



Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 04:48 pm GMT

PDB ID : 5LI0
EMDB ID : EMD-4050
Title : 70S ribosome from Staphylococcus aureus
Authors : Khusainov, I.; Vicens, Q.; Bochler, A.; Grosse, F.; Myasnikov, A.; Menetret, J.F.; Chicher, J.; Marzi, S.; Romby, P.; Yusupova, G.; Yusupov, M.; Hashem, Y.
Deposited on : 2016-07-13
Resolution : 3.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

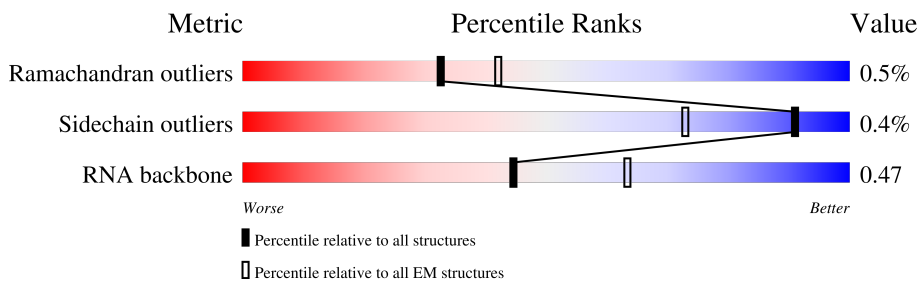
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	1547	
2	b	255	
3	c	217	
4	d	199	
5	e	165	
6	f	96	
7	g	150	
8	h	131	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	i	128	78% 99%
10	j	102	72% 100%
11	k	118	53% 100%
12	l	135	47% 100%
13	m	119	82% 96%
14	n	60	55% 97%
15	o	88	30% 100%
16	p	90	40% 100%
17	q	86	44% 95%
18	r	71	51% 100%
19	s	84	82% 96%
20	t	80	39% 100%
21	A	2918	9% 70% 27%
22	B	114	6% 82% 18%
23	D	275	20% 99%
24	E	218	18% 97%
25	F	199	21% 97%
26	G	166	64% 96%
27	H	164	51% 100%
28	M	145	19% 99%
29	N	122	24% 97%
30	O	131	31% 96%
31	P	141	29% 99%
32	Q	119	18% 100%
33	R	119	44% 98%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	S	110	33% 99%
35	T	116	15% 98%
36	U	102	26% 98%
37	V	112	20% 100%
38	W	89	39% 97%
39	X	100	33% 87% 13%
40	Y	94	61% 97%
41	Z	82	22% 95% 5%
42	0	46	22% 100%
43	1	65	34% 100%
44	2	57	16% 100%
45	3	84	79% 80% 19%
46	4	56	30% 96%
47	5	39	21% 62% 10% 28%
48	6	44	9% 93% 5%
49	7	60	20% 97%
50	8	37	24% 97%

2 Entry composition [i](#)

There are 54 unique types of molecules in this entry. The entry contains 140825 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 ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	a	1547	33126	14790	6036	10753	1547	0	0

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	b	224	1802	1147	315	333	7	0	0

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	c	208	1638	1032	306	298	2	0	0

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	d	197	1600	1009	300	289	2	0	0

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	e	165	1239	775	229	233	2	0	0

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	f	96	799	503	139	154	3	0	0

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	g	147	1189	744	227	214	4	0	0

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	h	131	1032	652	183	193	4	0	0

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	i	128	1017	629	203	184	1	0	0

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	j	102	813	512	148	150	3	0	0

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	k	118	881	543	169	166	3	0	0

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	l	135	1063	658	218	185	2	0	0

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	m	119	946	581	188	176	1	0	0

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	n	60	Total	C	N	O	S	0	0
			502	317	100	80	5		

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	o	88	Total	C	N	O	S	0	0
			738	454	153	130	1		

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	p	90	Total	C	N	O	S	0	0
			712	448	132	131	1		

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	86	Total	C	N	O	S	0	0
			707	447	126	133	1		

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	r	71	Total	C	N	O	S	0	0
			590	372	115	100	3		

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	s	84	Total	C	N	O	S	0	0
			678	434	120	122	2		

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	t	80	Total	C	N	O	S	0	0
			607	367	119	119	2		

- Molecule 21 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
21	A	2914	62475	27892	11424	20245	2914	0	0

- Molecule 22 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
22	B	114	2427	1086	436	792	113	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	D	275	2104	1309	417	373	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	E	218	1649	1030	304	310	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	F	199	1525	955	281	287	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	G	166	1312	832	223	251	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	H	164	1285	799	232	251	3	0	0

- Molecule 28 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	M	145	1151	717	211	220	3	0	0

- Molecule 29 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	N	122	920	572	174	170	4	0	0

- Molecule 30 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	O	131	998	618	197	182	1	0	0

- Molecule 31 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	P	141	1122	717	211	190	4	0	0

- Molecule 32 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	Q	119	940	575	181	183	1	0	0

- Molecule 33 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	R	119	922	574	174	173	1	0	0

- Molecule 34 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	S	110	886	557	177	151	1	0	0

- Molecule 35 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	T	116	Total	C	N	O	S	0	0
			944	593	189	158	4		

- Molecule 36 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	U	102	Total	C	N	O	S	0	0
			799	506	142	150	1		

- Molecule 37 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	V	112	Total	C	N	O	S	0	0
			863	537	164	159	3		

- Molecule 38 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	W	89	Total	C	N	O	S	0	0
			726	457	130	135	4		

- Molecule 39 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	X	87	Total	C	N	O	S	0	0
			669	423	122	123	1		

- Molecule 40 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Y	94	Total	C	N	O	S	0	0
			738	471	131	134	2		

- Molecule 41 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	Z	82	Total	C	N	O	0	0
			627	386	122	119		

- Molecule 42 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
42	0	46	374	231	83	60	0	0

- Molecule 43 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
43	1	65	537	330	101	106	0	0

- Molecule 44 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
44	2	57	442	274	83	85	0	0

- Molecule 45 is a protein called 50S ribosomal protein L31 type B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	3	83	677	430	116	128	3	0	0

- Molecule 46 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	4	56	444	268	92	79	5	0	0

- Molecule 47 is a protein called 50S ribosomal protein L33 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	5	28	229	137	45	43	4	0	0

- Molecule 48 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	6	44	373	228	90	54	1	0	0

- Molecule 49 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	7	60	Total	C	N	O	S	0	0
			488	300	108	78	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	8	37	Total	C	N	O	S	0	0
			297	186	60	46	5		

- Molecule 51 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
51	a	2	Total	Mg	0
			2	2	
51	A	29	Total	Mg	0
			29	29	

- Molecule 52 is OXYGEN ATOM (three-letter code: O) (formula: O).

Mol	Chain	Residues	Atoms		AltConf
52	A	9	Total	O	0
			9	9	

- Molecule 53 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
53	8	1	Total	Zn	0
			1	1	

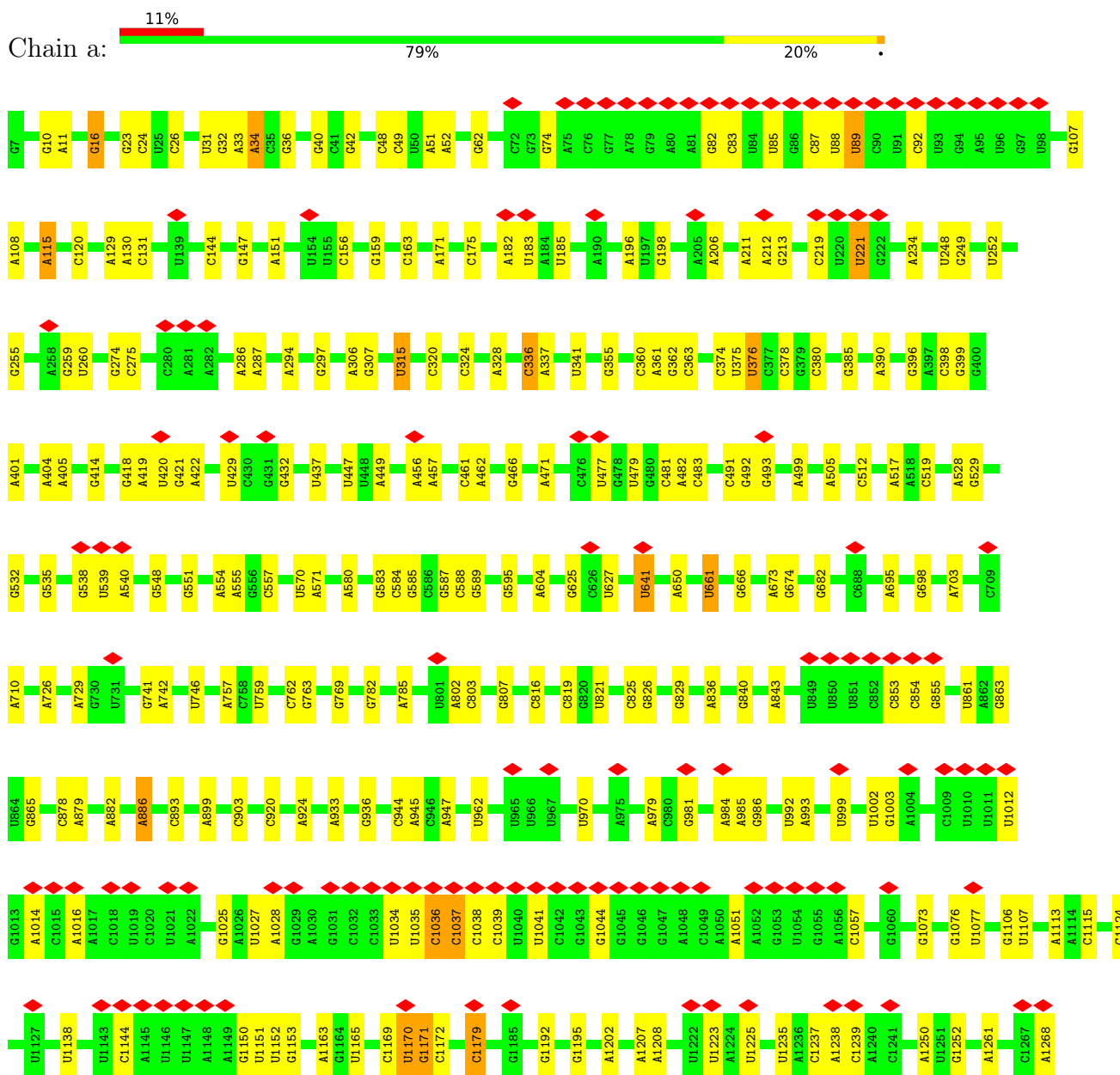
- Molecule 54 is water.

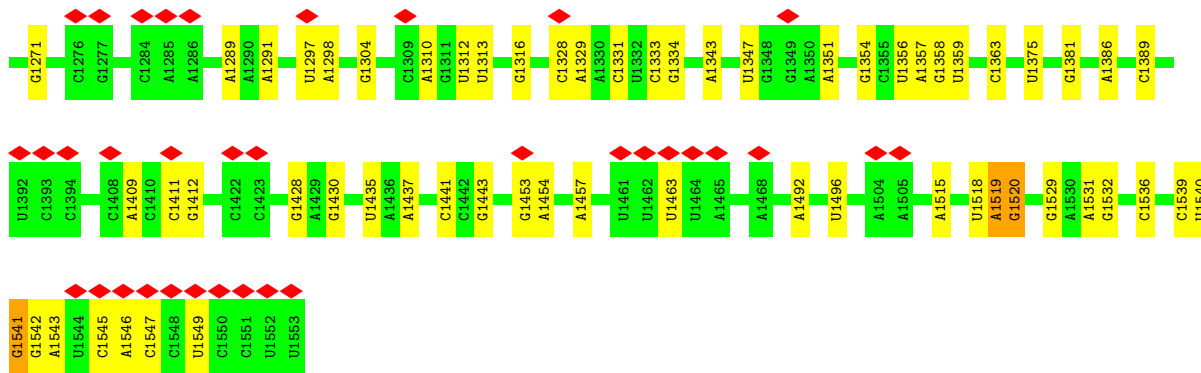
Mol	Chain	Residues	Atoms		AltConf
54	a	12	Total	O	0
			12	12	
54	A	143	Total	O	0
			143	143	
54	D	4	Total	O	0
			4	4	
54	T	2	Total	O	0
			2	2	
54	U	1	Total	O	0
			1	1	

3 Residue-property plots

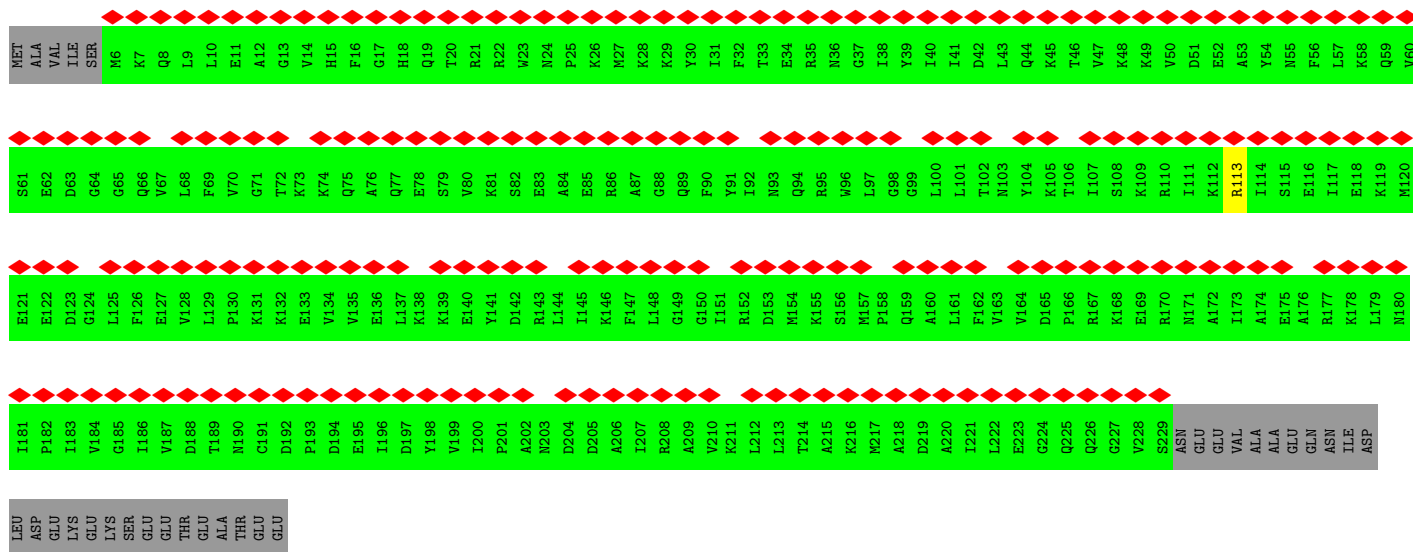
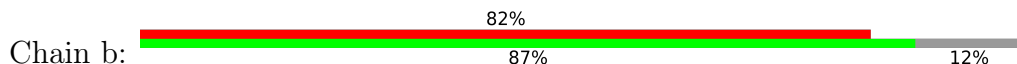
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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





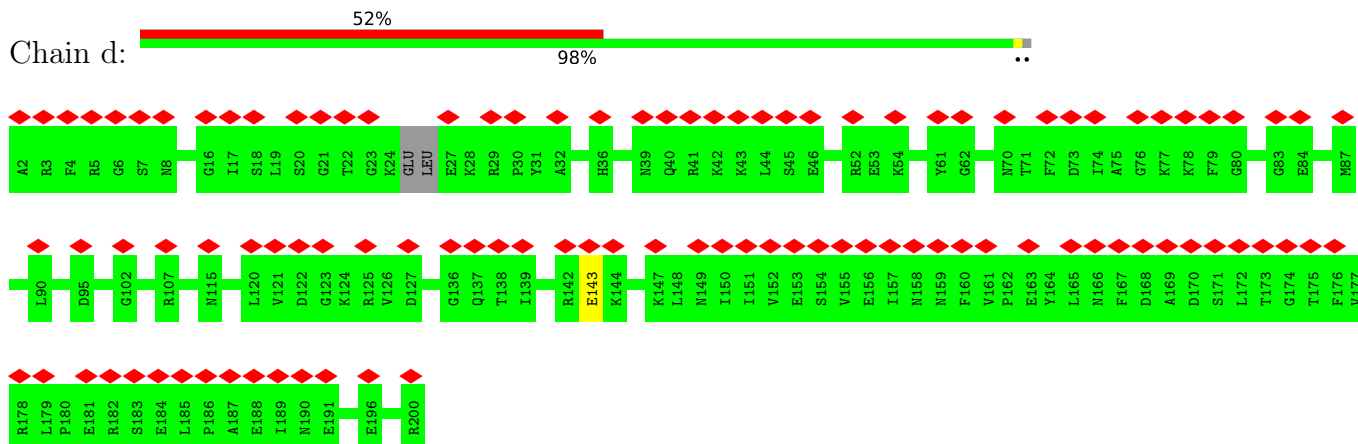
• Molecule 2: 30S ribosomal protein S2



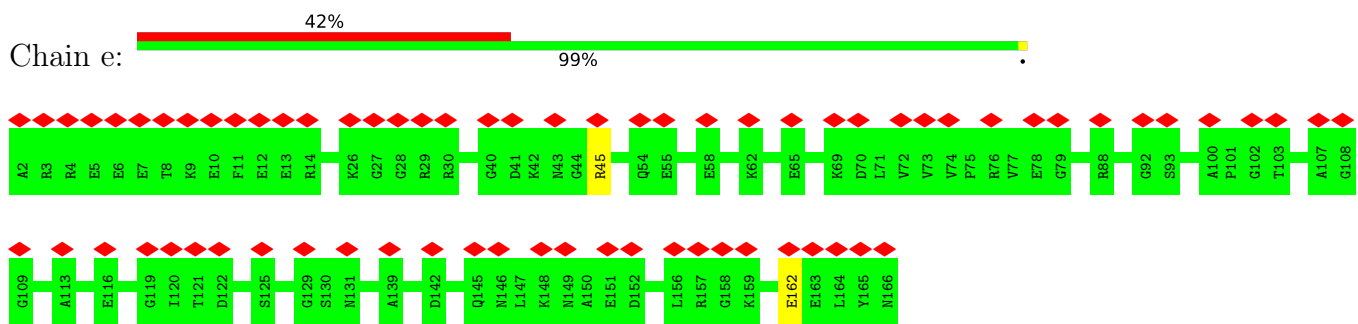
• Molecule 3: 30S ribosomal protein S3



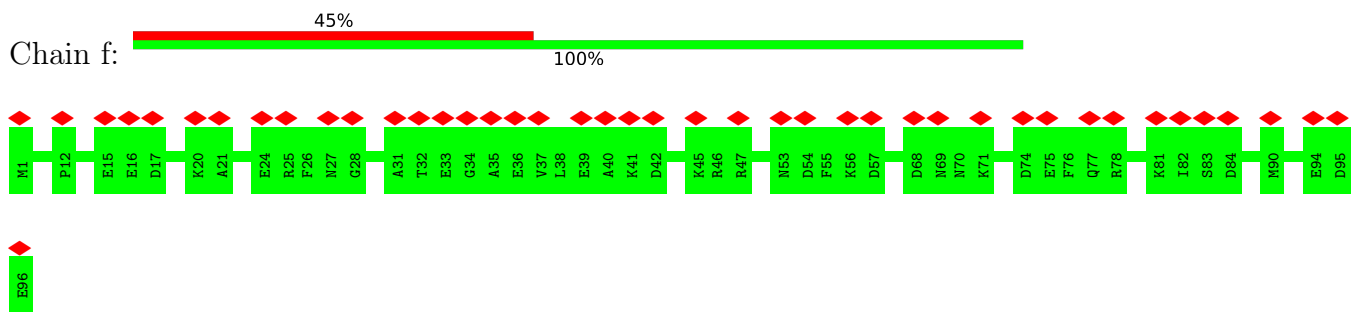
- Molecule 4: 30S ribosomal protein S4



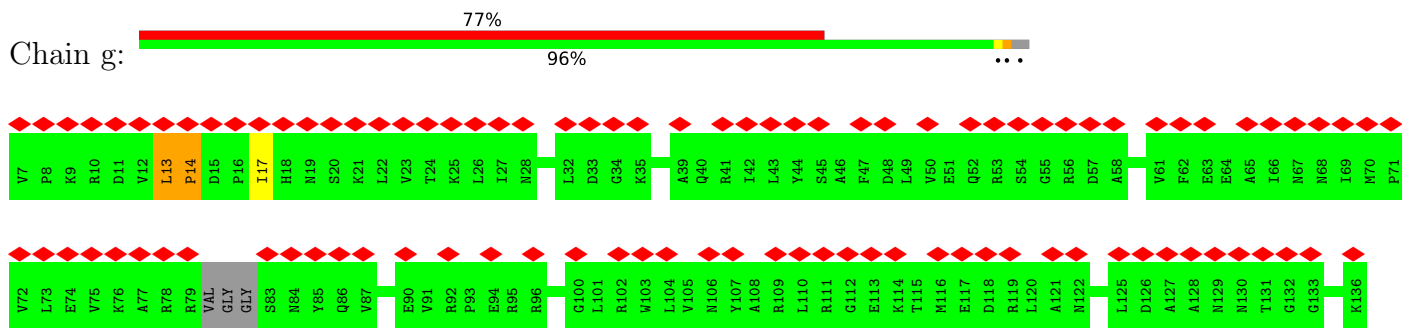
- Molecule 5: 30S ribosomal protein S5

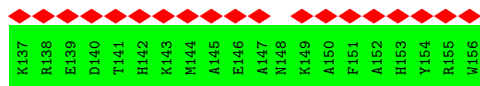


- Molecule 6: 30S ribosomal protein S6

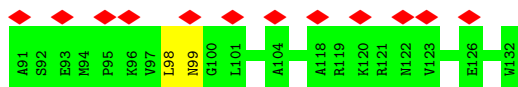
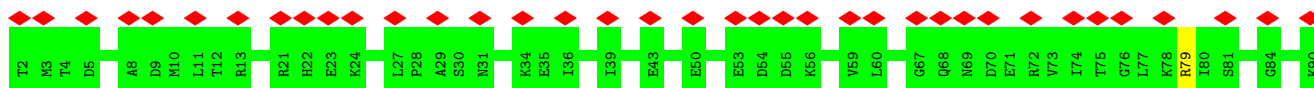


- Molecule 7: 30S ribosomal protein S7

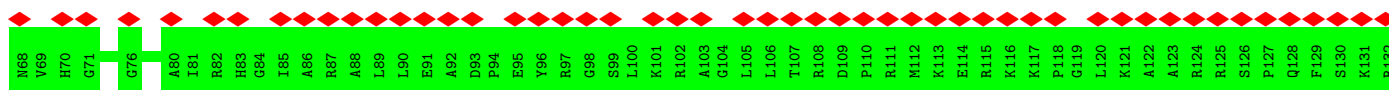
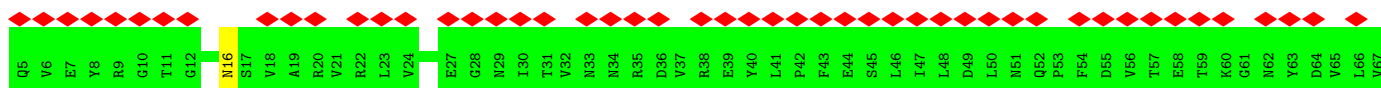
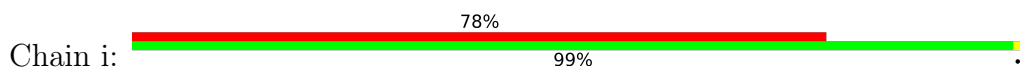




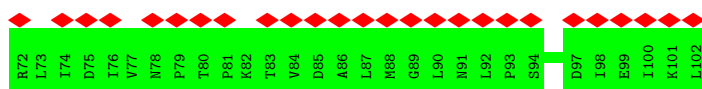
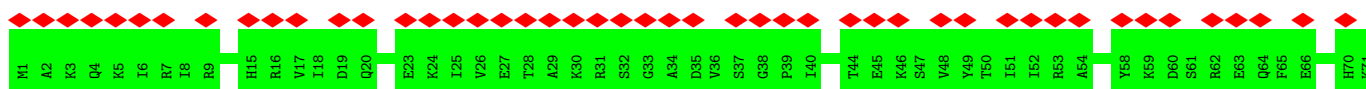
- Molecule 8: 30S ribosomal protein S8



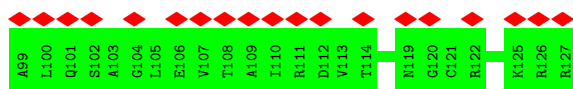
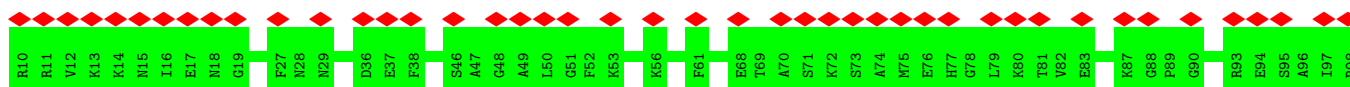
- Molecule 9: 30S ribosomal protein S9



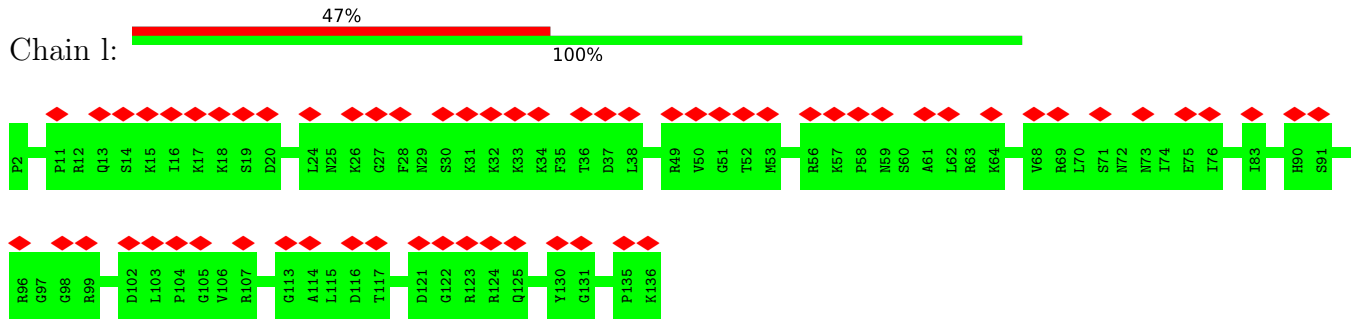
- Molecule 10: 30S ribosomal protein S10



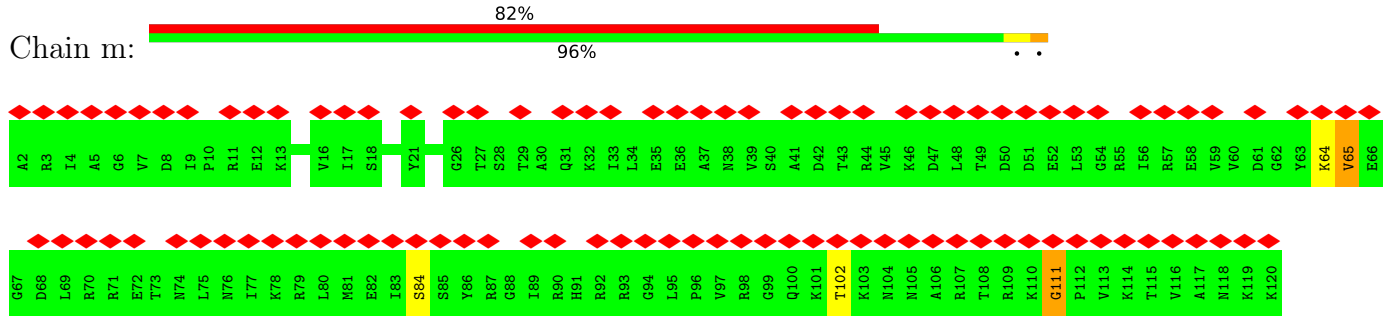
- Molecule 11: 30S ribosomal protein S11



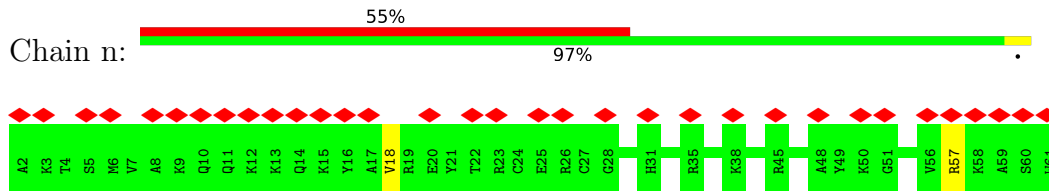
- Molecule 12: 30S ribosomal protein S12



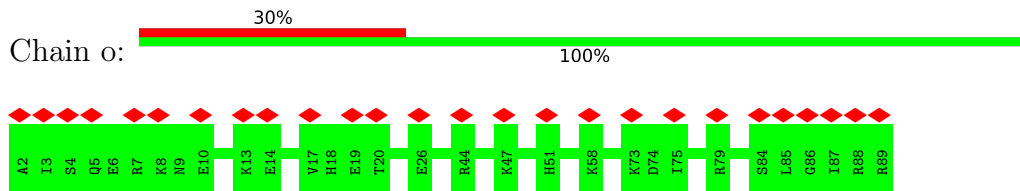
• Molecule 13: 30S ribosomal protein S13



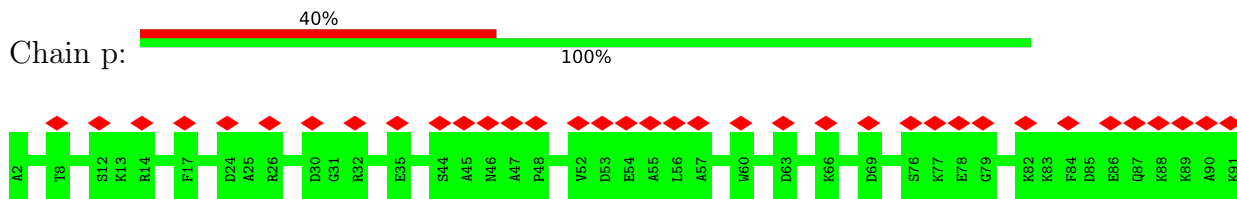
• Molecule 14: 30S ribosomal protein S14 type Z



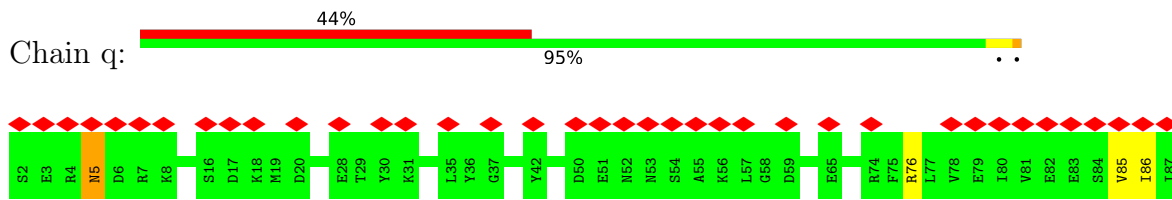
• Molecule 15: 30S ribosomal protein S15



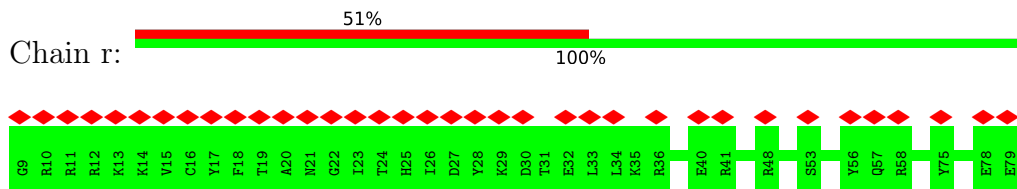
• Molecule 16: 30S ribosomal protein S16



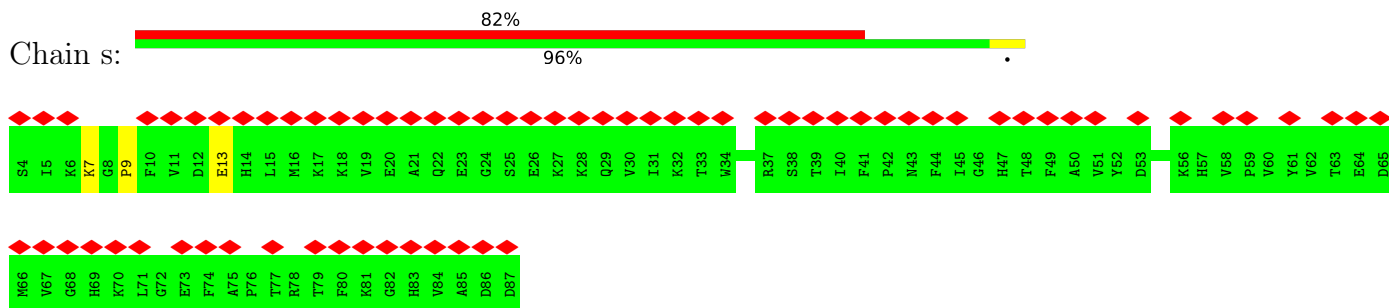
• Molecule 17: 30S ribosomal protein S17



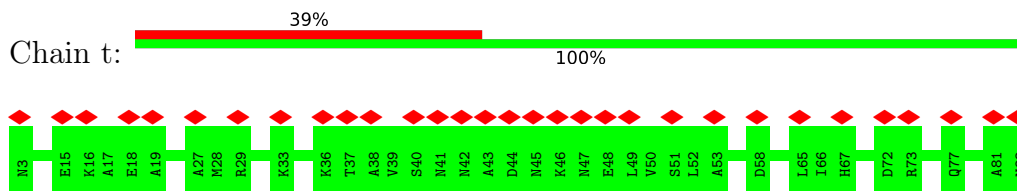
• Molecule 18: 30S ribosomal protein S18



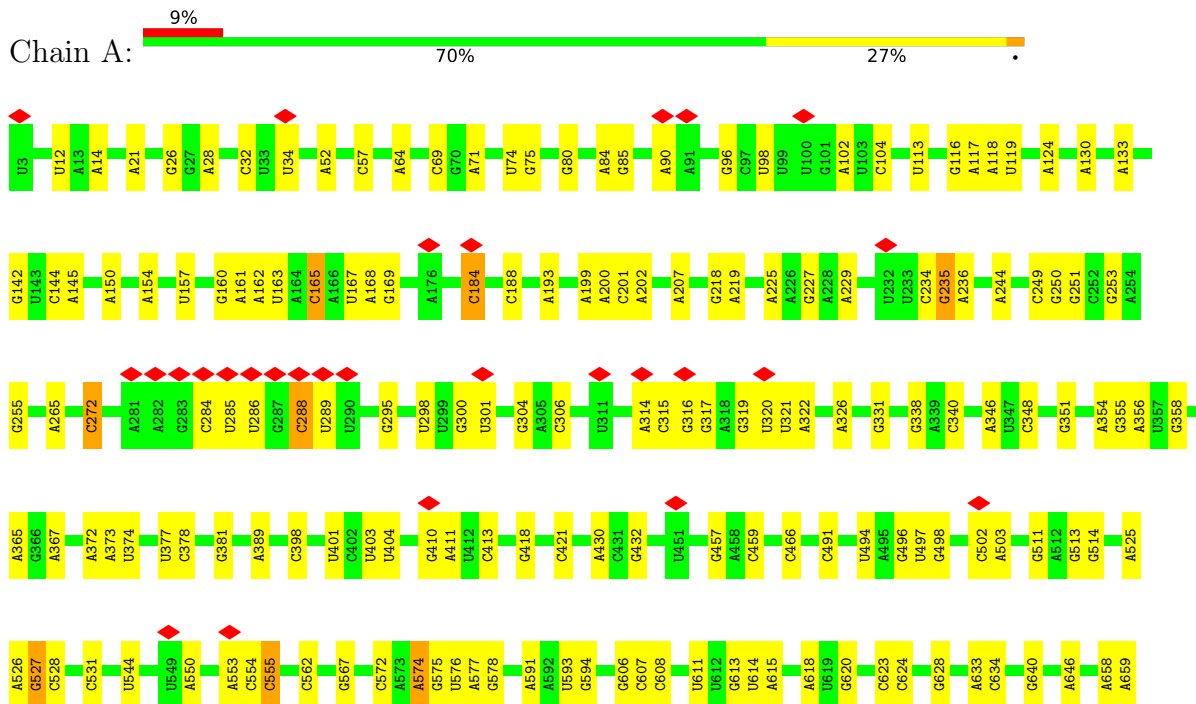
• Molecule 19: 30S ribosomal protein S19

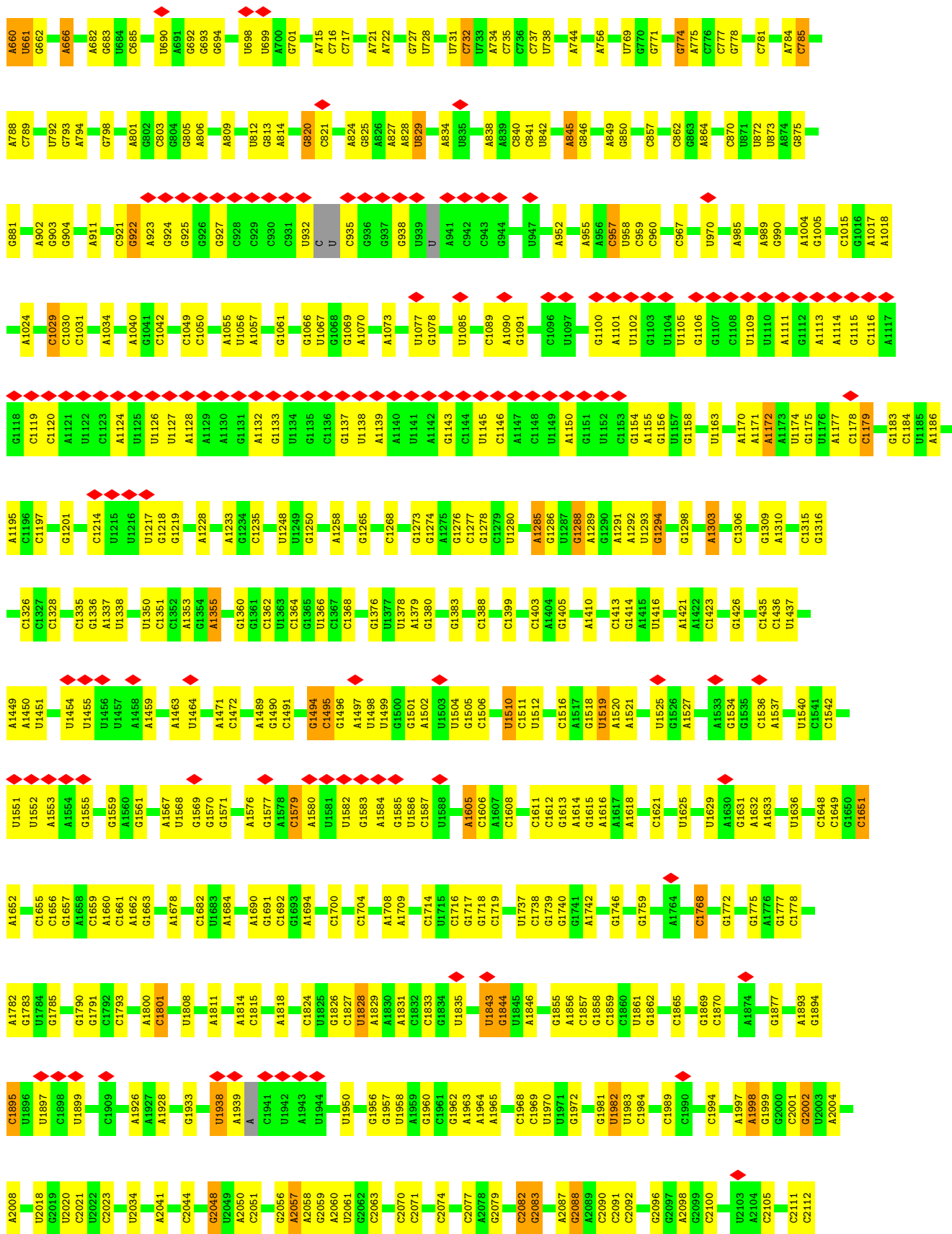


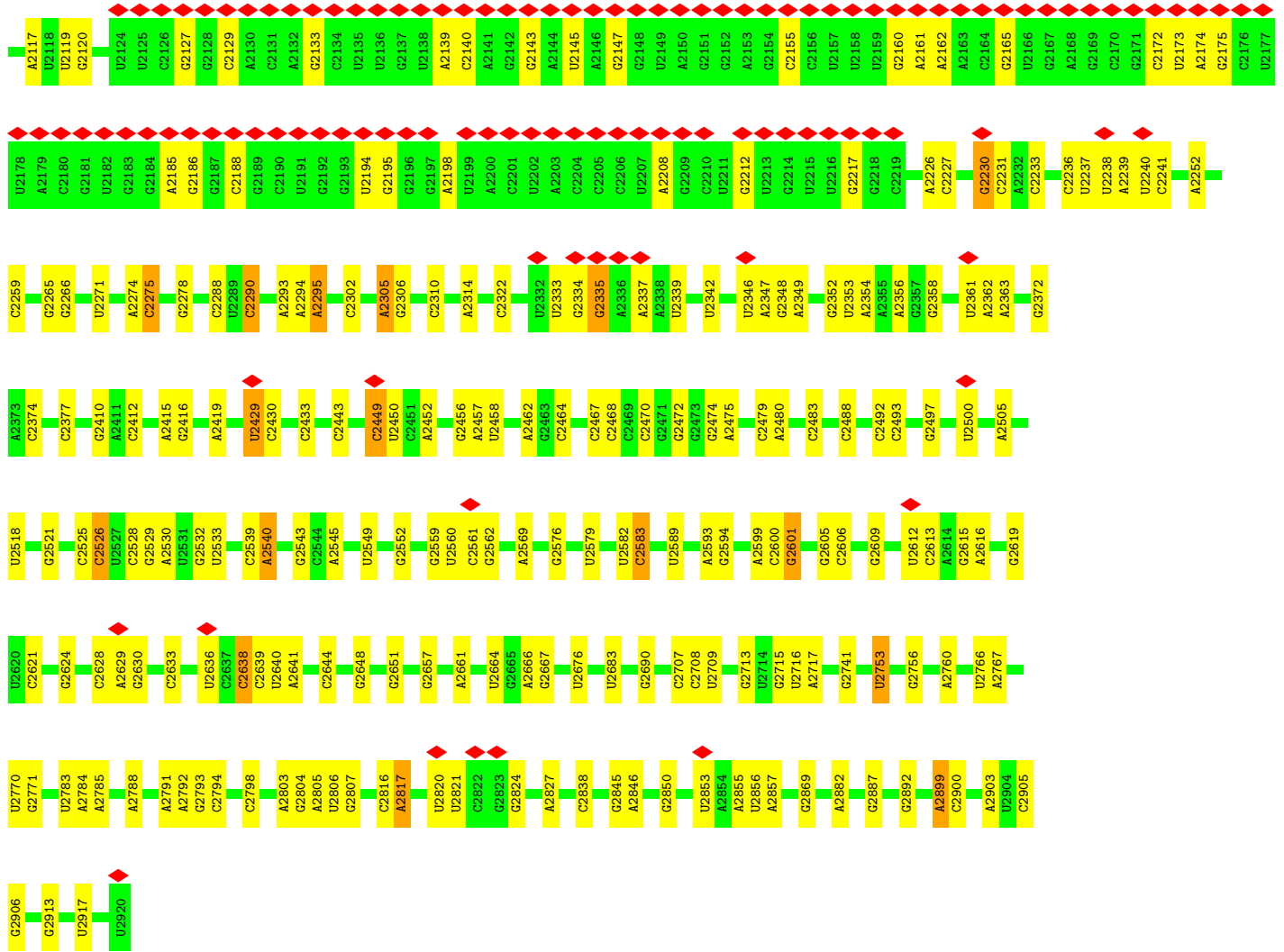
• Molecule 20: 30S ribosomal protein S20



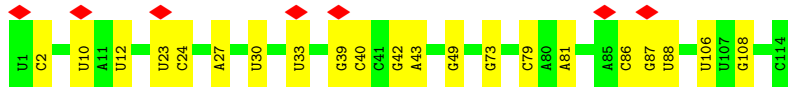
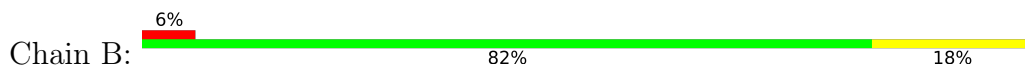
• Molecule 21: 23S ribosomal RNA



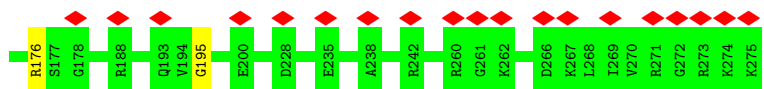




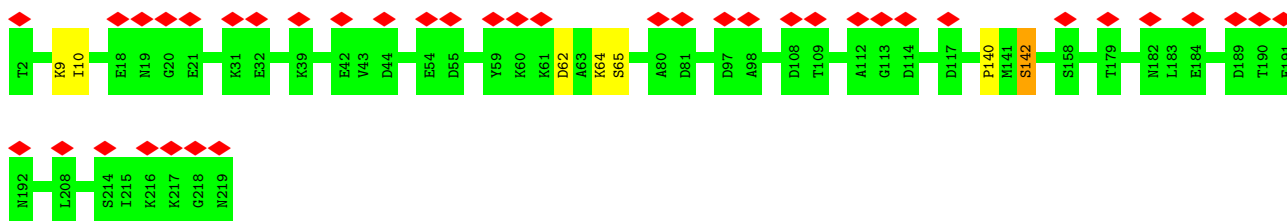
• Molecule 22: 5S ribosomal RNA



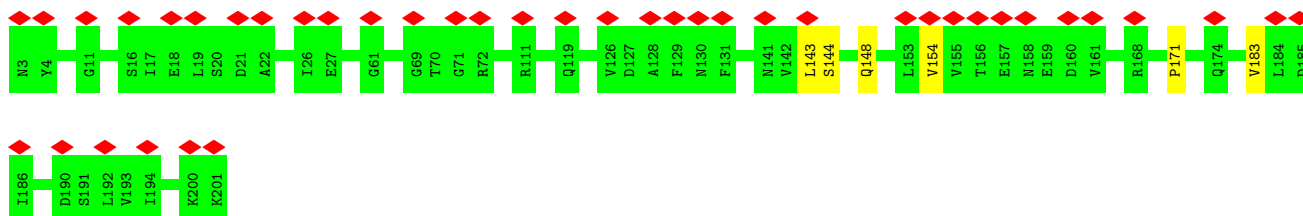
• Molecule 23: 50S ribosomal protein L2



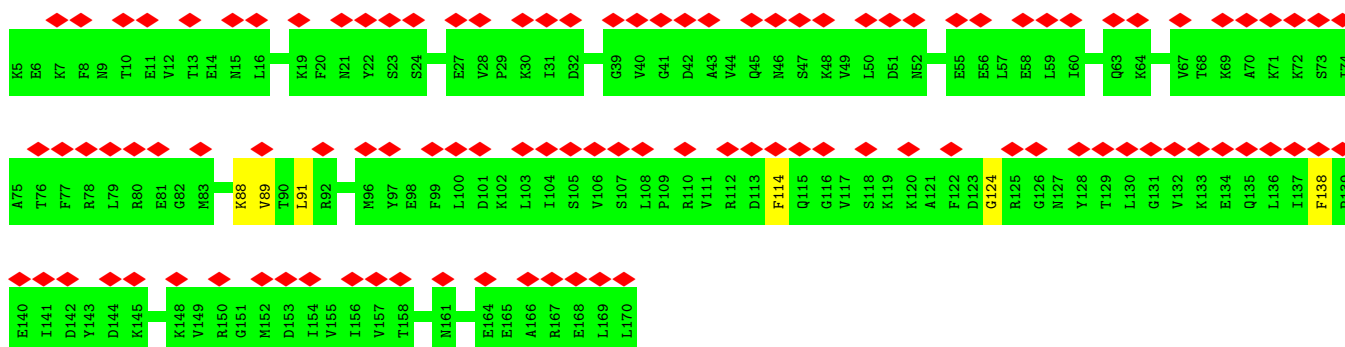
• Molecule 24: 50S ribosomal protein L3



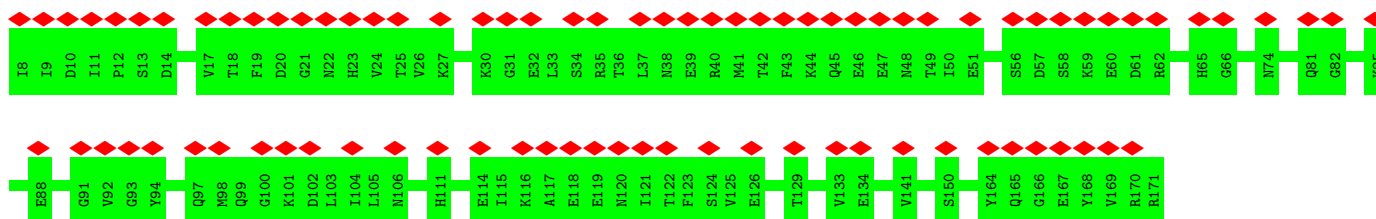
- Molecule 25: 50S ribosomal protein L4



- Molecule 26: 50S ribosomal protein L5

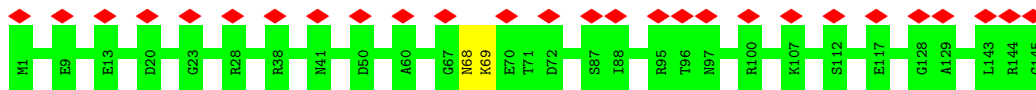


- Molecule 27: 50S ribosomal protein L6

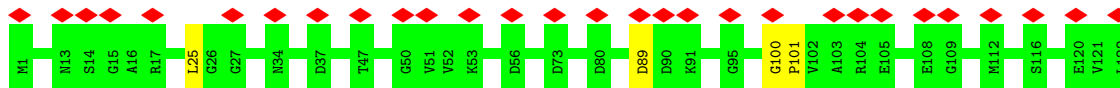


- Molecule 28: 50S ribosomal protein L13

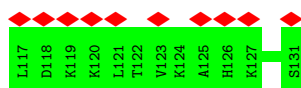
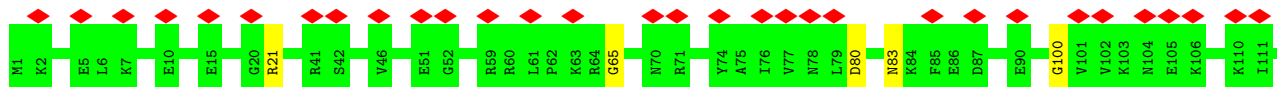




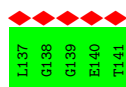
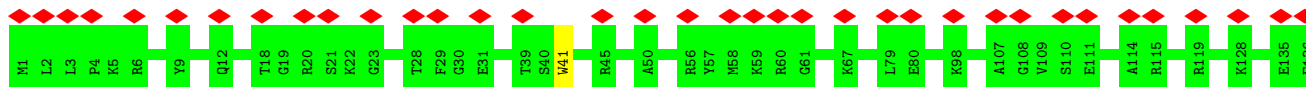
- Molecule 29: 50S ribosomal protein L14



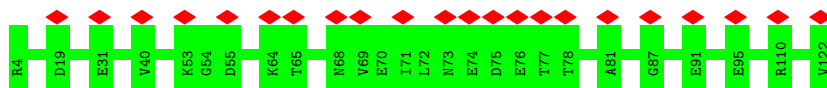
- Molecule 30: 50S ribosomal protein L15



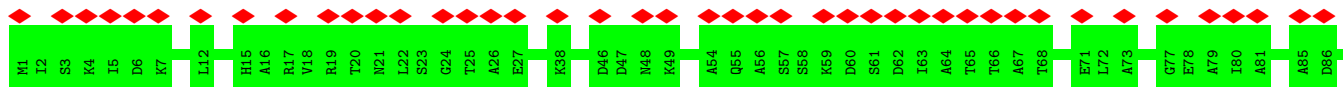
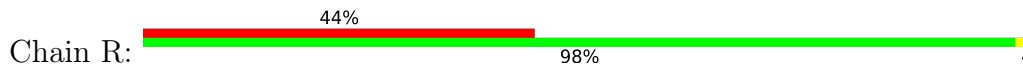
- Molecule 31: 50S ribosomal protein L16

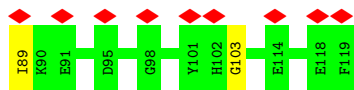


- Molecule 32: 50S ribosomal protein L17

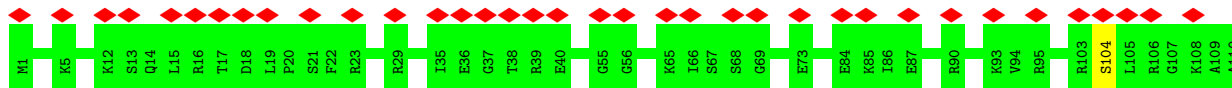


- Molecule 33: 50S ribosomal protein L18

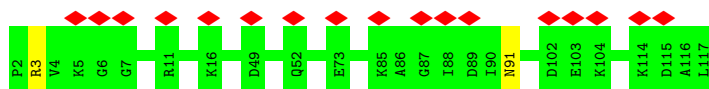




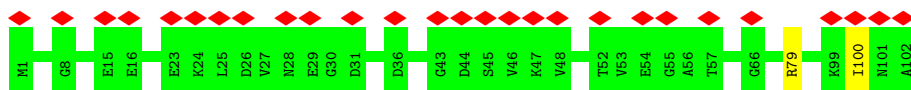
- Molecule 34: 50S ribosomal protein L19



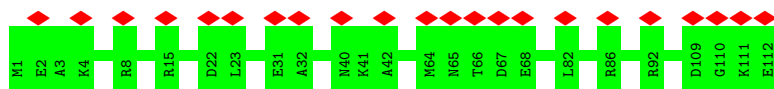
- Molecule 35: 50S ribosomal protein L20



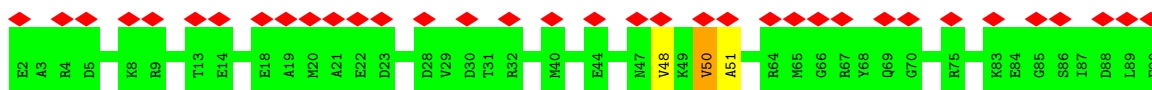
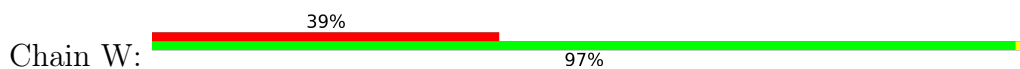
- Molecule 36: 50S ribosomal protein L21



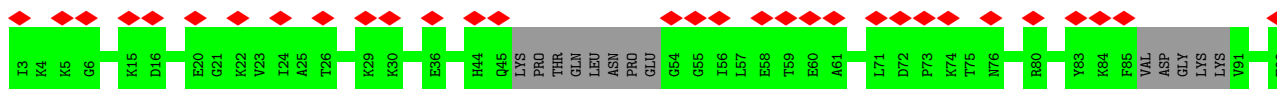
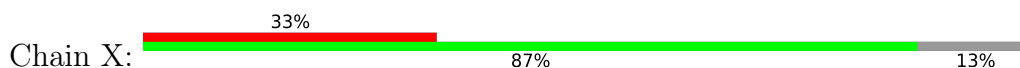
- Molecule 37: 50S ribosomal protein L22



- Molecule 38: 50S ribosomal protein L23

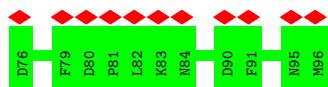
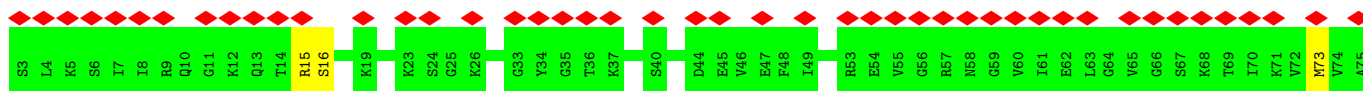


- Molecule 39: 50S ribosomal protein L24

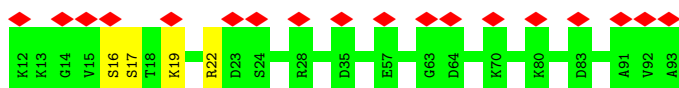
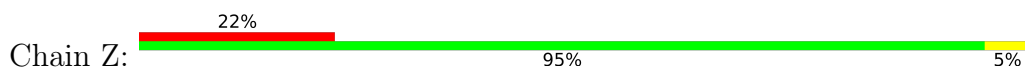




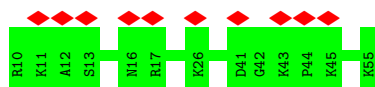
- Molecule 40: 50S ribosomal protein L25



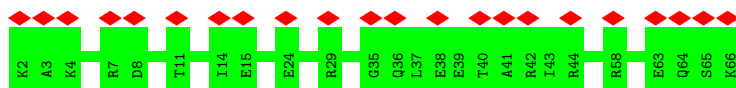
- Molecule 41: 50S ribosomal protein L27



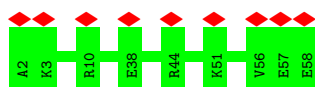
- Molecule 42: 50S ribosomal protein L28



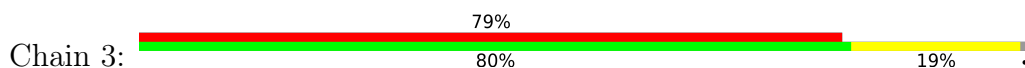
- Molecule 43: 50S ribosomal protein L29

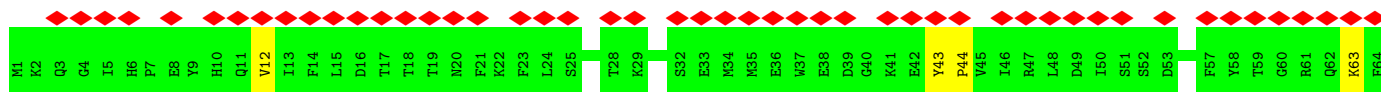


- Molecule 44: 50S ribosomal protein L30

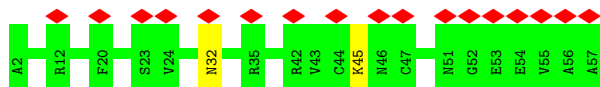


- Molecule 45: 50S ribosomal protein L31 type B

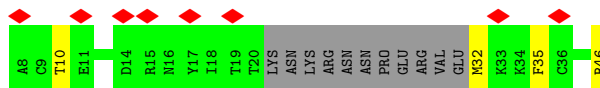




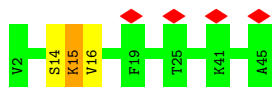
• Molecule 46: 50S ribosomal protein L32



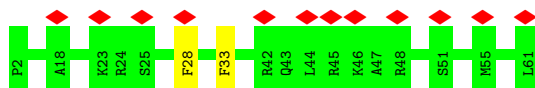
• Molecule 47: 50S ribosomal protein L33 2



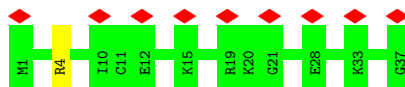
• Molecule 48: 50S ribosomal protein L34



• Molecule 49: 50S ribosomal protein L35



• Molecule 50: 50S ribosomal protein L36



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	110000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	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	0.447	Depositor
Minimum map value	-0.238	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.095	Depositor
Map size (Å)	365.2, 365.2, 365.2	wwPDB
Map dimensions	332, 332, 332	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: O, ZN, MG

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	0.89	0/37086	1.18	125/57833 (0.2%)
2	b	0.39	0/1829	0.63	1/2454 (0.0%)
3	c	0.44	0/1661	0.64	0/2233
4	d	0.51	0/1629	0.68	0/2185
5	e	0.55	0/1253	0.69	0/1687
6	f	0.60	0/810	0.63	0/1085
7	g	0.41	0/1207	0.65	0/1625
8	h	0.57	0/1044	0.72	0/1401
9	i	0.41	0/1033	0.70	0/1386
10	j	0.43	0/825	0.67	0/1110
11	k	0.46	0/896	0.69	0/1207
12	l	0.53	0/1080	0.78	0/1445
13	m	0.41	0/953	0.77	0/1275
14	n	0.54	0/512	0.70	0/678
15	o	0.51	0/747	0.68	0/996
16	p	0.55	0/723	0.67	0/971
17	q	0.57	0/715	0.79	0/955
18	r	0.45	0/599	0.72	0/797
19	s	0.41	0/696	0.73	0/934
20	t	0.44	0/607	0.61	0/810
21	A	2.04	70/69965 (0.1%)	1.80	586/109115 (0.5%)
22	B	0.85	0/2714	1.14	4/4228 (0.1%)
23	D	0.73	0/2139	0.75	0/2869
24	E	0.67	0/1673	0.69	0/2243
25	F	0.62	0/1548	0.66	0/2088
26	G	0.42	0/1327	0.70	1/1780 (0.1%)
27	H	0.47	0/1303	0.65	0/1757
28	M	0.65	0/1173	0.65	0/1578
29	N	0.71	0/927	0.76	0/1243
30	O	0.60	0/1011	0.80	1/1344 (0.1%)
31	P	0.66	0/1146	0.75	0/1536
32	Q	0.56	0/943	0.69	0/1259

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	R	0.53	0/931	0.69	0/1244
34	S	0.66	0/898	0.72	0/1199
35	T	0.73	0/956	0.77	1/1265 (0.1%)
36	U	0.63	0/809	0.69	1/1080 (0.1%)
37	V	0.63	0/871	0.76	0/1171
38	W	0.60	0/734	0.71	0/978
39	X	0.49	0/673	0.64	0/893
40	Y	0.50	0/746	0.69	0/1000
41	Z	0.72	0/633	0.77	0/838
42	0	0.54	0/379	0.78	0/504
43	1	0.49	0/538	0.63	0/714
44	2	0.58	0/444	0.66	0/597
45	3	0.46	0/694	0.74	1/930 (0.1%)
46	4	0.65	0/451	0.73	0/599
47	5	0.51	0/230	0.79	0/303
48	6	0.72	0/377	0.79	0/491
49	7	0.61	0/492	0.87	0/643
50	8	0.73	0/300	0.72	1/393 (0.3%)
All	All	1.48	70/152930 (0.0%)	1.43	722/228949 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	c	0	2
5	e	0	1
7	g	0	3
8	h	0	2
13	m	0	5
14	n	0	2
17	q	0	3
19	s	0	3
23	D	0	1
24	E	0	6
25	F	0	5
26	G	0	4
28	M	0	2
29	N	0	1
30	O	0	4
31	P	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
33	R	0	2
34	S	0	1
35	T	0	1
36	U	0	1
38	W	0	2
40	Y	0	1
41	Z	0	4
45	3	0	3
46	4	0	2
47	5	0	1
48	6	0	2
49	7	0	2
All	All	0	67

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	1288	G	C6-N1	171.20	2.59	1.39
21	A	1288	G	N3-C4	147.91	2.38	1.35
21	A	857	C	C5-C6	139.70	2.46	1.34
21	A	1288	G	N1-C2	138.56	2.48	1.37
21	A	1288	G	C2-N3	124.17	2.32	1.32
21	A	1288	G	C5-C4	122.56	2.24	1.38
21	A	1828	U	C2-N3	119.86	2.21	1.37
21	A	857	C	C2-N3	104.60	2.19	1.35
21	A	1828	U	N1-C2	98.17	2.27	1.38
21	A	1288	G	C5-C6	96.06	2.38	1.42
21	A	1828	U	N3-C4	92.48	2.21	1.38
21	A	1828	U	N1-C6	90.20	2.19	1.38
21	A	1828	U	C4-C5	83.56	2.18	1.43
21	A	1828	U	C5-C6	81.51	2.07	1.34
21	A	2230	G	C1'-N9	63.59	2.44	1.48
21	A	2230	G	N9-C4	38.43	1.68	1.38
21	A	857	C	N3-C4	37.14	1.59	1.33
21	A	2230	G	N9-C8	33.27	1.61	1.37
21	A	2230	G	N7-C5	-21.24	1.26	1.39
21	A	857	C	C4-C5	-18.54	1.28	1.43
21	A	1510	U	O3'-P	-17.20	1.40	1.61
21	A	1288	G	C8-N7	12.87	1.38	1.30
21	A	857	C	C2-O2	12.24	1.35	1.24
21	A	1288	G	N9-C4	-10.87	1.29	1.38
21	A	857	C	N1-C6	-10.07	1.31	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	2002	G	N3-C4	-9.93	1.28	1.35
21	A	1511	C	O3'-P	7.92	1.70	1.61
21	A	1858	G	N3-C4	-7.06	1.30	1.35
21	A	1815	C	C4-C5	-6.72	1.37	1.43
21	A	2002	G	C2-N3	-6.56	1.27	1.32
21	A	2230	G	N3-C4	6.12	1.39	1.35
21	A	1857	C	C2-N3	5.87	1.40	1.35
21	A	806	A	C5-C6	-5.85	1.35	1.41
21	A	2606	C	N1-C6	-5.80	1.33	1.37
21	A	824	A	N9-C4	-5.78	1.34	1.37
21	A	1024	A	N9-C4	-5.68	1.34	1.37
21	A	1031	C	C4-C5	-5.66	1.38	1.43
21	A	864	A	N9-C4	-5.62	1.34	1.37
21	A	2230	G	C8-N7	-5.54	1.27	1.30
21	A	1857	C	C4-C5	-5.52	1.38	1.43
21	A	1984	C	C4-C5	-5.51	1.38	1.43
21	A	903	G	N9-C4	-5.50	1.33	1.38
21	A	2644	C	N1-C6	-5.49	1.33	1.37
21	A	2230	G	C2'-C1'	5.48	1.59	1.53
21	A	2616	A	N9-C4	-5.46	1.34	1.37
21	A	2002	G	C2-N2	-5.46	1.29	1.34
21	A	2082	C	N1-C6	-5.43	1.33	1.37
21	A	2091	C	C4-C5	-5.43	1.38	1.43
21	A	1029	C	C4-C5	-5.41	1.38	1.43
21	A	2002	G	C5-C4	-5.41	1.34	1.38
21	A	2483	C	C4-C5	-5.38	1.38	1.43
21	A	1858	G	N9-C4	-5.33	1.33	1.38
21	A	2470	C	N1-C6	-5.30	1.33	1.37
21	A	903	G	N3-C4	-5.29	1.31	1.35
21	A	2002	G	N9-C4	-5.28	1.33	1.38
21	A	1708	A	N7-C5	-5.28	1.36	1.39
21	A	57	C	C4-C5	-5.27	1.38	1.43
21	A	555	C	C4-C5	-5.26	1.38	1.43
21	A	2443	C	C4-C5	-5.18	1.38	1.43
21	A	1858	G	C2-N3	-5.18	1.28	1.32
21	A	2001	C	N1-C6	-5.17	1.34	1.37
21	A	2474	G	N9-C8	-5.15	1.34	1.37
21	A	1435	C	C4-C5	-5.12	1.38	1.43
21	A	735	C	C4-C5	-5.11	1.38	1.43
21	A	2633	C	C4-C5	-5.09	1.38	1.43
21	A	1618	A	N9-C4	-5.06	1.34	1.37
21	A	1768	C	N1-C6	-5.02	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	1029	C	N3-C4	-5.02	1.30	1.33
21	A	201	C	C4-C5	-5.01	1.39	1.43
21	A	567	G	N7-C5	-5.00	1.36	1.39

All (722) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	857	C	N3-C4-C5	-238.20	26.62	121.90
21	A	857	C	C6-N1-C2	-227.33	29.37	120.30
21	A	2230	G	C8-N9-C4	-102.39	65.45	106.40
21	A	857	C	C2-N3-C4	83.55	161.67	119.90
21	A	857	C	C5-C6-N1	82.07	162.03	121.00
21	A	2230	G	N7-C8-N9	64.31	145.25	113.10
21	A	2230	G	N9-C4-C5	54.49	127.19	105.40
21	A	1288	G	C4-C5-N7	-52.34	89.86	110.80
21	A	857	C	C4-C5-C6	44.75	139.78	117.40
21	A	2230	G	N3-C4-C5	-42.21	107.50	128.60
21	A	2002	G	N3-C2-N2	-29.40	99.32	119.90
21	A	1288	G	C2-N3-C4	29.39	126.59	111.90
21	A	1288	G	N7-C8-N9	28.34	127.27	113.10
21	A	2230	G	C2-N3-C4	28.10	125.95	111.90
21	A	857	C	N3-C4-N4	27.49	137.24	118.00
21	A	1288	G	N1-C6-O6	-26.80	103.82	119.90
21	A	1288	G	C5-C6-O6	26.18	144.31	128.60
21	A	1288	G	C6-C5-N7	24.35	145.01	130.40
21	A	1288	G	N1-C2-N3	-20.86	111.39	123.90
21	A	1288	G	N3-C4-N9	20.13	138.08	126.00
21	A	2230	G	C4-C5-C6	19.20	130.32	118.80
21	A	1288	G	C5-N7-C8	18.78	113.69	104.30
21	A	1288	G	N3-C2-N2	18.02	132.51	119.90
21	A	2230	G	N9-C1'-C2'	17.32	136.51	114.00
21	A	857	C	C6-N1-C1'	17.22	141.46	120.80
21	A	1288	G	N3-C4-C5	-16.72	120.24	128.60
21	A	1858	G	N3-C2-N2	-16.17	108.58	119.90
21	A	2002	G	N1-C2-N2	16.09	130.68	116.20
21	A	2230	G	C8-N9-C1'	16.06	147.87	127.00
21	A	2002	G	C5-C6-O6	-15.95	119.03	128.60
21	A	2230	G	C5-N7-C8	-15.75	96.43	104.30
21	A	2230	G	C4-N9-C1'	15.52	146.68	126.50
21	A	857	C	N1-C2-N3	15.31	129.92	119.20
21	A	2002	G	C6-N1-C2	-14.81	116.21	125.10
21	A	1857	C	C2-N1-C1'	14.17	134.39	118.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	857	C	C5-C4-N4	-13.65	110.65	120.20
21	A	1511	C	OP2-P-O3'	13.65	135.22	105.20
21	A	1857	C	C6-N1-C2	-13.06	115.07	120.30
21	A	2230	G	C4-C5-N7	-12.92	105.63	110.80
21	A	806	A	C5-C6-N6	-12.01	114.09	123.70
21	A	1858	G	N1-C2-N2	11.65	126.68	116.20
21	A	1510	U	OP2-P-O3'	11.51	130.53	105.20
21	A	1510	U	P-O3'-C3'	-11.27	106.18	119.70
21	A	806	A	N1-C6-N6	11.22	125.33	118.60
21	A	2416	G	C5-C6-O6	-11.19	121.89	128.60
21	A	2002	G	N1-C6-O6	11.01	126.50	119.90
21	A	1235	C	C2-N3-C4	10.63	125.21	119.90
21	A	2230	G	C6-C5-N7	-10.60	124.04	130.40
21	A	1288	G	C4-C5-C6	10.51	125.11	118.80
21	A	2230	G	C6-N1-C2	-10.48	118.81	125.10
21	A	2416	G	N1-C6-O6	10.45	126.17	119.90
21	A	1235	C	N3-C4-C5	-10.03	117.89	121.90
21	A	857	C	N3-C2-O2	-9.94	114.94	121.90
21	A	1843	U	C2-N1-C1'	9.88	129.56	117.70
21	A	1828	U	N1-C2-N3	-9.81	109.02	114.90
21	A	1857	C	N3-C4-N4	9.74	124.82	118.00
21	A	2002	G	N1-C2-N3	9.74	129.75	123.90
21	A	1857	C	C5-C6-N1	9.48	125.74	121.00
21	A	2002	G	N9-C4-C5	9.42	109.17	105.40
21	A	903	G	N3-C4-N9	-9.41	120.35	126.00
21	A	2816	C	O4'-C1'-N1	9.41	115.73	108.20
21	A	1288	G	N9-C4-C5	-9.31	101.68	105.40
21	A	2105	C	N1-C2-O2	9.21	124.43	118.90
21	A	1857	C	C6-N1-C1'	-9.11	109.86	120.80
21	A	1858	G	N3-C4-N9	-9.06	120.56	126.00
21	A	806	A	C4-C5-N7	9.03	115.21	110.70
21	A	1656	C	N1-C2-O2	8.88	124.23	118.90
21	A	1364	C	C5-C4-N4	-8.84	114.01	120.20
21	A	1857	C	C5-C4-N4	-8.83	114.02	120.20
21	A	1004	A	N1-C6-N6	8.77	123.86	118.60
1	a	1536	C	C6-N1-C2	-8.76	116.80	120.30
21	A	857	C	N1-C2-O2	-8.69	113.68	118.90
21	A	806	A	C5-N7-C8	-8.56	99.62	103.90
21	A	2290	C	C6-N1-C2	-8.56	116.88	120.30
21	A	1235	C	C6-N1-C2	-8.51	116.90	120.30
21	A	2302	C	N1-C2-O2	8.51	124.01	118.90
21	A	737	C	C6-N1-C2	-8.47	116.91	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	735	C	C6-N1-C2	-8.46	116.92	120.30
21	A	165	C	C6-N1-C2	-8.40	116.94	120.30
21	A	1870	C	C6-N1-C2	-8.30	116.98	120.30
21	A	1368	C	N1-C2-O2	8.30	123.88	118.90
21	A	2063	C	C2-N1-C1'	8.28	127.90	118.80
21	A	201	C	N1-C2-O2	8.25	123.85	118.90
1	a	1179	C	C2-N1-C1'	8.21	127.83	118.80
22	B	79	C	C5-C4-N4	-8.19	114.47	120.20
1	a	1179	C	N1-C2-O2	8.18	123.81	118.90
21	A	1511	C	OP1-P-O3'	-8.06	87.47	105.20
21	A	1350	U	C2-N1-C1'	8.03	127.34	117.70
21	A	1815	C	C5-C4-N4	-8.00	114.60	120.20
21	A	1895	C	N3-C2-O2	-7.99	116.31	121.90
21	A	623	C	C5-C4-N4	-7.99	114.61	120.20
21	A	2057	A	N9-C4-C5	-7.96	102.62	105.80
21	A	1288	G	C4-N9-C1'	-7.89	116.25	126.50
21	A	1004	A	C5-C6-N6	-7.84	117.42	123.70
21	A	555	C	N1-C2-O2	7.70	123.52	118.90
21	A	1030	C	C6-N1-C2	-7.70	117.22	120.30
21	A	288	C	N1-C2-O2	7.64	123.48	118.90
21	A	1831	A	C5-C6-N6	-7.64	117.59	123.70
1	a	1179	C	N3-C2-O2	-7.60	116.58	121.90
21	A	788	A	C5-C6-N6	-7.58	117.64	123.70
21	A	935	C	C2-N1-C1'	7.52	127.08	118.80
21	A	1015	C	N1-C2-O2	7.52	123.41	118.90
21	A	2057	A	C8-N9-C4	7.50	108.80	105.80
21	A	2105	C	N3-C2-O2	-7.49	116.66	121.90
21	A	1895	C	N1-C2-O2	7.45	123.37	118.90
21	A	1984	C	N1-C2-O2	7.40	123.34	118.90
1	a	512	C	N1-C2-O2	7.37	123.32	118.90
1	a	115	A	N1-C6-N6	7.37	123.02	118.60
21	A	2063	C	C6-N1-C2	-7.37	117.35	120.30
1	a	399	G	C6-C5-N7	-7.37	125.98	130.40
21	A	845	A	N1-C6-N6	7.36	123.02	118.60
21	A	2619	G	C4-N9-C1'	7.35	136.05	126.50
1	a	641	U	C2-N1-C1'	7.24	126.39	117.70
21	A	1708	A	N1-C6-N6	7.23	122.94	118.60
21	A	234	C	N1-C2-O2	7.19	123.22	118.90
21	A	1843	U	N1-C2-O2	7.19	127.83	122.80
21	A	1828	U	C6-N1-C2	7.19	125.31	121.00
21	A	2105	C	C2-N1-C1'	7.17	126.68	118.80
21	A	732	C	C5-C4-N4	-7.15	115.20	120.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	1288	G	C8-N9-C1'	7.13	136.27	127.00
1	a	1519	A	C5-C6-N6	-7.12	118.00	123.70
21	A	574	A	N1-C2-N3	7.12	132.86	129.30
21	A	2543	G	N7-C8-N9	7.11	116.66	113.10
1	a	853	C	N3-C2-O2	-7.11	116.92	121.90
21	A	2021	C	C6-N1-C2	-7.10	117.46	120.30
21	A	2416	G	C4-C5-N7	7.08	113.63	110.80
21	A	1605	A	C5-C6-N6	-7.07	118.04	123.70
21	A	935	C	C6-N1-C2	-7.05	117.48	120.30
21	A	806	A	N9-C4-C5	-7.04	102.98	105.80
1	a	893	C	N1-C2-O2	7.04	123.12	118.90
21	A	692	G	N3-C2-N2	7.03	124.82	119.90
21	A	1435	C	C5-C4-N4	-7.03	115.28	120.20
21	A	721	A	N1-C6-N6	7.03	122.82	118.60
21	A	845	A	C5-C6-N6	-7.03	118.08	123.70
21	A	1315	C	N1-C2-O2	7.01	123.11	118.90
21	A	935	C	N3-C2-O2	-7.01	116.99	121.90
21	A	1843	U	N3-C2-O2	-7.01	117.29	122.20
1	a	115	A	C5-C6-N6	-6.99	118.11	123.70
1	a	819	C	C6-N1-C2	-6.97	117.51	120.30
21	A	1982	U	C5-C4-O4	-6.96	121.72	125.90
1	a	1541	G	C8-N9-C4	-6.96	103.62	106.40
21	A	2001	C	C2-N3-C4	-6.95	116.43	119.90
21	A	574	A	N1-C6-N6	-6.94	114.44	118.60
21	A	692	G	N1-C2-N2	-6.94	109.96	116.20
21	A	1778	C	N1-C2-O2	6.93	123.06	118.90
21	A	1042	C	N1-C2-O2	6.92	123.06	118.90
21	A	1298	G	C5-C6-O6	-6.92	124.45	128.60
21	A	661	U	C5-C6-N1	6.91	126.16	122.70
21	A	165	C	N3-C2-O2	-6.91	117.06	121.90
1	a	398	C	C6-N1-C2	-6.90	117.54	120.30
21	A	1414	G	C2-N3-C4	-6.89	108.45	111.90
1	a	1536	C	C2-N1-C1'	6.89	126.38	118.80
21	A	1843	U	C6-N1-C1'	-6.87	111.58	121.20
21	A	1648	C	N1-C2-O2	6.85	123.01	118.90
21	A	562	C	N3-C2-O2	-6.84	117.11	121.90
1	a	1171	G	O4'-C1'-N9	6.84	113.67	108.20
21	A	1201	G	C6-C5-N7	-6.83	126.30	130.40
1	a	399	G	N3-C4-N9	6.82	130.09	126.00
21	A	1235	C	C5-C6-N1	6.81	124.41	121.00
21	A	1029	C	N1-C2-O2	6.81	122.98	118.90
21	A	903	G	N3-C4-C5	6.80	132.00	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	819	C	C2-N1-C1'	6.76	126.24	118.80
21	A	12	U	C2-N1-C1'	6.76	125.81	117.70
21	A	735	C	C5-C6-N1	6.76	124.38	121.00
21	A	1029	C	C6-N1-C2	-6.75	117.60	120.30
21	A	2105	C	C6-N1-C2	-6.75	117.60	120.30
21	A	1815	C	N3-C4-N4	6.74	122.72	118.00
21	A	1998	A	N1-C6-N6	6.74	122.64	118.60
21	A	1605	A	N1-C6-N6	6.71	122.62	118.60
21	A	2023	C	N1-C2-O2	6.71	122.92	118.90
21	A	2288	C	N1-C2-O2	6.69	122.91	118.90
1	a	26	C	N1-C2-O2	6.67	122.90	118.90
21	A	2707	C	C6-N1-C2	-6.67	117.63	120.30
21	A	735	C	N3-C4-N4	6.64	122.65	118.00
21	A	2753	U	N3-C4-O4	-6.64	114.75	119.40
21	A	2077	C	N1-C2-O2	6.63	122.88	118.90
21	A	1858	G	N3-C4-C5	6.61	131.91	128.60
21	A	2227	C	C6-N1-C2	-6.61	117.66	120.30
21	A	2002	G	C8-N9-C4	-6.61	103.76	106.40
21	A	2322	C	N1-C2-O2	6.60	122.86	118.90
21	A	2302	C	N3-C2-O2	-6.60	117.28	121.90
21	A	2271	U	N3-C4-O4	6.59	124.01	119.40
21	A	555	C	C2-N1-C1'	6.58	126.04	118.80
21	A	2543	G	C4-N9-C1'	6.58	135.05	126.50
21	A	623	C	N3-C4-N4	6.56	122.59	118.00
35	T	3	ARG	NE-CZ-NH2	-6.54	117.03	120.30
21	A	2429	U	C2-N1-C1'	6.54	125.55	117.70
21	A	562	C	N1-C2-O2	6.54	122.82	118.90
1	a	920	C	N1-C2-O2	6.53	122.82	118.90
21	A	1815	C	C2-N1-C1'	6.53	125.98	118.80
21	A	2500	U	C2-N1-C1'	6.52	125.53	117.70
21	A	820	G	O4'-C1'-N9	6.51	113.41	108.20
21	A	2633	C	N1-C2-O2	6.51	122.81	118.90
21	A	935	C	N1-C2-O2	6.51	122.81	118.90
21	A	1984	C	C5-C4-N4	-6.50	115.65	120.20
21	A	633	A	N7-C8-N9	6.50	117.05	113.80
21	A	2133	G	C6-C5-N7	-6.49	126.50	130.40
21	A	1435	C	N3-C4-N4	6.49	122.54	118.00
21	A	2619	G	C8-N9-C1'	-6.49	118.57	127.00
21	A	2356	A	N7-C8-N9	6.48	117.04	113.80
21	A	1197	C	N1-C2-O2	6.48	122.78	118.90
21	A	1858	G	N1-C6-O6	6.47	123.78	119.90
21	A	1435	C	C2-N1-C1'	6.46	125.91	118.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	355	G	C6-C5-N7	-6.45	126.53	130.40
21	A	2606	C	N1-C2-O2	6.42	122.75	118.90
21	A	2416	G	C6-C5-N7	-6.41	126.55	130.40
21	A	2002	G	N3-C4-N9	-6.40	122.16	126.00
21	A	272	C	C6-N1-C2	-6.40	117.74	120.30
21	A	1960	G	N3-C2-N2	6.39	124.38	119.90
21	A	1364	C	N3-C4-N4	6.39	122.47	118.00
1	a	746	U	C5-C6-N1	6.39	125.89	122.70
21	A	2483	C	C5-C4-N4	-6.38	115.73	120.20
21	A	721	A	C5-C6-N6	-6.38	118.60	123.70
21	A	777	C	C6-N1-C2	-6.37	117.75	120.30
21	A	806	A	C6-C5-N7	-6.37	127.84	132.30
21	A	2034	U	C5-C4-O4	-6.36	122.08	125.90
21	A	1201	G	C4-C5-N7	6.35	113.34	110.80
1	a	933	A	N7-C8-N9	6.34	116.97	113.80
21	A	721	A	C5-N7-C8	-6.34	100.73	103.90
21	A	527	G	O4'-C1'-N9	6.33	113.27	108.20
1	a	625	G	C6-C5-N7	-6.33	126.60	130.40
21	A	2001	C	C5-C4-N4	-6.32	115.77	120.20
21	A	2483	C	N3-C4-N4	6.32	122.43	118.00
21	A	69	C	N3-C2-O2	-6.32	117.48	121.90
21	A	2464	C	N1-C2-O2	6.31	122.69	118.90
21	A	1015	C	N3-C2-O2	-6.30	117.49	121.90
1	a	361	A	N1-C6-N6	6.29	122.38	118.60
21	A	1368	C	N3-C2-O2	-6.29	117.50	121.90
21	A	1410	A	N9-C4-C5	-6.28	103.29	105.80
21	A	2023	C	N3-C2-O2	-6.27	117.51	121.90
1	a	1539	C	N3-C2-O2	-6.27	117.51	121.90
21	A	2133	G	N3-C4-N9	6.26	129.76	126.00
21	A	1708	A	C5-C6-N6	-6.26	118.69	123.70
21	A	496	G	N1-C2-N2	-6.26	110.56	116.20
21	A	608	C	C5-C4-N4	-6.26	115.82	120.20
21	A	1611	C	N1-C2-O2	6.26	122.66	118.90
1	a	1169	C	C6-N1-C2	-6.26	117.80	120.30
21	A	1029	C	C2-N1-C1'	6.26	125.68	118.80
1	a	762	C	C2-N1-C1'	6.24	125.66	118.80
21	A	2098	A	C5-C6-N6	-6.23	118.72	123.70
21	A	1801	C	C2-N3-C4	-6.22	116.79	119.90
1	a	843	A	C5-C6-N6	-6.22	118.73	123.70
21	A	2034	U	N3-C4-O4	6.21	123.75	119.40
1	a	1443	G	O4'-C1'-N9	6.21	113.17	108.20
21	A	2619	G	C6-C5-N7	-6.20	126.68	130.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	555	C	N3-C2-O2	-6.19	117.57	121.90
21	A	841	C	N1-C2-O2	6.19	122.61	118.90
21	A	1388	C	N1-C2-O2	6.18	122.61	118.90
21	A	2528	C	C6-N1-C2	-6.18	117.83	120.30
21	A	788	A	C6-C5-N7	-6.17	127.98	132.30
21	A	69	C	N1-C2-O2	6.17	122.60	118.90
21	A	2074	C	N1-C2-O2	6.17	122.60	118.90
21	A	903	G	C2-N3-C4	-6.16	108.82	111.90
1	a	1170	U	N1-C2-O2	6.16	127.11	122.80
1	a	726	A	N1-C6-N6	6.16	122.30	118.60
21	A	2305	A	C5-C6-N6	-6.16	118.78	123.70
21	A	870	C	N1-C2-O2	6.15	122.59	118.90
21	A	1651	C	N3-C4-C5	6.14	124.36	121.90
21	A	2044	C	C5-C4-N4	-6.14	115.90	120.20
21	A	2041	A	N1-C6-N6	-6.13	114.92	118.60
1	a	1536	C	C5-C6-N1	6.12	124.06	121.00
21	A	1219	G	N3-C4-N9	6.12	129.67	126.00
21	A	1608	C	N1-C2-O2	6.12	122.57	118.90
26	G	91	LEU	CA-CB-CG	6.12	129.37	115.30
21	A	1197	C	C2-N1-C1'	6.11	125.52	118.80
21	A	666	A	N1-C6-N6	6.10	122.26	118.60
21	A	1201	G	C4-N9-C1'	6.10	134.43	126.50
21	A	2271	U	C5-C4-O4	-6.10	122.24	125.90
21	A	528	C	C2-N1-C1'	6.09	125.50	118.80
21	A	57	C	C5-C4-N4	-6.09	115.94	120.20
21	A	1649	C	C2-N1-C1'	6.09	125.50	118.80
1	a	376	U	C2-N1-C1'	6.08	125.00	117.70
1	a	1441	C	N1-C2-O2	6.08	122.55	118.90
21	A	1350	U	C6-N1-C1'	-6.08	112.69	121.20
21	A	1414	G	C6-C5-N7	-6.08	126.75	130.40
21	A	2237	U	C5-C4-O4	-6.08	122.25	125.90
21	A	2443	C	C5-C4-N4	-6.08	115.95	120.20
1	a	903	C	C5-C4-N4	-6.07	115.95	120.20
21	A	732	C	N3-C4-N4	6.07	122.25	118.00
21	A	2117	A	N9-C4-C5	-6.06	103.38	105.80
21	A	735	C	C2-N1-C1'	6.06	125.46	118.80
21	A	528	C	C6-N1-C2	-6.05	117.88	120.30
21	A	1233	A	C5-C6-N1	6.05	120.73	117.70
21	A	1714	C	N3-C4-C5	6.05	124.32	121.90
1	a	89	U	C5-C4-O4	-6.04	122.28	125.90
50	8	4	ARG	NE-CZ-NH1	6.03	123.31	120.30
21	A	1984	C	N3-C2-O2	-6.02	117.68	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	1413	C	C5-C4-N4	-6.02	115.99	120.20
1	a	853	C	C6-N1-C2	-6.01	117.90	120.30
21	A	1938	U	P-O3'-C3'	6.01	126.91	119.70
21	A	1335	C	C2-N1-C1'	6.01	125.41	118.80
21	A	1984	C	C2-N1-C1'	6.00	125.40	118.80
21	A	2500	U	N3-C2-O2	-5.99	118.01	122.20
1	a	1343	A	N1-C6-N6	5.98	122.19	118.60
21	A	1778	C	N3-C2-O2	-5.97	117.72	121.90
1	a	1179	C	C6-N1-C2	-5.97	117.91	120.30
21	A	1831	A	N1-C6-N6	5.95	122.17	118.60
21	A	496	G	C2-N3-C4	-5.95	108.93	111.90
21	A	1351	C	C6-N1-C2	-5.95	117.92	120.30
21	A	1355	A	C5-C6-N6	-5.94	118.95	123.70
21	A	1031	C	C5-C4-N4	-5.93	116.05	120.20
21	A	1815	C	N1-C2-O2	5.93	122.46	118.90
1	a	341	U	C5-C4-O4	-5.93	122.34	125.90
21	A	555	C	C6-N1-C2	-5.90	117.94	120.30
21	A	1436	C	N1-C2-O2	5.90	122.44	118.90
45	3	80	LEU	C-N-CA	-5.90	106.95	121.70
21	A	1388	C	N3-C2-O2	-5.89	117.78	121.90
1	a	328	A	C5-C6-N1	5.89	120.64	117.70
21	A	1316	G	C6-C5-N7	-5.89	126.87	130.40
22	B	79	C	N3-C4-N4	5.88	122.12	118.00
21	A	661	U	C6-N1-C2	-5.88	117.47	121.00
21	A	201	C	N3-C2-O2	-5.88	117.78	121.90
1	a	1316	G	O4'-C1'-N9	5.88	112.90	108.20
21	A	2236	C	N1-C2-O2	5.88	122.42	118.90
21	A	355	G	C4-C5-N7	5.87	113.15	110.80
21	A	2002	G	C5-C6-N1	5.87	114.44	111.50
1	a	36	G	C4-N9-C1'	5.87	134.13	126.50
21	A	2236	C	N3-C2-O2	-5.87	117.79	121.90
21	A	2098	A	N1-C6-N6	5.86	122.11	118.60
21	A	2063	C	N3-C2-O2	-5.85	117.80	121.90
21	A	1502	A	N1-C6-N6	5.84	122.10	118.60
1	a	175	C	N1-C2-O2	5.83	122.40	118.90
21	A	1197	C	C5-C4-N4	-5.83	116.11	120.20
21	A	1612	C	C6-N1-C2	-5.83	117.97	120.30
21	A	2074	C	N3-C2-O2	-5.83	117.82	121.90
21	A	721	A	C4-C5-N7	5.83	113.61	110.70
1	a	399	G	C4-N9-C1'	5.83	134.07	126.50
21	A	144	C	C6-N1-C2	-5.83	117.97	120.30
21	A	1981	G	N3-C2-N2	5.83	123.98	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	399	G	C4-C5-N7	5.82	113.13	110.80
21	A	1360	G	C6-C5-N7	-5.81	126.92	130.40
21	A	1831	A	C4-C5-N7	5.80	113.60	110.70
21	A	531	C	N1-C2-O2	5.80	122.38	118.90
21	A	1814	A	C4-C5-N7	5.80	113.60	110.70
21	A	1494	G	C2-N3-C4	-5.79	109.00	111.90
21	A	2479	C	C5-C4-N4	-5.79	116.14	120.20
21	A	1360	G	N3-C4-N9	5.79	129.47	126.00
21	A	1869	G	C4-N9-C1'	5.79	134.03	126.50
21	A	1998	A	C5-C6-N6	-5.79	119.07	123.70
21	A	2100	C	C6-N1-C2	-5.79	117.98	120.30
21	A	1351	C	C5-C4-N4	-5.79	116.15	120.20
21	A	2569	A	C5-C6-N6	-5.79	119.07	123.70
21	A	2063	C	N1-C2-O2	5.77	122.36	118.90
1	a	320	C	N3-C2-O2	-5.77	117.86	121.90
1	a	1520	G	C4-N9-C1'	5.76	133.99	126.50
21	A	2077	C	C2-N1-C1'	5.76	125.13	118.80
21	A	1410	A	C8-N9-C4	5.76	108.10	105.80
21	A	1960	G	N1-C2-N2	-5.75	111.02	116.20
21	A	2063	C	C5-C4-N4	-5.75	116.17	120.20
21	A	2416	G	N9-C4-C5	-5.75	103.10	105.40
21	A	1831	A	N9-C4-C5	-5.75	103.50	105.80
21	A	2004	A	N9-C4-C5	-5.74	103.50	105.80
1	a	625	G	C4-N9-C1'	5.74	133.96	126.50
21	A	1828	U	N3-C2-O2	5.74	126.22	122.20
21	A	1004	A	C4-C5-N7	5.74	113.57	110.70
21	A	2112	C	C5-C4-N4	-5.74	116.18	120.20
21	A	2543	G	C8-N9-C4	-5.74	104.11	106.40
1	a	1536	C	N1-C2-O2	5.73	122.34	118.90
21	A	806	A	C5-C6-N1	5.73	120.56	117.70
21	A	1859	C	N1-C2-O2	5.73	122.34	118.90
21	A	2817	A	N1-C6-N6	-5.72	115.17	118.60
21	A	288	C	N3-C2-O2	-5.72	117.89	121.90
21	A	1661	C	C2-N1-C1'	5.72	125.09	118.80
21	A	2098	A	C6-C5-N7	-5.72	128.30	132.30
21	A	2290	C	C5-C6-N1	5.72	123.86	121.00
21	A	355	G	N3-C4-N9	5.71	129.43	126.00
21	A	1519	U	O4'-C1'-N1	5.71	112.77	108.20
21	A	1353	A	N7-C8-N9	5.71	116.66	113.80
21	A	2639	C	N1-C2-O2	5.70	122.32	118.90
1	a	878	C	N3-C2-O2	-5.70	117.91	121.90
21	A	788	A	C4-C5-N7	5.70	113.55	110.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	803	C	N3-C2-O2	-5.69	117.92	121.90
21	A	1828	U	C6-N1-C1'	-5.69	113.23	121.20
1	a	336	C	C6-N1-C2	-5.69	118.03	120.30
21	A	862	C	N1-C2-O2	5.69	122.31	118.90
1	a	878	C	N1-C2-O2	5.68	122.31	118.90
1	a	1536	C	N3-C2-O2	-5.68	117.92	121.90
21	A	608	C	C2-N3-C4	-5.68	117.06	119.90
1	a	491	C	C2-N1-C1'	5.68	125.05	118.80
21	A	57	C	C2-N1-C1'	5.67	125.04	118.80
21	A	1824	C	N3-C4-N4	5.67	121.97	118.00
21	A	1869	G	N7-C8-N9	5.67	115.94	113.10
21	A	2615	G	C4-C5-N7	5.67	113.07	110.80
21	A	2628	C	N1-C2-O2	5.67	122.30	118.90
1	a	479	U	N3-C2-O2	-5.66	118.24	122.20
21	A	2500	U	C6-N1-C2	-5.66	117.60	121.00
21	A	1414	G	C4-C5-N7	5.66	113.06	110.80
21	A	1351	C	C2-N1-C1'	5.66	125.02	118.80
1	a	1356	U	O4'-C1'-N1	5.65	112.72	108.20
21	A	737	C	C5-C6-N1	5.65	123.83	121.00
21	A	1649	C	N1-C2-O2	5.65	122.29	118.90
21	A	21	A	C5-C6-N6	-5.65	119.18	123.70
21	A	1984	C	N3-C4-N4	5.65	121.95	118.00
21	A	2449	C	C6-N1-C2	-5.65	118.04	120.30
21	A	1004	A	C6-C5-N7	-5.64	128.35	132.30
21	A	1542	C	C6-N1-C2	-5.64	118.04	120.30
21	A	2638	C	C5-C4-N4	-5.64	116.25	120.20
1	a	962	U	C5-C4-O4	-5.63	122.52	125.90
21	A	661	U	P-O3'-C3'	5.63	126.45	119.70
21	A	1858	G	C5-C6-O6	-5.63	125.22	128.60
21	A	2295	A	N7-C8-N9	5.63	116.61	113.80
21	A	2543	G	C6-C5-N7	-5.62	127.03	130.40
21	A	2092	C	C5-C4-N4	-5.62	116.27	120.20
21	A	903	G	N9-C4-C5	5.61	107.64	105.40
1	a	1354	G	C6-C5-N7	-5.61	127.04	130.40
21	A	1031	C	N1-C2-O2	5.61	122.26	118.90
1	a	36	G	C8-N9-C1'	-5.60	119.72	127.00
21	A	777	C	C2-N1-C1'	5.60	124.96	118.80
1	a	341	U	N3-C4-O4	5.59	123.31	119.40
21	A	774	G	C2-N3-C4	-5.58	109.11	111.90
21	A	2274	A	C5-C6-N6	-5.58	119.23	123.70
1	a	893	C	N3-C2-O2	-5.58	118.00	121.90
21	A	2239	A	O4'-C1'-N9	5.58	112.66	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	2559	G	C4-N9-C1'	5.58	133.75	126.50
21	A	1015	C	C2-N1-C1'	5.57	124.93	118.80
21	A	1869	G	C6-C5-N7	-5.57	127.06	130.40
21	A	1814	A	N9-C4-C5	-5.57	103.57	105.80
21	A	2233	C	C6-N1-C2	-5.56	118.08	120.30
21	A	1894	G	C6-C5-N7	-5.56	127.06	130.40
21	A	2048	G	C4-N9-C1'	5.56	133.73	126.50
21	A	2077	C	C5-C4-N4	-5.56	116.31	120.20
1	a	933	A	C5-N7-C8	-5.55	101.12	103.90
21	A	633	A	C6-C5-N7	-5.55	128.42	132.30
21	A	2707	C	N1-C2-O2	5.55	122.23	118.90
21	A	788	A	C6-N1-C2	-5.55	115.27	118.60
21	A	778	G	C2-N3-C4	-5.54	109.13	111.90
21	A	1435	C	N1-C2-O2	5.54	122.23	118.90
1	a	404	A	C5-C6-N6	-5.54	119.27	123.70
21	A	1870	C	C5-C6-N1	5.54	123.77	121.00
21	A	421	C	N1-C2-O2	5.54	122.22	118.90
21	A	1708	A	C4-C5-N7	5.54	113.47	110.70
1	a	588	C	N1-C2-O2	5.53	122.22	118.90
21	A	785	C	N1-C1'-C2'	5.53	121.19	114.00
21	A	2356	A	C5-N7-C8	-5.53	101.13	103.90
21	A	1801	C	C6-N1-C2	-5.53	118.09	120.30
21	A	624	C	N3-C2-O2	-5.53	118.03	121.90
21	A	1700	C	C6-N1-C2	-5.53	118.09	120.30
21	A	2090	C	C2-N1-C1'	5.53	124.88	118.80
21	A	2004	A	C8-N9-C4	5.52	108.01	105.80
21	A	1335	C	N3-C4-N4	5.52	121.86	118.00
1	a	933	A	C6-C5-N7	-5.52	128.44	132.30
21	A	788	A	C5-C6-N1	5.52	120.46	117.70
36	U	79	ARG	NE-CZ-NH1	5.52	123.06	120.30
21	A	737	C	N3-C4-N4	5.51	121.86	118.00
1	a	819	C	C5-C4-N4	-5.51	116.34	120.20
21	A	1661	C	C6-N1-C1'	-5.51	114.19	120.80
21	A	2117	A	C4-C5-N7	5.51	113.45	110.70
1	a	762	C	C6-N1-C1'	-5.51	114.19	120.80
21	A	829	U	O4'-C1'-N1	5.51	112.61	108.20
21	A	1360	G	C4-C5-N7	5.50	113.00	110.80
21	A	355	G	N9-C4-C5	-5.50	103.20	105.40
21	A	555	C	C5-C4-N4	-5.50	116.35	120.20
21	A	1844	G	C4-N9-C1'	5.49	133.63	126.50
21	A	1870	C	N1-C2-O2	5.49	122.19	118.90
21	A	57	C	N1-C2-O2	5.48	122.19	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	2569	A	N1-C6-N6	5.48	121.89	118.60
21	A	1268	C	C6-N1-C2	-5.48	118.11	120.30
1	a	625	G	N7-C8-N9	5.47	115.84	113.10
1	a	1428	G	C2-N3-C4	-5.47	109.16	111.90
21	A	57	C	N3-C4-N4	5.47	121.83	118.00
21	A	1336	G	C2-N3-C4	-5.47	109.16	111.90
21	A	666	A	C5-N7-C8	-5.47	101.17	103.90
21	A	1510	U	OP1-P-O3'	-5.47	93.17	105.20
21	A	2798	C	C6-N1-C2	-5.47	118.11	120.30
21	A	608	C	N3-C4-C5	5.47	124.09	121.90
21	A	2305	A	C4-C5-N7	5.47	113.43	110.70
21	A	628	G	N7-C8-N9	5.46	115.83	113.10
1	a	1237	C	C6-N1-C2	-5.46	118.12	120.30
1	a	1179	C	C6-N1-C1'	-5.45	114.25	120.80
21	A	514	G	C8-N9-C1'	-5.45	119.91	127.00
1	a	315	U	N3-C2-O2	-5.45	118.38	122.20
21	A	1179	C	C6-N1-C2	-5.45	118.12	120.30
1	a	1541	G	N7-C8-N9	5.45	115.82	113.10
21	A	737	C	C2-N1-C1'	5.45	124.79	118.80
21	A	1360	G	N9-C4-C5	-5.45	103.22	105.40
21	A	1828	U	C5-C6-N1	-5.45	119.98	122.70
21	A	2641	A	C5-C6-N1	5.45	120.42	117.70
21	A	1436	C	C2-N1-C1'	5.44	124.78	118.80
21	A	235	G	O4'-C1'-N9	5.44	112.55	108.20
21	A	1004	A	N9-C4-C5	-5.43	103.63	105.80
21	A	1315	C	N3-C2-O2	-5.43	118.10	121.90
21	A	2857	A	C5-C6-N6	-5.43	119.36	123.70
22	B	86	C	C6-N1-C2	-5.43	118.13	120.30
21	A	2480	A	C5-C6-N6	-5.42	119.36	123.70
21	A	957	C	N1-C2-O2	5.42	122.15	118.90
1	a	1036	C	C6-N1-C2	-5.42	118.13	120.30
21	A	2088	G	O4'-C1'-N9	5.41	112.53	108.20
21	A	2621	C	C5-C4-N4	-5.41	116.41	120.20
21	A	1511	C	P-O3'-C3'	-5.41	113.21	119.70
21	A	2539	C	C5-C4-N4	-5.41	116.42	120.20
21	A	2676	U	C5-C4-O4	-5.41	122.66	125.90
21	A	32	C	N1-C2-O2	5.40	122.14	118.90
21	A	12	U	N3-C2-O2	-5.40	118.42	122.20
21	A	1201	G	C8-N9-C1'	-5.40	119.98	127.00
1	a	819	C	C5-C6-N1	5.39	123.70	121.00
21	A	2083	G	C4-N9-C1'	5.39	133.50	126.50
21	A	1559	G	N3-C4-N9	-5.39	122.77	126.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	841	C	N3-C2-O2	-5.38	118.13	121.90
21	A	1368	C	C2-N1-C1'	5.38	124.72	118.80
21	A	1179	C	C2-N1-C1'	5.38	124.72	118.80
21	A	2117	A	C6-C5-N7	-5.38	128.53	132.30
1	a	816	C	C5-C4-N4	-5.38	116.44	120.20
21	A	1328	C	N1-C2-O2	5.38	122.13	118.90
21	A	2464	C	N3-C2-O2	-5.38	118.13	121.90
21	A	2664	U	C5-C6-N1	5.38	125.39	122.70
21	A	2090	C	N3-C2-O2	-5.38	118.14	121.90
21	A	1656	C	N3-C2-O2	-5.37	118.14	121.90
1	a	512	C	N3-C2-O2	-5.36	118.15	121.90
21	A	1303	A	C5-C6-N6	-5.36	119.42	123.70
21	A	2074	C	C6-N1-C2	-5.35	118.16	120.30
21	A	788	A	N1-C6-N6	5.35	121.81	118.60
21	A	2619	G	N7-C8-N9	5.35	115.78	113.10
21	A	1793	C	C5-C4-N4	-5.35	116.46	120.20
1	a	1354	G	N7-C8-N9	5.34	115.77	113.10
1	a	641	U	N1-C2-O2	5.34	126.53	122.80
21	A	801	A	C5-C6-N6	-5.34	119.43	123.70
21	A	728	U	C5-C4-O4	-5.33	122.70	125.90
21	A	1877	G	C4-C5-N7	5.33	112.93	110.80
21	A	2500	U	N1-C2-O2	5.33	126.53	122.80
21	A	633	A	C4-N9-C1'	5.33	135.89	126.30
21	A	2051	C	C6-N1-C2	-5.33	118.17	120.30
21	A	1858	G	N9-C4-C5	5.33	107.53	105.40
1	a	583	G	N3-C4-N9	-5.33	122.80	126.00
21	A	1029	C	C5-C4-N4	-5.33	116.47	120.20
1	a	627	U	C2-N1-C1'	5.32	124.08	117.70
21	A	1656	C	C2-N1-C1'	5.32	124.65	118.80
21	A	2098	A	C4-C5-N7	5.32	113.36	110.70
21	A	840	C	N3-C2-O2	-5.31	118.18	121.90
21	A	781	C	C5-C4-N4	-5.31	116.48	120.20
21	A	1648	C	N3-C2-O2	-5.31	118.18	121.90
21	A	1708	A	C6-C5-N7	-5.31	128.58	132.30
21	A	2117	A	C5-C6-N6	-5.31	119.45	123.70
21	A	250	G	C2-N3-C4	-5.31	109.25	111.90
21	A	2559	G	C8-N9-C1'	-5.30	120.12	127.00
1	a	320	C	N1-C2-O2	5.29	122.08	118.90
21	A	1410	A	C5-C6-N6	-5.29	119.47	123.70
1	a	399	G	C8-N9-C1'	-5.29	120.12	127.00
21	A	1380	G	C4-N9-C1'	5.29	133.38	126.50
21	A	2071	C	C6-N1-C2	-5.28	118.19	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1073	G	C4-N9-C1'	5.28	133.36	126.50
21	A	2651	G	C4-C5-N7	5.28	112.91	110.80
1	a	363	C	N1-C2-O2	5.28	122.06	118.90
21	A	788	A	N3-C4-N9	5.28	131.62	127.40
21	A	1719	C	N3-C4-C5	5.28	124.01	121.90
1	a	641	U	N3-C2-O2	-5.27	118.51	122.20
21	A	1579	C	C6-N1-C2	-5.27	118.19	120.30
21	A	2540	A	C6-N1-C2	-5.27	115.44	118.60
21	A	842	U	C5-C4-O4	-5.26	122.74	125.90
21	A	2083	G	C8-N9-C1'	-5.26	120.16	127.00
1	a	221	U	C2-N1-C1'	5.26	124.01	117.70
21	A	1280	U	N3-C4-O4	5.26	123.08	119.40
21	A	812	U	C5-C6-N1	5.26	125.33	122.70
21	A	1981	G	N1-C2-N2	-5.26	111.47	116.20
21	A	2063	C	C6-N1-C1'	-5.26	114.49	120.80
21	A	514	G	C4-N9-C1'	5.26	133.33	126.50
1	a	682	G	C6-C5-N7	-5.25	127.25	130.40
21	A	633	A	N3-C4-N9	5.25	131.60	127.40
21	A	1694	A	C5-C6-N6	-5.25	119.50	123.70
21	A	1050	C	C5-C4-N4	-5.25	116.53	120.20
1	a	1519	A	N1-C6-N6	5.25	121.75	118.60
21	A	1355	A	N1-C6-N6	5.25	121.75	118.60
21	A	788	A	C5-N7-C8	-5.24	101.28	103.90
21	A	2628	C	N3-C4-C5	5.24	124.00	121.90
1	a	399	G	N9-C4-C5	-5.24	103.30	105.40
21	A	1518	G	N3-C2-N2	5.24	123.57	119.90
21	A	1682	C	N1-C2-O2	5.24	122.04	118.90
21	A	2639	C	N3-C2-O2	-5.24	118.23	121.90
1	a	26	C	N3-C4-C5	5.23	123.99	121.90
21	A	346	A	C5-C6-N6	-5.23	119.51	123.70
21	A	1495	C	N3-C2-O2	-5.23	118.24	121.90
1	a	83	C	C6-N1-C2	-5.23	118.21	120.30
21	A	356	A	C5-C6-N6	-5.23	119.52	123.70
21	A	2295	A	C4-N9-C1'	5.23	135.71	126.30
1	a	447	U	N3-C2-O2	-5.22	118.54	122.20
21	A	249	C	C5-C4-N4	-5.22	116.54	120.20
1	a	1115	C	N1-C2-O2	5.22	122.03	118.90
21	A	2290	C	N3-C4-N4	5.22	121.65	118.00
21	A	735	C	C5-C4-N4	-5.22	116.55	120.20
21	A	781	C	N1-C2-O2	5.22	122.03	118.90
21	A	1228	A	C5-N7-C8	-5.22	101.29	103.90
21	A	1559	G	C2-N3-C4	-5.22	109.29	111.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	2601	G	C4-C5-N7	5.22	112.89	110.80
21	A	701	G	C6-C5-N7	-5.21	127.27	130.40
21	A	1894	G	N3-C4-N9	5.21	129.13	126.00
21	A	634	C	N1-C2-O2	5.21	122.03	118.90
21	A	666	A	C5-C6-N6	-5.21	119.53	123.70
21	A	721	A	C6-C5-N7	-5.21	128.66	132.30
21	A	2117	A	N1-C6-N6	5.21	121.72	118.60
1	a	315	U	C5-C6-N1	5.20	125.30	122.70
21	A	1399	C	C2-N1-C1'	5.20	124.52	118.80
2	b	113	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	a	1520	G	C8-N9-C1'	-5.19	120.25	127.00
21	A	2540	A	C5-C6-N6	-5.19	119.55	123.70
1	a	661	U	N1-C2-O2	5.19	126.43	122.80
21	A	777	C	C5-C6-N1	5.19	123.60	121.00
21	A	1315	C	C2-N1-C1'	5.19	124.51	118.80
1	a	171	A	N1-C6-N6	-5.18	115.49	118.60
21	A	771	G	C2-N3-C4	-5.18	109.31	111.90
21	A	666	A	C4-C5-N7	5.18	113.29	110.70
1	a	341	U	C5-C6-N1	5.18	125.29	122.70
21	A	738	U	N3-C4-O4	5.18	123.03	119.40
21	A	1201	G	N3-C4-N9	5.18	129.10	126.00
21	A	1351	C	N3-C4-N4	5.17	121.62	118.00
21	A	348	C	N1-C2-O2	5.17	122.00	118.90
21	A	1219	G	C6-C5-N7	-5.17	127.30	130.40
21	A	2111	C	C5-C4-N4	-5.17	116.58	120.20
21	A	193	A	C5-C6-N6	-5.16	119.57	123.70
21	A	2794	C	C6-N1-C2	-5.16	118.23	120.30
1	a	89	U	N3-C4-O4	5.16	123.01	119.40
1	a	491	C	C6-N1-C1'	-5.16	114.61	120.80
21	A	1235	C	N3-C2-O2	5.15	125.51	121.90
21	A	607	C	N1-C2-O2	5.15	121.99	118.90
21	A	1502	A	N7-C8-N9	5.15	116.38	113.80
21	A	2056	G	C4-C5-N7	5.15	112.86	110.80
21	A	1029	C	N3-C2-O2	-5.15	118.30	121.90
21	A	2090	C	N1-C2-O2	5.15	121.99	118.90
1	a	1363	C	N1-C2-O2	5.14	121.99	118.90
21	A	1217	U	C2-N1-C1'	5.14	123.87	117.70
21	A	1274	G	C2-N3-C4	-5.14	109.33	111.90
21	A	1326	C	C6-N1-C2	-5.14	118.24	120.30
21	A	265	A	C5-C6-N6	-5.14	119.59	123.70
21	A	2816	C	N3-C2-O2	-5.14	118.30	121.90
22	B	81	A	C5-C6-N6	-5.14	119.59	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	738	U	C5-C4-O4	-5.13	122.82	125.90
21	A	348	C	C5-C4-N4	-5.13	116.61	120.20
21	A	1657	G	N3-C4-C5	5.13	131.17	128.60
21	A	2899	A	C5-C6-N6	-5.13	119.60	123.70
1	a	34	A	C6-C5-N7	-5.12	128.71	132.30
1	a	548	G	C4-C5-N7	5.12	112.85	110.80
21	A	2488	C	C5-C4-N4	-5.12	116.61	120.20
21	A	2526	C	O4'-C1'-N1	-5.12	104.10	108.20
1	a	16	G	C4-N9-C1'	5.12	133.16	126.50
21	A	1197	C	N3-C4-N4	5.12	121.58	118.00
21	A	2770	U	C5-C4-O4	-5.12	122.83	125.90
21	A	1615	G	N3-C4-N9	-5.12	122.93	126.00
21	A	788	A	N9-C4-C5	-5.12	103.75	105.80
30	O	21	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	a	1536	C	N3-C4-N4	5.12	121.58	118.00
1	a	461	C	C6-N1-C2	-5.11	118.25	120.30
21	A	734	A	N7-C8-N9	5.11	116.36	113.80
21	A	2259	C	C5-C4-N4	-5.11	116.62	120.20
1	a	306	A	N9-C4-C5	-5.11	103.76	105.80
21	A	272	C	C2-N1-C1'	5.11	124.42	118.80
21	A	491	C	N1-C2-O2	5.10	121.96	118.90
21	A	857	C	C2-N1-C1'	-5.10	113.19	118.80
21	A	840	C	N1-C2-O2	5.10	121.96	118.90
21	A	355	G	C4-N9-C1'	5.10	133.13	126.50
21	A	967	C	N1-C2-O2	5.10	121.96	118.90
21	A	1435	C	C6-N1-C2	-5.10	118.26	120.30
21	A	567	G	C6-C5-N7	-5.09	127.34	130.40
21	A	1366	U	C5-C6-N1	5.09	125.25	122.70
21	A	555	C	N3-C4-N4	5.09	121.56	118.00
21	A	1426	G	C6-C5-N7	-5.09	127.34	130.40
21	A	2335	G	O4'-C1'-N9	5.09	112.27	108.20
21	A	2275	C	N1-C2-O2	5.09	121.95	118.90
1	a	24	C	N1-C2-O2	5.09	121.95	118.90
1	a	698	G	N1-C2-N2	-5.08	111.62	116.20
21	A	777	C	N3-C4-N4	5.08	121.56	118.00
1	a	315	U	N1-C2-O2	5.08	126.36	122.80
21	A	1870	C	N3-C2-O2	-5.08	118.34	121.90
21	A	2129	C	C6-N1-C2	-5.08	118.27	120.30
21	A	2493	C	N1-C2-O2	5.08	121.95	118.90
21	A	1831	A	C5-C6-N1	5.08	120.24	117.70
21	A	1612	C	N3-C2-O2	-5.08	118.35	121.90
21	A	620	G	N7-C8-N9	5.07	115.64	113.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	2290	C	C2-N1-C1'	5.07	124.38	118.80
21	A	184	C	C6-N1-C2	-5.07	118.27	120.30
21	A	778	G	N1-C2-N2	-5.07	111.64	116.20
21	A	1663	G	C6-C5-N7	-5.07	127.36	130.40
1	a	682	G	N7-C8-N9	5.07	115.63	113.10
21	A	1335	C	C6-N1-C2	-5.06	118.28	120.30
21	A	922	G	C8-N9-C1'	5.06	133.57	127.00
21	A	1285	A	C5-C6-N1	5.06	120.23	117.70
1	a	1037	C	C6-N1-C2	-5.06	118.28	120.30
21	A	188	C	C5-C4-N4	-5.05	116.66	120.20
21	A	1172	A	C5-C6-N6	-5.05	119.66	123.70
21	A	903	G	N3-C2-N2	-5.05	116.36	119.90
1	a	551	G	C4-N9-C1'	5.05	133.06	126.50
1	a	1519	A	C5-C6-N1	5.05	120.22	117.70
21	A	620	G	C6-C5-N7	-5.05	127.37	130.40
1	a	886	A	C5-C6-N6	-5.04	119.67	123.70
21	A	2715	G	C2-N3-C4	-5.04	109.38	111.90
21	A	116	G	C2-N3-C4	-5.04	109.38	111.90
21	A	491	C	C2-N1-C1'	5.04	124.34	118.80
21	A	685	C	N1-C2-O2	5.04	121.92	118.90
21	A	805	G	N3-C4-N9	5.04	129.02	126.00
21	A	2074	C	C2-N1-C1'	5.04	124.34	118.80
21	A	304	G	C4-C5-N7	5.03	112.81	110.80
21	A	1298	G	N3-C2-N2	-5.03	116.38	119.90
21	A	2077	C	N3-C4-N4	5.03	121.52	118.00
21	A	2356	A	C4-N9-C1'	5.03	135.36	126.30
21	A	660	A	N1-C6-N6	5.03	121.62	118.60
21	A	1353	A	C5-N7-C8	-5.03	101.39	103.90
21	A	2667	G	C6-C5-N7	-5.03	127.38	130.40
1	a	315	U	C6-N1-C2	-5.02	117.99	121.00
1	a	1435	U	C5-C4-O4	-5.02	122.89	125.90
21	A	26	G	C8-N9-C1'	-5.02	120.47	127.00
21	A	717	C	N1-C2-O2	5.02	121.91	118.90
21	A	2077	C	N3-C2-O2	-5.02	118.39	121.90
21	A	2899	A	N1-C6-N6	5.02	121.61	118.60
1	a	378	C	C5-C4-N4	-5.02	116.69	120.20
21	A	640	G	N1-C2-N2	-5.02	111.68	116.20
21	A	1859	C	C5-C4-N4	-5.02	116.69	120.20
1	a	1539	C	N1-C2-O2	5.01	121.91	118.90
21	A	250	G	N1-C2-N2	-5.01	111.69	116.20
21	A	814	A	C6-N1-C2	-5.01	115.59	118.60
21	A	1870	C	C2-N1-C1'	5.01	124.31	118.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	2048	G	C8-N9-C1'	-5.01	120.48	127.00
21	A	2583	C	C5-C4-N4	-5.01	116.69	120.20
1	a	147	G	C4-N9-C1'	5.01	133.01	126.50
21	A	2713	G	C6-C5-N7	-5.01	127.39	130.40
21	A	306	C	C6-N1-C2	-5.01	118.30	120.30
1	a	1520	G	C6-C5-N7	-5.01	127.39	130.40
1	a	1541	G	C6-C5-N7	-5.01	127.40	130.40
21	A	498	G	C4-N9-C1'	5.01	133.01	126.50
21	A	1294	G	C4-N9-C1'	5.01	133.01	126.50
21	A	1648	C	C2-N1-C1'	5.01	124.31	118.80
21	A	528	C	N3-C2-O2	-5.00	118.40	121.90
21	A	721	A	N7-C8-N9	5.00	116.30	113.80
21	A	789	C	N1-C2-O2	5.00	121.90	118.90
21	A	1501	G	C4-N9-C1'	5.00	133.00	126.50
21	A	340	C	C6-N1-C2	-5.00	118.30	120.30

There are no chirality outliers.

All (67) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
45	3	43	TYR	Peptide
45	3	44	PRO	Peptide
45	3	63	LYS	Peptide
46	4	32	ASN	Peptide
46	4	45	LYS	Peptide
47	5	10	THR	Peptide
48	6	14	SER	Peptide
48	6	15	LYS	Peptide
49	7	28	PHE	Peptide
49	7	33	PHE	Peptide
23	D	176	ARG	Peptide
24	E	140	PRO	Peptide
24	E	142	SER	Peptide
24	E	62	ASP	Peptide
24	E	64	LYS	Peptide
24	E	65	SER	Peptide
24	E	9	LYS	Peptide
25	F	143	LEU	Peptide
25	F	148	GLN	Peptide
25	F	154	VAL	Peptide
25	F	171	PRO	Peptide
25	F	183	VAL	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
26	G	114	PHE	Peptide
26	G	124	GLY	Peptide
26	G	138	PHE	Peptide
26	G	88	LYS	Peptide
28	M	68	ASN	Peptide
28	M	69	LYS	Peptide
29	N	89	ASP	Peptide
30	O	100	GLY	Peptide
30	O	65	GLY	Peptide
30	O	80	ASP	Peptide
30	O	83	ASN	Peptide
31	P	41	TRP	Peptide
33	R	103	GLY	Peptide
33	R	89	ILE	Peptide
34	S	104	SER	Peptide
35	T	91	ASN	Peptide
36	U	100	ILE	Peptide
38	W	48	VAL	Peptide
38	W	50	VAL	Peptide
40	Y	73	MET	Peptide
41	Z	16	SER	Peptide
41	Z	17	SER	Peptide
41	Z	19	LYS	Peptide
41	Z	22	ARG	Peptide
3	c	107	LYS	Peptide
3	c	24	ALA	Peptide
5	e	162	GLU	Peptide
7	g	13	LEU	Peptide
7	g	14	PRO	Peptide
7	g	17	ILE	Peptide
8	h	79	ARG	Peptide
8	h	98	LEU	Peptide
13	m	102	THR	Peptide
13	m	111	GLY	Peptide
13	m	64	LYS	Peptide
13	m	65	VAL	Peptide
13	m	84	SER	Peptide
14	n	18	VAL	Peptide
14	n	57	ARG	Peptide
17	q	5	ASN	Peptide
17	q	76	ARG	Peptide
17	q	85	VAL	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
19	s	13	GLU	Peptide
19	s	7	LYS	Peptide
19	s	9	PRO	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	b	222/255 (87%)	199 (90%)	23 (10%)	0	100	100
3	c	206/217 (95%)	172 (84%)	34 (16%)	0	100	100
4	d	193/199 (97%)	171 (89%)	21 (11%)	1 (0%)	29	66
5	e	163/165 (99%)	140 (86%)	23 (14%)	0	100	100
6	f	94/96 (98%)	85 (90%)	9 (10%)	0	100	100
7	g	143/150 (95%)	124 (87%)	17 (12%)	2 (1%)	11	46
8	h	129/131 (98%)	109 (84%)	19 (15%)	1 (1%)	19	57
9	i	126/128 (98%)	114 (90%)	12 (10%)	0	100	100
10	j	100/102 (98%)	89 (89%)	11 (11%)	0	100	100
11	k	116/118 (98%)	99 (85%)	17 (15%)	0	100	100
12	l	133/135 (98%)	103 (77%)	30 (23%)	0	100	100
13	m	117/119 (98%)	92 (79%)	23 (20%)	2 (2%)	9	43
14	n	58/60 (97%)	49 (84%)	9 (16%)	0	100	100
15	o	86/88 (98%)	75 (87%)	11 (13%)	0	100	100
16	p	88/90 (98%)	74 (84%)	14 (16%)	0	100	100
17	q	84/86 (98%)	66 (79%)	17 (20%)	1 (1%)	13	50

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	r	69/71 (97%)	58 (84%)	11 (16%)	0	100	100
19	s	82/84 (98%)	66 (80%)	16 (20%)	0	100	100
20	t	78/80 (98%)	71 (91%)	7 (9%)	0	100	100
23	D	273/275 (99%)	236 (86%)	36 (13%)	1 (0%)	34	70
24	E	216/218 (99%)	181 (84%)	33 (15%)	2 (1%)	17	54
25	F	197/199 (99%)	166 (84%)	30 (15%)	1 (0%)	29	66
26	G	164/166 (99%)	132 (80%)	31 (19%)	1 (1%)	25	62
27	H	162/164 (99%)	148 (91%)	14 (9%)	0	100	100
28	M	143/145 (99%)	126 (88%)	17 (12%)	0	100	100
29	N	120/122 (98%)	98 (82%)	19 (16%)	3 (2%)	5	36
30	O	129/131 (98%)	90 (70%)	39 (30%)	0	100	100
31	P	139/141 (99%)	106 (76%)	33 (24%)	0	100	100
32	Q	117/119 (98%)	104 (89%)	13 (11%)	0	100	100
33	R	117/119 (98%)	104 (89%)	13 (11%)	0	100	100
34	S	108/110 (98%)	97 (90%)	11 (10%)	0	100	100
35	T	114/116 (98%)	106 (93%)	8 (7%)	0	100	100
36	U	100/102 (98%)	82 (82%)	18 (18%)	0	100	100
37	V	110/112 (98%)	102 (93%)	8 (7%)	0	100	100
38	W	87/89 (98%)	75 (86%)	10 (12%)	2 (2%)	6	38
39	X	81/100 (81%)	66 (82%)	15 (18%)	0	100	100
40	Y	92/94 (98%)	73 (79%)	17 (18%)	2 (2%)	6	39
41	Z	80/82 (98%)	67 (84%)	13 (16%)	0	100	100
42	0	44/46 (96%)	30 (68%)	14 (32%)	0	100	100
43	1	63/65 (97%)	62 (98%)	1 (2%)	0	100	100
44	2	55/57 (96%)	48 (87%)	7 (13%)	0	100	100
45	3	81/84 (96%)	54 (67%)	24 (30%)	3 (4%)	3	29
46	4	54/56 (96%)	46 (85%)	8 (15%)	0	100	100
47	5	24/39 (62%)	15 (62%)	9 (38%)	0	100	100
48	6	42/44 (96%)	35 (83%)	5 (12%)	2 (5%)	2	24
49	7	58/60 (97%)	47 (81%)	11 (19%)	0	100	100
50	8	35/37 (95%)	29 (83%)	6 (17%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	5292/5466 (97%)	4481 (85%)	787 (15%)	24 (0%)	32	66

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	g	13	LEU
8	h	99	ASN
38	W	50	VAL
45	3	12	VAL
45	3	68	ASP
24	E	10	ILE
29	N	100	GLY
48	6	15	LYS
48	6	16	VAL
13	m	111	GLY
24	E	142	SER
4	d	143	GLU
25	F	144	SER
29	N	25	LEU
40	Y	15	ARG
7	g	14	PRO
38	W	51	ALA
40	Y	16	SER
23	D	195	GLY
45	3	71	VAL
29	N	101	PRO
13	m	65	VAL
26	G	89	VAL
17	q	86	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	b	194/221 (88%)	194 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	c	169/175 (97%)	169 (100%)	0	100	100
4	d	172/174 (99%)	172 (100%)	0	100	100
5	e	130/130 (100%)	129 (99%)	1 (1%)	81	89
6	f	84/84 (100%)	84 (100%)	0	100	100
7	g	126/127 (99%)	126 (100%)	0	100	100
8	h	112/112 (100%)	112 (100%)	0	100	100
9	i	106/106 (100%)	105 (99%)	1 (1%)	78	88
10	j	91/91 (100%)	91 (100%)	0	100	100
11	k	94/94 (100%)	94 (100%)	0	100	100
12	l	117/117 (100%)	117 (100%)	0	100	100
13	m	102/102 (100%)	102 (100%)	0	100	100
14	n	52/52 (100%)	52 (100%)	0	100	100
15	o	80/80 (100%)	80 (100%)	0	100	100
16	p	76/76 (100%)	76 (100%)	0	100	100
17	q	81/81 (100%)	80 (99%)	1 (1%)	71	84
18	r	63/63 (100%)	63 (100%)	0	100	100
19	s	73/73 (100%)	73 (100%)	0	100	100
20	t	67/67 (100%)	67 (100%)	0	100	100
23	D	222/222 (100%)	221 (100%)	1 (0%)	88	94
24	E	175/175 (100%)	175 (100%)	0	100	100
25	F	163/163 (100%)	163 (100%)	0	100	100
26	G	147/147 (100%)	147 (100%)	0	100	100
27	H	144/144 (100%)	144 (100%)	0	100	100
28	M	123/123 (100%)	123 (100%)	0	100	100
29	N	100/100 (100%)	100 (100%)	0	100	100
30	O	104/104 (100%)	104 (100%)	0	100	100
31	P	116/116 (100%)	116 (100%)	0	100	100
32	Q	100/100 (100%)	100 (100%)	0	100	100
33	R	95/95 (100%)	95 (100%)	0	100	100
34	S	96/96 (100%)	96 (100%)	0	100	100
35	T	96/96 (100%)	96 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	U	86/86 (100%)	86 (100%)	0	100	100
37	V	91/91 (100%)	91 (100%)	0	100	100
38	W	80/80 (100%)	80 (100%)	0	100	100
39	X	73/85 (86%)	73 (100%)	0	100	100
40	Y	83/83 (100%)	83 (100%)	0	100	100
41	Z	64/64 (100%)	64 (100%)	0	100	100
42	0	39/39 (100%)	39 (100%)	0	100	100
43	1	59/59 (100%)	59 (100%)	0	100	100
44	2	51/51 (100%)	51 (100%)	0	100	100
45	3	74/75 (99%)	65 (88%)	9 (12%)	5	25
46	4	49/49 (100%)	49 (100%)	0	100	100
47	5	26/37 (70%)	23 (88%)	3 (12%)	5	27
48	6	39/39 (100%)	39 (100%)	0	100	100
49	7	52/52 (100%)	52 (100%)	0	100	100
50	8	35/35 (100%)	35 (100%)	0	100	100
All	All	4571/4631 (99%)	4555 (100%)	16 (0%)	91	95

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	e	45	ARG
9	i	16	ASN
17	q	5	ASN
23	D	85	ASN
45	3	70	ARG
45	3	73	ARG
45	3	74	PHE
45	3	75	ASN
45	3	76	LYS
45	3	77	LYS
45	3	81	LYS
45	3	82	SER
45	3	83	ASN
47	5	32	MET
47	5	35	PHE
47	5	46	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
3	c	3	GLN
7	g	106	ASN
7	g	129	ASN
9	i	16	ASN
9	i	77	GLN
12	l	42	GLN
13	m	76	ASN
15	o	9	ASN
18	r	57	GLN
19	s	22	GLN
19	s	43	ASN
20	t	64	ASN
24	E	66	ASN
25	F	148	GLN
36	U	81	ASN
40	Y	38	ASN
40	Y	78	GLN
46	4	14	ASN
46	4	51	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1546/1547 (99%)	268 (17%)	0
21	A	2910/2918 (99%)	631 (21%)	8 (0%)
22	B	113/114 (99%)	18 (15%)	0
All	All	4569/4579 (99%)	917 (20%)	8 (0%)

All (917) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	10	G
1	a	11	A
1	a	16	G
1	a	23	G
1	a	31	U
1	a	32	G
1	a	33	A
1	a	34	A
1	a	40	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	a	42	G
1	a	48	C
1	a	49	C
1	a	51	A
1	a	52	A
1	a	62	G
1	a	74	G
1	a	82	G
1	a	85	U
1	a	87	C
1	a	88	U
1	a	89	U
1	a	92	C
1	a	107	G
1	a	108	A
1	a	115	A
1	a	120	C
1	a	129	A
1	a	130	A
1	a	131	C
1	a	144	C
1	a	151	A
1	a	156	C
1	a	159	G
1	a	163	C
1	a	182	A
1	a	183	U
1	a	185	U
1	a	196	A
1	a	198	G
1	a	206	A
1	a	211	A
1	a	212	A
1	a	213	G
1	a	219	C
1	a	221	U
1	a	234	A
1	a	248	U
1	a	249	G
1	a	252	U
1	a	255	G
1	a	259	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	a	260	U
1	a	274	G
1	a	275	C
1	a	286	A
1	a	287	A
1	a	294	A
1	a	297	G
1	a	307	G
1	a	315	U
1	a	324	C
1	a	336	C
1	a	337	A
1	a	355	G
1	a	360	C
1	a	362	G
1	a	374	C
1	a	375	U
1	a	376	U
1	a	380	C
1	a	385	G
1	a	390	A
1	a	396	G
1	a	401	A
1	a	405	A
1	a	414	G
1	a	418	G
1	a	419	A
1	a	420	U
1	a	421	G
1	a	422	A
1	a	429	U
1	a	432	G
1	a	437	U
1	a	449	A
1	a	456	A
1	a	457	A
1	a	462	A
1	a	466	G
1	a	471	A
1	a	477	U
1	a	481	C
1	a	482	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	a	483	C
1	a	492	G
1	a	493	G
1	a	499	A
1	a	505	A
1	a	517	A
1	a	519	C
1	a	528	A
1	a	529	G
1	a	532	G
1	a	535	G
1	a	538	G
1	a	539	U
1	a	540	A
1	a	554	A
1	a	555	A
1	a	557	C
1	a	570	U
1	a	571	A
1	a	580	A
1	a	584	C
1	a	585	G
1	a	587	G
1	a	589	G
1	a	595	G
1	a	604	A
1	a	641	U
1	a	650	A
1	a	661	U
1	a	666	G
1	a	673	A
1	a	674	G
1	a	695	A
1	a	703	A
1	a	710	A
1	a	729	A
1	a	741	G
1	a	742	A
1	a	757	A
1	a	759	U
1	a	763	G
1	a	769	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	a	782	G
1	a	785	A
1	a	802	A
1	a	803	C
1	a	807	G
1	a	821	U
1	a	825	C
1	a	826	G
1	a	829	G
1	a	836	A
1	a	840	G
1	a	854	C
1	a	855	G
1	a	861	U
1	a	863	G
1	a	865	G
1	a	879	A
1	a	882	A
1	a	886	A
1	a	899	A
1	a	924	A
1	a	936	G
1	a	944	C
1	a	945	A
1	a	947	A
1	a	970	U
1	a	979	A
1	a	981	G
1	a	984	A
1	a	985	A
1	a	986	G
1	a	992	U
1	a	993	A
1	a	999	U
1	a	1002	U
1	a	1003	G
1	a	1012	U
1	a	1014	A
1	a	1016	A
1	a	1025	G
1	a	1027	U
1	a	1028	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	a	1034	U
1	a	1035	U
1	a	1036	C
1	a	1037	C
1	a	1038	C
1	a	1039	C
1	a	1041	U
1	a	1044	G
1	a	1051	A
1	a	1057	C
1	a	1076	G
1	a	1077	U
1	a	1106	G
1	a	1107	U
1	a	1113	A
1	a	1124	C
1	a	1138	U
1	a	1144	C
1	a	1150	G
1	a	1151	U
1	a	1152	U
1	a	1153	G
1	a	1163	A
1	a	1165	U
1	a	1170	U
1	a	1171	G
1	a	1172	C
1	a	1179	C
1	a	1192	G
1	a	1195	G
1	a	1202	A
1	a	1207	A
1	a	1208	A
1	a	1223	U
1	a	1225	U
1	a	1235	U
1	a	1238	A
1	a	1239	C
1	a	1250	A
1	a	1252	G
1	a	1261	A
1	a	1268	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	a	1271	G
1	a	1289	A
1	a	1291	A
1	a	1297	U
1	a	1298	A
1	a	1304	G
1	a	1310	A
1	a	1312	U
1	a	1313	U
1	a	1328	C
1	a	1329	A
1	a	1331	C
1	a	1333	C
1	a	1334	G
1	a	1347	U
1	a	1351	A
1	a	1357	A
1	a	1358	G
1	a	1359	U
1	a	1375	U
1	a	1381	G
1	a	1386	A
1	a	1389	C
1	a	1409	A
1	a	1411	C
1	a	1412	G
1	a	1430	G
1	a	1437	A
1	a	1453	G
1	a	1454	A
1	a	1457	A
1	a	1463	U
1	a	1492	A
1	a	1496	U
1	a	1515	A
1	a	1518	U
1	a	1519	A
1	a	1520	G
1	a	1529	G
1	a	1531	A
1	a	1532	G
1	a	1540	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	a	1541	G
1	a	1542	G
1	a	1543	A
1	a	1545	C
1	a	1546	A
1	a	1547	C
1	a	1549	U
21	A	14	A
21	A	28	A
21	A	34	U
21	A	52	A
21	A	64	A
21	A	71	A
21	A	74	U
21	A	75	G
21	A	80	G
21	A	84	A
21	A	85	G
21	A	90	A
21	A	96	G
21	A	98	U
21	A	102	A
21	A	104	C
21	A	113	U
21	A	117	A
21	A	118	A
21	A	119	U
21	A	124	A
21	A	130	A
21	A	133	A
21	A	142	G
21	A	145	A
21	A	150	A
21	A	154	A
21	A	157	U
21	A	160	G
21	A	161	A
21	A	162	A
21	A	163	U
21	A	165	C
21	A	167	U
21	A	168	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	A	169	G
21	A	184	C
21	A	199	A
21	A	200	A
21	A	202	A
21	A	207	A
21	A	218	G
21	A	219	A
21	A	225	A
21	A	227	G
21	A	229	A
21	A	235	G
21	A	236	A
21	A	244	A
21	A	251	G
21	A	253	G
21	A	255	G
21	A	272	C
21	A	284	C
21	A	285	U
21	A	286	U
21	A	288	C
21	A	289	U
21	A	295	G
21	A	298	U
21	A	300	G
21	A	301	U
21	A	314	A
21	A	315	C
21	A	316	G
21	A	317	G
21	A	319	G
21	A	320	U
21	A	321	U
21	A	322	A
21	A	326	A
21	A	331	G
21	A	338	G
21	A	351	G
21	A	354	A
21	A	358	G
21	A	365	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	A	367	A
21	A	372	A
21	A	373	A
21	A	374	U
21	A	378	C
21	A	381	G
21	A	389	A
21	A	398	C
21	A	401	U
21	A	403	U
21	A	404	U
21	A	410	G
21	A	411	A
21	A	413	C
21	A	418	G
21	A	430	A
21	A	432	G
21	A	457	G
21	A	459	C
21	A	466	C
21	A	494	U
21	A	497	U
21	A	502	C
21	A	503	A
21	A	511	G
21	A	513	G
21	A	525	A
21	A	526	A
21	A	527	G
21	A	544	U
21	A	550	A
21	A	553	A
21	A	554	C
21	A	555	C
21	A	572	C
21	A	574	A
21	A	575	G
21	A	576	U
21	A	577	A
21	A	578	G
21	A	591	A
21	A	593	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	A	594	G
21	A	606	G
21	A	611	U
21	A	613	G
21	A	614	U
21	A	615	A
21	A	618	A
21	A	646	A
21	A	658	A
21	A	659	A
21	A	660	A
21	A	661	U
21	A	662	G
21	A	666	A
21	A	682	A
21	A	683	G
21	A	690	U
21	A	693	G
21	A	694	G
21	A	698	U
21	A	699	U
21	A	715	A
21	A	716	C
21	A	722	A
21	A	727	G
21	A	731	U
21	A	732	C
21	A	744	A
21	A	756	A
21	A	769	U
21	A	774	G
21	A	775	A
21	A	784	A
21	A	785	C
21	A	792	U
21	A	793	G
21	A	794	A
21	A	798	G
21	A	809	A
21	A	813	G
21	A	820	G
21	A	821	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	A	825	G
21	A	827	A
21	A	828	A
21	A	829	U
21	A	834	A
21	A	838	A
21	A	845	A
21	A	846	G
21	A	849	A
21	A	850	G
21	A	872	U
21	A	873	U
21	A	875	G
21	A	881	G
21	A	902	A
21	A	904	G
21	A	911	A
21	A	921	C
21	A	922	G
21	A	923	A
21	A	924	G
21	A	925	G
21	A	927	G
21	A	932	U
21	A	938	G
21	A	952	A
21	A	955	A
21	A	957	C
21	A	958	U
21	A	959	C
21	A	960	C
21	A	970	U
21	A	985	A
21	A	989	A
21	A	990	G
21	A	1005	G
21	A	1017	A
21	A	1018	A
21	A	1029	C
21	A	1034	A
21	A	1040	A
21	A	1049	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	A	1055	A
21	A	1056	U
21	A	1057	A
21	A	1061	G
21	A	1066	G
21	A	1067	U
21	A	1069	G
21	A	1070	A
21	A	1073	A
21	A	1077	U
21	A	1078	G
21	A	1085	U
21	A	1089	C
21	A	1090	A
21	A	1091	G
21	A	1100	G
21	A	1101	A
21	A	1102	U
21	A	1105	U
21	A	1106	G
21	A	1109	U
21	A	1111	A
21	A	1113	A
21	A	1114	A
21	A	1115	G
21	A	1116	C
21	A	1119	C
21	A	1120	C
21	A	1124	A
21	A	1126	U
21	A	1127	U
21	A	1128	A
21	A	1132	A
21	A	1133	G
21	A	1137	G
21	A	1138	U
21	A	1139	A
21	A	1143	G
21	A	1145	U
21	A	1146	C
21	A	1150	A
21	A	1154	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	A	1155	A
21	A	1156	G
21	A	1158	G
21	A	1163	U
21	A	1170	A
21	A	1171	A
21	A	1172	A
21	A	1174	U
21	A	1175	G
21	A	1177	A
21	A	1178	C
21	A	1179	C
21	A	1183	G
21	A	1184	C
21	A	1186	A
21	A	1195	A
21	A	1214	C
21	A	1218	G
21	A	1248	U
21	A	1250	G
21	A	1258	A
21	A	1265	G
21	A	1273	G
21	A	1276	G
21	A	1277	C
21	A	1278	G
21	A	1285	A
21	A	1286	G
21	A	1288	G
21	A	1289	A
21	A	1291	A
21	A	1292	A
21	A	1293	U
21	A	1294	G
21	A	1303	A
21	A	1306	C
21	A	1309	G
21	A	1310	A
21	A	1337	A
21	A	1338	U
21	A	1355	A
21	A	1362	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	A	1376	G
21	A	1378	U
21	A	1379	A
21	A	1383	G
21	A	1403	C
21	A	1405	G
21	A	1416	U
21	A	1421	A
21	A	1423	C
21	A	1437	U
21	A	1449	A
21	A	1450	A
21	A	1451	U
21	A	1454	U
21	A	1455	U
21	A	1459	A
21	A	1463	A
21	A	1464	U
21	A	1471	A
21	A	1472	C
21	A	1489	A
21	A	1490	G
21	A	1491	C
21	A	1494	G
21	A	1495	C
21	A	1496	G
21	A	1497	A
21	A	1498	U
21	A	1499	U
21	A	1504	U
21	A	1505	G
21	A	1506	C
21	A	1510	U
21	A	1512	U
21	A	1516	C
21	A	1519	U
21	A	1520	A
21	A	1521	A
21	A	1525	U
21	A	1527	A
21	A	1534	G
21	A	1536	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	A	1537	A
21	A	1540	U
21	A	1551	U
21	A	1552	U
21	A	1553	A
21	A	1555	G
21	A	1561	G
21	A	1567	A
21	A	1568	U
21	A	1569	G
21	A	1570	G
21	A	1571	G
21	A	1576	A
21	A	1577	G
21	A	1579	C
21	A	1580	A
21	A	1582	U
21	A	1583	G
21	A	1584	A
21	A	1585	G
21	A	1586	U
21	A	1587	C
21	A	1605	A
21	A	1606	C
21	A	1613	G
21	A	1614	A
21	A	1616	A
21	A	1621	C
21	A	1625	U
21	A	1629	U
21	A	1631	G
21	A	1632	A
21	A	1633	A
21	A	1636	U
21	A	1651	C
21	A	1652	A
21	A	1655	C
21	A	1659	C
21	A	1660	A
21	A	1662	A
21	A	1678	A
21	A	1684	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	A	1690	A
21	A	1691	G
21	A	1692	C
21	A	1704	C
21	A	1709	A
21	A	1716	C
21	A	1717	G
21	A	1718	G
21	A	1737	U
21	A	1738	C
21	A	1739	G
21	A	1740	G
21	A	1742	A
21	A	1746	G
21	A	1759	G
21	A	1768	C
21	A	1772	G
21	A	1775	G
21	A	1777	G
21	A	1782	A
21	A	1783	G
21	A	1785	G
21	A	1790	G
21	A	1791	G
21	A	1800	A
21	A	1801	C
21	A	1808	U
21	A	1811	A
21	A	1818	A
21	A	1826	G
21	A	1827	C
21	A	1828	U
21	A	1829	A
21	A	1833	C
21	A	1835	U
21	A	1843	U
21	A	1844	G
21	A	1846	A
21	A	1855	G
21	A	1856	A
21	A	1861	U
21	A	1862	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	A	1865	C
21	A	1893	A
21	A	1895	C
21	A	1897	U
21	A	1899	U
21	A	1926	A
21	A	1928	A
21	A	1933	G
21	A	1939	A
21	A	1950	U
21	A	1956	G
21	A	1957	G
21	A	1958	U
21	A	1963	A
21	A	1964	A
21	A	1965	A
21	A	1968	C
21	A	1969	C
21	A	1970	U
21	A	1972	G
21	A	1982	U
21	A	1983	U
21	A	1989	C
21	A	1994	C
21	A	1997	A
21	A	1998	A
21	A	1999	G
21	A	2002	G
21	A	2008	A
21	A	2018	U
21	A	2020	U
21	A	2048	G
21	A	2050	A
21	A	2057	A
21	A	2058	A
21	A	2059	G
21	A	2060	A
21	A	2061	U
21	A	2070	C
21	A	2079	G
21	A	2082	C
21	A	2083	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	A	2087	A
21	A	2088	G
21	A	2096	G
21	A	2119	U
21	A	2120	G
21	A	2127	G
21	A	2139	A
21	A	2140	C
21	A	2143	G
21	A	2145	U
21	A	2147	G
21	A	2155	C
21	A	2160	G
21	A	2161	A
21	A	2162	A
21	A	2165	G
21	A	2172	C
21	A	2173	U
21	A	2174	A
21	A	2175	G
21	A	2185	A
21	A	2186	G
21	A	2188	C
21	A	2194	U
21	A	2195	G
21	A	2198	A
21	A	2208	A
21	A	2212	G
21	A	2217	G
21	A	2226	A
21	A	2230	G
21	A	2231	C
21	A	2238	U
21	A	2240	U
21	A	2241	C
21	A	2252	A
21	A	2265	G
21	A	2266	G
21	A	2275	C
21	A	2278	G
21	A	2290	C
21	A	2293	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	A	2294	A
21	A	2295	A
21	A	2305	A
21	A	2306	G
21	A	2310	C
21	A	2314	A
21	A	2333	U
21	A	2334	G
21	A	2335	G
21	A	2337	A
21	A	2339	U
21	A	2342	U
21	A	2346	U
21	A	2347	A
21	A	2348	G
21	A	2349	A
21	A	2352	G
21	A	2353	U
21	A	2354	A
21	A	2358	G
21	A	2361	U
21	A	2362	A
21	A	2363	A
21	A	2372	G
21	A	2374	C
21	A	2377	C
21	A	2410	G
21	A	2412	C
21	A	2415	A
21	A	2419	A
21	A	2429	U
21	A	2430	C
21	A	2433	C
21	A	2449	C
21	A	2450	U
21	A	2452	A
21	A	2456	G
21	A	2457	A
21	A	2458	U
21	A	2462	A
21	A	2467	C
21	A	2468	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	A	2472	G
21	A	2475	A
21	A	2492	C
21	A	2497	G
21	A	2505	A
21	A	2518	U
21	A	2521	G
21	A	2525	C
21	A	2526	C
21	A	2529	G
21	A	2530	A
21	A	2532	G
21	A	2533	U
21	A	2540	A
21	A	2545	A
21	A	2549	U
21	A	2552	G
21	A	2560	U
21	A	2561	C
21	A	2562	G
21	A	2576	G
21	A	2579	U
21	A	2582	U
21	A	2583	C
21	A	2589	U
21	A	2593	A
21	A	2594	G
21	A	2599	A
21	A	2600	C
21	A	2601	G
21	A	2605	G
21	A	2609	G
21	A	2612	U
21	A	2613	C
21	A	2624	G
21	A	2629	A
21	A	2630	G
21	A	2636	U
21	A	2638	C
21	A	2640	U
21	A	2648	G
21	A	2657	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	A	2661	A
21	A	2666	A
21	A	2683	U
21	A	2690	G
21	A	2708	C
21	A	2709	U
21	A	2716	U
21	A	2717	A
21	A	2741	G
21	A	2753	U
21	A	2756	G
21	A	2760	A
21	A	2766	U
21	A	2767	A
21	A	2771	G
21	A	2783	U
21	A	2784	A
21	A	2785	A
21	A	2788	A
21	A	2791	A
21	A	2792	A
21	A	2793	G
21	A	2803	A
21	A	2804	G
21	A	2805	A
21	A	2806	U
21	A	2807	G
21	A	2817	A
21	A	2820	U
21	A	2821	U
21	A	2824	G
21	A	2827	A
21	A	2838	C
21	A	2845	G
21	A	2846	A
21	A	2850	G
21	A	2853	U
21	A	2855	A
21	A	2856	U
21	A	2869	G
21	A	2882	A
21	A	2887	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	A	2892	G
21	A	2899	A
21	A	2900	C
21	A	2903	A
21	A	2905	C
21	A	2906	G
21	A	2913	G
21	A	2917	U
22	B	2	C
22	B	10	U
22	B	12	U
22	B	23	U
22	B	24	C
22	B	27	A
22	B	30	U
22	B	33	U
22	B	39	G
22	B	40	C
22	B	42	G
22	B	43	A
22	B	49	G
22	B	73	G
22	B	87	G
22	B	88	U
22	B	106	U
22	B	108	G

All (8) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
21	A	160	G
21	A	199	A
21	A	377	U
21	A	661	U
21	A	1127	U
21	A	1938	U
21	A	1962	G
21	A	2230	G

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 41 ligands modelled in this entry, 41 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

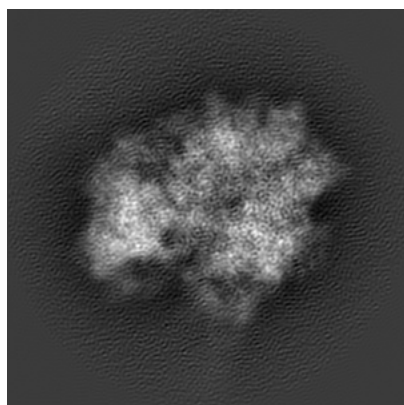
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4050. These allow visual inspection of the internal detail of the map and identification of artifacts.

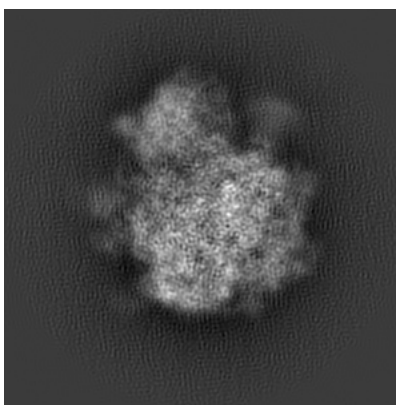
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

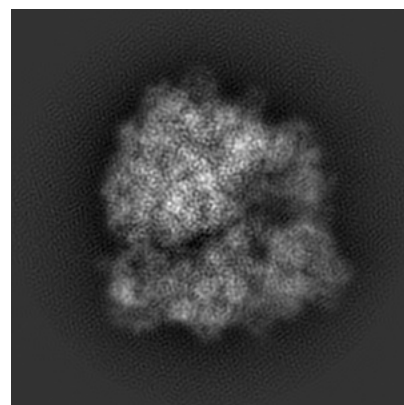
6.1.1 Primary map



X



Y

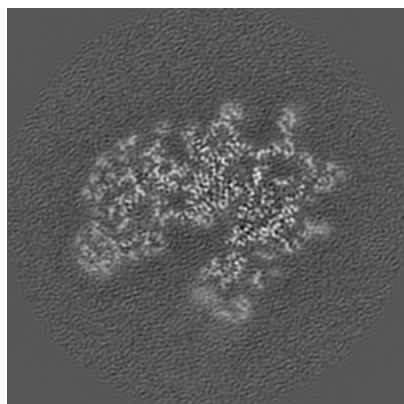


Z

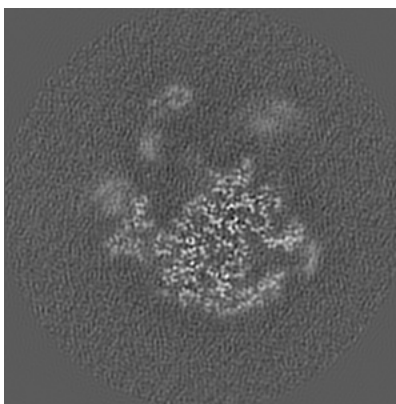
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

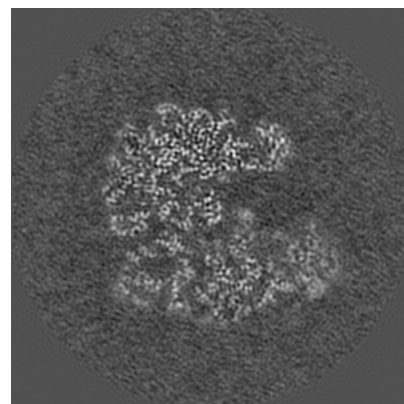
6.2.1 Primary map



X Index: 166



Y Index: 166

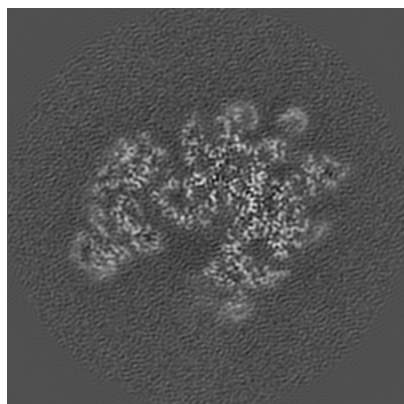


Z Index: 166

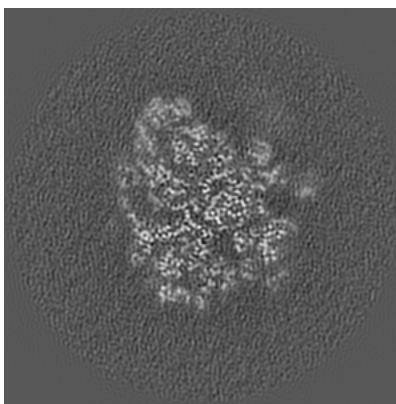
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

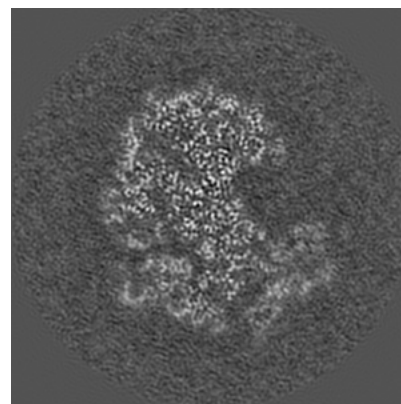
6.3.1 Primary map



X Index: 160



Y Index: 211



Z Index: 182

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

6.4 Orthogonal surface views [i](#)

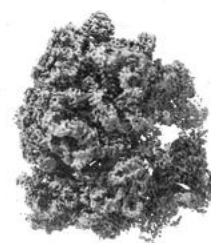
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.095. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

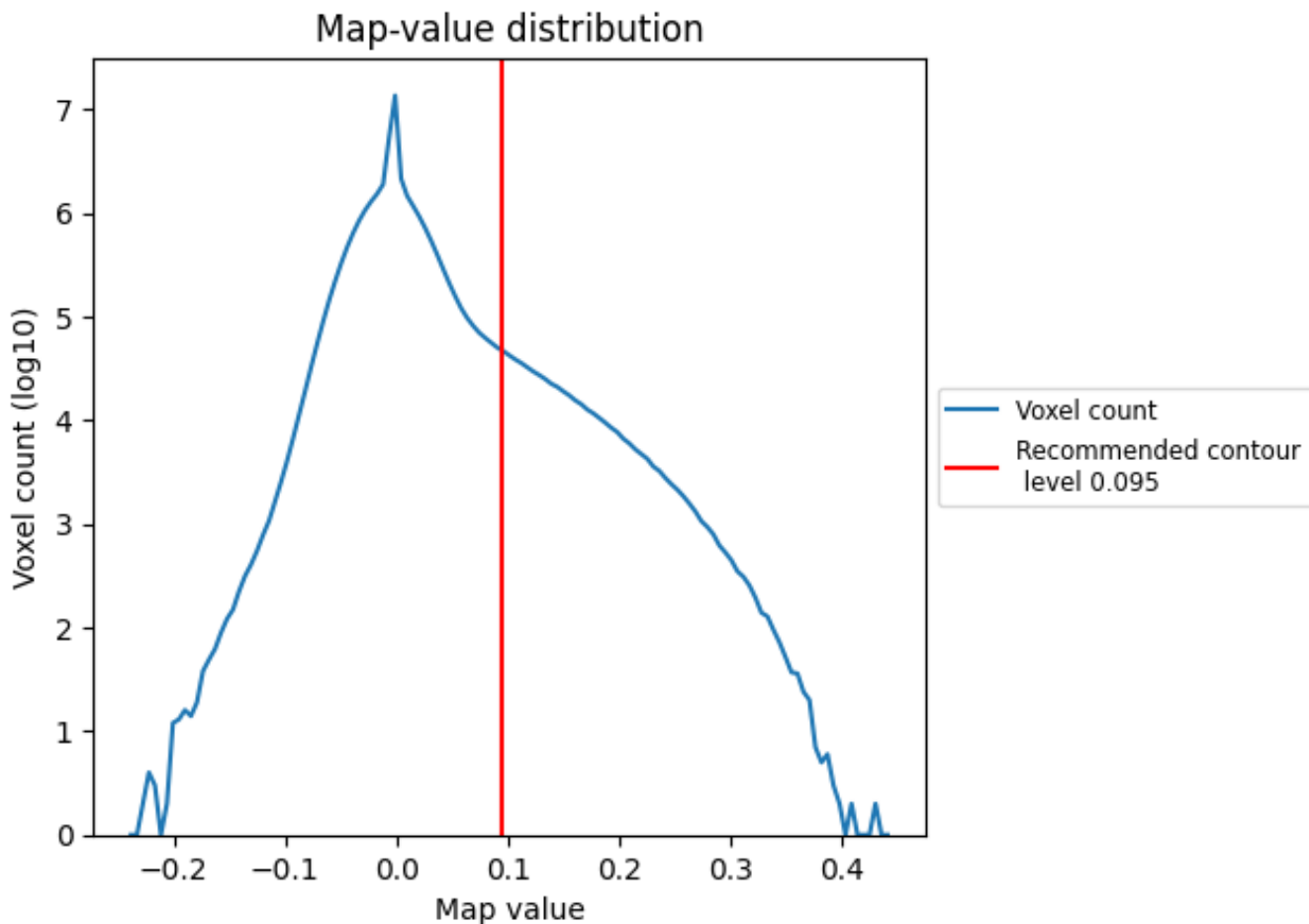
6.5 Mask visualisation

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

7 Map analysis [i](#)

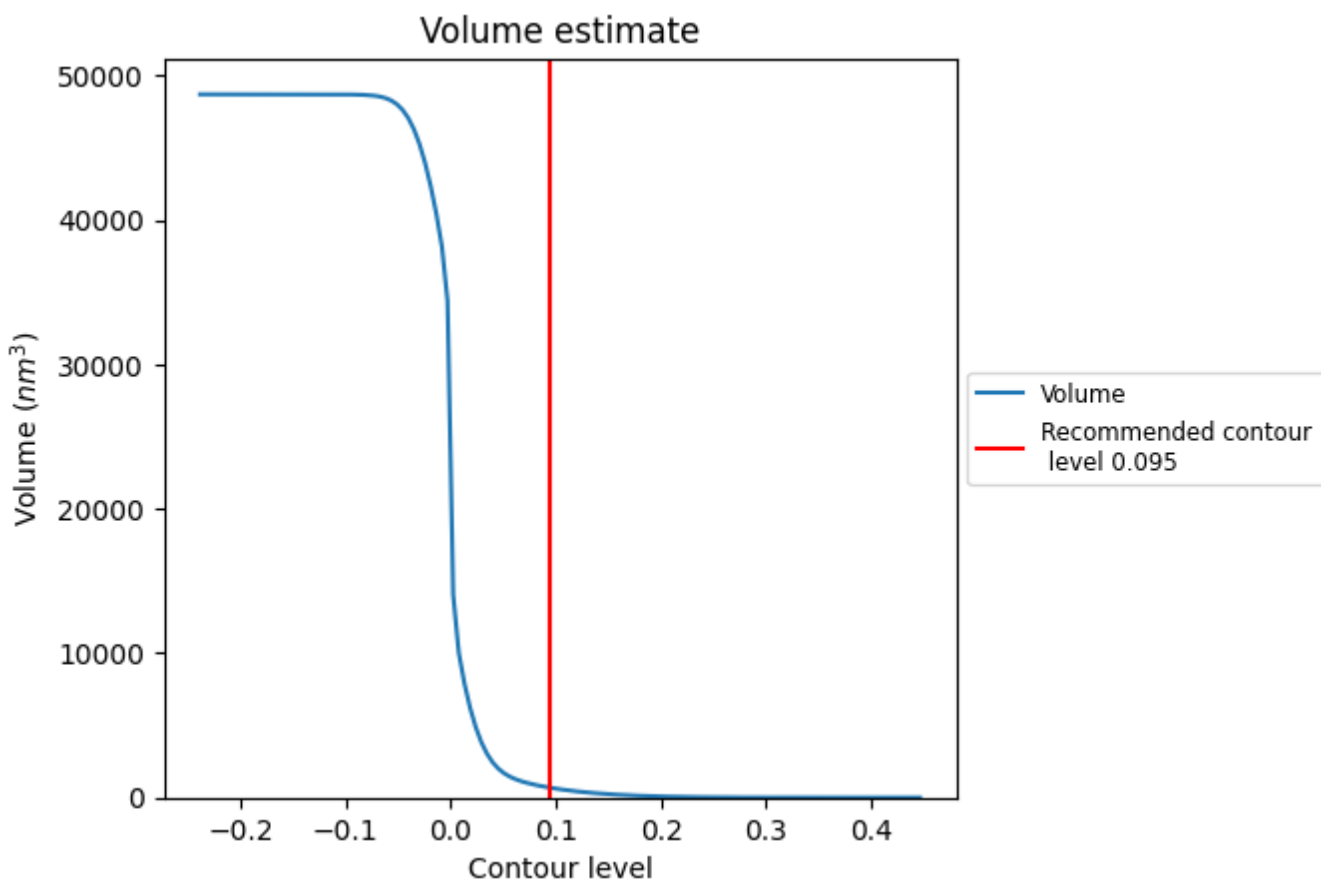
This section contains the results of statistical analysis of the map.

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.

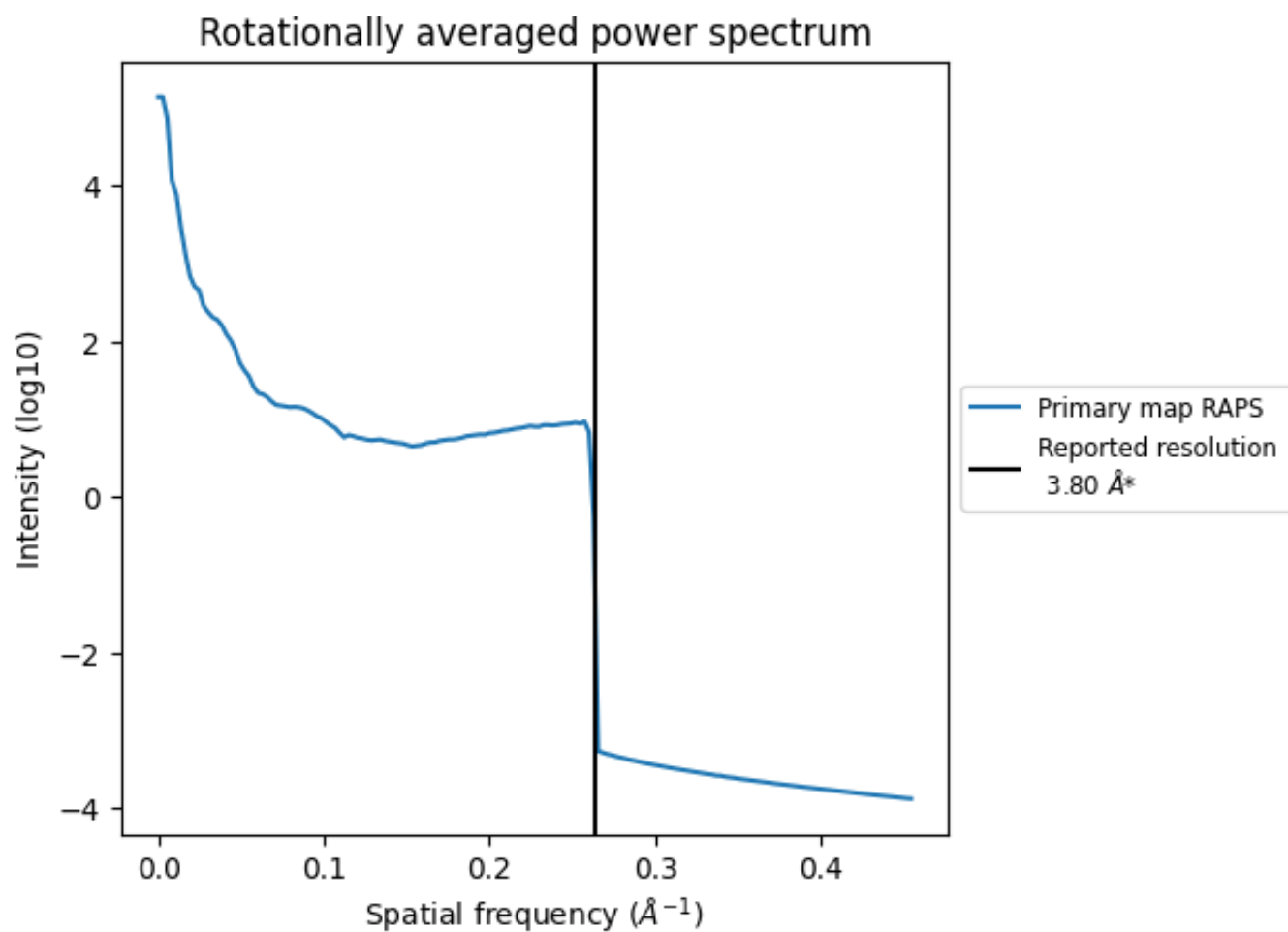
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 679 nm³; this corresponds to an approximate mass of 613 kDa.

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

7.3 Rotationally averaged power spectrum i



*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

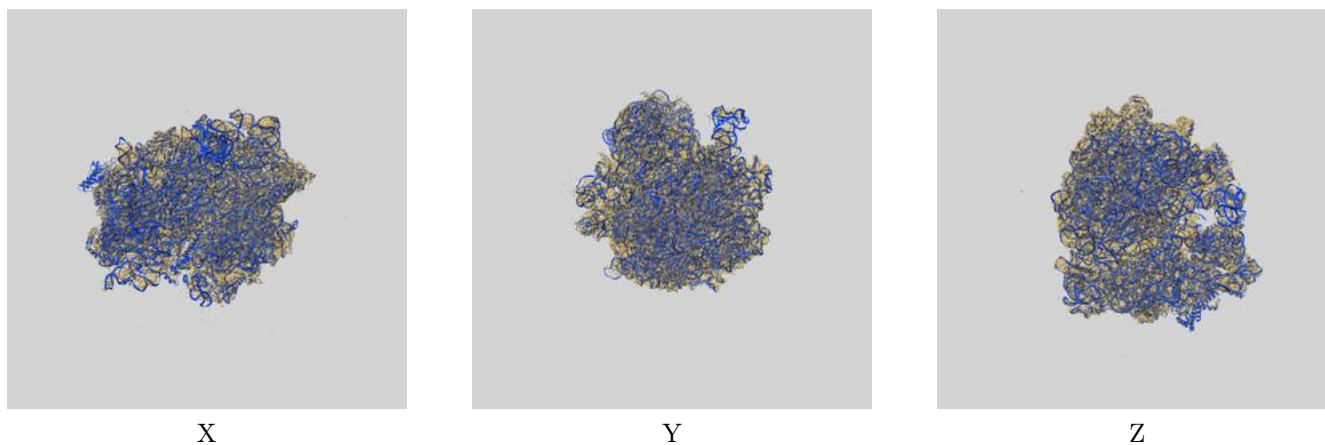
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

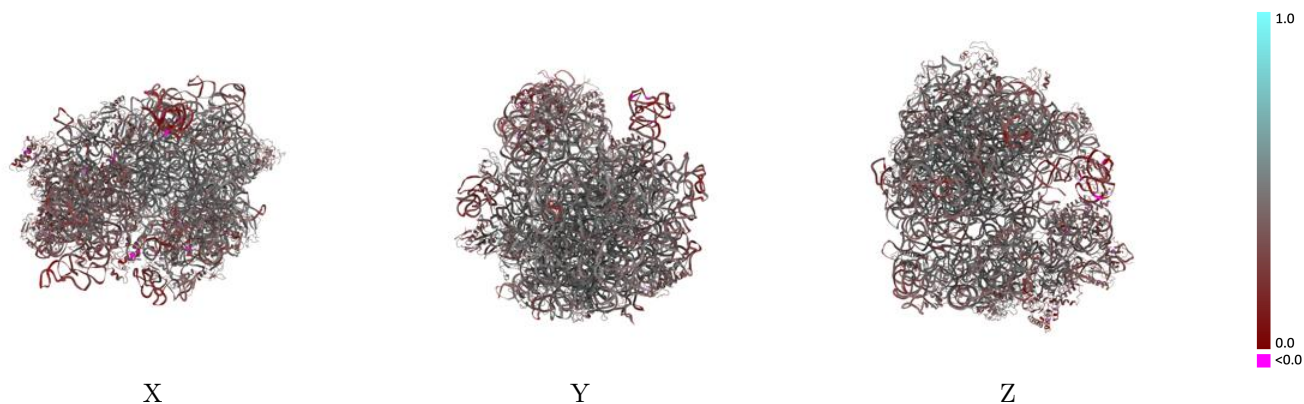
This section contains information regarding the fit between EMDB map EMD-4050 and PDB model 5LI0. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)



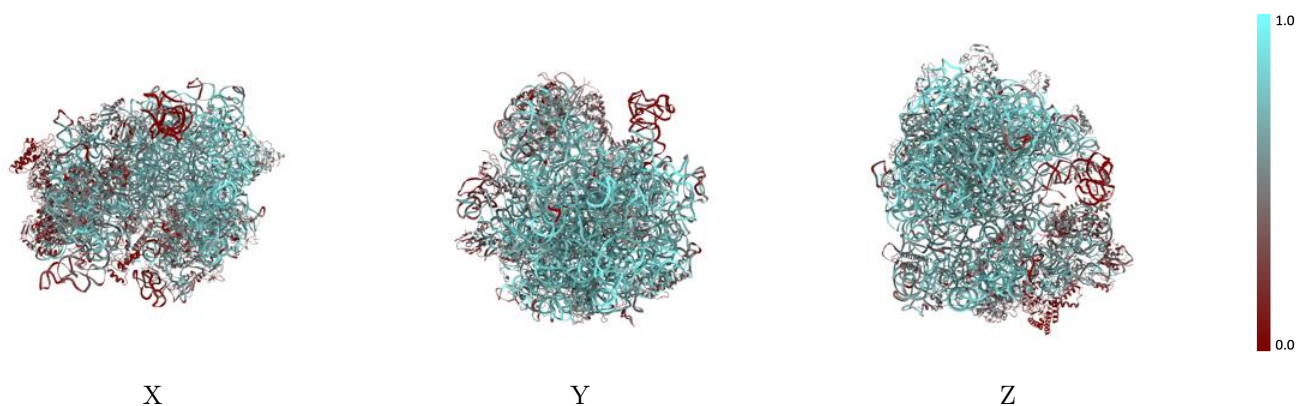
The images above show the 3D surface view of the map at the recommended contour level 0.095 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



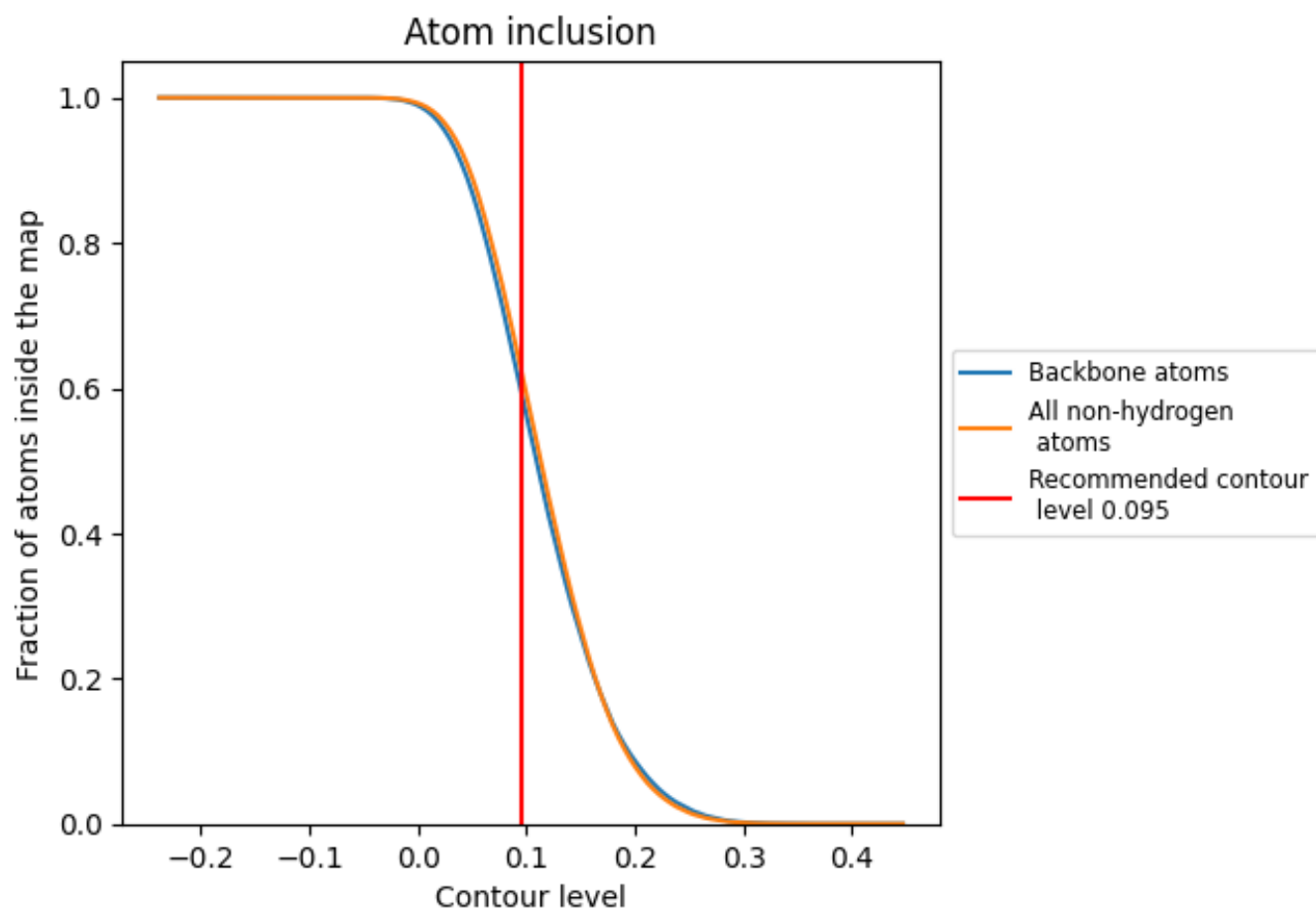
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.095).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 60% of all backbone atoms, 63% 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 (0.095) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6251	 0.4050
0	 0.5531	 0.4180
1	 0.4760	 0.3730
2	 0.5622	 0.4520
3	 0.1624	 0.2260
4	 0.5117	 0.4080
5	 0.5405	 0.3790
6	 0.6364	 0.4550
7	 0.5957	 0.4100
8	 0.5411	 0.4420
A	 0.7325	 0.4210
B	 0.7021	 0.3920
D	 0.5938	 0.4630
E	 0.5803	 0.4540
F	 0.5462	 0.4160
G	 0.3279	 0.2920
H	 0.3771	 0.3630
M	 0.5770	 0.4480
N	 0.5318	 0.4600
O	 0.5477	 0.3990
P	 0.5060	 0.4150
Q	 0.5529	 0.4200
R	 0.4378	 0.3590
S	 0.5141	 0.4400
T	 0.6202	 0.4490
U	 0.5311	 0.4440
V	 0.5529	 0.4470
W	 0.4944	 0.4010
X	 0.4471	 0.3890
Y	 0.3559	 0.3870
Z	 0.5625	 0.4420
a	 0.6685	 0.3980
b	 0.1336	 0.3060
c	 0.3010	 0.3470
d	 0.3813	 0.3530



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
e	 0.4335	 0.4010
f	 0.4374	 0.3970
g	 0.2693	 0.3330
h	 0.4747	 0.4040
i	 0.2768	 0.3380
j	 0.2594	 0.3530
k	 0.3666	 0.3690
l	 0.4060	 0.3860
m	 0.2055	 0.2880
n	 0.3534	 0.3370
o	 0.5106	 0.3950
p	 0.4604	 0.3860
q	 0.4348	 0.4070
r	 0.3657	 0.3720
s	 0.1889	 0.2760
t	 0.4374	 0.3600