



Full wwPDB EM Validation Report ⓘ

Mar 31, 2025 – 05:50 PM JST

PDB ID : 5ZEB / pdb_00005zeb
EMDB ID : EMD-6920
Title : M. Smegmatis P/P state 70S ribosome structure
Authors : Mishra, S.; Ahmed, T.; Tyagi, A.; Shi, J.; Bhushan, S.
Deposited on : 2018-02-27
Resolution : 3.40 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.dev117
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) : 2.42

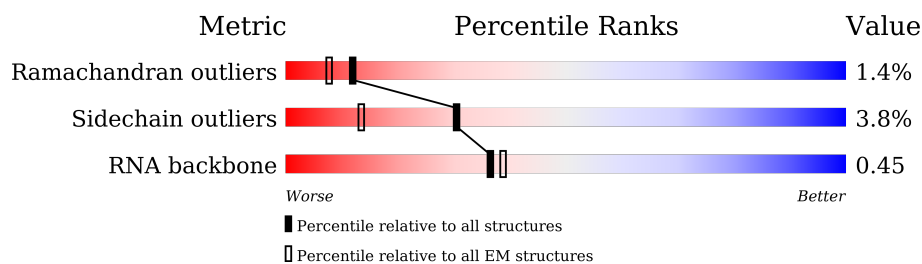
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

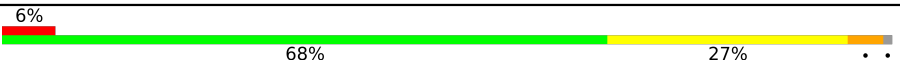
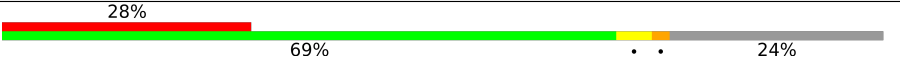

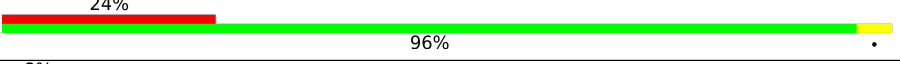
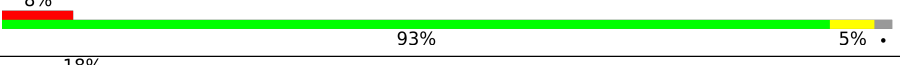
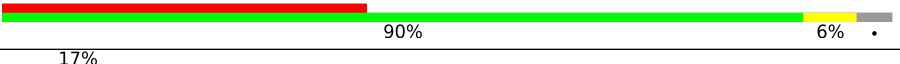
The reported resolution of this entry is 3.40 Å.

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	1528	
2	c	275	
3	e	214	
4	g	156	
5	h	132	
6	i	150	
7	j	101	
8	k	138	

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Mol	Chain	Length	Quality of chain
9	l	124	
10	o	89	
11	q	98	
12	r	84	
13	s	93	
14	t	86	
15	v	77	
16	n	61	
17	b	277	
18	d	201	
19	f	96	
20	m	124	
21	p	156	
22	u	33	
23	C	278	
24	D	217	
25	E	215	
26	F	187	
27	G	179	
28	H	151	
29	I	175	
30	J	142	
31	K	147	
32	L	122	
33	M	147	

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Mol	Chain	Length	Quality of chain
34	N	138	
35	O	199	
36	P	127	
37	Q	113	
38	R	129	
39	S	103	
40	T	153	
41	U	100	
42	V	105	
43	W	215	
44	X	88	
45	Y	64	
46	Z	77	
47	B	118	
48	A	3120	
49	1	61	
50	2	75	
51	3	57	
52	4	55	
53	5	47	
54	6	64	
55	7	37	
56	8	24	

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 150328 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 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	1506	Total	C	N	O	P	0	0
			32341	14404	5921	10510	1506		

- Molecule 2 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	c	210	Total	C	N	O	S	0	0
			1672	1043	324	300	5		

- Molecule 3 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	e	198	Total	C	N	O	S	0	0
			1433	885	282	262	4		

- Molecule 4 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	g	156	Total	C	N	O	S	0	0
			1240	773	242	222	3		

- Molecule 5 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	h	130	Total	C	N	O	S	0	0
			1003	629	188	185	1		

- Molecule 6 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	i	126	Total	C	N	O		0	0
			994	630	194	170			

- Molecule 7 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	j	97	Total	C	N	O	S	0	0
			775	488	143	141	3		

- Molecule 8 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	k	117	Total	C	N	O	S	0	0
			871	539	173	158	1		

- Molecule 9 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	l	122	Total	C	N	O	S	0	0
			958	594	197	165	2		

- Molecule 10 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	o	87	Total	C	N	O	0	0
			709	443	143	123		

- Molecule 11 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	q	92	Total	C	N	O	S	0	0
			730	458	138	132	2		

- Molecule 12 is a protein called 30S ribosomal protein S18 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	r	64	Total	C	N	O	S	0	0
			512	319	102	88	3		

- Molecule 13 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	s	78	Total	C	N	O	S	0	0
			630	405	117	107	1		

- Molecule 14 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	t	84	Total	C	N	O	0	0
			655	399	138	118		

- Molecule 15 is a RNA chain called P-tRNA^fMet.

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

- Molecule 16 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	n	60	Total	C	N	O	S	0	0
			477	302	97	73	5		

- Molecule 17 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	b	228	Total	C	N	O	S	0	0
			1793	1132	322	330	9		

- Molecule 18 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	d	200	Total	C	N	O	S	0	0
			1641	1028	316	295	2		

- Molecule 19 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	f	96	Total	C	N	O	S	0	0
			771	486	138	145	2		

- Molecule 20 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	m	116	Total	C	N	O	S	0	0
			935	572	191	169	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
21	p	113	Total	C	N	O		
			891	570	162	159	0	0

- Molecule 22 is a protein called Conserved domain protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	u	32	Total	C	N	O	S		
			280	172	71	36	1	0	0

- Molecule 23 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	C	273	Total	C	N	O	S		
			2097	1290	435	368	4	0	0

- Molecule 24 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	D	214	Total	C	N	O	S		
			1587	982	310	290	5	0	0

- Molecule 25 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	E	207	Total	C	N	O	S		
			1553	959	292	300	2	0	0

- Molecule 26 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	F	181	Total	C	N	O	S		
			1437	903	269	259	6	0	0

- Molecule 27 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	G	176	Total	C	N	O	S		
			1348	845	249	253	1	0	0

- Molecule 28 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	H	151	Total	C	N	O	S	0	0
			1018	635	188	194	1		

- Molecule 29 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	I	126	Total	C	N	O	S	0	0
			918	580	156	180	2		

- Molecule 30 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	J	133	Total	C	N	O	S	0	0
			990	625	175	187	3		

- Molecule 31 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	K	147	Total	C	N	O	S	0	0
			1138	727	208	201	2		

- Molecule 32 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	L	121	Total	C	N	O	S	0	0
			930	580	178	169	3		

- Molecule 33 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	M	145	Total	C	N	O	S	0	0
			1078	676	205	194	3		

- Molecule 34 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	N	134	Total	C	N	O	S	0	0
			1074	680	211	181	2		

- Molecule 35 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	O	117	Total	C	N	O	S	0	0
			919	577	178	162	2		

- Molecule 36 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	P	126	Total	C	N	O		0	0
			956	586	199	171			

- Molecule 37 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Q	113	Total	C	N	O	S	0	0
			907	570	171	165	1		

- Molecule 38 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	R	124	Total	C	N	O		0	0
			988	613	203	172			

- Molecule 39 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	S	102	Total	C	N	O		0	0
			768	487	140	141			

- Molecule 40 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	T	114	Total	C	N	O		0	0
			873	543	171	159			

- Molecule 41 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	U	94	Total	C	N	O		0	0
			739	469	135	135			

- Molecule 42 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	V	97	Total	C	N	O	S	0	0
			731	456	137	136	2		

- Molecule 43 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	W	188	Total	C	N	O		0	0
			1407	869	251	287			

- Molecule 44 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	X	82	Total	C	N	O		0	0
			604	372	127	105			

- Molecule 45 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Y	63	Total	C	N	O	S	0	0
			470	283	103	80	4		

- Molecule 46 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Z	63	Total	C	N	O	S	0	0
			527	322	102	102	1		

- Molecule 47 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	B	117	Total	C	N	O	P	0	0
			2501	1116	462	806	117		

- Molecule 48 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	A	3102	Total	C	N	O	P	0	0
			66623	29694	12253	21574	3102		

- Molecule 49 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	1	60	Total	C	N	O	0	0
			483	298	97	88		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	2	66	Total	C	N	O	S	0	0
			510	316	93	96	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
51	3	54	Total	C	N	O	S	0	0
			423	260	93	69	1		

- Molecule 52 is a protein called 50S ribosomal protein L33 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	4	50	Total	C	N	O	S	0	0
			416	254	86	72	4		

- Molecule 53 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	5	45	Total	C	N	O	S	0	0
			372	222	96	53	1		

- Molecule 54 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	6	63	Total	C	N	O	0	0
			502	302	115	85		

- Molecule 55 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	7	37	Total	C	N	O	S	0	0
			298	181	66	46	5		

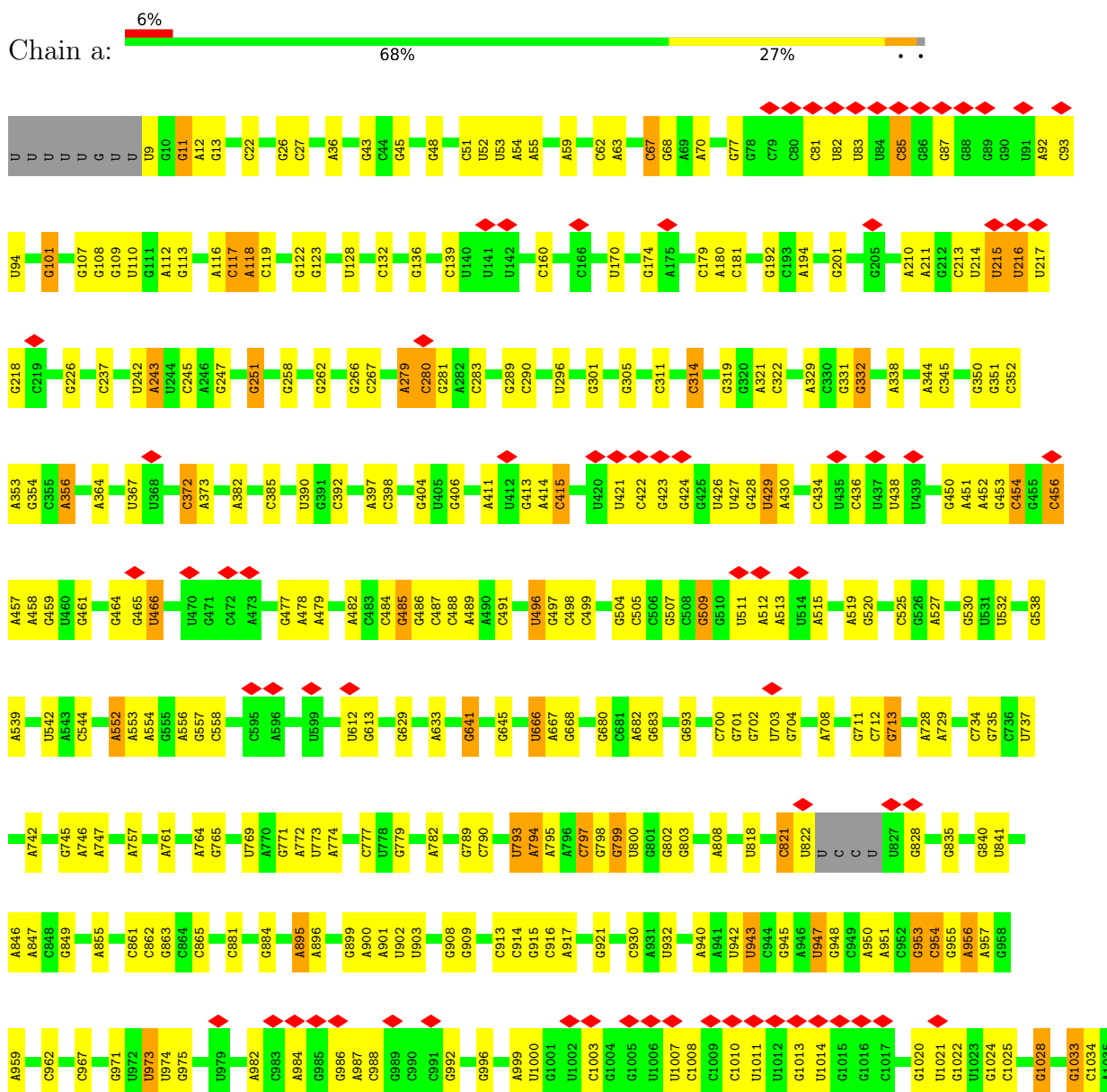
- Molecule 56 is a protein called Uncharacterized protein bL37.

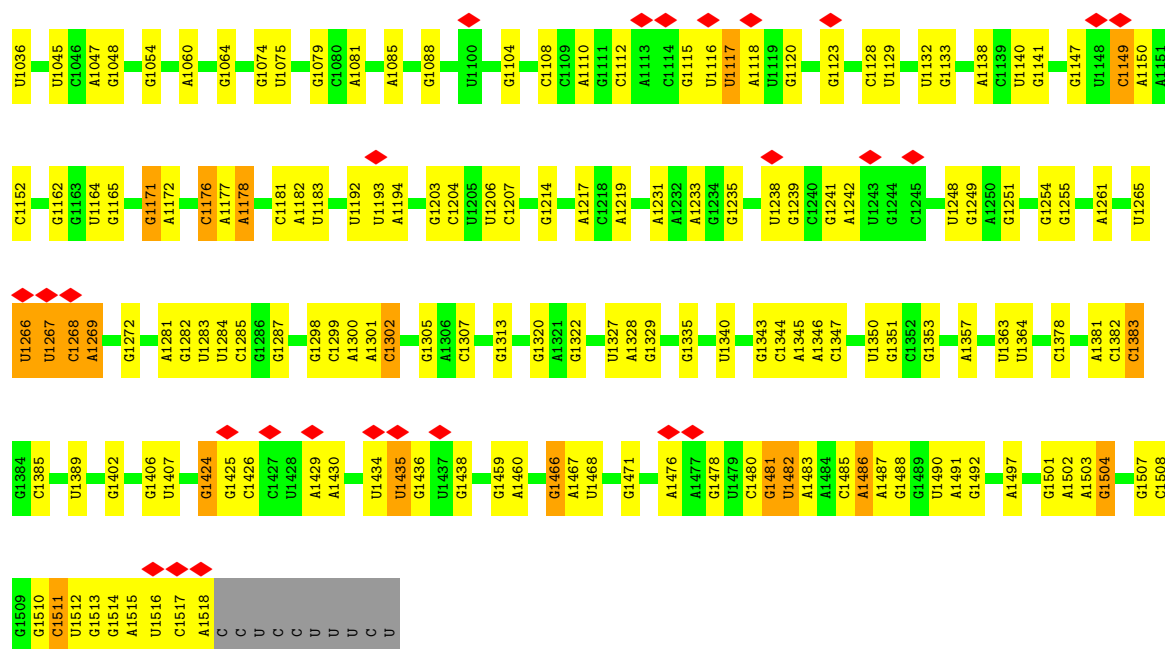
Mol	Chain	Residues	Atoms				AltConf	Trace
56	8	23	Total	C	N	O	0	0
			189	111	50	28		

3 Residue-property plots

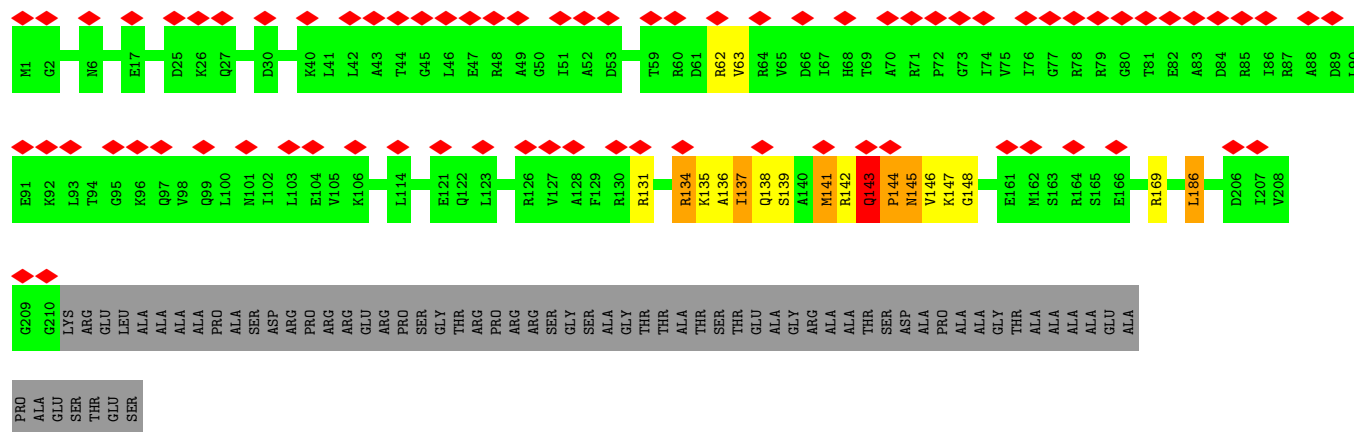
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 16S rRNA

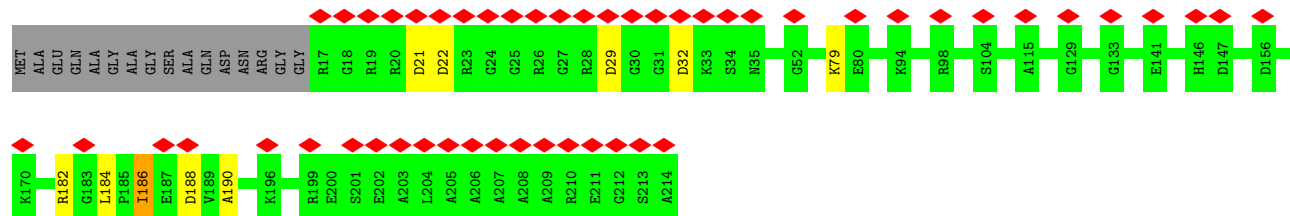
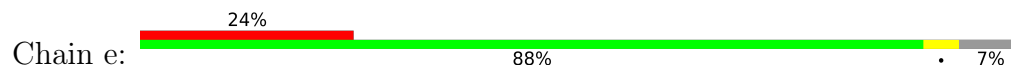




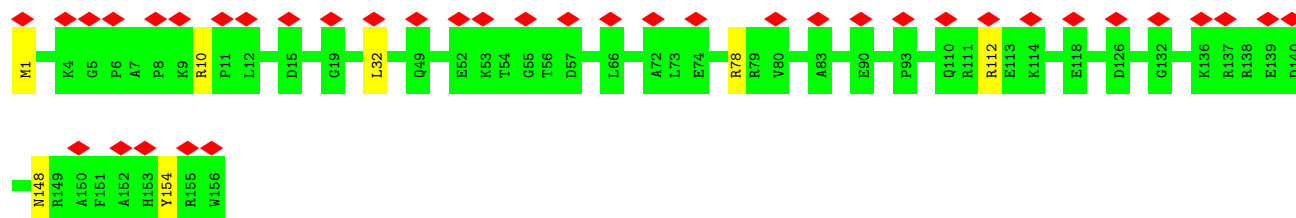
• Molecule 2: 30S ribosomal protein S3



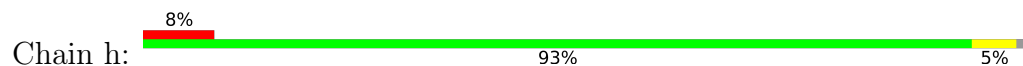
• Molecule 3: 30S ribosomal protein S5



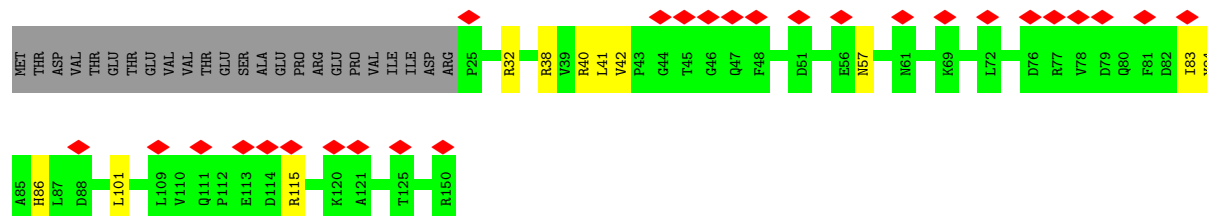
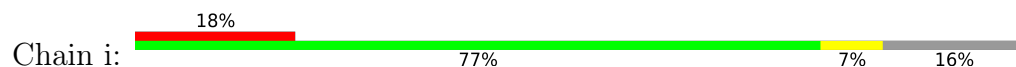
• Molecule 4: 30S ribosomal protein S7



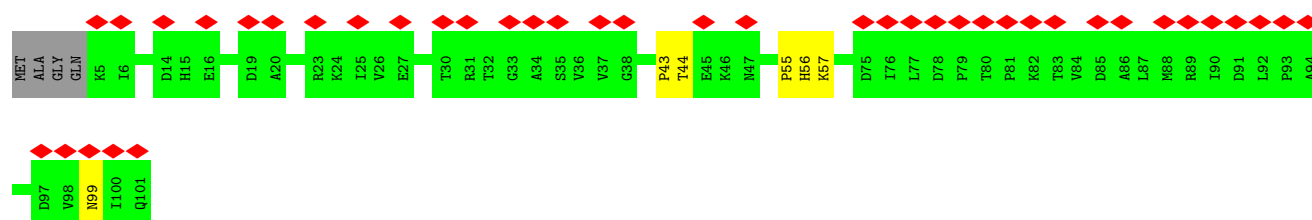
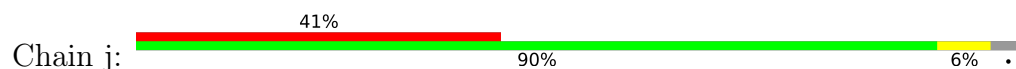
- Molecule 5: 30S ribosomal protein S8



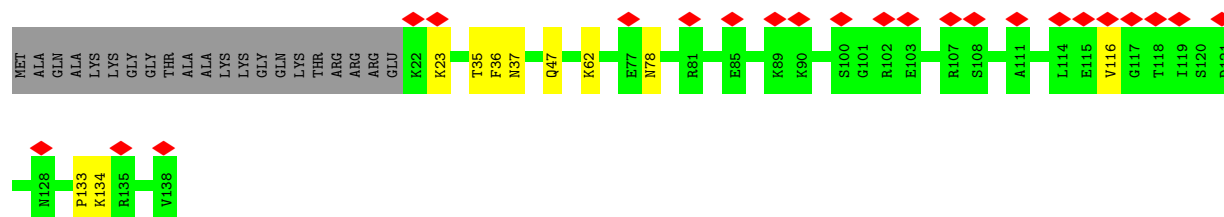
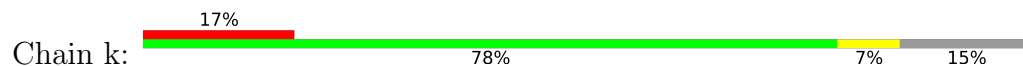
- Molecule 6: 30S ribosomal protein S9



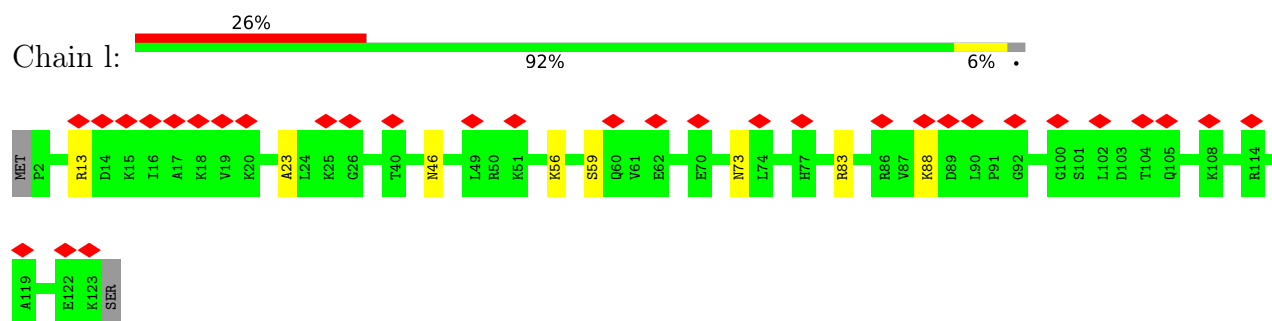
- Molecule 7: 30S ribosomal protein S10



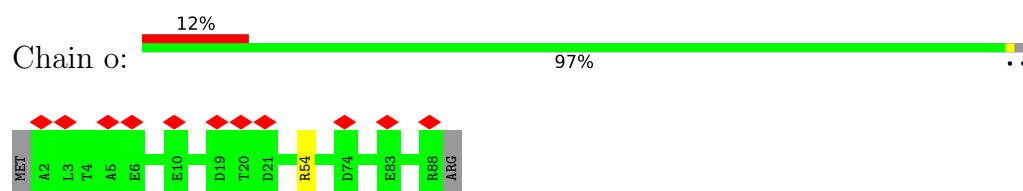
- Molecule 8: 30S ribosomal protein S11



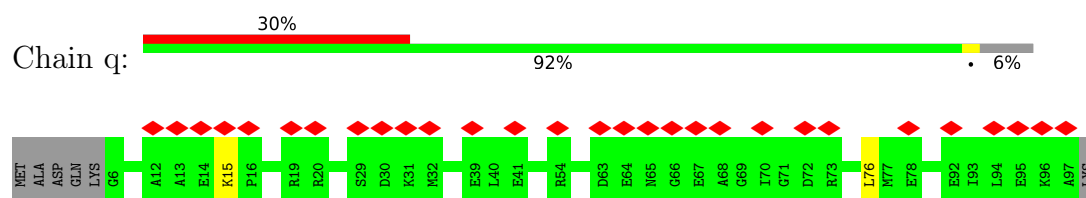
- Molecule 9: 30S ribosomal protein S12



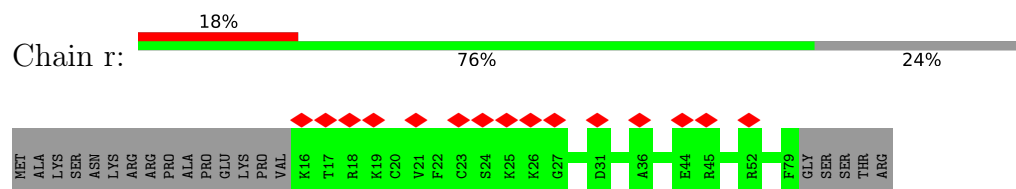
- Molecule 10: 30S ribosomal protein S15



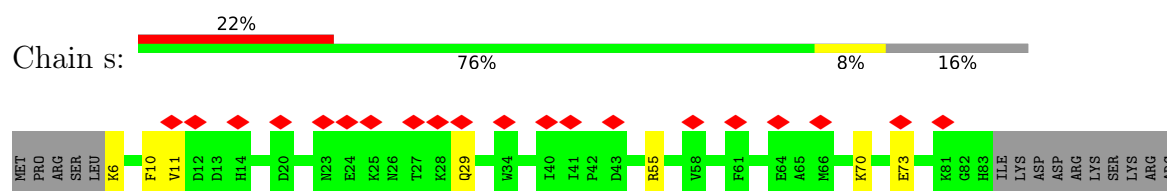
- Molecule 11: 30S ribosomal protein S17



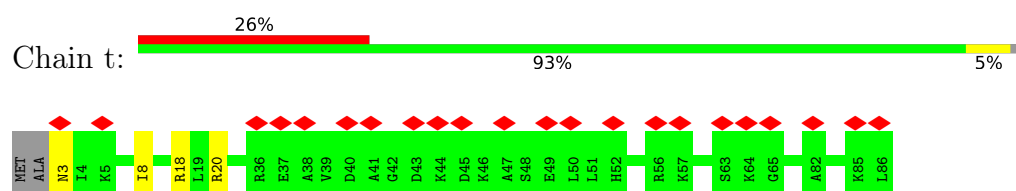
- Molecule 12: 30S ribosomal protein S18 2



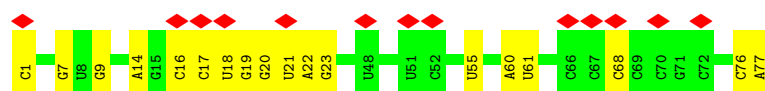
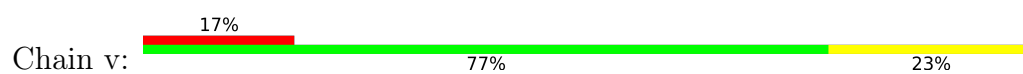
- Molecule 13: 30S ribosomal protein S19



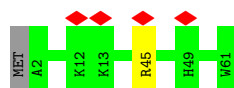
- Molecule 14: 30S ribosomal protein S20



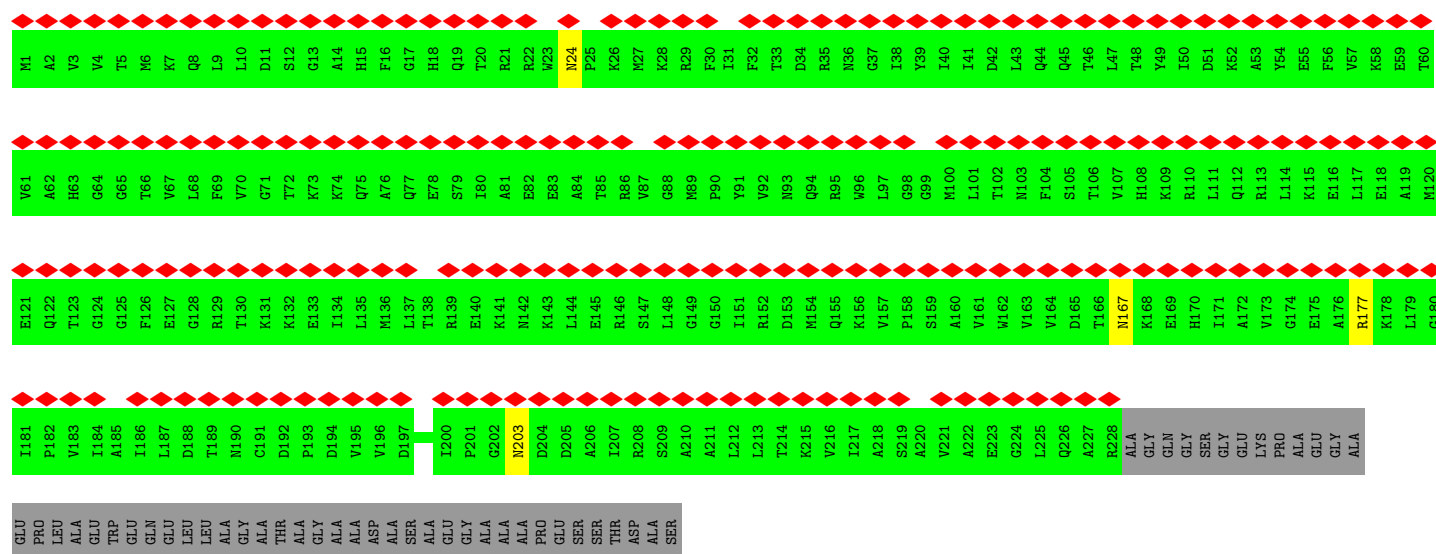
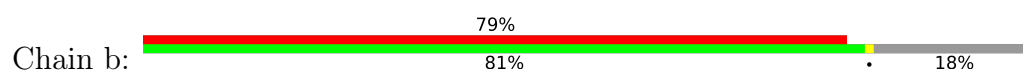
- Molecule 15: P-tRNA^{fMet}



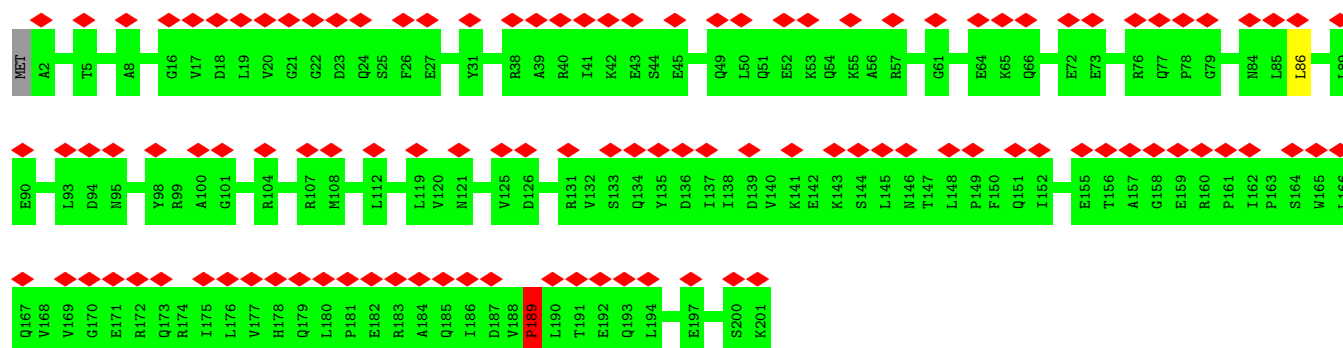
- Molecule 16: 30S ribosomal protein S14 type Z



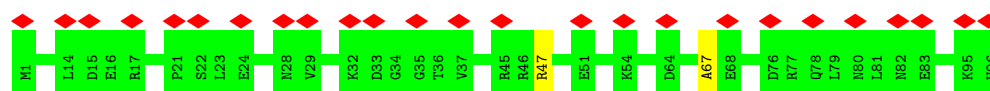
- Molecule 17: 30S ribosomal protein S2



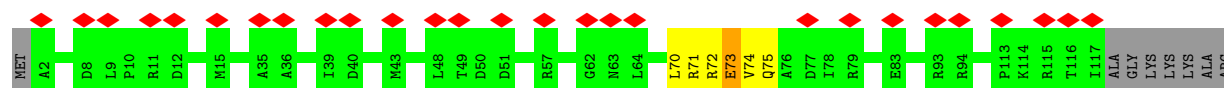
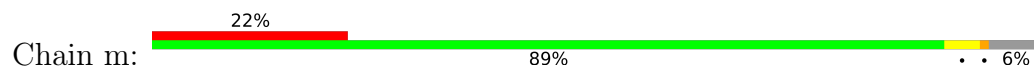
- Molecule 18: 30S ribosomal protein S4



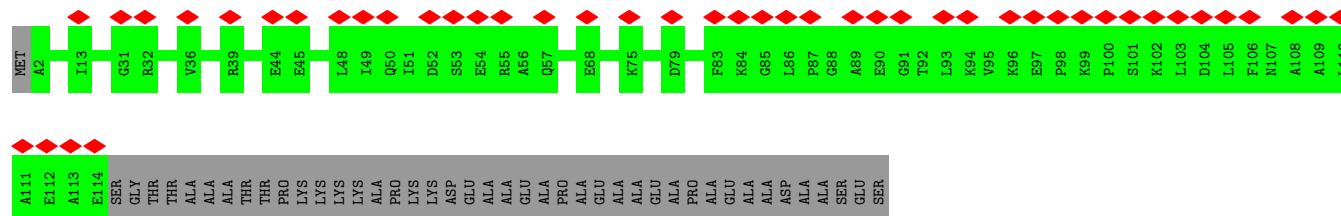
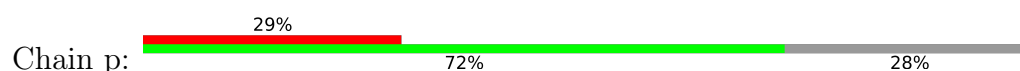
- Molecule 19: 30S ribosomal protein S6



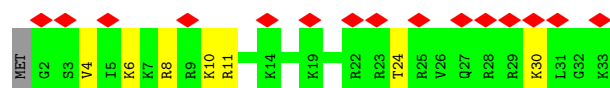
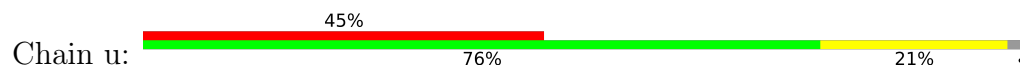
- Molecule 20: 30S ribosomal protein S13



- Molecule 21: 30S ribosomal protein S16



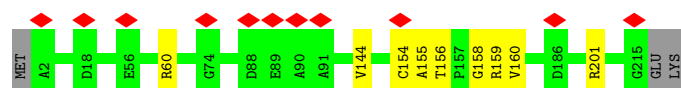
- Molecule 22: Conserved domain protein



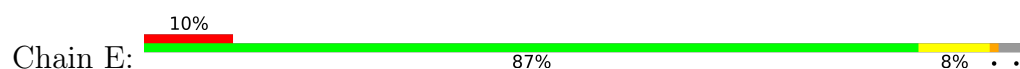
- Molecule 23: 50S ribosomal protein L2

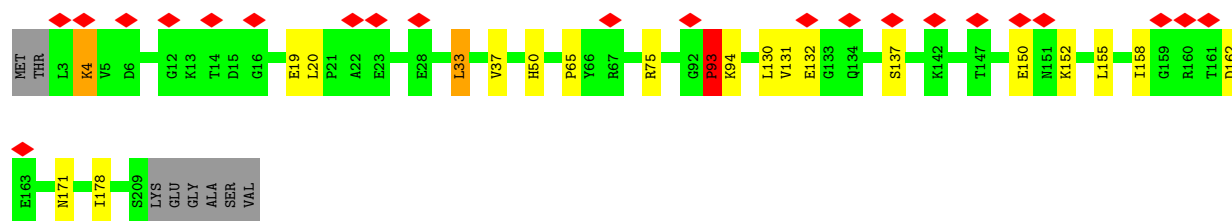


- Molecule 24: 50S ribosomal protein L3



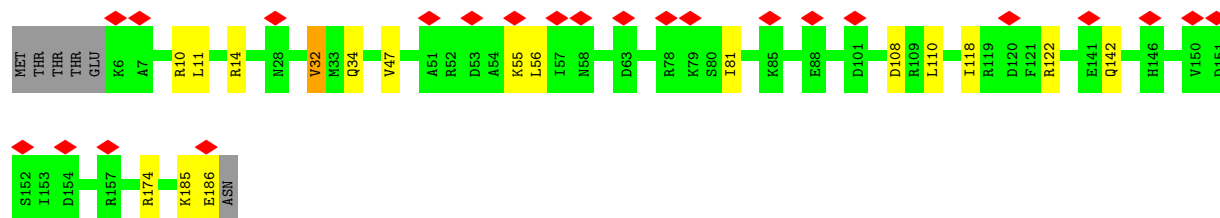
- Molecule 25: 50S ribosomal protein L4





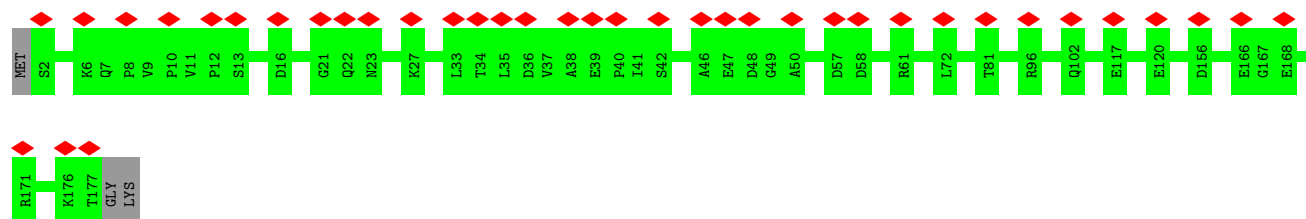
- Molecule 26: 50S ribosomal protein L5

Chain F: 12% 88% 9% . .



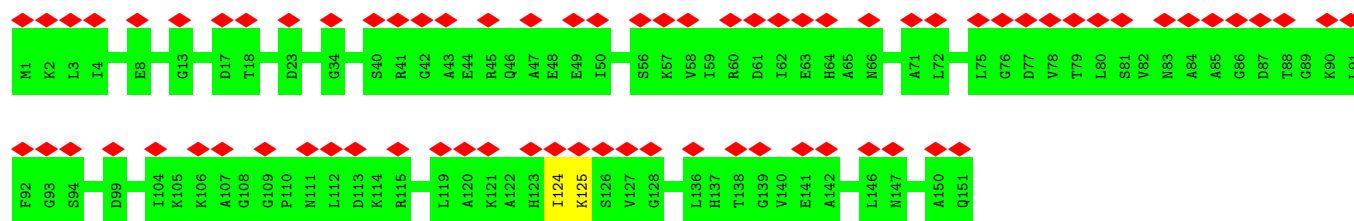
- Molecule 27: 50S ribosomal protein L6

Chain G: 21% 98% .



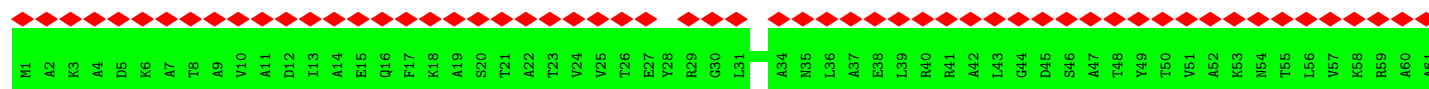
- Molecule 28: 50S ribosomal protein L9

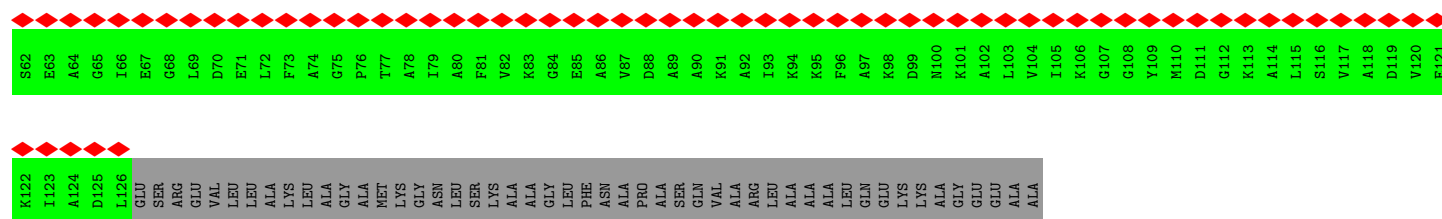
Chain H: 49% 99% .



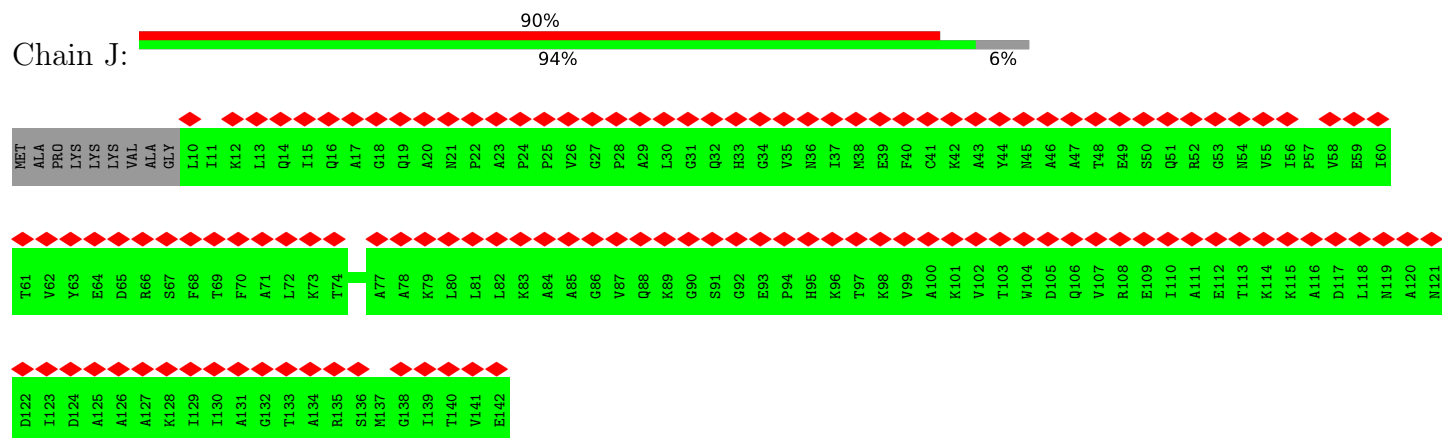
- Molecule 29: 50S ribosomal protein L10

Chain I: 70% 72% 28%

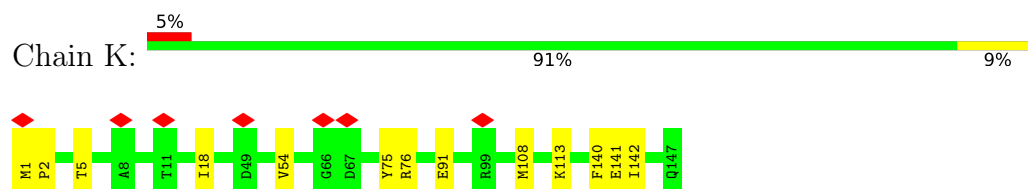




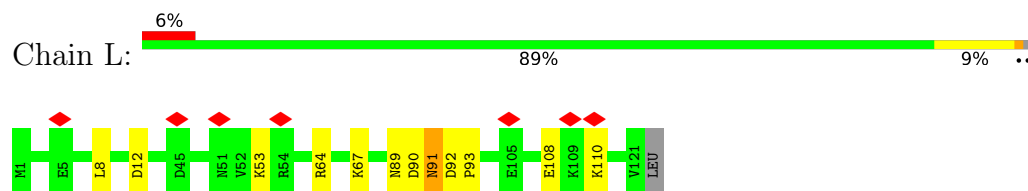
- Molecule 30: 50S ribosomal protein L11



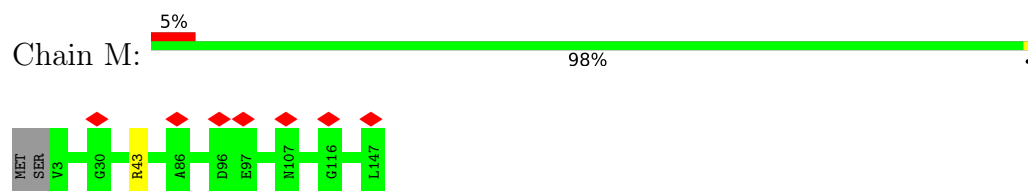
- Molecule 31: 50S ribosomal protein L13



- Molecule 32: 50S ribosomal protein L14

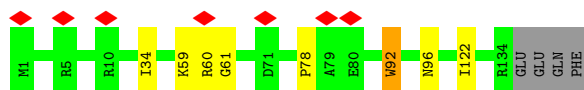


- Molecule 33: 50S ribosomal protein L15

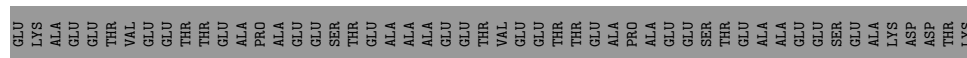
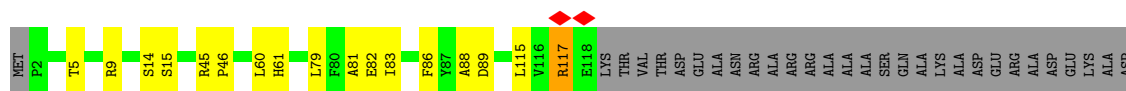


- Molecule 34: 50S ribosomal protein L16





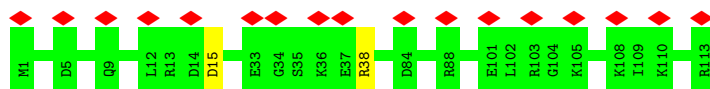
- Molecule 35: 50S ribosomal protein L17



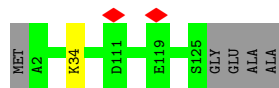
- Molecule 36: 50S ribosomal protein L18



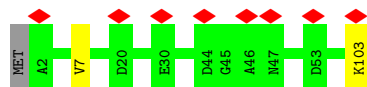
- Molecule 37: 50S ribosomal protein L19



- Molecule 38: 50S ribosomal protein L20

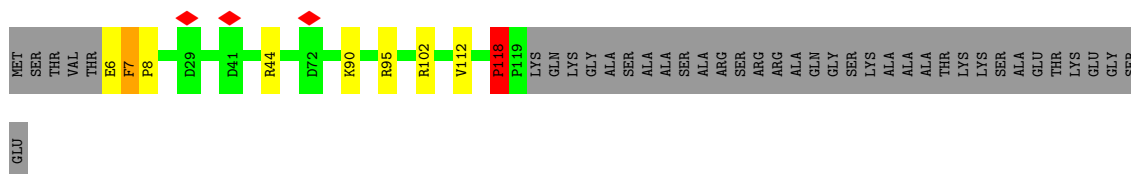


- Molecule 39: 50S ribosomal protein L21

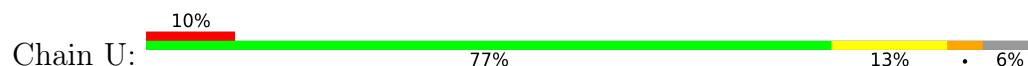


- Molecule 40: 50S ribosomal protein L22

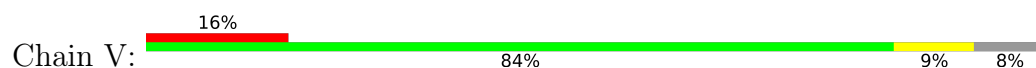




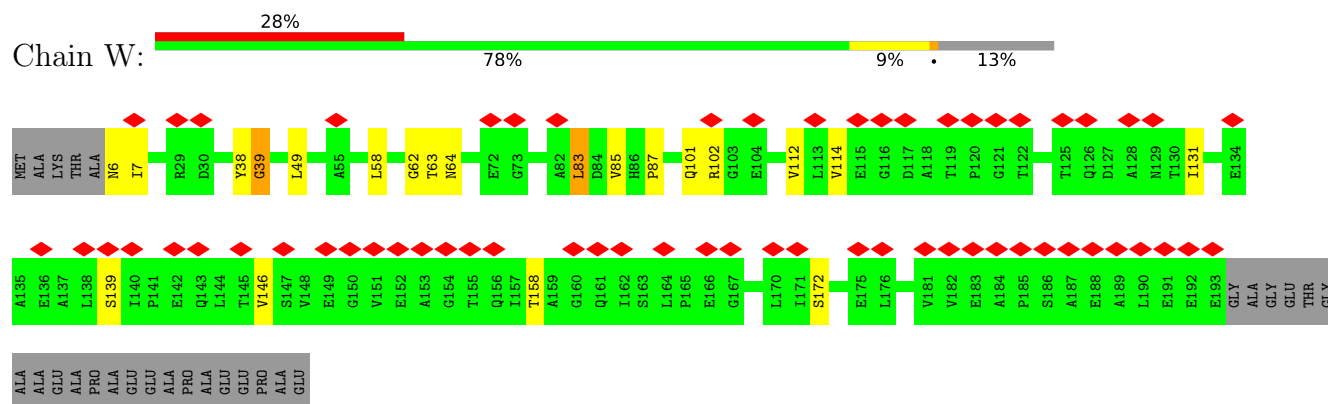
- Molecule 41: 50S ribosomal protein L23



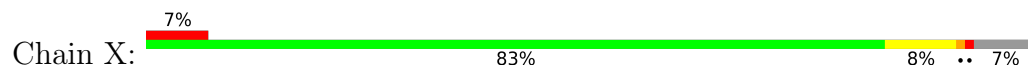
- Molecule 42: 50S ribosomal protein L24



- Molecule 43: 50S ribosomal protein L25



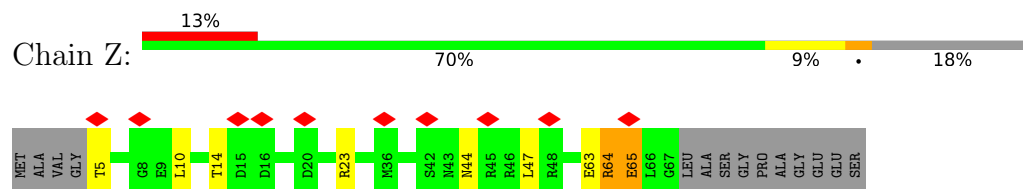
- Molecule 44: 50S ribosomal protein L27



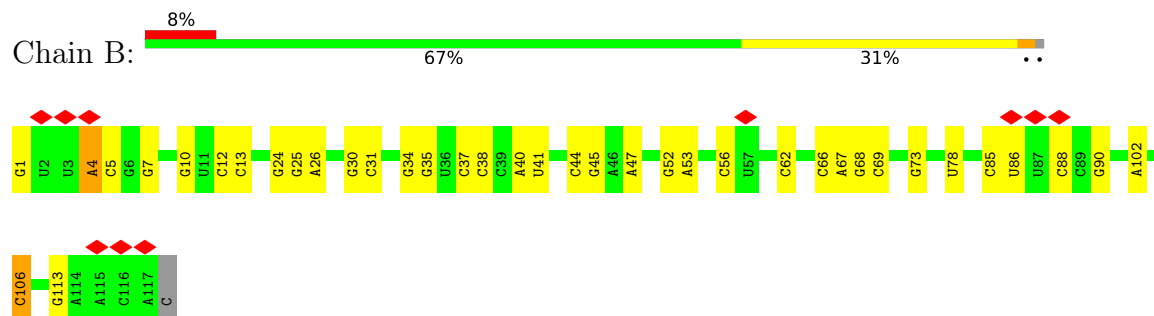
- Molecule 45: 50S ribosomal protein L28



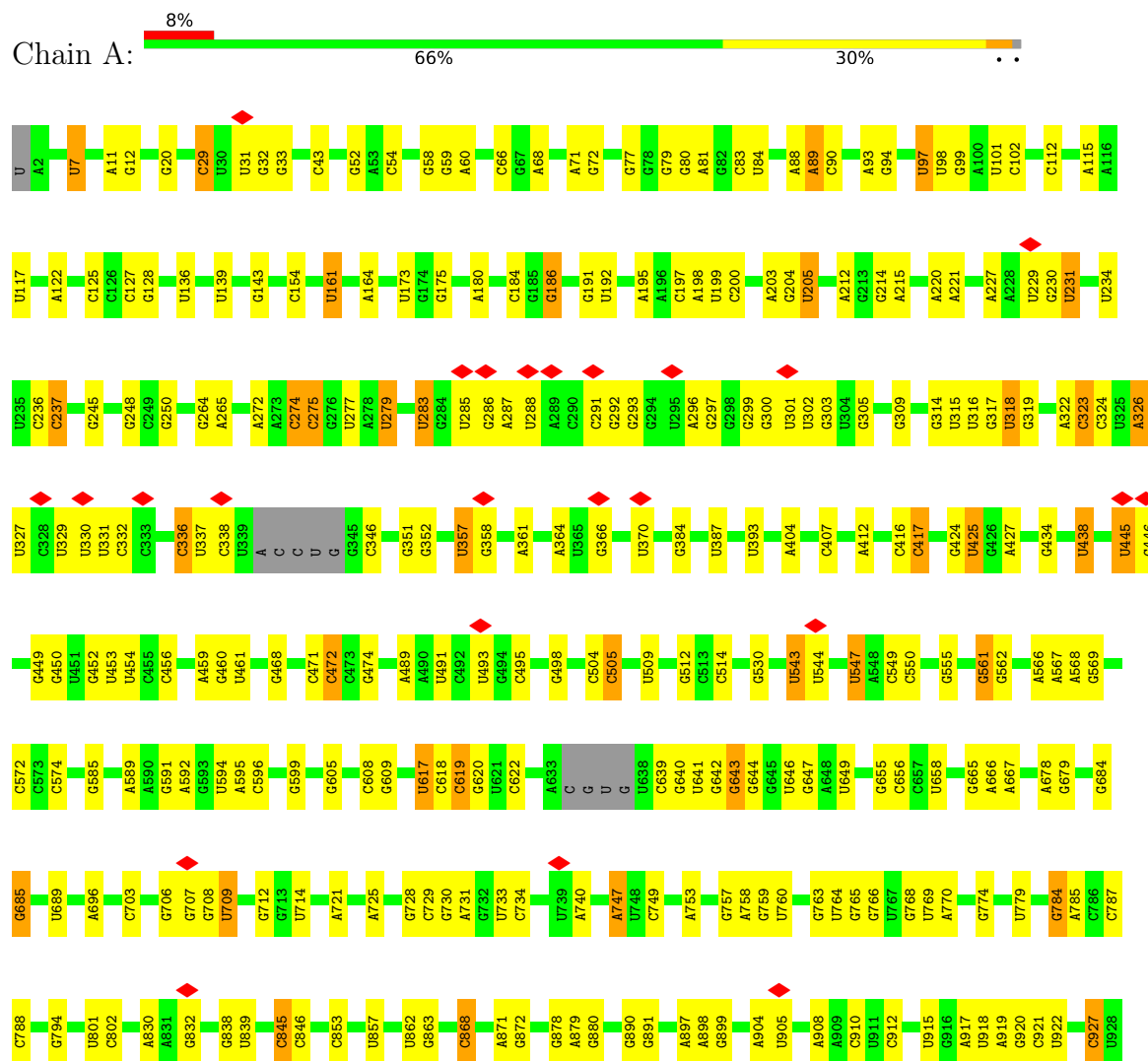
- Molecule 46: 50S ribosomal protein L29

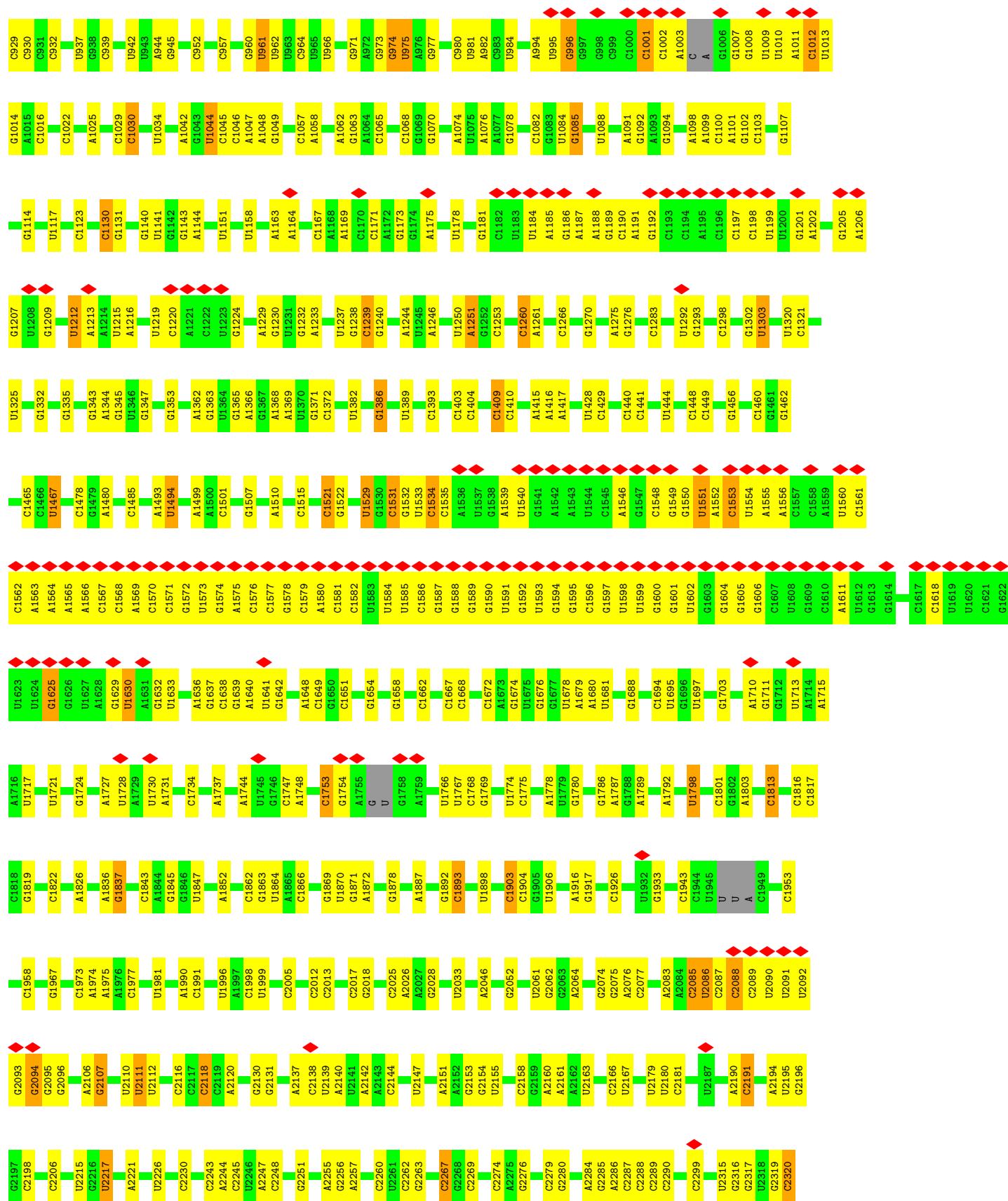


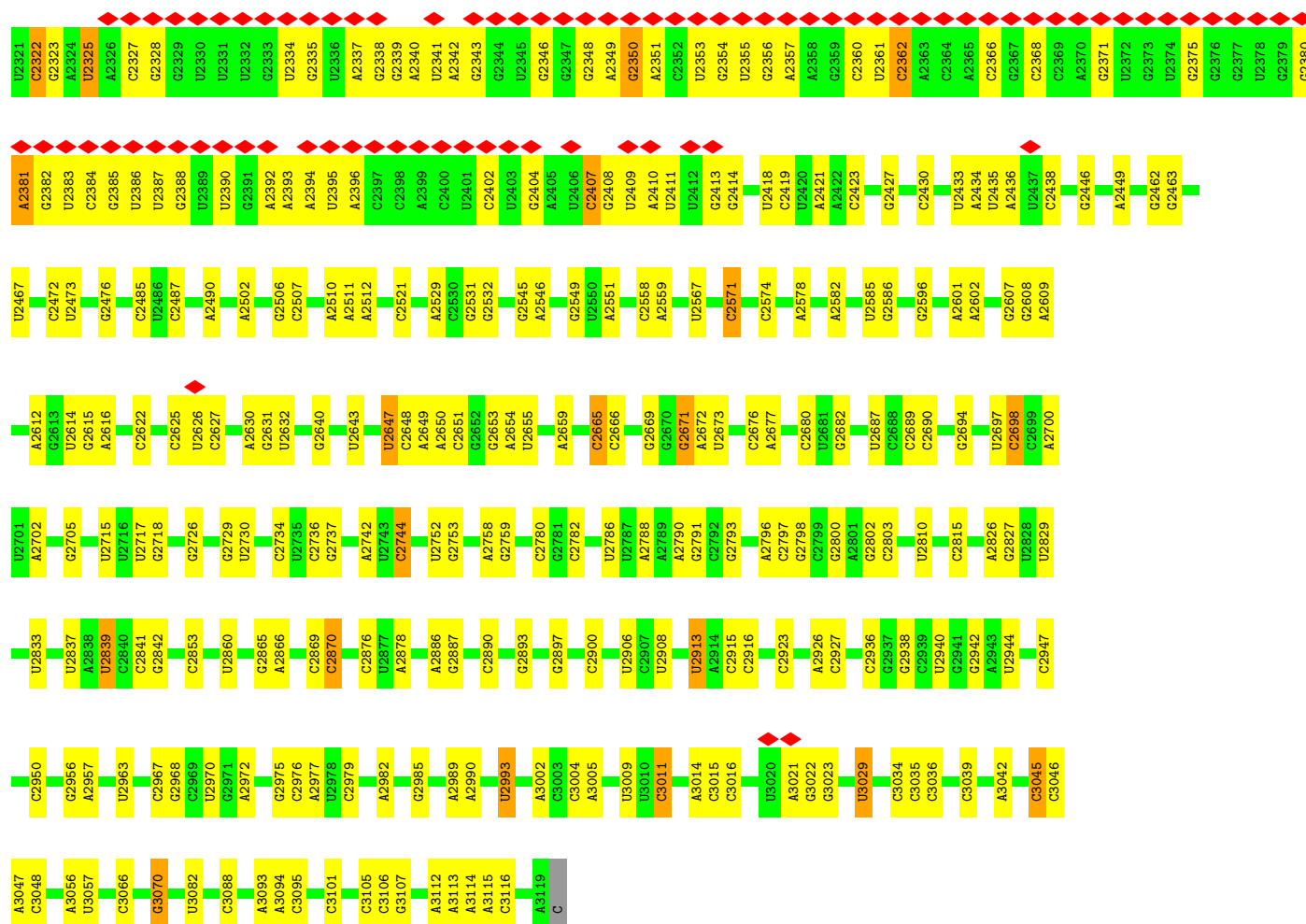
- Molecule 47: 5S rRNA



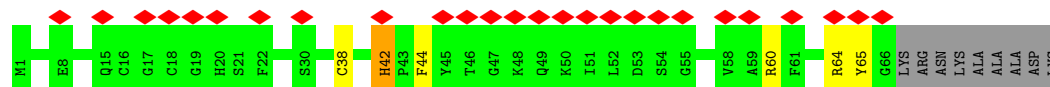
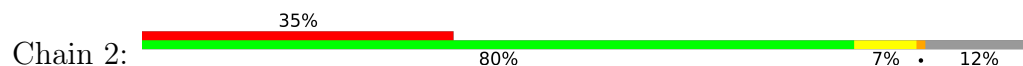
- Molecule 48: 23S rRNA





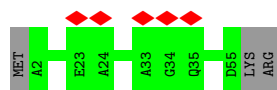


- Molecule 50: 50S ribosomal protein L31



- Molecule 51: 50S ribosomal protein L32

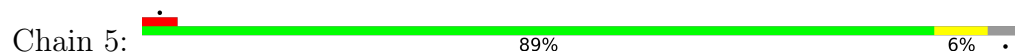




- Molecule 52: 50S ribosomal protein L33 1



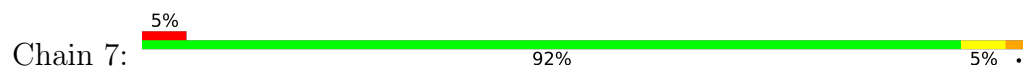
- Molecule 53: 50S ribosomal protein L34



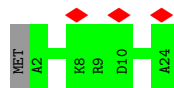
- Molecule 54: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L36



- Molecule 56: Uncharacterized protein bL37



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	391837	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.550	Depositor
Minimum map value	-0.382	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.07	Depositor
Map size (\AA)	419.99997, 419.99997, 419.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.05, 1.05, 1.05	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.81	23/36201 (0.1%)	1.27	219/56488 (0.4%)
2	c	0.37	0/1696	0.63	2/2276 (0.1%)
3	e	0.39	0/1449	0.67	5/1949 (0.3%)
4	g	0.35	0/1260	0.58	0/1701
5	h	0.41	0/1018	0.71	2/1375 (0.1%)
6	i	0.41	0/1012	0.79	2/1362 (0.1%)
7	j	0.41	0/789	0.64	0/1069
8	k	0.31	0/889	0.57	0/1201
9	l	0.38	0/969	0.76	0/1294
10	o	0.34	0/718	0.58	0/963
11	q	0.39	0/741	0.67	1/993 (0.1%)
12	r	0.35	0/517	0.59	0/691
13	s	0.39	0/647	0.68	0/871
14	t	0.33	0/658	0.52	0/875
15	v	0.40	1/1835 (0.1%)	0.79	0/2857
16	n	0.53	0/488	0.57	0/650
17	b	0.31	0/1822	0.55	0/2457
18	d	0.38	0/1672	0.61	1/2251 (0.0%)
19	f	0.38	0/782	0.62	1/1059 (0.1%)
20	m	0.35	0/942	0.63	0/1260
21	p	0.41	0/908	0.60	0/1226
22	u	0.49	0/280	0.67	0/359
23	C	1.01	5/2140 (0.2%)	0.93	5/2879 (0.2%)
24	D	0.55	0/1609	0.66	2/2165 (0.1%)
25	E	0.84	1/1576 (0.1%)	0.87	4/2132 (0.2%)
26	F	0.59	0/1459	0.78	0/1962
27	G	0.36	0/1369	0.57	0/1848
28	H	0.33	0/1027	0.61	1/1398 (0.1%)
29	I	0.29	0/925	0.52	0/1246
30	J	0.29	0/1006	0.60	0/1364
31	K	0.76	1/1165 (0.1%)	0.88	4/1578 (0.3%)
32	L	0.92	0/938	0.96	5/1257 (0.4%)
33	M	0.53	0/1091	0.65	0/1457
34	N	0.91	1/1100 (0.1%)	0.91	2/1482 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
35	O	0.73	0/936	0.87	2/1256 (0.2%)
36	P	0.43	0/966	0.57	0/1298
37	Q	0.51	0/921	0.60	1/1236 (0.1%)
38	R	0.55	0/1000	0.58	0/1341
39	S	0.48	0/778	0.56	0/1048
40	T	0.96	1/887 (0.1%)	0.93	3/1204 (0.2%)
41	U	0.75	0/749	0.88	2/1006 (0.2%)
42	V	0.65	0/737	0.78	1/987 (0.1%)
43	W	0.52	0/1422	0.80	4/1941 (0.2%)
44	X	0.96	0/613	0.88	1/821 (0.1%)
45	Y	0.55	0/478	0.70	0/641
46	Z	0.69	0/530	0.76	0/708
47	B	0.55	1/2797 (0.0%)	1.15	18/4357 (0.4%)
48	A	1.00	1/74597 (0.0%)	1.24	632/116386 (0.5%)
49	1	0.80	0/486	0.88	0/651
50	2	0.38	0/520	0.61	1/698 (0.1%)
51	3	0.55	0/427	0.61	0/572
52	4	0.74	1/424 (0.2%)	0.79	1/567 (0.2%)
53	5	0.84	0/375	1.00	1/493 (0.2%)
54	6	0.91	0/507	0.94	2/672 (0.3%)
55	7	0.85	0/302	0.84	0/401
56	8	0.44	0/191	0.60	0/247
All	All	0.84	36/163341 (0.0%)	1.13	925/244526 (0.4%)

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
2	c	0	10
3	e	0	1
4	g	0	2
5	h	0	2
7	j	0	1
8	k	0	2
9	l	0	2
11	q	0	1
13	s	0	2
18	d	0	1
20	m	0	1
23	C	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
25	E	0	5
26	F	0	3
31	K	0	1
32	L	0	2
34	N	0	1
35	O	0	4
40	T	0	1
43	W	0	2
44	X	0	4
50	2	0	1
52	4	0	1
All	All	0	55

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	v	1	C	OP3-P	-10.49	1.48	1.61
47	B	1	G	OP3-P	-10.45	1.48	1.61
1	a	861	C	N1-C6	-7.33	1.32	1.37
1	a	552	A	N9-C4	-7.10	1.33	1.37
23	C	79	VAL	CB-CG2	-6.93	1.38	1.52
40	T	112	VAL	CB-CG2	-6.66	1.38	1.52
1	a	552	A	N3-C4	-6.65	1.30	1.34
1	a	290	C	N1-C6	-6.24	1.33	1.37
23	C	224	VAL	CB-CG2	-6.24	1.39	1.52
1	a	1378	C	N1-C6	-6.15	1.33	1.37
1	a	746	A	N3-C4	-6.12	1.31	1.34
34	N	92	TRP	CB-CG	-5.99	1.39	1.50
1	a	1497	A	N9-C4	-5.97	1.34	1.37
1	a	746	A	N9-C4	-5.77	1.34	1.37
1	a	1204	C	N1-C6	-5.73	1.33	1.37
1	a	708	A	N9-C4	-5.67	1.34	1.37
52	4	42	CYS	CB-SG	-5.62	1.72	1.81
1	a	901	A	N9-C4	-5.50	1.34	1.37
23	C	247	VAL	CB-CG1	-5.49	1.41	1.52
1	a	22	C	N1-C6	-5.39	1.33	1.37
1	a	552	A	C5-C4	-5.38	1.34	1.38
1	a	797	C	N1-C6	-5.37	1.33	1.37
1	a	863	G	N9-C8	-5.36	1.34	1.37
1	a	777	C	N1-C6	-5.33	1.33	1.37
1	a	712	C	N1-C6	-5.25	1.33	1.37
1	a	1467	A	N3-C4	-5.25	1.31	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	A	1099	A	N7-C5	-5.25	1.36	1.39
1	a	119	C	N1-C6	-5.17	1.34	1.37
31	K	54	VAL	CB-CG2	-5.17	1.42	1.52
1	a	296	U	C2-N3	-5.15	1.34	1.37
1	a	746	A	C5-C4	-5.13	1.35	1.38
1	a	846	A	N3-C4	-5.13	1.31	1.34
25	E	37	VAL	CB-CG1	-5.13	1.42	1.52
23	C	224	VAL	CB-CG1	-5.12	1.42	1.52
1	a	899	G	C5-C4	-5.04	1.34	1.38
23	C	187	VAL	CB-CG1	-5.03	1.42	1.52

All (925) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	A	323	C	N1-C2-O2	11.57	125.84	118.90
48	A	1130	C	N1-C2-O2	11.21	125.63	118.90
48	A	2245	C	N1-C2-O2	11.09	125.55	118.90
48	A	2245	C	C2-N1-C1'	10.67	130.54	118.80
48	A	323	C	C2-N1-C1'	10.54	130.39	118.80
48	A	619	C	N1-C2-O2	10.29	125.07	118.90
48	A	2025	C	N3-C2-O2	-10.28	114.71	121.90
48	A	3046	C	C2-N1-C1'	10.19	130.01	118.80
48	A	1012	C	C2-N1-C1'	9.90	129.69	118.80
48	A	237	C	C6-N1-C2	-9.87	116.35	120.30
48	A	2245	C	N3-C2-O2	-9.68	115.12	121.90
48	A	1630	U	C5-C4-O4	9.65	131.69	125.90
5	h	94	LEU	N-CA-C	-9.60	85.09	111.00
48	A	1012	C	N1-C2-O2	9.60	124.66	118.90
48	A	1694	C	N1-C2-O2	9.58	124.65	118.90
48	A	1694	C	N3-C2-O2	-9.57	115.20	121.90
1	a	1482	U	P-O3'-C3'	9.54	131.14	119.70
48	A	1130	C	C2-N1-C1'	9.53	129.28	118.80
48	A	619	C	C2-N1-C1'	9.51	129.27	118.80
1	a	101	G	C8-N9-C4	-9.51	102.60	106.40
48	A	2025	C	N1-C2-O2	9.47	124.58	118.90
48	A	2407	C	N1-C2-O2	9.44	124.56	118.90
48	A	1001	C	C6-N1-C2	-9.41	116.53	120.30
48	A	1428	U	C2-N1-C1'	9.40	128.99	117.70
48	A	912	C	C5-C6-N1	9.36	125.68	121.00
48	A	323	C	N3-C2-O2	-9.33	115.37	121.90
6	i	101	LEU	CB-CG-CD2	-9.27	95.25	111.00
48	A	336	C	C2-N1-C1'	9.20	128.92	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	A	2025	C	C2-N1-C1'	9.19	128.91	118.80
1	a	70	A	N1-C2-N3	9.19	133.89	129.30
48	A	2407	C	C2-N1-C1'	9.18	128.90	118.80
1	a	489	A	N7-C8-N9	9.18	118.39	113.80
48	A	3046	C	N3-C2-O2	-9.17	115.48	121.90
1	a	108	G	C8-N9-C4	9.08	110.03	106.40
1	a	85	C	C2-N1-C1'	9.04	128.74	118.80
1	a	101	G	N7-C8-N9	9.02	117.61	113.10
1	a	332	G	C8-N9-C4	8.96	109.98	106.40
48	A	1428	U	N1-C2-O2	8.93	129.05	122.80
48	A	1130	C	N3-C2-O2	-8.92	115.65	121.90
48	A	1694	C	C6-N1-C2	-8.88	116.75	120.30
48	A	709	U	N3-C2-O2	-8.86	116.00	122.20
41	U	12	LEU	CA-CB-CG	8.79	135.52	115.30
1	a	1268	C	C2-N1-C1'	8.73	128.41	118.80
48	A	237	C	C5-C6-N1	8.70	125.35	121.00
48	A	1428	U	N3-C2-O2	-8.69	116.12	122.20
48	A	417	C	C6-N1-C2	-8.68	116.83	120.30
48	A	2697	U	N1-C2-O2	8.65	128.86	122.80
48	A	2870	C	C6-N1-C2	-8.57	116.87	120.30
48	A	3046	C	N1-C2-O2	8.47	123.98	118.90
48	A	709	U	N1-C2-O2	8.44	128.71	122.80
48	A	622	C	C5-C6-N1	8.42	125.21	121.00
35	O	45	ARG	C-N-CD	8.40	146.03	128.40
48	A	3011	C	N1-C2-O2	8.38	123.93	118.90
48	A	905	U	C2-N1-C1'	8.30	127.67	117.70
43	W	62	GLY	N-CA-C	8.29	133.83	113.10
48	A	2521	C	C2-N1-C1'	8.23	127.86	118.80
1	a	1486	A	C5-N7-C8	-8.21	99.79	103.90
48	A	703	C	C2-N1-C1'	8.17	127.79	118.80
48	A	2005	C	C6-N1-C2	-8.14	117.04	120.30
47	B	31	C	N1-C2-O2	8.05	123.73	118.90
48	A	845	C	N1-C2-O2	8.05	123.73	118.90
48	A	962	U	C2-N1-C1'	8.03	127.34	117.70
48	A	275	C	C2-N1-C1'	8.02	127.63	118.80
48	A	619	C	C6-N1-C1'	-8.00	111.21	120.80
48	A	2870	C	C5-C6-N1	7.96	124.98	121.00
48	A	1429	C	C2-N1-C1'	7.94	127.53	118.80
48	A	975	U	C2-N1-C1'	7.91	127.20	117.70
48	A	2689	C	C5-C6-N1	7.91	124.95	121.00
1	a	973	U	C6-N1-C2	-7.91	116.26	121.00
48	A	2267	C	C6-N1-C2	-7.90	117.14	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	A	323	C	C6-N1-C2	-7.89	117.14	120.30
1	a	85	C	N1-C2-O2	7.89	123.63	118.90
48	A	905	U	N1-C2-O2	7.88	128.31	122.80
48	A	2947	C	C6-N1-C2	-7.88	117.15	120.30
48	A	1521	C	C2-N1-C1'	7.87	127.45	118.80
48	A	1535	C	C6-N1-C2	-7.82	117.17	120.30
48	A	275	C	C6-N1-C2	-7.81	117.18	120.30
48	A	2325	U	N1-C2-O2	7.78	128.25	122.80
40	T	118	PRO	CA-N-CD	-7.78	100.61	111.50
1	a	489	A	C8-N9-C4	-7.78	102.69	105.80
48	A	275	C	N1-C2-O2	7.77	123.56	118.90
48	A	2289	C	C5-C6-N1	7.76	124.88	121.00
48	A	1694	C	C2-N1-C1'	7.75	127.33	118.80
48	A	543	U	N3-C2-O2	-7.75	116.78	122.20
48	A	1535	C	C2-N1-C1'	7.75	127.32	118.80
48	A	1403	C	N3-C2-O2	-7.74	116.48	121.90
48	A	2267	C	C5-C6-N1	7.71	124.85	121.00
48	A	2521	C	C6-N1-C2	-7.67	117.23	120.30
48	A	1302	G	C6-C5-N7	-7.66	125.80	130.40
48	A	2322	C	N1-C2-O2	7.66	123.50	118.90
48	A	2944	U	N1-C2-O2	7.62	128.13	122.80
48	A	29	C	C2-N1-C1'	7.62	127.18	118.80
48	A	2180	U	N1-C2-O2	7.61	128.13	122.80
48	A	2697	U	C2-N1-C1'	7.61	126.83	117.70
48	A	2245	C	C6-N1-C2	-7.60	117.26	120.30
48	A	102	C	C2-N1-C1'	7.59	127.15	118.80
48	A	1044	U	N1-C2-O2	7.59	128.11	122.80
1	a	1486	A	C6-C5-N7	-7.59	126.99	132.30
48	A	1130	C	C6-N1-C2	-7.57	117.27	120.30
1	a	67	C	C6-N1-C2	-7.56	117.27	120.30
48	A	472	C	C2-N1-C1'	7.56	127.12	118.80
48	A	932	C	C6-N1-C2	-7.56	117.28	120.30
48	A	2697	U	N3-C2-O2	-7.54	116.92	122.20
48	A	2288	C	C6-N1-C2	-7.53	117.29	120.30
1	a	862	C	C6-N1-C2	7.53	123.31	120.30
48	A	2180	U	N3-C2-O2	-7.51	116.94	122.20
48	A	1409	C	C6-N1-C2	-7.49	117.30	120.30
1	a	954	C	C5-C6-N1	-7.47	117.26	121.00
48	A	2111	U	N1-C2-O2	7.47	128.03	122.80
48	A	1123	C	C5-C6-N1	7.43	124.71	121.00
48	A	2287	C	C6-N1-C2	-7.40	117.34	120.30
48	A	1030	C	C2-N1-C1'	7.40	126.94	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	A	905	U	N3-C2-O2	-7.38	117.03	122.20
48	A	234	U	N3-C2-O2	-7.37	117.04	122.20
1	a	794	A	N1-C6-N6	7.37	123.02	118.60
1	a	311	C	N3-C2-O2	-7.36	116.75	121.90
48	A	1429	C	C5-C6-N1	7.36	124.68	121.00
48	A	1531	C	C2-N1-C1'	7.33	126.86	118.80
48	A	619	C	N3-C2-O2	-7.33	116.77	121.90
1	a	1302	C	C6-N1-C2	7.30	123.22	120.30
1	a	1486	A	C2-N3-C4	-7.30	106.95	110.60
48	A	2841	C	C6-N1-C2	-7.30	117.38	120.30
47	B	62	C	N1-C2-O2	7.25	123.25	118.90
1	a	1486	A	N7-C8-N9	7.25	117.42	113.80
1	a	305	G	N3-C4-N9	7.24	130.34	126.00
48	A	2325	U	N3-C2-O2	-7.23	117.14	122.20
48	A	1219	U	N3-C2-O2	-7.23	117.14	122.20
48	A	1822	C	C6-N1-C2	-7.23	117.41	120.30
1	a	1268	C	C5-C6-N1	7.22	124.61	121.00
1	a	954	C	C2-N1-C1'	-7.21	110.87	118.80
48	A	514	C	C2-N1-C1'	7.21	126.73	118.80
48	A	962	U	N1-C2-O2	7.21	127.84	122.80
48	A	2360	C	N1-C2-O2	7.21	123.22	118.90
1	a	794	A	N1-C2-N3	7.19	132.89	129.30
1	a	895	A	P-O3'-C3'	7.18	128.32	119.70
48	A	102	C	C6-N1-C2	-7.18	117.43	120.30
48	A	845	C	C6-N1-C2	-7.18	117.43	120.30
48	A	2087	C	C2-N1-C1'	7.18	126.70	118.80
48	A	2325	U	C2-N1-C1'	7.17	126.31	117.70
1	a	1033	G	C8-N9-C4	7.17	109.27	106.40
48	A	283	U	N3-C2-O2	-7.17	117.18	122.20
48	A	2245	C	C6-N1-C1'	-7.17	112.20	120.80
2	c	186	LEU	CA-CB-CG	7.16	131.76	115.30
1	a	803	G	N1-C6-O6	-7.12	115.63	119.90
48	A	279	U	N1-C2-O2	7.09	127.77	122.80
48	A	102	C	N1-C2-O2	7.08	123.15	118.90
48	A	3011	C	N3-C2-O2	-7.08	116.94	121.90
48	A	734	C	C5-C6-N1	7.08	124.54	121.00
48	A	543	U	N1-C2-O2	7.08	127.75	122.80
1	a	1350	U	C5-C6-N1	-7.07	119.17	122.70
48	A	1044	U	N3-C2-O2	-7.07	117.25	122.20
48	A	2320	C	N1-C2-O2	7.06	123.14	118.90
48	A	2005	C	C5-C6-N1	7.06	124.53	121.00
48	A	1044	U	C2-N1-C1'	7.05	126.16	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	A	1219	U	N1-C2-O2	7.04	127.73	122.80
48	A	1123	C	C6-N1-C2	-7.04	117.49	120.30
48	A	2322	C	C2-N1-C1'	7.03	126.53	118.80
47	B	31	C	N3-C2-O2	-7.01	116.99	121.90
48	A	336	C	C5-C6-N1	7.01	124.51	121.00
48	A	2085	C	P-O3'-C3'	7.01	128.11	119.70
48	A	445	U	P-O3'-C3'	7.00	128.10	119.70
48	A	709	U	C2-N1-C1'	7.00	126.11	117.70
48	A	1862	C	C6-N1-C2	-7.00	117.50	120.30
48	A	323	C	C6-N1-C1'	-7.00	112.40	120.80
48	A	2086	U	C5-C6-N1	6.99	126.19	122.70
48	A	2680	C	C5-C6-N1	6.99	124.49	121.00
48	A	283	U	N1-C2-O2	6.98	127.69	122.80
1	a	1149	C	C6-N1-C2	-6.98	117.51	120.30
1	a	793	U	C2-N1-C1'	6.98	126.08	117.70
48	A	2890	C	N1-C2-O2	6.97	123.08	118.90
1	a	314	C	C6-N1-C2	-6.97	117.51	120.30
48	A	2248	C	C5-C6-N1	6.97	124.48	121.00
48	A	3046	C	C6-N1-C1'	-6.96	112.44	120.80
48	A	2327	C	N1-C2-O2	6.96	123.08	118.90
1	a	1088	G	C8-N9-C4	-6.96	103.62	106.40
48	A	3046	C	C6-N1-C2	-6.95	117.52	120.30
1	a	216	U	N1-C2-O2	6.92	127.65	122.80
48	A	197	C	C5-C6-N1	6.92	124.46	121.00
48	A	714	U	N1-C2-O2	6.92	127.64	122.80
48	A	1012	C	C6-N1-C1'	-6.91	112.51	120.80
48	A	703	C	C6-N1-C2	-6.90	117.54	120.30
48	A	910	C	C5-C6-N1	6.89	124.45	121.00
48	A	2094	G	P-O3'-C3'	6.89	127.97	119.70
48	A	1298	C	C5-C6-N1	6.89	124.44	121.00
48	A	962	U	N3-C2-O2	-6.87	117.39	122.20
1	a	122	G	C8-N9-C4	6.86	109.14	106.40
48	A	1057	C	C6-N1-C2	-6.86	117.56	120.30
1	a	489	A	C5-N7-C8	-6.86	100.47	103.90
48	A	764	U	N3-C2-O2	-6.85	117.40	122.20
48	A	2327	C	C6-N1-C2	-6.85	117.56	120.30
48	A	472	C	N1-C2-O2	6.85	123.01	118.90
48	A	910	C	C6-N1-C2	-6.85	117.56	120.30
48	A	7	U	C2-N1-C1'	6.84	125.91	117.70
48	A	714	U	N3-C2-O2	-6.83	117.42	122.20
1	a	216	U	C2-N1-C1'	6.83	125.90	117.70
48	A	1303	U	C5-C6-N1	6.83	126.11	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	A	514	C	C6-N1-C2	-6.81	117.58	120.30
48	A	275	C	C5-C6-N1	6.81	124.41	121.00
48	A	1130	C	C5-C6-N1	6.79	124.40	121.00
1	a	849	G	N3-C4-C5	-6.79	125.21	128.60
48	A	2671	G	C6-N1-C2	-6.79	121.03	125.10
48	A	2890	C	N3-C2-O2	-6.77	117.16	121.90
48	A	784	G	C4-N9-C1'	6.77	135.30	126.50
48	A	656	C	C6-N1-C2	-6.76	117.59	120.30
48	A	2248	C	C6-N1-C2	-6.76	117.60	120.30
48	A	729	C	C6-N1-C2	-6.75	117.60	120.30
1	a	119	C	O5'-P-OP1	-6.75	99.63	105.70
48	A	1535	C	N3-C2-O2	-6.74	117.18	121.90
48	A	975	U	C5-C6-N1	6.74	126.07	122.70
1	a	216	U	N3-C2-O2	-6.74	117.48	122.20
48	A	1382	U	N1-C2-O2	6.74	127.52	122.80
48	A	1534	C	N1-C2-O2	6.74	122.94	118.90
1	a	9	U	C5-C6-N1	6.73	126.07	122.70
31	K	108	MET	CA-CB-CG	6.72	124.72	113.30
48	A	192	U	N3-C2-O2	-6.72	117.50	122.20
48	A	2289	C	C6-N1-C2	-6.71	117.61	120.30
48	A	975	U	N1-C2-O2	6.71	127.50	122.80
1	a	243	A	N1-C6-N6	6.70	122.62	118.60
48	A	2111	U	N3-C2-O2	-6.70	117.51	122.20
48	A	2689	C	C2-N1-C1'	6.70	126.17	118.80
1	a	847	A	C8-N9-C4	6.69	108.47	105.80
48	A	1667	C	C6-N1-C2	-6.69	117.62	120.30
48	A	2407	C	C5-C6-N1	6.68	124.34	121.00
1	a	943	U	O5'-P-OP2	-6.68	99.69	105.70
48	A	2647	U	N1-C2-O2	6.67	127.47	122.80
47	B	106	C	N1-C2-O2	6.67	122.90	118.90
1	a	101	G	C5-N7-C8	-6.67	100.97	104.30
1	a	1149	C	C2-N1-C1'	6.67	126.14	118.80
48	A	1630	U	N3-C4-O4	-6.66	114.74	119.40
1	a	895	A	C8-N9-C4	-6.65	103.14	105.80
48	A	417	C	C5-C6-N1	6.65	124.33	121.00
1	a	1269	A	C8-N9-C4	-6.65	103.14	105.80
1	a	429	U	P-O3'-C3'	6.65	127.68	119.70
1	a	1486	A	C4-C5-N7	6.64	114.02	110.70
1	a	331	G	C8-N9-C4	6.63	109.05	106.40
48	A	283	U	C2-N1-C1'	6.63	125.66	117.70
48	A	2717	U	C5-C6-N1	6.63	126.02	122.70
23	C	106	ILE	CG1-CB-CG2	-6.62	96.83	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	A	2327	C	C2-N1-C1'	6.61	126.07	118.80
48	A	2407	C	C6-N1-C1'	-6.61	112.86	120.80
48	A	2970	U	C5-C6-N1	6.61	126.01	122.70
19	f	67	ALA	C-N-CA	6.60	138.20	121.70
48	A	1302	G	N3-C4-N9	6.60	129.96	126.00
48	A	1239	C	C5-C6-N1	6.58	124.29	121.00
48	A	332	C	N3-C2-O2	-6.58	117.30	121.90
48	A	845	C	C5-C6-N1	6.57	124.29	121.00
48	A	2521	C	C5-C6-N1	6.57	124.28	121.00
1	a	1486	A	N1-C6-N6	6.57	122.54	118.60
48	A	1012	C	N3-C2-O2	-6.57	117.30	121.90
48	A	2913	U	N3-C2-O2	-6.56	117.61	122.20
48	A	2025	C	C6-N1-C1'	-6.56	112.93	120.80
48	A	1403	C	N1-C2-O2	6.55	122.83	118.90
48	A	7	U	N1-C2-O2	6.54	127.38	122.80
48	A	1219	U	C2-N1-C1'	6.53	125.54	117.70
48	A	2689	C	C6-N1-C2	-6.52	117.69	120.30
48	A	1123	C	C2-N1-C1'	6.52	125.97	118.80
48	A	1409	C	C5-C6-N1	6.51	124.25	121.00
48	A	2671	G	C5-C6-O6	-6.50	124.70	128.60
48	A	29	C	N1-C2-O2	6.49	122.80	118.90
48	A	1045	C	C2-N1-C1'	6.49	125.94	118.80
1	a	558	C	C5-C6-N1	-6.48	117.76	121.00
1	a	279	A	O4'-C1'-N9	-6.48	103.02	108.20
48	A	1302	G	C4-N9-C1'	6.47	134.91	126.50
48	A	2290	C	C6-N1-C2	-6.46	117.72	120.30
48	A	438	U	C2-N1-C1'	6.46	125.45	117.70
48	A	1893	C	N1-C2-O2	6.43	122.76	118.90
48	A	1991	C	C5-C6-N1	6.43	124.21	121.00
48	A	2407	C	N3-C2-O2	-6.43	117.40	121.90
48	A	764	U	N1-C2-O2	6.42	127.29	122.80
48	A	2269	C	C6-N1-C2	-6.41	117.73	120.30
1	a	85	C	C6-N1-C1'	-6.41	113.11	120.80
48	A	2916	C	C6-N1-C2	-6.41	117.74	120.30
48	A	2944	U	N3-C2-O2	-6.41	117.72	122.20
48	A	1197	C	C2-N1-C1'	6.40	125.84	118.80
1	a	1268	C	C6-N1-C1'	-6.39	113.13	120.80
48	A	139	U	N3-C2-O2	-6.39	117.73	122.20
1	a	1508	C	C6-N1-C2	-6.39	117.75	120.30
1	a	1266	U	C2-N1-C1'	6.38	125.36	117.70
48	A	1534	C	C2-N1-C1'	6.38	125.82	118.80
48	A	2734	C	N1-C2-O2	6.38	122.73	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	485	G	N7-C8-N9	6.37	116.29	113.10
48	A	336	C	C6-N1-C1'	-6.37	113.16	120.80
48	A	1428	U	C6-N1-C1'	-6.37	112.28	121.20
48	A	2947	C	C5-C6-N1	6.36	124.18	121.00
48	A	336	C	C6-N1-C2	-6.36	117.76	120.30
48	A	1551	U	C5-C6-N1	6.34	125.87	122.70
1	a	117	C	C6-N1-C2	6.34	122.83	120.30
48	A	336	C	N1-C2-O2	6.34	122.70	118.90
48	A	2360	C	C2-N1-C1'	6.34	125.77	118.80
48	A	1001	C	C5-C6-N1	6.33	124.17	121.00
1	a	332	G	N7-C8-N9	-6.33	109.94	113.10
1	a	364	A	C8-N9-C4	-6.33	103.27	105.80
48	A	550	C	C6-N1-C2	-6.33	117.77	120.30
48	A	2869	C	C2-N1-C1'	6.33	125.76	118.80
48	A	1212	U	C5-C6-N1	6.32	125.86	122.70
48	A	1837	G	C4-C5-N7	6.32	113.33	110.80
48	A	1012	C	C5-C6-N1	6.32	124.16	121.00
1	a	11	G	C5-N7-C8	-6.31	101.14	104.30
48	A	1012	C	C6-N1-C2	-6.31	117.78	120.30
24	D	144	VAL	CG1-CB-CG2	-6.31	100.81	110.90
48	A	514	C	C5-C6-N1	6.31	124.15	121.00
47	B	69	C	N1-C2-O2	6.30	122.68	118.90
48	A	279	U	N3-C2-O2	-6.30	117.79	122.20
48	A	461	U	N3-C2-O2	-6.30	117.79	122.20
48	A	1088	U	C5-C6-N1	6.29	125.85	122.70
35	O	46	PRO	CA-N-CD	-6.29	102.70	111.50
48	A	608	C	C5-C6-N1	6.29	124.14	121.00
48	A	192	U	N1-C2-O2	6.29	127.20	122.80
48	A	1197	C	N1-C2-O2	6.27	122.66	118.90
48	A	1816	C	C2-N1-C1'	6.26	125.69	118.80
48	A	2076	A	N1-C6-N6	6.26	122.36	118.60
48	A	2260	C	C6-N1-C2	-6.26	117.80	120.30
23	C	213	ARG	NE-CZ-NH2	-6.26	117.17	120.30
48	A	505	C	C5-C6-N1	6.26	124.13	121.00
1	a	1424	G	C4-N9-C1'	6.25	134.63	126.50
48	A	2841	C	C5-C6-N1	6.25	124.12	121.00
48	A	561	G	N3-C4-N9	6.25	129.75	126.00
48	A	2435	U	N3-C2-O2	-6.24	117.83	122.20
1	a	305	G	C4-N9-C1'	6.24	134.61	126.50
48	A	1893	C	N3-C2-O2	-6.24	117.53	121.90
1	a	305	G	N3-C4-C5	-6.23	125.48	128.60
48	A	102	C	C5-C6-N1	6.23	124.11	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	K	18	ILE	CG1-CB-CG2	-6.22	97.72	111.40
1	a	11	G	N3-C4-C5	6.22	131.71	128.60
48	A	2198	C	C5-C6-N1	6.22	124.11	121.00
48	A	1130	C	C6-N1-C1'	-6.21	113.35	120.80
1	a	485	G	C8-N9-C4	-6.21	103.92	106.40
48	A	2841	C	N1-C2-O2	6.21	122.62	118.90
48	A	1441	C	N1-C2-O2	6.21	122.62	118.90
48	A	1044	U	C5-C6-N1	6.20	125.80	122.70
48	A	2362	C	N1-C2-O2	6.20	122.62	118.90
48	A	3070	G	C4-N9-C1'	-6.20	118.44	126.50
48	A	1008	G	C4-N9-C1'	6.20	134.56	126.50
48	A	839	U	N3-C2-O2	-6.19	117.86	122.20
48	A	1429	C	C6-N1-C2	-6.19	117.82	120.30
48	A	898	A	C4-N9-C1'	6.19	137.44	126.30
1	a	305	G	C8-N9-C1'	-6.18	118.96	127.00
1	a	538	G	N3-C4-C5	-6.18	125.51	128.60
47	B	4	A	C8-N9-C4	-6.17	103.33	105.80
48	A	323	C	C5-C6-N1	6.17	124.08	121.00
34	N	61	GLY	N-CA-C	6.16	128.49	113.10
48	A	957	C	C6-N1-C2	-6.16	117.84	120.30
48	A	1057	C	C5-C6-N1	6.15	124.07	121.00
48	A	2487	C	C6-N1-C2	-6.15	117.84	120.30
48	A	2900	C	C6-N1-C2	-6.14	117.85	120.30
48	A	2320	C	C2-N1-C1'	6.13	125.55	118.80
34	N	122	ILE	CG1-CB-CG2	-6.13	97.92	111.40
48	A	1697	U	N3-C2-O2	-6.13	117.91	122.20
48	A	2366	C	N3-C2-O2	-6.12	117.61	121.90
48	A	2155	U	N1-C2-O2	6.11	127.08	122.80
1	a	1172	A	C8-N9-C4	-6.11	103.36	105.80
53	5	7	THR	N-CA-C	6.11	127.50	111.00
23	C	95	LEU	CB-CG-CD1	-6.11	100.62	111.00
47	B	4	A	N7-C8-N9	6.11	116.85	113.80
48	A	2900	C	C5-C6-N1	6.11	124.05	121.00
48	A	703	C	C5-C6-N1	6.10	124.05	121.00
48	A	1302	G	C8-N9-C1'	-6.10	119.07	127.00
48	A	549	C	C6-N1-C2	-6.10	117.86	120.30
1	a	794	A	C2-N3-C4	-6.09	107.55	110.60
1	a	1149	C	P-O3'-C3'	6.09	127.01	119.70
48	A	912	C	C6-N1-C2	-6.09	117.86	120.30
48	A	2320	C	N3-C2-O2	-6.09	117.64	121.90
40	T	102	ARG	NE-CZ-NH2	-6.09	117.25	120.30
48	A	1531	C	C5-C6-N1	6.09	124.04	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	A	2158	C	N1-C2-O2	6.09	122.55	118.90
48	A	3034	C	C6-N1-C2	-6.08	117.87	120.30
48	A	2166	C	C5-C6-N1	6.08	124.04	121.00
48	A	2680	C	C6-N1-C2	-6.07	117.87	120.30
48	A	853	C	C2-N1-C1'	6.06	125.47	118.80
48	A	2061	U	C5-C6-N1	6.06	125.73	122.70
42	V	10	LEU	CA-CB-CG	6.06	129.24	115.30
48	A	1535	C	N1-C2-O2	6.06	122.54	118.90
48	A	2438	C	N1-C2-O2	6.06	122.53	118.90
1	a	70	A	C6-N1-C2	-6.05	114.97	118.60
1	a	456	C	O5'-P-OP1	-6.05	100.25	105.70
48	A	918	U	C5-C6-N1	6.05	125.72	122.70
48	A	1251	A	O4'-C1'-N9	6.05	113.04	108.20
48	A	622	C	C6-N1-C2	-6.04	117.88	120.30
48	A	2782	C	C5-C6-N1	6.04	124.02	121.00
48	A	1103	C	C5-C6-N1	6.03	124.01	121.00
1	a	108	G	N3-C4-N9	6.03	129.62	126.00
48	A	1813	C	C5-C6-N1	6.02	124.01	121.00
1	a	101	G	C6-C5-N7	-6.02	126.79	130.40
47	B	62	C	N3-C2-O2	-6.02	117.69	121.90
1	a	108	G	N7-C8-N9	-6.02	110.09	113.10
48	A	3045	C	C6-N1-C2	-6.01	117.89	120.30
48	A	2993	U	N1-C2-O2	6.01	127.01	122.80
1	a	734	C	N3-C2-O2	-6.01	117.69	121.90
47	B	106	C	C2-N1-C1'	6.01	125.41	118.80
48	A	387	U	N1-C2-O2	6.01	127.01	122.80
48	A	2025	C	C6-N1-C2	-6.01	117.90	120.30
1	a	1178	A	N1-C2-N3	6.01	132.30	129.30
48	A	2940	U	N3-C2-O2	-6.01	118.00	122.20
1	a	861	C	C2-N3-C4	-6.00	116.90	119.90
1	a	404	G	N1-C6-O6	-6.00	116.30	119.90
48	A	293	G	N1-C6-O6	-6.00	116.30	119.90
48	A	2155	U	N3-C2-O2	-5.99	118.01	122.20
48	A	2689	C	N1-C2-O2	5.99	122.49	118.90
48	A	930	C	C6-N1-C2	-5.98	117.91	120.30
48	A	1553	C	N1-C2-O2	5.98	122.49	118.90
48	A	2381	A	P-O3'-C3'	5.98	126.88	119.70
48	A	461	U	N1-C2-O2	5.98	126.99	122.80
48	A	1798	U	N3-C2-O2	-5.98	118.01	122.20
48	A	237	C	C2-N1-C1'	5.98	125.38	118.80
48	A	2734	C	N3-C2-O2	-5.98	117.72	121.90
1	a	243	A	C5-N7-C8	-5.97	100.91	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	956	A	O4'-C1'-N9	5.97	112.98	108.20
1	a	1117	U	OP1-P-O3'	5.97	118.34	105.20
48	A	784	G	C8-N9-C1'	-5.97	119.23	127.00
48	A	1449	C	C6-N1-C2	-5.97	117.91	120.30
48	A	161	U	C2-N1-C1'	5.97	124.86	117.70
48	A	1410	C	C6-N1-C2	-5.96	117.92	120.30
48	A	1531	C	C6-N1-C2	-5.96	117.92	120.30
48	A	1531	C	N1-C2-O2	5.96	122.47	118.90
48	A	2622	C	C6-N1-C2	-5.96	117.92	120.30
48	A	2013	C	C6-N1-C2	-5.95	117.92	120.30
48	A	2602	A	N1-C6-N6	5.95	122.17	118.60
48	A	357	U	P-O3'-C3'	5.95	126.84	119.70
1	a	713	G	C4-N9-C1'	-5.95	118.77	126.50
47	B	31	C	C6-N1-C2	-5.95	117.92	120.30
1	a	1268	C	N3-C4-N4	5.95	122.16	118.00
25	E	33	LEU	CB-CG-CD2	-5.93	100.91	111.00
48	A	2111	U	C2-N1-C1'	5.93	124.82	117.70
48	A	2116	C	N1-C2-O2	5.93	122.46	118.90
1	a	532	U	C5-C6-N1	-5.93	119.74	122.70
48	A	1662	C	C6-N1-C2	-5.93	117.93	120.30
48	A	1158	U	N3-C2-O2	-5.93	118.05	122.20
48	A	617	U	N3-C2-O2	-5.92	118.05	122.20
48	A	2144	C	C6-N1-C2	-5.92	117.93	120.30
48	A	2327	C	N3-C2-O2	-5.92	117.75	121.90
48	A	1801	C	C2-N1-C1'	5.92	125.31	118.80
1	a	311	C	C2-N1-C1'	5.92	125.31	118.80
47	B	106	C	N3-C2-O2	-5.91	117.76	121.90
48	A	839	U	N1-C2-O2	5.90	126.93	122.80
48	A	845	C	C2-N3-C4	5.90	122.85	119.90
48	A	279	U	C2-N1-C1'	5.90	124.78	117.70
48	A	974	G	P-O3'-C3'	5.90	126.78	119.70
1	a	504	G	N3-C4-C5	-5.89	125.65	128.60
48	A	1529	U	C5-C6-N1	5.89	125.65	122.70
1	a	1204	C	C5-C6-N1	-5.89	118.06	121.00
48	A	66	C	C6-N1-C2	-5.89	117.94	120.30
48	A	1082	C	C6-N1-C2	-5.89	117.94	120.30
48	A	1467	U	N3-C2-O2	-5.88	118.08	122.20
48	A	714	U	C2-N1-C1'	5.88	124.75	117.70
48	A	1801	C	N1-C2-O2	5.88	122.43	118.90
48	A	2226	U	N1-C2-O2	5.88	126.91	122.80
48	A	2815	C	C6-N1-C2	-5.88	117.95	120.30
47	B	31	C	C2-N1-C1'	5.87	125.26	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	A	1302	G	C4-C5-N7	5.86	113.14	110.80
48	A	599	G	O4'-C1'-N9	5.86	112.89	108.20
1	a	1033	G	N7-C8-N9	-5.86	110.17	113.10
1	a	1350	U	C6-N1-C2	5.85	124.51	121.00
48	A	2419	C	C2-N1-C1'	5.85	125.24	118.80
48	A	324	C	N3-C2-O2	-5.85	117.81	121.90
1	a	769	U	C5-C4-O4	5.85	129.41	125.90
48	A	1030	C	N1-C2-O2	5.84	122.41	118.90
48	A	2110	U	C2-N1-C1'	5.83	124.70	117.70
48	A	1625	G	N7-C8-N9	5.83	116.02	113.10
48	A	1393	C	C6-N1-C2	-5.83	117.97	120.30
48	A	1747	C	C6-N1-C2	-5.82	117.97	120.30
1	a	107	G	N3-C4-C5	5.82	131.51	128.60
48	A	200	C	C6-N1-C2	-5.81	117.97	120.30
48	A	930	C	C5-C6-N1	5.81	123.91	121.00
48	A	1521	C	C6-N1-C2	-5.81	117.98	120.30
48	A	2430	C	N1-C2-O2	5.80	122.38	118.90
32	L	67	LYS	CD-CE-NZ	-5.80	98.36	111.70
48	A	1167	C	C6-N1-C2	-5.80	117.98	120.30
48	A	2690	C	C6-N1-C2	-5.80	117.98	120.30
1	a	1340	U	C5-C6-N1	-5.80	119.80	122.70
48	A	1082	C	C5-C6-N1	5.80	123.90	121.00
1	a	454	C	C2-N1-C1'	5.79	125.17	118.80
1	a	799	G	N3-C4-C5	5.78	131.49	128.60
48	A	2927	C	N1-C2-O2	5.78	122.37	118.90
48	A	1618	C	N1-C2-O2	5.78	122.37	118.90
43	W	49	LEU	CB-CG-CD2	-5.77	101.19	111.00
48	A	2407	C	C6-N1-C2	-5.77	117.99	120.30
48	A	1198	C	C6-N1-C2	-5.77	117.99	120.30
1	a	666	U	C6-N1-C1'	5.76	129.27	121.20
48	A	504	C	C5-C6-N1	5.76	123.88	121.00
48	A	7	U	N3-C2-O2	-5.76	118.17	122.20
48	A	2217	U	N3-C2-O2	-5.76	118.17	122.20
48	A	2890	C	C6-N1-C2	-5.75	118.00	120.30
1	a	1171	G	O5'-P-OP2	-5.75	100.53	105.70
1	a	1486	A	C5-C6-N1	-5.74	114.83	117.70
1	a	132	C	C6-N1-C2	5.74	122.59	120.30
48	A	1045	C	N1-C2-O2	5.73	122.34	118.90
48	A	2744	C	N1-C2-O2	5.73	122.34	118.90
1	a	666	U	C2-N1-C1'	-5.73	110.83	117.70
48	A	1775	C	C5-C6-N1	5.73	123.86	121.00
48	A	139	U	C2-N1-C1'	5.73	124.57	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	A	1321	C	C6-N1-C2	-5.73	118.01	120.30
48	A	1034	U	N3-C2-O2	-5.72	118.19	122.20
48	A	1560	U	N3-C2-O2	-5.72	118.20	122.20
48	A	2088	C	N1-C2-O2	5.72	122.33	118.90
1	a	488	C	C6-N1-C2	-5.72	118.01	120.30
48	A	417	C	N1-C2-O2	5.72	122.33	118.90
1	a	385	C	C6-N1-C2	-5.71	118.02	120.30
48	A	1668	C	C6-N1-C2	-5.71	118.02	120.30
48	A	1816	C	C5-C6-N1	5.70	123.85	121.00
48	A	2423	C	C5-C6-N1	5.70	123.85	121.00
48	A	1494	U	N3-C2-O2	-5.70	118.21	122.20
48	A	2191	C	N1-C2-O2	5.70	122.32	118.90
1	a	1481	G	C8-N9-C4	-5.69	104.12	106.40
48	A	191	G	C4-N9-C1'	5.69	133.90	126.50
48	A	332	C	N1-C2-O2	5.69	122.31	118.90
48	A	1001	C	N1-C2-O2	5.69	122.31	118.90
48	A	2803	C	N1-C2-O2	5.68	122.31	118.90
48	A	868	C	C6-N1-C2	-5.68	118.03	120.30
1	a	794	A	C4-C5-C6	5.68	119.84	117.00
48	A	975	U	N3-C2-O2	-5.67	118.23	122.20
48	A	1862	C	C5-C6-N1	5.67	123.83	121.00
48	A	2730	U	N3-C2-O2	-5.67	118.23	122.20
48	A	2666	C	N1-C2-O2	5.67	122.30	118.90
48	A	1651	C	C5-C6-N1	5.66	123.83	121.00
48	A	1197	C	C6-N1-C2	-5.66	118.04	120.30
1	a	693	G	N3-C4-C5	-5.65	125.77	128.60
48	A	2350	G	P-O3'-C3'	5.65	126.48	119.70
48	A	962	U	C6-N1-C1'	-5.65	113.29	121.20
1	a	413	G	O4'-C1'-N9	5.64	112.72	108.20
1	a	372	C	N3-C2-O2	-5.64	117.95	121.90
1	a	1117	U	P-O3'-C3'	5.64	126.47	119.70
1	a	745	G	C4-C5-N7	5.64	113.06	110.80
48	A	495	C	C6-N1-C2	-5.64	118.05	120.30
1	a	108	G	N9-C4-C5	-5.63	103.15	105.40
48	A	977	G	N3-C4-N9	5.63	129.38	126.00
48	A	1996	U	C2-N1-C1'	5.63	124.46	117.70
48	A	2144	C	C5-C6-N1	5.63	123.81	121.00
1	a	846	A	C2-N3-C4	-5.63	107.78	110.60
48	A	1386	G	C8-N9-C4	-5.63	104.15	106.40
43	W	49	LEU	CA-CB-CG	5.62	128.23	115.30
47	B	62	C	C2-N1-C1'	5.62	124.98	118.80
48	A	857	U	C5-C6-N1	5.62	125.51	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	A	1298	C	C2-N1-C1'	5.61	124.97	118.80
48	A	3066	C	C6-N1-C2	-5.61	118.06	120.30
48	A	839	U	C2-N1-C1'	5.61	124.43	117.70
47	B	69	C	N3-C2-O2	-5.61	117.98	121.90
48	A	788	C	C6-N1-C2	-5.61	118.06	120.30
48	A	2841	C	N3-C2-O2	-5.61	117.98	121.90
48	A	846	C	C6-N1-C2	-5.60	118.06	120.30
48	A	1467	U	C2-N1-C1'	5.60	124.42	117.70
1	a	243	A	C4-C5-N7	5.60	113.50	110.70
32	L	110	LYS	N-CA-C	5.60	126.12	111.00
48	A	1008	G	C6-C5-N7	-5.60	127.04	130.40
48	A	1813	C	C6-N1-C2	-5.60	118.06	120.30
48	A	939	C	C6-N1-C2	-5.60	118.06	120.30
48	A	1212	U	N1-C2-O2	5.60	126.72	122.80
1	a	466	U	C2-N1-C1'	5.60	124.42	117.70
48	A	898	A	N7-C8-N9	5.59	116.59	113.80
1	a	794	A	C6-C5-N7	-5.59	128.39	132.30
48	A	112	C	C6-N1-C2	-5.59	118.06	120.30
48	A	2842	G	N3-C4-C5	-5.59	125.81	128.60
48	A	2245	C	C5-C6-N1	5.58	123.79	121.00
48	A	3035	C	C6-N1-C2	-5.58	118.07	120.30
1	a	11	G	C4-C5-N7	5.58	113.03	110.80
48	A	922	U	N3-C2-O2	-5.58	118.29	122.20
48	A	29	C	C6-N1-C1'	-5.58	114.10	120.80
48	A	2687	U	C5-C6-N1	5.58	125.49	122.70
48	A	3048	C	N1-C2-O2	5.58	122.25	118.90
1	a	311	C	N1-C2-O2	5.58	122.25	118.90
48	A	1045	C	N3-C2-O2	-5.57	118.00	121.90
1	a	799	G	C8-N9-C4	5.57	108.63	106.40
48	A	2632	U	C5-C6-N1	5.57	125.49	122.70
48	A	1429	C	N1-C2-O2	5.57	122.24	118.90
48	A	1801	C	C6-N1-C2	-5.57	118.07	120.30
48	A	733	U	C5-C6-N1	5.56	125.48	122.70
48	A	1775	C	C2-N1-C1'	5.56	124.92	118.80
1	a	1214	G	C8-N9-C4	5.56	108.62	106.40
48	A	2290	C	C5-C6-N1	5.56	123.78	121.00
48	A	703	C	N1-C2-O2	5.56	122.23	118.90
48	A	2181	C	C6-N1-C2	-5.55	118.08	120.30
1	a	1507	G	C8-N9-C4	5.55	108.62	106.40
1	a	1117	U	O4'-C1'-N1	5.55	112.64	108.20
48	A	1843	C	C2-N1-C1'	5.54	124.90	118.80
1	a	70	A	N1-C6-N6	5.54	121.92	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	A	1548	C	N1-C2-O2	5.54	122.22	118.90
48	A	234	U	N1-C2-O2	5.53	126.67	122.80
48	A	929	C	C5-C6-N1	5.53	123.77	121.00
48	A	2198	C	C6-N1-C2	-5.53	118.09	120.30
31	K	5	THR	N-CA-C	-5.53	96.08	111.00
1	a	1383	C	C6-N1-C2	-5.52	118.09	120.30
48	A	2842	G	C2-N3-C4	5.52	114.66	111.90
48	A	43	C	C6-N1-C2	-5.52	118.09	120.30
1	a	902	U	C5-C6-N1	-5.51	119.94	122.70
1	a	243	A	C2-N3-C4	-5.50	107.85	110.60
1	a	85	C	N3-C2-O2	-5.49	118.06	121.90
1	a	666	U	C5-C4-O4	5.49	129.19	125.90
48	A	2979	C	C5-C6-N1	5.49	123.75	121.00
48	A	937	U	C5-C6-N1	5.48	125.44	122.70
48	A	154	C	C6-N1-C2	-5.48	118.11	120.30
48	A	1321	C	C5-C6-N1	5.48	123.74	121.00
48	A	3070	G	N3-C4-C5	5.48	131.34	128.60
48	A	2752	U	N1-C2-O2	5.48	126.63	122.80
1	a	953	G	O4'-C1'-N9	5.47	112.58	108.20
3	e	190	ALA	C-N-CD	5.47	139.90	128.40
1	a	821	C	N1-C2-O2	5.47	122.18	118.90
48	A	1158	U	N1-C2-O2	5.47	126.63	122.80
2	c	143	GLN	C-N-CD	5.47	139.88	128.40
48	A	918	U	C6-N1-C2	-5.47	117.72	121.00
37	Q	15	ASP	CB-CG-OD1	5.47	123.22	118.30
48	A	184	C	C6-N1-C2	-5.46	118.11	120.30
48	A	2886	A	C8-N9-C4	-5.46	103.61	105.80
1	a	641	G	C8-N9-C4	-5.46	104.22	106.40
48	A	2226	U	C5-C6-N1	5.46	125.43	122.70
1	a	415	C	C2-N1-C1'	5.46	124.80	118.80
48	A	2829	U	N3-C2-O2	-5.46	118.38	122.20
44	X	85	ARG	C-N-CD	5.46	139.86	128.40
48	A	1816	C	N1-C2-O2	5.45	122.17	118.90
1	a	489	A	C6-C5-N7	-5.45	128.48	132.30
32	L	12	ASP	CB-CG-OD1	5.45	123.21	118.30
48	A	425	U	C5-C6-N1	5.45	125.43	122.70
48	A	1515	C	C6-N1-C2	-5.45	118.12	120.30
48	A	2362	C	C6-N1-C2	-5.45	118.12	120.30
1	a	258	G	C8-N9-C4	-5.45	104.22	106.40
48	A	204	G	O4'-C1'-N9	5.45	112.56	108.20
48	A	2230	C	N1-C2-O2	5.45	122.17	118.90
1	a	954	C	C6-N1-C2	5.44	122.48	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	962	C	C5-C6-N1	5.43	123.72	121.00
48	A	97	U	P-O3'-C3'	5.43	126.22	119.70
48	A	1298	C	C6-N1-C2	-5.43	118.13	120.30
48	A	1366	A	C2-N3-C4	5.43	113.31	110.60
1	a	85	C	C5-C6-N1	5.43	123.72	121.00
48	A	1734	C	C6-N1-C2	-5.43	118.13	120.30
48	A	1302	G	N9-C4-C5	-5.42	103.23	105.40
1	a	296	U	N3-C2-O2	-5.42	118.40	122.20
1	a	1511	C	C5-C6-N1	5.42	123.71	121.00
48	A	1904	C	N3-C2-O2	-5.41	118.11	121.90
48	A	845	C	N3-C2-O2	-5.41	118.11	121.90
48	A	2647	U	N3-C2-O2	-5.41	118.41	122.20
48	A	1816	C	C6-N1-C2	-5.41	118.14	120.30
1	a	11	G	O4'-C1'-N9	5.40	112.52	108.20
48	A	2665	C	N1-C2-O2	5.40	122.14	118.90
48	A	1991	C	C6-N1-C2	-5.40	118.14	120.30
48	A	2521	C	N1-C2-O2	5.40	122.14	118.90
48	A	2625	C	N1-C2-O2	5.40	122.14	118.90
48	A	1926	C	C6-N1-C2	-5.39	118.14	120.30
48	A	2116	C	N3-C2-O2	-5.39	118.12	121.90
48	A	514	C	N1-C2-O2	5.39	122.13	118.90
48	A	1996	U	O4'-C1'-N1	5.39	112.51	108.20
48	A	1847	U	N1-C2-N3	5.39	118.13	114.90
1	a	85	C	C6-N1-C2	-5.38	118.15	120.30
48	A	2267	C	N1-C2-O2	5.38	122.13	118.90
48	A	2327	C	C5-C6-N1	5.38	123.69	121.00
48	A	1766	U	N1-C2-N3	5.38	118.13	114.90
48	A	1197	C	C5-C6-N1	5.38	123.69	121.00
47	B	38	C	N1-C2-O2	5.38	122.12	118.90
48	A	957	C	C5-C6-N1	5.38	123.69	121.00
48	A	3016	C	C6-N1-C2	-5.37	118.15	120.30
1	a	1028	G	C8-N9-C4	-5.37	104.25	106.40
48	A	191	G	C8-N9-C1'	-5.37	120.02	127.00
48	A	472	C	C6-N1-C2	-5.37	118.15	120.30
1	a	489	A	O4'-C1'-N9	5.37	112.49	108.20
48	A	324	C	C6-N1-C2	-5.37	118.15	120.30
48	A	1651	C	C6-N1-C2	-5.36	118.15	120.30
1	a	1204	C	C6-N1-C2	5.36	122.44	120.30
43	W	58	LEU	CB-CG-CD2	-5.36	101.89	111.00
48	A	802	C	N1-C2-O2	5.36	122.12	118.90
48	A	2472	C	C2-N1-C1'	5.36	124.70	118.80
48	A	2890	C	C2-N1-C1'	5.36	124.70	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	803	G	N9-C4-C5	5.36	107.54	105.40
1	a	1060	A	C8-N9-C4	5.36	107.94	105.80
1	a	496	U	C2-N1-C1'	5.36	124.13	117.70
48	A	1694	C	C5-C6-N1	5.36	123.68	121.00
48	A	905	U	C6-N1-C1'	-5.35	113.70	121.20
48	A	2360	C	C5-C6-N1	5.35	123.68	121.00
48	A	1102	G	N3-C4-C5	-5.35	125.92	128.60
48	A	1485	C	C5-C6-N1	5.35	123.67	121.00
1	a	1511	C	C6-N1-C2	-5.35	118.16	120.30
5	h	94	LEU	C-N-CD	5.34	139.62	128.40
18	d	189	PRO	C-N-CA	5.34	135.04	121.70
32	L	108	GLU	N-CA-C	-5.34	96.59	111.00
48	A	1898	U	N3-C2-O2	-5.34	118.46	122.20
48	A	2571	C	N1-C2-O2	5.33	122.10	118.90
1	a	947	U	C6-N1-C2	5.33	124.20	121.00
48	A	1260	C	C2-N1-C1'	5.33	124.67	118.80
48	A	1008	G	N3-C4-N9	5.33	129.20	126.00
1	a	1466	G	N3-C4-C5	-5.33	125.94	128.60
48	A	3116	C	C6-N1-C2	-5.32	118.17	120.30
1	a	1481	G	N3-C4-C5	-5.32	125.94	128.60
6	i	32	ARG	CB-CA-C	5.32	121.04	110.40
48	A	505	C	C6-N1-C2	-5.32	118.17	120.30
48	A	2322	C	C6-N1-C1'	-5.32	114.42	120.80
1	a	109	G	C5-C6-N1	5.32	114.16	111.50
1	a	110	U	C5-C6-N1	-5.32	120.04	122.70
48	A	984	U	C5-C6-N1	5.32	125.36	122.70
48	A	1943	C	N1-C2-O2	5.32	122.09	118.90
48	A	996	G	C4-N9-C1'	5.31	133.41	126.50
1	a	215	U	N3-C2-O2	-5.31	118.48	122.20
48	A	1521	C	C6-N1-C1'	-5.31	114.43	120.80
28	H	124	ILE	C-N-CA	5.31	134.97	121.70
54	6	15	ARG	CB-CG-CD	-5.31	97.80	111.60
48	A	1953	C	C6-N1-C2	-5.31	118.18	120.30
48	A	2690	C	C5-C6-N1	5.31	123.65	121.00
1	a	509	G	C5-N7-C8	-5.30	101.65	104.30
48	A	1220	C	C6-N1-C2	-5.30	118.18	120.30
48	A	1977	C	C6-N1-C2	-5.30	118.18	120.30
1	a	454	C	C6-N1-C2	-5.30	118.18	120.30
48	A	2012	C	C6-N1-C2	-5.30	118.18	120.30
48	A	2472	C	C5-C6-N1	5.30	123.65	121.00
25	E	19	GLU	C-N-CA	5.30	134.95	121.70
48	A	2435	U	C2-N1-C1'	5.30	124.06	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	251	G	N9-C4-C5	-5.30	103.28	105.40
48	A	2698	C	C2-N1-C1'	5.30	124.63	118.80
48	A	2736	C	C5-C6-N1	5.30	123.65	121.00
1	a	1203	G	N3-C4-N9	-5.29	122.82	126.00
31	K	1	MET	C-N-CD	5.29	139.52	128.40
48	A	102	C	N3-C2-O2	-5.29	118.19	121.90
1	a	903	U	C5-C6-N1	-5.29	120.05	122.70
48	A	231	U	C2-N1-C1'	5.29	124.05	117.70
48	A	2118	C	N1-C2-O2	5.29	122.08	118.90
1	a	322	C	N1-C2-O2	-5.29	115.73	118.90
1	a	1171	G	C5'-C4'-O4'	-5.29	102.75	109.10
48	A	274	C	C2-N1-C1'	5.29	124.61	118.80
48	A	1409	C	C2-N1-C1'	5.29	124.61	118.80
1	a	504	G	N3-C4-N9	5.28	129.17	126.00
48	A	2274	C	C6-N1-C2	-5.28	118.19	120.30
1	a	881	C	N3-C4-C5	5.28	124.01	121.90
48	A	324	C	N1-C2-O2	5.28	122.07	118.90
1	a	237	C	C6-N1-C2	-5.28	118.19	120.30
1	a	331	G	N9-C4-C5	-5.27	103.29	105.40
48	A	1266	C	C6-N1-C2	-5.27	118.19	120.30
1	a	846	A	N1-C2-N3	5.27	131.94	129.30
48	A	1065	C	C5-C6-N1	5.27	123.64	121.00
48	A	2487	C	N3-C2-O2	-5.27	118.21	121.90
48	A	2697	U	C5-C6-N1	5.27	125.33	122.70
48	A	2262	C	C5-C6-N1	5.26	123.63	121.00
48	A	101	U	N1-C2-O2	5.26	126.48	122.80
48	A	1276	G	C4-C5-N7	5.26	112.91	110.80
48	A	2087	C	C6-N1-C1'	-5.26	114.49	120.80
11	q	76	LEU	CA-CB-CG	5.26	127.39	115.30
48	A	2375	G	C6-C5-N7	-5.25	127.25	130.40
52	4	8	ARG	C-N-CD	5.25	139.44	128.40
48	A	417	C	N3-C2-O2	-5.25	118.22	121.90
48	A	927	C	C6-N1-C2	-5.25	118.20	120.30
48	A	2147	U	C5-C6-N1	5.25	125.33	122.70
1	a	799	G	N9-C4-C5	-5.25	103.30	105.40
48	A	275	C	N3-C2-O2	-5.25	118.22	121.90
47	B	78	U	N3-C2-O2	-5.25	118.53	122.20
48	A	929	C	C6-N1-C2	-5.25	118.20	120.30
1	a	1480	C	C6-N1-C2	-5.24	118.20	120.30
48	A	192	U	C2-N1-C1'	5.24	123.99	117.70
48	A	599	G	N1-C6-O6	-5.24	116.75	119.90
48	A	205	U	N1-C2-O2	5.24	126.47	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	A	1008	G	C8-N9-C1'	-5.24	120.19	127.00
48	A	1991	C	N3-C2-O2	-5.24	118.23	121.90
1	a	847	A	N7-C8-N9	-5.24	111.18	113.80
1	a	901	A	C2-N3-C4	-5.24	107.98	110.60
48	A	236	C	C5-C6-N1	5.24	123.62	121.00
48	A	3048	C	C5-C6-N1	5.24	123.62	121.00
1	a	737	U	C5-C6-N1	-5.23	120.08	122.70
48	A	2780	C	C6-N1-C2	-5.23	118.21	120.30
48	A	438	U	N1-C2-O2	5.23	126.46	122.80
48	A	2967	C	C6-N1-C2	-5.23	118.21	120.30
1	a	27	C	C6-N1-C2	5.23	122.39	120.30
48	A	2366	C	N1-C2-O2	5.23	122.04	118.90
1	a	747	A	C4-C5-C6	5.23	119.61	117.00
1	a	1510	G	N3-C4-C5	-5.23	125.99	128.60
48	A	472	C	C6-N1-C1'	-5.23	114.53	120.80
48	A	2260	C	N3-C2-O2	-5.23	118.24	121.90
48	A	802	C	C2-N1-C1'	5.23	124.55	118.80
1	a	1028	G	N7-C8-N9	5.22	115.71	113.10
48	A	1662	C	C5-C6-N1	5.22	123.61	121.00
1	a	509	G	N7-C8-N9	5.22	115.71	113.10
1	a	1307	C	C6-N1-C2	-5.22	118.21	120.30
48	A	1449	C	C5-C6-N1	5.22	123.61	121.00
54	6	62	LEU	CA-CB-CG	5.22	127.31	115.30
1	a	63	A	C8-N9-C4	-5.22	103.71	105.80
1	a	107	G	C8-N9-C4	5.22	108.49	106.40
48	A	1094	G	C4-C5-N7	5.22	112.89	110.80
48	A	1429	C	C6-N1-C1'	-5.22	114.54	120.80
3	e	22	ASP	CB-CG-OD2	5.21	122.99	118.30
40	T	7	PHE	C-N-CD	5.21	139.35	128.40
1	a	777	C	C6-N1-C1'	-5.21	114.54	120.80
3	e	21	ASP	CB-CG-OD2	5.21	122.99	118.30
3	e	32	ASP	CB-CG-OD2	5.21	122.99	118.30
48	A	1030	C	C6-N1-C1'	-5.21	114.55	120.80
48	A	1320	U	C5-C6-N1	5.21	125.30	122.70
48	A	952	C	C6-N1-C2	-5.21	118.22	120.30
48	A	1001	C	N3-C2-O2	-5.21	118.26	121.90
48	A	2780	C	N1-C2-O2	5.21	122.02	118.90
48	A	407	C	C6-N1-C2	-5.20	118.22	120.30
48	A	1553	C	N3-C2-O2	-5.20	118.26	121.90
48	A	1467	U	N1-C2-O2	5.19	126.44	122.80
1	a	895	A	N9-C4-C5	5.19	107.88	105.80
1	a	1435	U	O4'-C1'-N1	-5.19	104.05	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	A	2226	U	N3-C2-O2	-5.19	118.56	122.20
48	A	2260	C	N1-C2-O2	5.19	122.02	118.90
48	A	1478	C	N1-C2-O2	5.19	122.02	118.90
1	a	1510	G	C2-N3-C4	5.19	114.50	111.90
48	A	472	C	C5-C6-N1	5.19	123.59	121.00
48	A	277	U	C5-C6-N1	5.18	125.29	122.70
48	A	547	U	N1-C2-O2	5.18	126.43	122.80
1	a	485	G	C4-N9-C1'	5.18	133.24	126.50
3	e	29	ASP	CB-CG-OD2	5.18	122.96	118.30
48	A	1212	U	C2-N1-C1'	5.18	123.92	117.70
1	a	802	G	C8-N9-C4	-5.18	104.33	106.40
48	A	197	C	C2-N1-C1'	5.18	124.49	118.80
48	A	572	C	C5-C6-N1	5.18	123.59	121.00
48	A	472	C	N3-C2-O2	-5.17	118.28	121.90
48	A	658	U	C2-N1-C1'	5.17	123.91	117.70
48	A	2107	G	C2-N3-C4	-5.17	109.31	111.90
23	C	94	LEU	CB-CG-CD1	-5.17	102.21	111.00
48	A	685	G	C4-N9-C1'	5.17	133.22	126.50
48	A	1521	C	C5-C6-N1	5.17	123.58	121.00
48	A	2118	C	N3-C2-O2	-5.17	118.28	121.90
23	C	35	ARG	C-N-CD	5.17	139.25	128.40
48	A	79	G	C8-N9-C4	-5.17	104.33	106.40
48	A	184	C	C5-C6-N1	5.16	123.58	121.00
1	a	666	U	O4'-C1'-N1	5.16	112.33	108.20
48	A	83	C	C5-C6-N1	5.16	123.58	121.00
48	A	703	C	C6-N1-C1'	-5.16	114.61	120.80
48	A	912	C	C4-C5-C6	-5.16	114.82	117.40
48	A	318	U	N1-C2-O2	5.16	126.41	122.80
48	A	1817	C	C5-C6-N1	5.16	123.58	121.00
48	A	1953	C	C5-C6-N1	5.16	123.58	121.00
1	a	967	C	C6-N1-C2	5.15	122.36	120.30
48	A	608	C	N1-C2-O2	5.15	121.99	118.90
48	A	127	C	C5-C6-N1	5.15	123.58	121.00
48	A	326	A	C8-N9-C4	-5.15	103.74	105.80
48	A	2158	C	N3-C2-O2	-5.14	118.30	121.90
48	A	2940	U	N1-C2-O2	5.14	126.40	122.80
1	a	1340	U	C6-N1-C2	5.14	124.08	121.00
25	E	93	PRO	C-N-CA	5.14	134.55	121.70
1	a	530	G	C6-C5-N7	-5.14	127.32	130.40
48	A	1102	G	C2-N3-C4	5.14	114.47	111.90
48	A	1837	G	N9-C4-C5	-5.14	103.34	105.40
1	a	454	C	C5-C6-N1	5.13	123.57	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	A	1460	C	C2-N1-C1'	5.13	124.45	118.80
48	A	3034	C	C5-C6-N1	5.13	123.56	121.00
1	a	1515	A	C8-N9-C4	-5.13	103.75	105.80
48	A	387	U	N3-C2-O2	-5.13	118.61	122.20
48	A	2993	U	N3-C2-O2	-5.13	118.61	122.20
1	a	953	G	OP1-P-OP2	5.12	127.29	119.60
48	A	961	U	C2-N1-C1'	5.12	123.85	117.70
48	A	2680	C	C2-N1-C1'	5.12	124.44	118.80
48	A	3045	C	C5-C6-N1	5.12	123.56	121.00
41	U	6	ASP	C-N-CD	5.12	139.15	128.40
48	A	574	C	C6-N1-C2	-5.12	118.25	120.30
48	A	2485	C	N3-C2-O2	-5.12	118.32	121.90
1	a	415	C	C6-N1-C2	-5.12	118.25	120.30
48	A	1103	C	C2-N1-C1'	5.12	124.43	118.80
48	A	609	G	N3-C4-N9	5.11	129.07	126.00
48	A	1382	U	N3-C2-O2	-5.11	118.62	122.20
48	A	2839	U	N1-C2-O2	5.11	126.38	122.80
1	a	487	C	C6-N1-C2	-5.11	118.26	120.30
48	A	2782	C	C6-N1-C2	-5.11	118.26	120.30
48	A	2923	C	C5-C6-N1	5.11	123.55	121.00
48	A	3036	C	C6-N1-C2	-5.10	118.26	120.30
1	a	1504	G	C8-N9-C4	5.10	108.44	106.40
1	a	1302	C	C5-C6-N1	-5.10	118.45	121.00
48	A	2005	C	C2-N1-C1'	5.10	124.41	118.80
1	a	372	C	N1-C2-N3	5.10	122.77	119.20
48	A	186	G	C4-C5-N7	5.10	112.84	110.80
48	A	2243	C	C2-N1-C1'	5.10	124.41	118.80
48	A	787	C	C6-N1-C2	-5.09	118.26	120.30
48	A	2717	U	C6-N1-C2	-5.09	117.94	121.00
1	a	1192	U	O4'-C1'-N1	5.09	112.28	108.20
1	a	538	G	N3-C4-N9	5.09	129.06	126.00
48	A	1276	G	C6-C5-N7	-5.09	127.34	130.40
50	2	42	HIS	C-N-CD	5.09	139.09	128.40
48	A	1695	U	N1-C2-O2	5.09	126.36	122.80
47	B	4	A	N1-C6-N6	5.09	121.65	118.60
48	A	643	G	C4-C5-N7	5.09	112.83	110.80
48	A	964	C	C5-C6-N1	5.09	123.54	121.00
48	A	1903	C	N1-C2-O2	5.09	121.95	118.90
1	a	793	U	C5-C6-N1	5.08	125.24	122.70
48	A	2087	C	C5-C6-N1	5.08	123.54	121.00
48	A	197	C	N1-C2-O2	5.08	121.95	118.90
48	A	1819	G	N1-C6-O6	-5.08	116.85	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1269	A	N7-C8-N9	5.08	116.34	113.80
48	A	1862	C	N1-C2-O2	5.08	121.95	118.90
48	A	646	U	N3-C2-O2	-5.07	118.65	122.20
1	a	790	C	N3-C2-O2	-5.07	118.35	121.90
1	a	1485	C	C6-N1-C2	5.07	122.33	120.30
48	A	1837	G	N3-C4-N9	5.07	129.04	126.00
1	a	821	C	C2-N1-C1'	5.07	124.38	118.80
24	D	156	THR	C-N-CD	5.07	139.04	128.40
48	A	1102	G	N3-C4-N9	5.07	129.04	126.00
48	A	1534	C	N3-C2-O2	-5.07	118.36	121.90
48	A	2419	C	N1-C2-O2	5.06	121.94	118.90
48	A	2698	C	N1-C2-O2	5.06	121.94	118.90
1	a	798	G	O4'-C1'-N9	5.06	112.25	108.20
48	A	2361	U	C5-C6-N1	5.06	125.23	122.70
48	A	1403	C	C2-N1-C1'	5.06	124.36	118.80
48	A	1753	C	C6-N1-C2	-5.06	118.28	120.30
1	a	1171	G	P-O5'-C5'	-5.05	112.81	120.90
1	a	118	A	C5-C6-N1	5.05	120.23	117.70
48	A	2671	G	N3-C4-N9	5.05	129.03	126.00
1	a	1267	U	C5-C6-N1	5.05	125.22	122.70
48	A	2086	U	C6-N1-C2	-5.05	117.97	121.00
48	A	2118	C	C6-N1-C2	-5.05	118.28	120.30
48	A	2430	C	N3-C2-O2	-5.05	118.37	121.90
48	A	747	A	C4-C5-N7	5.04	113.22	110.70
48	A	2913	U	N1-C2-O2	5.04	126.33	122.80
1	a	280	C	C6-N1-C2	5.04	122.32	120.30
48	A	1298	C	N1-C2-O2	5.04	121.92	118.90
1	a	372	C	C6-N1-C2	-5.04	118.28	120.30
48	A	2320	C	C6-N1-C2	-5.04	118.28	120.30
1	a	855	A	N1-C6-N6	5.04	121.62	118.60
1	a	1176	C	C5-C6-N1	5.04	123.52	121.00
48	A	3029	U	N1-C2-O2	5.03	126.32	122.80
1	a	900	A	N1-C2-N3	5.03	131.81	129.30
48	A	54	C	C6-N1-C2	-5.03	118.29	120.30
1	a	973	U	C5-C6-N1	5.03	125.21	122.70
25	E	155	LEU	CB-CG-CD1	-5.03	102.45	111.00
48	A	1199	U	N3-C2-O2	-5.03	118.68	122.20
48	A	1283	C	C6-N1-C2	-5.03	118.29	120.30
1	a	799	G	C2-N3-C4	-5.03	109.39	111.90
48	A	199	U	N1-C2-O2	5.03	126.32	122.80
1	a	742	A	C4-C5-C6	5.02	119.51	117.00
47	B	73	G	N3-C4-N9	5.02	129.01	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	A	853	C	C6-N1-C2	-5.02	118.29	120.30
48	A	1085	G	O5'-P-OP2	-5.02	101.19	105.70
48	A	2402	C	N1-C2-O2	5.02	121.91	118.90
48	A	2800	G	C4-N9-C1'	5.02	133.02	126.50
48	A	2077	C	C5-C6-N1	5.02	123.51	121.00
48	A	749	C	C6-N1-C2	-5.01	118.29	120.30
48	A	89	A	P-O3'-C3'	5.01	125.72	119.70
48	A	759	G	N3-C4-C5	5.01	131.11	128.60
48	A	977	G	N3-C4-C5	-5.01	126.09	128.60
32	L	64	ARG	CB-CG-CD	-5.01	98.57	111.60
48	A	898	A	C8-N9-C1'	-5.01	118.68	127.70
48	A	1030	C	C5-C6-N1	5.01	123.50	121.00
48	A	779	U	N1-C2-O2	5.00	126.30	122.80
1	a	356	A	C4-C5-C6	5.00	119.50	117.00
48	A	1977	C	N1-C2-O2	5.00	121.90	118.90

There are no chirality outliers.

All (55) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
50	2	64	ARG	Peptide
52	4	52	LYS	Peptide
23	C	144	ALA	Peptide
23	C	229	VAL	Peptide
23	C	246	PRO	Peptide
23	C	35	ARG	Peptide
23	C	61	ALA	Peptide
25	E	131	VAL	Peptide
25	E	137	SER	Peptide
25	E	158	ILE	Peptide
25	E	162	ASP	Peptide
25	E	93	PRO	Peptide
26	F	32	VAL	Peptide
26	F	34	GLN	Peptide
26	F	81	ILE	Peptide
31	K	91	GLU	Peptide
32	L	89	ASN	Peptide
32	L	91	ASN	Peptide
34	N	78	PRO	Peptide
35	O	117	ARG	Peptide
35	O	61	HIS	Peptide
35	O	83	ILE	Peptide

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Mol	Chain	Res	Type	Group
35	O	88	ALA	Peptide
40	T	95	ARG	Peptide
43	W	38	TYR	Peptide
43	W	39	GLY	Peptide
44	X	80	ILE	Peptide
44	X	82	PRO	Peptide
44	X	84	ALA	Peptide
44	X	85	ARG	Peptide
2	c	136	ALA	Peptide
2	c	137	ILE	Peptide
2	c	141	MET	Peptide
2	c	142	ARG	Peptide
2	c	143	GLN	Peptide
2	c	144	PRO	Peptide
2	c	145	ASN	Peptide
2	c	146	VAL	Peptide
2	c	148	GLY	Peptide
2	c	62	ARG	Peptide
18	d	189	PRO	Peptide
3	e	186	ILE	Peptide
4	g	1	MET	Peptide
4	g	32	LEU	Peptide
5	h	126	GLU	Peptide
5	h	55	ARG	Peptide
7	j	44	THR	Peptide
8	k	133	PRO	Peptide
8	k	35	THR	Peptide
9	l	23	ALA	Peptide
9	l	88	LYS	Peptide
20	m	73	GLU	Peptide
11	q	15	LYS	Peptide
13	s	70	LYS	Peptide
13	s	73	GLU	Peptide

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	
2	c	208/275 (76%)	176 (85%)	24 (12%)	8 (4%)	2	15
3	e	196/214 (92%)	176 (90%)	19 (10%)	1 (0%)	25	54
4	g	154/156 (99%)	144 (94%)	9 (6%)	1 (1%)	22	50
5	h	128/132 (97%)	119 (93%)	8 (6%)	1 (1%)	16	44
6	i	124/150 (83%)	113 (91%)	11 (9%)	0	100	100
7	j	95/101 (94%)	82 (86%)	10 (10%)	3 (3%)	3	18
8	k	115/138 (83%)	103 (90%)	10 (9%)	2 (2%)	7	28
9	l	120/124 (97%)	94 (78%)	25 (21%)	1 (1%)	16	44
10	o	85/89 (96%)	81 (95%)	4 (5%)	0	100	100
11	q	90/98 (92%)	78 (87%)	12 (13%)	0	100	100
12	r	62/84 (74%)	55 (89%)	7 (11%)	0	100	100
13	s	76/93 (82%)	65 (86%)	9 (12%)	2 (3%)	4	22
14	t	82/86 (95%)	77 (94%)	5 (6%)	0	100	100
16	n	58/61 (95%)	53 (91%)	5 (9%)	0	100	100
17	b	226/277 (82%)	212 (94%)	14 (6%)	0	100	100
18	d	198/201 (98%)	185 (93%)	12 (6%)	1 (0%)	25	54
19	f	94/96 (98%)	90 (96%)	4 (4%)	0	100	100
20	m	114/124 (92%)	98 (86%)	15 (13%)	1 (1%)	14	41
21	p	111/156 (71%)	104 (94%)	7 (6%)	0	100	100
22	u	30/33 (91%)	28 (93%)	2 (7%)	0	100	100
23	C	271/278 (98%)	233 (86%)	32 (12%)	6 (2%)	5	24
24	D	212/217 (98%)	197 (93%)	13 (6%)	2 (1%)	14	41
25	E	205/215 (95%)	179 (87%)	20 (10%)	6 (3%)	3	19
26	F	179/187 (96%)	160 (89%)	16 (9%)	3 (2%)	7	28
27	G	174/179 (97%)	166 (95%)	8 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	H	149/151 (99%)	139 (93%)	9 (6%)	1 (1%)	19	47
29	I	124/175 (71%)	118 (95%)	6 (5%)	0	100	100
30	J	131/142 (92%)	118 (90%)	13 (10%)	0	100	100
31	K	145/147 (99%)	132 (91%)	10 (7%)	3 (2%)	5	24
32	L	119/122 (98%)	103 (87%)	13 (11%)	3 (2%)	4	22
33	M	143/147 (97%)	128 (90%)	15 (10%)	0	100	100
34	N	132/138 (96%)	113 (86%)	19 (14%)	0	100	100
35	O	115/199 (58%)	98 (85%)	12 (10%)	5 (4%)	2	14
36	P	124/127 (98%)	119 (96%)	5 (4%)	0	100	100
37	Q	111/113 (98%)	102 (92%)	9 (8%)	0	100	100
38	R	122/129 (95%)	120 (98%)	2 (2%)	0	100	100
39	S	100/103 (97%)	94 (94%)	5 (5%)	1 (1%)	13	39
40	T	112/153 (73%)	103 (92%)	6 (5%)	3 (3%)	4	21
41	U	92/100 (92%)	74 (80%)	12 (13%)	6 (6%)	1	7
42	V	93/105 (89%)	83 (89%)	8 (9%)	2 (2%)	5	24
43	W	186/215 (86%)	171 (92%)	10 (5%)	5 (3%)	4	21
44	X	80/88 (91%)	59 (74%)	15 (19%)	6 (8%)	1	5
45	Y	61/64 (95%)	57 (93%)	4 (7%)	0	100	100
46	Z	61/77 (79%)	56 (92%)	1 (2%)	4 (7%)	1	7
49	1	58/61 (95%)	53 (91%)	5 (9%)	0	100	100
50	2	64/75 (85%)	59 (92%)	4 (6%)	1 (2%)	8	29
51	3	52/57 (91%)	51 (98%)	1 (2%)	0	100	100
52	4	48/55 (87%)	41 (85%)	5 (10%)	2 (4%)	2	14
53	5	43/47 (92%)	41 (95%)	2 (5%)	0	100	100
54	6	61/64 (95%)	54 (88%)	7 (12%)	0	100	100
55	7	35/37 (95%)	33 (94%)	1 (3%)	1 (3%)	3	19
56	8	21/24 (88%)	20 (95%)	1 (5%)	0	100	100
All	All	5989/6679 (90%)	5407 (90%)	501 (8%)	81 (1%)	12	31

All (81) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	c	137	ILE

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Mol	Chain	Res	Type
2	c	138	GLN
2	c	143	GLN
2	c	144	PRO
2	c	145	ASN
4	g	154	TYR
8	k	116	VAL
23	C	58	HIS
23	C	145	VAL
23	C	262	LYS
24	D	155	ALA
25	E	94	LYS
25	E	152	LYS
26	F	32	VAL
26	F	47	VAL
31	K	142	ILE
32	L	91	ASN
32	L	92	ASP
35	O	81	ALA
35	O	89	ASP
40	T	7	PHE
40	T	118	PRO
41	U	68	ARG
43	W	83	LEU
46	Z	10	LEU
52	4	34	ASP
2	c	63	VAL
2	c	134	ARG
3	e	186	ILE
5	h	56	VAL
13	s	10	PHE
13	s	11	VAL
23	C	34	VAL
23	C	146	GLU
24	D	158	GLY
25	E	65	PRO
26	F	142	GLN
31	K	140	PHE
35	O	15	SER
35	O	82	GLU
41	U	75	LYS
43	W	39	GLY
43	W	63	THR

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Mol	Chain	Res	Type
44	X	12	ASN
44	X	16	SER
44	X	17	ALA
55	7	35	ARG
2	c	139	SER
9	l	59	SER
31	K	2	PRO
32	L	93	PRO
41	U	67	LYS
43	W	85	VAL
46	Z	65	GLU
7	j	56	HIS
8	k	36	PHE
18	d	189	PRO
25	E	4	LYS
25	E	93	PRO
28	H	125	LYS
35	O	60	LEU
40	T	8	PRO
41	U	6	ASP
42	V	90	GLU
42	V	101	ASN
43	W	87	PRO
44	X	85	ARG
46	Z	63	GLU
52	4	7	VAL
25	E	132	GLU
41	U	5	THR
44	X	81	VAL
7	j	43	PRO
46	Z	64	ARG
23	C	36	PRO
39	S	7	VAL
41	U	10	ILE
20	m	74	VAL
50	2	42	HIS
7	j	55	PRO
44	X	80	ILE

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	
2	c	171/212 (81%)	164 (96%)	7 (4%)	26	51
3	e	139/147 (95%)	135 (97%)	4 (3%)	37	61
4	g	132/132 (100%)	128 (97%)	4 (3%)	36	61
5	h	106/108 (98%)	103 (97%)	3 (3%)	38	62
6	i	102/125 (82%)	93 (91%)	9 (9%)	8	28
7	j	88/90 (98%)	86 (98%)	2 (2%)	45	67
8	k	91/105 (87%)	85 (93%)	6 (7%)	14	39
9	l	103/105 (98%)	98 (95%)	5 (5%)	21	48
10	o	75/77 (97%)	74 (99%)	1 (1%)	65	78
11	q	78/83 (94%)	78 (100%)	0	100	100
12	r	55/72 (76%)	55 (100%)	0	100	100
13	s	69/84 (82%)	66 (96%)	3 (4%)	25	50
14	t	69/70 (99%)	65 (94%)	4 (6%)	17	42
16	n	49/50 (98%)	48 (98%)	1 (2%)	50	70
17	b	191/218 (88%)	187 (98%)	4 (2%)	48	69
18	d	175/176 (99%)	174 (99%)	1 (1%)	84	90
19	f	85/85 (100%)	84 (99%)	1 (1%)	67	80
20	m	99/104 (95%)	94 (95%)	5 (5%)	20	46
21	p	92/118 (78%)	92 (100%)	0	100	100
22	u	30/31 (97%)	23 (77%)	7 (23%)	0	2
23	C	214/218 (98%)	207 (97%)	7 (3%)	33	58
24	D	160/163 (98%)	155 (97%)	5 (3%)	35	60
25	E	167/173 (96%)	158 (95%)	9 (5%)	18	44
26	F	150/156 (96%)	138 (92%)	12 (8%)	10	31
27	G	148/150 (99%)	148 (100%)	0	100	100
28	H	90/116 (78%)	90 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	I	89/120 (74%)	89 (100%)	0	100	100
30	J	102/108 (94%)	102 (100%)	0	100	100
31	K	120/120 (100%)	116 (97%)	4 (3%)	33	58
32	L	99/100 (99%)	96 (97%)	3 (3%)	36	61
33	M	112/114 (98%)	111 (99%)	1 (1%)	75	86
34	N	112/116 (97%)	107 (96%)	5 (4%)	23	50
35	O	96/158 (61%)	89 (93%)	7 (7%)	11	36
36	P	93/94 (99%)	93 (100%)	0	100	100
37	Q	100/100 (100%)	99 (99%)	1 (1%)	73	83
38	R	97/99 (98%)	96 (99%)	1 (1%)	73	83
39	S	82/83 (99%)	81 (99%)	1 (1%)	67	80
40	T	90/117 (77%)	86 (96%)	4 (4%)	24	50
41	U	82/85 (96%)	69 (84%)	13 (16%)	2	8
42	V	81/86 (94%)	75 (93%)	6 (7%)	11	35
43	W	154/168 (92%)	141 (92%)	13 (8%)	9	29
44	X	59/63 (94%)	57 (97%)	2 (3%)	32	57
45	Y	50/51 (98%)	50 (100%)	0	100	100
46	Z	58/66 (88%)	51 (88%)	7 (12%)	4	15
49	1	53/54 (98%)	51 (96%)	2 (4%)	28	54
50	2	57/63 (90%)	53 (93%)	4 (7%)	12	37
51	3	43/46 (94%)	43 (100%)	0	100	100
52	4	48/52 (92%)	38 (79%)	10 (21%)	1	2
53	5	35/36 (97%)	33 (94%)	2 (6%)	17	43
54	6	53/54 (98%)	53 (100%)	0	100	100
55	7	35/35 (100%)	32 (91%)	3 (9%)	8	29
56	8	18/19 (95%)	18 (100%)	0	100	100
All	All	4946/5375 (92%)	4757 (96%)	189 (4%)	30	54

All (189) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	c	131	ARG
2	c	134	ARG

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Mol	Chain	Res	Type
2	c	135	LYS
2	c	141	MET
2	c	147	LYS
2	c	169	ARG
2	c	186	LEU
3	e	79	LYS
3	e	182	ARG
3	e	184	LEU
3	e	188	ASP
4	g	10	ARG
4	g	78	ARG
4	g	112	ARG
4	g	148	ASN
5	h	41	LYS
5	h	50	ARG
5	h	96	ARG
6	i	38	ARG
6	i	40	ARG
6	i	41	LEU
6	i	42	VAL
6	i	57	ASN
6	i	83	ILE
6	i	84	TYR
6	i	86	HIS
6	i	115	ARG
7	j	57	LYS
7	j	99	ASN
8	k	23	LYS
8	k	37	ASN
8	k	47	GLN
8	k	62	LYS
8	k	78	ASN
8	k	134	LYS
9	l	13	ARG
9	l	46	ASN
9	l	56	LYS
9	l	73	ASN
9	l	83	ARG
10	o	54	ARG
13	s	6	LYS
13	s	29	GLN
13	s	55	ARG

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Mol	Chain	Res	Type
14	t	3	ASN
14	t	8	ILE
14	t	18	ARG
14	t	20	ARG
16	n	45	ARG
17	b	24	ASN
17	b	167	ASN
17	b	177	ARG
17	b	203	ASN
18	d	86	LEU
19	f	47	ARG
20	m	70	LEU
20	m	71	ARG
20	m	72	ARG
20	m	73	GLU
20	m	75	GLN
22	u	4	VAL
22	u	6	LYS
22	u	8	ARG
22	u	10	LYS
22	u	11	ARG
22	u	24	THR
22	u	30	LYS
23	C	35	ARG
23	C	36	PRO
23	C	71	ASP
23	C	73	ASP
23	C	168	LYS
23	C	256	ARG
23	C	258	ARG
24	D	60	ARG
24	D	154	CYS
24	D	159	ARG
24	D	160	VAL
24	D	201	ARG
25	E	4	LYS
25	E	20	LEU
25	E	33	LEU
25	E	50	HIS
25	E	75	ARG
25	E	130	LEU
25	E	150	GLU

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Mol	Chain	Res	Type
25	E	171	ASN
25	E	178	ILE
26	F	10	ARG
26	F	11	LEU
26	F	14	ARG
26	F	55	LYS
26	F	56	LEU
26	F	108	ASP
26	F	110	LEU
26	F	118	ILE
26	F	122	ARG
26	F	174	ARG
26	F	185	LYS
26	F	186	GLU
31	K	75	TYR
31	K	76	ARG
31	K	113	LYS
31	K	141	GLU
32	L	8	LEU
32	L	53	LYS
32	L	90	ASP
33	M	43	ARG
34	N	34	ILE
34	N	59	LYS
34	N	60	ARG
34	N	92	TRP
34	N	96	ASN
35	O	5	THR
35	O	9	ARG
35	O	14	SER
35	O	79	LEU
35	O	86	PHE
35	O	115	LEU
35	O	117	ARG
37	Q	38	ARG
38	R	34	LYS
39	S	103	LYS
40	T	6	GLU
40	T	44	ARG
40	T	90	LYS
40	T	118	PRO
41	U	9	ASP

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Mol	Chain	Res	Type
41	U	12	LEU
41	U	27	ASN
41	U	65	LYS
41	U	66	ARG
41	U	67	LYS
41	U	68	ARG
41	U	70	ARG
41	U	77	LYS
41	U	79	THR
41	U	94	ASP
41	U	95	LEU
41	U	96	PHE
42	V	20	LYS
42	V	22	LYS
42	V	39	ASN
42	V	89	ASP
42	V	96	ARG
42	V	99	LYS
43	W	6	ASN
43	W	7	ILE
43	W	64	ASN
43	W	83	LEU
43	W	101	GLN
43	W	102	ARG
43	W	112	VAL
43	W	114	VAL
43	W	131	ILE
43	W	139	SER
43	W	146	VAL
43	W	158	THR
43	W	172	SER
44	X	15	ASP
44	X	85	ARG
46	Z	5	THR
46	Z	14	THR
46	Z	23	ARG
46	Z	44	ASN
46	Z	47	LEU
46	Z	64	ARG
46	Z	65	GLU
49	1	8	GLN
49	1	51	HIS

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Mol	Chain	Res	Type
50	2	38	CYS
50	2	44	PHE
50	2	60	ARG
50	2	65	TYR
52	4	22	ASN
52	4	23	TYR
52	4	26	LYS
52	4	27	LYS
52	4	32	ASP
52	4	35	ARG
52	4	37	GLU
52	4	42	CYS
52	4	52	LYS
52	4	53	GLU
53	5	6	ARG
53	5	27	THR
55	7	20	HIS
55	7	34	GLN
55	7	35	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (94) such sidechains are listed below:

Mol	Chain	Res	Type
2	c	27	GLN
2	c	97	GLN
2	c	101	ASN
2	c	122	GLN
4	g	148	ASN
5	h	22	HIS
5	h	117	GLN
6	i	57	ASN
6	i	64	HIS
7	j	56	HIS
7	j	99	ASN
8	k	31	HIS
8	k	37	ASN
8	k	47	GLN
8	k	49	ASN
8	k	58	HIS
8	k	78	ASN
9	l	46	ASN
10	o	28	GLN

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Mol	Chain	Res	Type
11	q	33	GLN
12	r	70	ASN
13	s	22	GLN
13	s	29	GLN
14	t	3	ASN
14	t	7	GLN
17	b	24	ASN
17	b	167	ASN
17	b	203	ASN
18	d	49	GLN
19	f	80	ASN
23	C	58	HIS
23	C	96	HIS
23	C	130	ASN
23	C	135	ASN
23	C	205	ASN
24	D	34	ASN
25	E	35	HIS
25	E	76	GLN
25	E	121	ASN
25	E	176	HIS
25	E	184	ASN
25	E	202	ASN
26	F	44	ASN
26	F	142	GLN
26	F	146	HIS
27	G	66	HIS
30	J	33	HIS
30	J	119	ASN
31	K	47	ASN
31	K	132	HIS
31	K	135	GLN
32	L	4	GLN
32	L	91	ASN
33	M	58	HIS
33	M	76	GLN
33	M	84	ASN
33	M	127	ASN
34	N	96	ASN
35	O	16	HIS
35	O	77	HIS
36	P	41	ASN

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Mol	Chain	Res	Type
38	R	38	GLN
38	R	41	HIS
39	S	76	HIS
39	S	85	HIS
39	S	92	GLN
40	T	67	ASN
40	T	68	ASN
41	U	27	ASN
41	U	58	ASN
43	W	6	ASN
43	W	9	ASN
43	W	46	HIS
43	W	101	GLN
43	W	129	ASN
44	X	29	GLN
44	X	46	HIS
44	X	79	ASN
45	Y	22	HIS
46	Z	44	ASN
46	Z	52	GLN
49	1	8	GLN
49	1	42	GLN
49	1	51	HIS
50	2	40	GLN
52	4	48	HIS
52	4	49	GLN
52	4	51	HIS
53	5	11	ASN
53	5	19	HIS
54	6	7	HIS
54	6	28	ASN
54	6	31	HIS
56	8	17	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1504/1528 (98%)	393 (26%)	0
15	v	76/77 (98%)	17 (22%)	0
47	B	116/118 (98%)	31 (26%)	1 (0%)
48	A	3096/3120 (99%)	793 (25%)	45 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	4792/4843 (98%)	1234 (25%)	46 (0%)

All (1234) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	11	G
1	a	12	A
1	a	13	G
1	a	26	G
1	a	36	A
1	a	43	G
1	a	45	G
1	a	48	G
1	a	51	C
1	a	52	U
1	a	53	U
1	a	54	A
1	a	55	A
1	a	59	A
1	a	62	C
1	a	67	C
1	a	68	G
1	a	77	G
1	a	81	C
1	a	82	U
1	a	83	U
1	a	85	C
1	a	87	G
1	a	92	A
1	a	93	C
1	a	94	U
1	a	101	G
1	a	112	A
1	a	113	G
1	a	116	A
1	a	117	C
1	a	118	A
1	a	123	G
1	a	128	U
1	a	136	G
1	a	139	C
1	a	160	C

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Mol	Chain	Res	Type
1	a	170	U
1	a	174	G
1	a	179	C
1	a	180	A
1	a	181	C
1	a	192	G
1	a	194	A
1	a	201	G
1	a	210	A
1	a	211	A
1	a	213	C
1	a	214	U
1	a	215	U
1	a	216	U
1	a	217	U
1	a	218	G
1	a	226	G
1	a	242	U
1	a	243	A
1	a	245	C
1	a	247	G
1	a	251	G
1	a	262	G
1	a	266	G
1	a	267	C
1	a	279	A
1	a	280	C
1	a	281	G
1	a	283	C
1	a	289	G
1	a	301	G
1	a	314	C
1	a	319	G
1	a	321	A
1	a	329	A
1	a	332	G
1	a	338	A
1	a	344	A
1	a	345	C
1	a	350	G
1	a	351	G
1	a	352	C

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Mol	Chain	Res	Type
1	a	353	A
1	a	354	G
1	a	356	A
1	a	367	U
1	a	372	C
1	a	373	A
1	a	382	A
1	a	390	U
1	a	392	C
1	a	397	A
1	a	398	C
1	a	406	G
1	a	411	A
1	a	414	A
1	a	415	C
1	a	421	U
1	a	422	C
1	a	423	G
1	a	424	G
1	a	426	U
1	a	427	U
1	a	428	G
1	a	429	U
1	a	430	A
1	a	434	C
1	a	436	C
1	a	438	U
1	a	450	G
1	a	451	A
1	a	452	A
1	a	453	G
1	a	454	C
1	a	456	C
1	a	457	A
1	a	458	A
1	a	459	G
1	a	461	G
1	a	464	G
1	a	465	G
1	a	466	U
1	a	477	G
1	a	478	A

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Mol	Chain	Res	Type
1	a	479	A
1	a	482	A
1	a	484	C
1	a	485	G
1	a	486	G
1	a	491	C
1	a	496	U
1	a	497	G
1	a	498	C
1	a	499	C
1	a	505	C
1	a	507	G
1	a	509	G
1	a	511	U
1	a	512	A
1	a	513	A
1	a	515	A
1	a	519	A
1	a	520	G
1	a	525	C
1	a	527	A
1	a	539	A
1	a	542	U
1	a	544	C
1	a	552	A
1	a	553	A
1	a	554	A
1	a	556	A
1	a	557	G
1	a	612	U
1	a	613	G
1	a	629	G
1	a	633	A
1	a	641	G
1	a	645	G
1	a	666	U
1	a	667	A
1	a	668	G
1	a	680	G
1	a	682	A
1	a	683	G
1	a	700	C

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Mol	Chain	Res	Type
1	a	701	G
1	a	702	G
1	a	703	U
1	a	704	G
1	a	711	G
1	a	713	G
1	a	728	A
1	a	729	A
1	a	735	G
1	a	757	A
1	a	761	A
1	a	764	A
1	a	765	G
1	a	771	G
1	a	772	A
1	a	773	U
1	a	774	A
1	a	779	G
1	a	782	A
1	a	789	G
1	a	793	U
1	a	794	A
1	a	795	A
1	a	797	C
1	a	799	G
1	a	800	U
1	a	808	A
1	a	818	U
1	a	821	C
1	a	822	U
1	a	828	G
1	a	835	G
1	a	840	G
1	a	841	U
1	a	865	C
1	a	884	G
1	a	895	A
1	a	896	A
1	a	908	G
1	a	909	G
1	a	913	C
1	a	914	C

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Mol	Chain	Res	Type
1	a	915	G
1	a	916	C
1	a	917	A
1	a	921	G
1	a	930	C
1	a	932	U
1	a	940	A
1	a	942	U
1	a	943	U
1	a	945	G
1	a	947	U
1	a	948	G
1	a	950	A
1	a	951	A
1	a	953	G
1	a	954	C
1	a	955	G
1	a	956	A
1	a	957	A
1	a	959	A
1	a	971	G
1	a	973	U
1	a	974	U
1	a	975	G
1	a	982	A
1	a	984	A
1	a	986	G
1	a	987	A
1	a	988	C
1	a	992	G
1	a	996	G
1	a	999	A
1	a	1000	U
1	a	1003	C
1	a	1007	U
1	a	1008	C
1	a	1010	C
1	a	1011	U
1	a	1013	G
1	a	1014	U
1	a	1020	G
1	a	1021	U

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Mol	Chain	Res	Type
1	a	1022	G
1	a	1024	G
1	a	1025	C
1	a	1028	G
1	a	1033	G
1	a	1034	C
1	a	1036	U
1	a	1045	U
1	a	1047	A
1	a	1048	G
1	a	1054	G
1	a	1064	G
1	a	1074	G
1	a	1075	U
1	a	1079	G
1	a	1081	A
1	a	1085	A
1	a	1104	G
1	a	1108	C
1	a	1110	A
1	a	1112	C
1	a	1115	G
1	a	1116	U
1	a	1117	U
1	a	1118	A
1	a	1120	G
1	a	1123	G
1	a	1128	C
1	a	1129	U
1	a	1132	U
1	a	1133	G
1	a	1138	A
1	a	1140	U
1	a	1141	G
1	a	1147	G
1	a	1149	C
1	a	1150	A
1	a	1152	C
1	a	1162	G
1	a	1164	U
1	a	1165	G
1	a	1171	G

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Mol	Chain	Res	Type
1	a	1176	C
1	a	1177	A
1	a	1178	A
1	a	1181	C
1	a	1182	A
1	a	1183	U
1	a	1193	U
1	a	1194	A
1	a	1206	U
1	a	1207	C
1	a	1217	A
1	a	1219	A
1	a	1231	A
1	a	1233	A
1	a	1235	G
1	a	1238	U
1	a	1239	G
1	a	1241	G
1	a	1242	A
1	a	1248	U
1	a	1249	G
1	a	1251	G
1	a	1254	G
1	a	1255	G
1	a	1261	A
1	a	1265	U
1	a	1266	U
1	a	1267	U
1	a	1268	C
1	a	1269	A
1	a	1272	G
1	a	1281	A
1	a	1282	G
1	a	1283	U
1	a	1284	U
1	a	1285	C
1	a	1287	G
1	a	1298	G
1	a	1299	C
1	a	1300	A
1	a	1301	A
1	a	1302	C

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Mol	Chain	Res	Type
1	a	1305	G
1	a	1313	G
1	a	1320	G
1	a	1322	G
1	a	1327	U
1	a	1328	A
1	a	1329	G
1	a	1335	G
1	a	1343	G
1	a	1344	C
1	a	1345	A
1	a	1346	A
1	a	1347	C
1	a	1351	G
1	a	1353	G
1	a	1357	A
1	a	1363	U
1	a	1364	U
1	a	1381	A
1	a	1382	C
1	a	1383	C
1	a	1385	C
1	a	1389	U
1	a	1402	G
1	a	1406	G
1	a	1407	U
1	a	1424	G
1	a	1425	G
1	a	1426	C
1	a	1429	A
1	a	1430	A
1	a	1434	U
1	a	1435	U
1	a	1436	G
1	a	1438	G
1	a	1459	G
1	a	1460	A
1	a	1466	G
1	a	1468	U
1	a	1471	G
1	a	1476	A
1	a	1478	G

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Mol	Chain	Res	Type
1	a	1481	G
1	a	1482	U
1	a	1483	A
1	a	1486	A
1	a	1487	A
1	a	1488	G
1	a	1490	U
1	a	1491	A
1	a	1492	G
1	a	1501	G
1	a	1502	A
1	a	1503	A
1	a	1504	G
1	a	1511	C
1	a	1512	U
1	a	1513	G
1	a	1514	G
1	a	1516	U
1	a	1517	C
1	a	1518	A
15	v	7	G
15	v	9	G
15	v	14	A
15	v	16	C
15	v	17	C
15	v	18	U
15	v	19	G
15	v	20	G
15	v	21	U
15	v	22	A
15	v	23	G
15	v	55	U
15	v	60	A
15	v	61	U
15	v	68	C
15	v	76	C
15	v	77	A
47	B	4	A
47	B	5	C
47	B	7	G
47	B	10	G
47	B	12	C

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Mol	Chain	Res	Type
47	B	13	C
47	B	24	G
47	B	25	G
47	B	26	A
47	B	30	G
47	B	34	G
47	B	35	G
47	B	37	C
47	B	40	A
47	B	41	U
47	B	44	C
47	B	45	G
47	B	47	A
47	B	52	G
47	B	53	A
47	B	56	C
47	B	66	C
47	B	67	A
47	B	68	G
47	B	85	C
47	B	86	U
47	B	88	C
47	B	90	G
47	B	102	A
47	B	106	C
47	B	113	G
48	A	7	U
48	A	11	A
48	A	12	G
48	A	20	G
48	A	29	C
48	A	31	U
48	A	32	G
48	A	33	G
48	A	52	G
48	A	58	G
48	A	59	G
48	A	60	A
48	A	68	A
48	A	71	A
48	A	72	G
48	A	77	G

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Mol	Chain	Res	Type
48	A	80	G
48	A	81	A
48	A	88	A
48	A	89	A
48	A	90	C
48	A	93	A
48	A	94	G
48	A	98	U
48	A	99	G
48	A	115	A
48	A	117	U
48	A	122	A
48	A	125	C
48	A	128	G
48	A	136	U
48	A	143	G
48	A	161	U
48	A	164	A
48	A	173	U
48	A	175	G
48	A	180	A
48	A	186	G
48	A	195	A
48	A	198	A
48	A	203	A
48	A	205	U
48	A	212	A
48	A	214	G
48	A	215	A
48	A	220	A
48	A	221	A
48	A	227	A
48	A	229	U
48	A	230	G
48	A	231	U
48	A	237	C
48	A	245	G
48	A	248	G
48	A	250	G
48	A	264	G
48	A	265	A
48	A	272	A

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Mol	Chain	Res	Type
48	A	274	C
48	A	275	C
48	A	279	U
48	A	283	U
48	A	285	U
48	A	286	G
48	A	287	A
48	A	288	U
48	A	291	C
48	A	292	G
48	A	296	A
48	A	297	G
48	A	299	G
48	A	300	G
48	A	301	U
48	A	302	U
48	A	303	G
48	A	305	G
48	A	309	G
48	A	314	G
48	A	315	U
48	A	317	G
48	A	318	U
48	A	319	G
48	A	322	A
48	A	323	C
48	A	326	A
48	A	327	U
48	A	329	U
48	A	330	U
48	A	331	U
48	A	336	C
48	A	337	U
48	A	338	C
48	A	346	C
48	A	351	G
48	A	352	G
48	A	357	U
48	A	358	G
48	A	361	A
48	A	364	A
48	A	366	G

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Mol	Chain	Res	Type
48	A	370	U
48	A	384	G
48	A	393	U
48	A	404	A
48	A	412	A
48	A	416	C
48	A	417	C
48	A	424	G
48	A	425	U
48	A	427	A
48	A	434	G
48	A	438	U
48	A	445	U
48	A	446	G
48	A	449	G
48	A	450	G
48	A	452	G
48	A	453	U
48	A	454	U
48	A	459	A
48	A	460	G
48	A	468	G
48	A	471	C
48	A	472	C
48	A	474	G
48	A	489	A
48	A	491	U
48	A	493	U
48	A	498	G
48	A	505	C
48	A	509	U
48	A	512	G
48	A	530	G
48	A	543	U
48	A	544	U
48	A	547	U
48	A	555	G
48	A	561	G
48	A	562	G
48	A	566	A
48	A	567	A
48	A	568	A

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Mol	Chain	Res	Type
48	A	569	G
48	A	585	G
48	A	589	A
48	A	591	G
48	A	592	A
48	A	594	U
48	A	595	A
48	A	596	C
48	A	605	G
48	A	617	U
48	A	618	C
48	A	619	C
48	A	620	G
48	A	639	C
48	A	640	G
48	A	641	U
48	A	642	G
48	A	643	G
48	A	644	G
48	A	647	G
48	A	649	U
48	A	655	G
48	A	665	G
48	A	666	A
48	A	667	A
48	A	678	A
48	A	679	G
48	A	684	G
48	A	685	G
48	A	689	U
48	A	696	A
48	A	706	G
48	A	707	G
48	A	708	G
48	A	709	U
48	A	712	G
48	A	721	A
48	A	725	A
48	A	728	G
48	A	730	G
48	A	731	A
48	A	740	A

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Mol	Chain	Res	Type
48	A	747	A
48	A	753	A
48	A	757	G
48	A	758	A
48	A	760	U
48	A	763	G
48	A	765	G
48	A	766	G
48	A	768	G
48	A	769	U
48	A	770	A
48	A	774	G
48	A	784	G
48	A	785	A
48	A	794	G
48	A	801	U
48	A	830	A
48	A	832	G
48	A	838	G
48	A	845	C
48	A	862	U
48	A	863	G
48	A	868	C
48	A	871	A
48	A	872	G
48	A	878	G
48	A	879	A
48	A	880	G
48	A	890	G
48	A	891	G
48	A	897	A
48	A	899	G
48	A	904	A
48	A	908	A
48	A	915	U
48	A	917	A
48	A	919	A
48	A	920	G
48	A	921	C
48	A	927	C
48	A	942	U
48	A	944	A

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Mol	Chain	Res	Type
48	A	945	G
48	A	960	G
48	A	961	U
48	A	966	U
48	A	971	G
48	A	973	G
48	A	974	G
48	A	975	U
48	A	981	U
48	A	982	A
48	A	994	A
48	A	995	U
48	A	996	G
48	A	1001	C
48	A	1002	C
48	A	1003	A
48	A	1007	G
48	A	1009	U
48	A	1011	A
48	A	1012	C
48	A	1013	U
48	A	1014	G
48	A	1016	C
48	A	1022	C
48	A	1025	A
48	A	1029	C
48	A	1030	C
48	A	1042	A
48	A	1044	U
48	A	1046	C
48	A	1047	A
48	A	1048	A
48	A	1049	G
48	A	1058	A
48	A	1062	A
48	A	1063	G
48	A	1068	C
48	A	1070	G
48	A	1074	A
48	A	1076	A
48	A	1078	G
48	A	1085	G

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Mol	Chain	Res	Type
48	A	1091	A
48	A	1092	G
48	A	1098	A
48	A	1100	C
48	A	1101	A
48	A	1107	G
48	A	1114	G
48	A	1130	C
48	A	1131	G
48	A	1140	G
48	A	1141	U
48	A	1143	G
48	A	1144	A
48	A	1151	U
48	A	1163	A
48	A	1164	A
48	A	1169	A
48	A	1171	C
48	A	1173	G
48	A	1175	A
48	A	1178	U
48	A	1181	G
48	A	1184	U
48	A	1185	A
48	A	1186	G
48	A	1187	A
48	A	1188	A
48	A	1189	G
48	A	1190	C
48	A	1191	A
48	A	1192	G
48	A	1201	G
48	A	1202	A
48	A	1205	G
48	A	1206	A
48	A	1207	G
48	A	1209	G
48	A	1212	U
48	A	1213	A
48	A	1215	U
48	A	1216	A
48	A	1224	G

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Mol	Chain	Res	Type
48	A	1229	A
48	A	1230	G
48	A	1232	G
48	A	1233	A
48	A	1237	U
48	A	1238	G
48	A	1239	C
48	A	1240	G
48	A	1244	A
48	A	1246	A
48	A	1250	U
48	A	1251	A
48	A	1253	C
48	A	1260	C
48	A	1261	A
48	A	1270	G
48	A	1275	A
48	A	1292	U
48	A	1293	G
48	A	1303	U
48	A	1325	U
48	A	1332	G
48	A	1335	G
48	A	1343	G
48	A	1344	A
48	A	1345	G
48	A	1347	G
48	A	1353	G
48	A	1362	A
48	A	1363	G
48	A	1365	G
48	A	1368	A
48	A	1369	A
48	A	1371	G
48	A	1372	C
48	A	1386	G
48	A	1389	U
48	A	1404	C
48	A	1409	C
48	A	1415	A
48	A	1416	A
48	A	1417	A

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Mol	Chain	Res	Type
48	A	1440	C
48	A	1444	U
48	A	1448	C
48	A	1456	G
48	A	1462	G
48	A	1465	C
48	A	1467	U
48	A	1480	A
48	A	1493	A
48	A	1494	U
48	A	1499	A
48	A	1501	C
48	A	1507	G
48	A	1510	A
48	A	1521	C
48	A	1522	G
48	A	1529	U
48	A	1531	C
48	A	1532	G
48	A	1533	U
48	A	1534	C
48	A	1539	A
48	A	1540	U
48	A	1546	A
48	A	1549	G
48	A	1550	G
48	A	1551	U
48	A	1552	A
48	A	1553	C
48	A	1554	U
48	A	1555	A
48	A	1556	A
48	A	1561	C
48	A	1562	C
48	A	1563	A
48	A	1564	A
48	A	1565	A
48	A	1566	A
48	A	1567	C
48	A	1568	C
48	A	1569	A
48	A	1570	C

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Mol	Chain	Res	Type
48	A	1571	C
48	A	1572	G
48	A	1573	U
48	A	1574	G
48	A	1575	A
48	A	1576	C
48	A	1577	C
48	A	1578	G
48	A	1579	C
48	A	1580	A
48	A	1581	C
48	A	1582	C
48	A	1584	U
48	A	1585	U
48	A	1586	C
48	A	1587	G
48	A	1588	G
48	A	1589	G
48	A	1590	G
48	A	1591	U
48	A	1592	G
48	A	1593	U
48	A	1594	G
48	A	1595	G
48	A	1596	C
48	A	1597	G
48	A	1598	U
48	A	1599	U
48	A	1600	G
48	A	1601	G
48	A	1602	U
48	A	1604	G
48	A	1605	G
48	A	1606	G
48	A	1611	A
48	A	1625	G
48	A	1629	G
48	A	1630	U
48	A	1632	G
48	A	1633	U
48	A	1636	A
48	A	1637	G

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Mol	Chain	Res	Type
48	A	1638	C
48	A	1639	G
48	A	1640	A
48	A	1641	U
48	A	1642	G
48	A	1648	A
48	A	1649	C
48	A	1654	G
48	A	1658	G
48	A	1672	C
48	A	1674	G
48	A	1676	G
48	A	1678	U
48	A	1679	A
48	A	1680	A
48	A	1681	U
48	A	1688	G
48	A	1703	G
48	A	1710	A
48	A	1711	G
48	A	1713	U
48	A	1715	A
48	A	1717	U
48	A	1721	U
48	A	1724	G
48	A	1727	A
48	A	1728	U
48	A	1731	A
48	A	1737	A
48	A	1744	A
48	A	1748	A
48	A	1753	C
48	A	1754	G
48	A	1767	U
48	A	1768	C
48	A	1769	G
48	A	1774	U
48	A	1778	A
48	A	1780	G
48	A	1786	G
48	A	1787	A
48	A	1789	A

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Mol	Chain	Res	Type
48	A	1792	A
48	A	1798	U
48	A	1803	A
48	A	1813	C
48	A	1826	A
48	A	1836	A
48	A	1837	G
48	A	1845	G
48	A	1852	A
48	A	1863	G
48	A	1864	U
48	A	1866	C
48	A	1869	G
48	A	1870	U
48	A	1871	G
48	A	1872	A
48	A	1878	G
48	A	1887	A
48	A	1892	G
48	A	1893	C
48	A	1903	C
48	A	1906	U
48	A	1916	A
48	A	1917	G
48	A	1933	G
48	A	1958	C
48	A	1967	G
48	A	1973	C
48	A	1974	A
48	A	1975	A
48	A	1981	U
48	A	1990	A
48	A	1998	C
48	A	1999	U
48	A	2017	C
48	A	2018	G
48	A	2026	A
48	A	2028	G
48	A	2033	U
48	A	2046	A
48	A	2052	G
48	A	2062	G

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Mol	Chain	Res	Type
48	A	2064	A
48	A	2074	G
48	A	2075	G
48	A	2083	A
48	A	2085	C
48	A	2086	U
48	A	2088	C
48	A	2089	C
48	A	2090	U
48	A	2091	U
48	A	2092	U
48	A	2093	G
48	A	2094	G
48	A	2095	G
48	A	2096	G
48	A	2106	A
48	A	2107	G
48	A	2111	U
48	A	2112	U
48	A	2118	C
48	A	2120	A
48	A	2130	G
48	A	2131	G
48	A	2137	A
48	A	2138	C
48	A	2139	U
48	A	2140	A
48	A	2142	A
48	A	2151	A
48	A	2153	G
48	A	2154	G
48	A	2160	A
48	A	2161	A
48	A	2163	U
48	A	2167	U
48	A	2179	U
48	A	2190	A
48	A	2191	C
48	A	2194	A
48	A	2195	U
48	A	2196	G
48	A	2206	C

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Mol	Chain	Res	Type
48	A	2215	U
48	A	2217	U
48	A	2221	A
48	A	2244	A
48	A	2247	A
48	A	2251	G
48	A	2255	A
48	A	2256	G
48	A	2257	A
48	A	2263	G
48	A	2267	C
48	A	2276	G
48	A	2279	C
48	A	2280	G
48	A	2284	A
48	A	2285	G
48	A	2286	A
48	A	2299	C
48	A	2315	U
48	A	2316	G
48	A	2317	G
48	A	2319	G
48	A	2320	C
48	A	2322	C
48	A	2323	G
48	A	2325	U
48	A	2328	G
48	A	2334	U
48	A	2335	G
48	A	2337	A
48	A	2338	G
48	A	2339	G
48	A	2340	A
48	A	2341	U
48	A	2342	A
48	A	2343	G
48	A	2346	G
48	A	2348	G
48	A	2349	A
48	A	2351	A
48	A	2353	U
48	A	2354	G

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Mol	Chain	Res	Type
48	A	2355	U
48	A	2356	G
48	A	2357	A
48	A	2362	C
48	A	2368	C
48	A	2371	G
48	A	2380	G
48	A	2382	G
48	A	2383	U
48	A	2384	C
48	A	2385	G
48	A	2386	U
48	A	2387	U
48	A	2388	G
48	A	2390	U
48	A	2392	A
48	A	2393	A
48	A	2394	A
48	A	2395	U
48	A	2396	A
48	A	2404	G
48	A	2407	C
48	A	2408	G
48	A	2409	U
48	A	2410	A
48	A	2411	U
48	A	2413	G
48	A	2414	G
48	A	2418	U
48	A	2421	A
48	A	2427	G
48	A	2433	U
48	A	2434	A
48	A	2436	A
48	A	2446	G
48	A	2449	A
48	A	2462	G
48	A	2463	G
48	A	2467	U
48	A	2473	U
48	A	2476	G
48	A	2490	A

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Mol	Chain	Res	Type
48	A	2502	A
48	A	2506	G
48	A	2507	C
48	A	2510	A
48	A	2511	A
48	A	2512	A
48	A	2529	A
48	A	2531	G
48	A	2532	G
48	A	2545	G
48	A	2546	A
48	A	2549	G
48	A	2551	A
48	A	2558	C
48	A	2559	A
48	A	2567	U
48	A	2571	C
48	A	2574	C
48	A	2578	A
48	A	2582	A
48	A	2585	U
48	A	2586	G
48	A	2596	G
48	A	2601	A
48	A	2607	G
48	A	2608	G
48	A	2609	A
48	A	2612	A
48	A	2614	U
48	A	2615	G
48	A	2616	A
48	A	2626	U
48	A	2627	C
48	A	2630	A
48	A	2631	G
48	A	2640	G
48	A	2643	U
48	A	2647	U
48	A	2648	C
48	A	2649	A
48	A	2650	A
48	A	2651	C

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Mol	Chain	Res	Type
48	A	2653	G
48	A	2654	A
48	A	2655	U
48	A	2659	A
48	A	2665	C
48	A	2669	G
48	A	2671	G
48	A	2672	A
48	A	2673	U
48	A	2676	C
48	A	2677	A
48	A	2682	G
48	A	2694	G
48	A	2698	C
48	A	2700	A
48	A	2702	A
48	A	2705	G
48	A	2715	U
48	A	2718	G
48	A	2726	G
48	A	2729	G
48	A	2737	G
48	A	2742	A
48	A	2744	C
48	A	2753	G
48	A	2758	A
48	A	2759	G
48	A	2786	U
48	A	2788	A
48	A	2790	A
48	A	2791	G
48	A	2793	G
48	A	2796	A
48	A	2797	C
48	A	2798	G
48	A	2802	G
48	A	2810	U
48	A	2826	A
48	A	2827	G
48	A	2833	U
48	A	2837	U
48	A	2839	U

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Mol	Chain	Res	Type
48	A	2853	C
48	A	2860	U
48	A	2865	G
48	A	2866	A
48	A	2870	C
48	A	2876	C
48	A	2878	A
48	A	2887	G
48	A	2893	G
48	A	2897	G
48	A	2906	U
48	A	2908	U
48	A	2913	U
48	A	2915	C
48	A	2926	A
48	A	2936	C
48	A	2938	G
48	A	2942	G
48	A	2950	C
48	A	2956	G
48	A	2957	A
48	A	2963	U
48	A	2968	G
48	A	2972	A
48	A	2975	G
48	A	2976	C
48	A	2977	A
48	A	2982	A
48	A	2985	G
48	A	2989	A
48	A	2990	A
48	A	2993	U
48	A	3002	A
48	A	3004	C
48	A	3005	A
48	A	3009	U
48	A	3011	C
48	A	3014	A
48	A	3015	C
48	A	3021	A
48	A	3022	G
48	A	3023	G

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Mol	Chain	Res	Type
48	A	3029	U
48	A	3039	C
48	A	3042	A
48	A	3045	C
48	A	3047	A
48	A	3056	A
48	A	3057	U
48	A	3070	G
48	A	3082	U
48	A	3088	C
48	A	3093	A
48	A	3094	A
48	A	3095	C
48	A	3101	C
48	A	3105	C
48	A	3106	C
48	A	3107	G
48	A	3112	A
48	A	3113	A
48	A	3114	A
48	A	3115	A

All (46) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
47	B	66	C
48	A	84	U
48	A	89	A
48	A	97	U
48	A	316	U
48	A	336	C
48	A	357	U
48	A	445	U
48	A	456	C
48	A	567	A
48	A	974	G
48	A	980	C
48	A	981	U
48	A	1002	C
48	A	1010	U
48	A	1084	U
48	A	1117	U

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Mol	Chain	Res	Type
48	A	1186	G
48	A	1564	A
48	A	1565	A
48	A	1566	A
48	A	1567	C
48	A	1571	C
48	A	1572	G
48	A	1573	U
48	A	1574	G
48	A	1575	A
48	A	1576	C
48	A	1577	C
48	A	1578	G
48	A	1579	C
48	A	1580	A
48	A	1581	C
48	A	1590	G
48	A	1591	U
48	A	1592	G
48	A	1596	C
48	A	1597	G
48	A	1598	U
48	A	1599	U
48	A	1730	U
48	A	2085	C
48	A	2088	C
48	A	2094	G
48	A	2350	G
48	A	2381	A

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

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

5.5 Carbohydrates [i](#)

There are no 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](#)

There are no chain breaks in this entry.

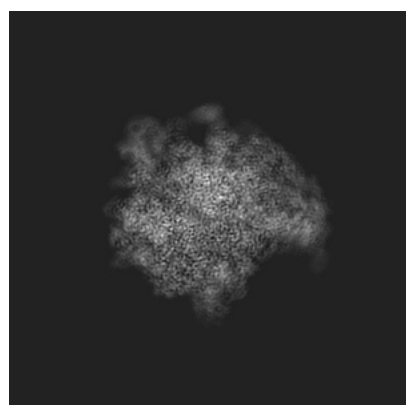
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6920. These allow visual inspection of the internal detail of the map and identification of artifacts.

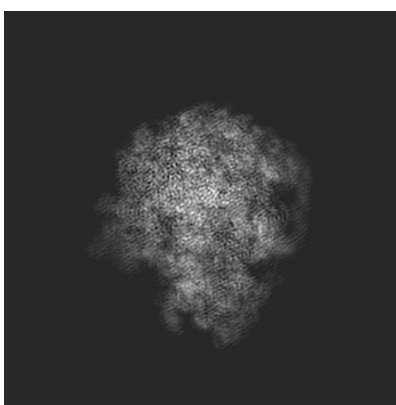
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

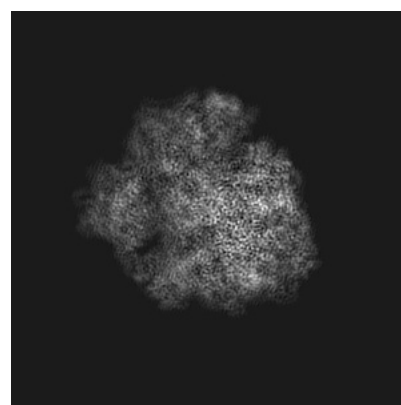
6.1.1 Primary map



X



Y

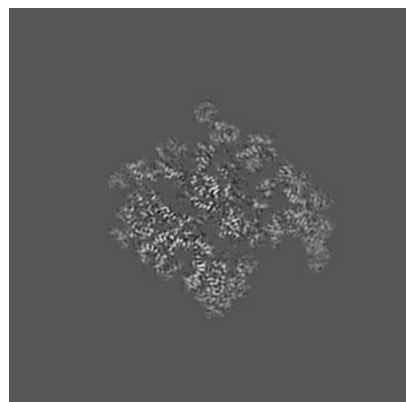


Z

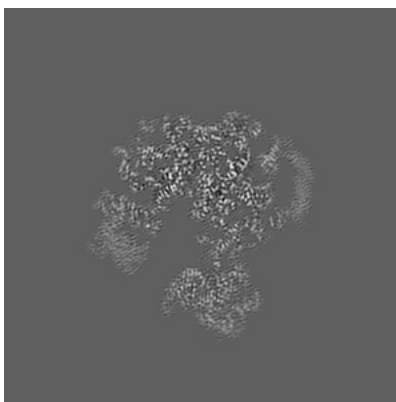
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

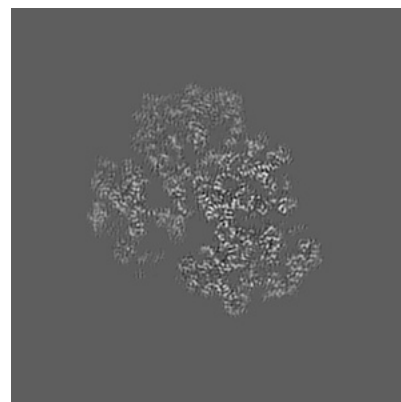
6.2.1 Primary map



X Index: 200



Y Index: 200

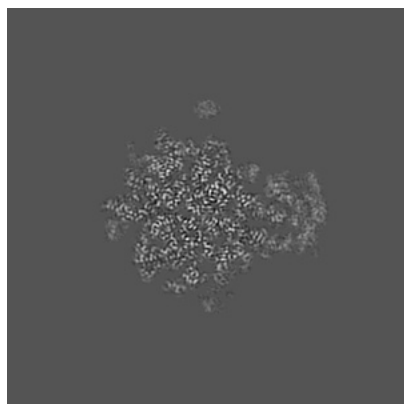


Z Index: 200

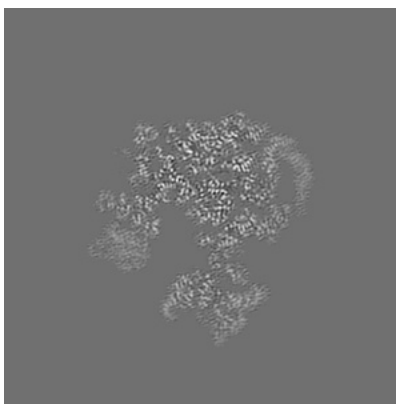
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

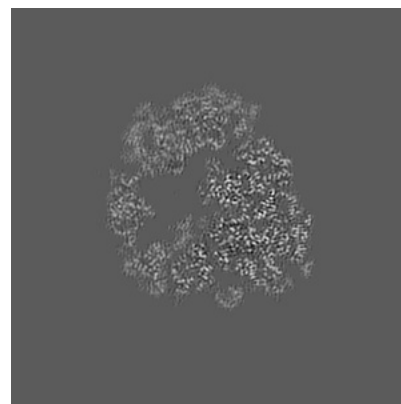
6.3.1 Primary map



X Index: 215



Y Index: 206

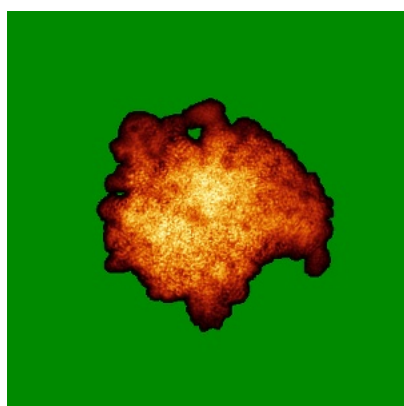


Z Index: 183

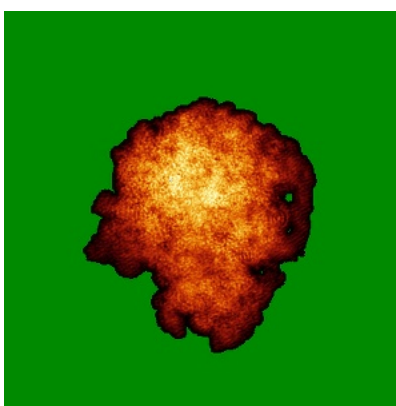
The images above show the largest variance slices of the map in three orthogonal directions.

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

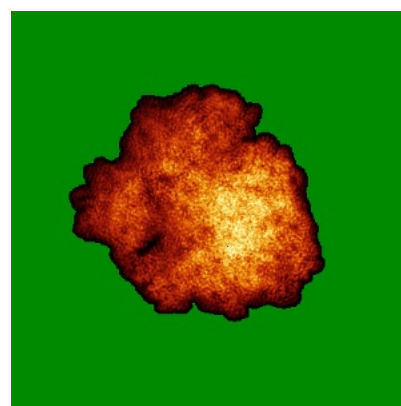
6.4.1 Primary map



X



Y

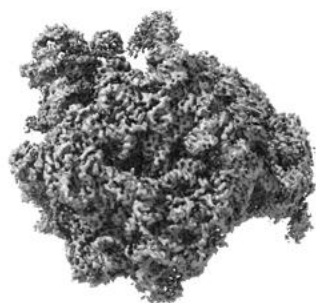


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

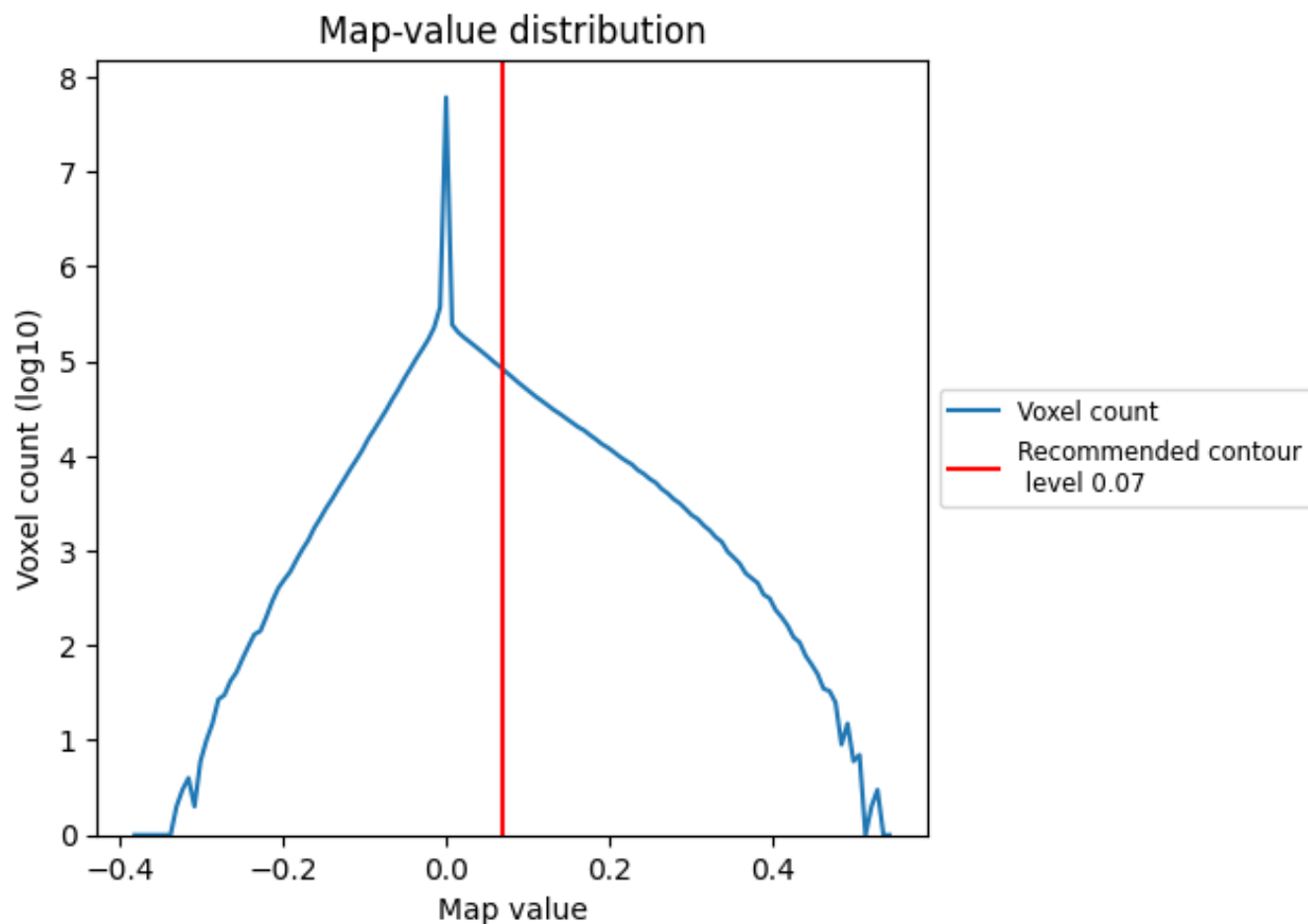
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

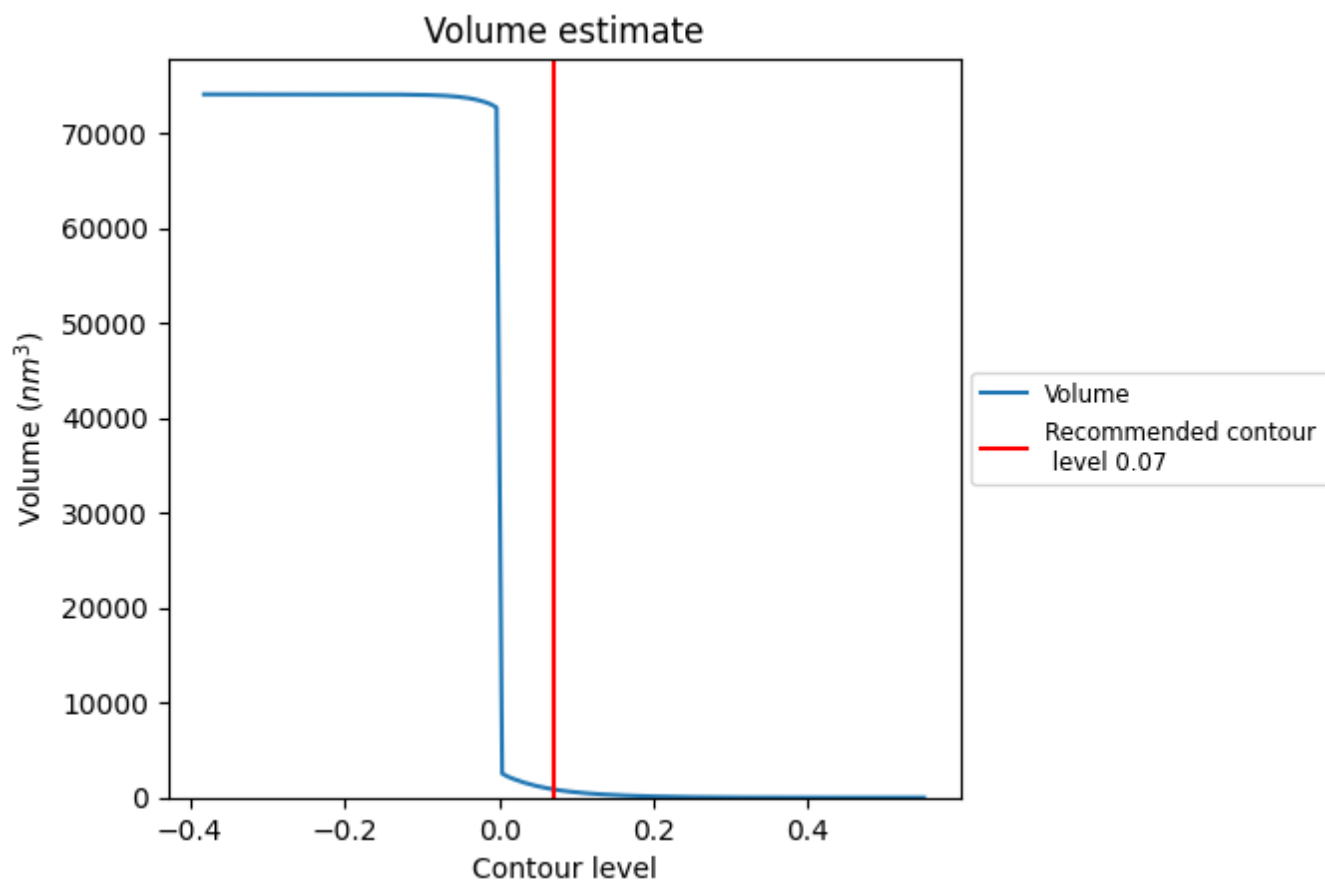
This section contains the results of statistical analysis of the map.

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.

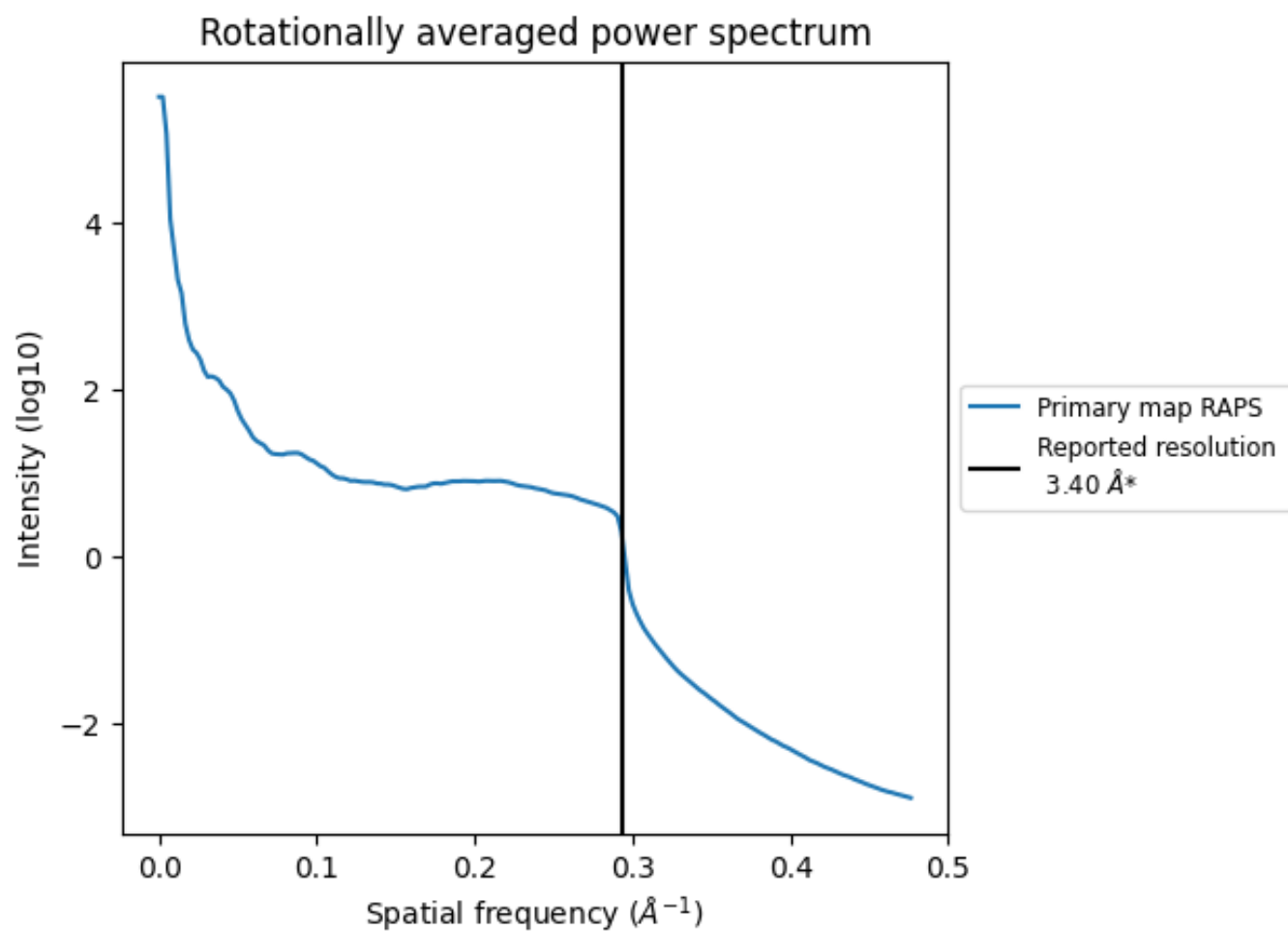
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 871 nm^3 ; this corresponds to an approximate mass of 787 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 0.294 Å⁻¹

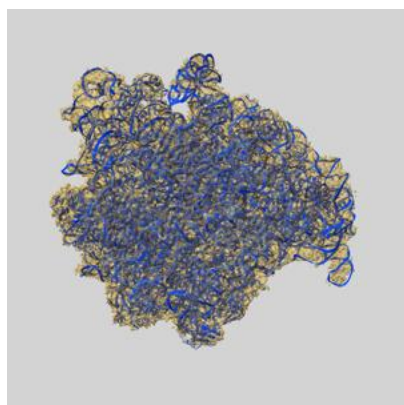
8 Fourier-Shell correlation

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

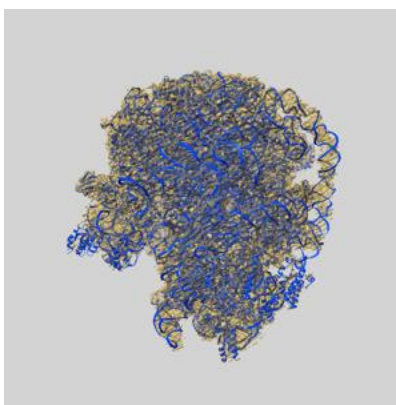
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6920 and PDB model 5ZEB. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

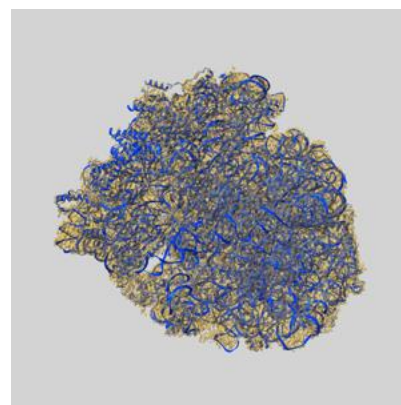
9.1 Map-model overlay [i](#)



X



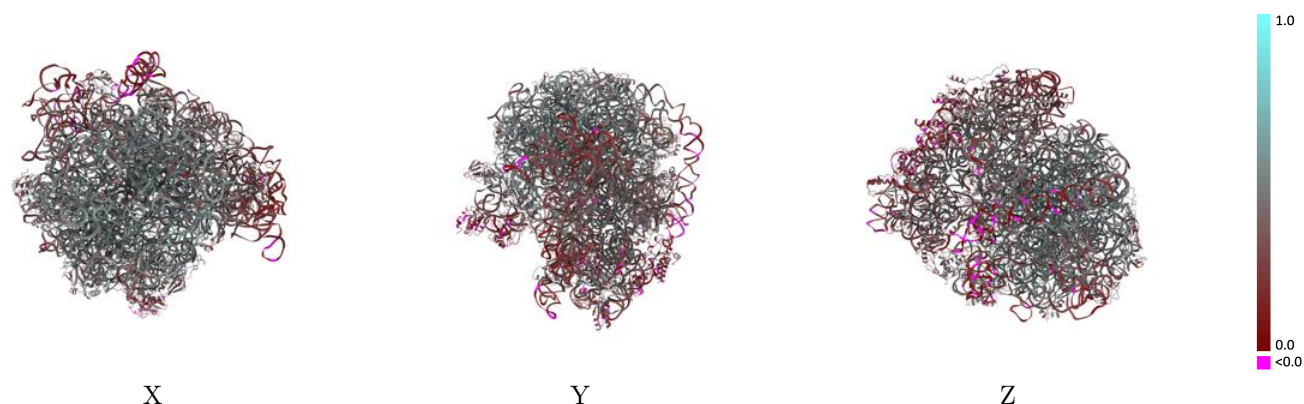
Y



Z

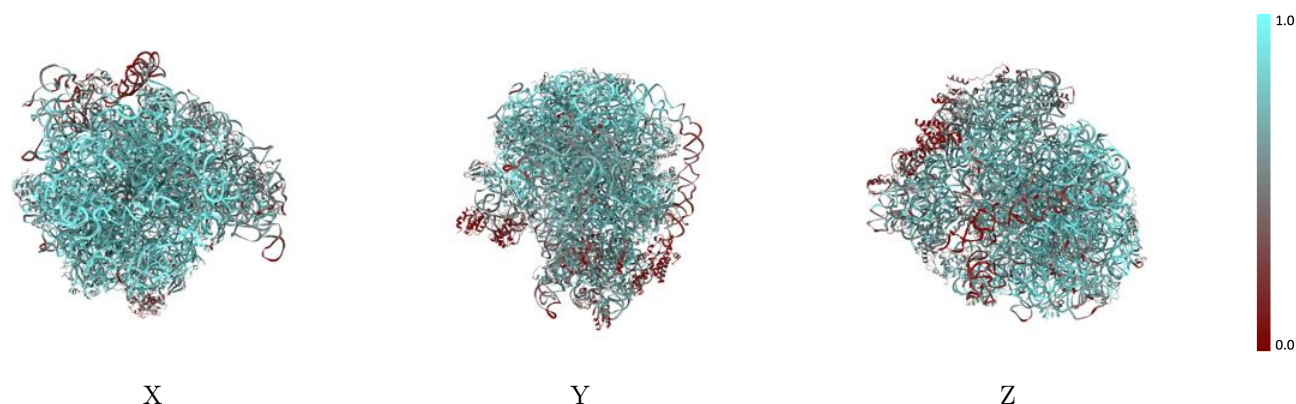
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



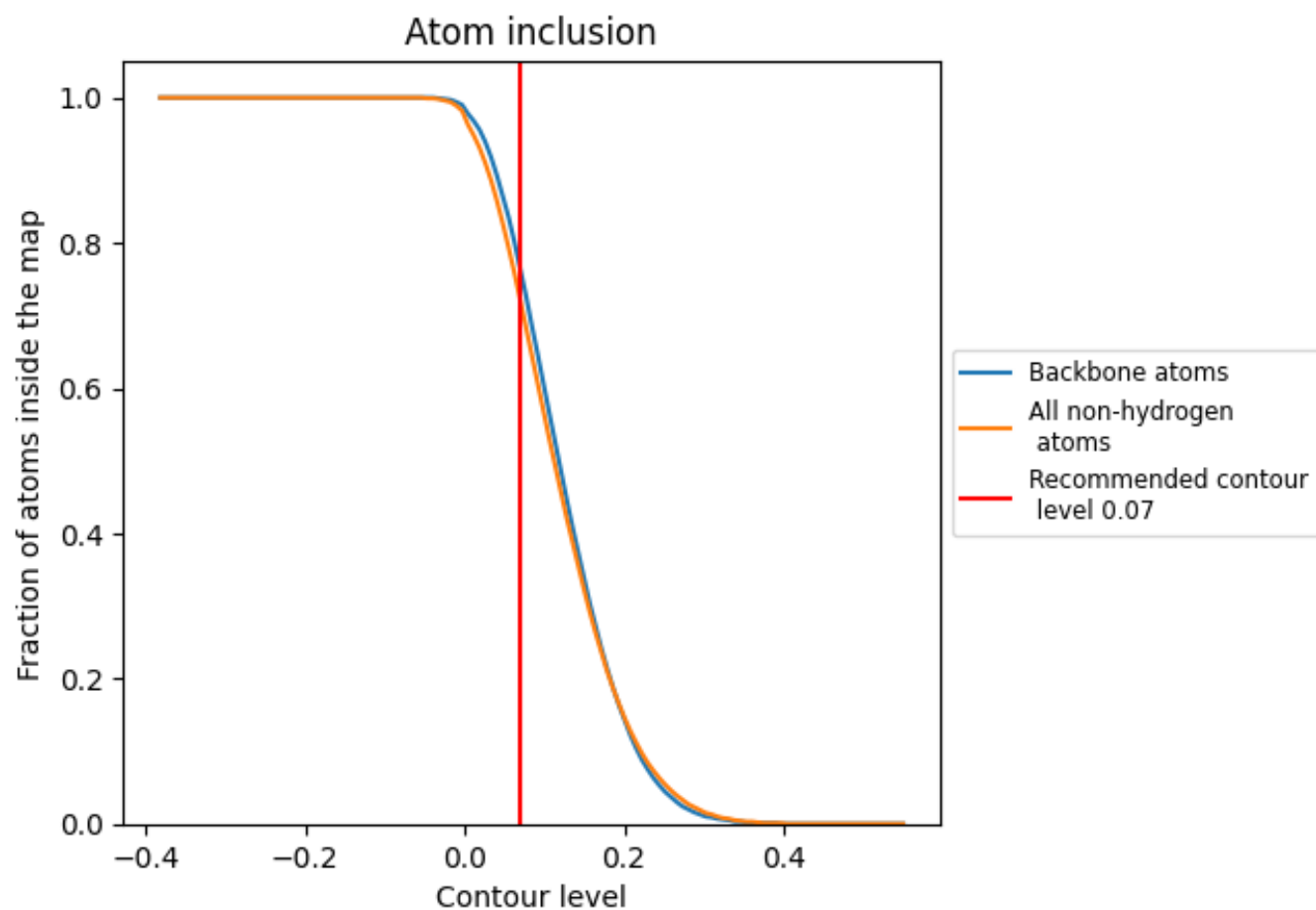
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.07).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 72% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7200	 0.4150
1	 0.7090	 0.4820
2	 0.4670	 0.2940
3	 0.7310	 0.4870
4	 0.6900	 0.4390
5	 0.7760	 0.5240
6	 0.8040	 0.5320
7	 0.7830	 0.5100
8	 0.6980	 0.5040
A	 0.8090	 0.4590
B	 0.7450	 0.4000
C	 0.7680	 0.5110
D	 0.7600	 0.4990
E	 0.7170	 0.4590
F	 0.6500	 0.4210
G	 0.5800	 0.3830
H	 0.4160	 0.3470
I	 0.0730	 0.1380
J	 0.0980	 0.1370
K	 0.7540	 0.5000
L	 0.7230	 0.4840
M	 0.7100	 0.4630
N	 0.7410	 0.5010
O	 0.7650	 0.4870
P	 0.7100	 0.4510
Q	 0.6760	 0.4500
R	 0.7850	 0.5020
S	 0.7180	 0.4950
T	 0.7510	 0.5120
U	 0.7050	 0.4680
V	 0.6250	 0.4400
W	 0.5320	 0.3570
X	 0.7410	 0.4930
Y	 0.7060	 0.4800
Z	 0.6660	 0.4120



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Chain	Atom inclusion	Q-score
a	 0.7230	 0.3610
b	 0.1100	 0.1740
c	 0.5060	 0.3440
d	 0.3890	 0.2660
e	 0.5280	 0.3480
f	 0.5590	 0.3710
g	 0.5470	 0.3400
h	 0.6780	 0.4170
i	 0.6000	 0.3650
j	 0.4710	 0.3300
k	 0.5980	 0.3630
l	 0.5360	 0.3630
m	 0.5720	 0.3610
n	 0.6950	 0.4410
o	 0.6840	 0.4230
p	 0.4700	 0.3130
q	 0.5280	 0.3410
r	 0.5910	 0.3640
s	 0.5470	 0.3320
t	 0.5450	 0.3150
u	 0.4240	 0.3470
v	 0.5860	 0.3080