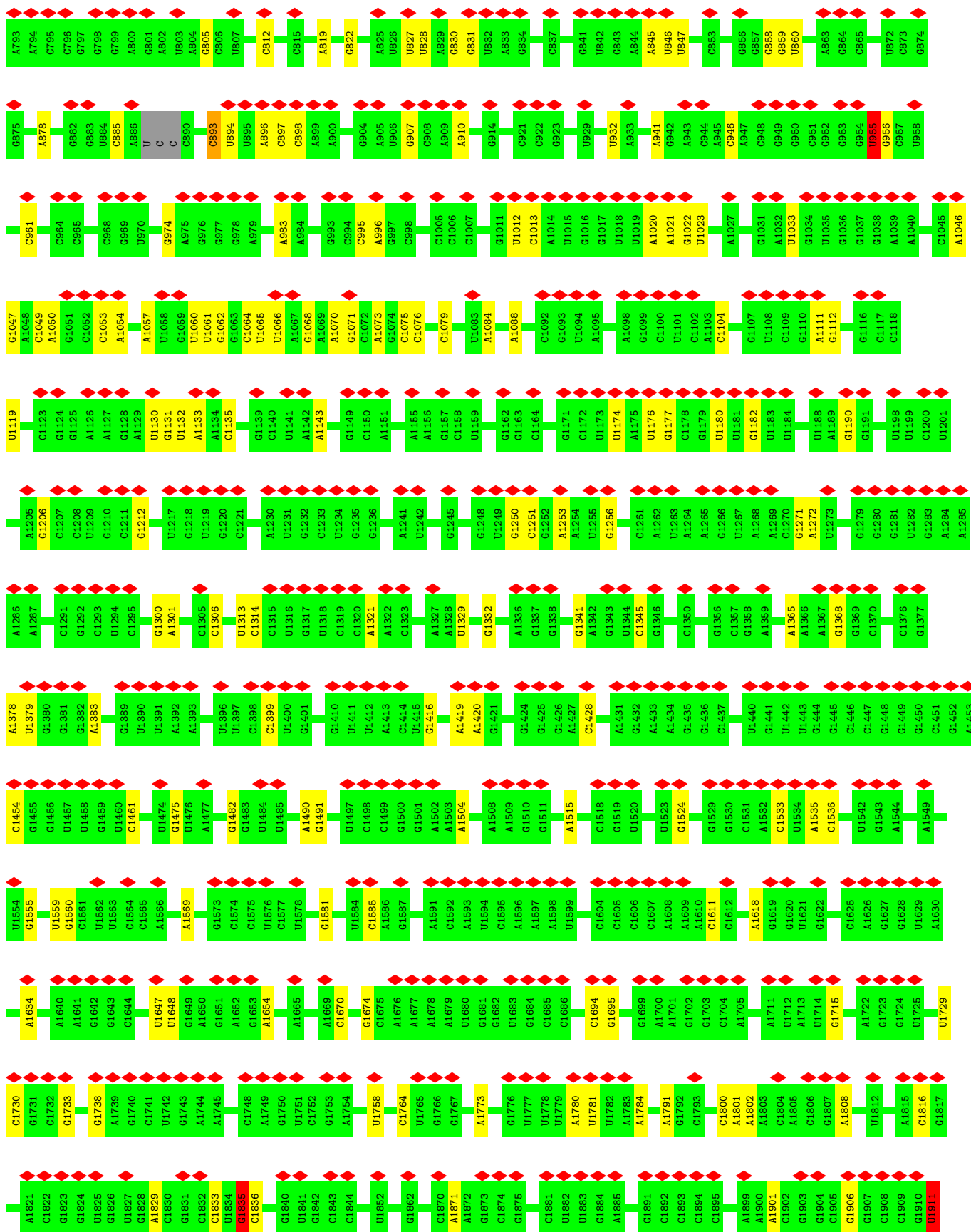
Mol	Chain	Residues	Atoms					AltConf	Trace
58	y	73	Total	C	N	O	P	0	0
			1581	709	280	519	73		

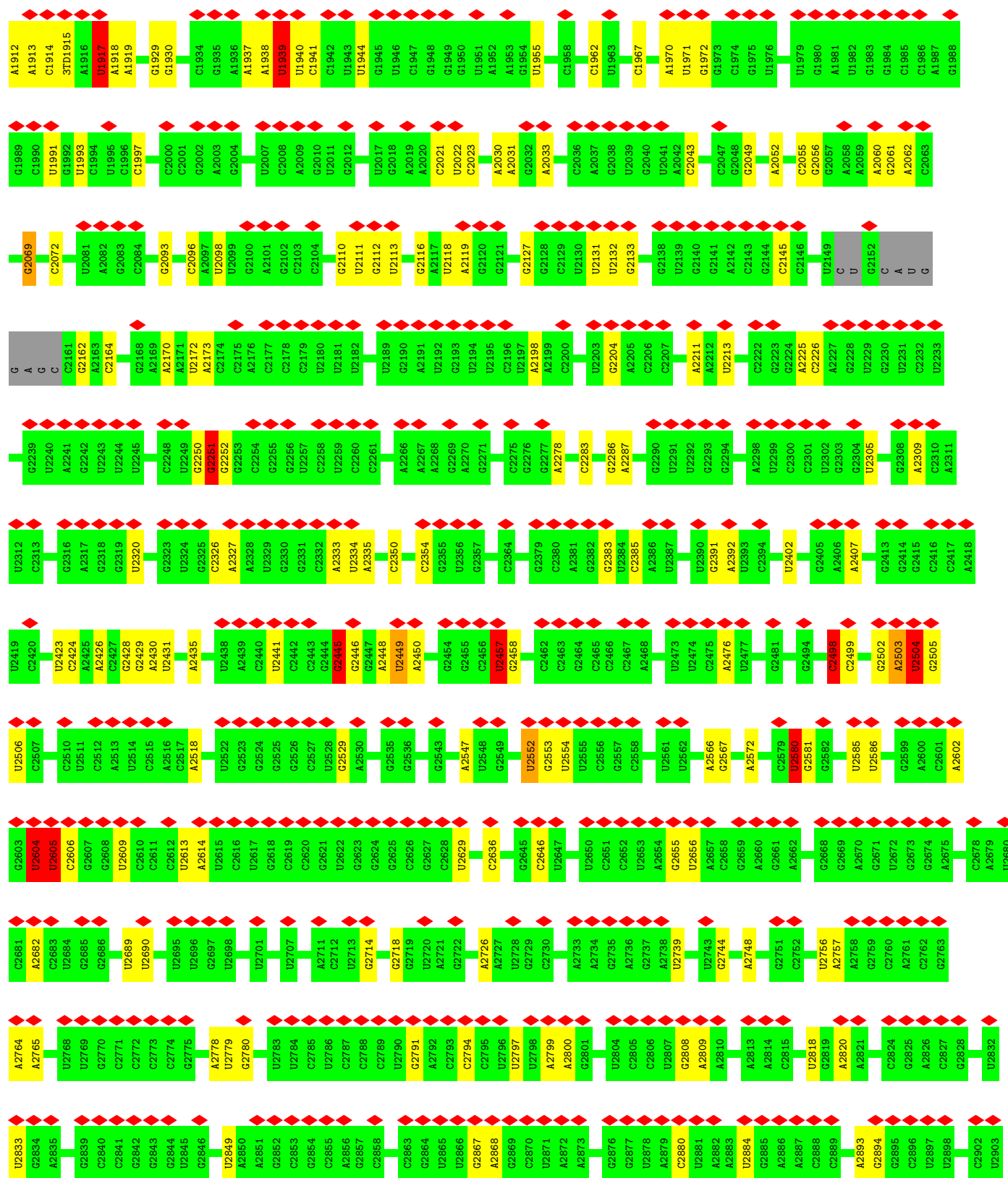
3 Residue-property plots

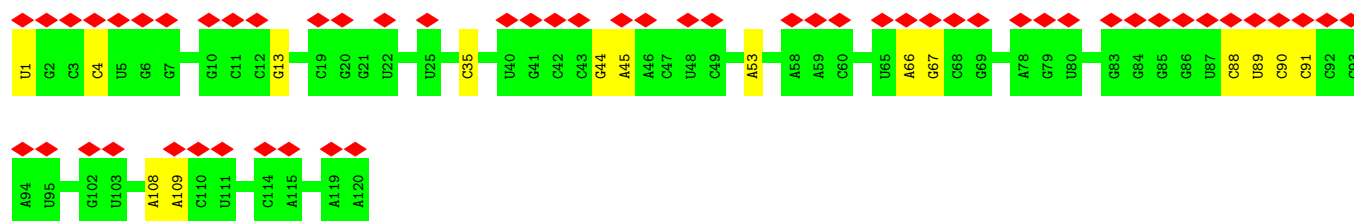
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: 23S ribosomal RNA

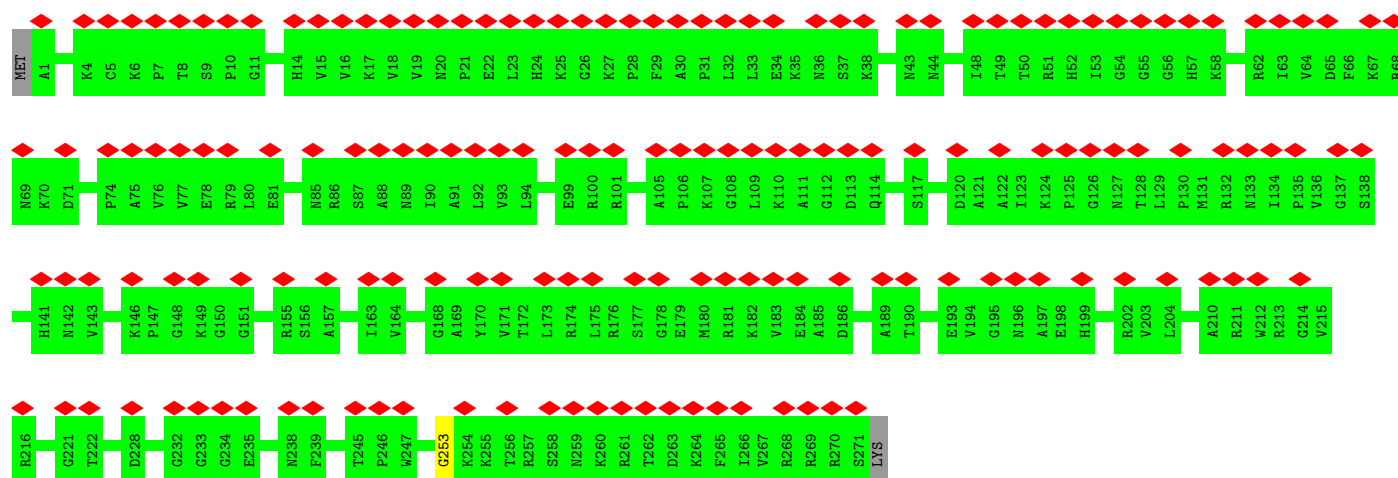




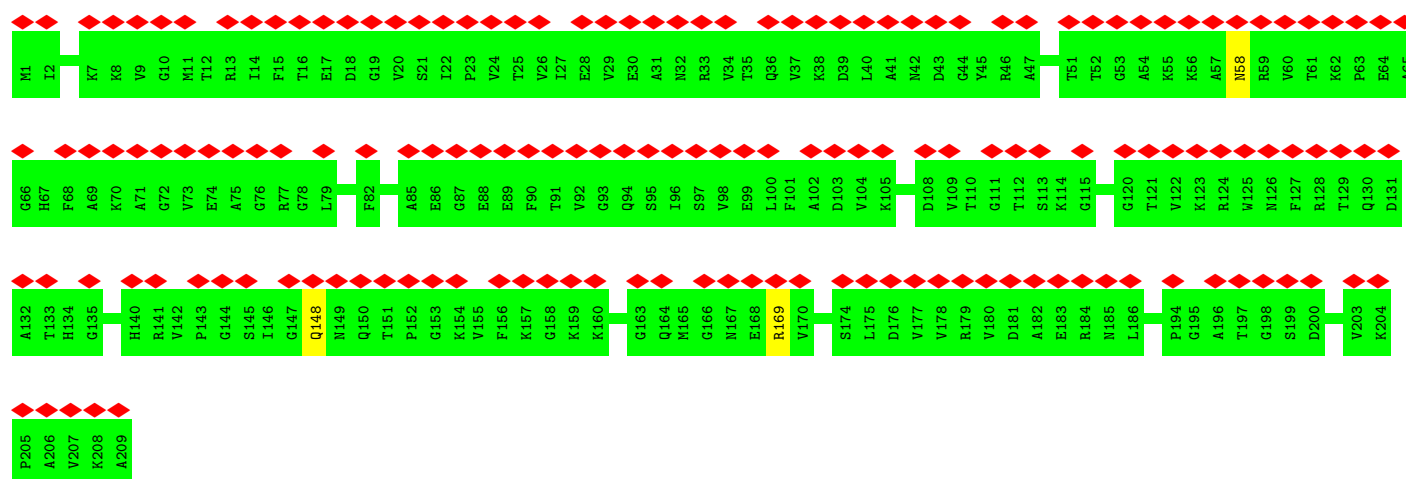
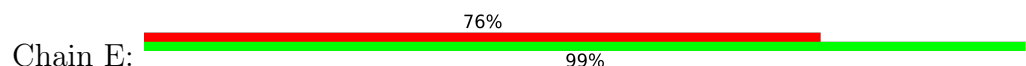




• Molecule 3: 50S ribosomal protein L2

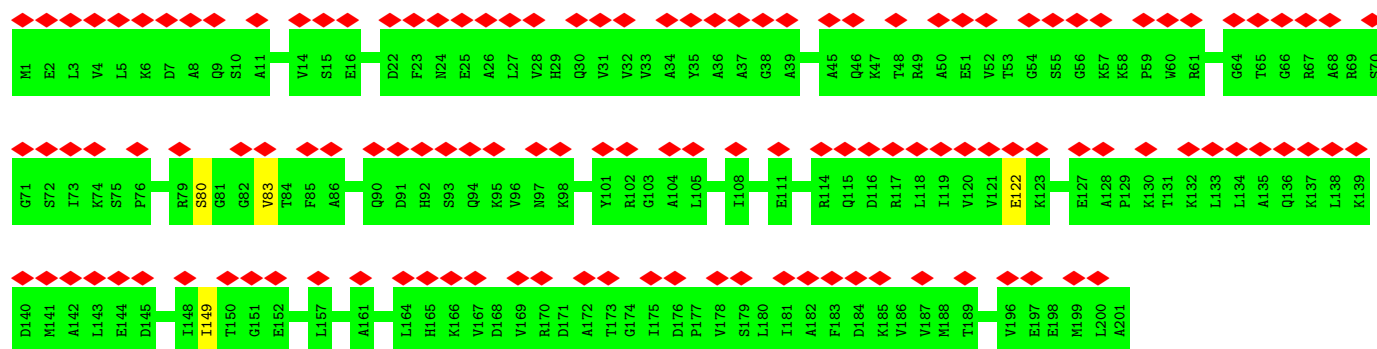


• Molecule 4: 50S ribosomal protein L3

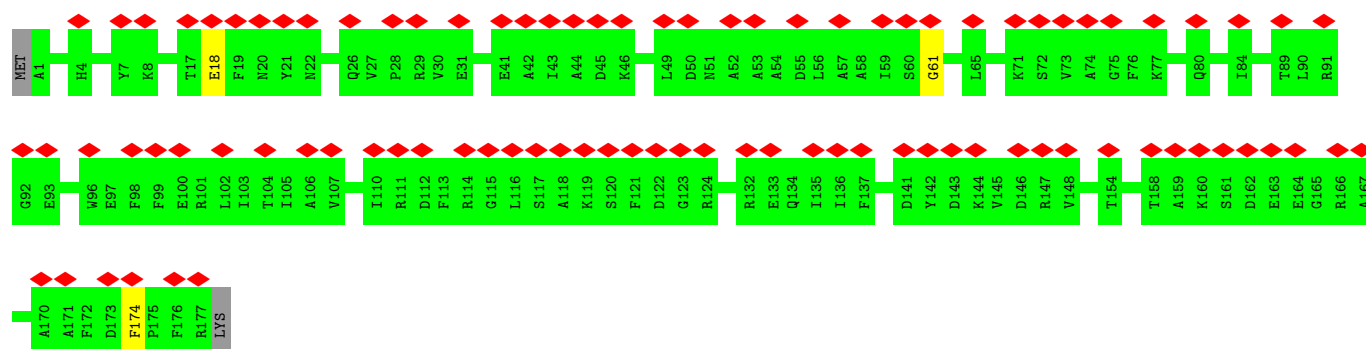


• Molecule 5: 50S ribosomal protein L4

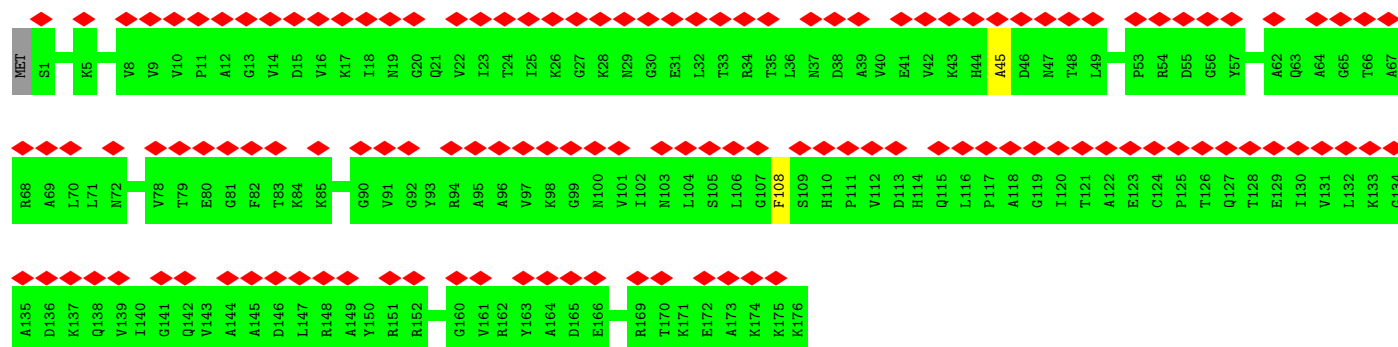
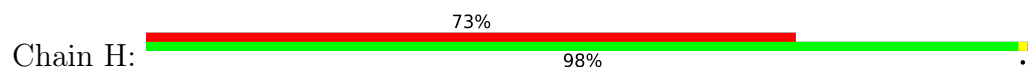




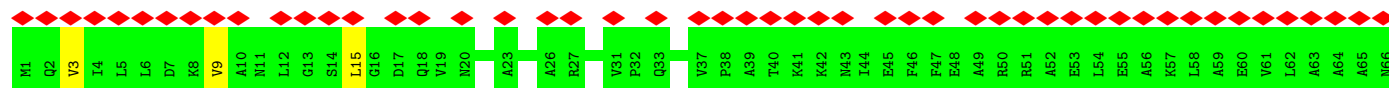
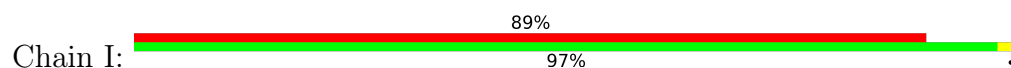
• Molecule 6: 50S ribosomal protein L5

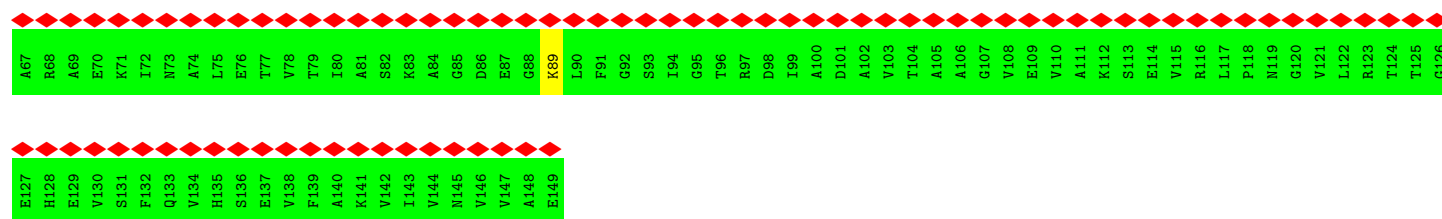


• Molecule 7: 50S ribosomal protein L6



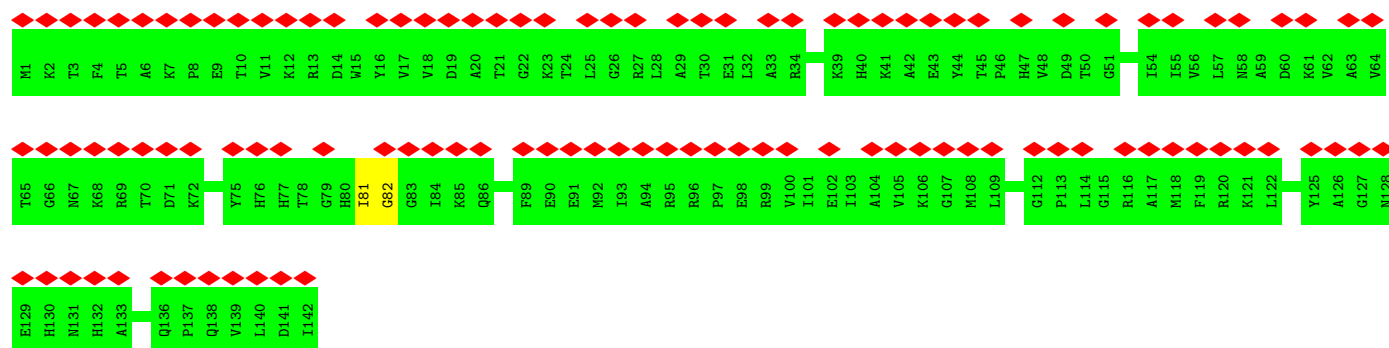
• Molecule 8: 50S ribosomal protein L9





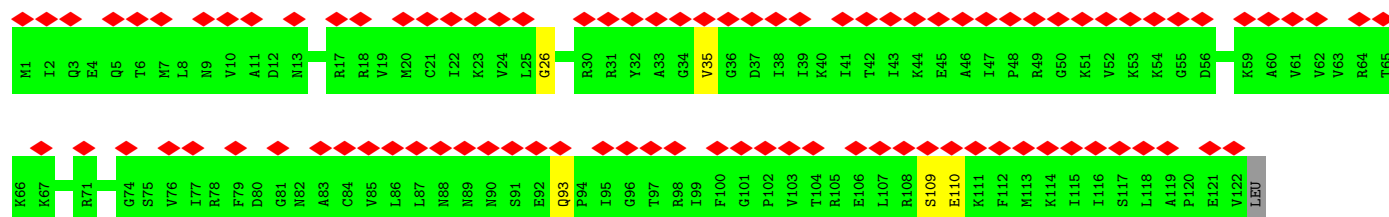
• Molecule 9: 50S ribosomal protein L13

Chain N: 77% 99%



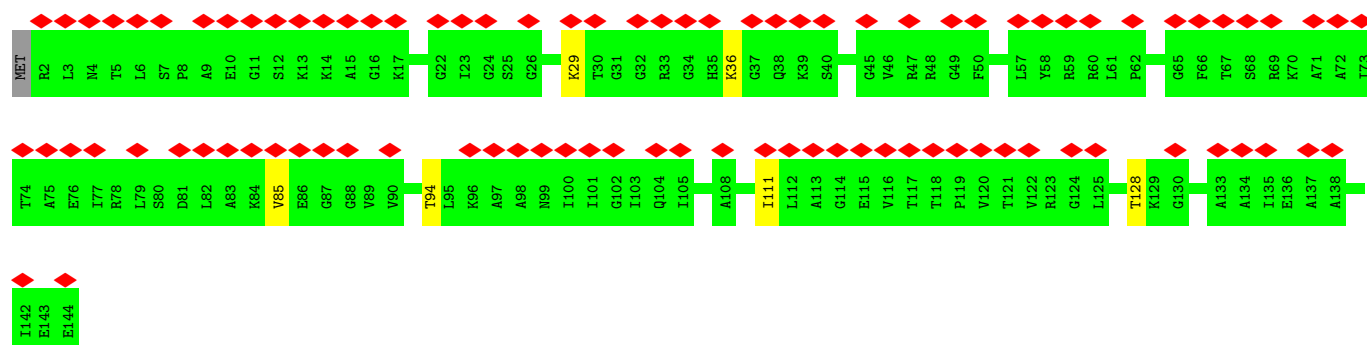
• Molecule 10: 50S ribosomal protein L14

Chain O: 76% 95%

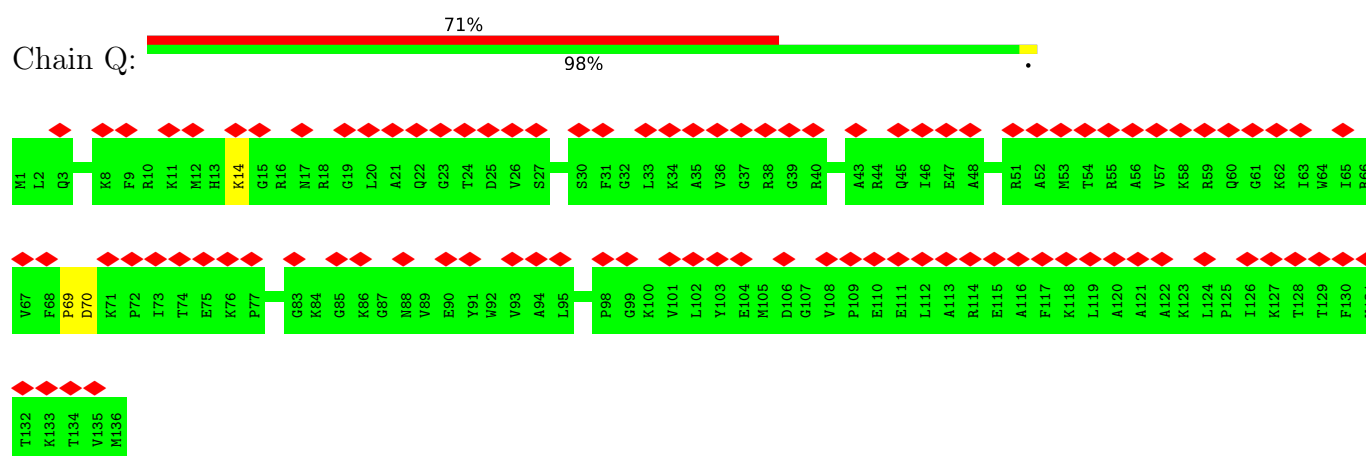


• Molecule 11: 50S ribosomal protein L15

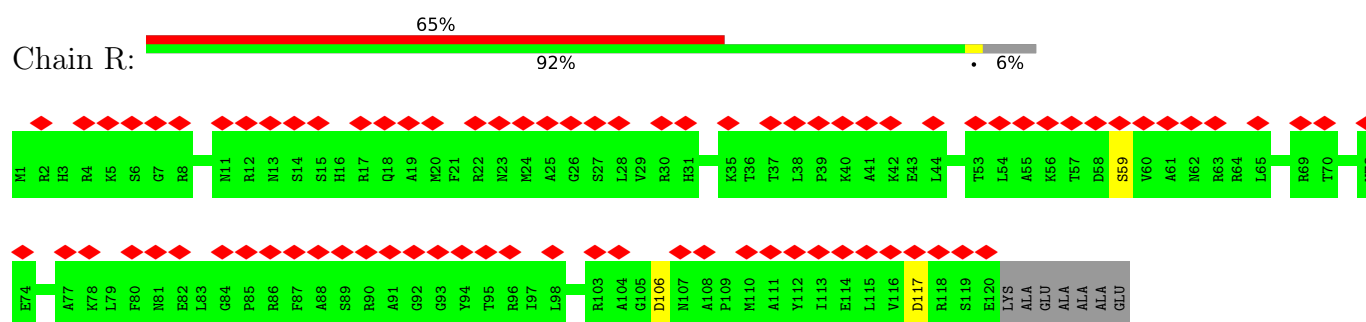
Chain P: 64% 95%



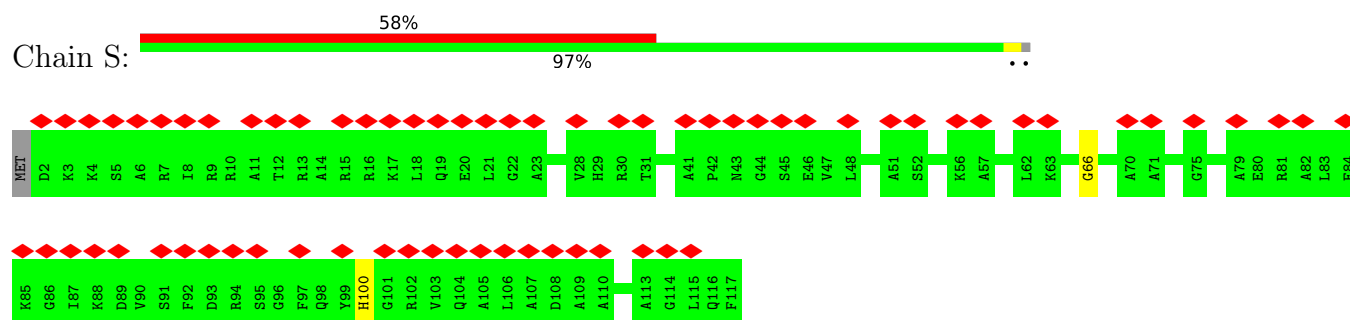
• Molecule 12: 50S ribosomal protein L16



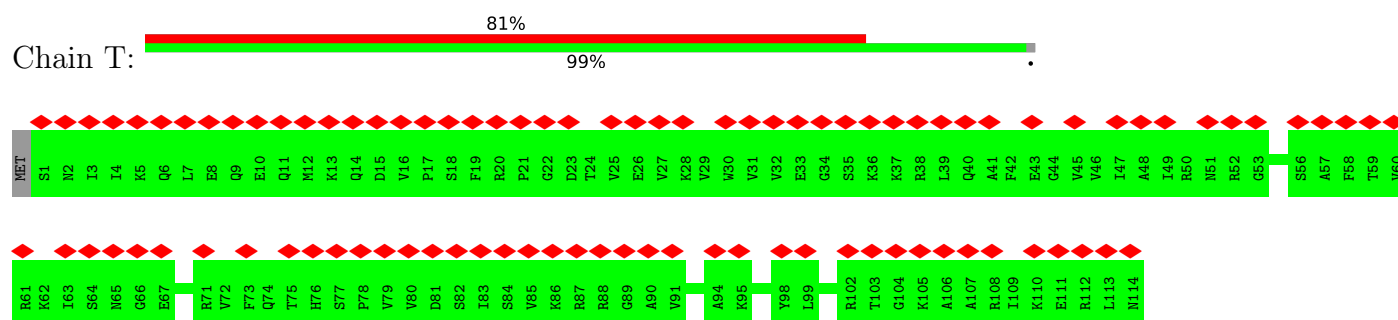
- Molecule 13: 50S ribosomal protein L17



- Molecule 14: 50S ribosomal protein L18

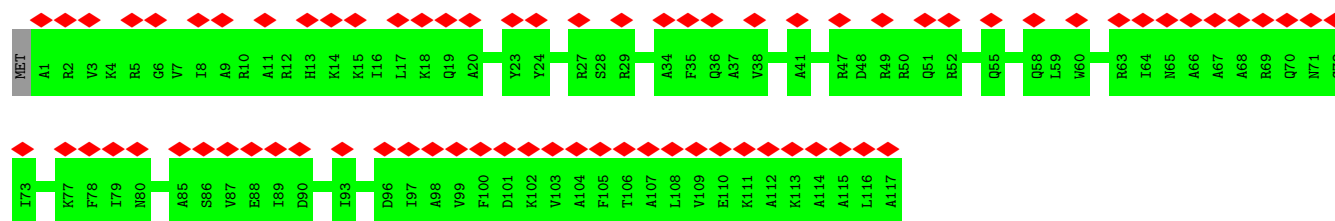


- Molecule 15: 50S ribosomal protein L19

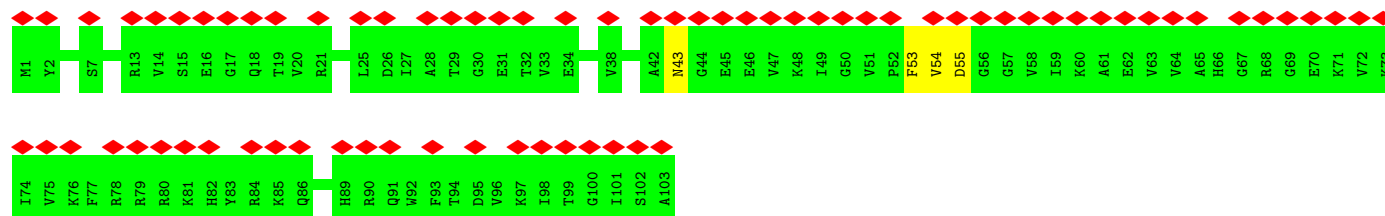


- Molecule 16: 50S ribosomal protein L20

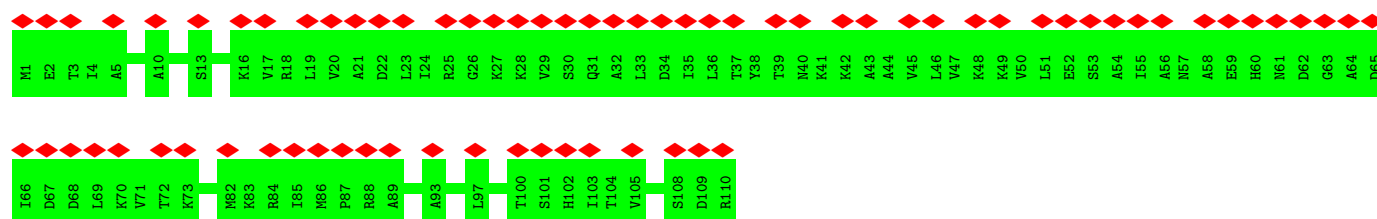




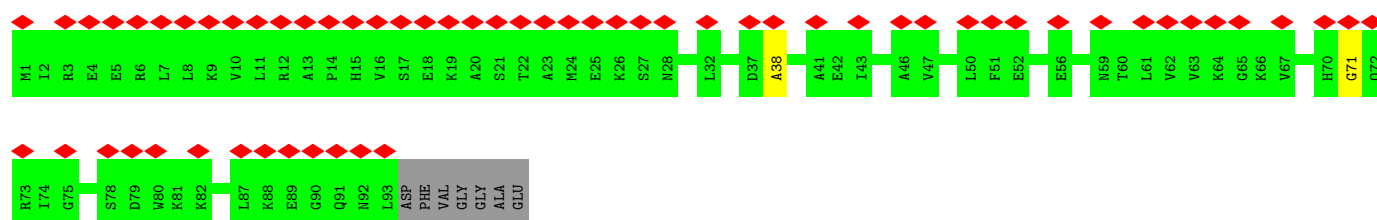
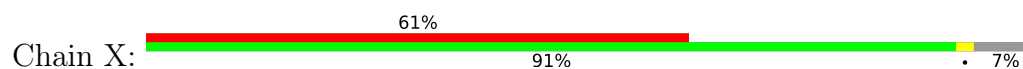
• Molecule 17: 50S ribosomal protein L21



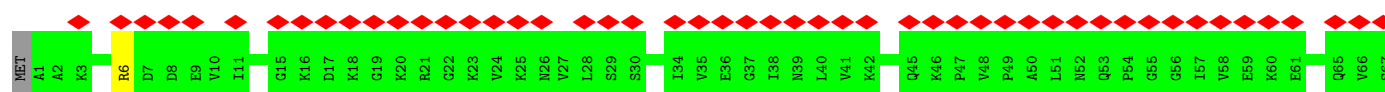
• Molecule 18: 50S ribosomal protein L22

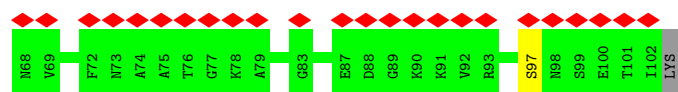


• Molecule 19: 50S ribosomal protein L23

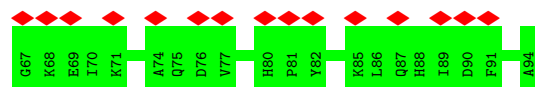
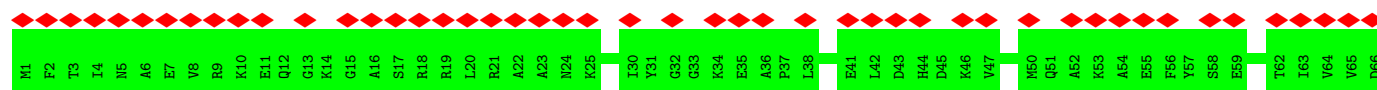


• Molecule 20: 50S ribosomal protein L24

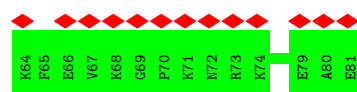
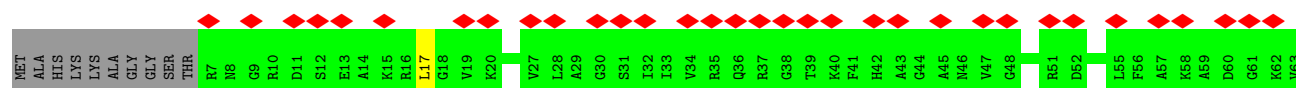
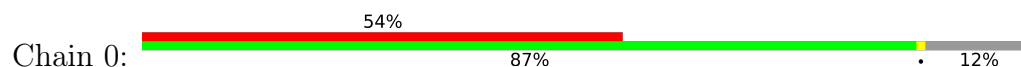




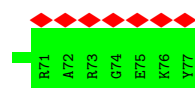
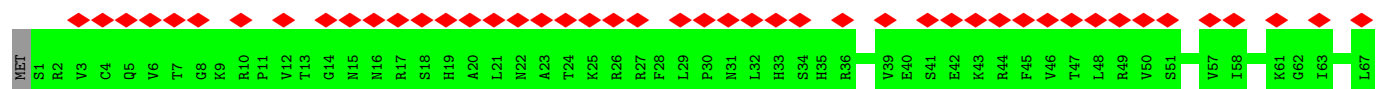
- Molecule 21: 50S ribosomal protein L25



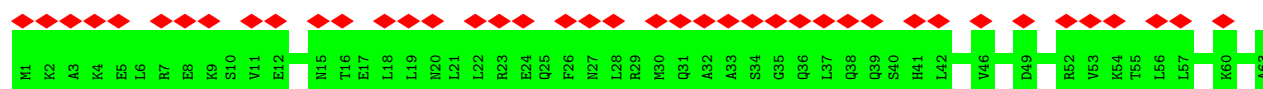
- Molecule 22: 50S ribosomal protein L27



- Molecule 23: 50S ribosomal protein L28

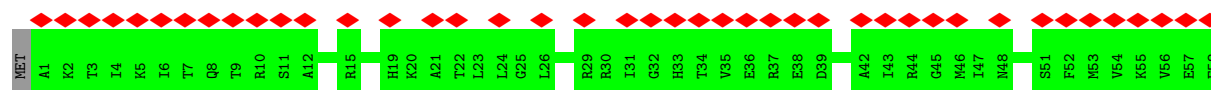


- Molecule 24: 50S ribosomal protein L29

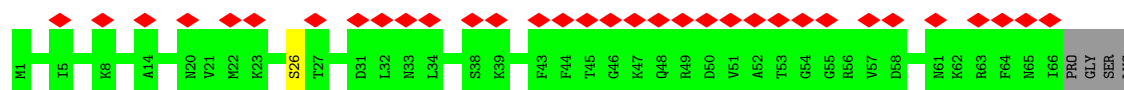
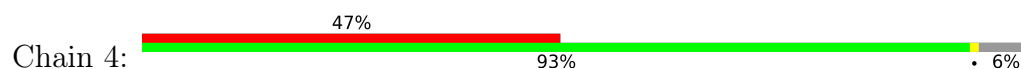


- Molecule 25: 50S ribosomal protein L30

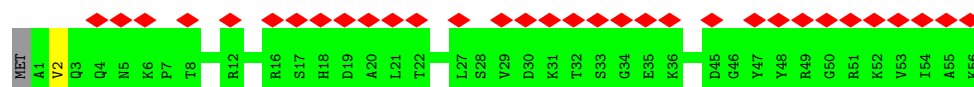




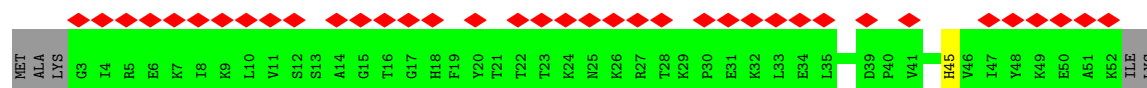
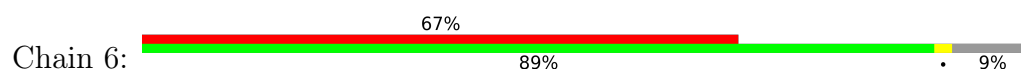
- Molecule 26: 50S ribosomal protein L31



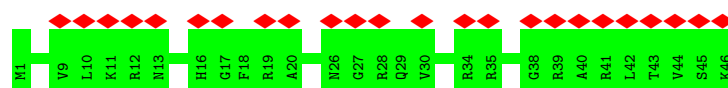
- Molecule 27: 50S ribosomal protein L32



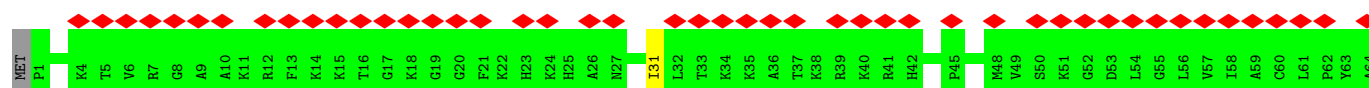
- Molecule 28: 50S ribosomal protein L33



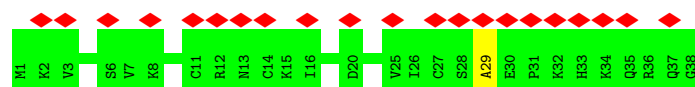
- Molecule 29: 50S ribosomal protein L34



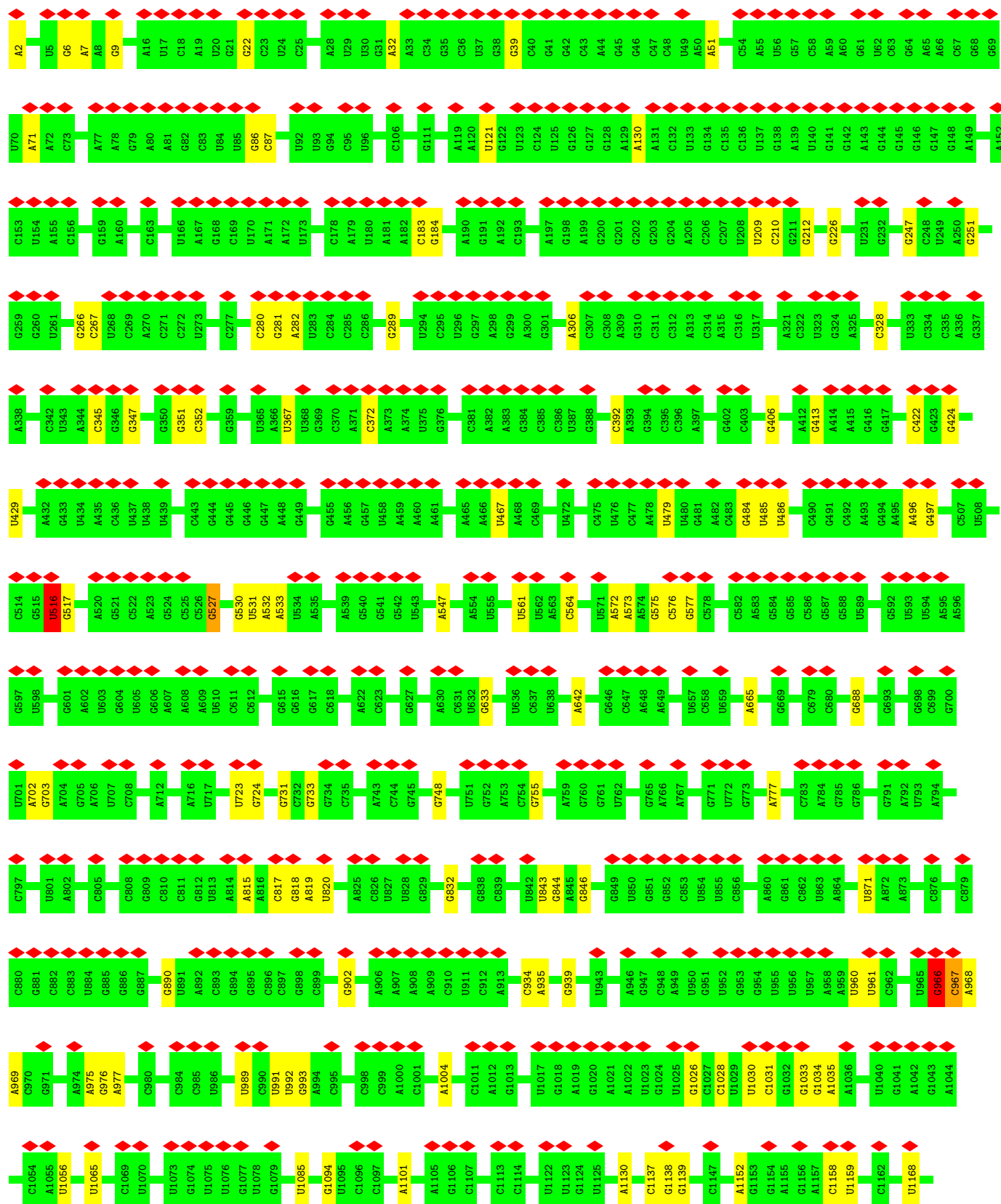
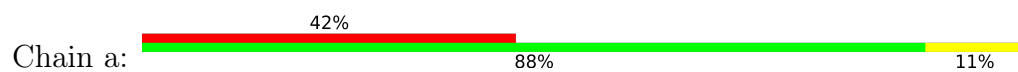
- Molecule 30: 50S ribosomal protein L35

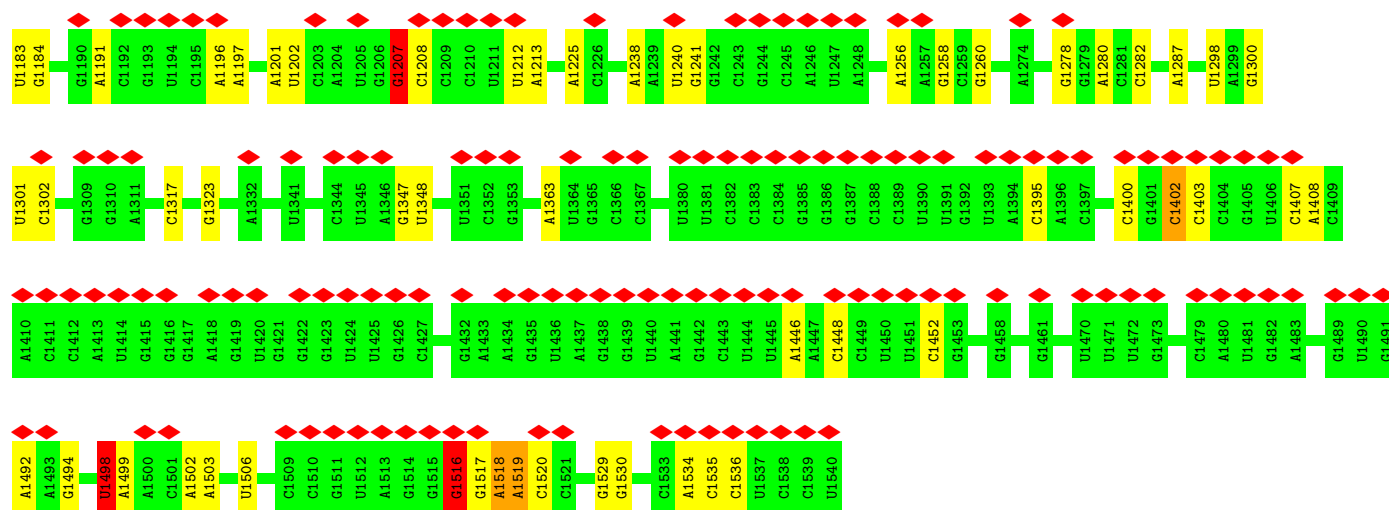


- Molecule 31: 50S ribosomal protein L36

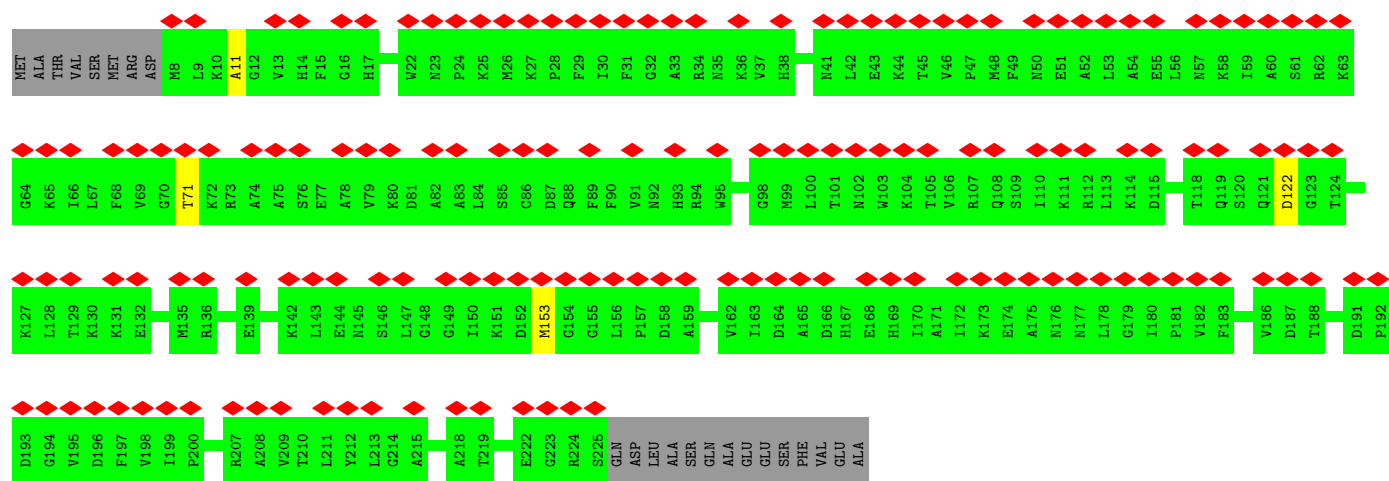
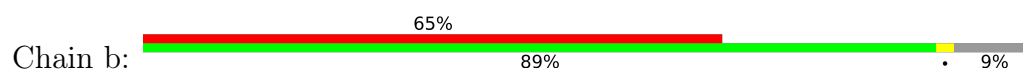


- Molecule 32: 16S ribosomal RNA

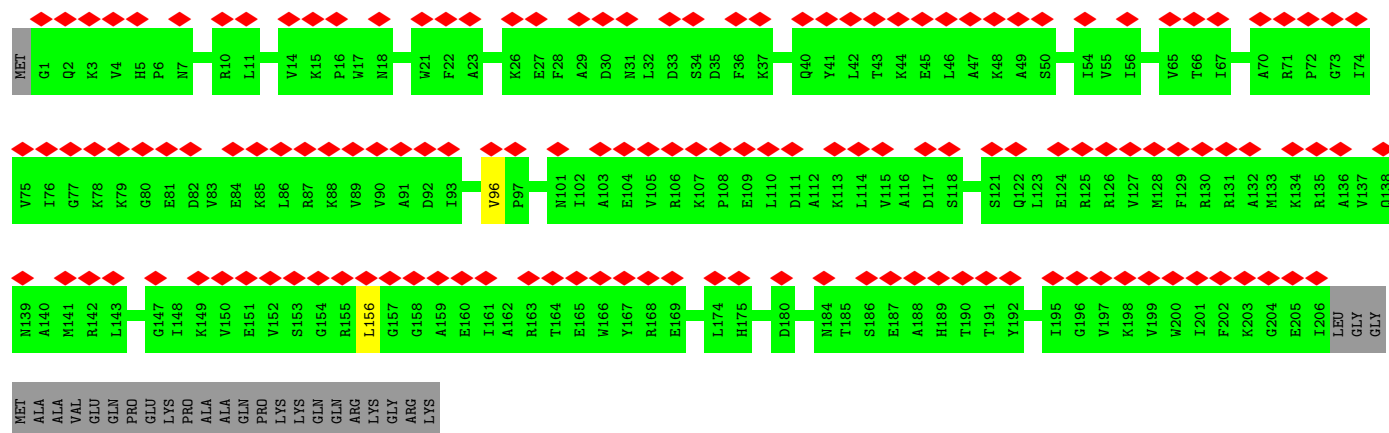
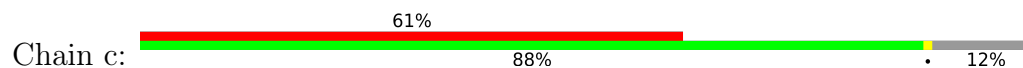




• Molecule 33: 30S ribosomal protein S2



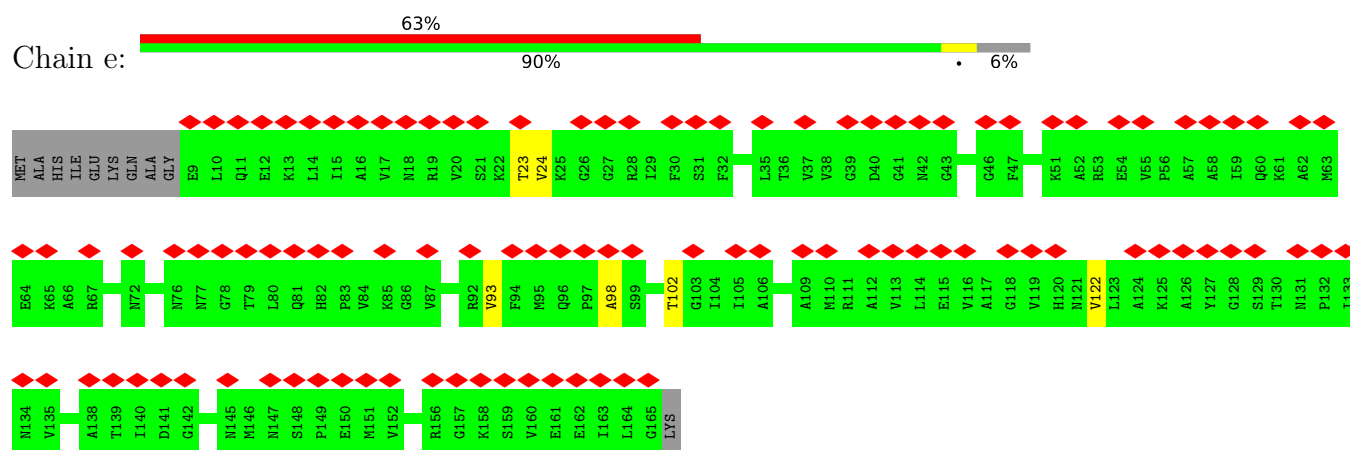
• Molecule 34: 30S ribosomal protein S3



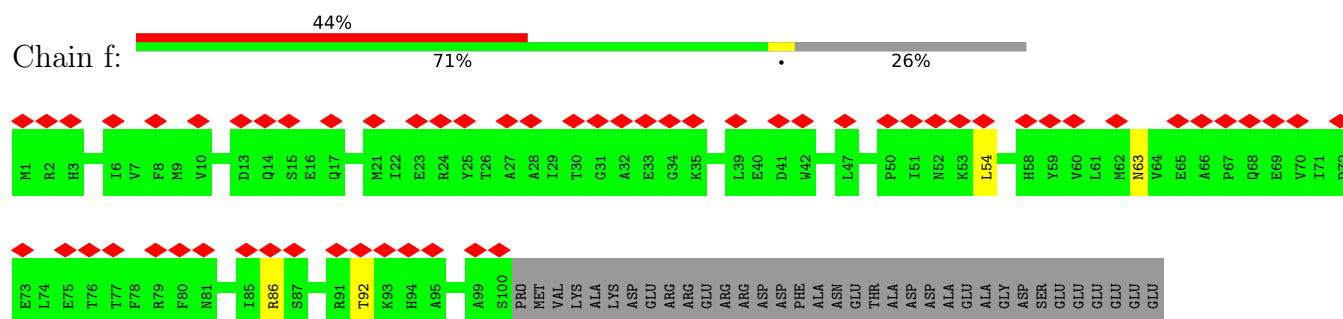
- Molecule 35: 30S ribosomal protein S4



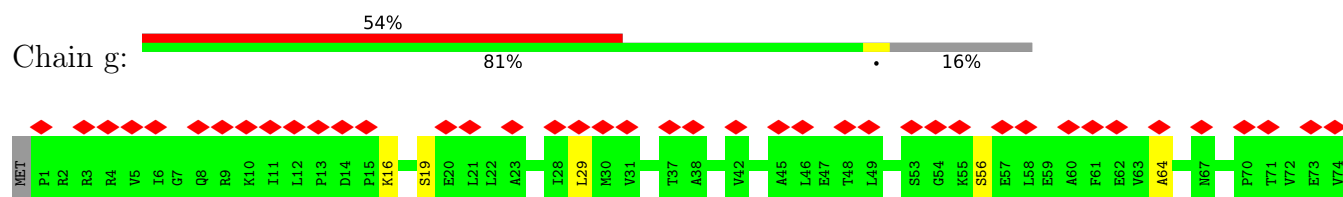
- Molecule 36: 30S ribosomal protein S5



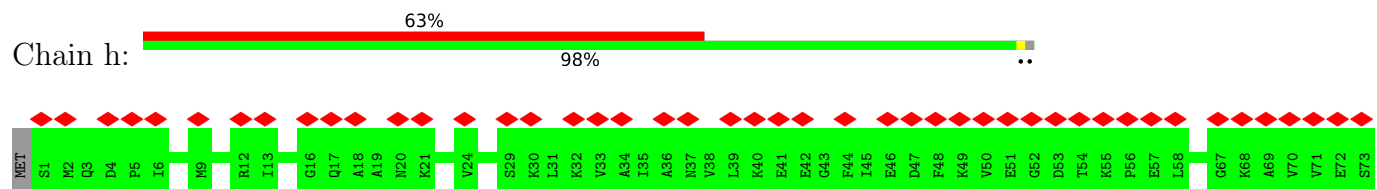
- Molecule 37: 30S ribosomal protein S6



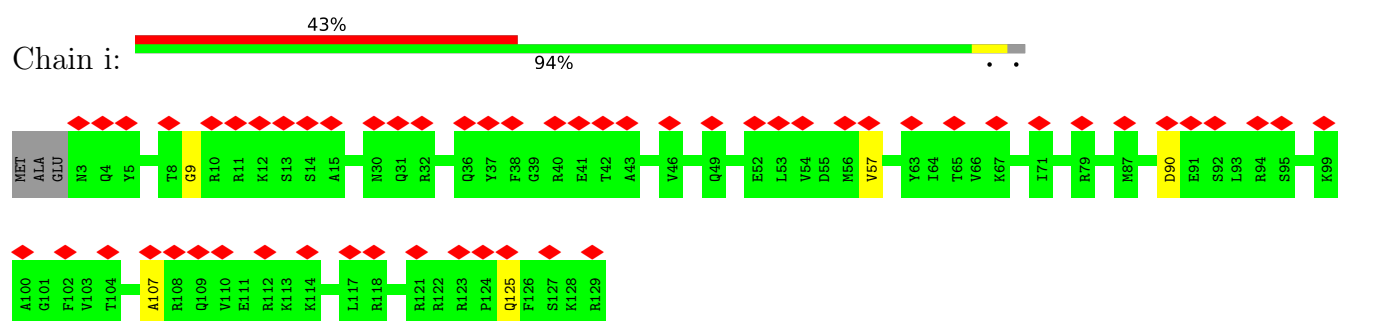
- Molecule 38: 30S ribosomal protein S7



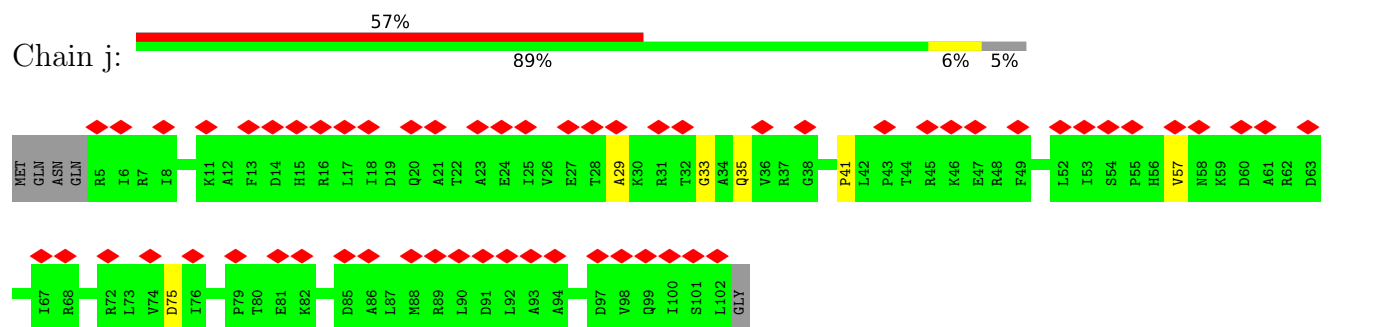
- Molecule 39: 30S ribosomal protein S8



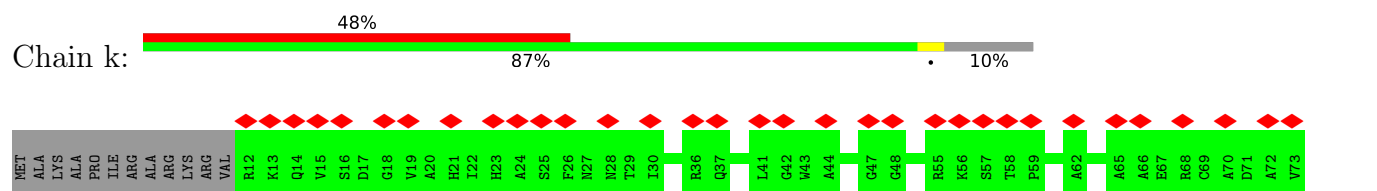
- Molecule 40: 30S ribosomal protein S9

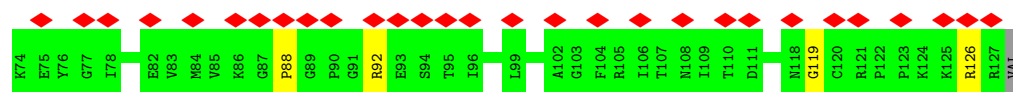


- Molecule 41: 30S ribosomal protein S10

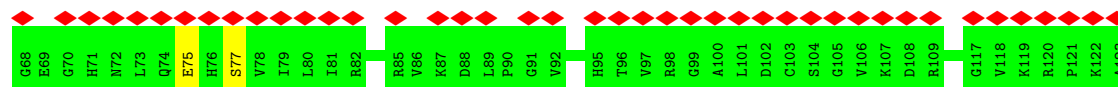
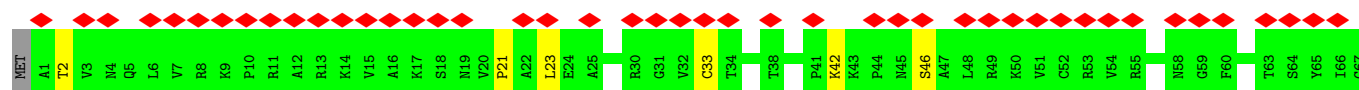
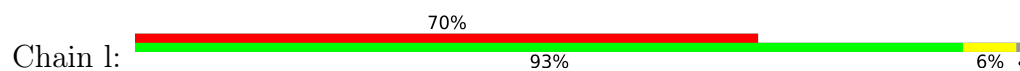


- Molecule 42: 30S ribosomal protein S11

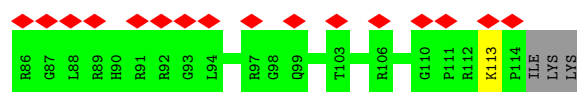
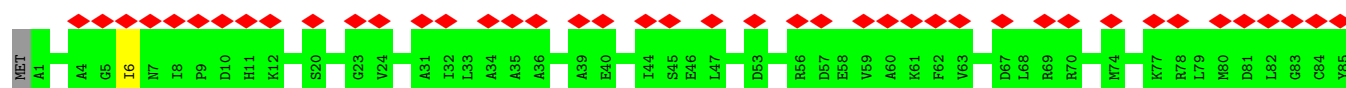




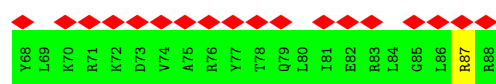
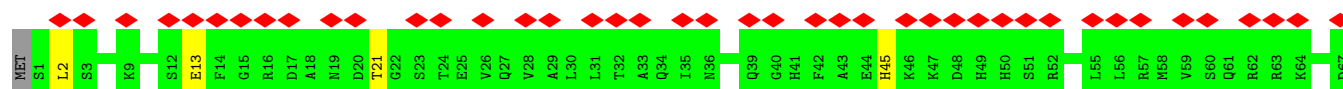
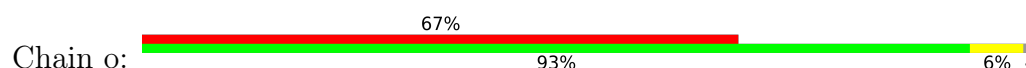
- Molecule 43: 30S ribosomal protein S12



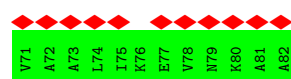
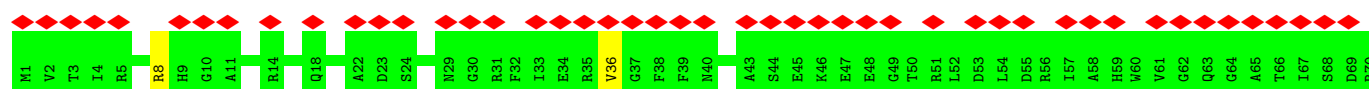
- Molecule 44: 30S ribosomal protein S13



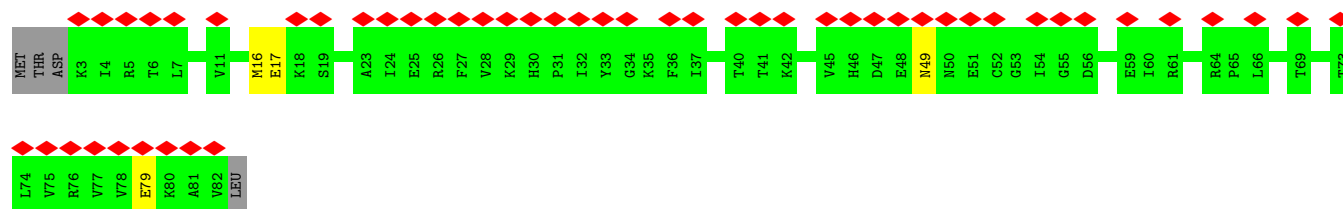
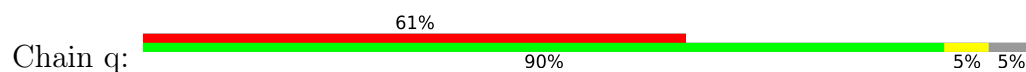
- Molecule 45: 30S ribosomal protein S15



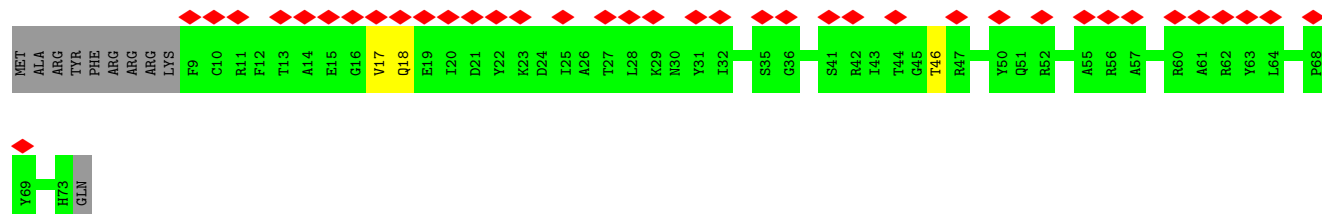
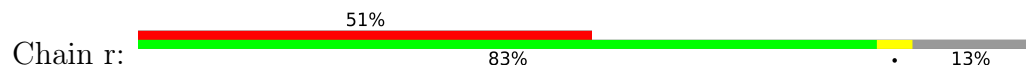
- Molecule 46: 30S ribosomal protein S16



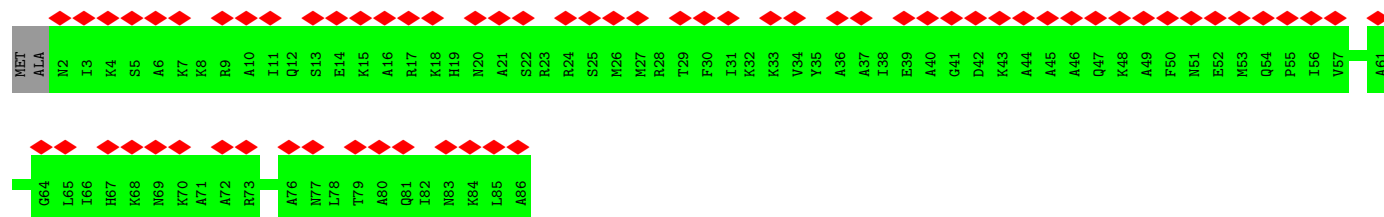
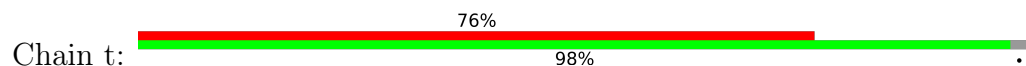
- Molecule 47: 30S ribosomal protein S17



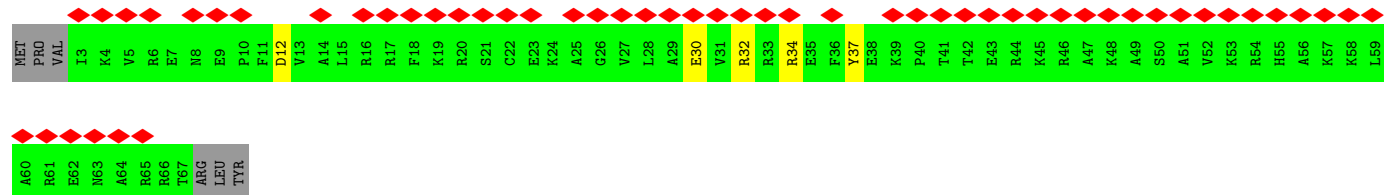
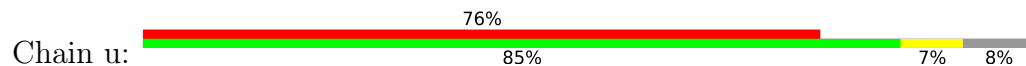
- Molecule 48: 30S ribosomal protein S18



- Molecule 49: 30S ribosomal protein S20

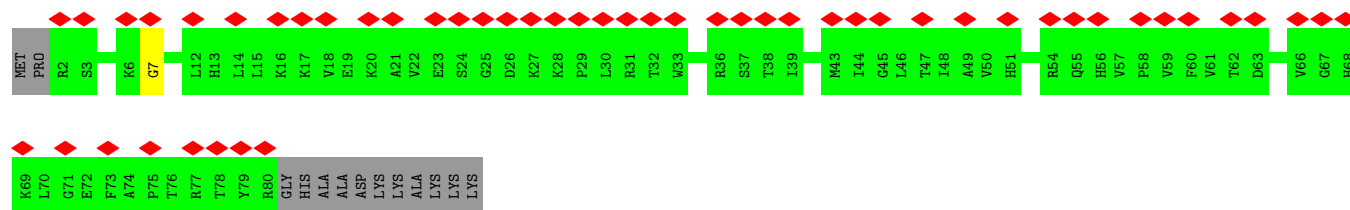
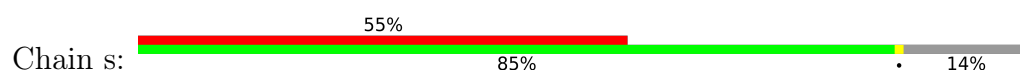


- Molecule 50: 30S ribosomal protein S21

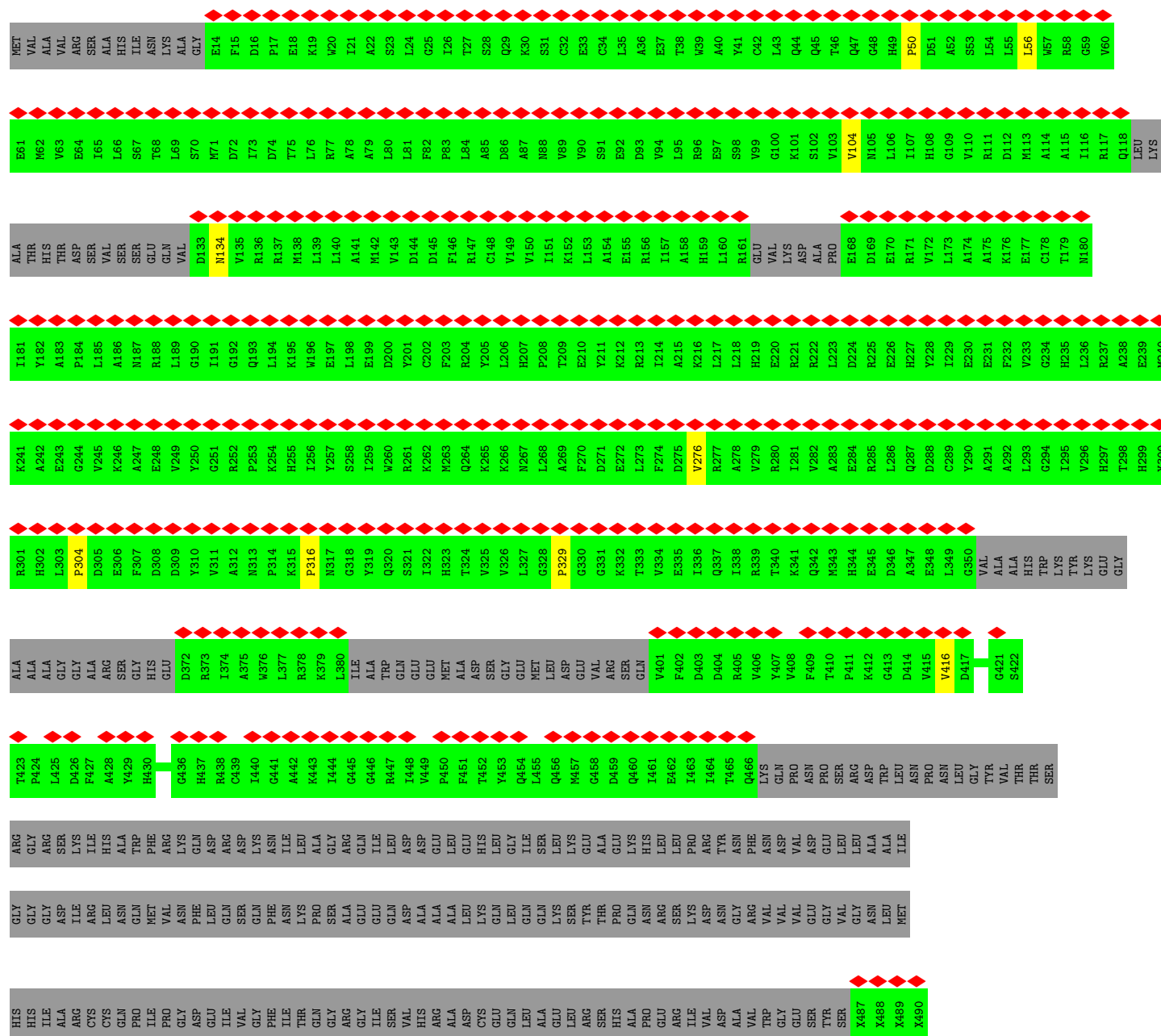


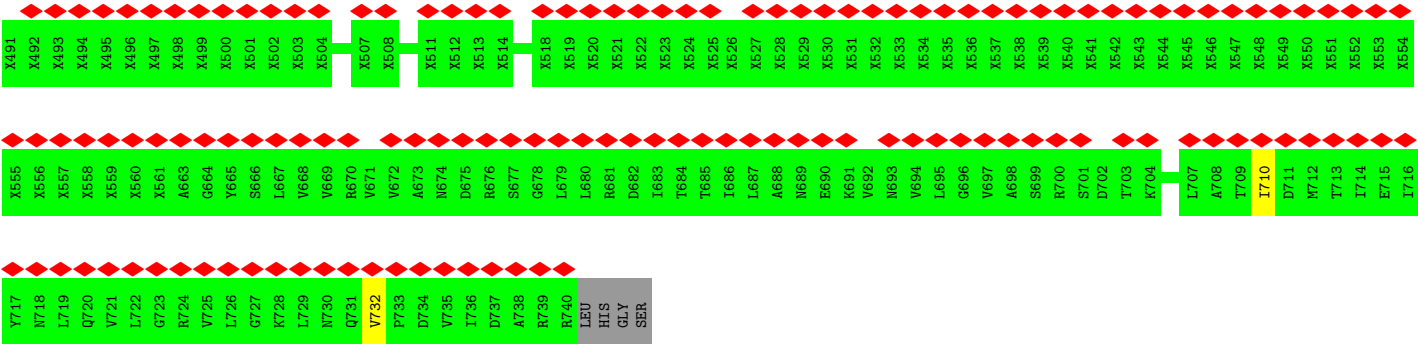
- Molecule 51: mRNA



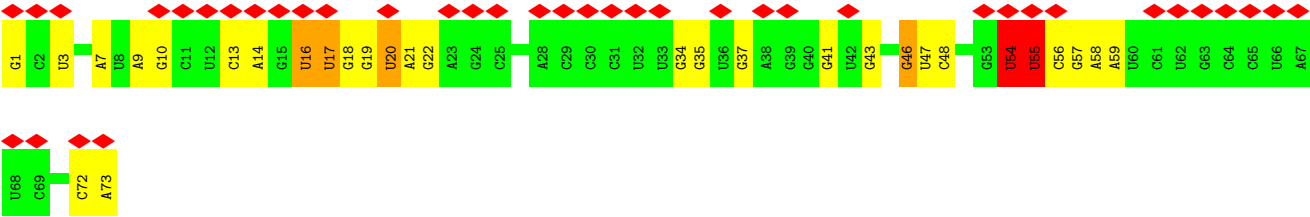


- Molecule 57: GTP pyrophosphokinase,GTP pyrophosphokinase,GTP pyrophosphokinase





● Molecule 58: deacylated A/R-tRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	24749	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 ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.003	Depositor
Minimum map value	-0.001	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.000	Depositor
Recommended contour level	0.00053	Depositor
Map size (Å)	391.92, 391.92, 391.92	wwPDB
Map dimensions	368, 368, 368	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.065, 1.065, 1.065	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MA6, 6MZ, H2U, 4OC, 7MG, OMG, PSU, 2MA, OMU, 3TD, OMC, UR3, 5MC, 5MU, 4SU, 1MG, YG, 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	A	0.12	1/68920 (0.0%)	0.67	20/107498 (0.0%)
2	B	0.23	1/2876 (0.0%)	0.65	0/4483
3	D	0.20	0/2121	0.39	0/2852
4	E	0.21	0/1586	0.38	0/2134
5	F	0.20	0/1571	0.37	0/2113
6	G	0.21	0/1434	0.40	0/1926
7	H	0.20	0/1343	0.37	0/1816
8	I	0.21	0/1122	0.38	0/1515
9	N	0.21	0/1152	0.39	0/1551
10	O	0.20	0/947	0.40	0/1268
11	P	0.20	0/1054	0.39	0/1403
12	Q	0.21	0/1093	0.41	0/1460
13	R	0.21	0/973	0.39	0/1301
14	S	0.20	0/902	0.35	0/1209
15	T	0.20	0/929	0.41	0/1242
16	U	0.21	0/960	0.35	0/1278
17	V	0.21	0/829	0.38	0/1107
18	W	0.19	0/864	0.39	0/1156
19	X	0.20	0/744	0.39	0/994
20	Y	0.21	0/787	0.37	0/1051
21	Z	0.20	0/766	0.36	0/1025
22	0	0.20	0/582	0.35	0/769
23	1	0.19	0/635	0.36	0/848
24	2	0.21	0/510	0.36	0/677
25	3	0.21	0/453	0.41	0/605
26	4	0.21	0/531	0.40	0/709
27	5	0.19	0/450	0.36	0/599
28	6	0.21	0/416	0.41	0/554
29	7	0.20	0/380	0.36	0/498
30	8	0.21	0/513	0.42	0/676
31	9	0.19	0/303	0.38	0/397

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	a	0.13	1/36701 (0.0%)	0.66	5/57246 (0.0%)
33	b	0.21	0/1735	0.39	0/2338
34	c	0.21	0/1651	0.41	0/2225
35	d	0.21	0/1665	0.38	0/2227
36	e	0.22	0/1154	0.41	0/1554
37	f	0.21	0/835	0.39	0/1128
38	g	0.20	0/1195	0.39	0/1602
39	h	0.21	0/989	0.40	0/1326
40	i	0.21	0/1034	0.40	0/1375
41	j	0.21	0/796	0.42	0/1077
42	k	0.20	0/885	0.39	0/1195
43	l	0.21	0/969	0.42	0/1300
44	m	0.20	0/892	0.41	0/1193
45	o	0.20	0/722	0.35	0/964
46	p	0.20	0/659	0.35	0/884
47	q	0.22	0/657	0.43	0/881
48	r	0.20	0/511	0.40	0/689
49	t	0.20	0/671	0.34	0/888
50	u	0.21	0/500	0.38	0/668
51	v	0.10	0/144	0.64	0/222
52	x	0.27	1/1747 (0.1%)	0.64	0/2721
53	J	0.22	0/1001	0.43	0/1350
54	K	0.21	0/1046	0.41	0/1410
55	n	0.20	0/811	0.37	0/1081
56	s	0.20	0/652	0.37	0/877
57	z	0.16	0/1874	0.32	0/2332
58	y	0.29	1/1585 (0.1%)	0.66	0/2469
All	All	0.16	5/160827 (0.0%)	0.60	25/239936 (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
1	A	35	0
32	a	17	0
52	x	9	0
58	y	9	0
All	All	70	0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	U	OP3-P	-10.62	1.48	1.61
58	y	1	G	OP3-P	-10.62	1.48	1.61
52	x	1	C	OP3-P	-10.58	1.48	1.61
32	a	2	A	OP3-P	-10.57	1.48	1.61
1	A	1	G	OP3-P	-10.54	1.48	1.61

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1049	C	C2-N3-C4	18.01	128.91	119.90
1	A	1050	A	N1-C2-N3	16.54	137.57	129.30
1	A	1073	A	N1-C2-N3	16.48	137.54	129.30
1	A	1050	A	C2-N3-C4	12.07	116.63	110.60
1	A	1073	A	C2-N3-C4	11.70	116.45	110.60
1	A	1049	C	N3-C4-C5	10.61	126.14	121.90
1	A	1073	A	C6-N1-C2	10.21	124.72	118.60
1	A	1050	A	C6-N1-C2	10.07	124.64	118.60
32	a	1158	C	N1-C2-O2	8.98	124.29	118.90
32	a	1158	C	C2-N1-C1'	8.38	128.02	118.80
1	A	1313	U	C2-N1-C1'	7.96	127.25	117.70
1	A	2884	U	C2-N1-C1'	7.82	127.09	117.70
32	a	1158	C	N3-C2-O2	-7.38	116.73	121.90
1	A	2884	U	N1-C2-O2	7.29	127.90	122.80
1	A	1313	U	N1-C2-O2	7.25	127.88	122.80
1	A	2884	U	N3-C2-O2	-6.77	117.46	122.20
1	A	1313	U	N3-C2-O2	-6.54	117.62	122.20
32	a	1158	C	C6-N1-C2	-5.82	117.97	120.30
1	A	51	G	OP2-P-O3'	5.76	117.88	105.20
1	A	1049	C	N1-C2-N3	5.75	123.22	119.20
32	a	1158	C	C6-N1-C1'	-5.73	113.93	120.80
1	A	893	C	P-O3'-C3'	5.42	126.20	119.70
1	A	1313	U	C6-N1-C1'	-5.19	113.94	121.20
1	A	51	G	P-O3'-C3'	5.14	125.87	119.70
1	A	2884	U	C6-N1-C1'	-5.01	114.19	121.20

All (70) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	746	PSU	C2',C4'
1	A	955	PSU	C2',C4'
1	A	1835	2MG	C2',C3'
1	A	1911	PSU	C2',C4'
1	A	1915	3TD	C4'

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Mol	Chain	Res	Type	Atom
1	A	1917	PSU	C2',C4'
1	A	1939	5MU	C2',C4',C3'
1	A	2069	7MG	C1'
1	A	2251	OMG	C3',C1'
1	A	2445	2MG	C2',C3'
1	A	2449	H2U	C1'
1	A	2457	PSU	C2',C4'
1	A	2498	OMC	C2',C4'
1	A	2503	2MA	C2',C1'
1	A	2504	PSU	C2',C4'
1	A	2552	OMU	C4'
1	A	2580	PSU	C2',C4'
1	A	2604	PSU	C2',C4'
1	A	2605	PSU	C2',C4'
32	a	516	PSU	C2',C4'
32	a	527	7MG	C1'
32	a	966	2MG	C2',C3'
32	a	1207	2MG	C2',C3'
32	a	1402	4OC	C2',C1'
32	a	1498	UR3	C2',C3'
32	a	1516	2MG	C2',C3'
32	a	1518	MA6	C2',C3'
32	a	1519	MA6	C2',C3'
52	x	8	4SU	C2',C4',C3'
52	x	20	H2U	C1'
52	x	54	5MU	C2',C4',C3'
52	x	55	PSU	C2',C4'
58	y	16	H2U	C1'
58	y	17	H2U	C1'
58	y	20	H2U	C1'
58	y	46	7MG	C1'
58	y	54	5MU	C2',C4',C3'
58	y	55	PSU	C2',C4'

There are no planarity outliers.

5.2 Too-close contacts

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	269/273 (98%)	243 (90%)	25 (9%)	1 (0%)	30	62
4	E	207/209 (99%)	187 (90%)	17 (8%)	3 (1%)	9	39
5	F	199/201 (99%)	184 (92%)	11 (6%)	4 (2%)	6	34
6	G	175/179 (98%)	154 (88%)	18 (10%)	3 (2%)	7	36
7	H	174/177 (98%)	149 (86%)	23 (13%)	2 (1%)	12	43
8	I	147/149 (99%)	129 (88%)	14 (10%)	4 (3%)	4	29
9	N	140/142 (99%)	130 (93%)	8 (6%)	2 (1%)	9	39
10	O	120/123 (98%)	108 (90%)	7 (6%)	5 (4%)	2	21
11	P	141/144 (98%)	122 (86%)	13 (9%)	6 (4%)	2	20
12	Q	134/136 (98%)	123 (92%)	8 (6%)	3 (2%)	5	32
13	R	118/127 (93%)	103 (87%)	12 (10%)	3 (2%)	4	30
14	S	114/117 (97%)	106 (93%)	6 (5%)	2 (2%)	7	35
15	T	112/115 (97%)	105 (94%)	7 (6%)	0	100	100
16	U	115/118 (98%)	113 (98%)	2 (2%)	0	100	100
17	V	101/103 (98%)	91 (90%)	6 (6%)	4 (4%)	2	22
18	W	108/110 (98%)	94 (87%)	14 (13%)	0	100	100
19	X	91/100 (91%)	81 (89%)	8 (9%)	2 (2%)	5	32
20	Y	100/104 (96%)	87 (87%)	11 (11%)	2 (2%)	6	34
21	Z	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
22	0	73/85 (86%)	68 (93%)	4 (6%)	1 (1%)	9	39
23	1	75/78 (96%)	71 (95%)	4 (5%)	0	100	100
24	2	61/63 (97%)	59 (97%)	2 (3%)	0	100	100
25	3	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
26	4	64/70 (91%)	56 (88%)	7 (11%)	1 (2%)	8	37
27	5	54/57 (95%)	51 (94%)	2 (4%)	1 (2%)	6	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	6	48/55 (87%)	43 (90%)	4 (8%)	1 (2%)	5	33
29	7	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
30	8	62/65 (95%)	58 (94%)	3 (5%)	1 (2%)	8	37
31	9	36/38 (95%)	32 (89%)	3 (8%)	1 (3%)	4	28
33	b	216/240 (90%)	187 (87%)	25 (12%)	4 (2%)	6	35
34	c	204/233 (88%)	188 (92%)	14 (7%)	2 (1%)	13	44
35	d	203/206 (98%)	180 (89%)	19 (9%)	4 (2%)	6	34
36	e	155/167 (93%)	132 (85%)	17 (11%)	6 (4%)	2	22
37	f	98/135 (73%)	85 (87%)	9 (9%)	4 (4%)	2	22
38	g	149/179 (83%)	130 (87%)	13 (9%)	6 (4%)	2	22
39	h	127/130 (98%)	115 (91%)	11 (9%)	1 (1%)	16	49
40	i	125/130 (96%)	107 (86%)	13 (10%)	5 (4%)	2	22
41	j	96/103 (93%)	79 (82%)	11 (12%)	6 (6%)	1	15
42	k	114/129 (88%)	99 (87%)	11 (10%)	4 (4%)	3	25
43	l	121/124 (98%)	104 (86%)	9 (7%)	8 (7%)	1	14
44	m	112/118 (95%)	103 (92%)	7 (6%)	2 (2%)	7	35
45	o	86/89 (97%)	76 (88%)	5 (6%)	5 (6%)	1	16
46	p	80/82 (98%)	71 (89%)	7 (9%)	2 (2%)	4	30
47	q	78/84 (93%)	65 (83%)	9 (12%)	4 (5%)	1	18
48	r	63/75 (84%)	56 (89%)	4 (6%)	3 (5%)	2	19
49	t	83/87 (95%)	80 (96%)	3 (4%)	0	100	100
50	u	63/71 (89%)	48 (76%)	10 (16%)	5 (8%)	1	10
53	J	129/165 (78%)	102 (79%)	21 (16%)	6 (5%)	2	19
54	K	139/142 (98%)	118 (85%)	14 (10%)	7 (5%)	1	18
55	n	99/102 (97%)	87 (88%)	8 (8%)	4 (4%)	2	22
56	s	77/92 (84%)	71 (92%)	5 (6%)	1 (1%)	10	40
57	z	458/819 (56%)	423 (92%)	24 (5%)	11 (2%)	5	30
All	All	6305/7039 (90%)	5637 (89%)	516 (8%)	152 (2%)	7	30

All (152) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	N	81	ILE

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Mol	Chain	Res	Type
11	P	128	THR
34	c	96	VAL
34	c	156	LEU
36	e	122	VAL
48	r	17	VAL
54	K	22	PRO
54	K	92	PRO
55	n	38	ASP
57	z	50	PRO
57	z	104	VAL
57	z	304	PRO
57	z	316	PRO
57	z	329	PRO
57	z	732	VAL
7	H	108	PHE
8	I	9	VAL
9	N	82	GLY
11	P	85	VAL
11	P	111	ILE
17	V	55	ASP
20	Y	97	SER
28	6	45	HIS
31	9	29	ALA
35	d	26	ALA
35	d	191	SER
37	f	92	THR
38	g	16	LYS
38	g	29	LEU
38	g	56	SER
39	h	74	ILE
40	i	90	ASP
41	j	57	VAL
42	k	88	PRO
43	l	42	LYS
44	m	6	ILE
46	p	8	ARG
50	u	30	GLU
50	u	37	TYR
53	J	55	VAL
53	J	90	GLY
54	K	12	VAL
55	n	54	ASP

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Mol	Chain	Res	Type
57	z	56	LEU
4	E	169	ARG
5	F	122	GLU
6	G	18	GLU
7	H	45	ALA
8	I	15	LEU
11	P	29	LYS
11	P	94	THR
13	R	59	SER
17	V	43	ASN
20	Y	6	ARG
22	0	17	LEU
33	b	11	ALA
35	d	152	SER
36	e	23	THR
36	e	98	ALA
37	f	54	LEU
37	f	63	ASN
37	f	86	ARG
38	g	64	ALA
38	g	145	GLU
40	i	57	VAL
40	i	107	ALA
40	i	125	GLN
42	k	92	ARG
43	l	2	THR
43	l	23	LEU
43	l	33	CYS
44	m	113	LYS
45	o	2	LEU
47	q	17	GLU
47	q	49	ASN
48	r	18	GLN
50	u	12	ASP
54	K	20	SER
54	K	64	ARG
54	K	100	ILE
55	n	2	LYS
4	E	58	ASN
4	E	148	GLN
5	F	80	SER
10	O	109	SER

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Mol	Chain	Res	Type
12	Q	14	LYS
12	Q	70	ASP
14	S	100	HIS
19	X	38	ALA
26	4	26	SER
33	b	71	THR
33	b	153	MET
35	d	166	LYS
36	e	102	THR
41	j	29	ALA
41	j	35	GLN
43	l	46	SER
45	o	13	GLU
45	o	45	HIS
47	q	16	MET
50	u	34	ARG
53	J	22	ALA
53	J	88	HIS
55	n	22	LYS
57	z	134	ASN
57	z	276	VAL
57	z	416	VAL
5	F	83	VAL
8	I	3	VAL
8	I	89	LYS
10	O	35	VAL
10	O	93	GLN
10	O	110	GLU
11	P	36	LYS
13	R	117	ASP
14	S	66	GLY
17	V	53	PHE
27	5	2	VAL
33	b	122	ASP
41	j	33	GLY
41	j	75	ASP
42	k	126	ARG
43	l	75	GLU
43	l	77	SER
45	o	21	THR
45	o	87	ARG
50	u	32	ARG

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Mol	Chain	Res	Type
53	J	71	CYS
53	J	118	ILE
54	K	3	LYS
6	G	61	GLY
13	R	106	ASP
38	g	19	SER
40	i	9	GLY
41	j	41	PRO
47	q	79	GLU
48	r	46	THR
57	z	710	ILE
3	D	253	GLY
19	X	71	GLY
42	k	119	GLY
30	8	31	ILE
43	l	21	PRO
56	s	7	GLY
5	F	149	ILE
6	G	174	PHE
12	Q	69	PRO
46	p	36	VAL
10	O	26	GLY
17	V	54	VAL
36	e	24	VAL
36	e	93	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	216/218 (99%)	216 (100%)	0	100	100
4	E	164/164 (100%)	164 (100%)	0	100	100
5	F	165/165 (100%)	165 (100%)	0	100	100
6	G	148/150 (99%)	148 (100%)	0	100	100
7	H	137/138 (99%)	137 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	I	114/114 (100%)	114 (100%)	0	100	100
9	N	116/116 (100%)	116 (100%)	0	100	100
10	O	103/104 (99%)	103 (100%)	0	100	100
11	P	102/103 (99%)	102 (100%)	0	100	100
12	Q	109/109 (100%)	109 (100%)	0	100	100
13	R	100/103 (97%)	100 (100%)	0	100	100
14	S	86/87 (99%)	86 (100%)	0	100	100
15	T	99/100 (99%)	99 (100%)	0	100	100
16	U	89/90 (99%)	89 (100%)	0	100	100
17	V	84/84 (100%)	84 (100%)	0	100	100
18	W	93/93 (100%)	93 (100%)	0	100	100
19	X	80/84 (95%)	80 (100%)	0	100	100
20	Y	83/85 (98%)	83 (100%)	0	100	100
21	Z	78/78 (100%)	78 (100%)	0	100	100
22	0	57/63 (90%)	57 (100%)	0	100	100
23	1	67/68 (98%)	67 (100%)	0	100	100
24	2	55/55 (100%)	55 (100%)	0	100	100
25	3	48/49 (98%)	48 (100%)	0	100	100
26	4	59/62 (95%)	59 (100%)	0	100	100
27	5	47/48 (98%)	47 (100%)	0	100	100
28	6	45/49 (92%)	45 (100%)	0	100	100
29	7	38/38 (100%)	38 (100%)	0	100	100
30	8	51/52 (98%)	51 (100%)	0	100	100
31	9	34/34 (100%)	34 (100%)	0	100	100
33	b	180/198 (91%)	180 (100%)	0	100	100
34	c	170/190 (90%)	170 (100%)	0	100	100
35	d	172/173 (99%)	172 (100%)	0	100	100
36	e	114/126 (90%)	114 (100%)	0	100	100
37	f	87/116 (75%)	87 (100%)	0	100	100
38	g	124/147 (84%)	124 (100%)	0	100	100
39	h	104/105 (99%)	104 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	i	105/107 (98%)	105 (100%)	0	100	100
41	j	86/90 (96%)	86 (100%)	0	100	100
42	k	89/99 (90%)	89 (100%)	0	100	100
43	l	103/104 (99%)	103 (100%)	0	100	100
44	m	92/96 (96%)	92 (100%)	0	100	100
45	o	76/77 (99%)	76 (100%)	0	100	100
46	p	65/65 (100%)	65 (100%)	0	100	100
47	q	74/78 (95%)	74 (100%)	0	100	100
48	r	48/65 (74%)	48 (100%)	0	100	100
49	t	65/66 (98%)	65 (100%)	0	100	100
50	u	44/61 (72%)	44 (100%)	0	100	100
53	J	100/123 (81%)	100 (100%)	0	100	100
54	K	109/110 (99%)	109 (100%)	0	100	100
55	n	79/84 (94%)	79 (100%)	0	100	100
56	s	70/79 (89%)	70 (100%)	0	100	100
All	All	4823/5062 (95%)	4823 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
3	D	225	ASN
4	E	32	ASN
4	E	173	GLN
5	F	41	GLN
5	F	165	HIS
6	G	4	HIS
7	H	138	GLN
10	O	3	GLN
11	P	99	ASN
12	Q	13	HIS
13	R	9	GLN
15	T	2	ASN
15	T	11	GLN
17	V	18	GLN

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Mol	Chain	Res	Type
18	W	7	HIS
18	W	40	ASN
18	W	61	ASN
20	Y	73	ASN
21	Z	87	GLN
22	0	42	HIS
23	1	16	ASN
24	2	25	GLN
24	2	58	ASN
25	3	19	HIS
28	6	18	HIS
28	6	45	HIS
31	9	35	GLN
33	b	18	GLN
33	b	41	ASN
35	d	119	HIS
35	d	125	ASN
36	e	145	ASN
37	f	11	HIS
37	f	58	HIS
38	g	141	HIS
39	h	3	GLN
40	i	4	GLN
41	j	70	HIS
42	k	27	ASN
43	l	4	ASN
44	m	11	HIS
44	m	90	HIS
45	o	39	GLN
46	p	9	HIS
46	p	63	GLN
46	p	79	ASN
47	q	30	HIS
49	t	2	ASN
49	t	74	HIS
53	J	4	ASN
53	J	88	HIS
56	s	55	GLN
56	s	68	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2881/2903 (99%)	415 (14%)	43 (1%)
2	B	119/120 (99%)	13 (10%)	2 (1%)
32	a	1535/1539 (99%)	176 (11%)	0
51	v	5/6 (83%)	0	0
52	x	76/77 (98%)	13 (17%)	0
58	y	72/73 (98%)	28 (38%)	0
All	All	4688/4718 (99%)	645 (13%)	45 (0%)

All (645) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	10	A
1	A	12	U
1	A	27	G
1	A	34	U
1	A	35	G
1	A	46	G
1	A	49	A
1	A	51	G
1	A	52	A
1	A	71	A
1	A	74	A
1	A	75	G
1	A	84	A
1	A	91	A
1	A	92	U
1	A	98	G
1	A	118	A
1	A	120	U
1	A	138	U
1	A	139	U
1	A	140	C
1	A	141	G
1	A	142	A
1	A	162	U
1	A	163	C
1	A	181	A
1	A	196	A
1	A	199	A
1	A	205	G
1	A	216	A
1	A	221	A
1	A	222	A

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Mol	Chain	Res	Type
1	A	242	G
1	A	243	U
1	A	248	G
1	A	249	C
1	A	255	A
1	A	266	G
1	A	267	C
1	A	276	U
1	A	278	A
1	A	294	A
1	A	310	A
1	A	311	A
1	A	323	C
1	A	329	G
1	A	330	A
1	A	353	C
1	A	361	G
1	A	367	G
1	A	371	A
1	A	373	U
1	A	386	G
1	A	387	U
1	A	391	A
1	A	404	A
1	A	406	G
1	A	411	G
1	A	424	G
1	A	451	U
1	A	456	C
1	A	457	A
1	A	458	G
1	A	459	U
1	A	480	A
1	A	481	G
1	A	491	G
1	A	504	A
1	A	505	A
1	A	506	G
1	A	529	A
1	A	530	G
1	A	532	A
1	A	533	G

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Mol	Chain	Res	Type
1	A	543	G
1	A	545	U
1	A	547	A
1	A	550	C
1	A	563	A
1	A	572	A
1	A	573	U
1	A	575	A
1	A	603	A
1	A	616	A
1	A	627	A
1	A	637	A
1	A	646	U
1	A	654	A
1	A	669	G
1	A	686	U
1	A	687	C
1	A	695	G
1	A	730	A
1	A	746	PSU
1	A	747	5MC
1	A	748	G
1	A	752	A
1	A	753	A
1	A	764	A
1	A	776	G
1	A	782	A
1	A	784	G
1	A	785	G
1	A	789	A
1	A	792	A
1	A	805	G
1	A	812	C
1	A	819	A
1	A	822	G
1	A	827	U
1	A	828	U
1	A	830	G
1	A	831	G
1	A	845	A
1	A	846	U
1	A	847	U

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Mol	Chain	Res	Type
1	A	858	G
1	A	859	G
1	A	860	U
1	A	878	A
1	A	885	C
1	A	894	U
1	A	896	A
1	A	897	C
1	A	898	C
1	A	907	G
1	A	910	A
1	A	932	U
1	A	941	A
1	A	946	C
1	A	955	PSU
1	A	956	G
1	A	961	C
1	A	974	G
1	A	983	A
1	A	995	C
1	A	996	A
1	A	1012	U
1	A	1013	C
1	A	1021	A
1	A	1022	G
1	A	1023	U
1	A	1033	U
1	A	1046	A
1	A	1047	G
1	A	1053	C
1	A	1054	A
1	A	1057	A
1	A	1060	U
1	A	1061	U
1	A	1062	G
1	A	1064	C
1	A	1065	U
1	A	1066	U
1	A	1068	G
1	A	1070	A
1	A	1071	G
1	A	1075	C

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Mol	Chain	Res	Type
1	A	1076	C
1	A	1079	C
1	A	1084	A
1	A	1088	A
1	A	1104	C
1	A	1111	A
1	A	1112	G
1	A	1119	U
1	A	1130	U
1	A	1131	G
1	A	1132	U
1	A	1133	A
1	A	1135	C
1	A	1143	A
1	A	1174	U
1	A	1176	U
1	A	1177	G
1	A	1180	U
1	A	1206	G
1	A	1212	G
1	A	1250	G
1	A	1251	C
1	A	1253	A
1	A	1256	G
1	A	1271	G
1	A	1272	A
1	A	1300	G
1	A	1301	A
1	A	1306	C
1	A	1314	C
1	A	1321	A
1	A	1329	U
1	A	1332	G
1	A	1341	G
1	A	1345	C
1	A	1365	A
1	A	1368	G
1	A	1378	A
1	A	1379	U
1	A	1383	A
1	A	1416	G
1	A	1419	A

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Mol	Chain	Res	Type
1	A	1420	A
1	A	1428	C
1	A	1454	C
1	A	1461	C
1	A	1475	G
1	A	1482	G
1	A	1490	A
1	A	1491	G
1	A	1504	A
1	A	1515	A
1	A	1524	G
1	A	1533	C
1	A	1535	A
1	A	1536	C
1	A	1555	G
1	A	1559	U
1	A	1560	G
1	A	1569	A
1	A	1581	G
1	A	1585	C
1	A	1611	C
1	A	1634	A
1	A	1647	U
1	A	1648	U
1	A	1654	A
1	A	1670	C
1	A	1674	G
1	A	1694	C
1	A	1695	G
1	A	1715	G
1	A	1729	U
1	A	1730	C
1	A	1733	G
1	A	1738	G
1	A	1758	U
1	A	1764	C
1	A	1773	A
1	A	1780	A
1	A	1781	U
1	A	1784	A
1	A	1791	A
1	A	1800	C

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Mol	Chain	Res	Type
1	A	1801	A
1	A	1802	A
1	A	1808	A
1	A	1816	C
1	A	1829	A
1	A	1833	C
1	A	1835	2MG
1	A	1836	C
1	A	1871	A
1	A	1901	A
1	A	1906	G
1	A	1911	PSU
1	A	1912	A
1	A	1913	A
1	A	1914	C
1	A	1917	PSU
1	A	1918	A
1	A	1919	A
1	A	1929	G
1	A	1930	G
1	A	1937	A
1	A	1938	A
1	A	1939	5MU
1	A	1940	U
1	A	1941	C
1	A	1944	U
1	A	1955	U
1	A	1967	C
1	A	1970	A
1	A	1971	U
1	A	1972	G
1	A	1991	U
1	A	1993	U
1	A	1997	C
1	A	2021	C
1	A	2022	U
1	A	2023	C
1	A	2031	A
1	A	2033	A
1	A	2043	C
1	A	2049	G
1	A	2052	A

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Mol	Chain	Res	Type
1	A	2055	C
1	A	2056	G
1	A	2060	A
1	A	2061	G
1	A	2062	A
1	A	2069	7MG
1	A	2072	C
1	A	2093	G
1	A	2096	C
1	A	2098	U
1	A	2110	G
1	A	2111	U
1	A	2112	G
1	A	2113	U
1	A	2116	G
1	A	2118	U
1	A	2119	A
1	A	2127	G
1	A	2131	U
1	A	2132	U
1	A	2133	G
1	A	2145	C
1	A	2162	G
1	A	2164	C
1	A	2170	A
1	A	2172	U
1	A	2173	A
1	A	2198	A
1	A	2204	G
1	A	2211	A
1	A	2213	U
1	A	2225	A
1	A	2226	C
1	A	2250	G
1	A	2251	OMG
1	A	2252	G
1	A	2278	A
1	A	2283	C
1	A	2286	G
1	A	2287	A
1	A	2305	U
1	A	2309	A

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Mol	Chain	Res	Type
1	A	2320	U
1	A	2327	A
1	A	2334	U
1	A	2335	A
1	A	2350	C
1	A	2354	C
1	A	2383	G
1	A	2385	C
1	A	2392	A
1	A	2402	U
1	A	2407	A
1	A	2423	U
1	A	2424	C
1	A	2426	A
1	A	2428	G
1	A	2429	G
1	A	2430	A
1	A	2431	U
1	A	2435	A
1	A	2441	U
1	A	2445	2MG
1	A	2446	G
1	A	2448	A
1	A	2449	H2U
1	A	2450	A
1	A	2457	PSU
1	A	2458	G
1	A	2476	A
1	A	2498	OMC
1	A	2499	C
1	A	2502	G
1	A	2504	PSU
1	A	2505	G
1	A	2506	U
1	A	2518	A
1	A	2529	G
1	A	2547	A
1	A	2552	OMU
1	A	2553	G
1	A	2554	U
1	A	2567	G
1	A	2572	A

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Mol	Chain	Res	Type
1	A	2580	PSU
1	A	2581	G
1	A	2585	U
1	A	2586	U
1	A	2602	A
1	A	2604	PSU
1	A	2605	PSU
1	A	2606	C
1	A	2609	U
1	A	2613	U
1	A	2614	A
1	A	2629	U
1	A	2636	C
1	A	2646	C
1	A	2655	G
1	A	2656	U
1	A	2682	A
1	A	2689	U
1	A	2690	U
1	A	2714	G
1	A	2718	G
1	A	2726	A
1	A	2739	U
1	A	2744	G
1	A	2748	A
1	A	2757	A
1	A	2764	A
1	A	2765	A
1	A	2778	A
1	A	2779	U
1	A	2780	G
1	A	2791	G
1	A	2794	C
1	A	2797	U
1	A	2799	A
1	A	2800	A
1	A	2808	G
1	A	2809	A
1	A	2818	U
1	A	2820	A
1	A	2833	U
1	A	2849	U

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Mol	Chain	Res	Type
1	A	2867	G
1	A	2868	A
1	A	2880	C
1	A	2893	A
1	A	2894	G
2	B	4	C
2	B	13	G
2	B	35	C
2	B	44	G
2	B	45	A
2	B	53	A
2	B	67	G
2	B	88	C
2	B	89	U
2	B	90	C
2	B	91	C
2	B	108	A
2	B	109	A
32	a	6	G
32	a	7	A
32	a	9	G
32	a	22	G
32	a	32	A
32	a	39	G
32	a	51	A
32	a	71	A
32	a	86	G
32	a	87	C
32	a	121	U
32	a	130	A
32	a	183	C
32	a	184	G
32	a	209	U
32	a	210	C
32	a	212	G
32	a	226	G
32	a	247	G
32	a	251	G
32	a	266	G
32	a	267	C
32	a	280	C
32	a	281	G

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Mol	Chain	Res	Type
32	a	282	A
32	a	289	G
32	a	306	A
32	a	328	C
32	a	345	C
32	a	347	G
32	a	351	G
32	a	352	C
32	a	367	U
32	a	372	C
32	a	392	C
32	a	406	G
32	a	413	G
32	a	422	C
32	a	424	G
32	a	429	U
32	a	467	U
32	a	479	U
32	a	484	G
32	a	485	U
32	a	486	U
32	a	496	A
32	a	497	G
32	a	516	PSU
32	a	517	G
32	a	527	7MG
32	a	530	G
32	a	531	U
32	a	532	A
32	a	533	A
32	a	547	A
32	a	561	U
32	a	564	C
32	a	572	A
32	a	573	A
32	a	575	G
32	a	576	C
32	a	577	G
32	a	633	G
32	a	642	A
32	a	665	A
32	a	688	G

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Mol	Chain	Res	Type
32	a	702	A
32	a	703	G
32	a	723	U
32	a	724	G
32	a	731	G
32	a	733	G
32	a	748	G
32	a	755	G
32	a	777	A
32	a	815	A
32	a	817	C
32	a	818	G
32	a	819	A
32	a	820	U
32	a	832	G
32	a	843	U
32	a	844	G
32	a	846	G
32	a	871	U
32	a	890	G
32	a	902	G
32	a	934	C
32	a	935	A
32	a	939	G
32	a	960	U
32	a	961	U
32	a	966	2MG
32	a	967	5MC
32	a	968	A
32	a	969	A
32	a	975	A
32	a	976	G
32	a	977	A
32	a	989	U
32	a	991	U
32	a	992	U
32	a	993	G
32	a	1004	A
32	a	1026	G
32	a	1028	C
32	a	1030	U
32	a	1031	C

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Mol	Chain	Res	Type
32	a	1033	G
32	a	1034	G
32	a	1035	A
32	a	1056	U
32	a	1065	U
32	a	1085	U
32	a	1094	G
32	a	1101	A
32	a	1130	A
32	a	1137	C
32	a	1138	G
32	a	1139	G
32	a	1152	A
32	a	1159	U
32	a	1168	U
32	a	1183	U
32	a	1184	G
32	a	1191	A
32	a	1196	A
32	a	1197	A
32	a	1201	A
32	a	1202	U
32	a	1207	2MG
32	a	1208	C
32	a	1212	U
32	a	1213	A
32	a	1225	A
32	a	1238	A
32	a	1240	U
32	a	1241	G
32	a	1256	A
32	a	1258	G
32	a	1260	G
32	a	1278	G
32	a	1280	A
32	a	1282	C
32	a	1287	A
32	a	1298	U
32	a	1300	G
32	a	1301	U
32	a	1302	C
32	a	1317	C

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Mol	Chain	Res	Type
32	a	1323	G
32	a	1347	G
32	a	1348	U
32	a	1363	A
32	a	1395	C
32	a	1400	C
32	a	1403	C
32	a	1408	A
32	a	1446	A
32	a	1448	C
32	a	1452	C
32	a	1492	A
32	a	1494	G
32	a	1498	UR3
32	a	1499	A
32	a	1502	A
32	a	1503	A
32	a	1506	U
32	a	1516	2MG
32	a	1517	G
32	a	1520	C
32	a	1529	G
32	a	1530	G
32	a	1534	A
32	a	1535	C
32	a	1536	C
52	x	8	4SU
52	x	9	G
52	x	16	C
52	x	17	C
52	x	17(A)	U
52	x	18	G
52	x	19	G
52	x	20	H2U
52	x	21	A
52	x	22	G
52	x	54	5MU
52	x	55	PSU
52	x	56	C
58	y	3	U
58	y	7	A
58	y	9	A

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Mol	Chain	Res	Type
58	y	10	G
58	y	13	C
58	y	14	A
58	y	16	H2U
58	y	17	H2U
58	y	18	G
58	y	19	G
58	y	20	H2U
58	y	21	A
58	y	22	G
58	y	34	G
58	y	35	G
58	y	41	G
58	y	43	G
58	y	46	7MG
58	y	47	U
58	y	48	C
58	y	54	5MU
58	y	55	PSU
58	y	56	C
58	y	57	G
58	y	58	A
58	y	59	A
58	y	72	C
58	y	73	A

All (45) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	51	G
1	A	86	G
1	A	204	A
1	A	242	G
1	A	372	G
1	A	458	G
1	A	479	A
1	A	490	C
1	A	746	PSU
1	A	752	A
1	A	858	G
1	A	859	G
1	A	893	C

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Mol	Chain	Res	Type
1	A	955	PSU
1	A	1020	A
1	A	1022	G
1	A	1070	A
1	A	1130	U
1	A	1182	G
1	A	1190	G
1	A	1300	G
1	A	1399	C
1	A	1835	2MG
1	A	1911	PSU
1	A	1917	PSU
1	A	1939	5MU
1	A	1940	U
1	A	2251	OMG
1	A	2286	G
1	A	2326	C
1	A	2333	A
1	A	2391	G
1	A	2445	2MG
1	A	2449	H2U
1	A	2457	PSU
1	A	2498	OMC
1	A	2504	PSU
1	A	2566	A
1	A	2580	PSU
1	A	2605	PSU
1	A	2655	G
1	A	2756	U
1	A	2808	G
2	B	66	A
2	B	88	C

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection.

RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	A	2604	1	18,21,22	1.68	3 (16%)	22,30,33	2.10	5 (22%)
52	H2U	x	20	52	18,21,22	3.10	5 (27%)	21,30,33	1.82	5 (23%)
32	2MG	a	1516	32	18,26,27	2.65	4 (22%)	16,38,41	1.55	3 (18%)
58	PSU	y	55	58	18,21,22	1.81	4 (22%)	22,30,33	2.09	5 (22%)
58	YG	y	37	58,1	31,42,43	1.40	3 (9%)	33,62,65	2.22	11 (33%)
1	2MG	A	1835	1	18,26,27	2.63	4 (22%)	16,38,41	1.53	3 (18%)
32	7MG	a	527	32	22,26,27	4.93	3 (13%)	29,39,42	2.50	9 (31%)
1	5MU	A	1939	1	19,22,23	2.16	5 (26%)	28,32,35	4.15	11 (39%)
32	2MG	a	1207	32	18,26,27	2.66	4 (22%)	16,38,41	1.47	3 (18%)
1	1MG	A	745	1	18,26,27	3.01	3 (16%)	19,39,42	1.31	2 (10%)
32	5MC	a	967	32	18,22,23	1.72	3 (16%)	26,32,35	1.26	3 (11%)
52	5MU	x	54	52	19,22,23	2.12	5 (26%)	28,32,35	4.12	11 (39%)
58	H2U	y	16	58	18,21,22	3.12	5 (27%)	21,30,33	1.90	5 (23%)
32	5MC	a	1407	32	18,22,23	1.70	3 (16%)	26,32,35	1.23	2 (7%)
1	OMC	A	2498	1	19,22,23	1.41	3 (15%)	26,31,34	0.89	2 (7%)
58	H2U	y	17	58	18,21,22	3.11	5 (27%)	21,30,33	1.94	5 (23%)
52	PSU	x	55	52	18,21,22	1.82	3 (16%)	22,30,33	2.06	5 (22%)
32	MA6	a	1518	32	18,26,27	0.75	0	19,38,41	1.24	3 (15%)
1	5MC	A	747	1	18,22,23	1.69	3 (16%)	26,32,35	1.24	2 (7%)
1	PSU	A	1917	1	18,21,22	1.83	4 (22%)	22,30,33	2.10	5 (22%)
1	PSU	A	2605	1	18,21,22	1.81	4 (22%)	22,30,33	2.09	5 (22%)
58	7MG	y	46	58	22,26,27	4.94	3 (13%)	29,39,42	2.37	9 (31%)
52	4SU	x	8	52	18,21,22	2.36	4 (22%)	26,30,33	2.42	7 (26%)
32	4OC	a	1402	32	20,23,24	2.60	4 (20%)	26,32,35	1.02	3 (11%)
1	2MA	A	2503	1	17,25,26	1.10	1 (5%)	17,37,40	1.18	2 (11%)
1	PSU	A	2504	1	18,21,22	1.71	3 (16%)	22,30,33	2.10	5 (22%)
1	7MG	A	2069	1	22,26,27	4.96	4 (18%)	29,39,42	2.59	9 (31%)
58	H2U	y	20	58	18,21,22	3.10	5 (27%)	21,30,33	1.80	5 (23%)
1	6MZ	A	1618	1	18,25,26	0.81	1 (5%)	16,36,39	2.17	4 (25%)
1	2MG	A	2445	1	18,26,27	2.64	4 (22%)	16,38,41	1.47	3 (18%)
1	PSU	A	2457	1	18,21,22	1.74	4 (22%)	22,30,33	2.13	5 (22%)
1	H2U	A	2449	1	18,21,22	3.10	5 (27%)	21,30,33	1.83	5 (23%)
32	UR3	a	1498	32	19,22,23	2.03	4 (21%)	26,32,35	1.61	4 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	A	1911	1	18,21,22	1.72	3 (16%)	22,30,33	2.13	5 (22%)
1	6MZ	A	2030	1	18,25,26	0.79	1 (5%)	16,36,39	2.21	4 (25%)
32	MA6	a	1519	32	18,26,27	0.70	0	19,38,41	1.38	3 (15%)
1	OMU	A	2552	1	19,22,23	2.66	7 (36%)	26,31,34	1.94	7 (26%)
58	5MU	y	54	58	19,22,23	2.16	5 (26%)	28,32,35	4.21	11 (39%)
32	PSU	a	516	32	18,21,22	1.73	3 (16%)	22,30,33	2.14	4 (18%)
1	PSU	A	955	1	18,21,22	1.77	4 (22%)	22,30,33	2.12	5 (22%)
1	PSU	A	2580	1	18,21,22	1.84	4 (22%)	22,30,33	2.13	5 (22%)
1	OMG	A	2251	52,1	18,26,27	2.88	4 (22%)	19,38,41	1.31	3 (15%)
1	PSU	A	746	1	18,21,22	1.67	3 (16%)	22,30,33	2.07	4 (18%)
1	5MC	A	1962	1	18,22,23	1.69	3 (16%)	26,32,35	1.23	3 (11%)
1	3TD	A	1915	1	18,22,23	2.85	5 (27%)	22,32,35	2.08	4 (18%)
32	2MG	a	966	32	18,26,27	2.64	4 (22%)	16,38,41	1.48	3 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	A	2604	1	2/2/5/5	3/7/25/26	0/2/2/2
52	H2U	x	20	52	1/1/8/9	5/7/38/39	0/2/2/2
32	2MG	a	1516	32	2/2/5/6	5/5/27/28	0/3/3/3
58	PSU	y	55	58	2/2/5/5	4/7/25/26	0/2/2/2
58	YG	y	37	58,1	-	1/20/42/43	0/3/4/4
1	2MG	A	1835	1	2/2/5/6	2/5/27/28	0/3/3/3
32	7MG	a	527	32	1/1/7/7	4/7/37/38	0/3/3/3
1	5MU	A	1939	1	3/3/5/5	1/7/25/26	0/2/2/2
32	2MG	a	1207	32	2/2/5/6	2/5/27/28	0/3/3/3
1	1MG	A	745	1	-	0/3/25/26	0/3/3/3
58	H2U	y	16	58	1/1/8/9	3/7/38/39	0/2/2/2
52	5MU	x	54	52	3/3/5/5	3/7/25/26	0/2/2/2
32	5MC	a	967	32	-	5/7/25/26	0/2/2/2
32	5MC	a	1407	32	-	4/7/25/26	0/2/2/2
1	OMC	A	2498	1	2/2/5/5	1/9/27/28	0/2/2/2
58	H2U	y	17	58	1/1/8/9	3/7/38/39	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	PSU	x	55	52	2/2/5/5	5/7/25/26	0/2/2/2
32	MA6	a	1518	32	2/2/6/6	6/7/29/30	0/3/3/3
1	PSU	A	1917	1	2/2/5/5	3/7/25/26	0/2/2/2
1	5MC	A	747	1	-	6/7/25/26	0/2/2/2
1	PSU	A	2605	1	2/2/5/5	2/7/25/26	0/2/2/2
58	7MG	y	46	58	1/1/7/7	3/7/37/38	0/3/3/3
52	4SU	x	8	52	3/3/5/5	3/7/25/26	0/2/2/2
32	4OC	a	1402	32	2/2/5/6	3/9/29/30	0/2/2/2
1	2MA	A	2503	1	2/2/5/5	2/3/25/26	0/3/3/3
1	PSU	A	2504	1	2/2/5/5	3/7/25/26	0/2/2/2
1	7MG	A	2069	1	1/1/7/7	3/7/37/38	0/3/3/3
58	H2U	y	20	58	1/1/8/9	5/7/38/39	0/2/2/2
1	6MZ	A	1618	1	-	2/5/27/28	0/3/3/3
1	2MG	A	2445	1	2/2/5/6	1/5/27/28	0/3/3/3
1	PSU	A	2457	1	2/2/5/5	3/7/25/26	0/2/2/2
1	H2U	A	2449	1	1/1/8/9	4/7/38/39	0/2/2/2
32	UR3	a	1498	32	2/2/5/5	5/7/25/26	0/2/2/2
1	PSU	A	1911	1	2/2/5/5	3/7/25/26	0/2/2/2
1	6MZ	A	2030	1	-	3/5/27/28	0/3/3/3
32	MA6	a	1519	32	2/2/6/6	3/7/29/30	0/3/3/3
1	OMU	A	2552	1	1/1/5/5	5/9/27/28	0/2/2/2
58	5MU	y	54	58	3/3/5/5	3/7/25/26	0/2/2/2
32	PSU	a	516	32	2/2/5/5	3/7/25/26	0/2/2/2
1	PSU	A	955	1	2/2/5/5	3/7/25/26	0/2/2/2
1	PSU	A	2580	1	2/2/5/5	3/7/25/26	0/2/2/2
1	OMG	A	2251	52,1	2/2/5/5	4/5/27/28	0/3/3/3
1	PSU	A	746	1	2/2/5/5	2/7/25/26	0/2/2/2
1	5MC	A	1962	1	-	3/7/25/26	0/2/2/2
1	3TD	A	1915	1	1/1/5/5	6/7/25/26	0/2/2/2
32	2MG	a	966	32	2/2/5/6	3/5/27/28	0/3/3/3

All (164) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	y	46	7MG	C8-N9	-20.28	1.34	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2069	7MG	C8-N9	-20.26	1.34	1.46
32	a	527	7MG	C8-N9	-20.21	1.34	1.46
1	A	2251	OMG	O6-C6	10.20	1.44	1.23
1	A	745	1MG	O6-C6	10.10	1.42	1.22
32	a	1402	4OC	O2-C2	10.04	1.42	1.23
1	A	2069	7MG	O6-C6	9.58	1.41	1.23
58	y	46	7MG	O6-C6	9.57	1.41	1.23
32	a	527	7MG	O6-C6	9.41	1.41	1.23
58	y	17	H2U	O4-C4	9.36	1.42	1.23
1	A	2449	H2U	O4-C4	9.35	1.42	1.23
58	y	20	H2U	O4-C4	9.33	1.42	1.23
52	x	20	H2U	O4-C4	9.32	1.42	1.23
58	y	16	H2U	O4-C4	9.32	1.42	1.23
32	a	1207	2MG	O6-C6	9.03	1.41	1.23
32	a	1516	2MG	O6-C6	9.02	1.41	1.23
32	a	966	2MG	O6-C6	9.01	1.41	1.23
1	A	2445	2MG	O6-C6	8.98	1.41	1.23
1	A	1835	2MG	O6-C6	8.94	1.41	1.23
1	A	2552	OMU	O4-C4	8.75	1.41	1.24
1	A	1915	3TD	O4-C4	8.63	1.41	1.23
52	x	8	4SU	O2-C2	8.35	1.38	1.23
58	y	16	H2U	C6-N1	-6.67	1.35	1.47
32	a	1498	UR3	O4-C4	6.59	1.37	1.23
1	A	2449	H2U	C6-N1	-6.57	1.35	1.47
52	x	20	H2U	C6-N1	-6.54	1.35	1.47
58	y	17	H2U	C6-N1	-6.54	1.35	1.47
58	y	20	H2U	C6-N1	-6.52	1.35	1.47
1	A	1915	3TD	C6-C5	6.30	1.42	1.35
1	A	745	1MG	C2-N2	5.80	1.44	1.34
1	A	1939	5MU	C6-C5	5.70	1.44	1.34
58	y	54	5MU	C6-C5	5.62	1.43	1.34
52	x	54	5MU	C6-C5	5.53	1.43	1.34
32	a	1516	2MG	C2-N2	5.34	1.45	1.33
1	A	2445	2MG	C2-N2	5.33	1.45	1.33
32	a	1207	2MG	C2-N2	5.33	1.45	1.33
1	A	1835	2MG	C2-N2	5.32	1.45	1.33
32	a	966	2MG	C2-N2	5.31	1.45	1.33
52	x	55	PSU	C6-C5	5.26	1.41	1.35
1	A	2580	PSU	C6-C5	5.21	1.41	1.35
1	A	2605	PSU	C6-C5	5.16	1.41	1.35
1	A	1917	PSU	C6-C5	5.13	1.41	1.35
1	A	2251	OMG	C2-N2	5.12	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	y	55	PSU	C6-C5	5.08	1.41	1.35
1	A	955	PSU	C6-C5	5.07	1.41	1.35
58	y	37	YG	O23-C21	-5.02	1.25	1.34
32	a	516	PSU	C6-C5	5.00	1.41	1.35
1	A	2504	PSU	C6-C5	4.98	1.41	1.35
1	A	746	PSU	C6-C5	4.97	1.41	1.35
1	A	2457	PSU	C6-C5	4.95	1.41	1.35
1	A	1911	PSU	C6-C5	4.95	1.41	1.35
1	A	2604	PSU	C6-C5	4.93	1.41	1.35
58	y	54	5MU	C2-N3	-4.67	1.29	1.38
1	A	1939	5MU	C2-N3	-4.67	1.29	1.38
52	x	54	5MU	C2-N3	-4.60	1.29	1.38
32	a	967	5MC	C6-C5	4.36	1.41	1.34
32	a	1407	5MC	C6-C5	4.32	1.41	1.34
1	A	2552	OMU	C2-N1	-4.29	1.31	1.38
1	A	1962	5MC	C6-C5	4.29	1.41	1.34
58	y	46	7MG	C2-N2	4.27	1.44	1.34
1	A	747	5MC	C6-C5	4.27	1.41	1.34
1	A	2069	7MG	C2-N2	4.26	1.44	1.34
32	a	527	7MG	C2-N2	4.24	1.44	1.34
1	A	745	1MG	CM1-N1	-4.23	1.39	1.47
52	x	20	H2U	C5-C4	-4.18	1.40	1.50
58	y	16	H2U	C5-C4	-4.17	1.40	1.50
58	y	20	H2U	C5-C4	-4.17	1.40	1.50
1	A	2449	H2U	C5-C4	-4.15	1.40	1.50
58	y	17	H2U	C5-C4	-4.14	1.40	1.50
58	y	54	5MU	C2-N1	-4.10	1.31	1.38
52	x	54	5MU	C2-N1	-3.94	1.32	1.38
1	A	1939	5MU	C2-N1	-3.83	1.32	1.38
1	A	955	PSU	C2-N1	-3.76	1.31	1.36
32	a	516	PSU	C2-N1	-3.75	1.31	1.36
1	A	2498	OMC	C4-N4	3.75	1.42	1.33
58	y	20	H2U	C6-C5	-3.74	1.42	1.52
1	A	2449	H2U	C6-C5	-3.74	1.42	1.52
52	x	20	H2U	C6-C5	-3.73	1.42	1.52
58	y	16	H2U	C6-C5	-3.73	1.42	1.52
58	y	55	PSU	C2-N1	-3.72	1.31	1.36
58	y	17	H2U	C6-C5	-3.71	1.42	1.52
1	A	1911	PSU	C2-N1	-3.71	1.31	1.36
1	A	1917	PSU	C2-N1	-3.71	1.31	1.36
52	x	55	PSU	C2-N1	-3.71	1.31	1.36
32	a	967	5MC	C4-N4	3.70	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2605	PSU	C2-N1	-3.69	1.31	1.36
32	a	1407	5MC	C4-N4	3.69	1.43	1.34
1	A	747	5MC	C4-N4	3.68	1.43	1.34
1	A	2580	PSU	C2-N1	-3.66	1.31	1.36
1	A	1962	5MC	C4-N4	3.66	1.43	1.34
1	A	2552	OMU	C4-N3	-3.65	1.32	1.38
1	A	2504	PSU	C2-N1	-3.65	1.31	1.36
1	A	2457	PSU	C2-N1	-3.63	1.31	1.36
1	A	2503	2MA	C6-N6	3.62	1.43	1.28
1	A	746	PSU	C2-N1	-3.61	1.31	1.36
1	A	2604	PSU	C2-N1	-3.59	1.31	1.36
32	a	1402	4OC	C4-N4	3.44	1.43	1.35
32	a	1498	UR3	C6-C5	3.36	1.42	1.35
1	A	1962	5MC	C2-N1	-3.21	1.33	1.40
1	A	747	5MC	C2-N1	-3.19	1.33	1.40
32	a	967	5MC	C2-N1	-3.19	1.33	1.40
32	a	1407	5MC	C2-N1	-3.17	1.33	1.40
58	y	37	YG	O18-C16	-3.15	1.25	1.33
1	A	2498	OMC	C2-N1	-3.15	1.33	1.40
1	A	1915	3TD	C10-N3	-3.09	1.41	1.47
1	A	1915	3TD	C2-N3	-3.06	1.31	1.38
52	x	20	H2U	C2-N3	-3.03	1.32	1.38
32	a	1498	UR3	C2-N3	-3.02	1.33	1.39
58	y	17	H2U	C2-N3	-3.02	1.32	1.38
58	y	16	H2U	C2-N3	-3.01	1.32	1.38
52	x	8	4SU	C2-N3	-3.01	1.32	1.38
58	y	20	H2U	C2-N3	-3.00	1.32	1.38
1	A	2449	H2U	C2-N3	-2.98	1.32	1.38
1	A	1939	5MU	C6-N1	-2.90	1.33	1.38
1	A	2552	OMU	C6-C5	2.89	1.41	1.35
58	y	54	5MU	C6-N1	-2.87	1.33	1.38
1	A	2498	OMC	C6-C5	2.84	1.41	1.35
52	x	54	5MU	C6-N1	-2.81	1.33	1.38
1	A	1917	PSU	O4'-C1'	-2.75	1.40	1.43
58	y	37	YG	C5-C6	-2.74	1.39	1.47
1	A	2580	PSU	O4'-C1'	-2.73	1.40	1.43
32	a	1402	4OC	C2-N1	-2.70	1.34	1.40
32	a	1498	UR3	O2-C2	2.70	1.27	1.22
32	a	1402	4OC	C6-C5	2.67	1.41	1.35
52	x	8	4SU	C4-N3	-2.66	1.34	1.37
1	A	2552	OMU	C2-N3	-2.59	1.33	1.38
58	y	55	PSU	C2-N3	-2.49	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	x	55	PSU	C2-N3	-2.45	1.33	1.37
52	x	8	4SU	C6-C5	2.43	1.40	1.35
1	A	1939	5MU	O4-C4	2.40	1.28	1.23
58	y	55	PSU	O4'-C1'	-2.39	1.40	1.43
1	A	2605	PSU	O4'-C1'	-2.38	1.40	1.43
1	A	2251	OMG	C5-C6	-2.38	1.42	1.47
1	A	1618	6MZ	C6-N6	2.38	1.39	1.35
1	A	1915	3TD	C2-N1	-2.37	1.34	1.37
1	A	1835	2MG	C2-N1	-2.35	1.33	1.36
1	A	2580	PSU	C2-N3	-2.35	1.33	1.37
32	a	1516	2MG	C2-N1	-2.33	1.33	1.36
1	A	2445	2MG	C2-N1	-2.33	1.33	1.36
32	a	1207	2MG	C2-N1	-2.32	1.33	1.36
58	y	54	5MU	O4-C4	2.31	1.28	1.23
32	a	1207	2MG	C5-C6	-2.30	1.42	1.47
52	x	54	5MU	O4-C4	2.30	1.28	1.23
1	A	2445	2MG	C5-C6	-2.27	1.42	1.47
1	A	2030	6MZ	C6-N6	2.27	1.38	1.35
1	A	2605	PSU	C2-N3	-2.27	1.33	1.37
1	A	1911	PSU	C2-N3	-2.27	1.33	1.37
32	a	966	2MG	C2-N1	-2.27	1.33	1.36
1	A	2457	PSU	C2-N3	-2.27	1.33	1.37
32	a	966	2MG	C5-C6	-2.25	1.42	1.47
1	A	1917	PSU	C2-N3	-2.25	1.33	1.37
32	a	1516	2MG	C5-C6	-2.24	1.42	1.47
1	A	2504	PSU	C2-N3	-2.24	1.33	1.37
1	A	2604	PSU	C2-N3	-2.23	1.33	1.37
32	a	516	PSU	C2-N3	-2.23	1.33	1.37
1	A	955	PSU	C2-N3	-2.21	1.33	1.37
1	A	746	PSU	C2-N3	-2.20	1.33	1.37
1	A	2251	OMG	C6-N1	-2.20	1.34	1.37
1	A	2552	OMU	C6-N1	-2.18	1.32	1.38
1	A	2457	PSU	O4'-C1'	-2.17	1.40	1.43
1	A	1835	2MG	C5-C6	-2.17	1.43	1.47
1	A	955	PSU	O4'-C1'	-2.16	1.40	1.43
1	A	2069	7MG	C4-N9	2.16	1.40	1.37
1	A	2552	OMU	C5-C4	-2.08	1.39	1.43

All (227) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	y	54	5MU	C4-N3-C2	-9.33	115.27	127.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	x	54	5MU	C4-N3-C2	-9.15	115.50	127.35
52	x	54	5MU	C5M-C5-C4	9.09	128.78	118.77
58	y	54	5MU	C5M-C5-C4	9.07	128.75	118.77
1	A	1939	5MU	C4-N3-C2	-9.04	115.65	127.35
1	A	1939	5MU	C5M-C5-C4	8.99	128.67	118.77
58	y	54	5MU	C5-C6-N1	-8.90	114.19	123.34
1	A	1939	5MU	C5-C6-N1	-8.60	114.50	123.34
1	A	1939	5MU	N3-C2-N1	8.53	126.22	114.89
52	x	54	5MU	N3-C2-N1	8.52	126.20	114.89
58	y	54	5MU	N3-C2-N1	8.50	126.17	114.89
52	x	54	5MU	C5-C6-N1	-8.38	114.72	123.34
1	A	1915	3TD	N1-C2-N3	8.08	122.52	116.14
58	y	54	5MU	C5-C4-N3	7.89	122.05	115.31
52	x	54	5MU	C5-C4-N3	7.71	121.89	115.31
1	A	1939	5MU	C5-C4-N3	7.48	121.69	115.31
1	A	2069	7MG	N9-C4-N3	6.89	135.78	125.47
1	A	1911	PSU	N1-C2-N3	6.74	122.76	115.13
1	A	1939	5MU	C5M-C5-C6	-6.73	113.86	122.85
32	a	516	PSU	N1-C2-N3	6.72	122.74	115.13
52	x	8	4SU	C4-N3-C2	-6.70	120.83	127.34
58	y	54	5MU	C5M-C5-C6	-6.69	113.91	122.85
52	x	54	5MU	C5M-C5-C6	-6.68	113.92	122.85
1	A	2457	PSU	N1-C2-N3	6.62	122.63	115.13
1	A	955	PSU	N1-C2-N3	6.59	122.60	115.13
1	A	2604	PSU	N1-C2-N3	6.56	122.56	115.13
1	A	2504	PSU	N1-C2-N3	6.54	122.54	115.13
1	A	746	PSU	N1-C2-N3	6.51	122.50	115.13
1	A	1917	PSU	N1-C2-N3	6.41	122.39	115.13
1	A	2605	PSU	N1-C2-N3	6.39	122.37	115.13
1	A	2580	PSU	N1-C2-N3	6.37	122.35	115.13
32	a	527	7MG	N9-C4-N3	6.36	134.97	125.47
58	y	55	PSU	N1-C2-N3	6.32	122.29	115.13
52	x	55	PSU	N1-C2-N3	6.27	122.23	115.13
58	y	46	7MG	N9-C4-N3	5.83	134.19	125.47
52	x	8	4SU	C5-C4-N3	5.71	119.98	114.69
52	x	8	4SU	N3-C2-N1	5.52	122.22	114.89
1	A	2552	OMU	N3-C2-N1	5.51	122.21	114.89
1	A	1618	6MZ	C2-N1-C6	5.49	121.29	116.59
1	A	2030	6MZ	C2-N1-C6	5.46	121.27	116.59
1	A	2069	7MG	C5-C4-N3	-5.45	117.75	128.13
58	y	37	YG	C3-N3-C2	-5.39	115.09	120.13
32	a	527	7MG	C5-C6-N1	5.37	120.46	110.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2069	7MG	C2-N3-C4	5.37	121.86	112.30
58	y	16	H2U	C4-N3-C2	-5.30	121.39	125.79
1	A	2069	7MG	C5-C6-N1	5.23	120.21	110.99
32	a	527	7MG	C2-N3-C4	5.22	121.61	112.30
58	y	17	H2U	C4-N3-C2	-5.16	121.51	125.79
58	y	46	7MG	C5-C6-N1	5.15	120.06	110.99
32	a	527	7MG	C5-C4-N3	-5.08	118.44	128.13
1	A	1618	6MZ	N3-C2-N1	-4.94	120.95	128.68
1	A	2030	6MZ	N3-C2-N1	-4.91	121.00	128.68
1	A	2069	7MG	N9-C8-N7	4.91	110.39	103.38
58	y	46	7MG	C2-N3-C4	4.87	120.98	112.30
58	y	17	H2U	N3-C2-N1	4.86	121.79	116.65
1	A	2449	H2U	C4-N3-C2	-4.84	121.78	125.79
52	x	20	H2U	C4-N3-C2	-4.84	121.78	125.79
58	y	20	H2U	C4-N3-C2	-4.74	121.86	125.79
58	y	46	7MG	C5-C4-N3	-4.67	119.24	128.13
52	x	20	H2U	N3-C2-N1	4.66	121.58	116.65
32	a	967	5MC	C5-C6-N1	-4.66	118.54	123.34
1	A	2449	H2U	N3-C2-N1	4.63	121.55	116.65
58	y	20	H2U	N3-C2-N1	4.63	121.55	116.65
58	y	16	H2U	N3-C2-N1	4.62	121.54	116.65
1	A	747	5MC	C5-C6-N1	-4.59	118.61	123.34
1	A	1962	5MC	C5-C6-N1	-4.59	118.62	123.34
32	a	1407	5MC	C5-C6-N1	-4.57	118.64	123.34
32	a	527	7MG	N9-C8-N7	4.47	109.77	103.38
32	a	1498	UR3	C1'-N1-C2	4.40	124.42	116.99
58	y	37	YG	C5-C6-N1	4.29	120.36	113.96
58	y	46	7MG	N9-C8-N7	4.26	109.48	103.38
1	A	1939	5MU	O4-C4-N3	-4.24	111.99	120.12
58	y	54	5MU	O4-C4-N3	-4.17	112.12	120.12
32	a	516	PSU	O2-C2-N1	-4.16	118.22	122.79
1	A	2552	OMU	C4-N3-C2	-4.10	121.17	126.58
58	y	37	YG	C3-N3-C4	4.09	123.98	116.71
1	A	2457	PSU	O2-C2-N1	-4.04	118.35	122.79
1	A	955	PSU	O2-C2-N1	-4.03	118.35	122.79
52	x	54	5MU	O4-C4-N3	-4.02	112.40	120.12
1	A	1911	PSU	O2-C2-N1	-4.00	118.38	122.79
1	A	2605	PSU	O2-C2-N1	-3.95	118.44	122.79
58	y	37	YG	O23-C21-N20	3.95	117.73	110.80
32	a	1498	UR3	O2-C2-N3	-3.93	115.81	121.34
58	y	37	YG	C24-O23-C21	3.91	120.28	115.66
1	A	2504	PSU	O2-C2-N1	-3.91	118.49	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2604	PSU	O2-C2-N1	-3.89	118.51	122.79
1	A	2604	PSU	C4-N3-C2	-3.86	120.78	126.34
1	A	2457	PSU	C4-N3-C2	-3.84	120.81	126.34
1	A	1911	PSU	C4-N3-C2	-3.83	120.82	126.34
1	A	2504	PSU	C4-N3-C2	-3.82	120.83	126.34
1	A	1917	PSU	O2-C2-N1	-3.79	118.61	122.79
32	a	516	PSU	C4-N3-C2	-3.79	120.88	126.34
1	A	746	PSU	O2-C2-N1	-3.78	118.63	122.79
52	x	8	4SU	C6-C5-C4	-3.76	116.69	119.95
1	A	746	PSU	C4-N3-C2	-3.76	120.92	126.34
1	A	1939	5MU	C1'-N1-C6	-3.76	114.86	121.12
1	A	955	PSU	C4-N3-C2	-3.76	120.93	126.34
1	A	1835	2MG	C5-C6-N1	3.75	120.57	113.95
58	y	54	5MU	O2-C2-N1	-3.73	117.82	122.79
1	A	2030	6MZ	C9-N6-C6	-3.73	119.66	122.87
58	y	37	YG	O23-C21-O22	-3.72	119.11	124.58
1	A	2580	PSU	C4-N3-C2	-3.70	121.00	126.34
1	A	2580	PSU	O2-C2-N1	-3.69	118.73	122.79
1	A	2605	PSU	C4-N3-C2	-3.66	121.07	126.34
52	x	55	PSU	C6-C5-C4	-3.66	115.64	118.20
58	y	54	5MU	C6-N1-C2	3.65	124.99	121.30
32	a	966	2MG	C5-C6-N1	3.63	120.37	113.95
1	A	1917	PSU	C4-N3-C2	-3.63	121.11	126.34
32	a	1498	UR3	C6-N1-C2	-3.61	118.55	121.79
1	A	2445	2MG	C5-C6-N1	3.60	120.31	113.95
32	a	1516	2MG	C5-C6-N1	3.60	120.30	113.95
32	a	1207	2MG	C5-C6-N1	3.59	120.29	113.95
58	y	55	PSU	C6-C5-C4	-3.55	115.71	118.20
1	A	1939	5MU	O2-C2-N3	-3.53	114.93	121.50
52	x	54	5MU	O2-C2-N1	-3.46	118.19	122.79
58	y	55	PSU	C4-N3-C2	-3.45	121.37	126.34
1	A	2552	OMU	C1'-N1-C2	3.45	123.81	117.57
52	x	55	PSU	C4-N3-C2	-3.42	121.41	126.34
1	A	1915	3TD	C4-N3-C2	-3.38	120.94	124.61
52	x	8	4SU	C5-C4-S4	-3.38	120.12	124.47
1	A	1618	6MZ	C9-N6-C6	-3.37	119.97	122.87
1	A	2503	2MA	C5-C6-N1	3.33	119.77	114.02
58	y	37	YG	O18-C16-C15	3.33	120.04	111.52
58	y	55	PSU	O2-C2-N1	-3.28	119.18	122.79
58	y	46	7MG	C6-C5-N7	3.28	137.07	131.91
1	A	745	1MG	C8-N7-C5	3.20	109.09	102.99
52	x	54	5MU	O2-C2-N3	-3.16	115.61	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	a	527	7MG	C6-C5-N7	3.16	136.88	131.91
58	y	37	YG	O6-C6-C5	-3.15	118.58	124.17
58	y	17	H2U	O2-C2-N1	-3.14	119.17	123.11
1	A	1939	5MU	C6-N1-C2	3.13	124.47	121.30
52	x	55	PSU	O2-C2-N1	-3.13	119.35	122.79
32	a	1519	MA6	N3-C2-N1	-3.11	123.82	128.68
32	a	1518	MA6	N1-C6-N6	3.09	120.31	117.06
1	A	745	1MG	C5-C6-N1	3.07	118.52	113.90
52	x	54	5MU	C6-N1-C2	3.06	124.39	121.30
1	A	1835	2MG	C8-N7-C5	3.03	108.76	102.99
58	y	37	YG	C8-N7-C5	3.00	108.70	102.99
32	a	966	2MG	C8-N7-C5	2.97	108.64	102.99
1	A	1939	5MU	O2-C2-N1	-2.96	118.85	122.79
52	x	54	5MU	C1'-N1-C6	-2.95	116.21	121.12
1	A	2251	OMG	C5-C6-N1	2.95	119.16	113.95
58	y	54	5MU	O2-C2-N3	-2.95	116.01	121.50
1	A	2445	2MG	C8-N7-C5	2.92	108.56	102.99
58	y	46	7MG	O6-C6-C5	-2.92	120.38	127.54
1	A	2503	2MA	C8-N7-C5	2.92	108.54	102.99
1	A	2552	OMU	O2-C2-N3	-2.91	116.08	121.50
1	A	2069	7MG	O6-C6-C5	-2.91	120.40	127.54
32	a	1518	MA6	N3-C2-N1	-2.89	124.16	128.68
58	y	54	5MU	C1'-N1-C6	-2.88	116.33	121.12
32	a	1207	2MG	C8-N7-C5	2.88	108.47	102.99
32	a	1516	2MG	C8-N7-C5	2.88	108.47	102.99
1	A	2605	PSU	C6-C5-C4	-2.87	116.19	118.20
32	a	527	7MG	O6-C6-C5	-2.83	120.60	127.54
1	A	2069	7MG	C2-N1-C6	-2.80	119.99	125.10
32	a	1519	MA6	C4-C5-N7	-2.80	106.48	109.40
1	A	2580	PSU	C6-C5-C4	-2.80	116.24	118.20
58	y	46	7MG	C6-C5-C4	-2.79	116.87	122.62
1	A	2552	OMU	C5-C4-N3	2.78	119.00	114.84
58	y	16	H2U	O2-C2-N1	-2.73	119.68	123.11
32	a	527	7MG	C6-C5-C4	-2.72	117.01	122.62
32	a	527	7MG	C2-N1-C6	-2.72	120.14	125.10
58	y	20	H2U	C5-C6-N1	2.70	120.53	111.61
1	A	2449	H2U	C5-C6-N1	2.70	120.52	111.61
52	x	20	H2U	C5-C6-N1	2.69	120.48	111.61
32	a	1519	MA6	N1-C6-N6	2.69	119.88	117.06
1	A	1911	PSU	C6-N1-C2	-2.68	119.94	122.68
1	A	2069	7MG	C6-C5-N7	2.68	136.13	131.91
1	A	2251	OMG	C8-N7-C5	2.65	108.04	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	a	516	PSU	C6-N1-C2	-2.65	119.97	122.68
1	A	955	PSU	C6-N1-C2	-2.63	119.99	122.68
58	y	17	H2U	C5-C6-N1	2.63	120.28	111.61
1	A	1917	PSU	C6-N1-C2	-2.62	120.00	122.68
1	A	2552	OMU	O4-C4-C5	-2.61	120.57	125.16
1	A	2605	PSU	C6-N1-C2	-2.60	120.02	122.68
58	y	46	7MG	C2-N1-C6	-2.60	120.36	125.10
58	y	55	PSU	C6-N1-C2	-2.56	120.07	122.68
1	A	1917	PSU	C6-C5-C4	-2.55	116.41	118.20
1	A	2030	6MZ	C4-C5-N7	-2.55	106.74	109.40
1	A	2457	PSU	C6-N1-C2	-2.54	120.08	122.68
32	a	1518	MA6	C4-C5-N7	-2.54	106.76	109.40
58	y	16	H2U	C5-C6-N1	2.53	119.94	111.61
1	A	2251	OMG	C2-N1-C6	-2.52	120.46	125.10
52	x	55	PSU	C6-N1-C2	-2.52	120.11	122.68
58	y	16	H2U	C5-C4-N3	2.51	119.47	116.65
1	A	2504	PSU	C6-N1-C2	-2.49	120.13	122.68
1	A	746	PSU	C6-N1-C2	-2.48	120.15	122.68
1	A	2580	PSU	C6-N1-C2	-2.47	120.16	122.68
32	a	1498	UR3	C4-N3-C2	-2.46	122.24	124.56
1	A	1618	6MZ	C4-C5-N7	-2.45	106.84	109.40
1	A	2069	7MG	C6-C5-C4	-2.43	117.60	122.62
58	y	17	H2U	C5-C4-N3	2.39	119.34	116.65
58	y	37	YG	O18-C16-O17	-2.37	119.20	123.84
58	y	37	YG	C11-C12-N1	-2.37	105.20	106.53
1	A	2604	PSU	C6-N1-C2	-2.36	120.27	122.68
32	a	1402	4OC	C5-C4-N3	-2.36	118.80	122.59
1	A	2552	OMU	C1'-N1-C6	-2.35	115.72	120.84
32	a	1207	2MG	O6-C6-C5	-2.34	119.81	124.37
1	A	955	PSU	C6-C5-C4	-2.33	116.57	118.20
32	a	1402	4OC	O2-C2-N3	-2.33	118.55	122.33
32	a	1516	2MG	O6-C6-C5	-2.32	119.84	124.37
1	A	2449	H2U	C5-C4-N3	2.32	119.26	116.65
32	a	966	2MG	O6-C6-C5	-2.31	119.85	124.37
52	x	20	H2U	C5-C4-N3	2.30	119.24	116.65
1	A	2445	2MG	O6-C6-C5	-2.28	119.92	124.37
1	A	2504	PSU	C6-C5-C4	-2.27	116.61	118.20
58	y	20	H2U	C5-C4-N3	2.25	119.18	116.65
1	A	2498	OMC	O2-C2-N3	-2.24	118.69	122.33
52	x	8	4SU	O2-C2-N1	-2.22	119.83	122.79
1	A	1962	5MC	C5-C4-N3	-2.15	119.36	121.67
1	A	747	5MC	C5-C4-N3	-2.13	119.37	121.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	a	1407	5MC	C5-C4-N3	-2.12	119.39	121.67
32	a	967	5MC	C5-C4-N3	-2.11	119.40	121.67
1	A	2457	PSU	C6-C5-C4	-2.10	116.73	118.20
1	A	1835	2MG	O6-C6-C5	-2.08	120.31	124.37
52	x	8	4SU	C1'-N1-C2	2.08	121.33	117.57
1	A	1915	3TD	O2-C2-N3	-2.07	118.77	121.83
1	A	2449	H2U	O2-C2-N3	-2.04	117.69	121.50
1	A	1911	PSU	C6-C5-C4	-2.04	116.77	118.20
32	a	967	5MC	O2-C2-N3	-2.02	119.05	122.33
1	A	2604	PSU	O4'-C1'-C2'	2.02	107.99	105.14
1	A	1962	5MC	O2-C2-N3	-2.02	119.05	122.33
58	y	20	H2U	O2-C2-N3	-2.01	117.75	121.50
32	a	1402	4OC	N1-C2-N3	2.01	122.46	118.81
1	A	2498	OMC	N1-C2-N3	2.00	122.46	118.81
1	A	1915	3TD	O4'-C1'-C2'	2.00	107.97	105.14
52	x	20	H2U	O2-C2-N1	-2.00	120.59	123.11

All (70) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	746	PSU	C2'
1	A	746	PSU	C4'
1	A	955	PSU	C2'
1	A	955	PSU	C4'
1	A	1835	2MG	C2'
1	A	1835	2MG	C3'
1	A	1911	PSU	C2'
1	A	1911	PSU	C4'
1	A	1915	3TD	C4'
1	A	1917	PSU	C2'
1	A	1917	PSU	C4'
1	A	1939	5MU	C2'
1	A	1939	5MU	C4'
1	A	1939	5MU	C3'
1	A	2069	7MG	C1'
1	A	2251	OMG	C3'
1	A	2251	OMG	C1'
1	A	2445	2MG	C2'
1	A	2445	2MG	C3'
1	A	2449	H2U	C1'
1	A	2457	PSU	C2'
1	A	2457	PSU	C4'

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Mol	Chain	Res	Type	Atom
1	A	2498	OMC	C2'
1	A	2498	OMC	C4'
1	A	2503	2MA	C2'
1	A	2503	2MA	C1'
1	A	2504	PSU	C2'
1	A	2504	PSU	C4'
1	A	2552	OMU	C4'
1	A	2580	PSU	C2'
1	A	2580	PSU	C4'
1	A	2604	PSU	C2'
1	A	2604	PSU	C4'
1	A	2605	PSU	C2'
1	A	2605	PSU	C4'
32	a	516	PSU	C2'
32	a	516	PSU	C4'
32	a	527	7MG	C1'
32	a	966	2MG	C2'
32	a	966	2MG	C3'
32	a	1207	2MG	C2'
32	a	1207	2MG	C3'
32	a	1402	4OC	C2'
32	a	1402	4OC	C1'
32	a	1498	UR3	C2'
32	a	1498	UR3	C3'
32	a	1516	2MG	C2'
32	a	1516	2MG	C3'
32	a	1518	MA6	C2'
32	a	1518	MA6	C3'
32	a	1519	MA6	C2'
32	a	1519	MA6	C3'
52	x	8	4SU	C2'
52	x	8	4SU	C4'
52	x	8	4SU	C3'
52	x	20	H2U	C1'
52	x	54	5MU	C2'
52	x	54	5MU	C4'
52	x	54	5MU	C3'
52	x	55	PSU	C2'
52	x	55	PSU	C4'
58	y	16	H2U	C1'
58	y	17	H2U	C1'
58	y	20	H2U	C1'

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Mol	Chain	Res	Type	Atom
58	y	46	7MG	C1'
58	y	54	5MU	C2'
58	y	54	5MU	C4'
58	y	54	5MU	C3'
58	y	55	PSU	C2'
58	y	55	PSU	C4'

All (149) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	746	PSU	C3'-C4'-C5'-O5'
1	A	747	5MC	C3'-C4'-C5'-O5'
1	A	747	5MC	C2'-C1'-N1-C2
1	A	747	5MC	C2'-C1'-N1-C6
1	A	955	PSU	C3'-C4'-C5'-O5'
1	A	955	PSU	O4'-C4'-C5'-O5'
1	A	955	PSU	C4'-C5'-O5'-P
1	A	1618	6MZ	C5-C6-N6-C9
1	A	1618	6MZ	N1-C6-N6-C9
1	A	1911	PSU	C3'-C4'-C5'-O5'
1	A	1911	PSU	C4'-C5'-O5'-P
1	A	1915	3TD	C2'-C1'-C5-C4
1	A	1915	3TD	O4'-C1'-C5-C4
1	A	1915	3TD	O4'-C1'-C5-C6
1	A	1915	3TD	C3'-C4'-C5'-O5'
1	A	1917	PSU	C3'-C4'-C5'-O5'
1	A	1917	PSU	C4'-C5'-O5'-P
1	A	1939	5MU	C4'-C5'-O5'-P
1	A	2030	6MZ	N1-C6-N6-C9
1	A	2251	OMG	C4'-C5'-O5'-P
1	A	2251	OMG	C3'-C2'-O2'-CM2
1	A	2449	H2U	O4'-C4'-C5'-O5'
1	A	2449	H2U	C3'-C4'-C5'-O5'
1	A	2449	H2U	O4'-C1'-N1-C6
1	A	2457	PSU	C3'-C4'-C5'-O5'
1	A	2457	PSU	C4'-C5'-O5'-P
1	A	2498	OMC	C4'-C5'-O5'-P
1	A	2552	OMU	O4'-C1'-N1-C2
1	A	2552	OMU	O4'-C1'-N1-C6
1	A	2552	OMU	C3'-C4'-C5'-O5'
1	A	2552	OMU	C4'-C5'-O5'-P
1	A	2604	PSU	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	A	2605	PSU	C3'-C4'-C5'-O5'
32	a	516	PSU	C3'-C4'-C5'-O5'
32	a	516	PSU	C4'-C5'-O5'-P
32	a	527	7MG	O4'-C4'-C5'-O5'
32	a	527	7MG	C3'-C4'-C5'-O5'
32	a	1207	2MG	C3'-C4'-C5'-O5'
32	a	1407	5MC	C2'-C1'-N1-C2
32	a	1407	5MC	C2'-C1'-N1-C6
32	a	1498	UR3	O4'-C4'-C5'-O5'
32	a	1498	UR3	C3'-C4'-C5'-O5'
32	a	1498	UR3	O4'-C1'-N1-C6
32	a	1498	UR3	O4'-C1'-N1-C2
32	a	1516	2MG	O4'-C4'-C5'-O5'
32	a	1516	2MG	C3'-C4'-C5'-O5'
32	a	1516	2MG	N1-C2-N2-CM2
32	a	1516	2MG	N3-C2-N2-CM2
32	a	1518	MA6	C5-C6-N6-C9
32	a	1518	MA6	C5-C6-N6-C10
32	a	1518	MA6	N1-C6-N6-C10
32	a	1519	MA6	C5-C6-N6-C10
32	a	1519	MA6	N1-C6-N6-C10
52	x	20	H2U	O4'-C1'-N1-C6
52	x	54	5MU	C3'-C4'-C5'-O5'
52	x	55	PSU	O4'-C1'-C5-C4
52	x	55	PSU	O4'-C1'-C5-C6
52	x	55	PSU	C3'-C4'-C5'-O5'
58	y	16	H2U	C3'-C4'-C5'-O5'
58	y	20	H2U	O4'-C4'-C5'-O5'
58	y	20	H2U	O4'-C1'-N1-C6
58	y	54	5MU	C3'-C4'-C5'-O5'
58	y	54	5MU	C4'-C5'-O5'-P
58	y	55	PSU	O4'-C1'-C5-C6
58	y	55	PSU	C3'-C4'-C5'-O5'
58	y	55	PSU	O4'-C4'-C5'-O5'
58	y	55	PSU	C4'-C5'-O5'-P
1	A	2449	H2U	O4'-C1'-N1-C2
52	x	20	H2U	O4'-C1'-N1-C2
58	y	20	H2U	O4'-C1'-N1-C2
1	A	1915	3TD	C4'-C5'-O5'-P
1	A	2580	PSU	C4'-C5'-O5'-P
1	A	2604	PSU	C4'-C5'-O5'-P
1	A	2030	6MZ	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	A	2030	6MZ	C3'-C4'-C5'-O5'
1	A	2069	7MG	C3'-C4'-C5'-O5'
1	A	2503	2MA	O4'-C4'-C5'-O5'
1	A	2503	2MA	C3'-C4'-C5'-O5'
1	A	2504	PSU	C3'-C4'-C5'-O5'
1	A	2580	PSU	C3'-C4'-C5'-O5'
1	A	2580	PSU	O4'-C4'-C5'-O5'
52	x	8	4SU	C3'-C4'-C5'-O5'
58	y	20	H2U	C3'-C4'-C5'-O5'
1	A	747	5MC	O4'-C4'-C5'-O5'
1	A	1911	PSU	O4'-C4'-C5'-O5'
1	A	1917	PSU	O4'-C4'-C5'-O5'
1	A	2069	7MG	O4'-C4'-C5'-O5'
1	A	2457	PSU	O4'-C4'-C5'-O5'
1	A	2504	PSU	O4'-C4'-C5'-O5'
1	A	2552	OMU	O4'-C4'-C5'-O5'
1	A	2605	PSU	O4'-C4'-C5'-O5'
32	a	516	PSU	O4'-C4'-C5'-O5'
32	a	1207	2MG	O4'-C4'-C5'-O5'
52	x	8	4SU	O4'-C4'-C5'-O5'
52	x	54	5MU	O4'-C4'-C5'-O5'
52	x	55	PSU	O4'-C4'-C5'-O5'
58	y	17	H2U	O4'-C4'-C5'-O5'
58	y	54	5MU	O4'-C4'-C5'-O5'
32	a	966	2MG	O4'-C4'-C5'-O5'
58	y	17	H2U	C3'-C4'-C5'-O5'
32	a	967	5MC	C2'-C1'-N1-C6
32	a	527	7MG	C2'-C1'-N9-C8
1	A	1915	3TD	O4'-C4'-C5'-O5'
32	a	966	2MG	C3'-C4'-C5'-O5'
58	y	37	YG	C12-C13-C14-C15
52	x	54	5MU	C4'-C5'-O5'-P
1	A	746	PSU	O4'-C4'-C5'-O5'
1	A	2604	PSU	O4'-C4'-C5'-O5'
52	x	20	H2U	O4'-C4'-C5'-O5'
58	y	16	H2U	O4'-C4'-C5'-O5'
52	x	20	H2U	C3'-C4'-C5'-O5'
58	y	16	H2U	C4'-C5'-O5'-P
1	A	2069	7MG	C2'-C1'-N9-C8
1	A	2504	PSU	C4'-C5'-O5'-P
32	a	967	5MC	C2'-C1'-N1-C2
32	a	527	7MG	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
58	y	46	7MG	C4'-C5'-O5'-P
58	y	46	7MG	C2'-C1'-N9-C8
32	a	967	5MC	O4'-C1'-N1-C6
1	A	2445	2MG	C4'-C5'-O5'-P
58	y	20	H2U	C4'-C5'-O5'-P
32	a	1402	4OC	C3'-C4'-C5'-O5'
58	y	46	7MG	C3'-C4'-C5'-O5'
32	a	967	5MC	O4'-C1'-N1-C2
32	a	1518	MA6	N1-C6-N6-C9
32	a	1407	5MC	O4'-C1'-N1-C6
32	a	967	5MC	C4'-C5'-O5'-P
32	a	1516	2MG	C4'-C5'-O5'-P
32	a	1519	MA6	C5-C6-N6-C9
52	x	8	4SU	C4'-C5'-O5'-P
52	x	55	PSU	C4'-C5'-O5'-P
58	y	17	H2U	C4'-C5'-O5'-P
32	a	1402	4OC	O4'-C4'-C5'-O5'
1	A	747	5MC	O4'-C1'-N1-C6
1	A	1962	5MC	C2'-C1'-N1-C6
32	a	1407	5MC	O4'-C1'-N1-C2
32	a	966	2MG	C4'-C5'-O5'-P
52	x	20	H2U	C4'-C5'-O5'-P
32	a	1518	MA6	O4'-C4'-C5'-O5'
1	A	747	5MC	O4'-C1'-N1-C2
1	A	1962	5MC	O4'-C1'-N1-C6
1	A	2251	OMG	O4'-C4'-C5'-O5'
1	A	2251	OMG	C3'-C4'-C5'-O5'
32	a	1498	UR3	C2'-C1'-N1-C6
1	A	1835	2MG	O4'-C4'-C5'-O5'
32	a	1518	MA6	C3'-C4'-C5'-O5'
1	A	1962	5MC	O4'-C1'-N1-C2
1	A	1835	2MG	C3'-C4'-C5'-O5'
32	a	1402	4OC	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
57	z	6

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	z	517:UNK	C	518:UNK	N	39.33
1	z	561:UNK	C	663:ALA	N	37.34
1	z	493:UNK	C	494:UNK	N	34.24
1	z	547:UNK	C	548:UNK	N	30.19
1	z	526:UNK	C	527:UNK	N	18.32
1	z	535:UNK	C	536:UNK	N	8.04

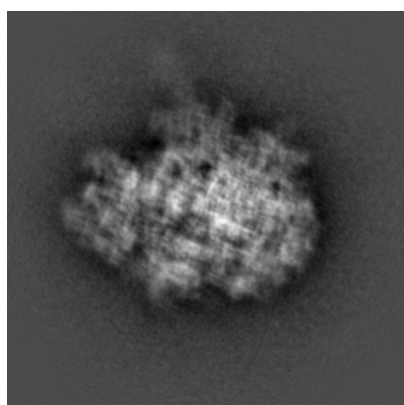
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4001. These allow visual inspection of the internal detail of the map and identification of artifacts.

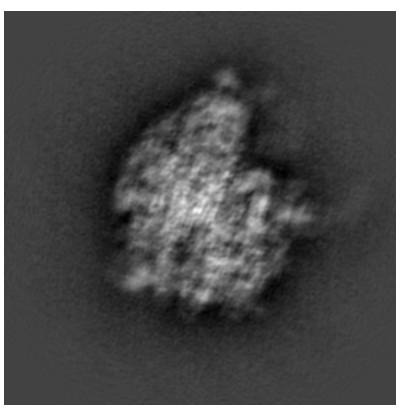
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

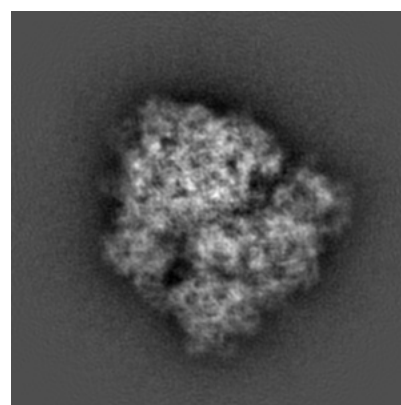
6.1.1 Primary map



X



Y

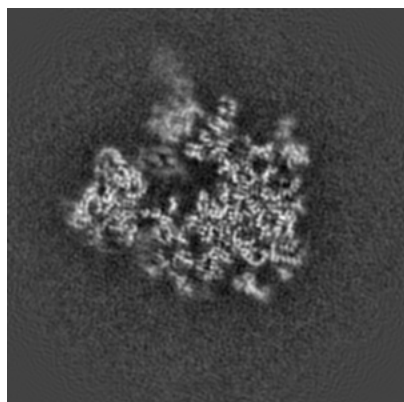


Z

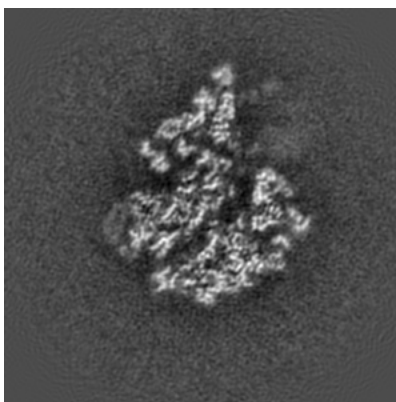
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

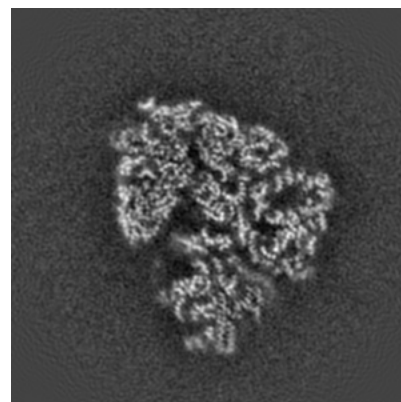
6.2.1 Primary map



X Index: 184



Y Index: 184

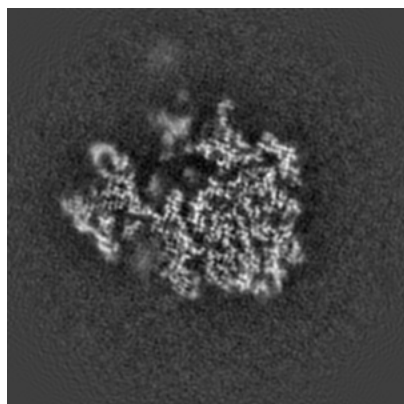


Z Index: 184

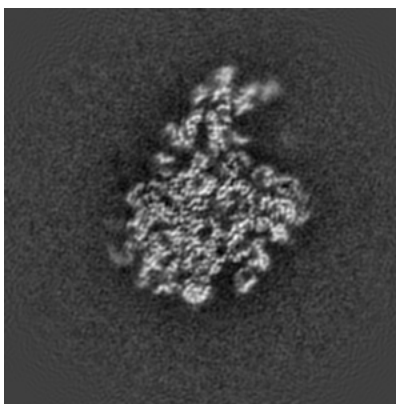
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

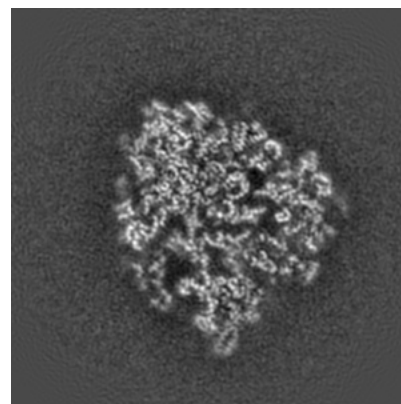
6.3.1 Primary map



X Index: 193



Y Index: 194

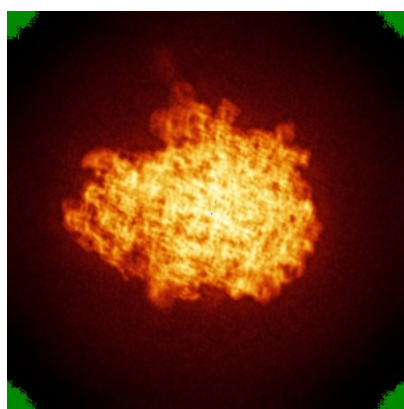


Z Index: 191

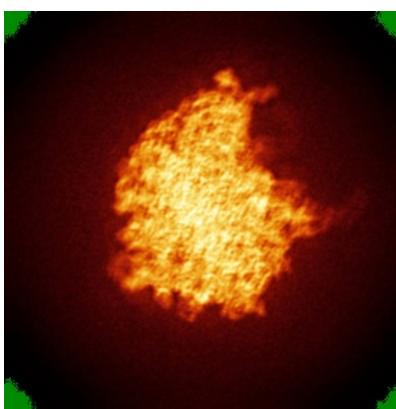
The images above show the largest variance slices of the map in three orthogonal directions.

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

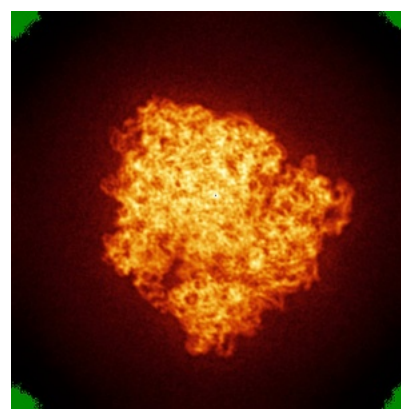
6.4.1 Primary map



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 0.00053. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

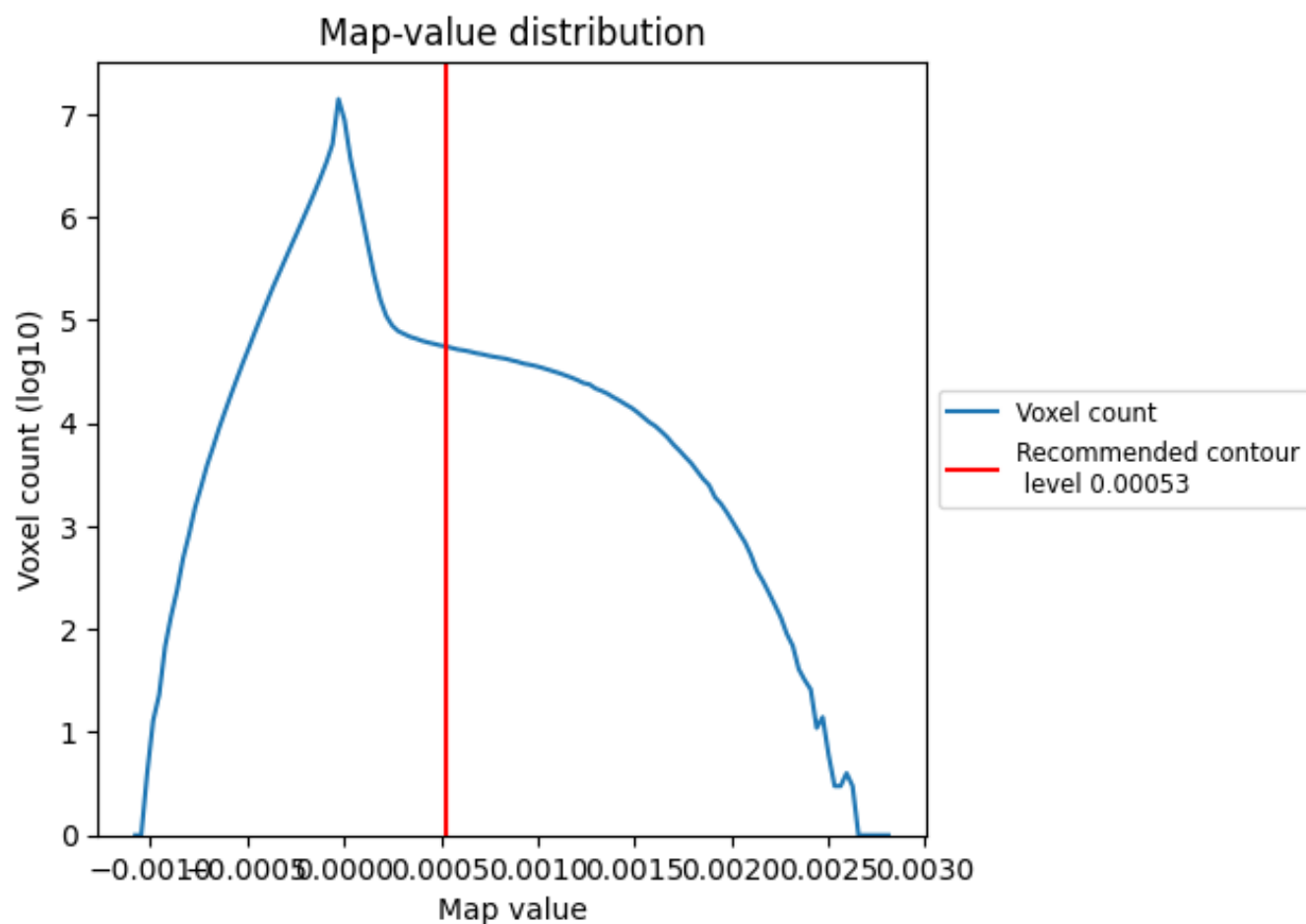
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

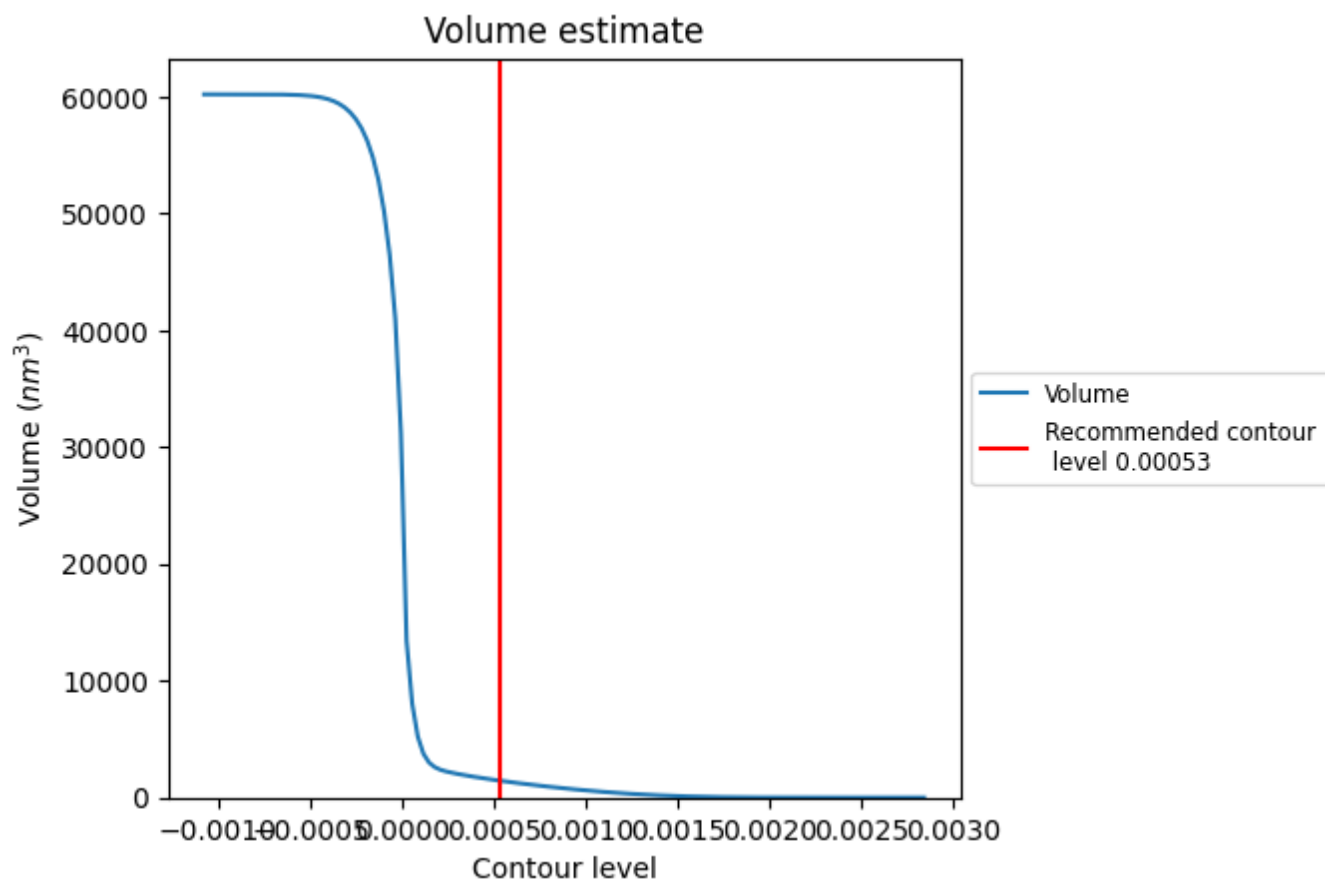
This section contains the results of statistical analysis of the map.

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.

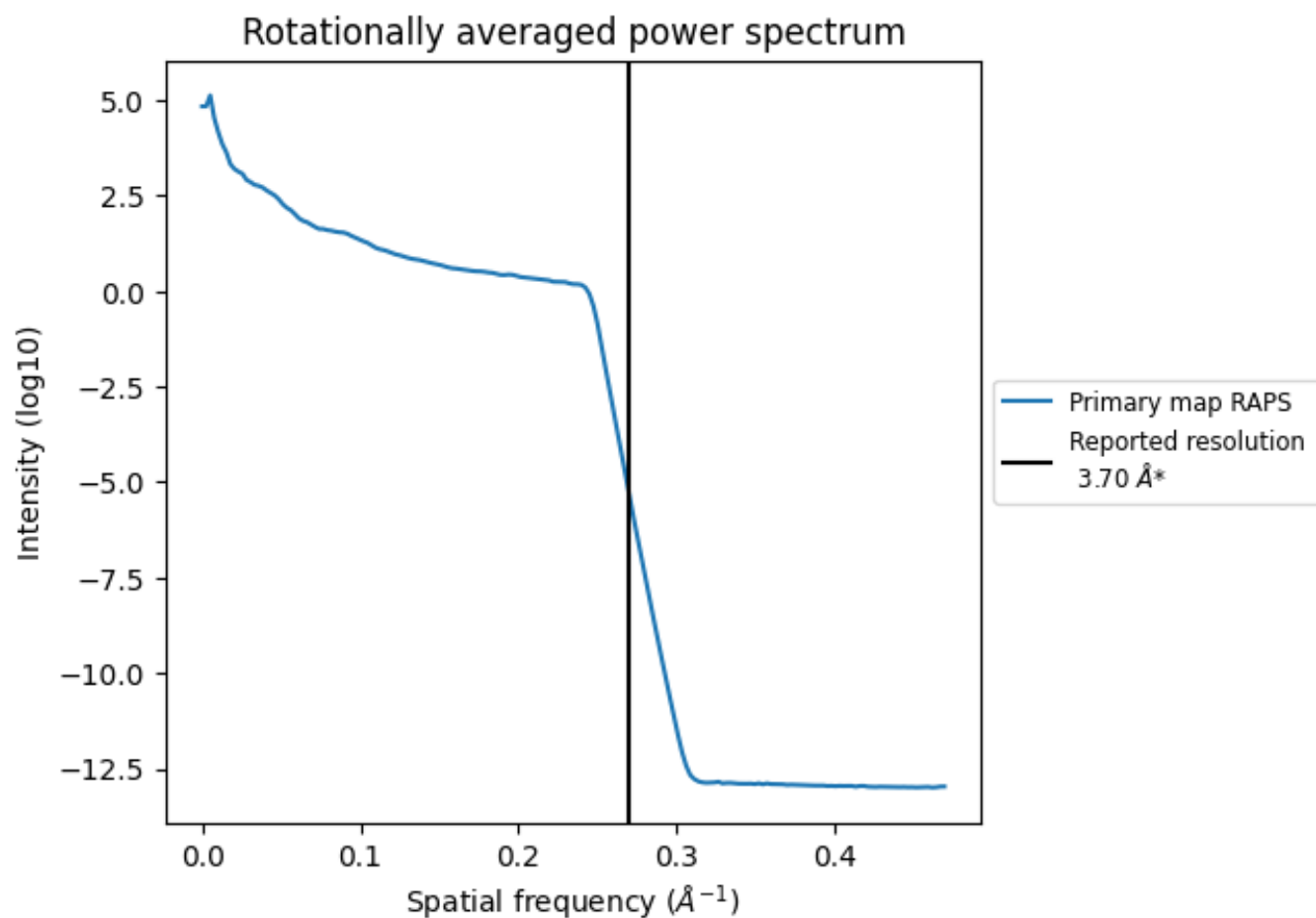
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1451 nm³; this corresponds to an approximate mass of 1311 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 0.270 Å⁻¹

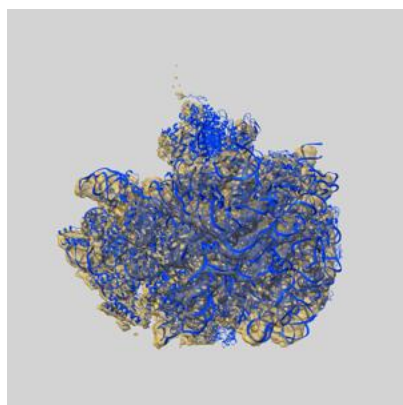
8 Fourier-Shell correlation

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

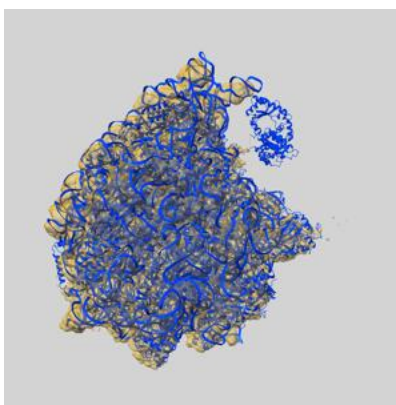
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4001 and PDB model 5L3P. Per-residue inclusion information can be found in section [3](#) on page [15](#).

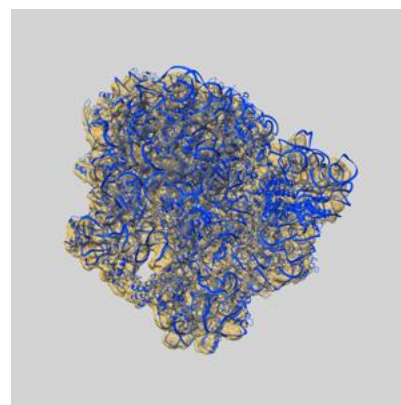
9.1 Map-model overlay [i](#)



X



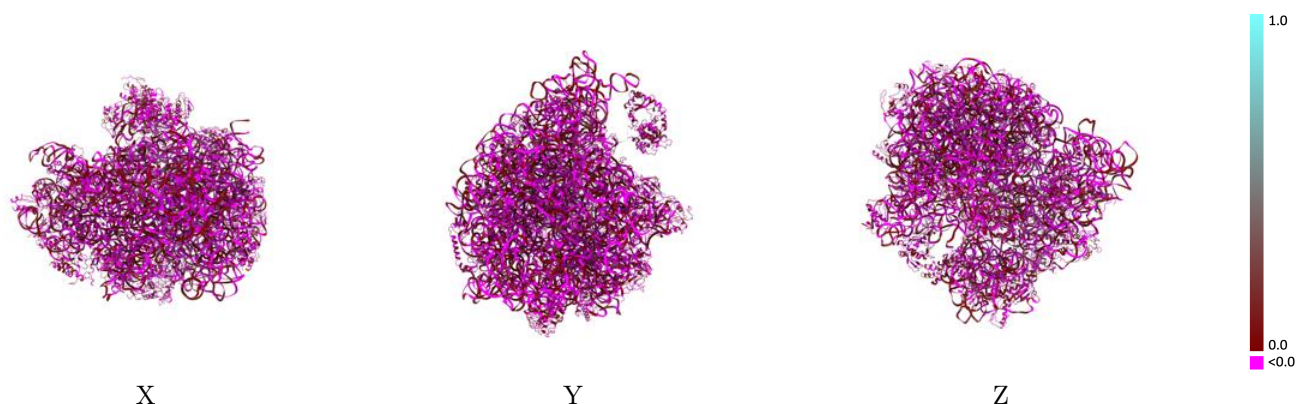
Y



Z

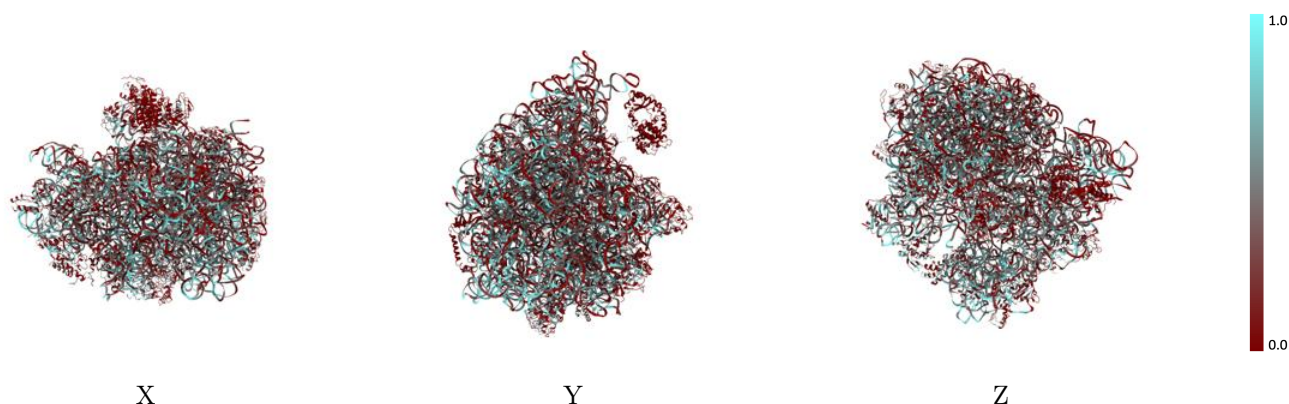
The images above show the 3D surface view of the map at the recommended contour level 0.00053 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



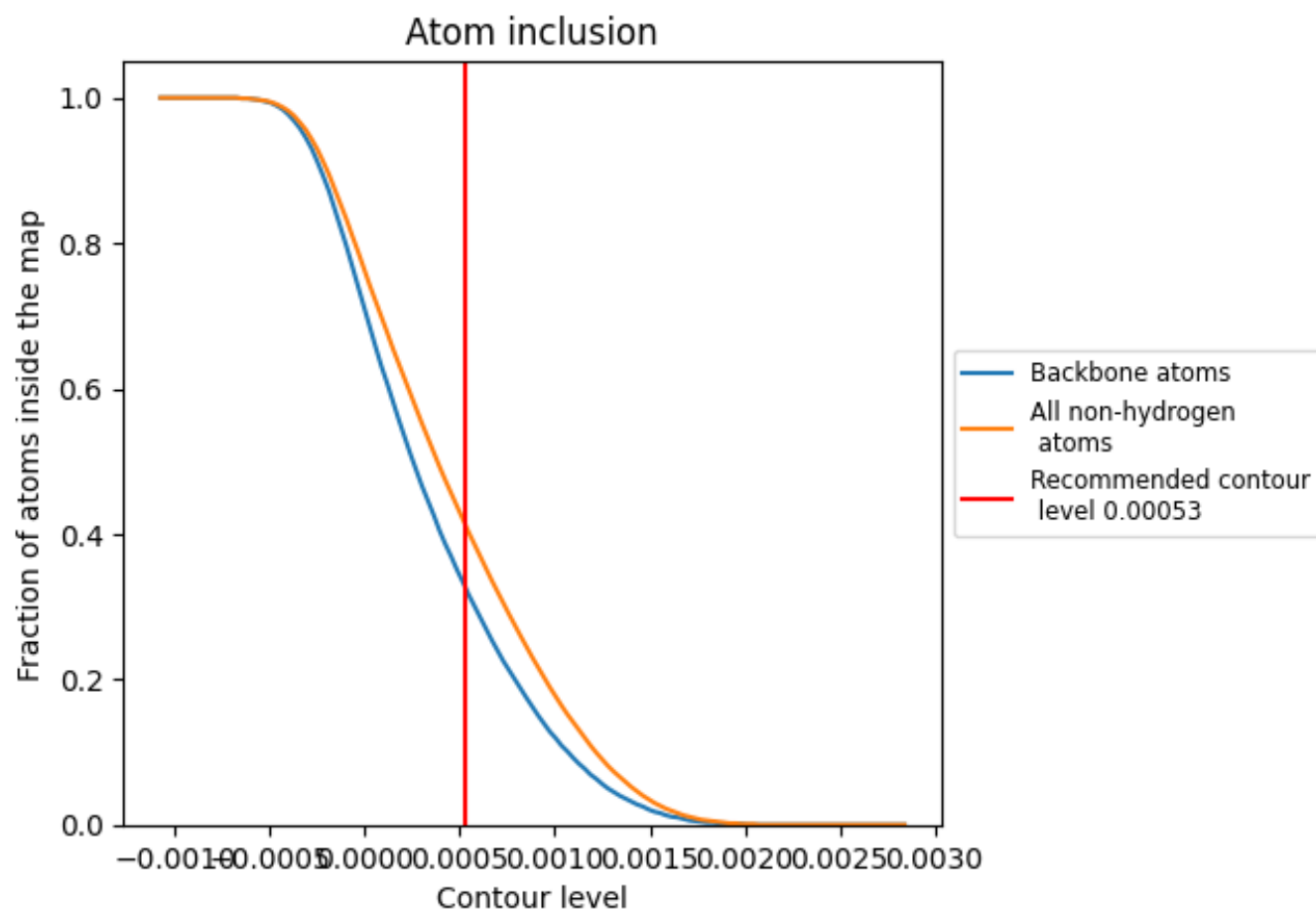
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00053).

9.4 Atom inclusion ⓘ



At the recommended contour level, 33% of all backbone atoms, 41% 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 (0.00053) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4120	-0.0010
0	0.3490	-0.0060
1	0.3010	-0.0000
2	0.3240	0.0300
3	0.2150	-0.0270
4	0.4150	0.0430
5	0.3670	-0.0130
6	0.2670	-0.0130
7	0.4370	0.0170
8	0.2850	-0.0010
9	0.3900	-0.0350
A	0.4690	-0.0020
B	0.4800	-0.0090
D	0.3410	-0.0150
E	0.2130	-0.0300
F	0.3120	-0.0340
G	0.4220	0.0170
H	0.2470	-0.0020
I	0.0680	-0.0080
J	0.1760	0.0100
K	0.2400	0.0410
N	0.2180	-0.0400
O	0.2400	-0.0180
P	0.3300	0.0020
Q	0.2510	-0.0360
R	0.2850	-0.0300
S	0.3930	-0.0190
T	0.1590	-0.0420
U	0.3000	-0.0340
V	0.2600	-0.0080
W	0.2810	0.0050
X	0.2960	-0.0210
Y	0.2420	-0.0210
Z	0.2710	-0.0100
a	0.4880	0.0120



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Chain	Atom inclusion	Q-score
b	 0.2610	 0.0160
c	 0.2690	 0.0130
d	 0.3240	 -0.0190
e	 0.2910	 0.0010
f	 0.3730	 0.0180
g	 0.3200	 0.0070
h	 0.3190	 -0.0120
i	 0.4490	 -0.0260
j	 0.3230	 -0.0190
k	 0.4120	 -0.0190
l	 0.2550	 -0.0170
m	 0.4350	 0.0540
n	 0.3280	 -0.0270
o	 0.2730	 -0.0040
p	 0.3080	 -0.0170
q	 0.3320	 -0.0140
r	 0.3880	 -0.0070
s	 0.3240	 -0.0020
t	 0.2430	 -0.0630
u	 0.1830	 0.0000
v	 0.5040	 0.0520
x	 0.3530	 -0.0030
y	 0.3620	 0.0360
z	 0.0540	 -0.0040