



Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 04:08 pm GMT

PDB ID : 5ND9
EMDB ID : EMD-3625
Title : Hibernating ribosome from Staphylococcus aureus (Rotated state)
Authors : Khusainov, I.; Vicens, Q.; Ayupov, R.; Usachev, K.; Myasnikov, A.; Simonetti, A.; Validov, S.; Kieffer, B.; Yusupova, G.; Yusupov, M.; Hashem, Y.
Deposited on : 2017-03-07
Resolution : 3.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

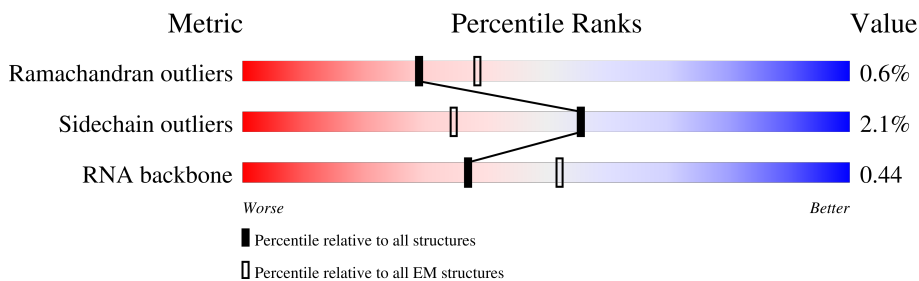
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance

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

The reported resolution of this entry is 3.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	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	1556	
2	b	255	
3	c	217	
4	d	200	
5	e	166	
6	f	98	
7	g	156	
8	h	132	

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Mol	Chain	Length	Quality of chain
9	i	132	77% 97%
10	j	102	78% 94%
11	k	129	34% 87% 11%
12	l	137	23% 93% 6%
13	m	121	77% 89% 9%
14	n	61	66% 93% 5%
15	o	89	22% 96%
16	p	91	19% 97%
17	q	87	31% 95%
18	r	80	30% 69% 30%
19	s	92	66% 90% 9%
20	t	83	27% 95%
21	u	58	76% 59% 19% 22%
22	v	190	46% 35% 15% 47%
23	A	2923	7% 63% 33%
24	B	114	73% 27%
25	D	277	9% 96%
26	E	220	10% 95%
27	F	207	9% 94%
28	G	179	54% 92% 7%
29	H	178	30% 91% 8%
30	M	145	8% 99%
31	N	122	16% 99%
32	O	146	8% 84% 6% 10%
33	P	144	10% 86% 6% 8%

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Mol	Chain	Length	Quality of chain
34	Q	122	13% 95% ..
35	R	119	28% 97% .
36	S	116	12% 89% .. 8%
37	T	118	. 96% ..
38	U	102	15% 97% .
39	V	117	9% 96% .
40	W	91	19% 98% .
41	X	105	18% 82% .. 17%
42	Y	217	39% 42% 57%
43	Z	94	5% 79% .. 18%
44	0	62	15% 71% .. 26%
45	1	69	19% 94% 6%
46	2	59	7% 90% 7% .
47	3	84	82% 88% 8% .
48	4	58	24% 72% .. 24%
49	5	49	53% 55% 43%
50	6	45	. 89% 7% ..
51	7	66	8% 82% 9% 9%
52	8	37	8% 97% .

2 Entry composition [i](#)

There are 52 unique types of molecules in this entry. The entry contains 141051 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	1541	33006	14736	6021	10708	1541	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	222	1788	1139	313	330	6	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	203	1600	1007	301	290	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	160	1194	750	218	224	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	94	781	494	137	147	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	143	1142	712	216	210	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	99	791	498	144	147	2	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	115	851	526	160	162	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	1058	658	214	184	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	110	877	537	175	164	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	85	Total	C	N	O	S	0	0
			698	441	125	131	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	r	56	Total	C	N	O	S	0	0
			466	295	88	81	2		

- 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
			677	434	120	121	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
			606	367	119	118	2		

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
21	u	45	377	233	76	68	0	0

- Molecule 22 is a protein called Ribosome hibernation promotion factor.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
22	v	101	831	518	156	157	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
23	A	2914	62480	27894	11427	20245	2914	0	0

- Molecule 24 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
24	B	114	2430	1086	436	794	114	0	0

- Molecule 25 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	D	275	2103	1309	417	372	5	0	0

- Molecule 26 is a protein called 50S ribosomal protein L3.

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

- Molecule 27 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	F	199	1524	955	281	286	2	0	0

- Molecule 28 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	G	166	1311	832	223	250	6	0	0

- Molecule 29 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	H	164	1284	799	232	250	3	0	0

- Molecule 30 is a protein called 50S ribosomal protein L13.

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

- Molecule 31 is a protein called 50S ribosomal protein L14.

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

- Molecule 32 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	O	131	997	618	197	181	1	0	0

- Molecule 33 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	P	133	1065	681	203	178	3	0	0

- Molecule 34 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	Q	117	924	564	179	180	1	0	0

- Molecule 35 is a protein called 50S ribosomal protein L18.

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

- Molecule 36 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	S	107	862	544	173	145		0	0

- Molecule 37 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	T	116	943	593	189	157	4	0	0

- Molecule 38 is a protein called 50S ribosomal protein L21.

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

- Molecule 39 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	V	112	862	537	164	158	3	0	0

- Molecule 40 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	W	89	725	457	130	134	4	0	0

- Molecule 41 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	X	87	668	423	122	122	1	0	0

- Molecule 42 is a protein called 50S ribosomal protein L25.

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

- Molecule 43 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Z	77	Total	C	N	O		0	0
			591	364	115	112			

- Molecule 44 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	0	46	Total	C	N	O		0	0
			373	231	83	59			

- Molecule 45 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	1	65	Total	C	N	O		0	0
			536	330	101	105			

- Molecule 46 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	2	57	Total	C	N	O		0	0
			441	274	83	84			

- Molecule 47 is a protein called 50S ribosomal protein L31 type B.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	3	81	Total	C	N	O	S	0	0
			663	423	113	124	3		

- Molecule 48 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	4	44	Total	C	N	O	S	0	0
			360	220	78	58	4		

- Molecule 49 is a protein called 50S ribosomal protein L33 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	5	28	229	137	45	43	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	6	44	373	228	90	54	1	0	0

- Molecule 51 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	7	60	487	300	108	77	2	0	0

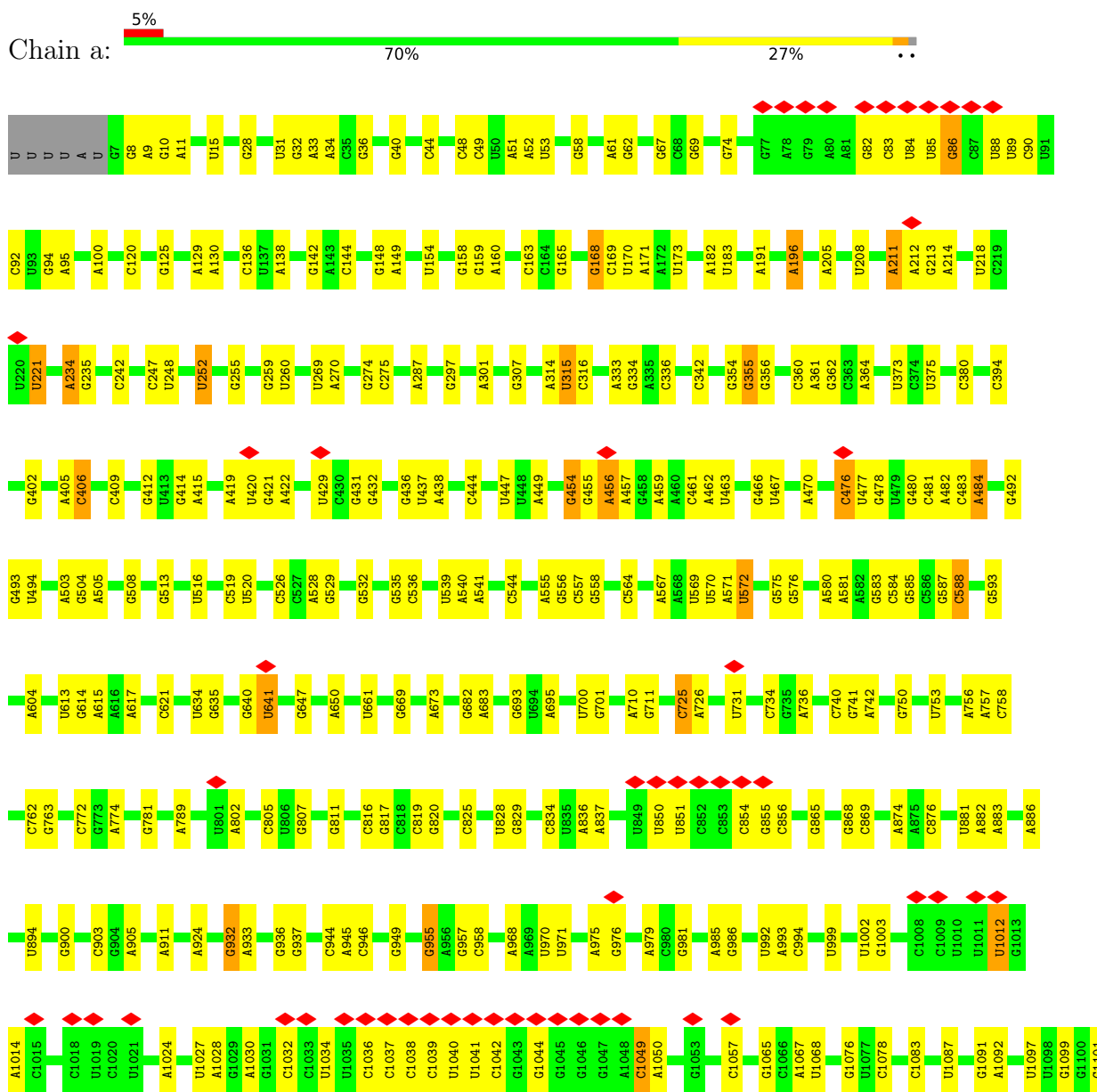
- Molecule 52 is a protein called 50S ribosomal protein L36.

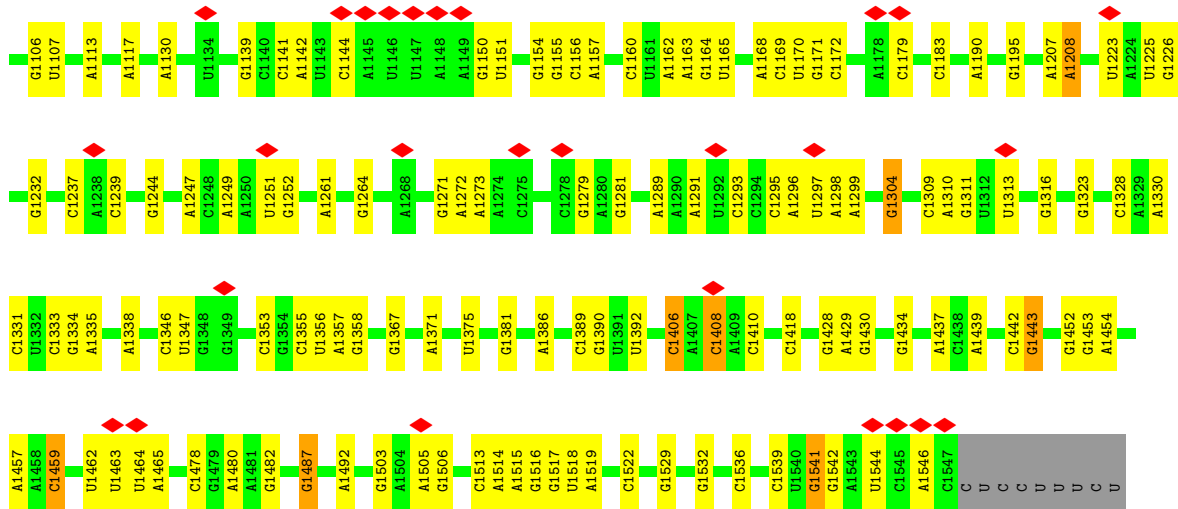
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	8	37	297	186	60	46	5	0	0

3 Residue-property plots

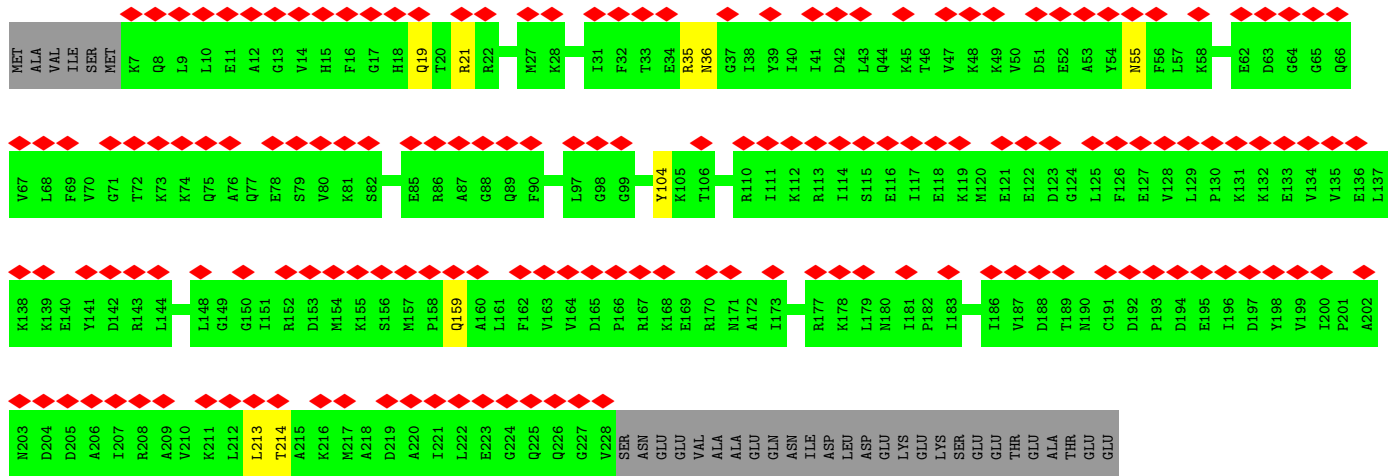
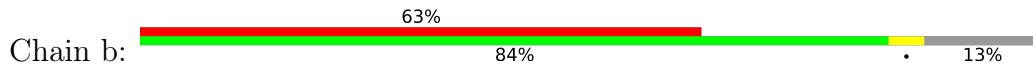
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

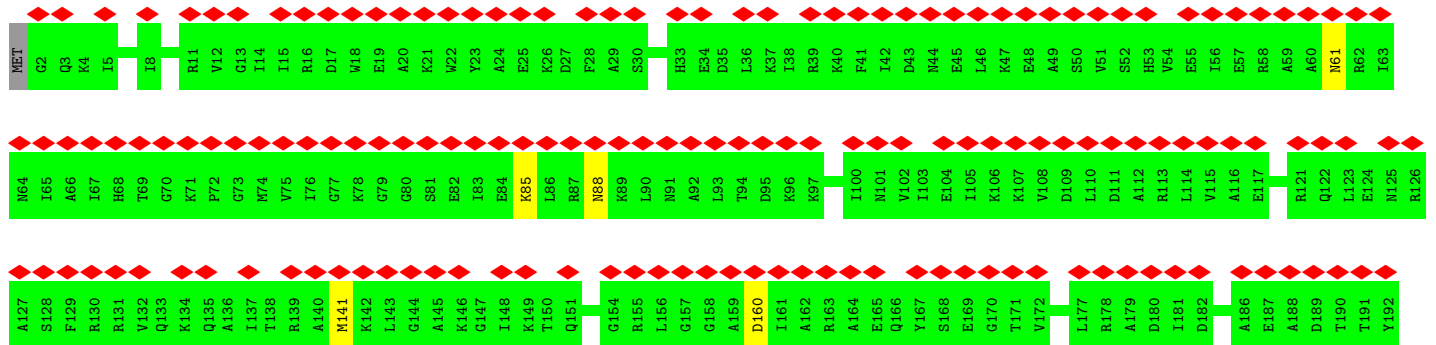
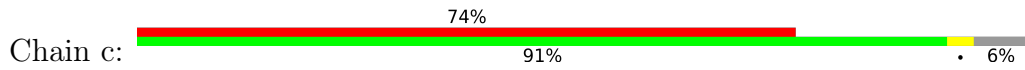


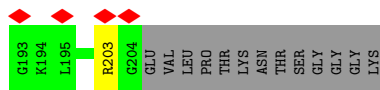


• Molecule 2: 30S ribosomal protein S2

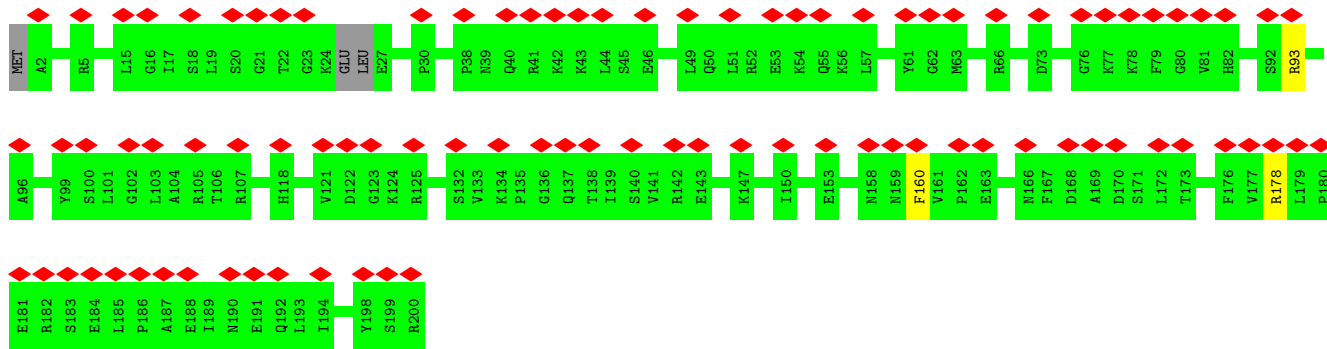


• Molecule 3: 30S ribosomal protein S3

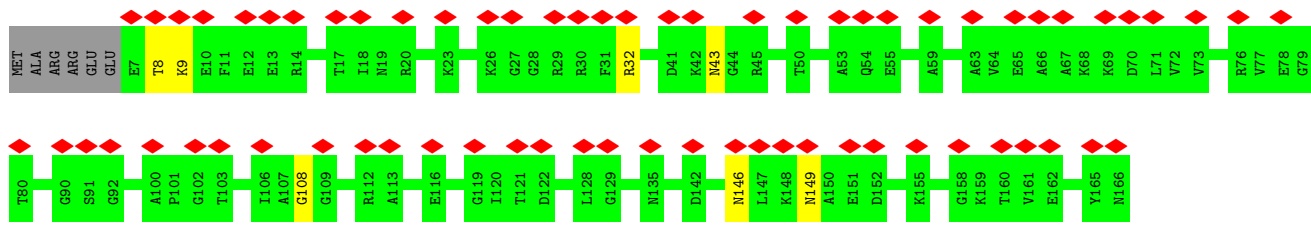
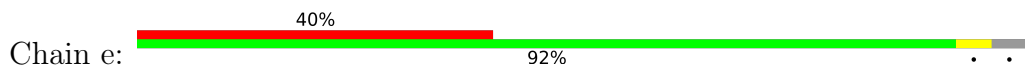




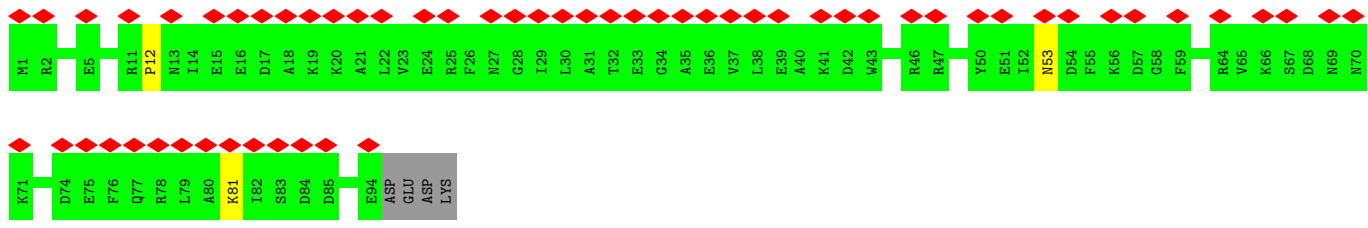
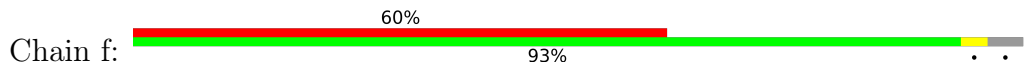
• Molecule 4: 30S ribosomal protein S4



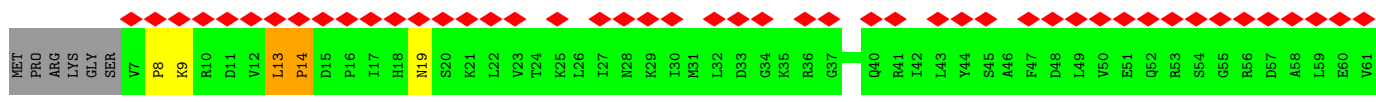
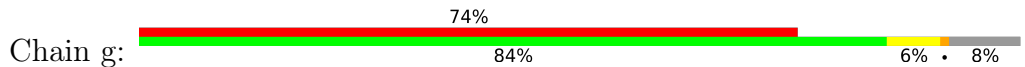
• Molecule 5: 30S ribosomal protein S5

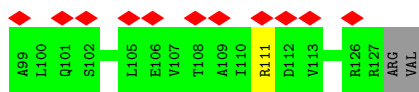


• Molecule 6: 30S ribosomal protein S6

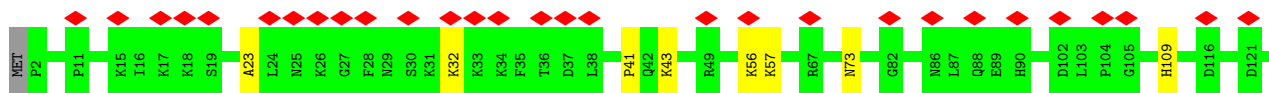
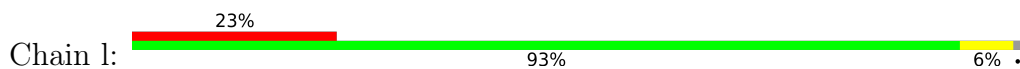


• Molecule 7: 30S ribosomal protein S7

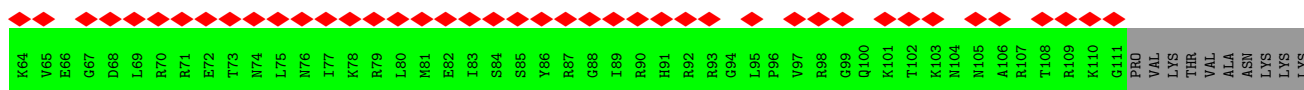
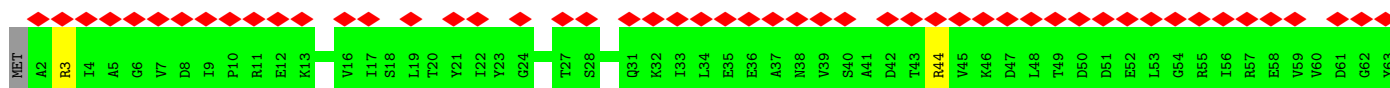
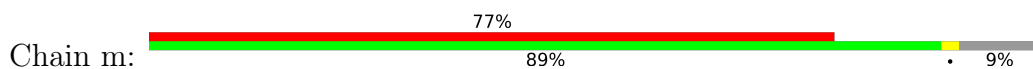




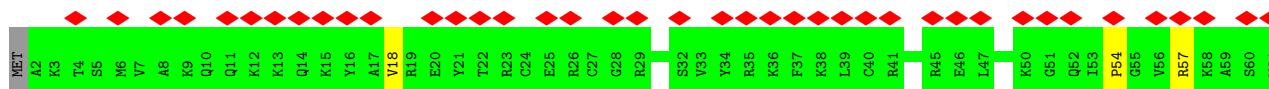
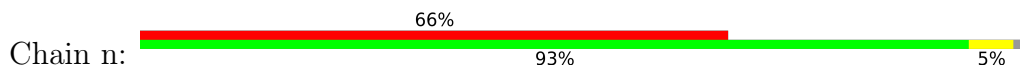
- Molecule 12: 30S ribosomal protein S12



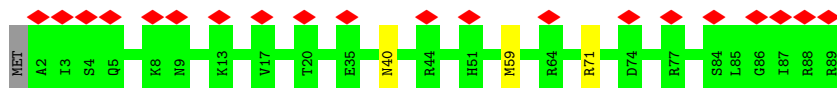
- Molecule 13: 30S ribosomal protein S13



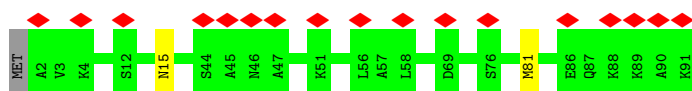
- Molecule 14: 30S ribosomal protein S14 type Z



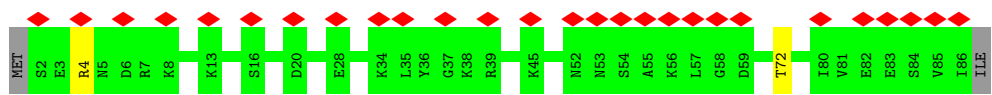
- Molecule 15: 30S ribosomal protein S15



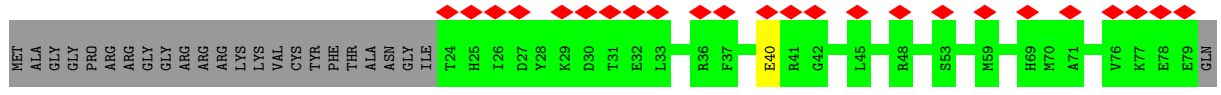
- Molecule 16: 30S ribosomal protein S16



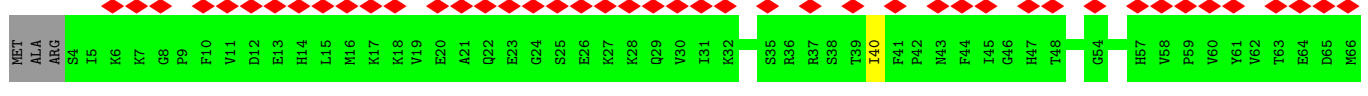
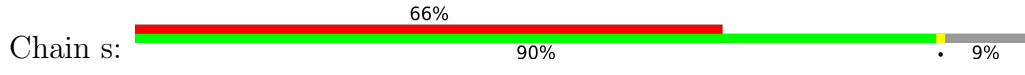
- Molecule 17: 30S ribosomal protein S17



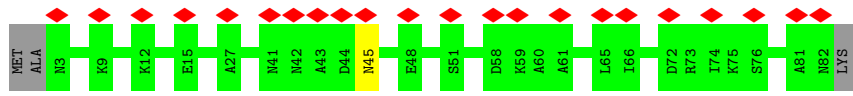
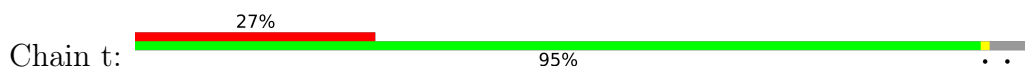
• Molecule 18: 30S ribosomal protein S18



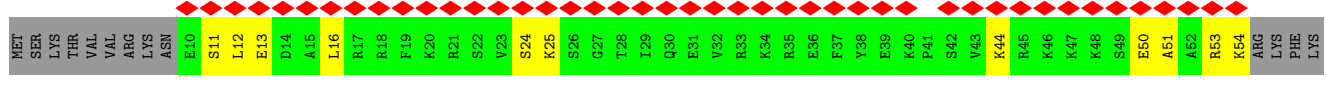
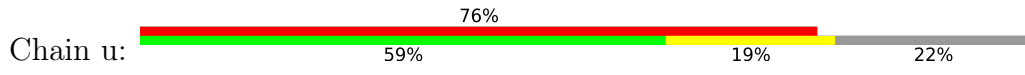
• Molecule 19: 30S ribosomal protein S19



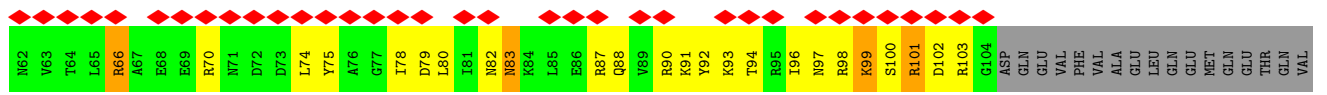
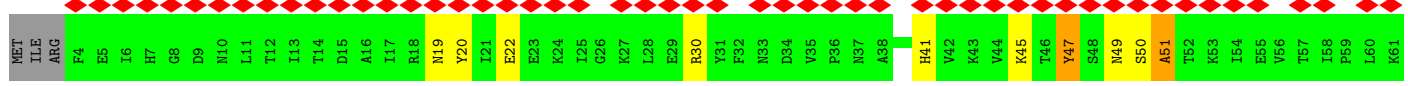
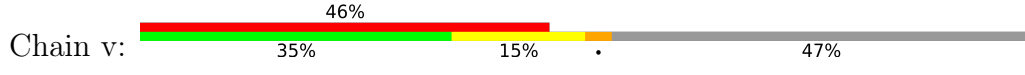
• Molecule 20: 30S ribosomal protein S20



• Molecule 21: 30S ribosomal protein S21



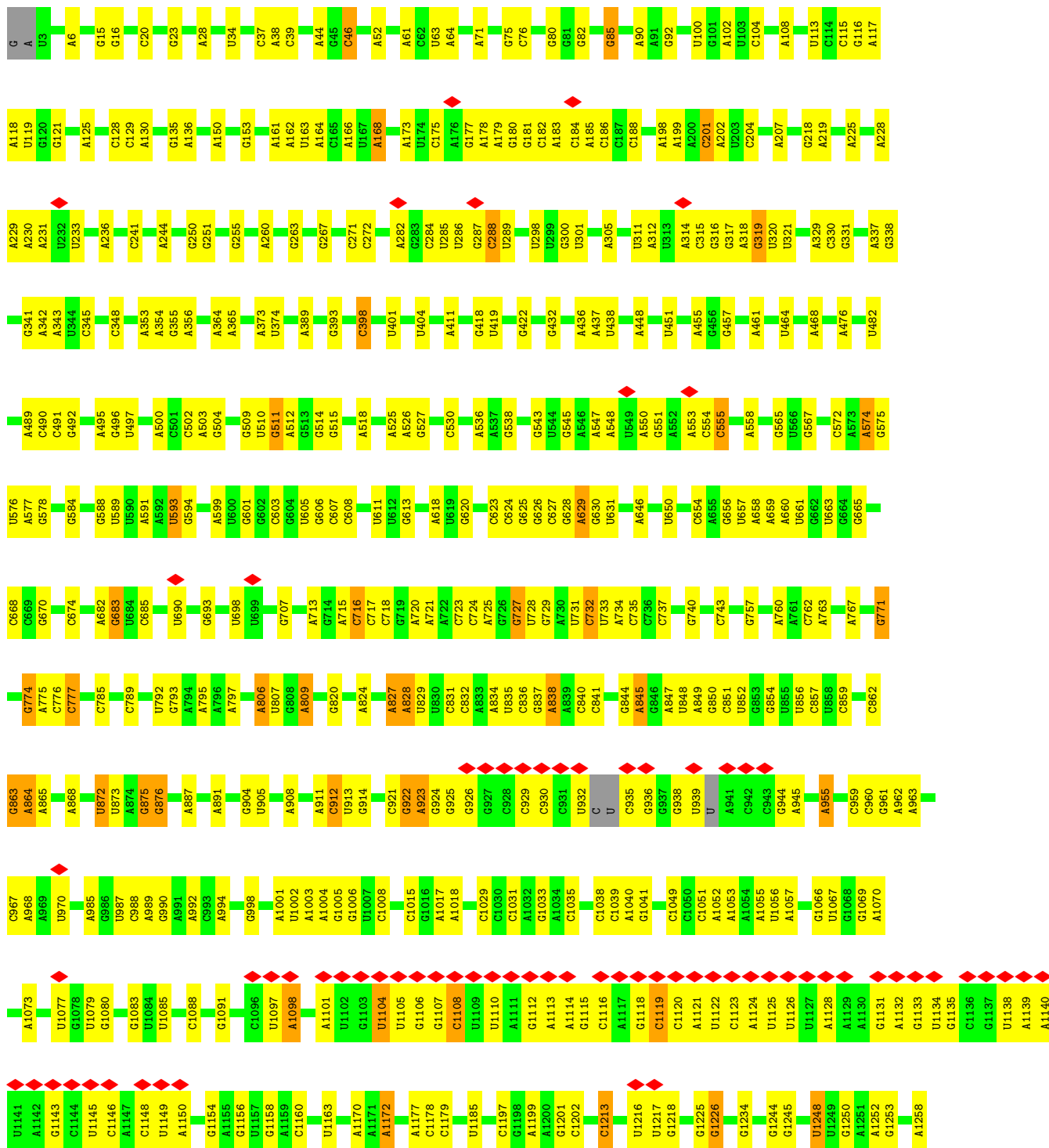
• Molecule 22: Ribosome hibernation promotion factor

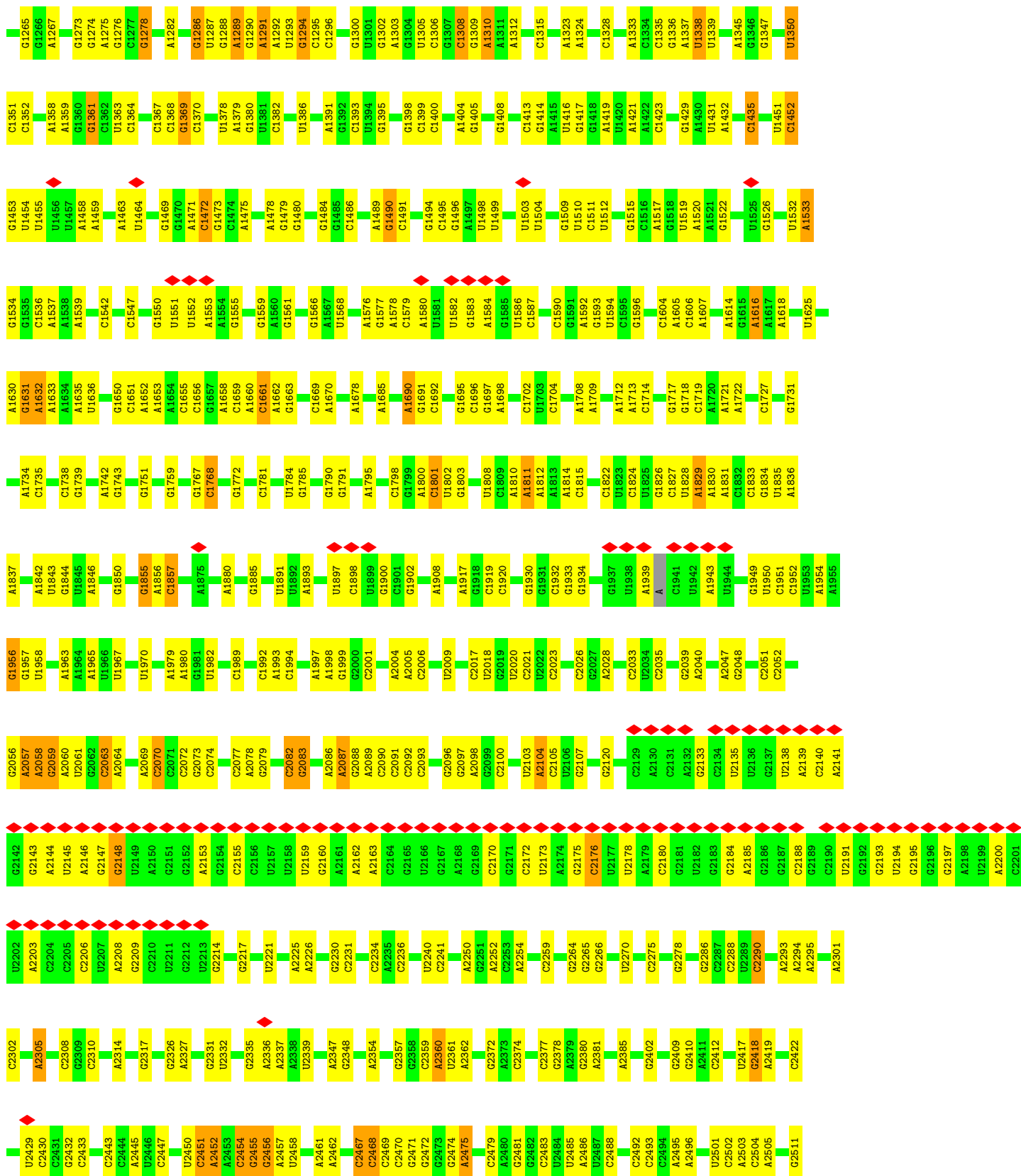


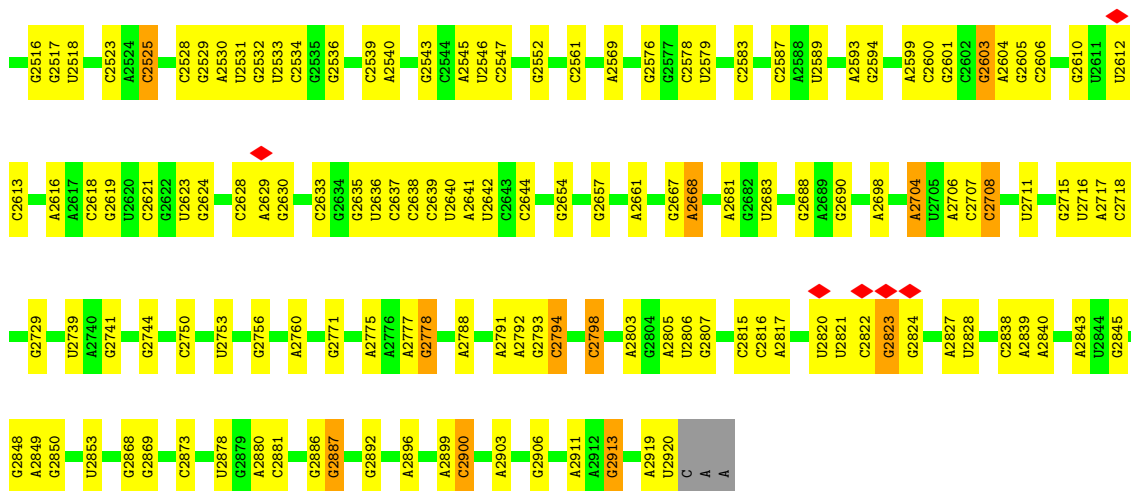
ASP	ASN	ALA	ASP	ASP	ASP	GLU	GLU	ILE	ILE	ILE	ARG	SER	LYS	LYS	PHE	PHE	LEU	SER	LEU	PRO	MET	ASP	SER	GLU	GLU	ALA	VAL	LEU	GLN	MET	ASN	LEU	LEU	GLY	HIS	ASP	PHE	PHE	VAL	THR	ASP	ARG	GLU	THR	ASP	GLY	THR	SER	ILE	VAL	ARG	ARG	LYS	ASP	GLY	LYS
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

TYR	GLY	LEU	ILE	GLN	THR	SER	GLU	GLN
-----	-----	-----	-----	-----	-----	-----	-----	-----

• Molecule 23: 23S ribosomal RNA



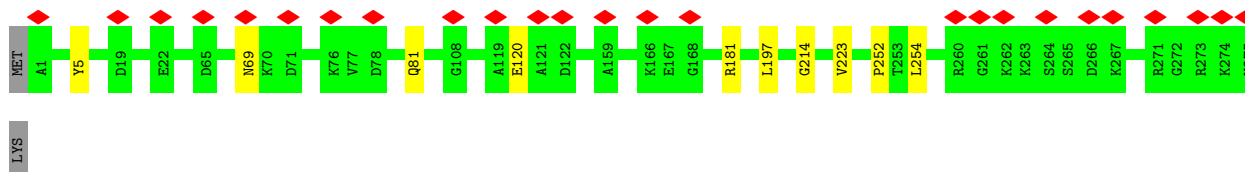




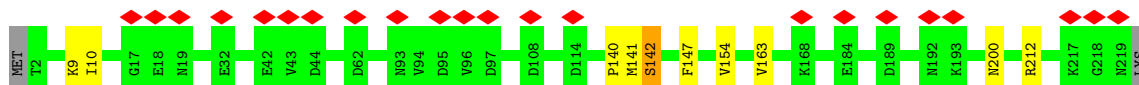
• Molecule 24: 5S ribosomal RNA



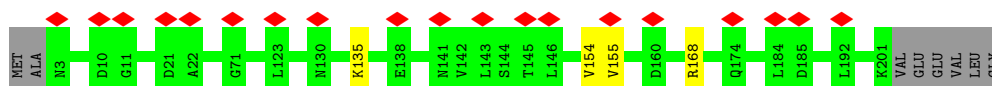
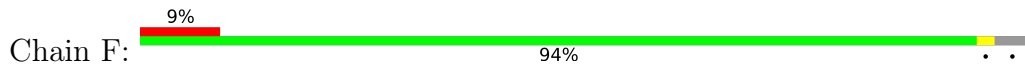
• Molecule 25: 50S ribosomal protein L2



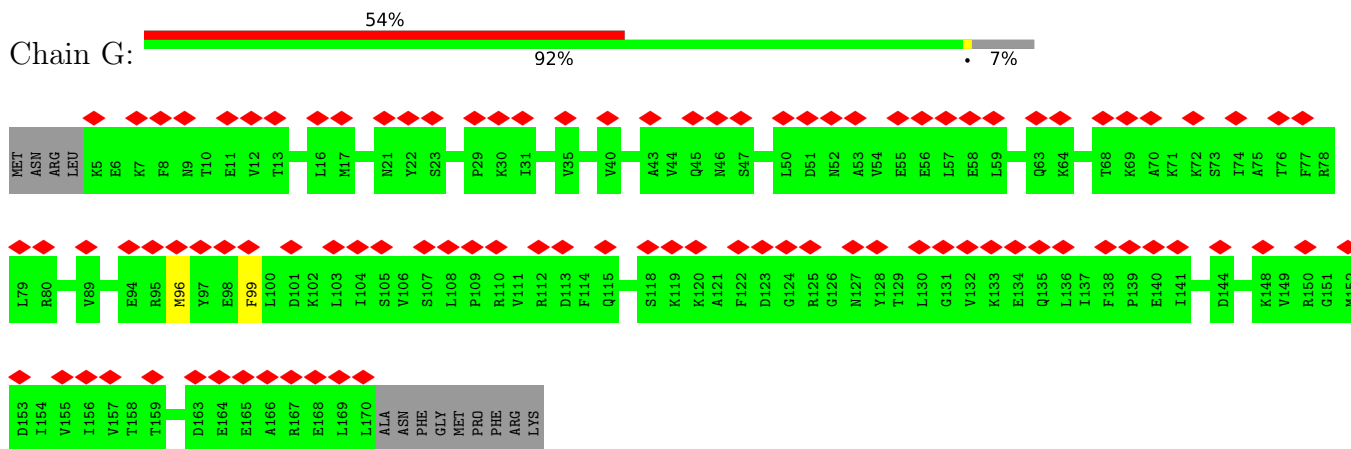
• Molecule 26: 50S ribosomal protein L3



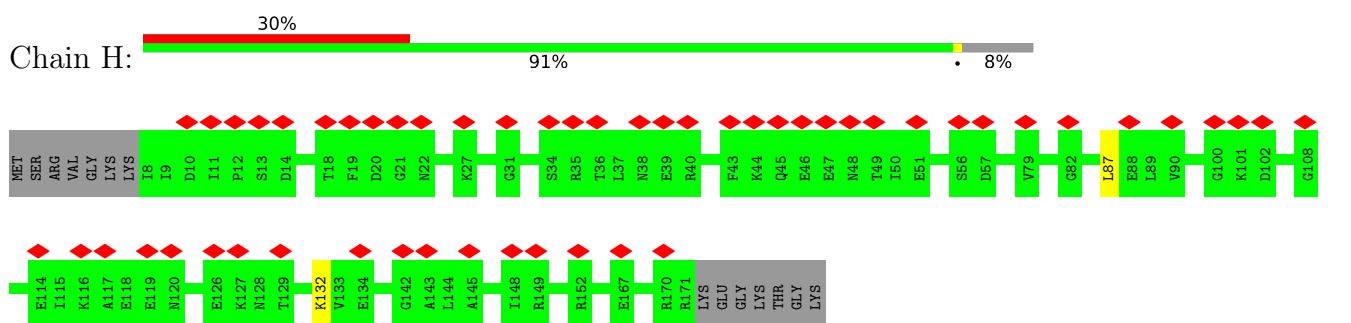
• Molecule 27: 50S ribosomal protein L4



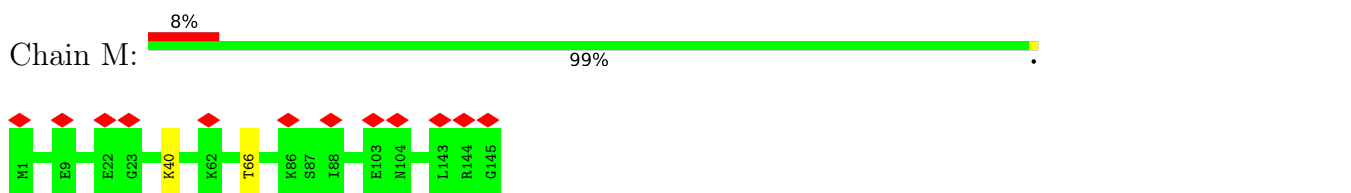
• Molecule 28: 50S ribosomal protein L5



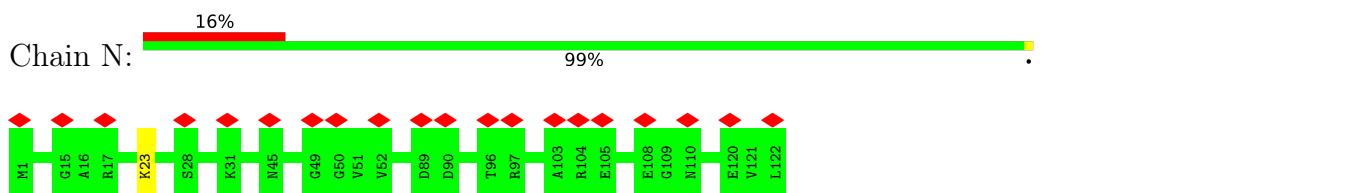
• Molecule 29: 50S ribosomal protein L6



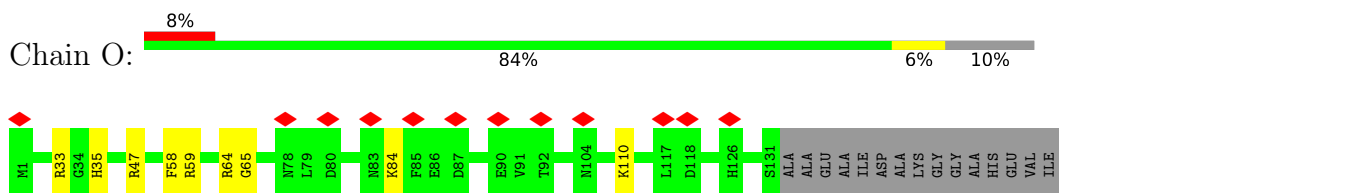
• Molecule 30: 50S ribosomal protein L13



• Molecule 31: 50S ribosomal protein L14

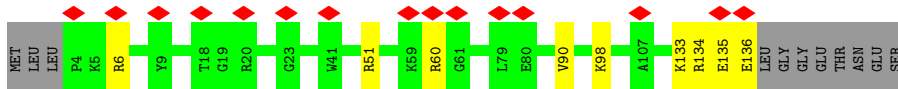


• Molecule 32: 50S ribosomal protein L15

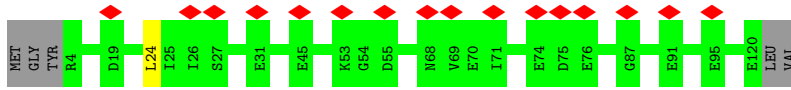


• Molecule 33: 50S ribosomal protein L16

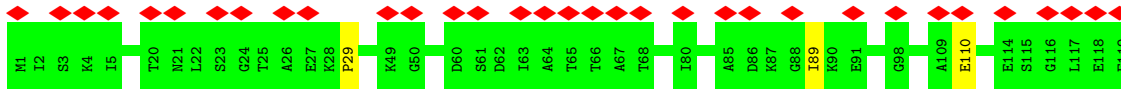




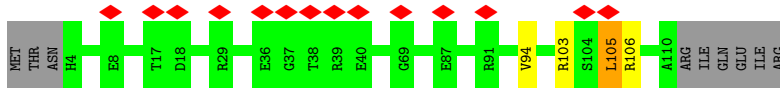
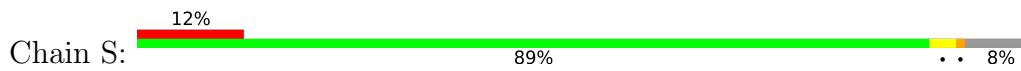
- Molecule 34: 50S ribosomal protein L17



- Molecule 35: 50S ribosomal protein L18



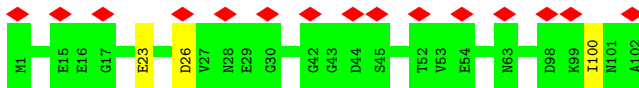
- Molecule 36: 50S ribosomal protein L19



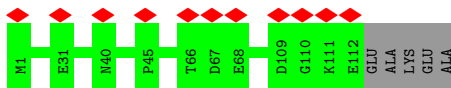
- Molecule 37: 50S ribosomal protein L20



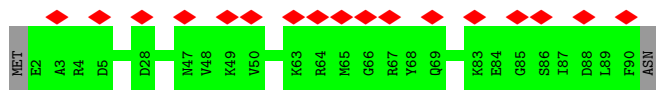
- Molecule 38: 50S ribosomal protein L21



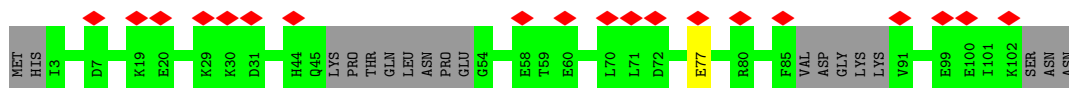
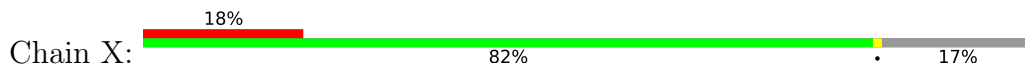
- Molecule 39: 50S ribosomal protein L22



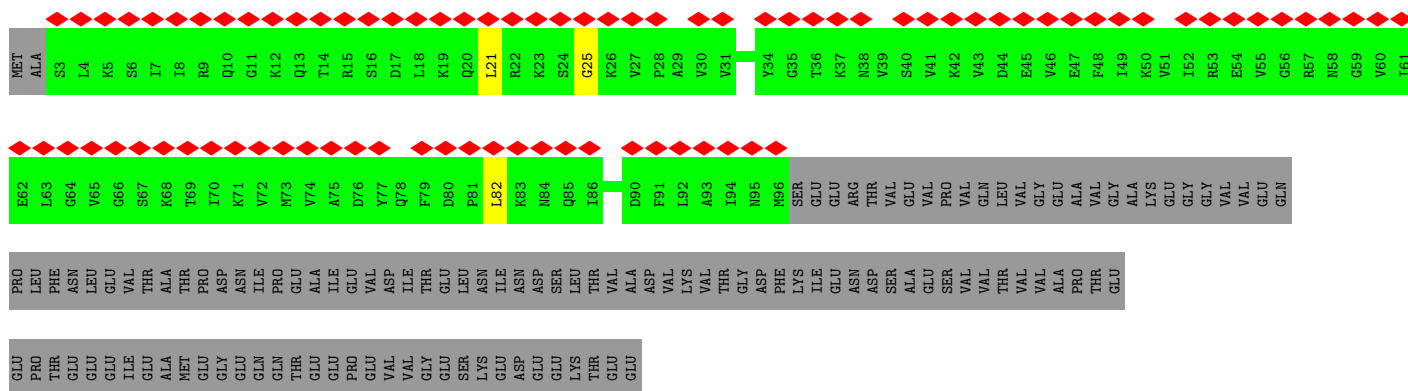
- Molecule 40: 50S ribosomal protein L23



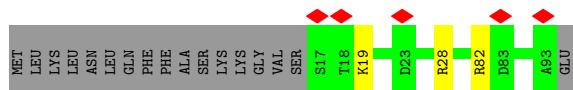
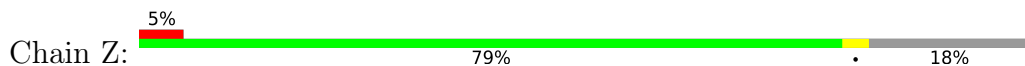
- Molecule 41: 50S ribosomal protein L24



- Molecule 42: 50S ribosomal protein L25



- Molecule 43: 50S ribosomal protein L27

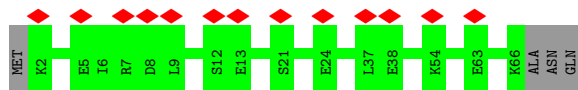


- Molecule 44: 50S ribosomal protein L28

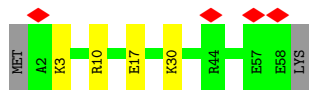
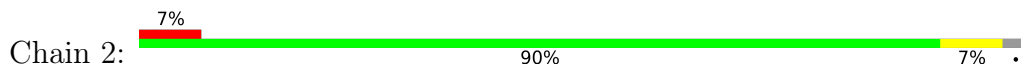


- Molecule 45: 50S ribosomal protein L29

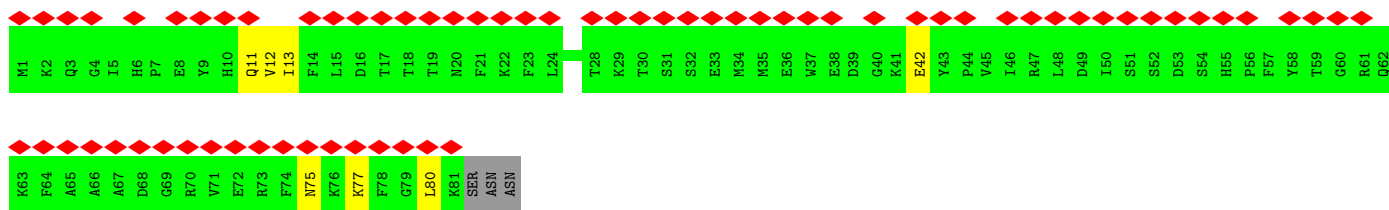
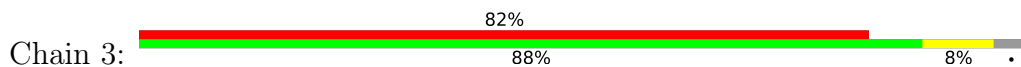




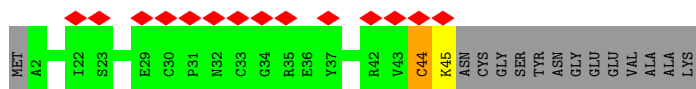
• Molecule 46: 50S ribosomal protein L30



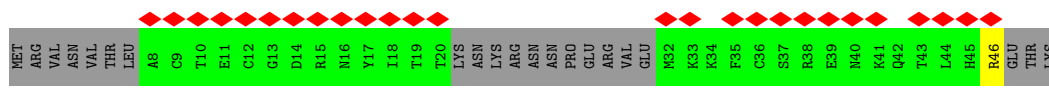
• Molecule 47: 50S ribosomal protein L31 type B



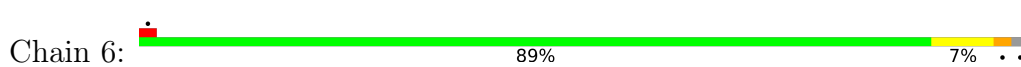
• Molecule 48: 50S ribosomal protein L32



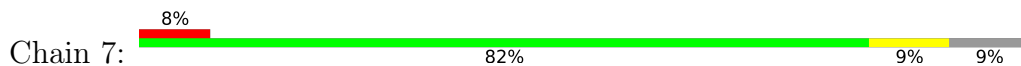
• Molecule 49: 50S ribosomal protein L33 2



• Molecule 50: 50S ribosomal protein L34



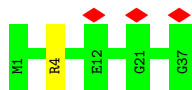
• Molecule 51: 50S ribosomal protein L35





- Molecule 52: 50S ribosomal protein L36

Chain 8: 8% 97%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	83000	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	0.299	Depositor
Minimum map value	-0.132	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	374.0, 374.0, 374.0	wwPDB
Map dimensions	340, 340, 340	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

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	0.97	3/36954 (0.0%)	1.25	166/57629 (0.3%)
2	b	0.47	0/1815	0.72	3/2436 (0.1%)
3	c	0.39	0/1622	0.68	0/2178
4	d	0.46	0/1629	0.69	0/2185
5	e	0.53	0/1208	0.73	0/1628
6	f	0.54	0/792	0.68	0/1062
7	g	0.45	0/1157	0.73	2/1557 (0.1%)
8	h	0.58	0/1044	0.75	0/1401
9	i	0.41	0/1033	0.71	0/1386
10	j	0.42	0/803	0.69	0/1082
11	k	0.48	0/866	0.67	1/1169 (0.1%)
12	l	0.62	0/1075	0.80	0/1439
13	m	0.42	0/883	0.79	0/1182
14	n	0.46	0/512	0.81	0/678
15	o	0.53	0/747	0.80	0/996
16	p	0.56	0/723	0.69	0/971
17	q	0.57	0/706	0.73	0/944
18	r	0.51	0/473	0.76	0/632
19	s	0.40	0/695	0.68	0/934
20	t	0.43	0/606	0.69	0/810
21	u	0.35	0/380	0.53	0/498
22	v	0.37	0/841	0.72	0/1131
23	A	1.33	155/69971 (0.2%)	1.40	719/109124 (0.7%)
24	B	0.94	1/2717 (0.0%)	1.26	19/4232 (0.4%)
25	D	0.86	2/2138 (0.1%)	0.82	2/2869 (0.1%)
26	E	0.78	2/1673 (0.1%)	0.73	0/2243
27	F	0.72	0/1547	0.76	1/2088 (0.0%)
28	G	0.42	0/1326	0.73	0/1780
29	H	0.51	1/1302 (0.1%)	0.70	0/1757
30	M	0.68	0/1173	0.71	0/1578
31	N	0.77	0/927	0.83	0/1243
32	O	0.70	0/1010	0.89	4/1344 (0.3%)
33	P	0.75	0/1089	0.84	0/1460
34	Q	0.63	0/927	0.77	1/1238 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
35	R	0.48	0/931	0.74	0/1244
36	S	0.70	0/874	0.86	2/1168 (0.2%)
37	T	0.81	0/955	0.82	3/1265 (0.2%)
38	U	0.72	0/809	0.75	1/1080 (0.1%)
39	V	0.69	0/870	0.78	0/1171
40	W	0.69	0/733	0.76	0/978
41	X	0.50	0/672	0.66	0/893
42	Y	0.76	1/746 (0.1%)	1.56	4/1000 (0.4%)
43	Z	0.72	0/597	0.69	0/793
44	0	0.59	0/378	0.90	0/504
45	1	0.53	0/537	0.71	0/714
46	2	0.64	0/443	0.76	1/597 (0.2%)
47	3	0.47	0/680	0.83	1/911 (0.1%)
48	4	0.73	0/366	0.76	0/485
49	5	0.40	0/230	0.85	0/303
50	6	0.91	0/377	0.89	1/491 (0.2%)
51	7	0.73	0/491	0.96	2/643 (0.3%)
52	8	0.70	0/300	0.88	2/393 (0.5%)
All	All	1.08	165/153353 (0.1%)	1.23	935/229517 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	b	0	2
3	c	0	1
4	d	0	2
5	e	0	1
6	f	0	1
7	g	0	6
11	k	0	1
12	l	0	3
13	m	0	1
14	n	0	2
17	q	0	2
19	s	0	1
22	v	0	7
25	D	0	2
26	E	0	5
27	F	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
30	M	0	1
31	N	0	1
32	O	0	4
33	P	0	3
35	R	0	3
36	S	0	2
37	T	0	1
38	U	0	1
41	X	0	1
43	Z	0	1
46	2	0	1
47	3	0	3
50	6	0	2
51	7	0	2
All	All	0	65

All (165) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	Y	25	GLY	C-N	17.38	1.74	1.34
26	E	147	PHE	CA-CB	-8.04	1.36	1.53
23	A	806	A	C5-C6	-7.55	1.34	1.41
23	A	2606	C	N1-C6	-7.36	1.32	1.37
23	A	2503	A	N9-C4	-7.23	1.33	1.37
25	D	5	TYR	C-N	-7.06	1.17	1.34
23	A	732	C	C4-C5	-6.91	1.37	1.43
23	A	2708	C	N1-C6	-6.83	1.33	1.37
23	A	2082	C	N1-C6	-6.72	1.33	1.37
23	A	2021	C	C4-C5	-6.69	1.37	1.43
23	A	2451	C	N3-C4	-6.60	1.29	1.33
23	A	840	C	N1-C6	-6.54	1.33	1.37
23	A	558	A	N9-C4	-6.53	1.33	1.37
23	A	2078	A	N9-C4	-6.51	1.33	1.37
23	A	2017	C	N1-C6	-6.34	1.33	1.37
23	A	201	C	C4-C5	-6.32	1.37	1.43
23	A	827	A	N9-C4	-6.30	1.34	1.37
23	A	2616	A	N9-C4	-6.25	1.34	1.37
23	A	1618	A	N9-C4	-6.25	1.34	1.37
23	A	623	C	C4-C5	-6.23	1.38	1.43
23	A	2051	C	C4-C5	-6.18	1.38	1.43
23	A	629	A	N9-C4	-6.13	1.34	1.37
23	A	841	C	N1-C6	-6.12	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	491	C	N1-C6	-6.10	1.33	1.37
23	A	1714	C	C4-C5	-6.05	1.38	1.43
23	A	849	A	N9-C4	-6.05	1.34	1.37
23	A	721	A	N9-C4	-6.03	1.34	1.37
23	A	2021	C	N1-C6	-6.03	1.33	1.37
23	A	1029	C	C4-C5	-6.02	1.38	1.43
26	E	163	VAL	CB-CG1	-6.01	1.40	1.52
23	A	718	C	N1-C6	-5.98	1.33	1.37
23	A	2098	A	N9-C4	-5.96	1.34	1.37
23	A	737	C	C4-C5	-5.89	1.38	1.43
23	A	859	C	N1-C6	-5.85	1.33	1.37
23	A	836	C	N1-C6	-5.84	1.33	1.37
23	A	2052	C	C4-C5	-5.83	1.38	1.43
23	A	716	C	N1-C6	-5.83	1.33	1.37
23	A	1296	C	N1-C6	-5.79	1.33	1.37
23	A	1008	C	N1-C6	-5.78	1.33	1.37
23	A	716	C	C4-C5	-5.78	1.38	1.43
23	A	1850	G	N9-C8	-5.78	1.33	1.37
23	A	845	A	N9-C4	-5.77	1.34	1.37
23	A	1815	C	C4-C5	-5.75	1.38	1.43
23	A	2454	C	C4-C5	-5.74	1.38	1.43
23	A	716	C	N3-C4	-5.71	1.29	1.33
23	A	809	A	C6-N6	-5.70	1.29	1.33
23	A	1798	C	C4-C5	-5.70	1.38	1.43
23	A	1824	C	C4-C5	-5.69	1.38	1.43
23	A	2467	C	N1-C6	-5.68	1.33	1.37
23	A	2250	A	N9-C4	-5.68	1.34	1.37
23	A	1802	U	C4-C5	-5.67	1.38	1.43
23	A	2483	C	C4-C5	-5.67	1.38	1.43
23	A	832	C	N1-C6	-5.65	1.33	1.37
23	A	2091	C	C4-C5	-5.64	1.38	1.43
23	A	2079	G	N9-C8	-5.63	1.33	1.37
23	A	1721	A	N9-C4	-5.62	1.34	1.37
23	A	774	G	C6-N1	-5.61	1.35	1.39
23	A	1202	C	C4-C5	-5.58	1.38	1.43
23	A	511	G	N9-C8	-5.58	1.33	1.37
23	A	1712	A	N9-C4	-5.57	1.34	1.37
23	A	1172	A	N9-C4	-5.56	1.34	1.37
23	A	1370	C	C4-C5	-5.55	1.38	1.43
23	A	1616	A	N9-C4	-5.54	1.34	1.37
23	A	512	A	N9-C4	-5.53	1.34	1.37
23	A	2301	A	N9-C4	-5.53	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	2750	C	C4-C5	-5.52	1.38	1.43
23	A	1734	A	N9-C4	-5.51	1.34	1.37
23	A	2525	C	C4-C5	-5.50	1.38	1.43
23	A	2481	G	N9-C8	-5.48	1.34	1.37
23	A	2707	C	C4-C5	-5.48	1.38	1.43
23	A	2523	C	N1-C6	-5.46	1.33	1.37
23	A	743	C	N1-C6	-5.45	1.33	1.37
23	A	500	A	N9-C4	-5.45	1.34	1.37
23	A	865	A	N9-C4	-5.45	1.34	1.37
23	A	515	G	C6-N1	-5.43	1.35	1.39
23	A	625	G	N9-C8	-5.43	1.34	1.37
23	A	1566	G	N9-C4	-5.43	1.33	1.38
23	A	2470	C	N1-C6	-5.43	1.33	1.37
23	A	1661	C	N1-C6	-5.41	1.33	1.37
23	A	1347	G	N1-C2	-5.41	1.33	1.37
23	A	717	C	C4-C5	-5.40	1.38	1.43
23	A	1038	C	N1-C6	-5.39	1.33	1.37
23	A	603	C	N1-C6	-5.39	1.33	1.37
23	A	724	C	C4-C5	-5.39	1.38	1.43
23	A	201	C	N3-C4	-5.37	1.30	1.33
23	A	1833	C	N1-C6	-5.37	1.33	1.37
23	A	2057	A	N9-C4	-5.36	1.34	1.37
23	A	1367	C	N1-C6	-5.35	1.33	1.37
23	A	789	C	C4-C5	-5.34	1.38	1.43
23	A	2618	C	C4-C5	-5.33	1.38	1.43
23	A	2569	A	N9-C4	-5.33	1.34	1.37
23	A	735	C	N1-C6	-5.32	1.33	1.37
23	A	2471	G	N9-C8	-5.32	1.34	1.37
23	A	732	C	N1-C6	-5.31	1.33	1.37
23	A	836	C	C4-C5	-5.31	1.38	1.43
23	A	607	C	N1-C6	-5.29	1.33	1.37
23	A	2093	C	N1-C6	-5.29	1.33	1.37
23	A	720	A	N9-C4	-5.29	1.34	1.37
1	a	270	A	N7-C5	-5.29	1.36	1.39
23	A	627	C	N1-C6	-5.29	1.33	1.37
23	A	723	C	N1-C6	-5.28	1.33	1.37
23	A	876	G	N9-C4	-5.28	1.33	1.38
23	A	2536	G	N9-C4	-5.27	1.33	1.38
23	A	2288	C	C4-C5	-5.27	1.38	1.43
23	A	1829	A	N9-C4	-5.27	1.34	1.37
23	A	2026	C	N1-C6	-5.26	1.33	1.37
23	A	831	C	N1-C6	-5.26	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	844	G	N3-C4	-5.25	1.31	1.35
23	A	624	C	N1-C6	-5.24	1.34	1.37
23	A	2090	C	C4-C5	-5.24	1.38	1.43
23	A	670	G	C2-N3	-5.23	1.28	1.32
23	A	998	G	N9-C8	-5.23	1.34	1.37
23	A	1393	C	C4-C5	-5.23	1.38	1.43
23	A	1855	G	C2-N2	-5.22	1.29	1.34
23	A	2644	C	C4-C5	-5.21	1.38	1.43
23	A	2644	C	N1-C6	-5.19	1.34	1.37
23	A	1702	C	C4-C5	-5.19	1.38	1.43
23	A	1768	C	N1-C6	-5.18	1.34	1.37
23	A	1539	A	N9-C4	-5.17	1.34	1.37
23	A	1695	G	N7-C5	-5.17	1.36	1.39
23	A	2092	C	N1-C6	-5.16	1.34	1.37
23	A	2091	C	N1-C6	-5.16	1.34	1.37
23	A	2539	C	N1-C6	-5.16	1.34	1.37
23	A	116	G	N9-C8	-5.16	1.34	1.37
23	A	717	C	N1-C6	-5.16	1.34	1.37
25	D	223	VAL	CB-CG1	-5.16	1.42	1.52
23	A	2275	C	C4-C5	-5.15	1.38	1.43
23	A	1830	A	N9-C4	-5.14	1.34	1.37
23	A	1932	C	N1-C6	-5.14	1.34	1.37
1	a	911	A	N7-C5	-5.14	1.36	1.39
23	A	1855	G	N3-C4	-5.14	1.31	1.35
23	A	509	G	N9-C4	-5.13	1.33	1.38
23	A	2445	A	N9-C4	-5.13	1.34	1.37
23	A	2619	G	N9-C8	-5.12	1.34	1.37
23	A	1822	C	N1-C6	-5.11	1.34	1.37
23	A	2006	C	N1-C6	-5.11	1.34	1.37
23	A	854	G	N9-C4	-5.11	1.33	1.38
23	A	1336	G	N9-C8	-5.11	1.34	1.37
23	A	1814	A	N7-C5	-5.11	1.36	1.39
23	A	1391	A	N9-C4	-5.10	1.34	1.37
23	A	838	A	C6-N6	-5.10	1.29	1.33
23	A	230	A	N9-C4	-5.09	1.34	1.37
23	A	2100	C	N1-C6	-5.09	1.34	1.37
29	H	87	LEU	CA-CB	-5.09	1.42	1.53
23	A	2474	G	N9-C8	-5.08	1.34	1.37
23	A	1335	C	C4-C5	-5.08	1.38	1.43
23	A	2077	C	C4-C5	-5.08	1.38	1.43
23	A	1435	C	C4-C5	-5.07	1.38	1.43
23	A	1810	A	N9-C4	-5.07	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	79	C	C4-C5	-5.06	1.38	1.43
23	A	988	C	N1-C6	-5.06	1.34	1.37
23	A	1324	A	N9-C4	-5.06	1.34	1.37
23	A	2469	C	N3-C4	-5.06	1.30	1.33
23	A	806	A	N7-C5	-5.05	1.36	1.39
23	A	228	A	N9-C4	-5.04	1.34	1.37
23	A	1015	C	C4-C5	-5.04	1.39	1.43
23	A	1368	C	N1-C6	-5.03	1.34	1.37
23	A	864	A	N9-C4	-5.03	1.34	1.37
23	A	1292	A	N9-C4	-5.03	1.34	1.37
1	a	740	C	N1-C6	-5.03	1.34	1.37
23	A	844	G	N9-C8	-5.02	1.34	1.37
23	A	1857	C	C4-C5	-5.01	1.39	1.43
23	A	1039	C	N1-C6	-5.01	1.34	1.37
23	A	734	A	C6-N6	-5.00	1.29	1.33
23	A	1414	G	N1-C2	-5.00	1.33	1.37

All (935) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	Y	25	GLY	CA-C-N	-26.58	58.73	117.20
42	Y	25	GLY	O-C-N	25.46	163.44	122.70
42	Y	25	GLY	C-N-CA	-23.37	63.28	121.70
23	A	806	A	N1-C6-N6	18.77	129.86	118.60
23	A	2451	C	C6-N1-C2	-17.47	113.31	120.30
23	A	260	A	C5'-C4'-C3'	-14.85	92.23	116.00
23	A	2451	C	N3-C2-O2	-14.79	111.54	121.90
23	A	806	A	C5-C6-N6	-14.73	111.92	123.70
23	A	198	A	N1-C6-N6	13.88	126.93	118.60
23	A	806	A	C4-C5-N7	11.66	116.53	110.70
23	A	806	A	C6-C5-N7	-11.04	124.58	132.30
23	A	201	C	N1-C2-O2	10.90	125.44	118.90
23	A	806	A	C5-N7-C8	-10.64	98.58	103.90
23	A	1347	G	N1-C2-N2	-10.42	106.82	116.20
23	A	1714	C	C5-C4-N4	-10.16	113.08	120.20
23	A	806	A	N9-C4-C5	-9.89	101.84	105.80
23	A	2275	C	N1-C2-O2	9.63	124.68	118.90
23	A	2451	C	N1-C2-O2	9.47	124.58	118.90
23	A	732	C	C5-C4-N4	-9.40	113.62	120.20
1	a	136	C	N1-C2-O2	9.13	124.38	118.90
23	A	2090	C	C5-C4-N4	-9.00	113.90	120.20
23	A	1382	C	N1-C2-O2	8.95	124.27	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	1857	C	N1-C2-O2	8.93	124.26	118.90
23	A	857	C	C5-C4-N4	-8.90	113.97	120.20
23	A	1347	G	N3-C2-N2	8.89	126.12	119.90
23	A	955	A	N1-C6-N6	-8.84	113.30	118.60
1	a	1541	G	N7-C8-N9	8.58	117.39	113.10
23	A	2033	C	N1-C2-O2	8.57	124.04	118.90
23	A	2290	C	C6-N1-C2	-8.55	116.88	120.30
23	A	840	C	N1-C2-O2	8.54	124.02	118.90
23	A	201	C	N3-C2-O2	-8.49	115.95	121.90
23	A	2451	C	C2-N1-C1'	8.49	128.14	118.80
23	A	198	A	C5-C6-N6	-8.41	116.97	123.70
24	B	79	C	N3-C4-N4	8.41	123.89	118.00
23	A	198	A	N9-C4-C5	-8.35	102.46	105.80
23	A	260	A	C5'-C4'-O4'	8.30	119.06	109.10
1	a	617	A	N1-C6-N6	8.24	123.55	118.60
23	A	1351	C	C6-N1-C2	-8.23	117.01	120.30
23	A	2452	A	N1-C6-N6	-8.22	113.67	118.60
23	A	1395	G	N1-C2-N2	-8.21	108.81	116.20
23	A	476	A	N1-C6-N6	-8.15	113.71	118.60
1	a	641	U	C2-N1-C1'	8.15	127.48	117.70
23	A	1248	U	C5-C4-O4	-8.13	121.02	125.90
1	a	1541	G	C8-N9-C4	-8.09	103.16	106.40
23	A	1604	C	N3-C2-O2	-8.09	116.24	121.90
24	B	79	C	C6-N1-C2	-8.08	117.07	120.30
23	A	1566	G	N3-C4-N9	-8.05	121.17	126.00
23	A	2052	C	C6-N1-C2	-8.05	117.08	120.30
23	A	1509	G	O4'-C1'-N9	8.02	114.62	108.20
23	A	1509	G	N3-C2-N2	7.98	125.48	119.90
1	a	1506	G	C4-C5-N7	7.95	113.98	110.80
23	A	2052	C	N1-C2-O2	7.91	123.64	118.90
23	A	1857	C	N3-C2-O2	-7.88	116.38	121.90
23	A	1395	G	N3-C2-N2	7.88	125.42	119.90
23	A	774	G	C6-C5-N7	-7.87	125.68	130.40
37	T	3	ARG	NE-CZ-NH2	-7.83	116.39	120.30
1	a	476	C	C6-N1-C2	-7.82	117.17	120.30
1	a	415	A	N1-C6-N6	7.82	123.29	118.60
23	A	1119	C	N1-C2-O2	7.80	123.58	118.90
23	A	806	A	N7-C8-N9	7.74	117.67	113.80
23	A	1197	C	N1-C2-O2	7.74	123.54	118.90
1	a	394	C	N1-C2-O2	7.73	123.54	118.90
23	A	1658	A	C5-C6-N6	-7.70	117.54	123.70
23	A	857	C	N3-C4-C5	7.63	124.95	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	2058	A	C5-C6-N6	-7.59	117.63	123.70
23	A	2058	A	N1-C6-N6	7.58	123.15	118.60
23	A	623	C	N1-C2-O2	7.56	123.44	118.90
23	A	774	G	C4-C5-N7	7.55	113.82	110.80
23	A	1604	C	N1-C2-O2	7.54	123.42	118.90
23	A	1658	A	N1-C6-N6	7.54	123.12	118.60
23	A	2051	C	C6-N1-C2	-7.54	117.28	120.30
1	a	571	A	N1-C6-N6	-7.53	114.08	118.60
23	A	1920	C	N3-C2-O2	-7.52	116.64	121.90
23	A	2467	C	C2-N1-C1'	7.48	127.02	118.80
23	A	832	C	C6-N1-C2	-7.47	117.31	120.30
23	A	1008	C	N3-C2-O2	-7.43	116.70	121.90
23	A	2587	C	N3-C4-C5	7.41	124.86	121.90
1	a	572	U	N3-C2-O2	-7.41	117.02	122.20
23	A	2528	C	C6-N1-C2	-7.37	117.35	120.30
23	A	201	C	C6-N1-C2	-7.36	117.36	120.30
23	A	836	C	N3-C4-C5	7.36	124.84	121.90
23	A	841	C	N1-C2-O2	7.34	123.30	118.90
23	A	515	G	C8-N9-C1'	-7.34	117.46	127.00
23	A	1275	A	N1-C6-N6	7.31	122.99	118.60
1	a	1443	G	O4'-C1'-N9	7.31	114.05	108.20
23	A	2540	A	C5-C6-N6	-7.29	117.86	123.70
23	A	1382	C	N3-C2-O2	-7.28	116.81	121.90
23	A	774	G	N9-C4-C5	-7.25	102.50	105.40
36	S	94	VAL	CG1-CB-CG2	7.25	122.49	110.90
23	A	1857	C	C6-N1-C2	-7.23	117.41	120.30
23	A	1351	C	C2-N1-C1'	7.22	126.74	118.80
23	A	2409	G	C8-N9-C1'	-7.22	117.61	127.00
1	a	762	C	C2-N1-C1'	7.22	126.74	118.80
23	A	624	C	N1-C2-O2	7.21	123.22	118.90
23	A	2305	A	C5-C6-N6	-7.20	117.94	123.70
23	A	2051	C	C5-C4-N4	-7.19	115.17	120.20
23	A	1837	A	C5-C6-N6	-7.19	117.95	123.70
23	A	840	C	N3-C2-O2	-7.16	116.89	121.90
23	A	2057	A	C4-C5-C6	-7.12	113.44	117.00
24	B	79	C	C2-N1-C1'	7.12	126.63	118.80
23	A	2033	C	N3-C2-O2	-7.08	116.94	121.90
32	O	33	ARG	NE-CZ-NH1	7.08	123.84	120.30
23	A	2517	G	N1-C2-N2	-7.07	109.84	116.20
23	A	845	A	N1-C6-N6	7.07	122.84	118.60
23	A	2305	A	C5-C6-N1	7.06	121.23	117.70
23	A	491	C	N1-C2-O2	7.04	123.12	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	1413	C	N1-C2-O2	7.04	123.12	118.90
1	a	1480	A	N1-C6-N6	7.03	122.81	118.60
23	A	2288	C	C5-C4-N4	-7.02	115.29	120.20
23	A	2569	A	C5-C6-N6	-7.02	118.08	123.70
23	A	1714	C	N3-C4-N4	7.02	122.91	118.00
1	a	894	U	C5-C6-N1	7.02	126.21	122.70
23	A	1119	C	N3-C2-O2	-7.01	116.99	121.90
23	A	1509	G	N1-C2-N2	-7.01	109.89	116.20
1	a	572	U	N1-C2-O2	7.00	127.70	122.80
23	A	198	A	C6-C5-N7	-7.00	127.40	132.30
1	a	1506	G	N9-C4-C5	-6.99	102.61	105.40
23	A	2504	C	C6-N1-C2	-6.99	117.50	120.30
23	A	1566	G	N3-C4-C5	6.98	132.09	128.60
23	A	2058	A	N9-C4-C5	-6.97	103.01	105.80
42	Y	82	LEU	CA-CB-CG	6.97	131.33	115.30
23	A	2275	C	C2-N1-C1'	6.93	126.42	118.80
1	a	211	A	N1-C6-N6	-6.90	114.46	118.60
1	a	196	A	N1-C6-N6	6.90	122.74	118.60
23	A	2017	C	N1-C2-O2	6.90	123.04	118.90
1	a	1408	C	C2-N1-C1'	6.89	126.38	118.80
23	A	2485	U	C5-C6-N1	6.88	126.14	122.70
23	A	2052	C	C5-C6-N1	6.88	124.44	121.00
23	A	1029	C	C2-N1-C1'	6.88	126.36	118.80
23	A	175	C	N3-C2-O2	-6.84	117.11	121.90
23	A	1347	G	N1-C6-O6	-6.84	115.80	119.90
23	A	1837	A	N1-C6-N6	6.82	122.69	118.60
23	A	1029	C	C6-N1-C2	-6.81	117.58	120.30
23	A	1920	C	N1-C2-O2	6.81	122.99	118.90
23	A	1004	A	C5-C6-N6	-6.80	118.26	123.70
23	A	2275	C	C6-N1-C2	-6.78	117.59	120.30
23	A	1029	C	N1-C2-O2	6.78	122.97	118.90
24	B	79	C	N1-C2-O2	6.78	122.97	118.90
23	A	2523	C	N3-C2-O2	-6.78	117.16	121.90
23	A	2004	A	C5-C6-N6	-6.78	118.28	123.70
23	A	2057	A	C5-C6-N1	6.77	121.09	117.70
1	a	86	G	N3-C4-N9	-6.76	121.94	126.00
23	A	1880	A	N1-C6-N6	6.75	122.65	118.60
23	A	1248	U	N3-C4-O4	6.75	124.13	119.40
23	A	2409	G	C4-N9-C1'	6.75	135.27	126.50
23	A	2628	C	N1-C2-O2	6.72	122.93	118.90
23	A	515	G	C4-N9-C1'	6.72	135.23	126.50
23	A	603	C	N1-C2-O2	6.72	122.93	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	3	80	LEU	CA-CB-CG	6.72	130.75	115.30
23	A	2078	A	N1-C6-N6	6.71	122.63	118.60
23	A	2052	C	N3-C2-O2	-6.71	117.20	121.90
23	A	2275	C	N3-C2-O2	-6.70	117.21	121.90
23	A	1004	A	C5-C6-N1	6.70	121.05	117.70
23	A	717	C	C2-N1-C1'	6.69	126.16	118.80
23	A	1148	C	C6-N1-C2	-6.67	117.63	120.30
23	A	2706	A	C5-C6-N6	-6.65	118.38	123.70
23	A	128	C	N1-C2-O2	6.64	122.89	118.90
23	A	1802	U	C5-C6-N1	6.61	126.00	122.70
23	A	136	A	C5-C6-N6	-6.60	118.42	123.70
23	A	1347	G	C5-C6-O6	6.60	132.56	128.60
24	B	79	C	C5-C4-N4	-6.60	115.58	120.20
23	A	1932	C	N3-C4-C5	6.59	124.54	121.90
23	A	1393	C	C6-N1-C2	-6.58	117.67	120.30
23	A	2619	G	C4-N9-C1'	6.58	135.05	126.50
23	A	832	C	C2-N1-C1'	6.57	126.02	118.80
23	A	2097	G	C2-N3-C4	-6.56	108.62	111.90
23	A	717	C	N1-C2-O2	6.56	122.83	118.90
23	A	994	A	C5-C6-N6	-6.55	118.46	123.70
23	A	1364	C	C5-C4-N4	-6.55	115.61	120.20
23	A	1393	C	N1-C2-O2	6.55	122.83	118.90
23	A	1798	C	C5-C4-N4	-6.55	115.61	120.20
23	A	2523	C	N1-C2-O2	6.53	122.82	118.90
23	A	2729	G	C4-N9-C1'	6.53	134.99	126.50
23	A	1695	G	C4-N9-C1'	6.53	134.99	126.50
23	A	178	A	N9-C4-C5	-6.52	103.19	105.80
23	A	1515	G	N3-C2-N2	6.51	124.46	119.90
23	A	1333	A	C5-N7-C8	-6.51	100.65	103.90
1	a	315	U	C6-N1-C2	-6.50	117.10	121.00
23	A	548	A	N1-C6-N6	6.50	122.50	118.60
1	a	1408	C	N1-C2-O2	6.50	122.80	118.90
23	A	2536	G	N3-C4-C5	6.49	131.84	128.60
23	A	515	G	O4'-C1'-N9	6.49	113.39	108.20
23	A	2456	G	C6-C5-N7	-6.49	126.51	130.40
23	A	2644	C	C5-C4-N4	-6.48	115.66	120.20
23	A	2873	C	N1-C2-O2	6.48	122.79	118.90
23	A	1289	A	C5-C6-N1	6.47	120.94	117.70
23	A	1695	G	C6-C5-N7	-6.47	126.52	130.40
23	A	491	C	C2-N1-C1'	6.47	125.91	118.80
23	A	1690	A	C5-C6-N6	-6.46	118.53	123.70
23	A	1202	C	N1-C2-O2	6.44	122.76	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	484	A	C5-C6-N6	-6.43	118.56	123.70
23	A	2051	C	N3-C4-N4	6.42	122.49	118.00
23	A	2517	G	C2-N3-C4	-6.37	108.72	111.90
1	a	641	U	N3-C2-O2	-6.36	117.75	122.20
23	A	1719	C	C5-C4-N4	-6.36	115.75	120.20
23	A	1274	G	N1-C2-N2	-6.35	110.48	116.20
23	A	1201	G	C4-N9-C1'	6.33	134.73	126.50
1	a	805	C	N1-C2-O2	6.32	122.69	118.90
23	A	718	C	N3-C4-C5	6.32	124.43	121.90
23	A	1880	A	C5-C6-N6	-6.32	118.64	123.70
32	O	47	ARG	NE-CZ-NH1	6.32	123.46	120.30
23	A	500	A	N1-C6-N6	6.32	122.39	118.60
23	A	1472	C	C5-C4-N4	-6.32	115.78	120.20
23	A	2569	A	N1-C6-N6	6.31	122.39	118.60
23	A	1831	A	C5-C6-N1	6.30	120.85	117.70
23	A	1855	G	N1-C2-N3	6.30	127.68	123.90
23	A	1380	G	C4-N9-C1'	6.30	134.69	126.50
23	A	876	G	N3-C4-C5	6.29	131.75	128.60
24	B	114	C	N1-C2-O2	6.28	122.67	118.90
23	A	436	A	C5-C6-N6	-6.27	118.68	123.70
23	A	1880	A	N9-C4-C5	-6.27	103.29	105.80
23	A	515	G	C2-N3-C4	-6.26	108.77	111.90
1	a	874	A	N1-C6-N6	-6.26	114.84	118.60
1	a	1452	G	N3-C2-N2	-6.26	115.52	119.90
23	A	548	A	C5-C6-N6	-6.25	118.70	123.70
1	a	412	G	C2-N3-C4	-6.25	108.78	111.90
23	A	732	C	N3-C4-N4	6.24	122.37	118.00
1	a	409	C	N1-C2-O2	6.24	122.64	118.90
23	A	2578	C	N1-C2-O2	6.23	122.64	118.90
23	A	558	A	C8-N9-C4	6.23	108.29	105.80
23	A	1607	A	N1-C6-N6	-6.23	114.86	118.60
23	A	2074	C	N1-C2-O2	6.22	122.63	118.90
23	A	2668	A	C5-C6-N1	6.22	120.81	117.70
23	A	1824	C	C5-C4-N4	-6.22	115.85	120.20
1	a	1160	C	C6-N1-C2	-6.20	117.82	120.30
1	a	1459	C	C6-N1-C2	-6.20	117.82	120.30
23	A	728	U	C5-C4-O4	-6.20	122.18	125.90
23	A	241	C	C6-N1-C2	-6.19	117.82	120.30
23	A	668	C	N1-C2-O2	6.19	122.61	118.90
23	A	436	A	N1-C6-N6	6.19	122.31	118.60
23	A	125	A	N1-C6-N6	6.19	122.31	118.60
23	A	2070	C	N1-C2-O2	6.18	122.61	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	O	47	ARG	NE-CZ-NH2	-6.18	117.21	120.30
23	A	1414	G	N1-C2-N2	-6.18	110.64	116.20
23	A	509	G	C2-N3-C4	-6.17	108.82	111.90
1	a	160	A	N1-C6-N6	6.17	122.30	118.60
23	A	2077	C	C6-N1-C2	-6.16	117.83	120.30
23	A	2528	C	C5-C4-N4	-6.16	115.89	120.20
23	A	2468	C	C5-C4-N4	-6.16	115.89	120.20
23	A	1031	C	N3-C4-C5	6.15	124.36	121.90
1	a	196	A	C6-C5-N7	-6.15	127.99	132.30
23	A	1956	G	C4-N9-C1'	6.15	134.50	126.50
1	a	168	G	C4-C5-N7	6.15	113.26	110.80
23	A	1393	C	C2-N1-C1'	6.14	125.56	118.80
23	A	2451	C	N1-C2-N3	6.14	123.50	119.20
23	A	1857	C	C2-N1-C1'	6.14	125.56	118.80
23	A	201	C	C2-N1-C1'	6.14	125.56	118.80
1	a	682	G	C2-N3-C4	-6.13	108.83	111.90
1	a	36	G	C4-N9-C1'	6.13	134.47	126.50
23	A	1798	C	C2-N1-C1'	6.13	125.54	118.80
1	a	725	C	N1-C2-O2	6.13	122.58	118.90
23	A	608	C	C5-C4-N4	-6.12	115.92	120.20
24	B	98	G	C6-C5-N7	-6.12	126.73	130.40
23	A	670	G	N3-C4-N9	-6.11	122.33	126.00
23	A	2479	C	C5-C4-N4	-6.11	115.92	120.20
1	a	762	C	C6-N1-C1'	-6.11	113.47	120.80
23	A	1685	A	N1-C6-N6	-6.11	114.94	118.60
23	A	153	G	C5-C6-O6	6.10	132.26	128.60
1	a	316	C	N1-C2-O2	6.09	122.55	118.90
1	a	315	U	C5-C6-N1	6.09	125.74	122.70
24	B	114	C	N3-C2-O2	-6.09	117.64	121.90
23	A	734	A	C5-C6-N1	6.08	120.74	117.70
23	A	789	C	C5-C4-N4	-6.08	115.94	120.20
23	A	1350	U	C2-N1-C1'	6.08	124.99	117.70
23	A	2707	C	C5-C4-N4	-6.08	115.95	120.20
23	A	1727	C	N3-C4-C5	6.08	124.33	121.90
23	A	2063	C	N1-C2-O2	6.08	122.55	118.90
1	a	932	G	C2-N3-C4	-6.07	108.86	111.90
23	A	656	G	N3-C4-C5	6.07	131.63	128.60
23	A	992	A	N9-C4-C5	-6.07	103.37	105.80
23	A	129	C	N1-C2-O2	6.07	122.54	118.90
23	A	198	A	C4-C5-N7	6.06	113.73	110.70
23	A	2028	A	C5-C6-N1	6.06	120.73	117.70
23	A	2456	G	N1-C6-O6	6.05	123.53	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	851	C	C6-N1-C2	-6.04	117.88	120.30
23	A	844	G	N3-C4-N9	-6.04	122.38	126.00
23	A	584	G	N3-C4-N9	-6.04	122.38	126.00
23	A	1148	C	C2-N1-C1'	6.04	125.44	118.80
23	A	2729	G	N3-C4-C5	-6.04	125.58	128.60
23	A	1049	C	C6-N1-C2	-6.03	117.89	120.30
23	A	1029	C	C5-C4-N4	-6.03	115.98	120.20
23	A	343	A	N1-C6-N6	6.03	122.22	118.60
23	A	1795	A	C5-C6-N1	6.03	120.71	117.70
23	A	2467	C	C6-N1-C1'	-6.03	113.57	120.80
1	a	621	C	N3-C4-C5	6.03	124.31	121.90
23	A	496	G	C2-N3-C4	-6.03	108.89	111.90
23	A	1768	C	C5-C6-N1	6.03	124.01	121.00
23	A	767	A	N9-C4-C5	-6.02	103.39	105.80
1	a	136	C	N3-C2-O2	-6.02	117.69	121.90
23	A	1658	A	N9-C4-C5	-6.02	103.39	105.80
23	A	2503	A	N3-C4-N9	-6.01	122.59	127.40
23	A	729	G	C2-N3-C4	-6.01	108.89	111.90
23	A	1336	G	C2-N3-C4	-6.01	108.89	111.90
23	A	1201	G	C6-C5-N7	-6.01	126.79	130.40
23	A	1338	U	C6-N1-C2	-6.00	117.40	121.00
23	A	2418	G	C5-C6-O6	-6.00	125.00	128.60
23	A	115	C	N1-C2-O2	5.99	122.49	118.90
23	A	419	U	N3-C2-O2	-5.99	118.01	122.20
23	A	728	U	N3-C4-O4	5.99	123.59	119.40
23	A	1333	A	C4-C5-N7	5.99	113.69	110.70
23	A	1369	G	C8-N9-C1'	-5.99	119.22	127.00
23	A	565	G	N3-C2-N2	5.98	124.09	119.90
1	a	641	U	N1-C2-O2	5.98	126.98	122.80
23	A	776	C	N1-C2-O2	5.98	122.49	118.90
23	A	2090	C	N3-C4-N4	5.98	122.19	118.00
23	A	1727	C	C5-C4-N4	-5.97	116.02	120.20
1	a	415	A	C5-C6-N6	-5.96	118.93	123.70
23	A	1980	A	N1-C6-N6	-5.96	115.03	118.60
23	A	2618	C	C5-C4-N4	-5.95	116.03	120.20
23	A	2077	C	C5-C4-N4	-5.95	116.03	120.20
1	a	911	A	C5-C6-N6	-5.95	118.94	123.70
23	A	994	A	C5-C6-N1	5.95	120.68	117.70
23	A	2063	C	C6-N1-C2	-5.95	117.92	120.30
1	a	394	C	N3-C2-O2	-5.95	117.74	121.90
23	A	777	C	C6-N1-C2	-5.95	117.92	120.30
1	a	196	A	N7-C8-N9	5.94	116.77	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	933	A	C5-C6-N6	-5.94	118.94	123.70
23	A	1289	A	N1-C6-N6	-5.94	115.03	118.60
23	A	2528	C	C5-C6-N1	5.94	123.97	121.00
1	a	911	A	N1-C6-N6	5.94	122.16	118.60
23	A	1295	C	N3-C4-C5	5.93	124.27	121.90
23	A	455	A	C5-C6-N6	-5.93	118.95	123.70
23	A	1475	A	C5-C6-N6	-5.93	118.95	123.70
1	a	1439	A	C5-C6-N6	-5.93	118.95	123.70
23	A	1713	A	C8-N9-C4	-5.93	103.43	105.80
23	A	2004	A	N1-C6-N6	5.93	122.16	118.60
38	U	26	ASP	CB-CG-OD1	5.93	123.64	118.30
23	A	960	C	C6-N1-C2	-5.93	117.93	120.30
23	A	2843	A	C5-C6-N6	-5.92	118.96	123.70
23	A	2488	C	N1-C2-O2	5.91	122.45	118.90
23	A	2704	A	C5-C6-N1	5.91	120.66	117.70
23	A	2706	A	C5-N7-C8	-5.91	100.95	103.90
1	a	1032	C	N3-C2-O2	-5.91	117.77	121.90
1	a	1522	C	N1-C2-O2	5.91	122.44	118.90
23	A	46	C	C6-N1-C2	-5.91	117.94	120.30
23	A	2517	G	N7-C8-N9	5.91	116.05	113.10
23	A	623	C	C2-N1-C1'	5.90	125.29	118.80
52	8	4	ARG	NE-CZ-NH1	5.90	123.25	120.30
23	A	863	G	C6-C5-N7	-5.90	126.86	130.40
23	A	1414	G	C4-C5-N7	5.90	113.16	110.80
23	A	271	C	N3-C4-C5	5.89	124.26	121.90
1	a	1408	C	C6-N1-C1'	-5.89	113.73	120.80
23	A	1393	C	C5-C4-N4	-5.89	116.08	120.20
25	D	181	ARG	NE-CZ-NH1	5.89	123.25	120.30
23	A	1370	C	N1-C2-O2	5.89	122.43	118.90
23	A	1956	G	C6-C5-N7	-5.88	126.87	130.40
23	A	168	A	N1-C6-N6	5.88	122.13	118.60
23	A	492	G	N1-C2-N2	-5.88	110.91	116.20
23	A	186	C	N1-C2-O2	5.88	122.43	118.90
23	A	824	A	C5-C6-N6	-5.88	119.00	123.70
23	A	2063	C	N3-C2-O2	-5.88	117.79	121.90
1	a	1539	C	N3-C2-O2	-5.87	117.79	121.90
1	a	476	C	C2-N1-C1'	5.86	125.24	118.80
23	A	509	G	N3-C4-C5	5.85	131.52	128.60
23	A	1291	A	C5-C6-N1	5.85	120.62	117.70
23	A	2359	C	N1-C2-O2	5.85	122.41	118.90
23	A	2661	A	C5-C6-N6	-5.84	119.03	123.70
23	A	2290	C	C2-N1-C1'	5.84	125.22	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1304	G	C4-C5-N7	5.84	113.14	110.80
23	A	250	G	N1-C2-N2	-5.84	110.95	116.20
23	A	2091	C	N3-C4-N4	5.83	122.08	118.00
1	a	1049	C	C6-N1-C2	-5.83	117.97	120.30
23	A	2587	C	N1-C2-O2	5.83	122.40	118.90
23	A	2360	A	N1-C6-N6	-5.82	115.11	118.60
23	A	2063	C	C2-N1-C1'	5.82	125.20	118.80
23	A	832	C	N3-C4-N4	5.82	122.07	118.00
23	A	2536	G	N3-C4-N9	-5.82	122.51	126.00
23	A	771	G	C2-N3-C4	-5.82	108.99	111.90
23	A	836	C	N1-C2-O2	5.82	122.39	118.90
1	a	1480	A	C5-C6-N6	-5.81	119.05	123.70
1	a	1506	G	C6-C5-N7	-5.81	126.91	130.40
1	a	1252	G	N7-C8-N9	5.81	116.00	113.10
23	A	2668	A	C5-C6-N6	-5.81	119.05	123.70
37	T	53	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	a	1418	C	N1-C2-O2	5.80	122.38	118.90
23	A	774	G	C8-N9-C1'	-5.80	119.46	127.00
24	B	104	C	N3-C4-C5	5.80	124.22	121.90
23	A	1253	G	N3-C2-N2	5.80	123.96	119.90
23	A	1369	G	C4-N9-C1'	5.80	134.04	126.50
23	A	2357	G	N3-C4-N9	-5.80	122.52	126.00
23	A	1855	G	C2-N3-C4	-5.79	109.00	111.90
23	A	2052	C	C2-N1-C1'	5.79	125.17	118.80
23	A	1811	A	N9-C4-C5	-5.79	103.48	105.80
1	a	1429	A	C5-C6-N6	-5.79	119.07	123.70
1	a	86	G	C8-N9-C1'	5.79	134.53	127.00
23	A	2017	C	N3-C2-O2	-5.79	117.85	121.90
23	A	876	G	N3-C4-N9	-5.79	122.53	126.00
23	A	128	C	N3-C2-O2	-5.79	117.85	121.90
23	A	1413	C	N3-C2-O2	-5.79	117.85	121.90
1	a	125	G	C2-N3-C4	-5.78	109.01	111.90
23	A	1308	C	C5-C4-N4	-5.78	116.15	120.20
1	a	1452	G	N3-C4-N9	-5.78	122.53	126.00
23	A	1453	G	N1-C2-N2	-5.78	111.00	116.20
23	A	1658	A	C4-C5-N7	5.78	113.59	110.70
1	a	725	C	N3-C2-O2	-5.78	117.86	121.90
23	A	1708	A	C5-C6-N6	-5.77	119.08	123.70
23	A	2288	C	N3-C4-N4	5.77	122.04	118.00
23	A	2816	C	N1-C2-O2	5.77	122.36	118.90
1	a	1487	G	N1-C2-N2	-5.77	111.01	116.20
23	A	2105	C	C2-N1-C1'	5.76	125.14	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	2913	G	C5-C6-O6	5.76	132.06	128.60
1	a	221	U	N3-C2-O2	-5.76	118.17	122.20
23	A	624	C	N3-C2-O2	-5.75	117.87	121.90
23	A	1731	G	C2-N3-C4	-5.75	109.02	111.90
23	A	601	G	C4-C5-N7	5.75	113.10	110.80
1	a	34	A	C6-C5-N7	-5.75	128.28	132.30
23	A	824	A	C5-C6-N1	5.75	120.57	117.70
23	A	1798	C	N1-C2-O2	5.75	122.35	118.90
1	a	1428	G	C2-N3-C4	-5.75	109.03	111.90
23	A	2578	C	C2-N1-C1'	5.74	125.12	118.80
23	A	2528	C	N3-C4-N4	5.74	122.02	118.00
23	A	2706	A	C4-C5-N7	5.74	113.57	110.70
1	a	762	C	N1-C2-O2	5.73	122.34	118.90
1	a	903	C	C5-C4-N4	-5.73	116.19	120.20
1	a	1012	U	C2-N1-C1'	5.73	124.58	117.70
23	A	1029	C	N3-C2-O2	-5.73	117.89	121.90
23	A	1950	U	C5-C6-N1	5.73	125.56	122.70
23	A	2105	C	C6-N1-C2	-5.73	118.01	120.30
1	a	1155	G	N3-C2-N2	-5.73	115.89	119.90
23	A	1253	G	N1-C2-N2	-5.73	111.05	116.20
23	A	2409	G	N3-C4-N9	5.73	129.44	126.00
1	a	753	U	C5-C6-N1	5.72	125.56	122.70
1	a	1247	A	C5-C6-N6	-5.72	119.12	123.70
23	A	1956	G	C8-N9-C1'	-5.72	119.56	127.00
27	F	168	ARG	NE-CZ-NH2	5.72	123.16	120.30
23	A	2004	A	C4-C5-N7	5.72	113.56	110.70
23	A	623	C	C5-C4-N4	-5.72	116.20	120.20
1	a	536	C	N3-C2-O2	-5.71	117.90	121.90
23	A	1695	G	C8-N9-C1'	-5.71	119.57	127.00
23	A	188	C	C5-C4-N4	-5.71	116.20	120.20
23	A	1542	C	N3-C2-O2	-5.71	117.91	121.90
23	A	2919	A	N9-C4-C5	-5.71	103.52	105.80
23	A	175	C	C6-N1-C2	-5.70	118.02	120.30
1	a	315	U	N3-C2-O2	-5.70	118.21	122.20
23	A	1104	U	P-O3'-C3'	5.70	126.54	119.70
1	a	641	U	C6-N1-C1'	-5.70	113.23	121.20
23	A	1934	G	C6-C5-N7	-5.69	126.98	130.40
23	A	1108	C	C6-N1-C2	-5.69	118.02	120.30
1	a	34	A	C5-N7-C8	-5.69	101.06	103.90
1	a	493	G	N3-C4-C5	5.69	131.44	128.60
1	a	1252	G	C4-N9-C1'	5.69	133.89	126.50
23	A	1517	A	C5-C6-N6	-5.69	119.15	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	2148	G	N3-C4-N9	5.69	129.41	126.00
23	A	2456	G	C4-N9-C1'	5.68	133.89	126.50
23	A	500	A	C5-C6-N6	-5.68	119.15	123.70
23	A	856	U	N3-C2-O2	-5.68	118.22	122.20
23	A	2021	C	C5-C4-N4	-5.68	116.22	120.20
23	A	2451	C	C5-C4-N4	5.68	124.18	120.20
51	7	13	ARG	NE-CZ-NH2	5.68	123.14	120.30
23	A	1822	C	N1-C2-O2	5.67	122.30	118.90
23	A	2635	G	C2-N3-C4	-5.67	109.06	111.90
24	B	98	G	C4-N9-C1'	5.67	133.87	126.50
23	A	2628	C	C2-N1-C1'	5.67	125.04	118.80
23	A	514	G	C8-N9-C1'	-5.67	119.64	127.00
23	A	876	G	C2-N3-C4	-5.67	109.07	111.90
23	A	1294	G	C4-N9-C1'	5.67	133.87	126.50
23	A	845	A	C5-C6-N6	-5.66	119.17	123.70
23	A	315	C	C6-N1-C2	-5.66	118.03	120.30
23	A	2798	C	N3-C4-C5	5.65	124.16	121.90
23	A	863	G	C2-N3-C4	-5.65	109.08	111.90
23	A	2091	C	C6-N1-C2	-5.65	118.04	120.30
23	A	2525	C	C6-N1-C2	-5.65	118.04	120.30
1	a	700	U	C5-C4-O4	-5.64	122.51	125.90
23	A	1811	A	C5-C6-N6	-5.64	119.19	123.70
23	A	828	A	C5-C6-N1	5.64	120.52	117.70
2	b	213	LEU	CA-CB-CG	5.63	128.25	115.30
23	A	1484	G	C2-N3-C4	-5.63	109.08	111.90
23	A	2077	C	C2-N1-C1'	5.63	124.99	118.80
23	A	398	C	N3-C4-C5	5.63	124.15	121.90
23	A	654	C	C5-C4-N4	-5.62	116.26	120.20
1	a	409	C	N3-C2-O2	-5.62	117.97	121.90
23	A	2839	A	N9-C4-C5	-5.62	103.55	105.80
23	A	1274	G	N3-C2-N2	5.62	123.83	119.90
1	a	1482	G	C2-N3-C4	-5.62	109.09	111.90
1	a	772	C	C5-C4-N4	-5.61	116.27	120.20
23	A	260	A	O4'-C4'-C3'	-5.61	98.39	104.00
23	A	1008	C	N1-C2-O2	5.61	122.27	118.90
23	A	1380	G	C8-N9-C1'	-5.61	119.70	127.00
23	A	2021	C	N3-C4-C5	5.61	124.15	121.90
23	A	2603	G	N3-C2-N2	-5.61	115.97	119.90
23	A	2707	C	C2-N1-C1'	5.61	124.97	118.80
1	a	34	A	C4-C5-N7	5.61	113.50	110.70
23	A	2051	C	N1-C2-O2	5.61	122.27	118.90
23	A	2619	G	C8-N9-C1'	-5.61	119.71	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	1547	C	N3-C2-O2	-5.61	117.97	121.90
1	a	86	G	C4-N9-C1'	-5.61	119.21	126.50
23	A	514	G	C4-N9-C1'	5.61	133.79	126.50
23	A	992	A	C4-C5-N7	5.61	113.50	110.70
23	A	838	A	C5-C6-N6	-5.60	119.22	123.70
23	A	1517	A	N3-C4-N9	5.60	131.88	127.40
23	A	757	G	N3-C4-C5	5.60	131.40	128.60
1	a	463	U	C2-N1-C1'	5.60	124.42	117.70
23	A	620	G	C4-N9-C1'	5.59	133.77	126.50
23	A	497	U	C5-C6-N1	5.59	125.50	122.70
23	A	555	C	C6-N1-C2	-5.59	118.06	120.30
23	A	565	G	N1-C2-N2	-5.59	111.17	116.20
23	A	1414	G	C5-N7-C8	-5.59	101.50	104.30
23	A	2059	G	N3-C4-N9	-5.59	122.65	126.00
1	a	484	A	N1-C6-N6	5.58	121.95	118.60
23	A	1490	G	N3-C2-N2	5.58	123.81	119.90
23	A	178	A	C4-C5-N7	5.58	113.49	110.70
23	A	1419	A	N1-C6-N6	5.58	121.95	118.60
23	A	718	C	C6-N1-C2	5.58	122.53	120.30
23	A	1542	C	N1-C2-O2	5.58	122.25	118.90
23	A	2057	A	N1-C6-N6	-5.58	115.25	118.60
23	A	1695	G	N3-C4-N9	5.58	129.35	126.00
23	A	865	A	C5-C6-N1	5.57	120.48	117.70
23	A	2848	G	N3-C4-N9	-5.57	122.66	126.00
23	A	2051	C	C2-N1-C1'	5.57	124.92	118.80
23	A	2729	G	C8-N9-C1'	-5.56	119.77	127.00
23	A	1803	G	C4-N9-C1'	5.56	133.73	126.50
23	A	2234	C	N1-C2-O2	5.56	122.24	118.90
23	A	288	C	C6-N1-C2	-5.56	118.08	120.30
23	A	2288	C	N1-C2-O2	5.56	122.23	118.90
23	A	1393	C	N3-C2-O2	-5.56	118.01	121.90
1	a	1183	C	C6-N1-C2	-5.55	118.08	120.30
23	A	955	A	C5-C6-N6	5.55	128.14	123.70
23	A	1414	G	N7-C8-N9	5.55	115.87	113.10
1	a	36	G	C8-N9-C1'	-5.54	119.80	127.00
23	A	272	C	C6-N1-C2	-5.54	118.08	120.30
23	A	2729	G	N1-C2-N2	-5.54	111.22	116.20
23	A	707	G	C2-N3-C4	-5.54	109.13	111.90
23	A	2540	A	C5-C6-N1	5.53	120.47	117.70
23	A	1696	C	C5-C4-N4	-5.53	116.33	120.20
23	A	2610	G	N3-C4-N9	-5.53	122.68	126.00
23	A	515	G	N1-C2-N2	-5.53	111.23	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	2778	G	N3-C4-N9	-5.53	122.68	126.00
23	A	935	C	C2-N1-C1'	5.52	124.88	118.80
23	A	626	G	C4-N9-C1'	5.52	133.67	126.50
23	A	125	A	C5-C6-N6	-5.52	119.29	123.70
23	A	1286	G	N3-C4-C5	5.51	131.36	128.60
1	a	86	G	C6-C5-N7	5.51	133.71	130.40
23	A	1202	C	C2-N1-C1'	5.51	124.86	118.80
23	A	1547	C	N1-C2-O2	5.51	122.21	118.90
23	A	2503	A	N3-C4-C5	5.51	130.66	126.80
23	A	260	A	O4'-C1'-N9	5.51	112.61	108.20
23	A	1197	C	N3-C2-O2	-5.51	118.04	121.90
23	A	623	C	N3-C2-O2	-5.51	118.05	121.90
23	A	2059	G	N3-C4-C5	5.51	131.35	128.60
23	A	2409	G	N1-C2-N2	-5.51	111.24	116.20
23	A	1515	G	N1-C2-N2	-5.50	111.25	116.20
23	A	1333	A	N7-C8-N9	5.50	116.55	113.80
1	a	734	C	N1-C2-O2	5.50	122.20	118.90
23	A	2455	G	N3-C4-C5	5.50	131.35	128.60
23	A	1308	C	N3-C4-C5	5.49	124.10	121.90
23	A	2409	G	N3-C2-N2	5.49	123.75	119.90
23	A	1656	C	N1-C2-O2	5.49	122.19	118.90
23	A	1031	C	N1-C2-O2	5.48	122.19	118.90
1	a	564	C	N1-C2-O2	5.48	122.19	118.90
1	a	1367	G	C4-N9-C1'	5.48	133.62	126.50
23	A	584	G	N3-C4-C5	5.48	131.34	128.60
23	A	175	C	C6-N1-C1'	5.47	127.37	120.80
23	A	1472	C	N3-C4-N4	5.47	121.83	118.00
23	A	2409	G	N9-C4-C5	-5.47	103.21	105.40
23	A	1201	G	C8-N9-C1'	-5.47	119.89	127.00
23	A	2077	C	N1-C2-O2	5.47	122.18	118.90
23	A	85	G	N3-C4-C5	5.46	131.33	128.60
23	A	1811	A	N1-C6-N6	5.46	121.88	118.60
23	A	724	C	C5-C4-N4	-5.46	116.38	120.20
23	A	1880	A	C4-C5-N7	5.46	113.43	110.70
23	A	2900	C	N3-C2-O2	-5.46	118.08	121.90
23	A	1049	C	N1-C2-O2	5.46	122.17	118.90
1	a	1299	A	N1-C6-N6	5.45	121.87	118.60
23	A	2078	A	C5-N7-C8	-5.45	101.17	103.90
50	6	40	ARG	NE-CZ-NH2	5.45	123.03	120.30
52	8	4	ARG	NE-CZ-NH2	-5.45	117.57	120.30
23	A	1148	C	N3-C2-O2	-5.45	118.08	121.90
23	A	1213	C	N1-C2-O2	5.45	122.17	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	456	A	C2-N3-C4	5.45	113.33	110.60
1	a	593	G	C6-C5-N7	-5.45	127.13	130.40
24	B	98	G	C8-N9-C1'	-5.44	119.92	127.00
23	A	854	G	N3-C4-C5	5.44	131.32	128.60
23	A	2668	A	C6-N1-C2	-5.44	115.34	118.60
1	a	454	G	C4-N9-C1'	5.43	133.56	126.50
23	A	1302	G	C2-N3-C4	-5.43	109.18	111.90
23	A	2308	C	N3-C4-N4	-5.43	114.20	118.00
23	A	718	C	C5-C4-N4	-5.43	116.40	120.20
23	A	1393	C	N3-C4-N4	5.43	121.80	118.00
23	A	1956	G	N1-C2-N2	-5.43	111.31	116.20
23	A	2479	C	C2-N3-C4	-5.43	117.19	119.90
1	a	750	G	N3-C4-N9	-5.42	122.75	126.00
1	a	252	U	C2-N1-C1'	5.42	124.20	117.70
23	A	832	C	N3-C2-O2	-5.42	118.11	121.90
1	a	1156	C	N1-C2-O2	5.42	122.15	118.90
23	A	348	C	N1-C2-O2	5.42	122.15	118.90
23	A	1294	G	C5-C6-O6	5.41	131.85	128.60
23	A	1803	G	N7-C8-N9	5.41	115.81	113.10
23	A	2452	A	C8-N9-C4	-5.41	103.64	105.80
23	A	44	A	C5-N7-C8	-5.41	101.19	103.90
23	A	2778	G	N3-C2-N2	-5.41	116.11	119.90
36	S	94	VAL	CA-CB-CG2	5.41	119.01	110.90
23	A	113	U	C2-N1-C1'	5.40	124.19	117.70
23	A	2058	A	C4-C5-N7	5.40	113.40	110.70
23	A	2236	C	N1-C2-O2	5.40	122.14	118.90
23	A	2750	C	C5-C4-N4	-5.40	116.42	120.20
23	A	2621	C	C5-C4-N4	-5.40	116.42	120.20
23	A	476	A	C5-C6-N1	5.39	120.40	117.70
23	A	2082	C	C6-N1-C2	5.39	122.46	120.30
23	A	2503	A	C2-N3-C4	-5.39	107.90	110.60
1	a	1355	C	N3-C2-O2	-5.39	118.13	121.90
23	A	1435	C	C5-C4-N4	-5.39	116.43	120.20
23	A	1767	G	O4'-C1'-N9	5.39	112.51	108.20
23	A	2275	C	C5-C6-N1	5.39	123.69	121.00
23	A	1435	C	N1-C2-O2	5.39	122.13	118.90
1	a	196	A	C4-N9-C1'	5.38	135.99	126.30
1	a	415	A	C6-C5-N7	-5.38	128.53	132.30
1	a	1367	G	N7-C8-N9	5.38	115.79	113.10
23	A	574	A	N1-C6-N6	5.38	121.83	118.60
23	A	1395	G	C4-C5-N7	5.38	112.95	110.80
23	A	2176	C	N3-C4-N4	5.38	121.77	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1541	G	N3-C2-N2	5.38	123.66	119.90
23	A	2004	A	N9-C4-C5	-5.38	103.65	105.80
23	A	491	C	N3-C2-O2	-5.37	118.14	121.90
23	A	922	G	O4'-C1'-N9	5.37	112.50	108.20
23	A	1290	G	N1-C2-N2	-5.37	111.37	116.20
23	A	2456	G	N7-C8-N9	5.37	115.78	113.10
23	A	1669	C	N3-C4-C5	5.37	124.05	121.90
23	A	2083	G	C4-N9-C1'	5.37	133.47	126.50
23	A	627	C	C6-N1-C2	-5.36	118.15	120.30
23	A	1291	A	C5-C6-N6	-5.36	119.41	123.70
23	A	2059	G	C8-N9-C1'	5.36	133.97	127.00
34	Q	24	LEU	CA-CB-CG	5.36	127.63	115.30
23	A	1452	C	N3-C4-C5	5.36	124.04	121.90
23	A	319	G	N1-C2-N2	-5.35	111.38	116.20
23	A	2072	C	N1-C2-O2	5.35	122.11	118.90
23	A	1469	G	C2-N3-C4	-5.35	109.23	111.90
1	a	1156	C	N3-C2-O2	-5.35	118.16	121.90
51	7	44	LEU	CA-CB-CG	5.35	127.60	115.30
23	A	912	C	N3-C4-C5	5.34	124.04	121.90
23	A	1631	G	N1-C2-N2	5.34	121.01	116.20
23	A	2048	G	C4-N9-C1'	5.34	133.44	126.50
23	A	2082	C	N3-C4-C5	5.34	124.03	121.90
23	A	2654	G	C2-N3-C4	-5.34	109.23	111.90
23	A	1370	C	C5-C4-N4	-5.34	116.46	120.20
23	A	1917	A	N1-C6-N6	5.34	121.80	118.60
23	A	518	A	N1-C6-N6	5.33	121.80	118.60
23	A	2711	U	C5-C4-O4	-5.33	122.70	125.90
23	A	1347	G	C4-N9-C1'	5.33	133.44	126.50
23	A	2534	C	N1-C2-O2	5.33	122.10	118.90
23	A	774	G	C5-N7-C8	-5.33	101.63	104.30
23	A	914	G	N3-C4-N9	-5.33	122.80	126.00
23	A	1197	C	C2-N1-C1'	5.33	124.67	118.80
1	a	252	U	N3-C2-O2	-5.33	118.47	122.20
23	A	356	A	N9-C4-C5	-5.33	103.67	105.80
23	A	511	G	C2-N3-C4	-5.33	109.24	111.90
1	a	158	G	N3-C4-N9	-5.33	122.80	126.00
23	A	1490	G	N1-C6-O6	-5.33	116.70	119.90
23	A	1798	C	N3-C4-N4	5.32	121.73	118.00
23	A	2409	G	C6-C5-N7	-5.32	127.21	130.40
23	A	2919	A	C6-C5-N7	-5.32	128.57	132.30
1	a	100	A	N1-C6-N6	5.32	121.79	118.60
23	A	1226	G	C2-N3-C4	-5.31	109.24	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1295	C	N3-C2-O2	-5.31	118.18	121.90
23	A	181	G	N3-C4-N9	-5.31	122.81	126.00
23	A	1431	U	O4'-C1'-N1	-5.31	103.95	108.20
23	A	574	A	C5-N7-C8	-5.31	101.25	103.90
23	A	2302	C	C6-N1-C2	-5.31	118.18	120.30
23	A	767	A	C4-C5-N7	5.31	113.35	110.70
1	a	461	C	C5-C4-N4	-5.30	116.49	120.20
23	A	1663	G	C4-N9-C1'	5.30	133.40	126.50
23	A	2327	A	C5-C6-N6	-5.30	119.46	123.70
23	A	603	C	N3-C2-O2	-5.30	118.19	121.90
1	a	1304	G	N9-C4-C5	-5.30	103.28	105.40
23	A	178	A	C6-C5-N7	-5.30	128.59	132.30
23	A	186	C	N3-C2-O2	-5.30	118.19	121.90
23	A	685	C	N1-C2-O2	5.30	122.08	118.90
23	A	1934	G	C4-C5-N7	5.30	112.92	110.80
23	A	2456	G	C8-N9-C1'	-5.30	120.11	127.00
1	a	168	G	N3-C2-N2	5.30	123.61	119.90
23	A	656	G	N3-C4-N9	-5.30	122.82	126.00
23	A	1051	C	N3-C4-C5	5.29	124.02	121.90
23	A	1690	A	N1-C6-N6	5.29	121.77	118.60
23	A	548	A	C5-N7-C8	-5.29	101.25	103.90
1	a	905	A	C5-C6-N1	5.29	120.34	117.70
1	a	1353	C	N1-C2-O2	5.29	122.07	118.90
23	A	1950	U	C6-N1-C2	-5.29	117.83	121.00
23	A	2452	A	N9-C4-C5	5.29	107.91	105.80
1	a	168	G	C5-N7-C8	-5.28	101.66	104.30
23	A	1004	A	C6-N1-C2	-5.28	115.43	118.60
23	A	732	C	N3-C4-C5	5.28	124.01	121.90
1	a	1208	A	N9-C4-C5	-5.28	103.69	105.80
23	A	1274	G	C2-N3-C4	-5.28	109.26	111.90
1	a	493	G	N3-C4-N9	-5.28	122.83	126.00
1	a	614	G	N3-C4-N9	-5.28	122.83	126.00
23	A	436	A	N9-C4-C5	-5.28	103.69	105.80
23	A	2707	C	N1-C2-O2	5.27	122.06	118.90
23	A	1382	C	C2-N1-C1'	5.27	124.59	118.80
23	A	2385	A	N9-C4-C5	-5.27	103.69	105.80
23	A	2471	G	C8-N9-C1'	-5.27	120.16	127.00
1	a	1439	A	C4-C5-N7	5.26	113.33	110.70
23	A	1347	G	N1-C2-N3	5.26	127.06	123.90
24	B	114	C	C2-N1-C1'	5.26	124.59	118.80
1	a	415	A	C4-C5-N7	5.26	113.33	110.70
37	T	53	ARG	NE-CZ-NH2	-5.26	117.67	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	2001	C	C5-C4-N4	-5.26	116.52	120.20
23	A	2275	C	N3-C4-N4	5.26	121.68	118.00
23	A	38	A	C6-N1-C2	-5.25	115.45	118.60
1	a	588	C	C5-C4-N4	-5.25	116.52	120.20
1	a	100	A	C5-N7-C8	-5.25	101.27	103.90
23	A	863	G	C4-N9-C1'	5.25	133.33	126.50
23	A	1815	C	N1-C2-O2	5.25	122.05	118.90
23	A	2706	A	C6-C5-N7	-5.25	128.63	132.30
23	A	567	G	C6-C5-N7	-5.24	127.25	130.40
23	A	862	C	C5-C4-N4	-5.24	116.53	120.20
1	a	355	G	C8-N9-C4	5.24	108.50	106.40
23	A	1932	C	C2-N3-C4	-5.24	117.28	119.90
23	A	2422	C	N1-C2-O2	5.24	122.05	118.90
23	A	1731	G	N3-C4-C5	5.24	131.22	128.60
23	A	729	G	N1-C2-N2	-5.24	111.48	116.20
23	A	872	U	C6-N1-C2	-5.24	117.86	121.00
46	2	10	ARG	NE-CZ-NH1	5.24	122.92	120.30
23	A	1919	C	N1-C2-O2	5.24	122.04	118.90
23	A	2654	G	N7-C8-N9	5.23	115.72	113.10
1	a	1099	G	C2-N3-C4	-5.23	109.28	111.90
23	A	341	G	N3-C4-C5	5.23	131.22	128.60
1	a	34	A	N7-C8-N9	5.23	116.42	113.80
23	A	908	A	C4-C5-N7	5.23	113.31	110.70
23	A	1453	G	N3-C2-N2	5.23	123.56	119.90
23	A	2064	A	C5-C6-N6	-5.23	119.52	123.70
23	A	1400	C	N1-C2-O2	5.22	122.03	118.90
23	A	2816	C	O4'-C1'-N1	5.22	112.38	108.20
1	a	1434	G	N3-C4-N9	-5.22	122.87	126.00
23	A	988	C	C5-C4-N4	-5.21	116.55	120.20
23	A	2788	A	C5-C6-N1	5.21	120.31	117.70
1	a	196	A	C5-C6-N6	-5.21	119.53	123.70
23	A	923	A	O4'-C1'-N9	5.21	112.37	108.20
23	A	2543	G	C4-N9-C1'	5.21	133.28	126.50
23	A	1035	C	N1-C2-O2	5.21	122.03	118.90
23	A	1202	C	C5-C4-N4	-5.21	116.55	120.20
23	A	1812	A	C5-C6-N1	5.21	120.30	117.70
23	A	2849	A	C5-C6-N6	-5.21	119.53	123.70
25	D	197	LEU	CB-CG-CD1	-5.21	102.15	111.00
23	A	1517	A	N9-C4-C5	-5.20	103.72	105.80
23	A	2074	C	C6-N1-C2	-5.20	118.22	120.30
23	A	2278	G	N3-C4-C5	5.20	131.20	128.60
1	a	876	C	N3-C4-C5	5.20	123.98	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	O	64	ARG	NE-CZ-NH2	5.20	122.90	120.30
23	A	777	C	N3-C2-O2	-5.20	118.26	121.90
23	A	1951	C	C6-N1-C2	-5.20	118.22	120.30
23	A	500	A	C5-N7-C8	-5.19	101.30	103.90
23	A	601	G	C5-N7-C8	-5.19	101.70	104.30
23	A	939	U	C5-C4-O4	5.19	129.01	125.90
23	A	136	A	N1-C6-N6	5.19	121.71	118.60
23	A	670	G	N3-C4-C5	5.19	131.19	128.60
23	A	2878	U	O4'-C1'-N1	-5.19	104.05	108.20
23	A	1695	G	N3-C2-N2	5.19	123.53	119.90
23	A	1735	C	N1-C2-O2	5.18	122.01	118.90
23	A	1352	C	N1-C2-O2	5.18	122.01	118.90
1	a	1513	C	N3-C2-O2	-5.18	118.27	121.90
23	A	727	G	C2-N3-C4	-5.18	109.31	111.90
23	A	1596	G	N3-C2-N2	-5.18	116.28	119.90
23	A	2715	G	N3-C4-C5	5.18	131.19	128.60
23	A	518	A	C5-C6-N6	-5.18	119.56	123.70
23	A	1148	C	N1-C2-O2	5.18	122.01	118.90
1	a	933	A	N1-C6-N6	5.18	121.71	118.60
23	A	241	C	C2-N1-C1'	5.18	124.49	118.80
23	A	2214	G	N9-C4-C5	-5.17	103.33	105.40
1	a	1439	A	N1-C6-N6	5.17	121.70	118.60
23	A	1361	G	C8-N9-C4	-5.17	104.33	106.40
23	A	1414	G	C6-C5-N7	-5.17	127.30	130.40
23	A	1328	C	C5-C4-N4	-5.17	116.58	120.20
23	A	1596	G	N3-C4-N9	-5.17	122.90	126.00
23	A	2104	A	C5-N7-C8	-5.17	101.32	103.90
23	A	668	C	N3-C2-O2	-5.17	118.28	121.90
23	A	2610	G	C2-N3-C4	-5.16	109.32	111.90
1	a	805	C	N3-C2-O2	-5.16	118.29	121.90
23	A	2706	A	N9-C4-C5	-5.16	103.74	105.80
23	A	1278	G	C8-N9-C4	-5.16	104.34	106.40
23	A	574	A	C5-C6-N6	-5.15	119.58	123.70
1	a	342	C	N1-C2-O2	5.15	121.99	118.90
23	A	548	A	N7-C8-N9	5.15	116.38	113.80
23	A	668	C	C2-N1-C1'	5.15	124.47	118.80
23	A	1802	U	C6-N1-C2	-5.15	117.91	121.00
23	A	2035	C	C5-C4-N4	-5.15	116.59	120.20
23	A	809	A	C6-N1-C2	-5.15	115.51	118.60
23	A	2493	C	C5-C4-N4	-5.15	116.60	120.20
1	a	316	C	N3-C2-O2	-5.14	118.30	121.90
23	A	448	A	C5-C6-N6	-5.14	119.58	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	547	A	C5-C6-N6	-5.14	119.58	123.70
23	A	593	U	P-O3'-C3'	5.14	125.87	119.70
23	A	624	C	C2-N1-C1'	5.14	124.46	118.80
23	A	1714	C	N3-C4-C5	5.14	123.96	121.90
23	A	2104	A	C4-C5-N7	5.14	113.27	110.70
23	A	1098	A	N1-C6-N6	-5.14	115.52	118.60
1	a	208	U	C2-N3-C4	5.14	130.08	127.00
1	a	1247	A	N1-C6-N6	5.13	121.68	118.60
1	a	955	G	N3-C2-N2	5.13	123.49	119.90
23	A	844	G	C2-N3-C4	-5.13	109.33	111.90
11	k	111	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	a	750	G	N3-C4-C5	5.13	131.16	128.60
2	b	214	THR	CA-CB-CG2	5.13	119.58	112.40
23	A	2578	C	N3-C2-O2	-5.12	118.31	121.90
23	A	809	A	C5-C6-N1	5.12	120.26	117.70
23	A	2729	G	N3-C4-N9	5.12	129.07	126.00
24	B	96	G	C4-N9-C1'	5.12	133.16	126.50
24	B	111	A	O4'-C1'-N9	5.12	112.30	108.20
23	A	1414	G	N3-C2-N2	5.12	123.48	119.90
23	A	2639	C	C2-N1-C1'	5.12	124.43	118.80
1	a	834	C	N1-C2-O2	5.11	121.97	118.90
23	A	1963	A	N1-C6-N6	5.11	121.67	118.60
23	A	2540	A	N1-C6-N6	5.11	121.67	118.60
23	A	2456	G	C5-C6-O6	-5.11	125.53	128.60
23	A	777	C	N1-C2-O2	5.11	121.97	118.90
24	B	81	A	C5-C6-N6	-5.11	119.61	123.70
1	a	235	G	N9-C4-C5	-5.11	103.36	105.40
23	A	967	C	N1-C2-O2	5.11	121.96	118.90
23	A	1282	A	C5-C6-N1	5.11	120.25	117.70
23	A	1632	A	O4'-C1'-N9	-5.11	104.11	108.20
23	A	1650	G	C2-N3-C4	-5.11	109.35	111.90
23	A	2698	A	C4-C5-N7	5.11	113.25	110.70
1	a	1439	A	N9-C4-C5	-5.11	103.76	105.80
23	A	2706	A	N1-C6-N6	5.11	121.66	118.60
23	A	674	C	N3-C4-C5	5.10	123.94	121.90
1	a	1544	U	C2-N1-C1'	5.10	123.82	117.70
23	A	44	A	C4-C5-N7	5.10	113.25	110.70
23	A	863	G	C8-N9-C1'	-5.10	120.37	127.00
23	A	2074	C	N3-C2-O2	-5.10	118.33	121.90
23	A	757	G	N3-C4-N9	-5.10	122.94	126.00
23	A	2539	C	N1-C2-O2	5.10	121.96	118.90
1	a	242	C	N1-C2-O2	5.10	121.96	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	2069	A	N1-C6-N6	5.10	121.66	118.60
23	A	2718	C	N1-C2-O2	5.10	121.96	118.90
23	A	774	G	C4-N9-C1'	5.10	133.13	126.50
23	A	2887	G	O4'-C1'-N9	5.10	112.28	108.20
1	a	544	C	N1-C2-O2	5.09	121.96	118.90
23	A	37	C	C5-C4-N4	-5.09	116.63	120.20
23	A	868	A	C5-C6-N6	-5.09	119.62	123.70
23	A	1834	G	C2-N3-C4	-5.09	109.35	111.90
23	A	2633	C	N3-C4-C5	5.09	123.94	121.90
23	A	1310	A	C5-C6-N6	-5.09	119.63	123.70
23	A	725	A	C5-C6-N6	-5.09	119.63	123.70
23	A	724	C	N3-C4-N4	5.09	121.56	118.00
23	A	1408	G	C2-N3-C4	-5.09	109.36	111.90
23	A	1419	A	C5-N7-C8	-5.08	101.36	103.90
1	a	1101	G	N1-C6-O6	-5.08	116.85	119.90
1	a	1353	C	N3-C2-O2	-5.08	118.34	121.90
2	b	214	THR	OG1-CB-CG2	5.08	121.69	110.00
23	A	1294	G	N1-C6-O6	-5.08	116.85	119.90
23	A	1533	A	O4'-C1'-N9	5.08	112.27	108.20
23	A	1934	G	N9-C4-C5	-5.08	103.37	105.40
23	A	2900	C	N1-C2-O2	5.08	121.95	118.90
23	A	348	C	C2-N1-C1'	5.08	124.39	118.80
23	A	1880	A	C5-N7-C8	-5.08	101.36	103.90
23	A	2378	G	C2-N3-C4	-5.08	109.36	111.90
23	A	2048	G	C8-N9-C1'	-5.08	120.40	127.00
23	A	859	C	C5-C4-N4	-5.07	116.65	120.20
23	A	2816	C	N3-C2-O2	-5.07	118.35	121.90
23	A	574	A	N7-C8-N9	5.07	116.33	113.80
23	A	1399	C	N3-C4-C5	5.07	123.93	121.90
23	A	2214	G	C6-C5-N7	-5.07	127.36	130.40
23	A	2744	G	N1-C2-N2	-5.07	111.64	116.20
23	A	2839	A	C5-C6-N6	-5.07	119.64	123.70
1	a	837	A	C5-C6-N6	-5.07	119.64	123.70
23	A	250	G	C2-N3-C4	-5.07	109.36	111.90
23	A	1801	C	C5-C4-N4	-5.07	116.65	120.20
1	a	456	A	N1-C6-N6	-5.07	115.56	118.60
23	A	492	G	N3-C2-N2	5.07	123.45	119.90
23	A	2642	U	N3-C4-O4	5.07	122.95	119.40
1	a	234	A	N9-C4-C5	-5.07	103.77	105.80
23	A	461	A	N7-C8-N9	5.06	116.33	113.80
23	A	515	G	C6-C5-N7	-5.06	127.36	130.40
23	A	1118	G	N3-C4-N9	-5.06	122.96	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	2056	G	N7-C8-N9	5.06	115.63	113.10
1	a	208	U	C2-N1-C1'	5.06	123.77	117.70
23	A	1708	A	N1-C6-N6	5.06	121.64	118.60
23	A	2087	A	O4'-C1'-N9	5.06	112.25	108.20
23	A	2452	A	C5-C6-N1	5.06	120.23	117.70
1	a	683	A	N1-C6-N6	5.06	121.63	118.60
23	A	6	A	C5-N7-C8	-5.06	101.37	103.90
23	A	555	C	C2-N1-C1'	5.06	124.36	118.80
23	A	862	C	N3-C4-N4	5.06	121.54	118.00
23	A	740	G	N3-C4-N9	-5.06	122.97	126.00
23	A	16	G	C2-N3-C4	-5.05	109.37	111.90
23	A	1826	G	N3-C4-N9	-5.05	122.97	126.00
23	A	2078	A	C5-C6-N6	-5.05	119.66	123.70
23	A	2317	G	C4-N9-C1'	5.05	133.07	126.50
23	A	20	C	N1-C2-O2	5.05	121.93	118.90
23	A	495	A	N9-C4-C5	-5.05	103.78	105.80
23	A	2475	A	C5-C6-N6	-5.05	119.66	123.70
23	A	136	A	N9-C4-C5	-5.05	103.78	105.80
23	A	436	A	C4-C5-N7	5.05	113.22	110.70
23	A	683	G	N7-C8-N9	5.05	115.62	113.10
1	a	406	C	N1-C2-O2	5.04	121.93	118.90
1	a	1541	G	C5-N7-C8	-5.04	101.78	104.30
23	A	767	A	C5-C6-N6	-5.04	119.67	123.70
23	A	1315	C	N1-C2-O2	5.04	121.92	118.90
23	A	2091	C	C2-N1-C1'	5.04	124.34	118.80
23	A	2264	G	C2-N3-C4	-5.04	109.38	111.90
23	A	2628	C	C6-N1-C1'	-5.04	114.75	120.80
23	A	1781	C	C5-C4-N4	-5.04	116.67	120.20
1	a	221	U	C6-N1-C2	-5.04	117.98	121.00
7	g	101	LEU	CA-CB-CG	5.04	126.88	115.30
23	A	1080	G	C2-N3-C4	-5.04	109.38	111.90
23	A	2097	G	N1-C2-N2	-5.04	111.67	116.20
23	A	2214	G	C4-C5-N7	5.04	112.81	110.80
24	B	86	C	C6-N1-C2	-5.03	118.29	120.30
23	A	1435	C	N3-C4-N4	5.03	121.52	118.00
1	a	1406	C	C5-C4-N4	-5.03	116.68	120.20
24	B	96	G	N1-C2-N2	-5.03	111.67	116.20
23	A	2823	G	C8-N9-C1'	5.03	133.54	127.00
23	A	875	G	N3-C2-N2	-5.03	116.38	119.90
23	A	2794	C	N1-C2-O2	5.03	121.92	118.90
23	A	2845	G	N3-C4-C5	5.03	131.11	128.60
23	A	1335	C	N1-C2-O2	5.03	121.92	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	2540	A	C4-C5-N7	5.03	113.21	110.70
23	A	92	G	N3-C4-N9	-5.02	122.98	126.00
23	A	1414	G	C2-N3-C4	-5.02	109.39	111.90
23	A	2843	A	C5-C6-N1	5.02	120.21	117.70
1	a	252	U	N1-C2-O2	5.02	126.31	122.80
23	A	178	A	C5-C6-N6	-5.02	119.68	123.70
23	A	422	G	N7-C8-N9	5.02	115.61	113.10
23	A	2348	G	C4-N9-C1'	5.02	133.02	126.50
23	A	2815	C	C2-N1-C1'	5.02	124.32	118.80
23	A	1486	C	N3-C4-N4	-5.02	114.49	118.00
23	A	1658	A	C5-N7-C8	-5.01	101.39	103.90
23	A	2005	A	C5-N7-C8	-5.01	101.39	103.90
23	A	1386	U	O4'-C1'-N1	5.01	112.21	108.20
23	A	2610	G	N3-C4-C5	5.01	131.11	128.60
1	a	588	C	N1-C2-O2	5.01	121.91	118.90
1	a	1513	C	N1-C2-O2	5.01	121.91	118.90
23	A	1213	C	C6-N1-C2	-5.01	118.30	120.30
23	A	2698	A	C5-C6-N6	-5.01	119.69	123.70
7	g	95	ARG	NE-CZ-NH1	5.01	122.80	120.30
23	A	912	C	C5-C4-N4	-5.01	116.69	120.20
1	a	933	A	C4-C5-N7	5.01	113.20	110.70
23	A	545	G	C2-N3-C4	-5.01	109.40	111.90
23	A	1656	C	C2-N1-C1'	5.01	124.31	118.80
1	a	816	C	N1-C2-O2	5.00	121.90	118.90
23	A	37	C	N1-C2-O2	5.00	121.90	118.90
23	A	1370	C	N3-C4-N4	5.00	121.50	118.00
24	B	111	A	C4-C5-N7	5.00	113.20	110.70
23	A	2259	C	N1-C2-O2	5.00	121.90	118.90
23	A	2090	C	N3-C4-C5	5.00	123.90	121.90
23	A	2443	C	C5-C4-N4	-5.00	116.70	120.20
24	B	111	A	C5-N7-C8	-5.00	101.40	103.90

There are no chirality outliers.

All (65) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
46	2	17	GLU	Peptide
47	3	11	GLN	Peptide
47	3	13	ILE	Peptide
47	3	42	GLU	Peptide
50	6	15	LYS	Peptide
50	6	7	GLN	Peptide

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Mol	Chain	Res	Type	Group
51	7	28	PHE	Peptide
51	7	33	PHE	Peptide
25	D	120	GLU	Peptide
25	D	214	GLY	Peptide
26	E	140	PRO	Peptide
26	E	141	MET	Peptide
26	E	142	SER	Peptide
26	E	200	ASN	Peptide
26	E	9	LYS	Peptide
27	F	154	VAL	Peptide
27	F	155	VAL	Peptide
30	M	40	LYS	Peptide
31	N	23	LYS	Peptide
32	O	110	LYS	Peptide
32	O	35	HIS	Peptide
32	O	58	PHE	Peptide
32	O	65	GLY	Peptide
33	P	134	ARG	Sidechain
33	P	90	VAL	Peptide
33	P	98	LYS	Peptide
35	R	110	GLU	Peptide
35	R	29	PRO	Peptide
35	R	89	ILE	Peptide
36	S	103	ARG	Peptide
36	S	105	LEU	Peptide
37	T	85	LYS	Peptide
38	U	100	ILE	Peptide
41	X	77	GLU	Peptide
43	Z	82	ARG	Peptide
2	b	19	GLN	Peptide
2	b	21	ARG	Peptide
3	c	160	ASP	Peptide
4	d	160	PHE	Peptide
4	d	93	ARG	Peptide
5	e	108	GLY	Peptide
6	f	81	LYS	Peptide
7	g	13	LEU	Peptide
7	g	14	PRO	Peptide
7	g	146	GLU	Peptide
7	g	73	LEU	Peptide
7	g	8	PRO	Peptide
7	g	9	LYS	Peptide

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Mol	Chain	Res	Type	Group
11	k	53	LYS	Peptide
12	l	109	HIS	Peptide
12	l	23	ALA	Peptide
12	l	32	LYS	Peptide
13	m	44	ARG	Peptide
14	n	18	VAL	Peptide
14	n	54	PRO	Peptide
17	q	4	ARG	Peptide
17	q	72	THR	Peptide
19	s	40	ILE	Peptide
22	v	47	TYR	Peptide
22	v	49	ASN	Peptide
22	v	50	SER	Peptide
22	v	51	ALA	Peptide
22	v	66	ARG	Sidechain
22	v	87	ARG	Sidechain
22	v	98	ARG	Sidechain

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	220/255 (86%)	192 (87%)	27 (12%)	1 (0%)	29	66
3	c	201/217 (93%)	166 (83%)	34 (17%)	1 (0%)	29	66
4	d	193/200 (96%)	163 (84%)	30 (16%)	0	100	100
5	e	158/166 (95%)	124 (78%)	34 (22%)	0	100	100
6	f	92/98 (94%)	73 (79%)	18 (20%)	1 (1%)	14	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	g	139/156 (89%)	117 (84%)	20 (14%)	2 (1%)	11	45
8	h	129/132 (98%)	107 (83%)	21 (16%)	1 (1%)	19	56
9	i	126/132 (96%)	107 (85%)	19 (15%)	0	100	100
10	j	97/102 (95%)	87 (90%)	10 (10%)	0	100	100
11	k	113/129 (88%)	89 (79%)	24 (21%)	0	100	100
12	l	133/137 (97%)	98 (74%)	33 (25%)	2 (2%)	10	44
13	m	108/121 (89%)	87 (81%)	21 (19%)	0	100	100
14	n	58/61 (95%)	40 (69%)	18 (31%)	0	100	100
15	o	86/89 (97%)	78 (91%)	8 (9%)	0	100	100
16	p	88/91 (97%)	69 (78%)	19 (22%)	0	100	100
17	q	83/87 (95%)	64 (77%)	19 (23%)	0	100	100
18	r	54/80 (68%)	41 (76%)	13 (24%)	0	100	100
19	s	82/92 (89%)	63 (77%)	19 (23%)	0	100	100
20	t	78/83 (94%)	73 (94%)	5 (6%)	0	100	100
21	u	43/58 (74%)	31 (72%)	9 (21%)	3 (7%)	1	15
22	v	99/190 (52%)	70 (71%)	21 (21%)	8 (8%)	1	11
25	D	273/277 (99%)	228 (84%)	44 (16%)	1 (0%)	34	69
26	E	216/220 (98%)	172 (80%)	41 (19%)	3 (1%)	11	45
27	F	197/207 (95%)	157 (80%)	40 (20%)	0	100	100
28	G	164/179 (92%)	123 (75%)	40 (24%)	1 (1%)	25	62
29	H	162/178 (91%)	140 (86%)	22 (14%)	0	100	100
30	M	143/145 (99%)	117 (82%)	25 (18%)	1 (1%)	22	59
31	N	120/122 (98%)	83 (69%)	37 (31%)	0	100	100
32	O	129/146 (88%)	90 (70%)	39 (30%)	0	100	100
33	P	131/144 (91%)	101 (77%)	30 (23%)	0	100	100
34	Q	115/122 (94%)	89 (77%)	26 (23%)	0	100	100
35	R	117/119 (98%)	95 (81%)	22 (19%)	0	100	100
36	S	105/116 (90%)	86 (82%)	17 (16%)	2 (2%)	8	40
37	T	114/118 (97%)	102 (90%)	12 (10%)	0	100	100
38	U	100/102 (98%)	79 (79%)	20 (20%)	1 (1%)	15	51
39	V	110/117 (94%)	98 (89%)	12 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	W	87/91 (96%)	68 (78%)	19 (22%)	0	100	100
41	X	81/105 (77%)	50 (62%)	31 (38%)	0	100	100
42	Y	92/217 (42%)	68 (74%)	24 (26%)	0	100	100
43	Z	75/94 (80%)	65 (87%)	9 (12%)	1 (1%)	12	47
44	0	44/62 (71%)	33 (75%)	11 (25%)	0	100	100
45	1	63/69 (91%)	56 (89%)	7 (11%)	0	100	100
46	2	55/59 (93%)	48 (87%)	6 (11%)	1 (2%)	8	41
47	3	79/84 (94%)	47 (60%)	31 (39%)	1 (1%)	12	47
48	4	42/58 (72%)	36 (86%)	5 (12%)	1 (2%)	6	35
49	5	24/49 (49%)	19 (79%)	5 (21%)	0	100	100
50	6	42/45 (93%)	34 (81%)	6 (14%)	2 (5%)	2	22
51	7	58/66 (88%)	38 (66%)	20 (34%)	0	100	100
52	8	35/37 (95%)	27 (77%)	8 (23%)	0	100	100
All	All	5353/6024 (89%)	4288 (80%)	1031 (19%)	34 (1%)	29	62

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
21	u	13	GLU
21	u	50	GLU
22	v	97	ASN
22	v	99	LYS
22	v	100	SER
22	v	102	ASP
2	b	104	TYR
21	u	51	ALA
22	v	51	ALA
22	v	79	ASP
22	v	83	ASN
22	v	101	ARG
26	E	10	ILE
26	E	142	SER
36	S	105	LEU
43	Z	28	ARG
47	3	12	VAL
50	6	16	VAL
7	g	14	PRO

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Mol	Chain	Res	Type
50	6	15	LYS
7	g	13	LEU
36	S	106	ARG
48	4	44	CYS
3	c	203	ARG
12	l	57	LYS
28	G	99	PHE
30	M	66	THR
38	U	23	GLU
8	h	100	GLY
46	2	30	LYS
12	l	41	PRO
6	f	12	PRO
25	D	252	PRO
26	E	154	VAL

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	192/221 (87%)	188 (98%)	4 (2%)	53	74
3	c	164/175 (94%)	160 (98%)	4 (2%)	49	71
4	d	172/175 (98%)	171 (99%)	1 (1%)	86	93
5	e	126/131 (96%)	120 (95%)	6 (5%)	25	56
6	f	82/86 (95%)	81 (99%)	1 (1%)	71	84
7	g	122/132 (92%)	118 (97%)	4 (3%)	38	64
8	h	112/113 (99%)	110 (98%)	2 (2%)	59	77
9	i	106/109 (97%)	106 (100%)	0	100	100
10	j	89/91 (98%)	86 (97%)	3 (3%)	37	64
11	k	91/104 (88%)	90 (99%)	1 (1%)	73	85
12	l	117/119 (98%)	114 (97%)	3 (3%)	46	69
13	m	94/104 (90%)	93 (99%)	1 (1%)	73	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	n	52/53 (98%)	51 (98%)	1 (2%)	57	76
15	o	80/81 (99%)	77 (96%)	3 (4%)	33	61
16	p	76/77 (99%)	74 (97%)	2 (3%)	46	69
17	q	80/82 (98%)	80 (100%)	0	100	100
18	r	51/68 (75%)	50 (98%)	1 (2%)	55	74
19	s	73/80 (91%)	73 (100%)	0	100	100
20	t	67/69 (97%)	66 (98%)	1 (2%)	65	81
21	u	41/54 (76%)	33 (80%)	8 (20%)	1	9
22	v	91/173 (53%)	66 (72%)	25 (28%)	0	3
25	D	222/224 (99%)	219 (99%)	3 (1%)	67	82
26	E	175/177 (99%)	174 (99%)	1 (1%)	86	93
27	F	163/169 (96%)	162 (99%)	1 (1%)	86	93
28	G	147/158 (93%)	146 (99%)	1 (1%)	84	91
29	H	144/155 (93%)	143 (99%)	1 (1%)	84	91
30	M	123/123 (100%)	123 (100%)	0	100	100
31	N	100/100 (100%)	100 (100%)	0	100	100
32	O	104/112 (93%)	102 (98%)	2 (2%)	57	76
33	P	110/119 (92%)	104 (94%)	6 (6%)	21	53
34	Q	98/102 (96%)	98 (100%)	0	100	100
35	R	95/95 (100%)	95 (100%)	0	100	100
36	S	93/102 (91%)	93 (100%)	0	100	100
37	T	96/98 (98%)	96 (100%)	0	100	100
38	U	86/86 (100%)	86 (100%)	0	100	100
39	V	91/94 (97%)	91 (100%)	0	100	100
40	W	80/82 (98%)	80 (100%)	0	100	100
41	X	73/90 (81%)	73 (100%)	0	100	100
42	Y	83/190 (44%)	82 (99%)	1 (1%)	71	84
43	Z	60/75 (80%)	59 (98%)	1 (2%)	60	79
44	0	39/52 (75%)	37 (95%)	2 (5%)	24	55
45	1	59/62 (95%)	59 (100%)	0	100	100
46	2	51/53 (96%)	50 (98%)	1 (2%)	55	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	3	72/75 (96%)	70 (97%)	2 (3%)	43	67
48	4	41/51 (80%)	39 (95%)	2 (5%)	25	56
49	5	26/47 (55%)	25 (96%)	1 (4%)	33	61
50	6	39/40 (98%)	39 (100%)	0	100	100
51	7	52/57 (91%)	50 (96%)	2 (4%)	33	61
52	8	35/35 (100%)	35 (100%)	0	100	100
All	All	4635/5120 (90%)	4537 (98%)	98 (2%)	56	74

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	35	ARG
2	b	36	ASN
2	b	55	ASN
2	b	159	GLN
3	c	61	ASN
3	c	85	LYS
3	c	88	ASN
3	c	141	MET
4	d	178	ARG
5	e	8	THR
5	e	9	LYS
5	e	32	ARG
5	e	43	ASN
5	e	146	ASN
5	e	149	ASN
6	f	53	ASN
7	g	19	ASN
7	g	109	ARG
7	g	137	LYS
7	g	148	ASN
8	h	96	LYS
8	h	99	ASN
10	j	4	GLN
10	j	5	LYS
10	j	16	ARG
11	k	14	LYS
12	l	43	LYS
12	l	56	LYS
12	l	73	ASN

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Mol	Chain	Res	Type
13	m	3	ARG
14	n	57	ARG
15	o	40	ASN
15	o	59	MET
15	o	71	ARG
16	p	15	ASN
16	p	81	MET
18	r	40	GLU
20	t	45	ASN
21	u	11	SER
21	u	12	LEU
21	u	16	LEU
21	u	24	SER
21	u	25	LYS
21	u	44	LYS
21	u	53	ARG
21	u	54	LYS
22	v	19	ASN
22	v	20	TYR
22	v	22	GLU
22	v	30	ARG
22	v	41	HIS
22	v	45	LYS
22	v	47	TYR
22	v	66	ARG
22	v	70	ARG
22	v	74	LEU
22	v	75	TYR
22	v	78	ILE
22	v	80	LEU
22	v	82	ASN
22	v	83	ASN
22	v	88	GLN
22	v	90	ARG
22	v	91	LYS
22	v	92	TYR
22	v	93	LYS
22	v	94	THR
22	v	96	ILE
22	v	99	LYS
22	v	101	ARG
22	v	103	ARG

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Mol	Chain	Res	Type
25	D	69	ASN
25	D	81	GLN
25	D	254	LEU
26	E	212	ARG
27	F	135	LYS
28	G	96	MET
29	H	132	LYS
32	O	59	ARG
32	O	84	LYS
33	P	6	ARG
33	P	51	ARG
33	P	60	ARG
33	P	133	LYS
33	P	135	GLU
33	P	136	GLU
42	Y	21	LEU
43	Z	19	LYS
44	0	23	ASN
44	0	32	ASN
46	2	3	LYS
47	3	75	ASN
47	3	77	LYS
48	4	44	CYS
48	4	45	LYS
49	5	46	ARG
51	7	26	ARG
51	7	45	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
2	b	19	GLN
2	b	36	ASN
2	b	55	ASN
2	b	77	GLN
2	b	159	GLN
3	c	6	ASN
3	c	44	ASN
3	c	88	ASN
4	d	159	ASN
5	e	43	ASN
5	e	146	ASN

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Mol	Chain	Res	Type
5	e	149	ASN
6	f	53	ASN
7	g	19	ASN
7	g	40	GLN
8	h	31	ASN
8	h	68	GLN
9	i	33	ASN
12	l	25	ASN
12	l	73	ASN
13	m	76	ASN
16	p	15	ASN
20	t	21	ASN
20	t	62	GLN
22	v	19	ASN
22	v	41	HIS
22	v	71	ASN
22	v	82	ASN
22	v	88	GLN
22	v	97	ASN
25	D	43	ASN
25	D	193	GLN
26	E	50	GLN
26	E	103	GLN
27	F	75	GLN
27	F	148	GLN
29	H	23	HIS
29	H	106	ASN
29	H	120	ASN
29	H	165	GLN
31	N	82	ASN
32	O	114	ASN
33	P	35	GLN
34	Q	61	ASN
35	R	37	ASN
39	V	90	GLN
41	X	76	ASN
42	Y	10	GLN
43	Z	20	ASN
44	0	32	ASN
44	0	34	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1540/1556 (98%)	373 (24%)	0
23	A	2909/2923 (99%)	727 (24%)	18 (0%)
24	B	113/114 (99%)	23 (20%)	0
All	All	4562/4593 (99%)	1123 (24%)	18 (0%)

All (1123) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	8	G
1	a	9	A
1	a	10	G
1	a	11	A
1	a	15	U
1	a	28	G
1	a	31	U
1	a	32	G
1	a	33	A
1	a	40	G
1	a	44	C
1	a	48	C
1	a	49	C
1	a	51	A
1	a	52	A
1	a	53	U
1	a	58	G
1	a	61	A
1	a	62	G
1	a	67	G
1	a	69	G
1	a	74	G
1	a	82	G
1	a	83	C
1	a	84	U
1	a	85	U
1	a	86	G
1	a	88	U
1	a	89	U
1	a	90	C
1	a	92	C
1	a	94	G
1	a	95	A
1	a	120	C
1	a	129	A

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Mol	Chain	Res	Type
1	a	130	A
1	a	138	A
1	a	142	G
1	a	144	C
1	a	148	G
1	a	149	A
1	a	154	U
1	a	159	G
1	a	163	C
1	a	165	G
1	a	168	G
1	a	169	C
1	a	170	U
1	a	171	A
1	a	173	U
1	a	182	A
1	a	183	U
1	a	191	A
1	a	196	A
1	a	205	A
1	a	211	A
1	a	212	A
1	a	213	G
1	a	214	A
1	a	218	U
1	a	221	U
1	a	234	A
1	a	247	C
1	a	248	U
1	a	252	U
1	a	255	G
1	a	259	G
1	a	260	U
1	a	269	U
1	a	274	G
1	a	275	C
1	a	287	A
1	a	297	G
1	a	301	A
1	a	307	G
1	a	314	A
1	a	315	U

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Mol	Chain	Res	Type
1	a	333	A
1	a	334	G
1	a	336	C
1	a	354	G
1	a	355	G
1	a	356	G
1	a	360	C
1	a	361	A
1	a	362	G
1	a	364	A
1	a	373	U
1	a	375	U
1	a	380	C
1	a	402	G
1	a	405	A
1	a	406	C
1	a	414	G
1	a	419	A
1	a	420	U
1	a	421	G
1	a	422	A
1	a	429	U
1	a	431	G
1	a	432	G
1	a	436	G
1	a	437	U
1	a	438	A
1	a	444	C
1	a	447	U
1	a	449	A
1	a	454	G
1	a	455	G
1	a	456	A
1	a	457	A
1	a	459	A
1	a	462	A
1	a	466	G
1	a	467	U
1	a	470	A
1	a	476	C
1	a	477	U
1	a	478	G

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Mol	Chain	Res	Type
1	a	480	G
1	a	481	C
1	a	482	A
1	a	483	C
1	a	484	A
1	a	492	G
1	a	494	U
1	a	503	A
1	a	504	G
1	a	505	A
1	a	508	G
1	a	513	G
1	a	516	U
1	a	519	C
1	a	520	U
1	a	526	C
1	a	528	A
1	a	529	G
1	a	532	G
1	a	535	G
1	a	539	U
1	a	540	A
1	a	541	A
1	a	555	A
1	a	556	G
1	a	557	C
1	a	558	G
1	a	567	A
1	a	569	U
1	a	570	U
1	a	572	U
1	a	575	G
1	a	576	G
1	a	580	A
1	a	581	A
1	a	583	G
1	a	584	C
1	a	585	G
1	a	587	G
1	a	588	C
1	a	604	A
1	a	613	U

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Mol	Chain	Res	Type
1	a	615	A
1	a	634	U
1	a	635	G
1	a	640	G
1	a	641	U
1	a	647	G
1	a	650	A
1	a	661	U
1	a	669	G
1	a	673	A
1	a	693	G
1	a	695	A
1	a	701	G
1	a	710	A
1	a	711	G
1	a	725	C
1	a	726	A
1	a	731	U
1	a	736	A
1	a	741	G
1	a	742	A
1	a	756	A
1	a	757	A
1	a	758	C
1	a	763	G
1	a	774	A
1	a	781	G
1	a	789	A
1	a	802	A
1	a	807	G
1	a	811	G
1	a	817	G
1	a	819	C
1	a	820	G
1	a	825	C
1	a	828	U
1	a	829	G
1	a	836	A
1	a	850	U
1	a	851	U
1	a	854	C
1	a	855	G

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Mol	Chain	Res	Type
1	a	856	C
1	a	865	G
1	a	868	G
1	a	869	C
1	a	881	U
1	a	882	A
1	a	883	A
1	a	886	A
1	a	900	G
1	a	924	A
1	a	932	G
1	a	936	G
1	a	937	G
1	a	944	C
1	a	945	A
1	a	946	C
1	a	949	G
1	a	955	G
1	a	957	G
1	a	958	C
1	a	968	A
1	a	970	U
1	a	971	U
1	a	975	A
1	a	976	G
1	a	979	A
1	a	981	G
1	a	985	A
1	a	986	G
1	a	992	U
1	a	993	A
1	a	994	C
1	a	999	U
1	a	1002	U
1	a	1003	G
1	a	1012	U
1	a	1014	A
1	a	1024	A
1	a	1027	U
1	a	1028	A
1	a	1030	A
1	a	1034	U

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Mol	Chain	Res	Type
1	a	1036	C
1	a	1037	C
1	a	1038	C
1	a	1039	C
1	a	1040	U
1	a	1041	U
1	a	1042	C
1	a	1044	G
1	a	1049	C
1	a	1050	A
1	a	1057	C
1	a	1065	G
1	a	1067	A
1	a	1068	U
1	a	1076	G
1	a	1078	C
1	a	1083	C
1	a	1087	U
1	a	1091	G
1	a	1092	A
1	a	1097	U
1	a	1106	G
1	a	1107	U
1	a	1113	A
1	a	1117	A
1	a	1130	A
1	a	1139	G
1	a	1141	C
1	a	1142	A
1	a	1144	C
1	a	1150	G
1	a	1151	U
1	a	1154	G
1	a	1157	A
1	a	1162	A
1	a	1163	A
1	a	1164	G
1	a	1165	U
1	a	1168	A
1	a	1169	C
1	a	1170	U
1	a	1171	G

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Mol	Chain	Res	Type
1	a	1172	C
1	a	1179	C
1	a	1190	A
1	a	1195	G
1	a	1207	A
1	a	1208	A
1	a	1223	U
1	a	1225	U
1	a	1226	G
1	a	1232	G
1	a	1237	C
1	a	1239	C
1	a	1244	G
1	a	1249	A
1	a	1251	U
1	a	1261	A
1	a	1264	G
1	a	1271	G
1	a	1272	A
1	a	1273	A
1	a	1279	G
1	a	1281	G
1	a	1289	A
1	a	1291	A
1	a	1293	C
1	a	1296	A
1	a	1297	U
1	a	1298	A
1	a	1304	G
1	a	1309	C
1	a	1310	A
1	a	1311	G
1	a	1313	U
1	a	1316	G
1	a	1323	G
1	a	1328	C
1	a	1330	A
1	a	1331	C
1	a	1333	C
1	a	1334	G
1	a	1335	A
1	a	1338	A

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Mol	Chain	Res	Type
1	a	1346	C
1	a	1347	U
1	a	1356	U
1	a	1357	A
1	a	1358	G
1	a	1371	A
1	a	1375	U
1	a	1381	G
1	a	1386	A
1	a	1389	C
1	a	1390	G
1	a	1392	U
1	a	1406	C
1	a	1408	C
1	a	1410	C
1	a	1430	G
1	a	1437	A
1	a	1442	C
1	a	1443	G
1	a	1453	G
1	a	1454	A
1	a	1457	A
1	a	1459	C
1	a	1462	U
1	a	1463	U
1	a	1464	U
1	a	1465	A
1	a	1478	C
1	a	1487	G
1	a	1492	A
1	a	1503	G
1	a	1505	A
1	a	1514	A
1	a	1515	A
1	a	1516	G
1	a	1517	G
1	a	1518	U
1	a	1519	A
1	a	1529	G
1	a	1532	G
1	a	1536	C
1	a	1541	G

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Mol	Chain	Res	Type
1	a	1542	G
1	a	1546	A
23	A	15	G
23	A	23	G
23	A	28	A
23	A	34	U
23	A	39	C
23	A	46	C
23	A	52	A
23	A	61	A
23	A	63	U
23	A	64	A
23	A	71	A
23	A	75	G
23	A	76	C
23	A	80	G
23	A	82	G
23	A	85	G
23	A	90	A
23	A	100	U
23	A	102	A
23	A	104	C
23	A	108	A
23	A	117	A
23	A	118	A
23	A	119	U
23	A	121	G
23	A	130	A
23	A	135	G
23	A	150	A
23	A	161	A
23	A	162	A
23	A	163	U
23	A	164	A
23	A	166	A
23	A	168	A
23	A	173	A
23	A	177	G
23	A	180	G
23	A	182	C
23	A	183	A
23	A	184	C

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Mol	Chain	Res	Type
23	A	185	A
23	A	199	A
23	A	201	C
23	A	202	A
23	A	204	C
23	A	207	A
23	A	218	G
23	A	219	A
23	A	225	A
23	A	229	A
23	A	231	A
23	A	233	U
23	A	236	A
23	A	244	A
23	A	251	G
23	A	255	G
23	A	263	G
23	A	267	G
23	A	282	A
23	A	284	C
23	A	285	U
23	A	286	U
23	A	287	G
23	A	288	C
23	A	289	U
23	A	298	U
23	A	300	G
23	A	301	U
23	A	305	A
23	A	312	A
23	A	314	A
23	A	316	G
23	A	317	G
23	A	318	A
23	A	319	G
23	A	320	U
23	A	321	U
23	A	329	A
23	A	330	C
23	A	331	G
23	A	337	A
23	A	338	G

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Mol	Chain	Res	Type
23	A	342	A
23	A	345	C
23	A	353	A
23	A	354	A
23	A	355	G
23	A	364	A
23	A	365	A
23	A	373	A
23	A	374	U
23	A	389	A
23	A	393	G
23	A	398	C
23	A	401	U
23	A	404	U
23	A	411	A
23	A	418	G
23	A	432	G
23	A	438	U
23	A	451	U
23	A	457	G
23	A	464	U
23	A	468	A
23	A	482	U
23	A	489	A
23	A	490	C
23	A	502	C
23	A	503	A
23	A	504	G
23	A	510	U
23	A	511	G
23	A	525	A
23	A	526	A
23	A	527	G
23	A	530	C
23	A	536	A
23	A	538	G
23	A	543	G
23	A	550	A
23	A	551	G
23	A	553	A
23	A	554	C
23	A	555	C

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Mol	Chain	Res	Type
23	A	572	C
23	A	574	A
23	A	575	G
23	A	576	U
23	A	577	A
23	A	578	G
23	A	588	G
23	A	589	U
23	A	591	A
23	A	593	U
23	A	594	G
23	A	599	A
23	A	605	U
23	A	606	G
23	A	611	U
23	A	613	G
23	A	618	A
23	A	628	G
23	A	629	A
23	A	630	G
23	A	631	U
23	A	646	A
23	A	650	U
23	A	657	U
23	A	658	A
23	A	659	A
23	A	660	A
23	A	661	U
23	A	663	U
23	A	665	G
23	A	682	A
23	A	683	G
23	A	690	U
23	A	693	G
23	A	698	U
23	A	713	A
23	A	715	A
23	A	716	C
23	A	727	G
23	A	731	U
23	A	732	C
23	A	733	U

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Mol	Chain	Res	Type
23	A	760	A
23	A	762	C
23	A	763	A
23	A	771	G
23	A	774	G
23	A	775	A
23	A	777	C
23	A	785	C
23	A	792	U
23	A	793	G
23	A	795	A
23	A	797	A
23	A	806	A
23	A	807	U
23	A	809	A
23	A	820	G
23	A	827	A
23	A	828	A
23	A	829	U
23	A	834	A
23	A	835	U
23	A	837	G
23	A	838	A
23	A	845	A
23	A	847	A
23	A	848	U
23	A	850	G
23	A	852	U
23	A	864	A
23	A	872	U
23	A	873	U
23	A	875	G
23	A	876	G
23	A	887	A
23	A	891	A
23	A	904	G
23	A	905	U
23	A	911	A
23	A	912	C
23	A	913	U
23	A	921	C
23	A	922	G

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Mol	Chain	Res	Type
23	A	923	A
23	A	924	G
23	A	925	G
23	A	926	G
23	A	929	C
23	A	930	C
23	A	932	U
23	A	936	G
23	A	938	G
23	A	944	G
23	A	945	A
23	A	955	A
23	A	959	C
23	A	962	A
23	A	963	A
23	A	968	A
23	A	970	U
23	A	985	A
23	A	987	U
23	A	989	A
23	A	990	G
23	A	1001	A
23	A	1002	U
23	A	1003	A
23	A	1005	G
23	A	1006	G
23	A	1017	A
23	A	1018	A
23	A	1033	G
23	A	1040	A
23	A	1041	G
23	A	1052	A
23	A	1053	A
23	A	1055	A
23	A	1056	U
23	A	1057	A
23	A	1066	G
23	A	1067	U
23	A	1069	G
23	A	1070	A
23	A	1073	A
23	A	1077	U

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Mol	Chain	Res	Type
23	A	1079	U
23	A	1083	G
23	A	1085	U
23	A	1088	C
23	A	1091	G
23	A	1097	U
23	A	1098	A
23	A	1101	A
23	A	1104	U
23	A	1105	U
23	A	1106	G
23	A	1107	G
23	A	1108	C
23	A	1110	U
23	A	1112	G
23	A	1113	A
23	A	1114	A
23	A	1115	G
23	A	1116	C
23	A	1119	C
23	A	1120	C
23	A	1121	A
23	A	1122	U
23	A	1123	C
23	A	1124	A
23	A	1125	U
23	A	1126	U
23	A	1128	A
23	A	1131	G
23	A	1132	A
23	A	1133	G
23	A	1134	U
23	A	1135	G
23	A	1138	U
23	A	1139	A
23	A	1140	A
23	A	1143	G
23	A	1145	U
23	A	1146	C
23	A	1149	U
23	A	1150	A
23	A	1154	G

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Mol	Chain	Res	Type
23	A	1156	G
23	A	1158	G
23	A	1160	C
23	A	1163	U
23	A	1170	A
23	A	1172	A
23	A	1177	A
23	A	1178	C
23	A	1179	C
23	A	1185	U
23	A	1199	A
23	A	1213	C
23	A	1216	U
23	A	1217	U
23	A	1218	G
23	A	1225	G
23	A	1226	G
23	A	1234	G
23	A	1244	G
23	A	1245	G
23	A	1248	U
23	A	1250	G
23	A	1252	A
23	A	1258	A
23	A	1265	G
23	A	1267	A
23	A	1273	G
23	A	1276	G
23	A	1278	G
23	A	1286	G
23	A	1287	U
23	A	1288	G
23	A	1289	A
23	A	1291	A
23	A	1293	U
23	A	1294	G
23	A	1300	G
23	A	1303	A
23	A	1305	U
23	A	1306	C
23	A	1308	C
23	A	1309	G

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Mol	Chain	Res	Type
23	A	1310	A
23	A	1312	A
23	A	1323	A
23	A	1337	A
23	A	1338	U
23	A	1339	U
23	A	1345	A
23	A	1350	U
23	A	1358	A
23	A	1359	A
23	A	1361	G
23	A	1363	U
23	A	1369	G
23	A	1378	U
23	A	1379	A
23	A	1398	G
23	A	1404	A
23	A	1405	G
23	A	1416	U
23	A	1417	G
23	A	1421	A
23	A	1423	C
23	A	1429	G
23	A	1432	A
23	A	1435	C
23	A	1451	U
23	A	1452	C
23	A	1454	U
23	A	1455	U
23	A	1458	A
23	A	1459	A
23	A	1463	A
23	A	1464	U
23	A	1471	A
23	A	1472	C
23	A	1473	G
23	A	1479	G
23	A	1480	G
23	A	1489	A
23	A	1490	G
23	A	1491	C
23	A	1494	G

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Mol	Chain	Res	Type
23	A	1495	C
23	A	1496	G
23	A	1498	U
23	A	1499	U
23	A	1503	U
23	A	1504	U
23	A	1510	U
23	A	1511	C
23	A	1512	U
23	A	1519	U
23	A	1520	A
23	A	1522	G
23	A	1526	G
23	A	1533	A
23	A	1534	G
23	A	1536	C
23	A	1537	A
23	A	1550	G
23	A	1551	U
23	A	1552	U
23	A	1553	A
23	A	1555	G
23	A	1559	G
23	A	1561	G
23	A	1568	U
23	A	1576	A
23	A	1577	G
23	A	1578	A
23	A	1579	C
23	A	1580	A
23	A	1582	U
23	A	1583	G
23	A	1584	A
23	A	1586	U
23	A	1587	C
23	A	1590	C
23	A	1592	A
23	A	1593	G
23	A	1594	U
23	A	1605	A
23	A	1606	C
23	A	1614	A

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Mol	Chain	Res	Type
23	A	1616	A
23	A	1625	U
23	A	1630	A
23	A	1631	G
23	A	1632	A
23	A	1633	A
23	A	1635	A
23	A	1636	U
23	A	1651	C
23	A	1652	A
23	A	1653	A
23	A	1655	C
23	A	1659	C
23	A	1660	A
23	A	1661	C
23	A	1662	A
23	A	1670	A
23	A	1678	A
23	A	1690	A
23	A	1691	G
23	A	1692	C
23	A	1697	G
23	A	1698	A
23	A	1704	C
23	A	1709	A
23	A	1717	G
23	A	1718	G
23	A	1722	A
23	A	1738	C
23	A	1739	G
23	A	1742	A
23	A	1743	G
23	A	1751	G
23	A	1759	G
23	A	1768	C
23	A	1772	G
23	A	1784	U
23	A	1785	G
23	A	1790	G
23	A	1791	G
23	A	1800	A
23	A	1801	C

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Mol	Chain	Res	Type
23	A	1808	U
23	A	1811	A
23	A	1827	C
23	A	1828	U
23	A	1829	A
23	A	1835	U
23	A	1836	A
23	A	1842	A
23	A	1843	U
23	A	1844	G
23	A	1846	A
23	A	1855	G
23	A	1856	A
23	A	1857	C
23	A	1885	G
23	A	1891	U
23	A	1893	A
23	A	1897	U
23	A	1898	C
23	A	1900	G
23	A	1902	G
23	A	1908	A
23	A	1930	G
23	A	1933	G
23	A	1939	A
23	A	1943	A
23	A	1949	G
23	A	1952	C
23	A	1954	A
23	A	1956	G
23	A	1957	G
23	A	1958	U
23	A	1965	A
23	A	1967	U
23	A	1970	U
23	A	1979	A
23	A	1982	U
23	A	1989	C
23	A	1992	C
23	A	1993	A
23	A	1994	C
23	A	1997	A

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Mol	Chain	Res	Type
23	A	1998	A
23	A	1999	G
23	A	2009	U
23	A	2018	U
23	A	2020	U
23	A	2023	C
23	A	2040	A
23	A	2047	A
23	A	2057	A
23	A	2058	A
23	A	2059	G
23	A	2060	A
23	A	2061	U
23	A	2063	C
23	A	2070	C
23	A	2073	G
23	A	2082	C
23	A	2083	G
23	A	2086	A
23	A	2087	A
23	A	2088	G
23	A	2089	A
23	A	2096	G
23	A	2103	U
23	A	2104	A
23	A	2107	G
23	A	2120	G
23	A	2133	G
23	A	2135	U
23	A	2138	U
23	A	2139	A
23	A	2140	C
23	A	2141	A
23	A	2143	G
23	A	2144	A
23	A	2145	U
23	A	2146	A
23	A	2147	G
23	A	2148	G
23	A	2153	A
23	A	2155	C
23	A	2159	U

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Mol	Chain	Res	Type
23	A	2160	G
23	A	2162	A
23	A	2163	A
23	A	2170	C
23	A	2172	C
23	A	2173	U
23	A	2175	G
23	A	2176	C
23	A	2178	U
23	A	2180	C
23	A	2184	G
23	A	2185	A
23	A	2188	C
23	A	2191	U
23	A	2193	G
23	A	2194	U
23	A	2195	G
23	A	2197	G
23	A	2200	A
23	A	2203	A
23	A	2206	C
23	A	2208	A
23	A	2209	G
23	A	2217	G
23	A	2221	U
23	A	2225	A
23	A	2226	A
23	A	2230	G
23	A	2231	C
23	A	2240	U
23	A	2241	C
23	A	2252	A
23	A	2254	A
23	A	2265	G
23	A	2266	G
23	A	2270	U
23	A	2286	G
23	A	2290	C
23	A	2293	A
23	A	2294	A
23	A	2295	A
23	A	2305	A

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Mol	Chain	Res	Type
23	A	2310	C
23	A	2314	A
23	A	2326	G
23	A	2331	G
23	A	2332	U
23	A	2335	G
23	A	2336	A
23	A	2337	A
23	A	2339	U
23	A	2347	A
23	A	2354	A
23	A	2360	A
23	A	2361	U
23	A	2362	A
23	A	2372	G
23	A	2374	C
23	A	2377	C
23	A	2380	G
23	A	2381	A
23	A	2402	G
23	A	2410	G
23	A	2412	C
23	A	2417	U
23	A	2418	G
23	A	2419	A
23	A	2429	U
23	A	2430	C
23	A	2433	C
23	A	2447	C
23	A	2450	U
23	A	2451	C
23	A	2452	A
23	A	2454	C
23	A	2455	G
23	A	2456	G
23	A	2457	A
23	A	2458	U
23	A	2461	A
23	A	2462	A
23	A	2468	C
23	A	2472	G
23	A	2475	A

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Mol	Chain	Res	Type
23	A	2486	A
23	A	2492	C
23	A	2495	A
23	A	2496	A
23	A	2502	C
23	A	2505	A
23	A	2511	G
23	A	2516	G
23	A	2518	U
23	A	2525	C
23	A	2529	G
23	A	2530	A
23	A	2531	U
23	A	2532	G
23	A	2533	U
23	A	2545	A
23	A	2546	U
23	A	2547	C
23	A	2552	G
23	A	2561	C
23	A	2576	G
23	A	2579	U
23	A	2583	C
23	A	2589	U
23	A	2593	A
23	A	2594	G
23	A	2599	A
23	A	2600	C
23	A	2601	G
23	A	2603	G
23	A	2604	A
23	A	2605	G
23	A	2612	U
23	A	2613	C
23	A	2623	U
23	A	2624	G
23	A	2629	A
23	A	2630	G
23	A	2636	U
23	A	2637	C
23	A	2638	C
23	A	2640	U

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Mol	Chain	Res	Type
23	A	2641	A
23	A	2657	G
23	A	2667	G
23	A	2668	A
23	A	2681	A
23	A	2683	U
23	A	2688	G
23	A	2690	G
23	A	2704	A
23	A	2708	C
23	A	2716	U
23	A	2717	A
23	A	2739	U
23	A	2741	G
23	A	2753	U
23	A	2756	G
23	A	2760	A
23	A	2771	G
23	A	2775	A
23	A	2777	A
23	A	2778	G
23	A	2791	A
23	A	2792	A
23	A	2793	G
23	A	2794	C
23	A	2798	C
23	A	2803	A
23	A	2805	A
23	A	2806	U
23	A	2807	G
23	A	2817	A
23	A	2820	U
23	A	2821	U
23	A	2822	C
23	A	2823	G
23	A	2824	G
23	A	2827	A
23	A	2828	U
23	A	2838	C
23	A	2840	A
23	A	2850	G
23	A	2853	U

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Mol	Chain	Res	Type
23	A	2868	G
23	A	2869	G
23	A	2880	A
23	A	2881	C
23	A	2886	G
23	A	2887	G
23	A	2892	G
23	A	2896	A
23	A	2899	A
23	A	2900	C
23	A	2903	A
23	A	2906	G
23	A	2911	A
23	A	2913	G
23	A	2920	U
24	B	8	A
24	B	10	U
24	B	13	A
24	B	23	U
24	B	24	C
24	B	33	U
24	B	35	C
24	B	38	U
24	B	39	G
24	B	40	C
24	B	42	G
24	B	49	G
24	B	51	A
24	B	55	A
24	B	60	C
24	B	67	G
24	B	84	U
24	B	87	G
24	B	88	U
24	B	92	G
24	B	93	C
24	B	106	U
24	B	113	G

All (18) RNA pucker outliers are listed below:

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Mol	Chain	Res	Type
23	A	162	A
23	A	179	A
23	A	300	G
23	A	311	U
23	A	437	A
23	A	593	U
23	A	863	G
23	A	961	G
23	A	1104	U
23	A	1288	G
23	A	1478	A
23	A	1532	U
23	A	2039	G
23	A	2360	A
23	A	2418	G
23	A	2432	G
23	A	2467	C
23	A	2501	U

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
23	A	1
42	Y	1
25	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1569:G	O3'	1570:G	P	3.00
1	Y	25:GLY	C	26:LYS	N	1.74
1	D	5:TYR	C	6:LYS	N	1.17

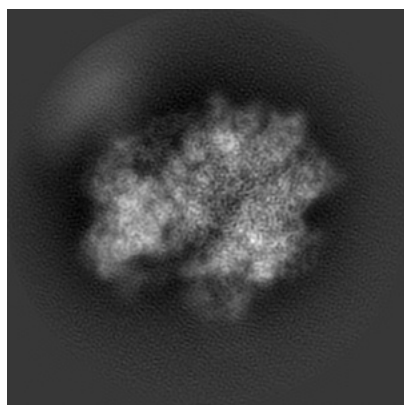
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3625. These allow visual inspection of the internal detail of the map and identification of artifacts.

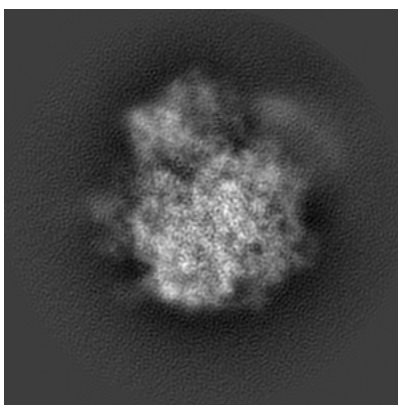
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

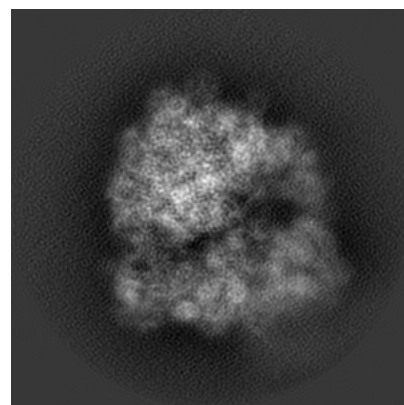
6.1.1 Primary map



X



Y

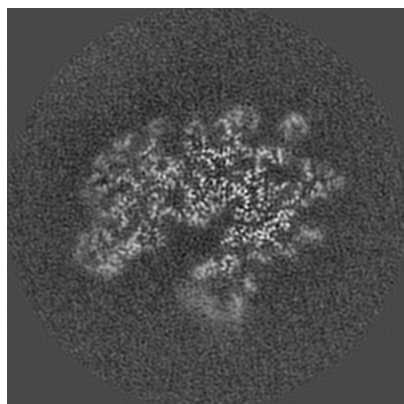


Z

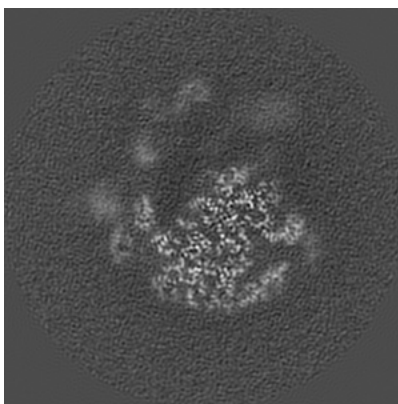
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

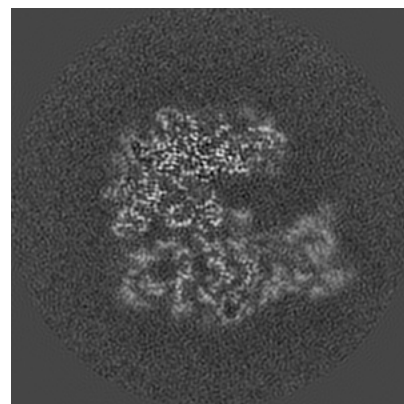
6.2.1 Primary map



X Index: 170



Y Index: 170

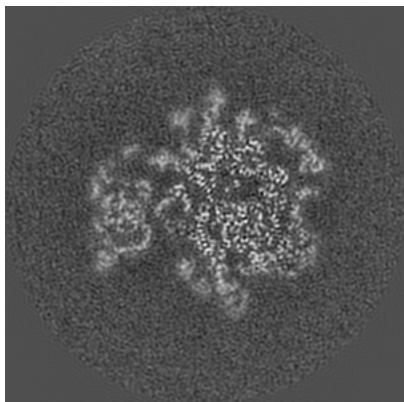


Z Index: 170

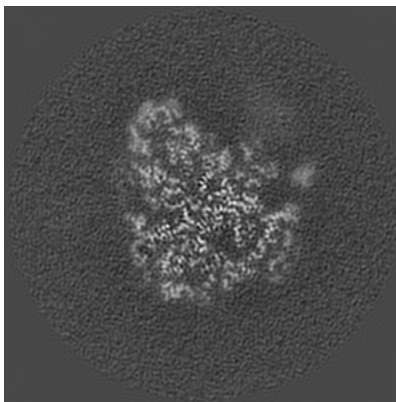
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

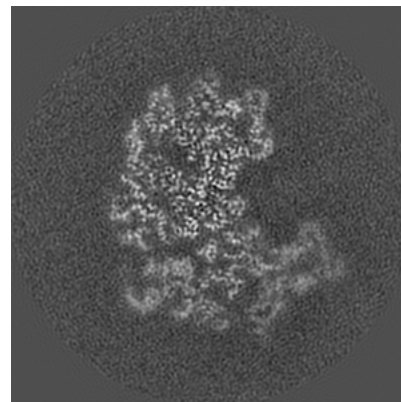
6.3.1 Primary map



X Index: 144



Y Index: 212



Z Index: 187

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

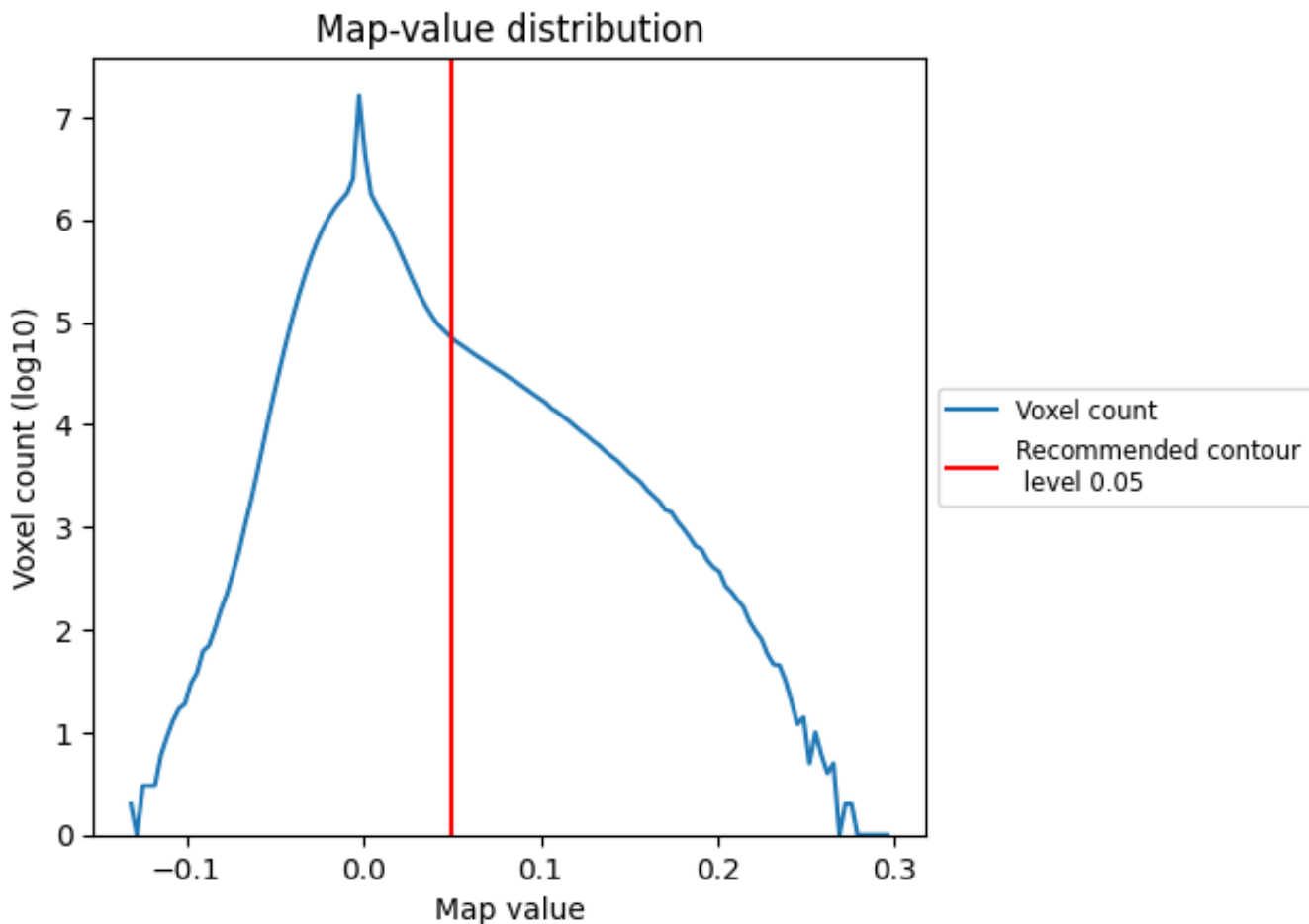
6.5 Mask visualisation

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

7 Map analysis [i](#)

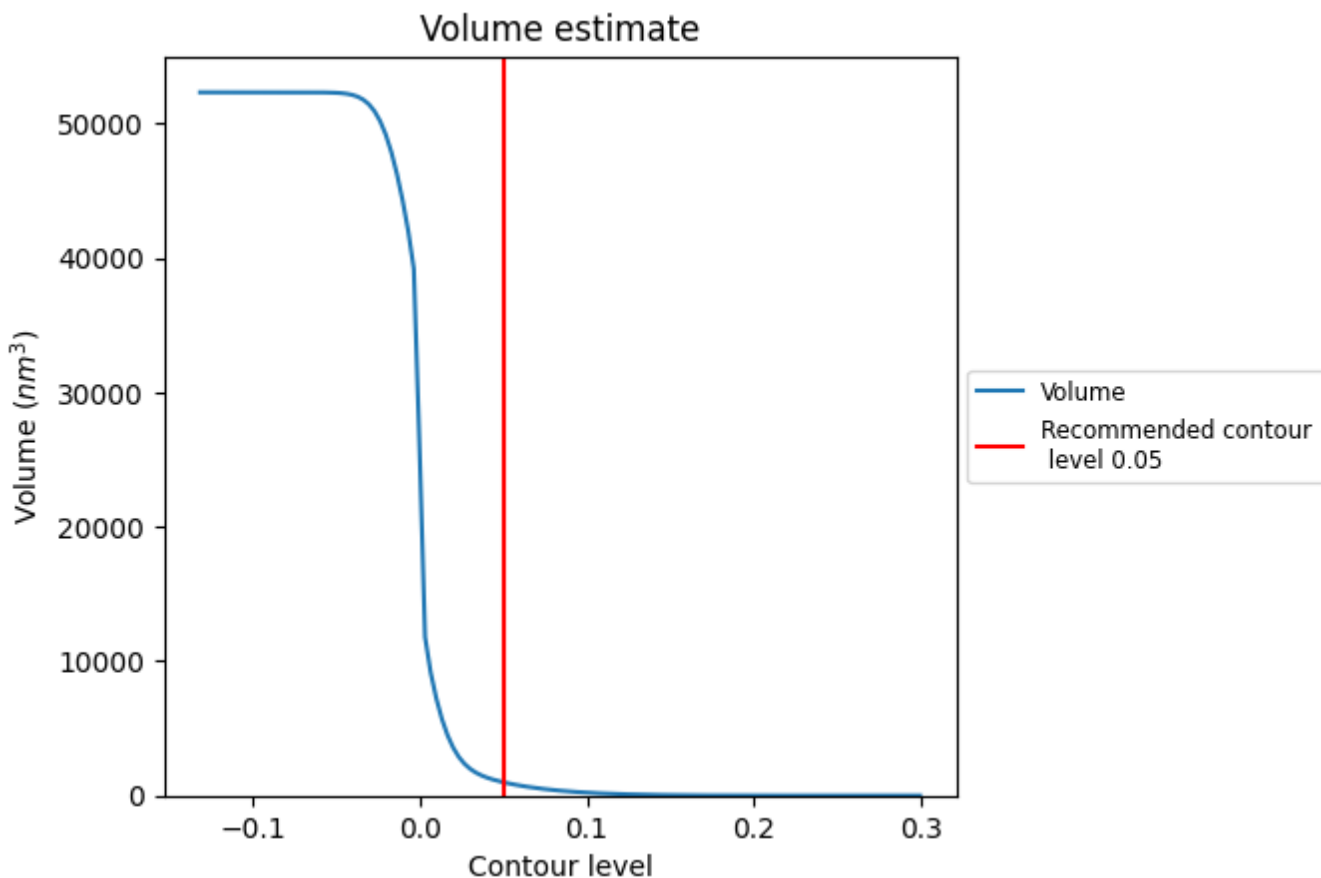
This section contains the results of statistical analysis of the map.

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.

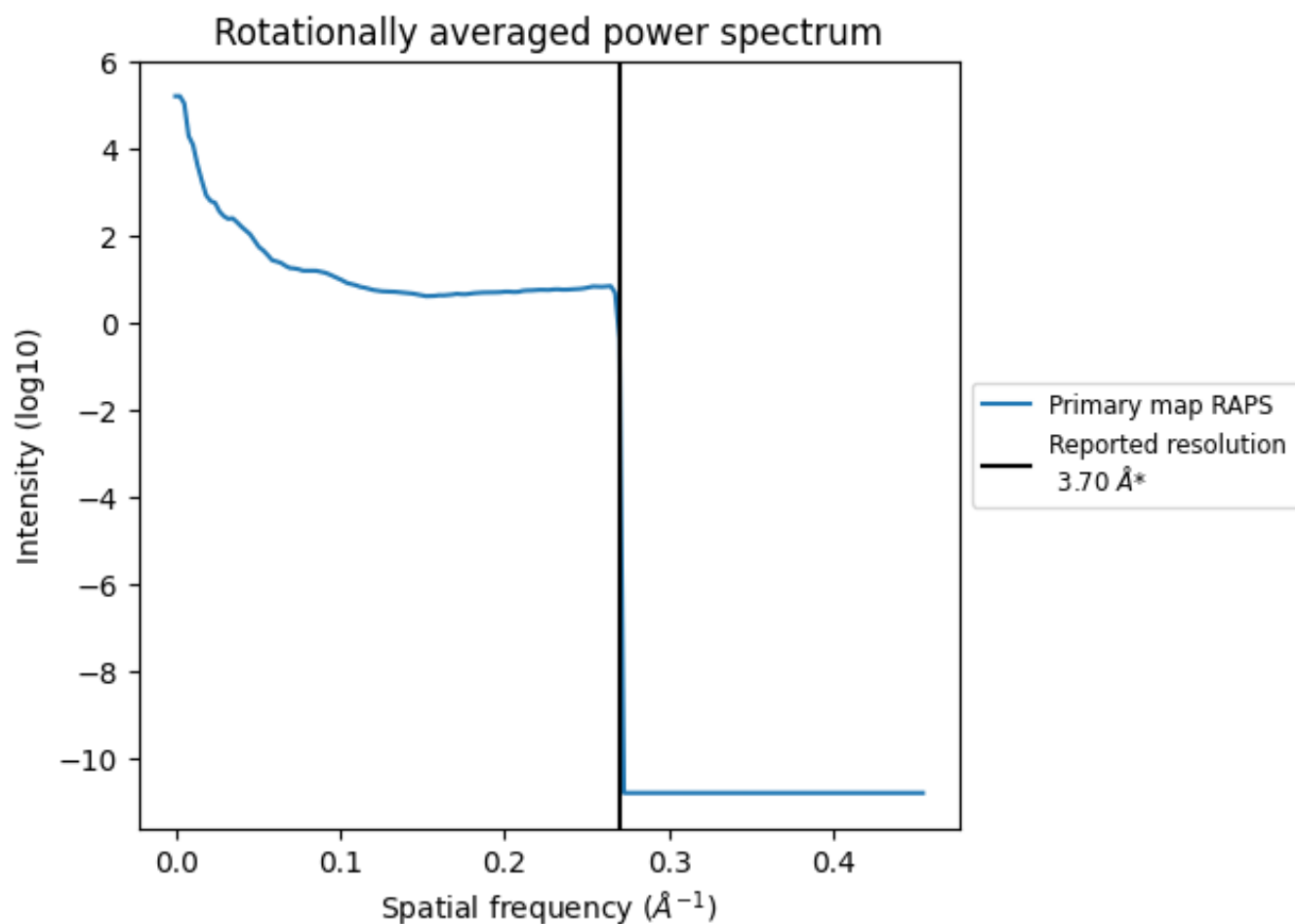
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 989 nm^3 ; this corresponds to an approximate mass of 894 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 0.270 Å⁻¹

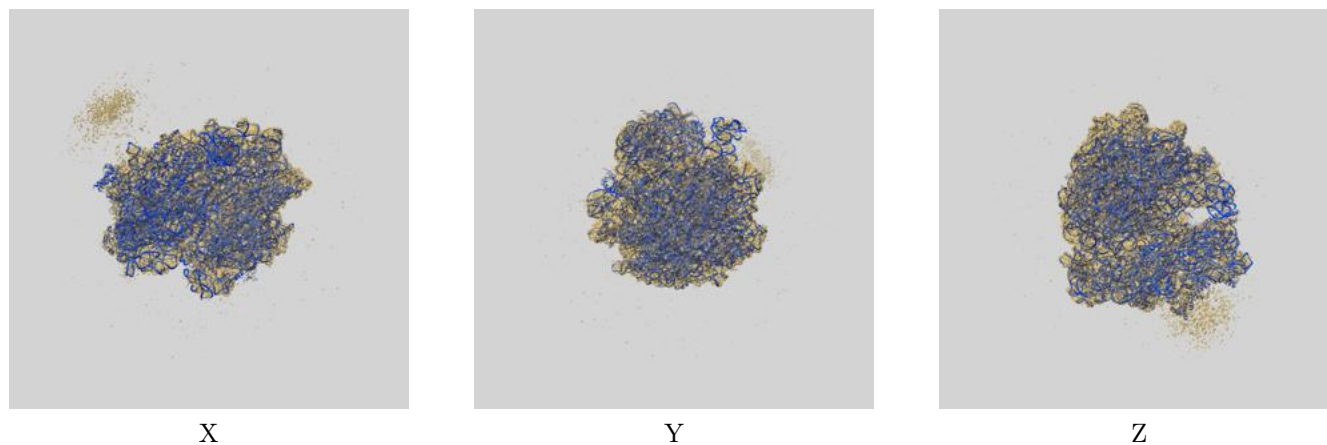
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

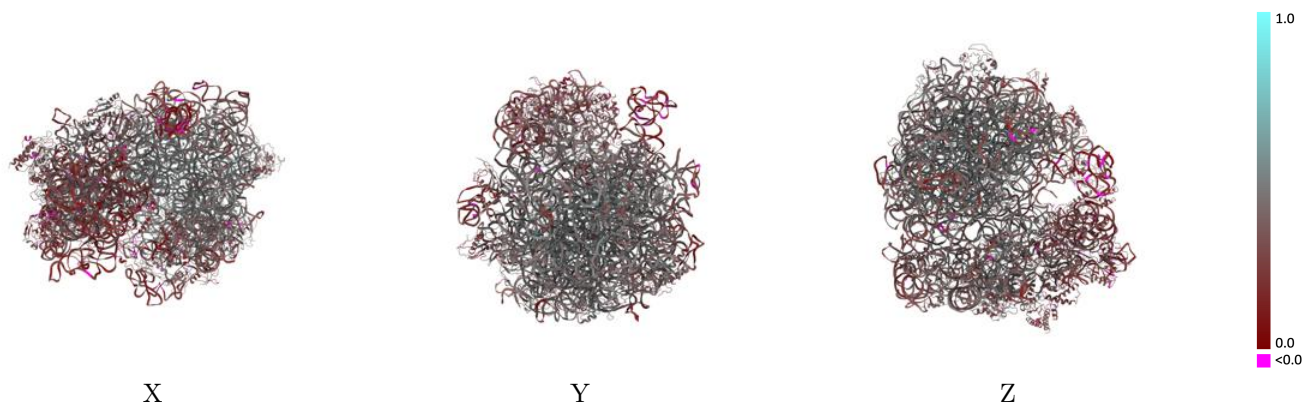
This section contains information regarding the fit between EMDB map EMD-3625 and PDB model 5ND9. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)



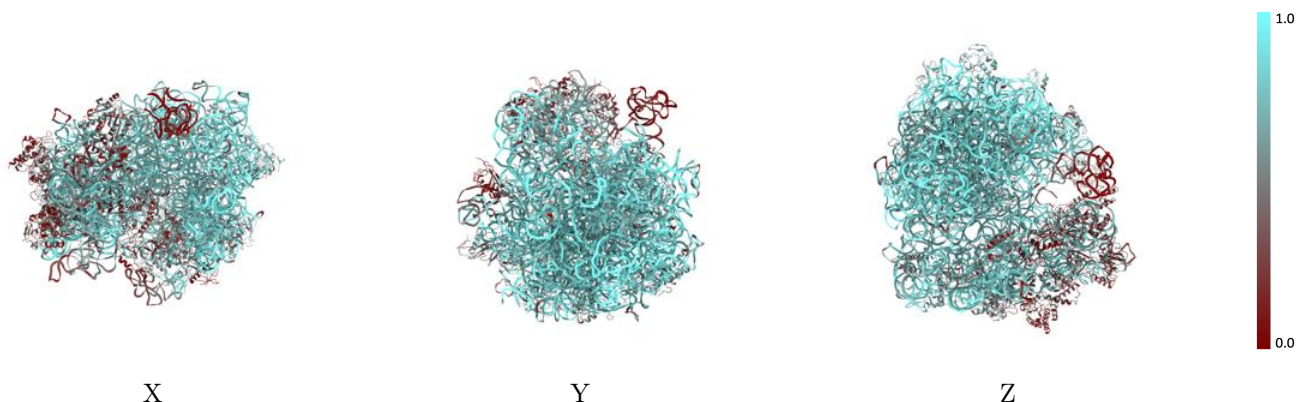
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



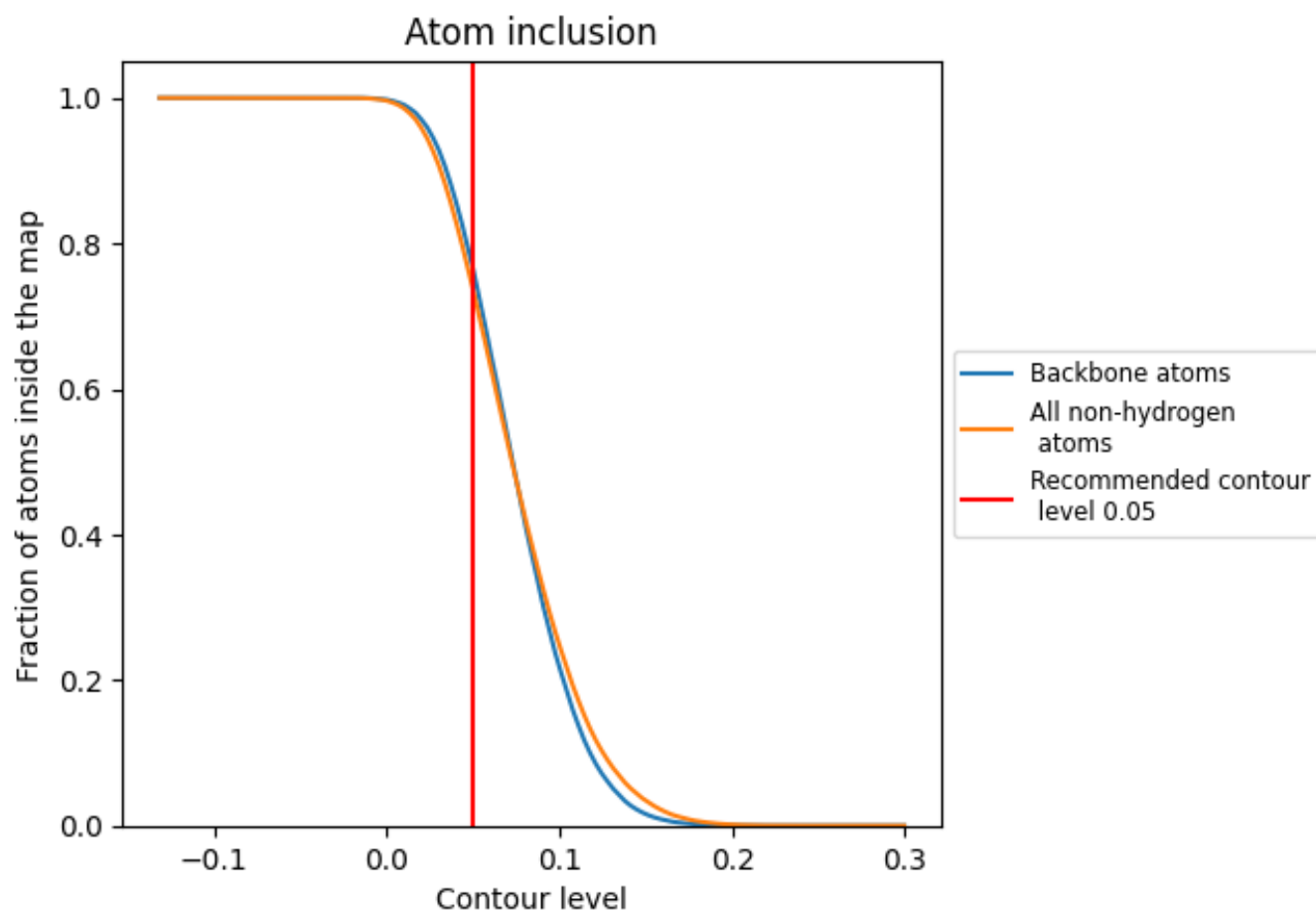
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 73% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7350	 0.3860
0	 0.5854	 0.4000
1	 0.5923	 0.3850
2	 0.6744	 0.4350
3	 0.1659	 0.2440
4	 0.5710	 0.4250
5	 0.1622	 0.3020
6	 0.7330	 0.4740
7	 0.6951	 0.4180
8	 0.6323	 0.4370
A	 0.8542	 0.4220
B	 0.8737	 0.3600
D	 0.7000	 0.4740
E	 0.6911	 0.4530
F	 0.6752	 0.4230
G	 0.3561	 0.2770
H	 0.5151	 0.3260
M	 0.7044	 0.4470
N	 0.5964	 0.4550
O	 0.6869	 0.4070
P	 0.6641	 0.4230
Q	 0.6614	 0.4210
R	 0.5611	 0.3230
S	 0.6389	 0.4310
T	 0.7330	 0.4450
U	 0.6518	 0.4290
V	 0.6833	 0.4580
W	 0.6153	 0.4130
X	 0.5825	 0.3730
Y	 0.1214	 0.3050
Z	 0.7203	 0.4400
a	 0.8055	 0.3510
b	 0.2801	 0.3130
c	 0.2192	 0.2750
d	 0.4103	 0.2760



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Chain	Atom inclusion	Q-score
e	 0.4342	 0.3600
f	 0.3646	 0.3660
g	 0.2342	 0.2470
h	 0.5302	 0.3770
i	 0.2431	 0.2360
j	 0.2085	 0.2290
k	 0.4844	 0.3560
l	 0.5712	 0.3890
m	 0.1998	 0.2280
n	 0.3222	 0.2550
o	 0.5416	 0.3410
p	 0.6014	 0.3850
q	 0.5242	 0.3650
r	 0.4321	 0.3540
s	 0.2568	 0.1900
t	 0.5401	 0.3160
u	 0.0801	 0.2820
v	 0.1948	 0.2990