Full wwPDB EM Validation Report ⓘ

Nov 6, 2023 – 12:26 PM JST

PDB ID	:	8INK
EMDB ID	:	EMD-35599
Title	:	human nuclear pre-60S ribosomal particle - State D
Authors	:	Zhang, Y.; Gao, N.
Deposited on	:	2023-03-10
Resolution	:	3.20 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:

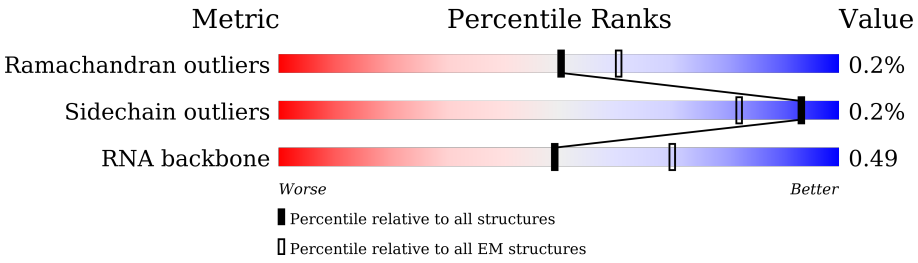
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 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 <=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	N	687	46% 48% · 52%
2	6	245	5% 99%
3	7	163	· 83% 17%
4	8	156	· 71% 26% ·
5	9	134	39% 63% · 36%
6	A	159	9% 28% · 72%
7	B	403	· 99%
8	D	427	· 83% · 16%

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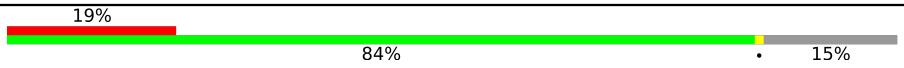
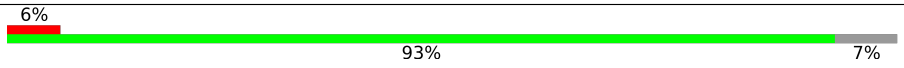
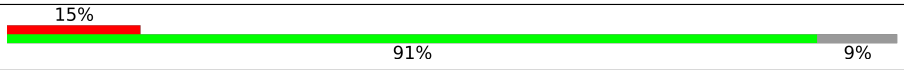
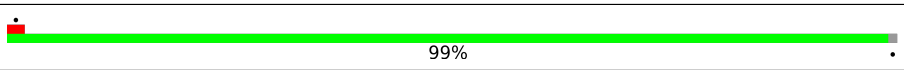
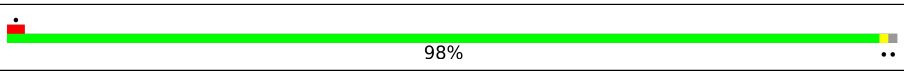
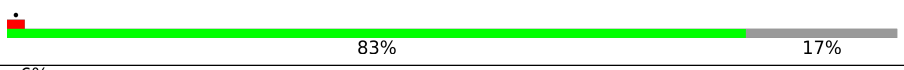
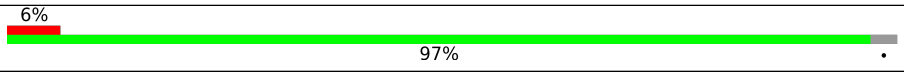
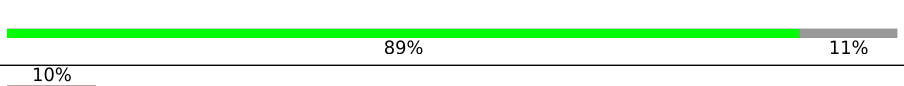
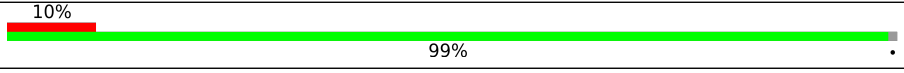
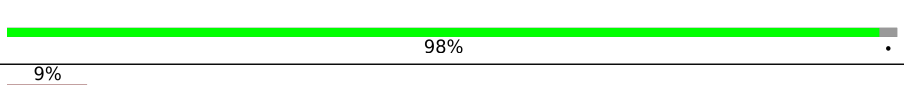
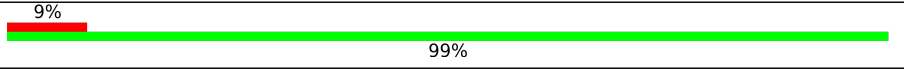
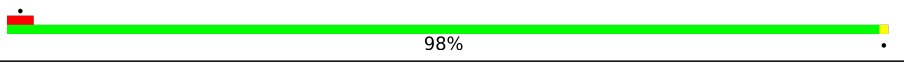
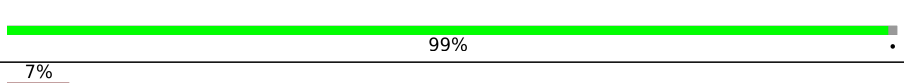
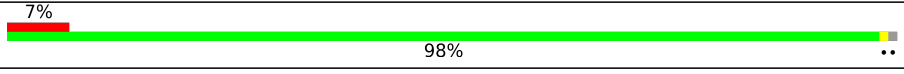
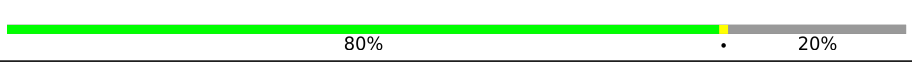
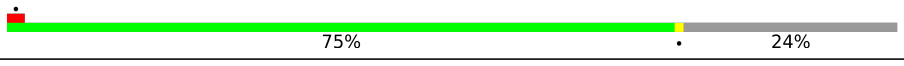
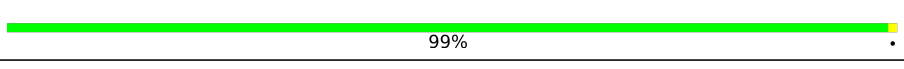
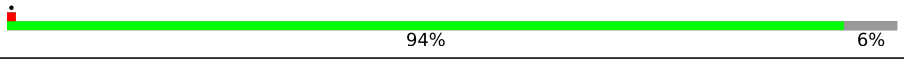
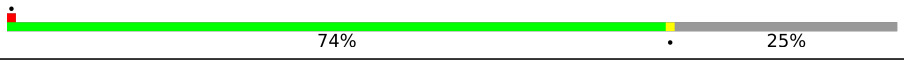
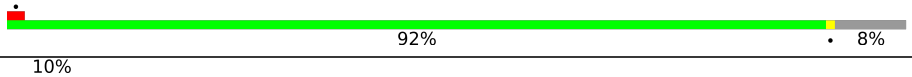
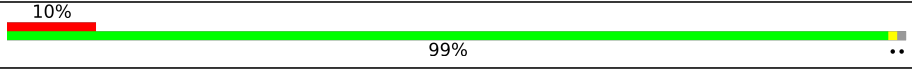
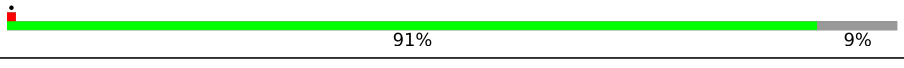
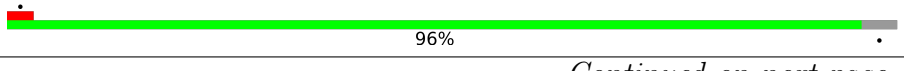
Mol	Chain	Length	Quality of chain
9	E	115	
10	F	117	
11	G	266	
12	H	123	
13	I	192	
14	J	260	
15	K	105	
16	L	148	
17	M	97	
18	O	70	
19	P	51	
20	Q	211	
21	S	215	
22	U	204	
23	V	203	
24	X	92	
25	Z	188	
26	a	196	
27	b	176	
28	e	140	
29	g	156	
30	h	145	
31	i	136	
32	l	137	
33	m	257	

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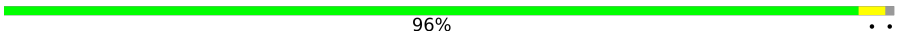
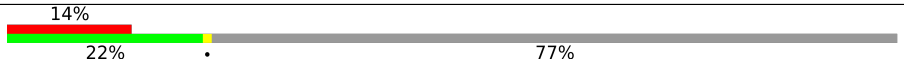
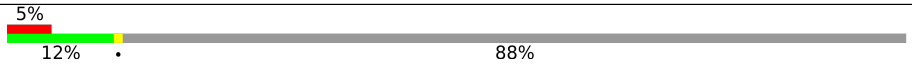
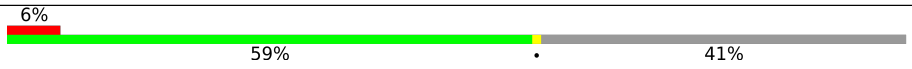
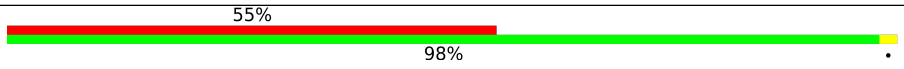
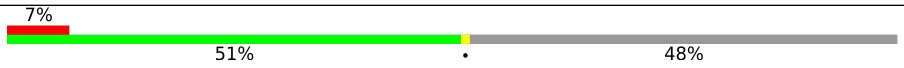
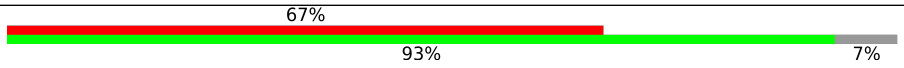
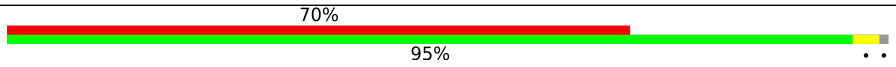
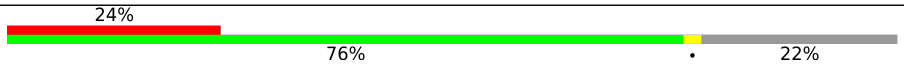
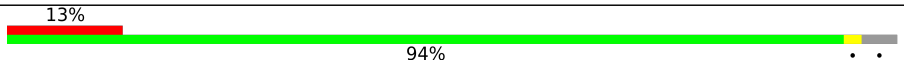
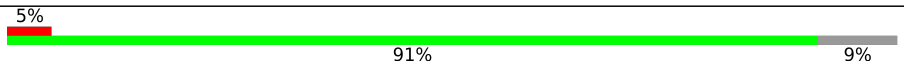
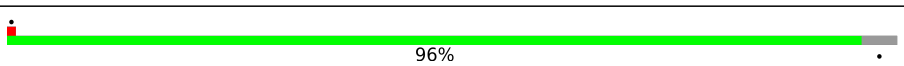
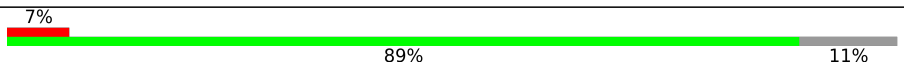
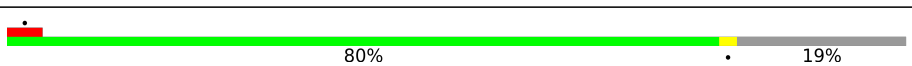
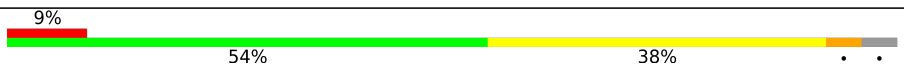
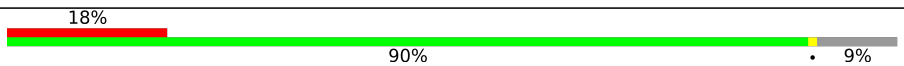
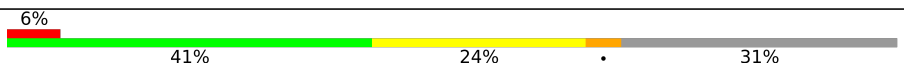
Mol	Chain	Length	Quality of chain
34	n	110	
35	o	288	
36	p	248	
37	r	360	
38	u	549	
39	w	731	
40	y	165	
41	z	129	
42	C	178	
43	R	297	
44	W	485	
45	T	160	
46	4	634	
47	Y	184	
48	k	135	
49	j	125	
50	d	128	
51	3	120	
52	v	239	
53	2	5054	

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 152807 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Protein SDA1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	N	332	2719	1762	461	475	21	0	0

- Molecule 2 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	6	244	1852	1149	318	372	13	0	0

- Molecule 3 is a protein called Probable ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	7	135	1159	737	225	187	10	0	0

- Molecule 4 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	8	156	3315	1481	585	1094	155	0	0

- Molecule 5 is a protein called Zinc finger protein 593.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	9	86	711	433	154	121	3	0	0

- Molecule 6 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	A	45	352	221	76	52	3	0	0

- Molecule 7 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	402	Total	C	N	O	S	1	0
			3244	2065	609	556	14		

- Molecule 8 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	358	Total	C	N	O	S	0	0
			2853	1797	570	473	13		

- Molecule 9 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	98	Total	C	N	O	S	0	0
			764	485	135	138	6		

- Molecule 10 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	109	Total	C	N	O	S	0	0
			868	544	179	139	6		

- Molecule 11 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	241	Total	C	N	O	S	0	0
			1927	1228	371	324	4		

- Molecule 12 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	122	Total	C	N	O	S	0	0
			1015	641	205	168	1		

- Molecule 13 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	190	Total	C	N	O	S	0	0
			1518	956	284	272	6		

- Molecule 14 is a protein called Ribosome biogenesis protein NSA2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	217	Total	C	N	O	S	0	0
			1772	1134	334	296	8		

- Molecule 15 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	102	Total	C	N	O	S	0	0
			832	521	177	129	5		

- Molecule 16 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	112	Total	C	N	O	S	0	0
			877	557	172	145	3		

- Molecule 17 is a protein called 60S ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	86	Total	C	N	O	S	0	0
			705	434	155	111	5		

- Molecule 18 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

- Molecule 19 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	P	50	Total	C	N	O	S	0	0
			444	281	98	64	1		

- Molecule 20 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Q	210	Total	C	N	O	S	0	0
			1701	1064	352	281	4		

- Molecule 21 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	S	135	Total	C	N	O	S	0	0
			1111	713	213	178	7		

- Molecule 22 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	U	203	Total	C	N	O	S	0	0
			1701	1072	359	266	4		

- Molecule 23 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	V	201	Total	C	N	O	S	0	0
			1650	1063	321	261	5		

- Molecule 24 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	91	Total	C	N	O	S	0	0
			708	445	136	120	7		

- Molecule 25 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	151	Total	C	N	O	S	0	0
			1223	768	247	203	5		

- Molecule 26 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	148	Total	C	N	O	S	0	0
			1239	772	266	192	9		

- Molecule 27 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	176	Total	C	N	O	S	0	0
			1461	930	284	236	11		

- Molecule 28 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	e	131	Total	C	N	O	S	0	0
			979	618	184	172	5		

- Molecule 29 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	g	117	Total	C	N	O	S	0	0
			958	612	179	166	1		

- Molecule 30 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	h	134	Total	C	N	O	S	0	0
			1115	700	226	186	3		

- Molecule 31 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	i	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 32 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	l	125	Total	C	N	O	S	0	0
			1002	622	207	168	5		

- Molecule 33 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	m	248	Total	C	N	O	S	0	0
			1898	1189	389	314	6		

- Molecule 34 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	n	109	Total	C	N	O	S	0	0
			876	555	174	144	3		

- Molecule 35 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	o	235	Total	C	N	O	S	0	0
			1897	1217	360	316	4		

- Molecule 36 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	p	225	Total	C	N	O	S	1	0
			1878	1207	361	301	9		

- Molecule 37 is a protein called Coiled-coil domain-containing protein 86.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	r	82	Total	C	N	O	S	0	0
			723	442	158	121	2		

- Molecule 38 is a protein called Guanine nucleotide-binding protein-like 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	u	68	Total	C	N	O	S	0	0
			578	362	121	92	3		

- Molecule 39 is a protein called G Protein Nucleolar 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	w	433	Total	C	N	O	S	0	0
			3472	2201	615	643	13		

- Molecule 40 is a protein called 60S ribosomal protein L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	y	165	Total	C	N	O	S	0	0
			1250	779	232	234	5		

- Molecule 41 is a protein called Protein LLP homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	z	67	Total	C	N	O	S	0	0
			581	363	128	88	2		

- Molecule 42 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	C	165	Total	C	N	O	S	0	0
			1319	836	245	233	5		

- Molecule 43 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	R	293	Total	C	N	O	S	0	0
			2382	1507	434	427	14		

- Molecule 44 is a protein called Notchless protein homolog 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	W	388	Total	C	N	O	S	0	0
			3018	1889	556	562	11		

- Molecule 45 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	T	124	Total	C	N	O	S	0	0
			1001	632	194	171	4		

- Molecule 46 is a protein called GTP-binding protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	4	611	Total	C	N	O	S	0	0
			5016	3151	918	920	27		

- Molecule 47 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Y	167	Total	C	N	O	S	0	0
			1355	848	260	238	9		

- Molecule 48 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	k	129	Total	C	N	O	S	0	0
			1064	673	220	166	5		

- Molecule 49 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	j	111	Total	C	N	O	S	0	0
			918	578	178	160	2		

- Molecule 50 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	d	104	Total	C	N	O	S	0	0
			850	542	149	157	2		

- Molecule 51 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	3	115	Total	C	N	O	P	0	0
			2453	1093	437	808	115		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	92	C	G	conflict	GB NR_023363
3	93	G	C	conflict	GB NR_023363
3	95	C	U	conflict	GB NR_023363
3	96	U	G	conflict	GB NR_023363

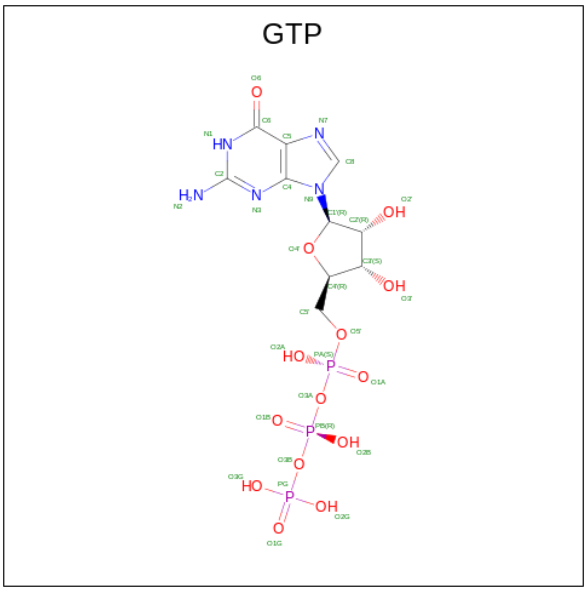
- Molecule 52 is a protein called mRNA turnover protein 4 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	v	217	Total	C	N	O	S	0	0
			1771	1129	311	320	11		

- Molecule 53 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	2	3495	Total	C	N	O	P	0	0
			75023	33449	13712	24368	3494		

- Molecule 54 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
54	w	1	Total	C	N	O	P	0
			32	10	5	14	3	

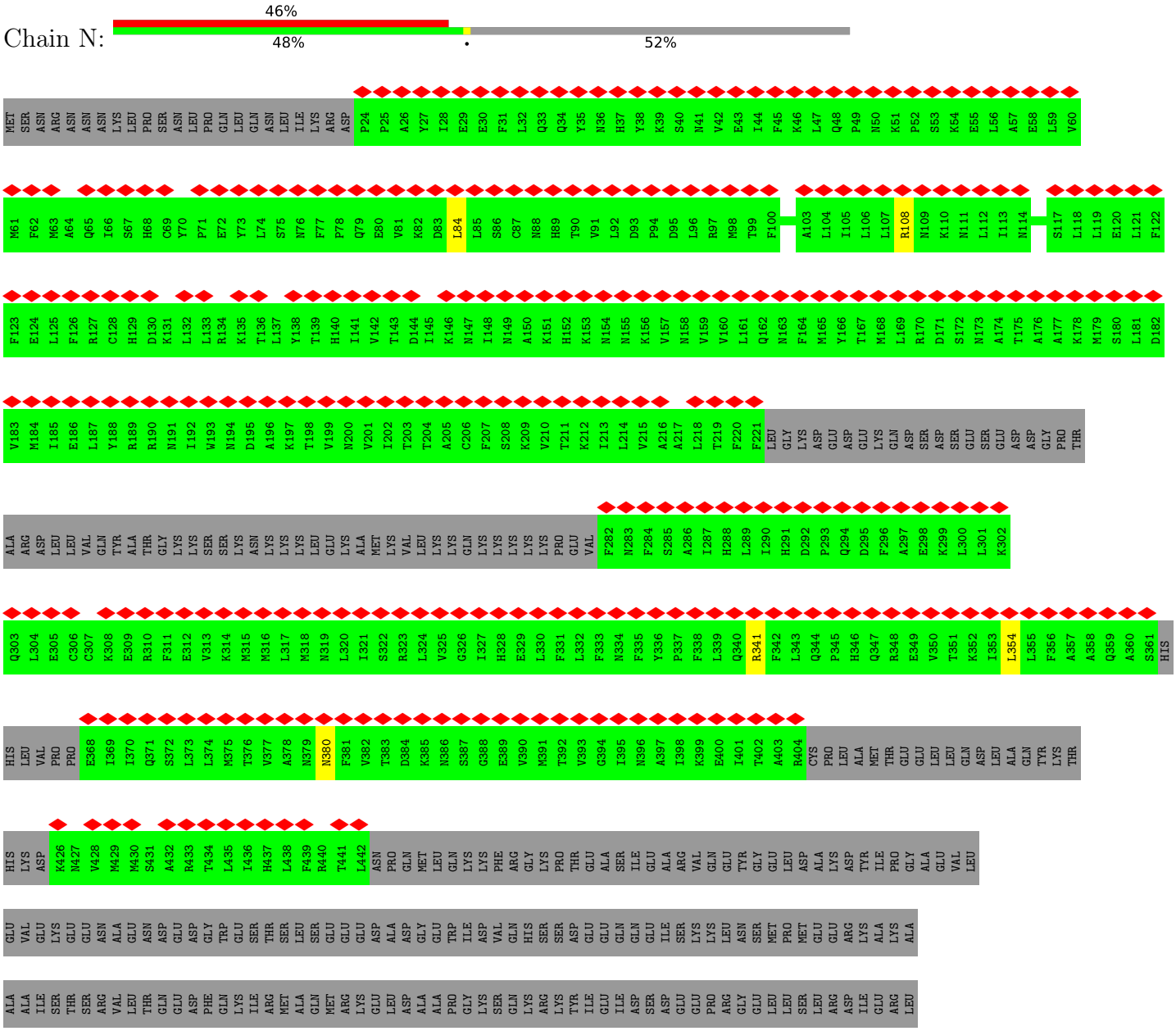
- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

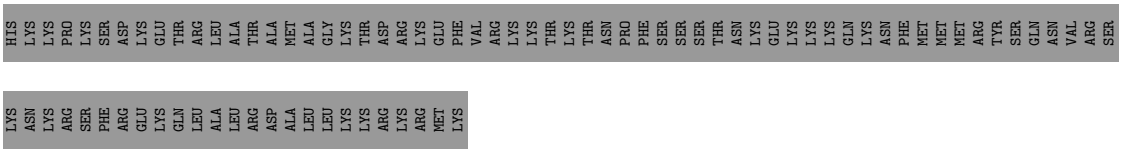
Mol	Chain	Residues	Atoms		AltConf
55	w	1	Total	Mg	0
			1	1	

3 Residue-property plots (i)

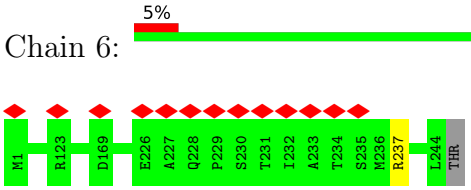
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Protein SDA1 homolog

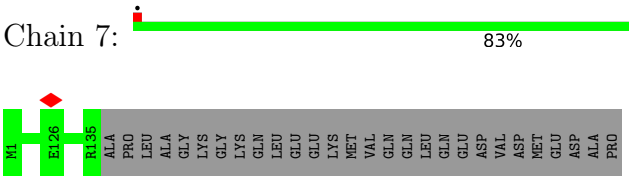




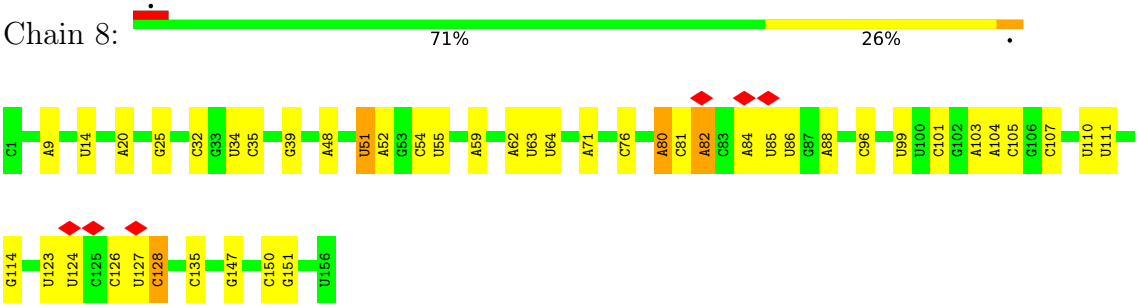
• Molecule 2: Eukaryotic translation initiation factor 6



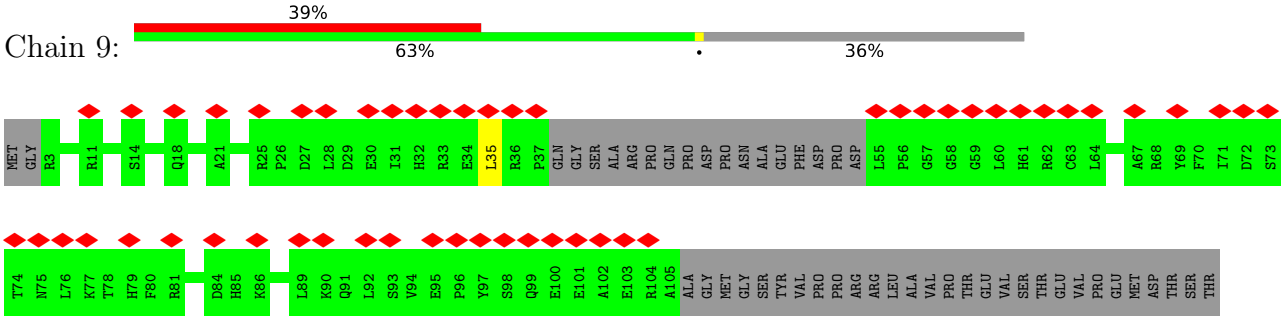
• Molecule 3: Probable ribosome biogenesis protein RLP24



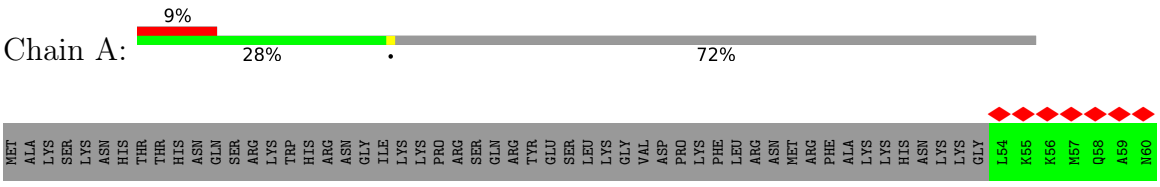
• Molecule 4: 5.8S rRNA

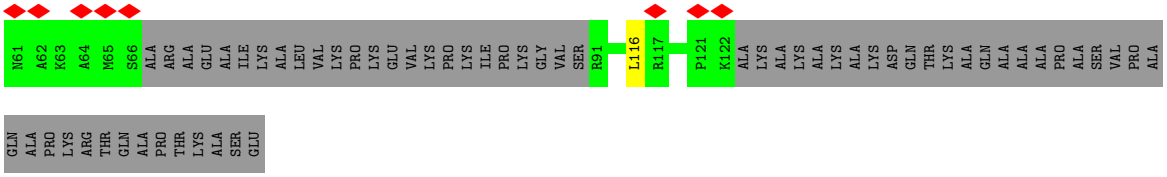


• Molecule 5: Zinc finger protein 593



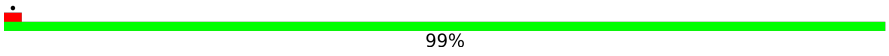
• Molecule 6: 60S ribosomal protein L29

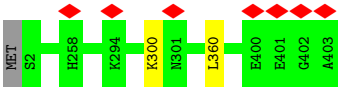




• Molecule 7: 60S ribosomal protein L3

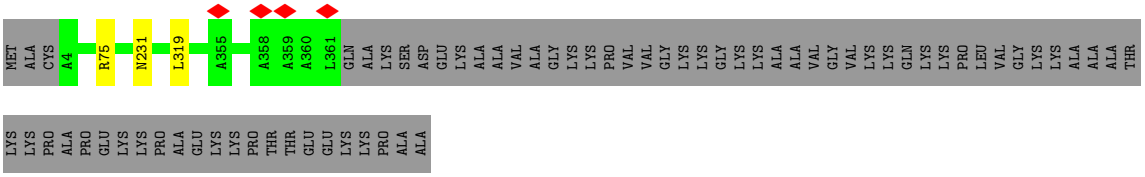
Chain B:





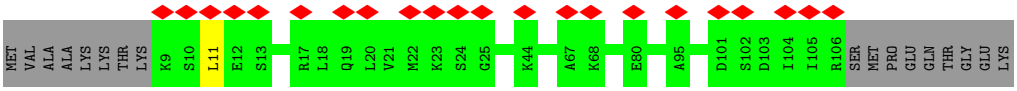
• Molecule 8: 60S ribosomal protein L4

Chain D:



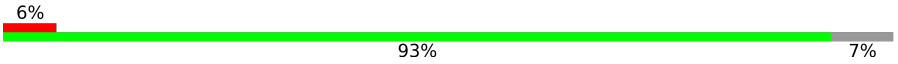
• Molecule 9: 60S ribosomal protein L30

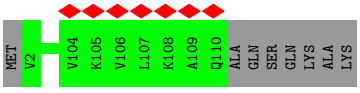
Chain E:



• Molecule 10: 60S ribosomal protein L34

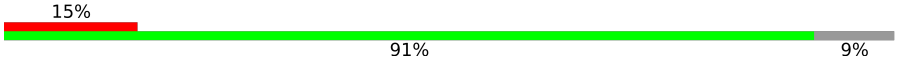
Chain F:

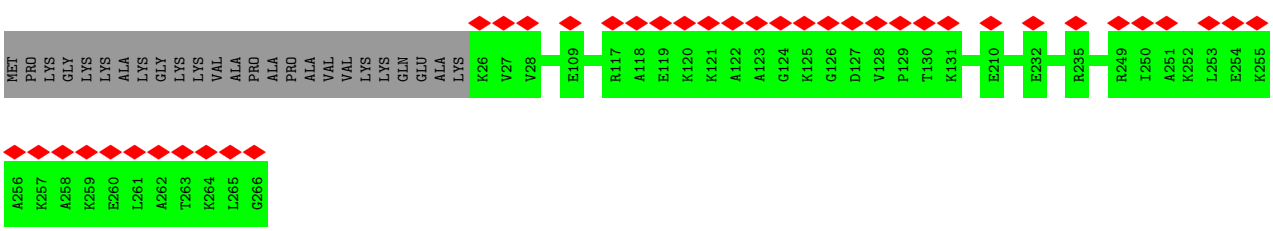




• Molecule 11: 60S ribosomal protein L7a

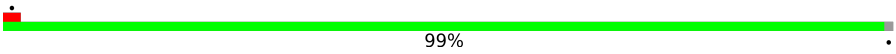
Chain G:





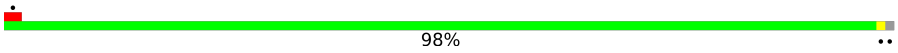
• Molecule 12: 60S ribosomal protein L35

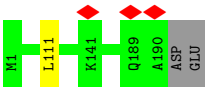
Chain H:



• Molecule 13: 60S ribosomal protein L9

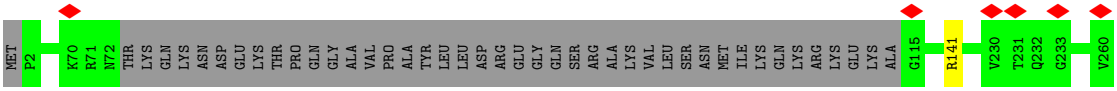
Chain I:





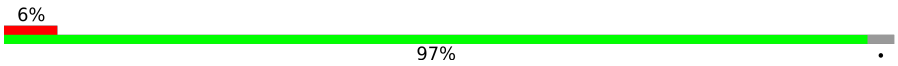
• Molecule 14: Ribosome biogenesis protein NSA2 homolog

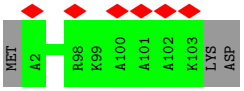
Chain J:



• Molecule 15: 60S ribosomal protein L36

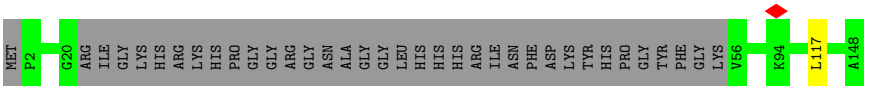
Chain K:





• Molecule 16: 60S ribosomal protein L27a

Chain L:

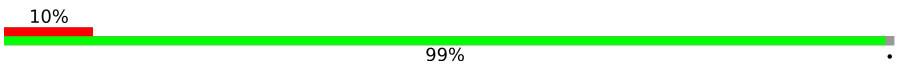


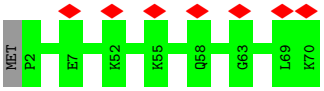
• Molecule 17: 60S ribosomal protein L37

Chain M:

• Molecule 18: 60S ribosomal protein L38

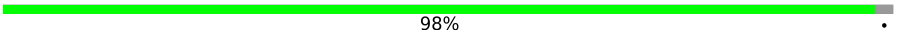
Chain O:





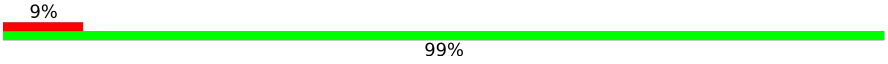
• Molecule 19: 60S ribosomal protein L39

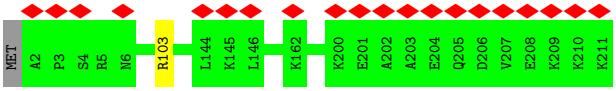
Chain P:



• Molecule 20: 60S ribosomal protein L13

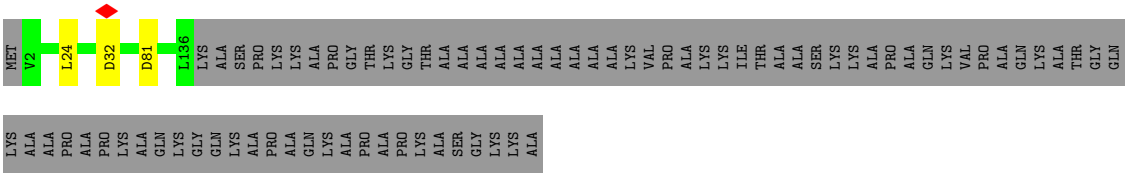
Chain Q:





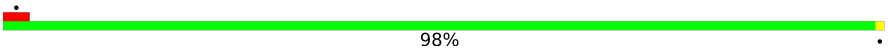
• Molecule 21: 60S ribosomal protein L14

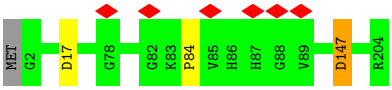
Chain S:



• Molecule 22: 60S ribosomal protein L15

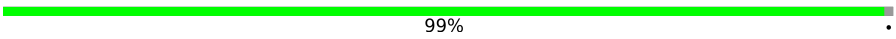
Chain U:

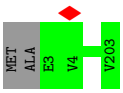




• Molecule 23: 60S ribosomal protein L13a

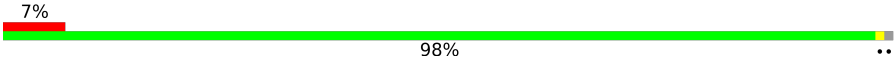
Chain V:

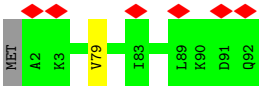




• Molecule 24: 60S ribosomal protein L37a

Chain X:



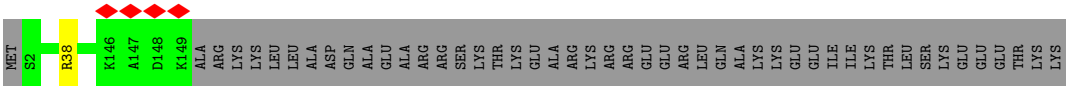


• Molecule 25: 60S ribosomal protein L18

Chain Z:

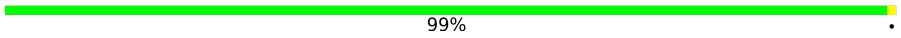
• Molecule 26: 60S ribosomal protein L19

Chain a:



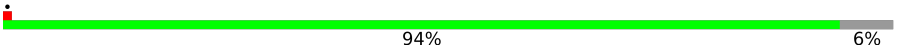
• Molecule 27: 60S ribosomal protein L18a

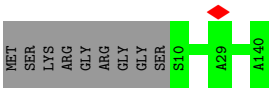
Chain b:



• Molecule 28: 60S ribosomal protein L23

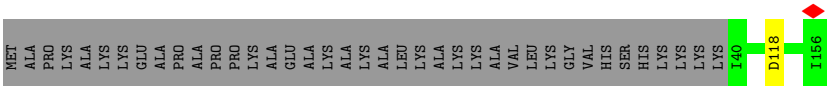
Chain e:





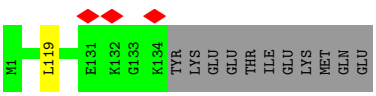
• Molecule 29: 60S ribosomal protein L23a

Chain g:



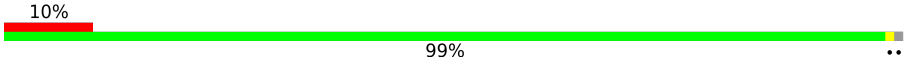
• Molecule 30: 60S ribosomal protein L26

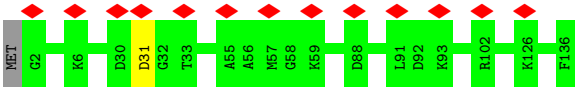
Chain h:



• Molecule 31: 60S ribosomal protein L27

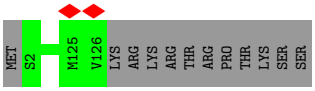
Chain i:





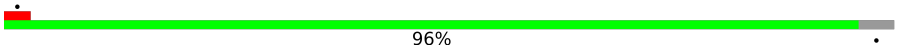
• Molecule 32: 60S ribosomal protein L28

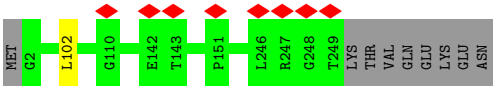
Chain l:



• Molecule 33: 60S ribosomal protein L8

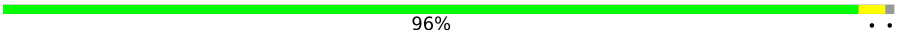
Chain m:

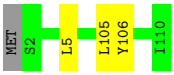




• Molecule 34: 60S ribosomal protein L35a

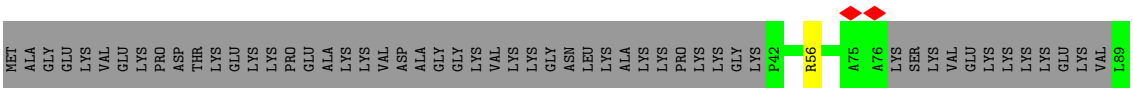
Chain n:

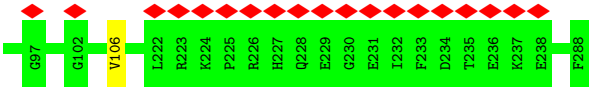




• Molecule 35: 60S ribosomal protein L6

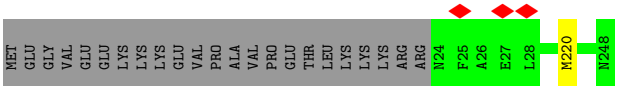
Chain o:





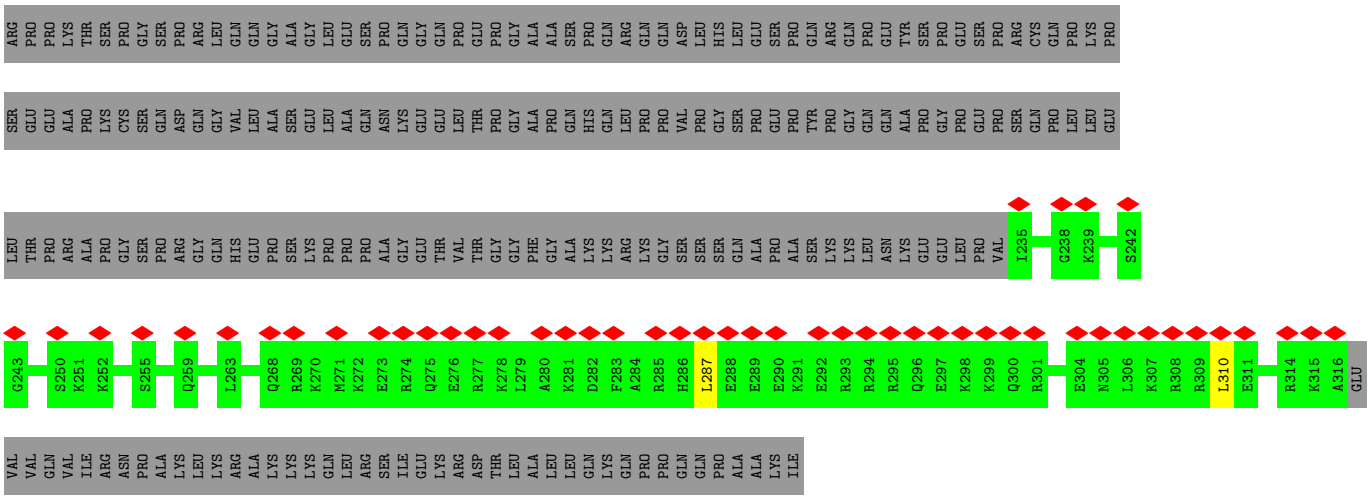
• Molecule 36: 60S ribosomal protein L7

Chain p:

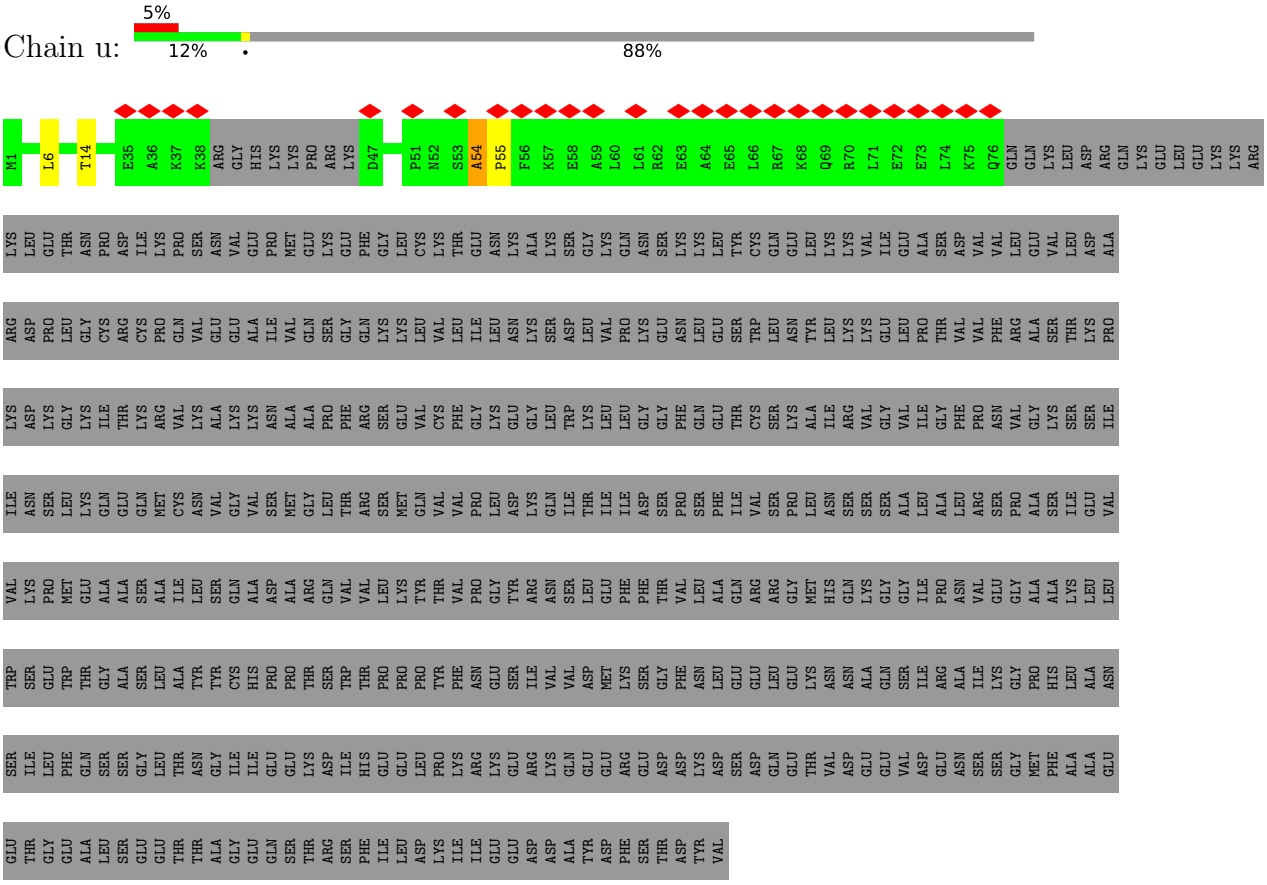


• Molecule 37: Coiled-coil domain-containing protein 86

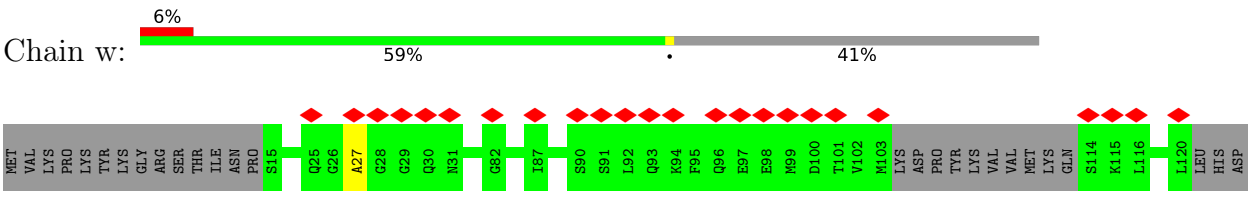
Chain r:

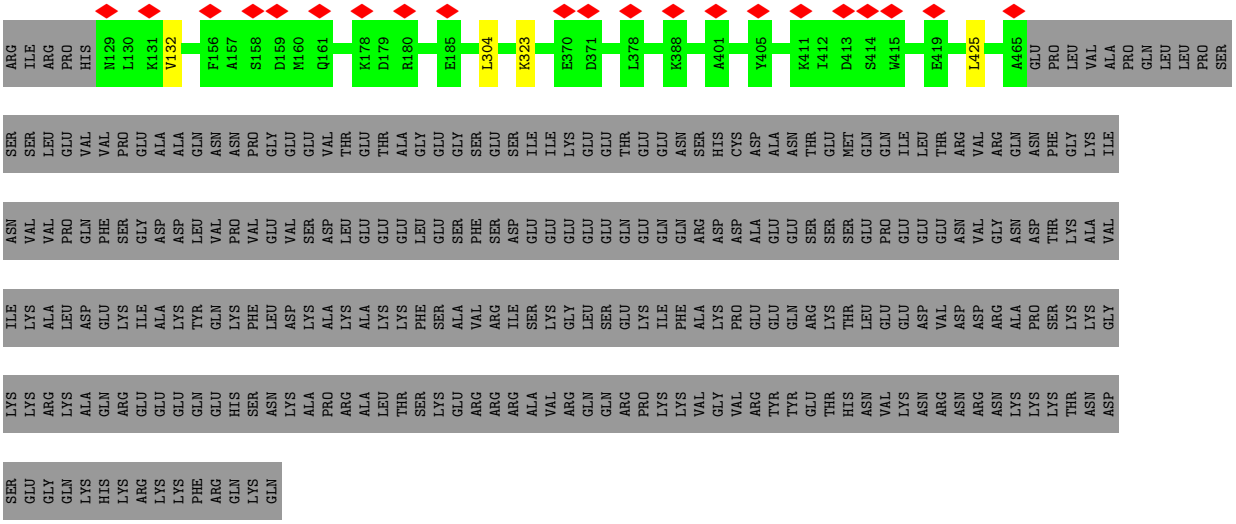


• Molecule 38: Guanine nucleotide-binding protein-like 3



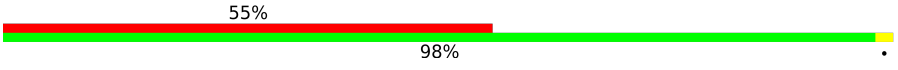
• Molecule 39: G Protein Nucleolar 2

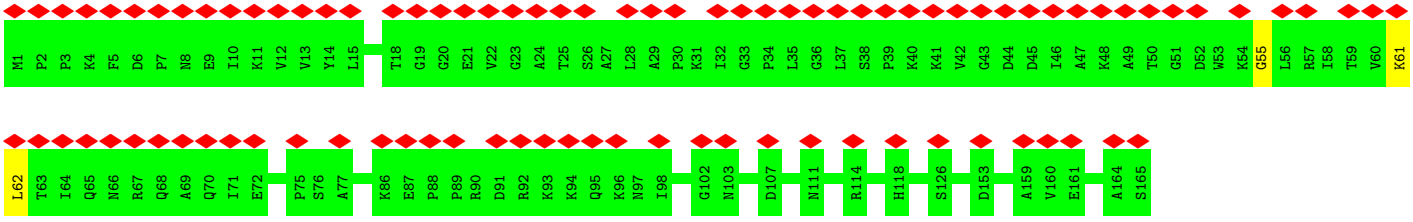




• Molecule 40: 60S ribosomal protein L12

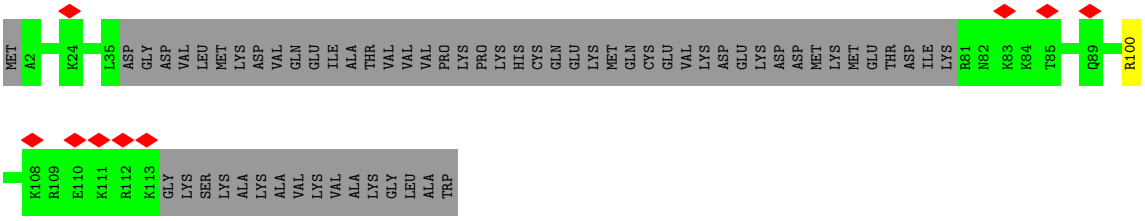
Chain y:





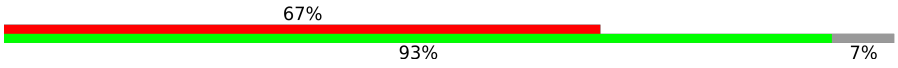
• Molecule 41: Protein LLP homolog

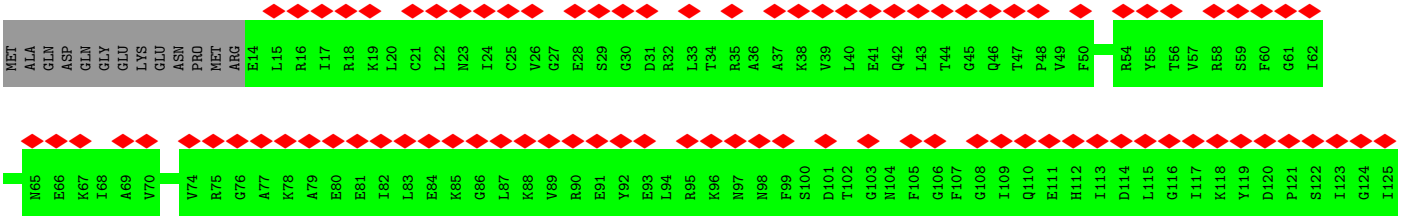
Chain z:

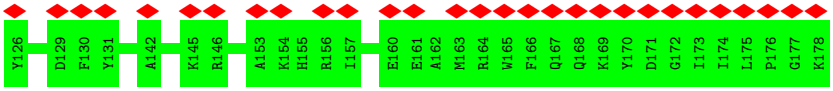


• Molecule 42: 60S ribosomal protein L11

Chain C:

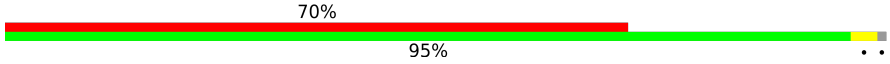


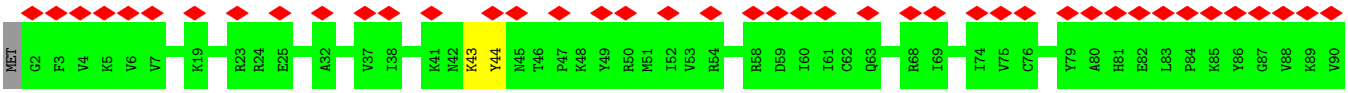


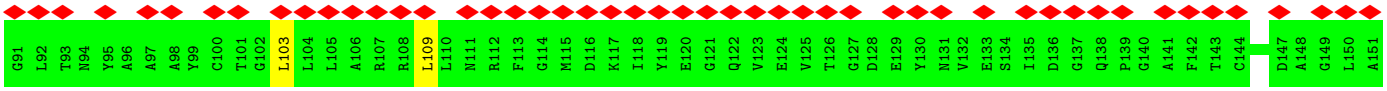


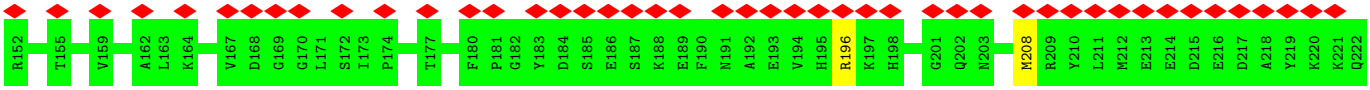
• Molecule 43: 60S ribosomal protein L5

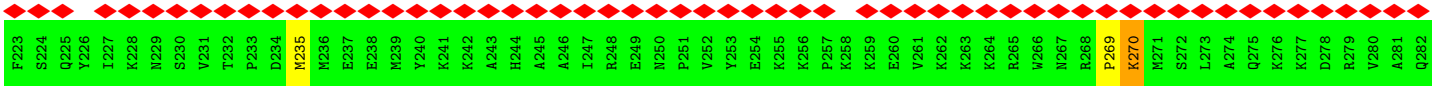
Chain R:

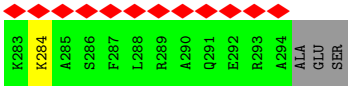






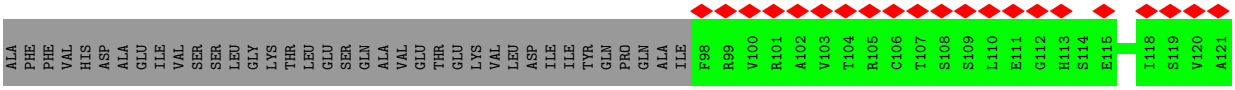


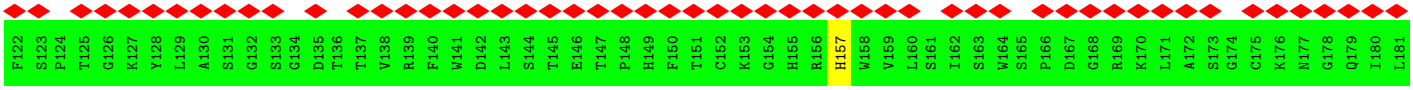


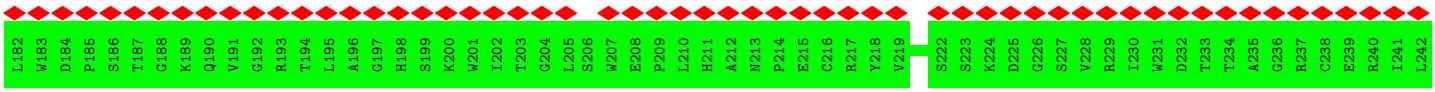


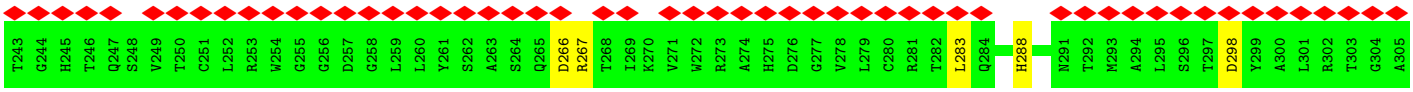
• Molecule 44: Notchless protein homolog 1

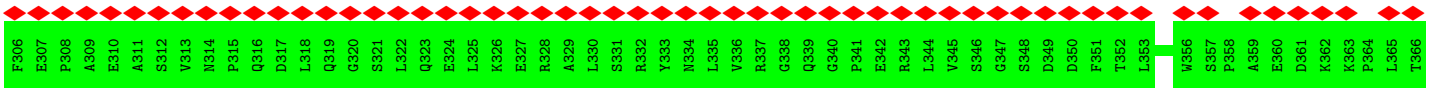
Chain W:





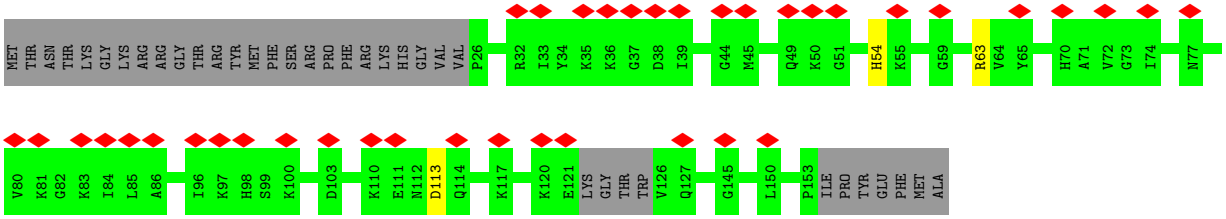






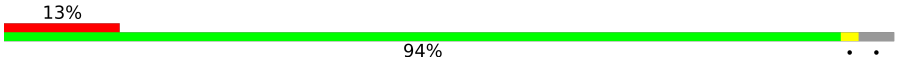
• Molecule 45: 60S ribosomal protein L21

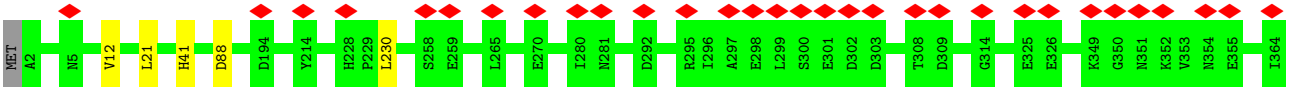
Chain T:

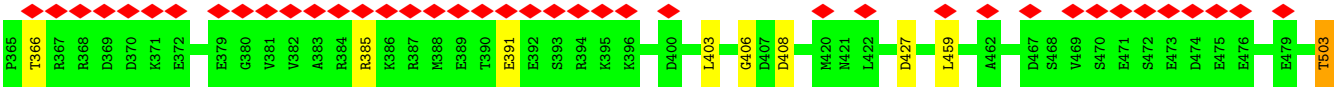


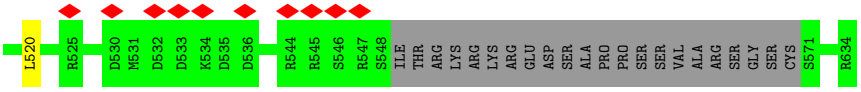
• Molecule 46: GTP-binding protein 4

Chain 4:



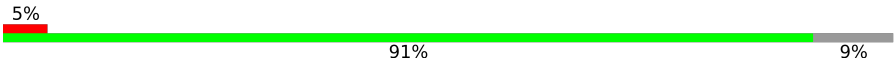


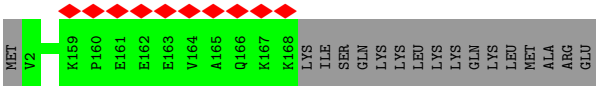




• Molecule 47: 60S ribosomal protein L17

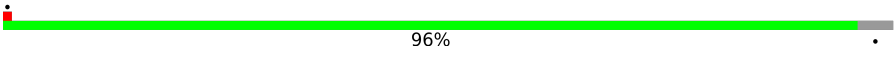
Chain Y:

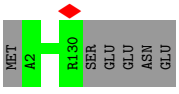




• Molecule 48: 60S ribosomal protein L32

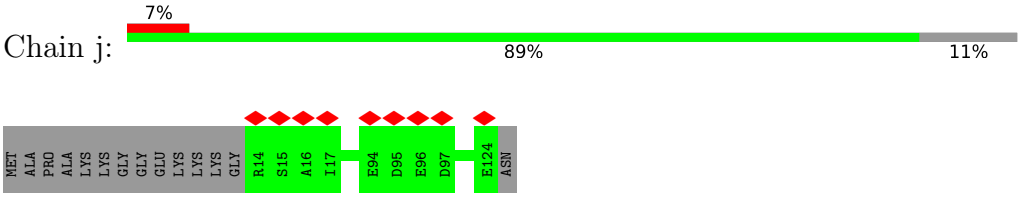
Chain k:





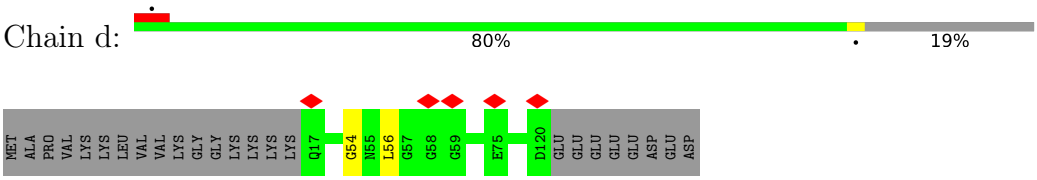
• Molecule 49: 60S ribosomal protein L31

Chain j:



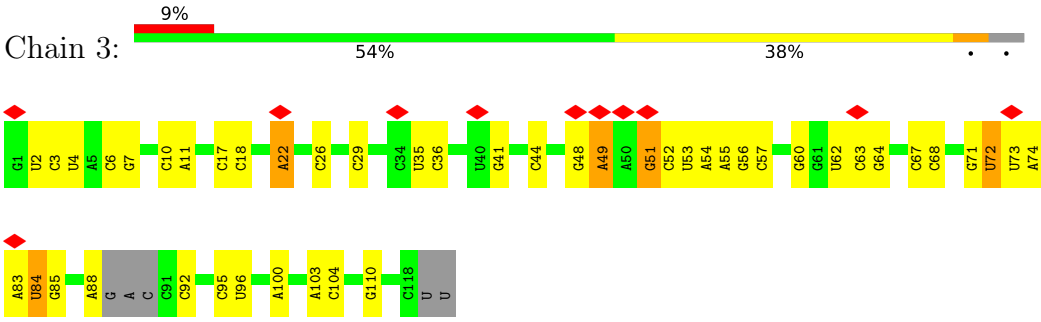
• Molecule 50: 60S ribosomal protein L22

Chain d:



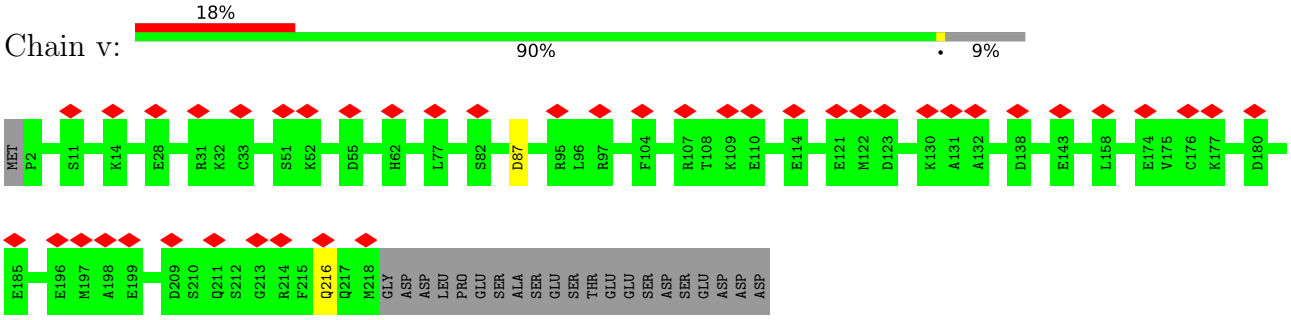
• Molecule 51: 5S rRNA

Chain 3:



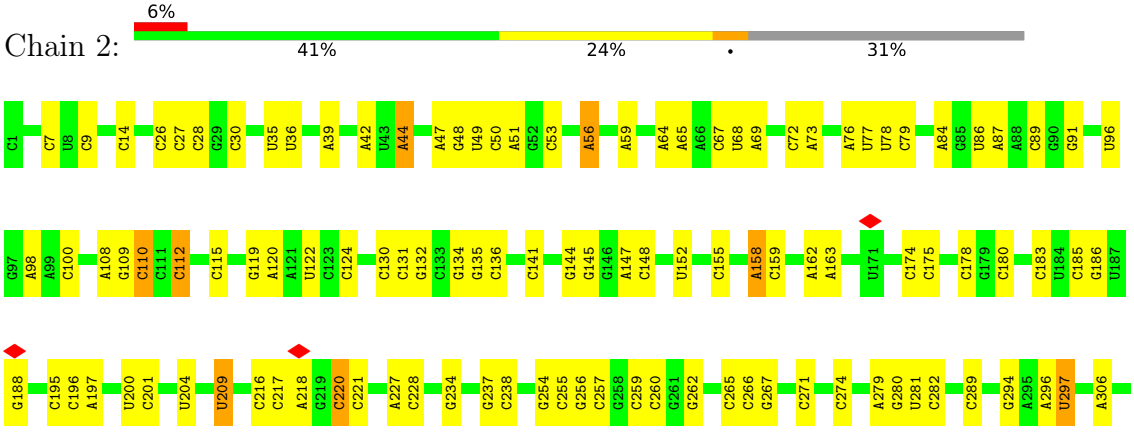
• Molecule 52: mRNA turnover protein 4 homolog

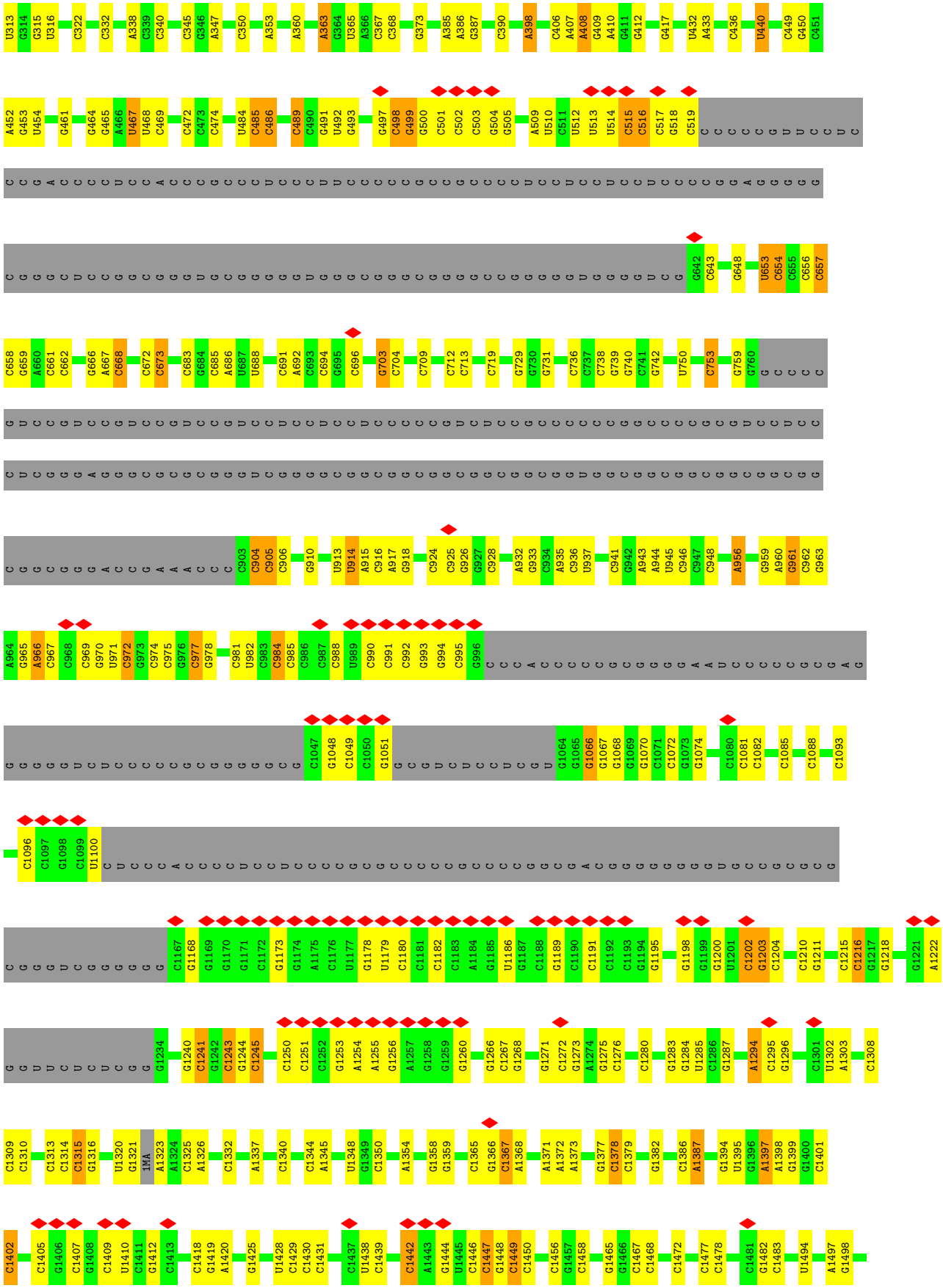
Chain v:

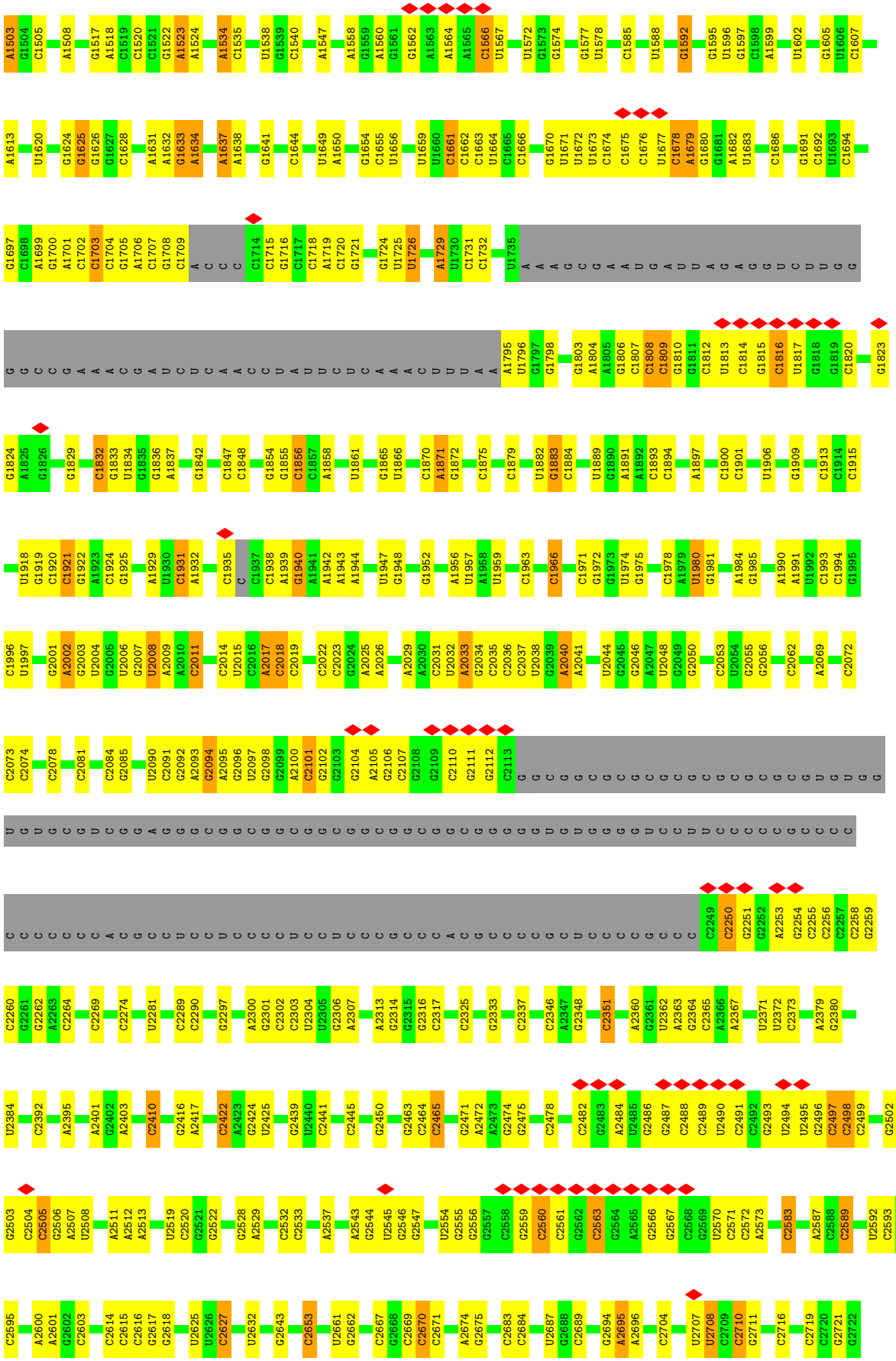


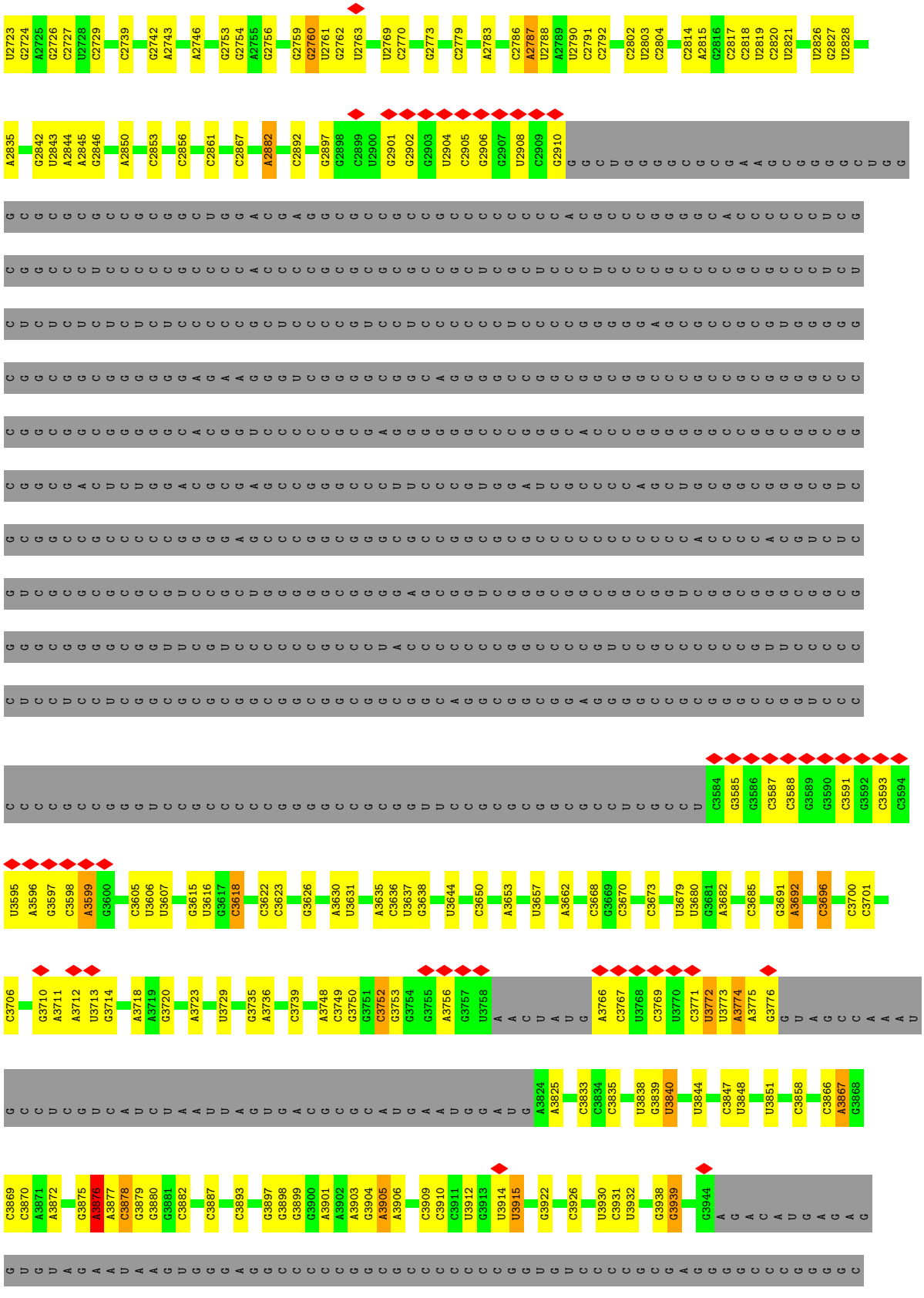
• Molecule 53: 28S rRNA

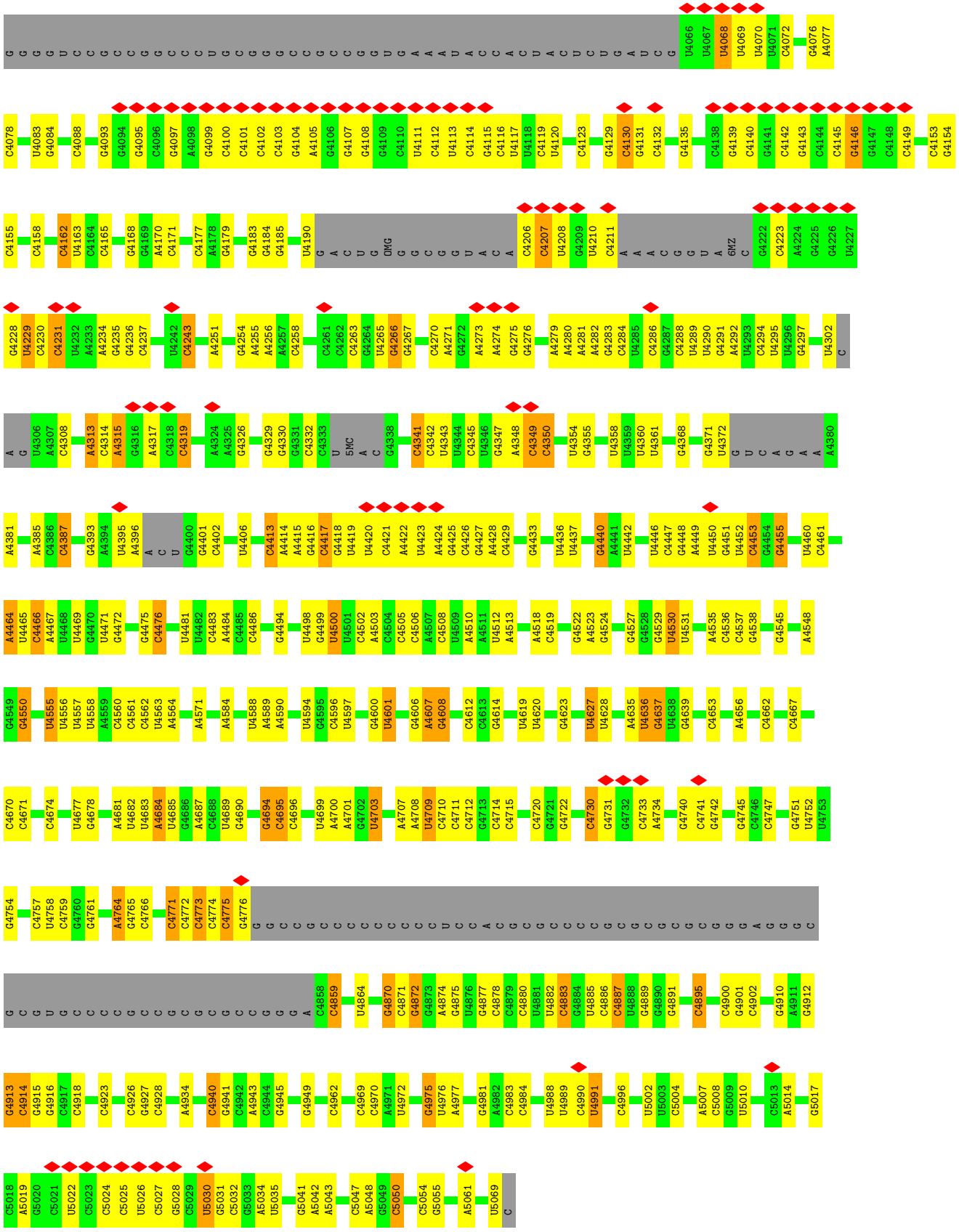
Chain 2:











4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	24229	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 ($e^-/Å^2$)	1.8	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.205	Depositor
Minimum map value	-0.070	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.031	Depositor
Map size (Å)	548.0, 548.0, 548.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.37, 1.37, 1.37	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: E7G, OMG, I4U, 2MG, MG, B8Q, B8T, P7G, GTP, P4U, B9B, 7MG, A2M, 5MU, B8W, OMU, M7A, OMC, B9H, BGH, UR3, B8K

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	N	0.37	0/2772	0.72	2/3738 (0.1%)
2	6	0.32	0/1877	0.68	0/2554
3	7	0.36	0/1181	0.64	0/1563
4	8	0.39	0/3679	1.27	33/5732 (0.6%)
5	9	0.32	0/723	0.82	1/961 (0.1%)
6	A	0.30	0/354	0.83	1/465 (0.2%)
7	B	0.32	0/3315	0.67	1/4435 (0.0%)
8	D	0.30	0/2907	0.65	1/3905 (0.0%)
9	E	0.34	0/774	0.76	1/1038 (0.1%)
10	F	0.29	0/878	0.69	0/1170
11	G	0.36	0/1960	0.66	0/2637
12	H	0.32	0/1023	0.65	0/1351
13	I	0.32	0/1537	0.71	1/2066 (0.0%)
14	J	0.30	0/1808	0.61	0/2414
15	K	0.32	0/843	0.72	0/1115
16	L	0.31	0/893	0.66	1/1193 (0.1%)
17	M	0.30	0/720	0.68	0/952
18	O	0.39	0/575	0.76	0/761
19	P	0.29	0/454	0.62	0/599
20	Q	0.33	0/1732	0.67	0/2315
21	S	0.37	0/1133	0.72	3/1516 (0.2%)
22	U	0.46	1/1746 (0.1%)	0.86	6/2338 (0.3%)
23	V	0.33	0/1682	0.62	0/2250
24	X	0.31	0/718	0.68	1/953 (0.1%)
25	Z	0.29	0/1239	0.69	1/1658 (0.1%)
26	a	0.32	0/1255	0.75	1/1662 (0.1%)
27	b	0.34	0/1501	0.64	0/2013
28	e	0.32	0/993	0.65	0/1332
29	g	0.31	0/975	0.68	1/1312 (0.1%)
30	h	0.30	0/1132	0.70	1/1504 (0.1%)
31	i	0.34	0/1130	0.67	0/1507

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	l	0.31	0/1017	0.65	0/1364
33	m	0.33	0/1936	0.74	1/2596 (0.0%)
34	n	0.31	0/895	0.72	2/1198 (0.2%)
35	o	0.31	0/1935	0.70	1/2596 (0.0%)
36	p	0.35	0/1916	0.66	1/2553 (0.0%)
37	r	0.38	0/732	0.82	2/960 (0.2%)
38	u	0.41	0/585	0.83	2/767 (0.3%)
39	w	0.32	0/3541	0.65	2/4775 (0.0%)
40	y	0.34	0/1269	0.75	1/1712 (0.1%)
41	z	0.35	0/587	0.76	0/767
42	C	0.40	0/1341	0.80	0/1793
43	R	0.36	0/2428	0.78	4/3252 (0.1%)
44	W	0.30	0/3093	0.72	7/4196 (0.2%)
45	T	0.33	0/1018	0.78	1/1357 (0.1%)
46	4	0.34	0/5099	0.77	11/6840 (0.2%)
47	Y	0.29	0/1383	0.60	0/1856
48	k	0.29	0/1082	0.67	0/1443
49	j	0.32	0/933	0.70	0/1256
50	d	0.42	0/864	0.79	2/1160 (0.2%)
51	3	0.48	0/2739	1.47	61/4266 (1.4%)
52	v	0.34	0/1806	0.73	1/2420 (0.0%)
53	2	0.49	5/82131 (0.0%)	1.42	1418/128040 (1.1%)
All	All	0.42	6/161839 (0.0%)	1.17	1573/236176 (0.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	N	0	1
8	D	0	1
34	n	0	1
38	u	0	1
40	y	0	1
43	R	0	2
45	T	0	1
46	4	0	1
53	2	0	1
All	All	0	10

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	2	3876	A	N9-C4	24.06	1.52	1.37
22	U	84	PRO	CG-CD	-13.30	1.06	1.50
53	2	3876	A	N7-C5	-8.34	1.34	1.39
53	2	3876	A	N3-C4	6.90	1.39	1.34
53	2	3876	A	N9-C8	6.13	1.42	1.37
53	2	1929	A	N9-C4	5.32	1.41	1.37

All (1573) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	2	3876	A	C8-N9-C4	-52.09	84.96	105.80
53	2	3876	A	N7-C8-N9	33.88	130.74	113.80
53	2	1872	G	OP1-P-OP2	-26.83	79.36	119.60
53	2	1872	G	O5'-P-OP1	-26.05	79.44	110.70
53	2	3876	A	C2-N3-C4	25.94	123.57	110.60
53	2	3876	A	N3-C4-C5	-19.64	113.06	126.80
22	U	84	PRO	N-CD-CG	-18.54	75.38	103.20
53	2	3876	A	N9-C4-C5	16.86	112.54	105.80
53	2	1872	G	O5'-P-OP2	15.82	129.68	110.70
53	2	1871	A2M	OP2-P-O3'	-15.77	70.50	105.20
53	2	1871	A2M	OP1-P-O3'	14.46	137.01	105.20
53	2	753	C	N1-C2-O2	13.73	127.14	118.90
53	2	3876	A	C5-N7-C8	-13.72	97.04	103.90
53	2	4775	C	N1-C2-O2	12.69	126.51	118.90
53	2	753	C	N3-C2-O2	-12.39	113.22	121.90
53	2	3876	A	C8-N9-C1'	12.36	149.95	127.70
53	2	4926	C	N1-C2-O2	12.29	126.28	118.90
53	2	2710	C	C6-N1-C2	-12.27	115.39	120.30
46	4	230	LEU	CA-CB-CG	12.11	143.16	115.30
53	2	4476	C	N1-C2-O2	11.83	126.00	118.90
51	3	78	C	N1-C2-O2	11.70	125.92	118.90
53	2	2820	C	N1-C2-O2	11.66	125.89	118.90
22	U	84	PRO	CA-CB-CG	-11.52	82.11	104.00
53	2	4775	C	C2-N1-C1'	11.43	131.38	118.80
53	2	4926	C	C6-N1-C2	-11.33	115.77	120.30
53	2	2710	C	N3-C2-O2	-11.22	114.05	121.90
53	2	753	C	C6-N1-C2	-11.20	115.82	120.30
53	2	100	C	C2-N1-C1'	11.00	130.90	118.80
53	2	2710	C	N1-C2-O2	11.00	125.50	118.90
53	2	4926	C	N3-C2-O2	-10.70	114.41	121.90
53	2	2499	C	N1-C2-O2	10.69	125.31	118.90
53	2	100	C	N1-C2-O2	10.67	125.30	118.90
53	2	4476	C	C2-N1-C1'	10.65	130.52	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	3	78	C	C6-N1-C2	-10.59	116.06	120.30
53	2	1994	C	C2-N1-C1'	10.45	130.30	118.80
53	2	1816	C	N1-C2-O2	10.44	125.17	118.90
53	2	2627	C	C6-N1-C2	-10.38	116.15	120.30
53	2	4775	C	N3-C2-O2	-10.31	114.69	121.90
53	2	1994	C	N1-C2-O2	10.29	125.07	118.90
53	2	1671	U	N1-C2-O2	10.22	129.96	122.80
53	2	467	U	N1-C2-O2	10.20	129.94	122.80
53	2	4714	C	N1-C2-O2	10.18	125.01	118.90
53	2	1671	U	N3-C2-O2	-10.16	115.09	122.20
53	2	1402	C	N1-C2-O2	10.12	124.97	118.90
53	2	467	U	N3-C2-O2	-10.02	115.19	122.20
53	2	1241	C	N1-C2-O2	9.98	124.89	118.90
53	2	4709	U	N3-C2-O2	-9.95	115.24	122.20
53	2	4758	U	N3-C2-O2	-9.94	115.24	122.20
51	3	95	C	C2-N1-C1'	9.93	129.72	118.80
53	2	4608	G	N7-C8-N9	9.92	118.06	113.10
51	3	78	C	N3-C2-O2	-9.91	114.97	121.90
53	2	2820	C	N3-C2-O2	-9.82	115.03	121.90
53	2	115	C	N1-C2-O2	9.74	124.75	118.90
51	3	95	C	N1-C2-O2	9.74	124.75	118.90
53	2	4476	C	N3-C2-O2	-9.72	115.09	121.90
53	2	4709	U	N1-C2-O2	9.71	129.60	122.80
51	3	78	C	C2-N1-C1'	9.65	129.41	118.80
53	2	2710	C	C2-N1-C1'	9.56	129.32	118.80
53	2	5035	U	N3-C2-O2	-9.55	115.51	122.20
53	2	4158	C	N3-C2-O2	-9.54	115.22	121.90
53	2	4608	G	C8-N9-C4	-9.54	102.58	106.40
53	2	3636	C	C6-N1-C2	-9.51	116.50	120.30
53	2	516	C	N1-C2-O2	9.46	124.58	118.90
53	2	35	U	N3-C2-O2	-9.43	115.60	122.20
53	2	1405	C	N1-C2-O2	9.42	124.55	118.90
53	2	904	C	N1-C2-O2	9.41	124.55	118.90
53	2	2439	G	C4-N9-C1'	9.38	138.69	126.50
53	2	2571	C	N3-C2-O2	-9.29	115.40	121.90
53	2	282	C	N1-C2-O2	9.29	124.47	118.90
53	2	1671	U	C2-N1-C1'	9.27	128.82	117.70
53	2	1216	C	N1-C2-O2	9.27	124.46	118.90
46	4	408	ASP	CB-CG-OD1	9.26	126.63	118.30
53	2	1921	C	N1-C2-O2	9.26	124.46	118.90
53	2	2410	C	C6-N1-C2	-9.26	116.60	120.30
53	2	1276	C	C6-N1-C2	-9.25	116.60	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	2	2022	C	N1-C2-O2	9.25	124.45	118.90
53	2	516	C	C6-N1-C2	-9.23	116.61	120.30
53	2	4758	U	N1-C2-O2	9.21	129.25	122.80
53	2	3876	A	N9-C1'-C2'	9.20	125.95	114.00
53	2	77	U	N3-C2-O2	-9.19	115.77	122.20
53	2	2262	G	C4-N9-C1'	9.16	138.41	126.50
53	2	472	C	C6-N1-C2	-9.14	116.64	120.30
53	2	2499	C	C6-N1-C2	-9.13	116.65	120.30
53	2	115	C	C2-N1-C1'	9.08	128.79	118.80
53	2	100	C	N3-C2-O2	-9.06	115.56	121.90
53	2	4864	U	N3-C2-O2	-9.05	115.86	122.20
53	2	2627	C	N1-C2-O2	9.04	124.33	118.90
53	2	4880	C	N1-C2-O2	9.03	124.32	118.90
52	v	87	ASP	CB-CG-OD1	9.01	126.41	118.30
53	2	499	G	N3-C4-C5	-9.01	124.10	128.60
53	2	3622	C	N1-C2-O2	8.99	124.29	118.90
53	2	4471	U	N3-C2-O2	-8.98	115.91	122.20
53	2	963	G	C4-N9-C1'	8.98	138.17	126.50
53	2	2499	C	C2-N1-C1'	8.98	128.67	118.80
53	2	972	C	N1-C2-O2	8.97	124.28	118.90
53	2	4766	C	C6-N1-C2	-8.93	116.73	120.30
53	2	499	G	C4-N9-C1'	8.92	138.10	126.50
53	2	3876	A	N1-C2-N3	-8.92	124.84	129.30
53	2	35	U	N1-C2-O2	8.89	129.03	122.80
53	2	1243	C	C6-N1-C2	-8.89	116.74	120.30
53	2	1929	A	C2-N3-C4	8.89	115.04	110.60
53	2	4926	C	C2-N1-C1'	8.89	128.58	118.80
53	2	961	G	C4-N9-C1'	8.88	138.05	126.50
53	2	2410	C	C2-N1-C1'	8.88	128.57	118.80
53	2	467	U	C2-N1-C1'	8.86	128.33	117.70
53	2	1216	C	C2-N1-C1'	8.85	128.53	118.80
53	2	4714	C	C6-N1-C2	-8.84	116.76	120.30
53	2	1402	C	N3-C2-O2	-8.84	115.71	121.90
53	2	499	G	N3-C4-N9	8.81	131.28	126.00
53	2	516	C	N3-C2-O2	-8.80	115.74	121.90
53	2	4864	U	N1-C2-O2	8.79	128.95	122.80
53	2	753	C	C2-N1-C1'	8.76	128.44	118.80
53	2	178	C	C6-N1-C2	-8.65	116.84	120.30
53	2	1726	U	N3-C2-O2	-8.63	116.16	122.20
53	2	1994	C	N3-C2-O2	-8.62	115.87	121.90
53	2	3876	A	C5-C6-N1	8.61	122.01	117.70
53	2	515	C	N1-C2-O2	8.60	124.06	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	2	4682	U	N3-C2-O2	-8.59	116.19	122.20
53	2	1494	U	N3-C2-O2	-8.57	116.20	122.20
53	2	1458	C	N1-C2-O2	8.56	124.04	118.90
53	2	4350	C	C6-N1-C2	-8.56	116.88	120.30
53	2	96	U	N3-C2-O2	-8.56	116.21	122.20
22	U	147	ASP	CB-CG-OD1	8.53	125.97	118.30
53	2	4476	C	C6-N1-C2	-8.52	116.89	120.30
53	2	2627	C	C2-N1-C1'	8.51	128.16	118.80
53	2	4885	U	N3-C2-O2	-8.51	116.24	122.20
53	2	4112	C	N1-C2-O2	8.48	123.99	118.90
53	2	1243	C	C2-N1-C1'	8.48	128.13	118.80
53	2	5035	U	N1-C2-O2	8.43	128.70	122.80
53	2	2497	C	C6-N1-C2	-8.43	116.93	120.30
53	2	4662	C	C6-N1-C2	-8.40	116.94	120.30
53	2	4266	G	C4-N9-C1'	8.38	137.40	126.50
53	2	904	C	N3-C2-O2	-8.38	116.03	121.90
51	3	84	U	C2-N1-C1'	8.38	127.75	117.70
53	2	3772	U	N3-C2-O2	-8.36	116.35	122.20
53	2	961	G	N3-C4-N9	8.34	131.01	126.00
53	2	2560	C	C6-N1-C2	-8.34	116.96	120.30
53	2	2022	C	N3-C2-O2	-8.34	116.06	121.90
53	2	2031	C	C6-N1-C2	-8.33	116.97	120.30
53	2	2627	C	C5-C6-N1	8.32	125.16	121.00
53	2	4714	C	N3-C2-O2	-8.30	116.09	121.90
53	2	3657	U	N3-C2-O2	-8.30	116.39	122.20
53	2	2499	C	N3-C2-O2	-8.28	116.10	121.90
53	2	4859	C	N1-C2-O2	8.27	123.86	118.90
53	2	220	C	N1-C2-O2	8.27	123.86	118.90
22	U	84	PRO	CB-CG-CD	8.26	138.72	106.50
53	2	1494	U	N1-C2-O2	8.25	128.58	122.80
53	2	1978	C	N1-C2-O2	8.24	123.85	118.90
53	2	2589	C	C6-N1-C2	-8.23	117.01	120.30
53	2	2856	C	N1-C2-O2	8.21	123.83	118.90
53	2	2439	G	C8-N9-C1'	-8.20	116.34	127.00
53	2	4266	G	N3-C4-C5	-8.20	124.50	128.60
53	2	4758	U	C2-N1-C1'	8.20	127.54	117.70
53	2	4682	U	N1-C2-O2	8.20	128.54	122.80
53	2	4266	G	N3-C4-N9	8.18	130.91	126.00
53	2	4360	U	N3-C2-O2	-8.17	116.48	122.20
53	2	672	C	N1-C2-O2	8.16	123.80	118.90
53	2	469	C	N1-C2-O2	8.16	123.80	118.90
53	2	472	C	C2-N1-C1'	8.13	127.75	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	2	4926	C	C5-C6-N1	8.13	125.06	121.00
53	2	1241	C	C2-N1-C1'	8.12	127.73	118.80
53	2	2262	G	N3-C4-C5	-8.08	124.56	128.60
51	3	78	C	C5-C6-N1	8.07	125.03	121.00
8	D	319	LEU	CA-CB-CG	8.06	133.85	115.30
53	2	2820	C	C6-N1-C2	-8.06	117.08	120.30
53	2	2760	G	P-O3'-C3'	8.05	129.37	119.70
51	3	95	C	N3-C2-O2	-8.05	116.26	121.90
53	2	1671	U	C5-C6-N1	8.04	126.72	122.70
53	2	4674	C	C6-N1-C2	-8.04	117.08	120.30
53	2	1889	U	N3-C2-O2	-8.03	116.58	122.20
53	2	906	C	C6-N1-C2	-8.02	117.09	120.30
53	2	1402	C	C6-N1-C2	-8.00	117.10	120.30
53	2	77	U	N1-C2-O2	7.98	128.38	122.80
53	2	4295	U	N3-C2-O2	-7.98	116.61	122.20
53	2	282	C	N3-C2-O2	-7.97	116.32	121.90
53	2	2262	G	N3-C4-N9	7.97	130.78	126.00
53	2	115	C	N3-C2-O2	-7.96	116.33	121.90
53	2	2791	C	C6-N1-C2	-7.95	117.12	120.30
53	2	112	C	C6-N1-C2	-7.95	117.12	120.30
53	2	2571	C	N1-C2-O2	7.95	123.67	118.90
53	2	1966	C	C6-N1-C2	-7.94	117.12	120.30
53	2	4171	C	N1-C2-O2	7.94	123.66	118.90
53	2	972	C	N3-C2-O2	-7.92	116.35	121.90
53	2	961	G	N3-C4-C5	-7.92	124.64	128.60
53	2	195	C	C6-N1-C2	-7.90	117.14	120.30
1	N	84	LEU	CA-CB-CG	7.90	133.47	115.30
53	2	1191	C	N3-C2-O2	-7.89	116.38	121.90
53	2	220	C	C6-N1-C2	-7.88	117.15	120.30
53	2	1726	U	N1-C2-O2	7.88	128.32	122.80
53	2	2561	C	C6-N1-C2	-7.88	117.15	120.30
53	2	2410	C	C5-C6-N1	7.86	124.93	121.00
53	2	4775	C	C6-N1-C1'	-7.85	111.38	120.80
53	2	4885	U	N1-C2-O2	7.85	128.29	122.80
53	2	1732	C	C6-N1-C2	-7.84	117.16	120.30
53	2	4284	C	C5-C6-N1	7.84	124.92	121.00
53	2	322	C	C6-N1-C2	-7.83	117.17	120.30
53	2	4471	U	N1-C2-O2	7.82	128.27	122.80
53	2	2290	C	C6-N1-C2	-7.81	117.17	120.30
53	2	112	C	C2-N1-C1'	7.81	127.39	118.80
53	2	201	C	C6-N1-C2	-7.81	117.18	120.30
4	8	64	U	N3-C2-O2	-7.80	116.74	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	2	2410	C	N1-C2-O2	7.80	123.58	118.90
53	2	2528	G	C4-N9-C1'	7.80	136.64	126.50
53	2	2497	C	C2-N1-C1'	7.79	127.37	118.80
53	2	1325	C	N1-C2-O2	7.78	123.57	118.90
53	2	2592	U	N3-C2-O2	-7.77	116.76	122.20
53	2	1889	U	N1-C2-O2	7.76	128.23	122.80
53	2	1816	C	N3-C2-O2	-7.75	116.47	121.90
53	2	50	C	N1-C2-O2	7.74	123.55	118.90
53	2	4158	C	N1-C2-O2	7.74	123.55	118.90
51	3	95	C	C6-N1-C1'	-7.74	111.51	120.80
53	2	4206	C	N1-C2-O2	7.74	123.54	118.90
53	2	515	C	C6-N1-C2	-7.74	117.21	120.30
53	2	2561	C	C5-C6-N1	7.73	124.86	121.00
53	2	2814	C	N1-C2-O2	7.73	123.54	118.90
53	2	1678	C	P-O3'-C3'	7.73	128.97	119.70
53	2	3606	U	N3-C2-O2	-7.73	116.79	122.20
53	2	963	G	N3-C4-N9	7.72	130.63	126.00
53	2	100	C	C6-N1-C1'	-7.72	111.54	120.80
53	2	1655	C	C6-N1-C2	-7.71	117.22	120.30
53	2	49	U	N3-C2-O2	-7.71	116.80	122.20
53	2	1703	C	N1-C2-O2	7.71	123.53	118.90
53	2	3774	A	P-O3'-C3'	7.71	128.95	119.70
53	2	4695	C	N1-C2-O2	7.71	123.53	118.90
53	2	4505	C	C6-N1-C2	-7.71	117.22	120.30
53	2	4522	G	C4-N9-C1'	7.70	136.51	126.50
53	2	2281	U	N3-C2-O2	-7.69	116.81	122.20
53	2	1996	C	C6-N1-C2	-7.69	117.22	120.30
53	2	4766	C	C2-N1-C1'	7.69	127.26	118.80
53	2	472	C	C5-C6-N1	7.68	124.84	121.00
53	2	963	G	C8-N9-C1'	-7.68	117.01	127.00
53	2	1243	C	N1-C2-O2	7.68	123.51	118.90
53	2	2362	U	N3-C2-O2	-7.68	116.82	122.20
53	2	1245	C	C6-N1-C2	-7.67	117.23	120.30
53	2	1607	C	C6-N1-C2	-7.67	117.23	120.30
53	2	4453	C	N1-C2-O2	7.67	123.50	118.90
53	2	1731	C	C6-N1-C2	-7.67	117.23	120.30
53	2	2107	C	C6-N1-C2	-7.67	117.23	120.30
53	2	4112	C	C6-N1-C2	-7.67	117.23	120.30
53	2	4775	C	C6-N1-C2	-7.66	117.23	120.30
29	g	118	ASP	CB-CG-OD1	7.65	125.19	118.30
53	2	914	U	P-O3'-C3'	7.65	128.88	119.70
36	p	220	MET	CA-CB-CG	7.63	126.28	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	2	1245	C	C5-C6-N1	7.63	124.81	121.00
53	2	3876	A	N3-C4-N9	7.63	133.50	127.40
53	2	668	C	N1-C2-O2	7.63	123.48	118.90
53	2	1607	C	N1-C2-O2	7.62	123.47	118.90
53	2	259	C	N1-C2-O2	7.60	123.46	118.90
53	2	4295	U	N1-C2-O2	7.60	128.12	122.80
53	2	4207	C	N1-C2-O2	7.59	123.46	118.90
53	2	1251	C	C6-N1-C2	-7.59	117.26	120.30
53	2	1832	C	N1-C2-O2	7.59	123.45	118.90
53	2	4766	C	C5-C6-N1	7.59	124.79	121.00
53	2	2281	U	N1-C2-O2	7.59	128.11	122.80
53	2	2262	G	C8-N9-C1'	-7.58	117.14	127.00
53	2	2445	C	C6-N1-C2	-7.58	117.27	120.30
53	2	4709	U	C2-N1-C1'	7.57	126.79	117.70
53	2	1632	A	C2-N3-C4	7.57	114.38	110.60
53	2	753	C	C5-C6-N1	7.56	124.78	121.00
53	2	3636	C	N1-C2-O2	7.56	123.44	118.90
53	2	3926	C	N1-C2-O2	7.56	123.43	118.90
53	2	112	C	N1-C2-O2	7.55	123.43	118.90
53	2	961	G	C8-N9-C1'	-7.55	117.18	127.00
4	8	54	C	N1-C2-O2	7.54	123.43	118.90
53	2	1966	C	C5-C6-N1	7.53	124.77	121.00
53	2	2337	C	N1-C2-O2	7.52	123.41	118.90
53	2	390	C	C6-N1-C2	-7.51	117.30	120.30
53	2	365	U	N3-C2-O2	-7.50	116.95	122.20
53	2	2072	C	C6-N1-C2	-7.49	117.30	120.30
53	2	1963	C	C6-N1-C2	-7.49	117.31	120.30
53	2	4895	C	N1-C2-O2	7.48	123.39	118.90
53	2	4171	C	C6-N1-C2	-7.46	117.31	120.30
53	2	2351	C	C6-N1-C2	-7.46	117.32	120.30
53	2	4112	C	N3-C2-O2	-7.46	116.68	121.90
53	2	96	U	N1-C2-O2	7.45	128.01	122.80
53	2	499	G	C8-N9-C1'	-7.45	117.32	127.00
53	2	2528	G	N3-C4-N9	7.44	130.47	126.00
53	2	1340	C	C6-N1-C2	-7.44	117.32	120.30
53	2	49	U	N1-C2-O2	7.43	128.00	122.80
53	2	1216	C	N3-C2-O2	-7.43	116.70	121.90
53	2	1405	C	N3-C2-O2	-7.42	116.70	121.90
53	2	2008	U	N3-C2-O2	-7.42	117.00	122.20
53	2	1203	G	C4-N9-C1'	7.42	136.14	126.50
53	2	175	C	C6-N1-C2	-7.40	117.34	120.30
53	2	3587	C	N1-C2-O2	7.39	123.33	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	2	9	C	C6-N1-C2	-7.38	117.35	120.30
53	2	4747	C	C2-N1-C1'	7.37	126.91	118.80
53	2	2667	C	N1-C2-O2	7.37	123.32	118.90
53	2	365	U	N1-C2-O2	7.34	127.94	122.80
53	2	963	G	N3-C4-C5	-7.34	124.93	128.60
53	2	2439	G	N3-C4-N9	7.33	130.40	126.00
53	2	4308	C	N1-C2-O2	7.33	123.30	118.90
53	2	4636	U	N3-C2-O2	-7.32	117.07	122.20
53	2	2528	G	N3-C4-C5	-7.32	124.94	128.60
53	2	4453	C	C2-N1-C1'	7.32	126.85	118.80
53	2	2627	C	N3-C2-O2	-7.32	116.78	121.90
53	2	1458	C	N3-C2-O2	-7.31	116.78	121.90
53	2	2505	C	C6-N1-C2	-7.31	117.38	120.30
53	2	3606	U	N1-C2-O2	7.31	127.92	122.80
53	2	30	C	C6-N1-C2	-7.31	117.38	120.30
53	2	178	C	C5-C6-N1	7.29	124.64	121.00
53	2	1344	C	C6-N1-C2	-7.29	117.39	120.30
53	2	1241	C	N3-C2-O2	-7.28	116.81	121.90
53	2	2033	A	P-O3'-C3'	7.27	128.42	119.70
53	2	4880	C	C6-N1-C2	-7.26	117.39	120.30
53	2	3876	A	C4-N9-C1'	-7.26	113.23	126.30
53	2	972	C	C6-N1-C2	-7.26	117.39	120.30
53	2	1472	C	C6-N1-C2	-7.26	117.40	120.30
53	2	1367	C	N1-C2-O2	7.25	123.25	118.90
53	2	1921	C	N3-C2-O2	-7.25	116.82	121.90
53	2	1402	C	C2-N1-C1'	7.25	126.78	118.80
53	2	1812	C	C6-N1-C2	-7.25	117.40	120.30
53	2	4284	C	C6-N1-C2	-7.24	117.40	120.30
53	2	3636	C	N3-C2-O2	-7.24	116.83	121.90
53	2	1315	C	C6-N1-C2	-7.23	117.41	120.30
53	2	4162	C	N1-C2-O2	7.23	123.24	118.90
53	2	2031	C	C5-C6-N1	7.22	124.61	121.00
53	2	1276	C	N1-C2-O2	7.22	123.23	118.90
53	2	112	C	C5-C6-N1	7.22	124.61	121.00
53	2	1340	C	C5-C6-N1	7.22	124.61	121.00
53	2	2499	C	C5-C6-N1	7.22	124.61	121.00
53	2	4505	C	C2-N1-C1'	7.22	126.74	118.80
53	2	3622	C	N3-C2-O2	-7.21	116.85	121.90
53	2	2850	A	C2-N3-C4	7.20	114.20	110.60
53	2	3915	U	N3-C2-O2	-7.20	117.16	122.20
53	2	178	C	C2-N1-C1'	7.19	126.71	118.80
53	2	4747	C	C6-N1-C2	-7.19	117.42	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	2	4880	C	N3-C2-O2	-7.19	116.87	121.90
53	2	259	C	C6-N1-C2	-7.18	117.43	120.30
53	2	2532	C	C6-N1-C2	-7.18	117.43	120.30
53	2	472	C	N1-C2-O2	7.17	123.20	118.90
53	2	2710	C	C5-C6-N1	7.17	124.59	121.00
53	2	1367	C	C2-N1-C1'	7.16	126.68	118.80
53	2	5002	U	N3-C2-O2	-7.16	117.19	122.20
53	2	2031	C	C2-N1-C1'	7.15	126.67	118.80
53	2	1994	C	C6-N1-C1'	-7.15	112.22	120.80
53	2	3769	C	C5-C6-N1	7.15	124.57	121.00
53	2	5030	U	C2-N1-C1'	7.15	126.28	117.70
53	2	3905	A	P-O3'-C3'	7.14	128.27	119.70
53	2	4508	C	N1-C2-O2	7.13	123.18	118.90
53	2	657	C	N1-C2-O2	7.12	123.17	118.90
53	2	4387	C	N1-C2-O2	7.12	123.17	118.90
53	2	4636	U	N1-C2-O2	7.12	127.78	122.80
53	2	1980	U	P-O3'-C3'	7.12	128.24	119.70
53	2	906	C	C2-N1-C1'	7.12	126.63	118.80
53	2	2362	U	N1-C2-O2	7.11	127.78	122.80
53	2	1921	C	C2-N1-C1'	7.11	126.62	118.80
53	2	3622	C	C6-N1-C2	-7.11	117.46	120.30
53	2	2011	C	N1-C2-O2	7.10	123.16	118.90
53	2	1477	C	C6-N1-C2	-7.10	117.46	120.30
53	2	178	C	N1-C2-O2	7.10	123.16	118.90
53	2	1607	C	N3-C2-O2	-7.10	116.93	121.90
53	2	1994	C	C6-N1-C2	-7.09	117.46	120.30
53	2	4764	A	N1-C2-N3	-7.09	125.76	129.30
53	2	2011	C	C6-N1-C2	-7.08	117.47	120.30
53	2	4563	U	N3-C2-O2	-7.08	117.24	122.20
53	2	1250	C	N1-C2-O2	7.08	123.14	118.90
53	2	1702	C	C2-N1-C1'	7.07	126.58	118.80
53	2	4562	C	N1-C2-O2	7.07	123.14	118.90
53	2	4972	U	N3-C2-O2	-7.07	117.25	122.20
53	2	4132	C	C6-N1-C2	-7.06	117.47	120.30
53	2	4505	C	N1-C2-O2	7.06	123.14	118.90
53	2	2867	C	C6-N1-C2	-7.05	117.48	120.30
53	2	1243	C	C5-C6-N1	7.04	124.52	121.00
53	2	1915	C	N1-C2-O2	7.04	123.12	118.90
53	2	2592	U	N1-C2-O2	7.04	127.73	122.80
53	2	1203	G	N3-C4-C5	-7.04	125.08	128.60
53	2	3769	C	C6-N1-C2	-7.04	117.48	120.30
53	2	4360	U	N1-C2-O2	7.04	127.73	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	2	1276	C	C5-C6-N1	7.04	124.52	121.00
53	2	1978	C	C6-N1-C2	-7.03	117.49	120.30
53	2	2814	C	C2-N1-C1'	7.03	126.53	118.80
53	2	4505	C	C5-C6-N1	7.03	124.52	121.00
34	n	5	LEU	CA-CB-CG	7.03	131.47	115.30
53	2	499	G	C2-N3-C4	7.02	115.41	111.90
53	2	4714	C	C5-C6-N1	7.01	124.51	121.00
53	2	4502	C	N1-C2-O2	7.01	123.11	118.90
53	2	2532	C	N1-C2-O2	7.00	123.10	118.90
53	2	4996	C	C6-N1-C2	-7.00	117.50	120.30
53	2	2856	C	N3-C2-O2	-6.99	117.00	121.90
53	2	3772	U	C2-N1-C1'	6.99	126.09	117.70
53	2	1663	C	C6-N1-C2	-6.99	117.50	120.30
53	2	3926	C	C6-N1-C2	-6.99	117.50	120.30
53	2	4864	U	C2-N1-C1'	6.97	126.07	117.70
53	2	2532	C	C5-C6-N1	6.97	124.49	121.00
38	u	6	LEU	CA-CB-CG	6.97	131.33	115.30
53	2	4341	C	N1-C2-O2	6.96	123.08	118.90
53	2	3848	U	N3-C2-O2	-6.96	117.33	122.20
53	2	259	C	C5-C6-N1	6.96	124.48	121.00
53	2	1472	C	C2-N1-C1'	6.96	126.45	118.80
53	2	44	A	C2-N3-C4	6.96	114.08	110.60
53	2	3878	C	N1-C2-O2	6.95	123.07	118.90
53	2	4266	G	C8-N9-C1'	-6.95	117.96	127.00
7	B	360	LEU	CA-CB-CG	6.93	131.23	115.30
53	2	1931	C	P-O3'-C3'	6.92	128.01	119.70
53	2	2008	U	N1-C2-O2	6.92	127.65	122.80
53	2	4402	C	N1-C2-O2	6.92	123.05	118.90
53	2	1592	G	C4-N9-C1'	6.91	135.48	126.50
53	2	4627	U	N3-C2-O2	-6.91	117.36	122.20
53	2	673	C	C6-N1-C2	-6.90	117.54	120.30
53	2	1671	U	C6-N1-C2	-6.90	116.86	121.00
51	3	51	G	P-O3'-C3'	6.90	127.98	119.70
53	2	281	U	N3-C2-O2	-6.89	117.38	122.20
53	2	36	U	N3-C2-O2	-6.88	117.39	122.20
53	2	3876	A	C4-C5-C6	6.88	120.44	117.00
53	2	100	C	C6-N1-C2	-6.87	117.55	120.30
53	2	1720	C	N1-C2-O2	6.87	123.02	118.90
53	2	4913	G	P-O3'-C3'	6.87	127.94	119.70
53	2	1442	C	C6-N1-C2	-6.87	117.55	120.30
53	2	4349	C	N1-C2-O2	6.86	123.02	118.90
53	2	4476	C	C6-N1-C1'	-6.85	112.58	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	2	4771	C	C6-N1-C2	-6.85	117.56	120.30
53	2	515	C	N3-C2-O2	-6.85	117.11	121.90
53	2	4508	C	C6-N1-C2	-6.85	117.56	120.30
53	2	1732	C	N1-C2-O2	6.84	123.00	118.90
53	2	4426	C	C6-N1-C2	-6.83	117.57	120.30
53	2	4766	C	N1-C2-O2	6.83	123.00	118.90
53	2	2532	C	C2-N1-C1'	6.83	126.31	118.80
53	2	4991	U	N3-C2-O2	-6.83	117.42	122.20
53	2	985	C	C6-N1-C2	-6.82	117.57	120.30
53	2	2867	C	C2-N1-C1'	6.82	126.30	118.80
53	2	2372	U	N3-C2-O2	-6.82	117.43	122.20
53	2	4914	C	C6-N1-C2	-6.81	117.58	120.30
53	2	26	C	C6-N1-C2	-6.81	117.58	120.30
53	2	204	U	N3-C2-O2	-6.80	117.44	122.20
53	2	1893	C	C6-N1-C2	-6.80	117.58	120.30
53	2	2439	G	N3-C4-C5	-6.80	125.20	128.60
53	2	4481	U	N3-C2-O2	-6.80	117.44	122.20
53	2	906	C	C5-C6-N1	6.80	124.40	121.00
53	2	4158	C	C6-N1-C2	-6.80	117.58	120.30
53	2	50	C	C6-N1-C2	-6.79	117.58	120.30
53	2	1655	C	N1-C2-O2	6.79	122.98	118.90
53	2	4231	C	N1-C2-O2	6.79	122.97	118.90
53	2	4522	G	N3-C4-C5	-6.79	125.20	128.60
53	2	155	C	N3-C2-O2	-6.79	117.15	121.90
53	2	2497	C	N1-C2-O2	6.78	122.97	118.90
53	2	122	U	N3-C2-O2	-6.78	117.45	122.20
53	2	220	C	N3-C2-O2	-6.77	117.16	121.90
53	2	1978	C	C2-N1-C1'	6.76	126.24	118.80
53	2	220	C	C5-C6-N1	6.76	124.38	121.00
51	3	67	C	C6-N1-C2	-6.75	117.60	120.30
53	2	977	C	C6-N1-C2	-6.75	117.60	120.30
53	2	3631	U	N3-C2-O2	-6.75	117.47	122.20
53	2	4563	U	N1-C2-O2	6.75	127.52	122.80
53	2	4207	C	N3-C2-O2	-6.75	117.18	121.90
53	2	1310	C	C6-N1-C2	-6.74	117.60	120.30
53	2	1666	C	C6-N1-C2	-6.74	117.60	120.30
53	2	1344	C	C2-N1-C1'	6.74	126.21	118.80
53	2	3637	U	N3-C2-O2	-6.74	117.48	122.20
53	2	1816	C	C6-N1-C2	-6.73	117.61	120.30
22	U	84	PRO	CA-N-CD	-6.73	102.08	111.50
53	2	1991	A	C2-N3-C4	6.73	113.97	110.60
53	2	3587	C	C6-N1-C2	-6.72	117.61	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	2	1812	C	C5-C6-N1	6.72	124.36	121.00
53	2	1731	C	C5-C6-N1	6.71	124.36	121.00
53	2	3870	C	C6-N1-C2	-6.71	117.61	120.30
53	2	2038	U	N3-C2-O2	-6.71	117.50	122.20
53	2	1993	C	C6-N1-C2	-6.70	117.62	120.30
53	2	3650	C	C6-N1-C2	-6.68	117.63	120.30
53	2	2589	C	C5-C6-N1	6.68	124.34	121.00
51	3	29	C	C6-N1-C2	-6.68	117.63	120.30
53	2	694	C	C6-N1-C2	-6.67	117.63	120.30
53	2	719	C	C6-N1-C2	-6.67	117.63	120.30
53	2	4627	U	N1-C2-O2	6.67	127.47	122.80
53	2	1929	A	C4-N9-C1'	6.66	138.29	126.30
53	2	4319	C	C6-N1-C2	-6.66	117.64	120.30
4	8	64	U	N1-C2-O2	6.65	127.46	122.80
53	2	4522	G	N3-C4-N9	6.64	129.99	126.00
53	2	3772	U	N1-C2-O2	6.64	127.45	122.80
53	2	4991	U	N1-C2-O2	6.63	127.44	122.80
53	2	5002	U	N1-C2-O2	6.63	127.44	122.80
53	2	1191	C	N1-C2-O2	6.62	122.87	118.90
53	2	4508	C	C5-C6-N1	6.61	124.31	121.00
53	2	4350	C	C5-C6-N1	6.61	124.30	121.00
53	2	4476	C	C5-C6-N1	6.60	124.30	121.00
53	2	1505	C	C5-C6-N1	6.59	124.30	121.00
53	2	1795	A	C2-N3-C4	6.59	113.90	110.60
53	2	4771	C	N1-C2-O2	6.59	122.86	118.90
53	2	2670	C	C6-N1-C2	-6.58	117.67	120.30
53	2	3774	A	OP1-P-O3'	6.58	119.68	105.20
53	2	1378	C	C2-N1-C1'	6.58	126.03	118.80
53	2	4207	C	C6-N1-C2	-6.57	117.67	120.30
53	2	1915	C	N3-C2-O2	-6.57	117.30	121.90
53	2	1309	C	C6-N1-C2	-6.57	117.67	120.30
53	2	2019	C	C6-N1-C2	-6.57	117.67	120.30
53	2	86	U	N3-C2-O2	-6.56	117.61	122.20
53	2	2704	C	C6-N1-C2	-6.56	117.68	120.30
53	2	4417	C	C6-N1-C2	-6.55	117.68	120.30
53	2	155	C	N1-C2-O2	6.55	122.83	118.90
53	2	2528	G	C8-N9-C1'	-6.55	118.48	127.00
53	2	1663	C	C5-C6-N1	6.55	124.27	121.00
53	2	2062	C	C6-N1-C2	-6.55	117.68	120.30
53	2	4859	C	N3-C2-O2	-6.55	117.32	121.90
53	2	486	C	C6-N1-C2	-6.54	117.68	120.30
53	2	4171	C	N3-C2-O2	-6.54	117.32	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	2	906	C	N1-C2-O2	6.54	122.83	118.90
53	2	4653	C	C6-N1-C2	-6.54	117.68	120.30
53	2	4406	U	C2-N1-C1'	6.54	125.55	117.70
53	2	78	U	N3-C2-O2	-6.54	117.63	122.20
53	2	2008	U	C2-N1-C1'	6.54	125.54	117.70
53	2	3685	C	C6-N1-C2	-6.53	117.69	120.30
53	2	36	U	N1-C2-O2	6.52	127.36	122.80
51	3	72	U	O5'-P-OP2	-6.51	99.84	105.70
53	2	1276	C	N3-C2-O2	-6.51	117.34	121.90
53	2	1875	C	N1-C2-O2	6.51	122.81	118.90
53	2	1325	C	N3-C2-O2	-6.51	117.34	121.90
53	2	1656	U	N3-C2-O2	-6.51	117.65	122.20
34	n	105	LEU	C-N-CA	6.50	137.96	121.70
53	2	4393	G	C5-C6-O6	6.50	132.50	128.60
53	2	1494	U	C2-N1-C1'	6.50	125.50	117.70
53	2	2820	C	C2-N1-C1'	6.49	125.94	118.80
53	2	2031	C	N1-C2-O2	6.49	122.79	118.90
53	2	2667	C	C6-N1-C2	-6.49	117.70	120.30
53	2	1931	C	C6-N1-C2	-6.49	117.70	120.30
53	2	4387	C	C6-N1-C2	-6.48	117.71	120.30
53	2	2560	C	N1-C2-O2	6.48	122.79	118.90
53	2	4350	C	C2-N1-C1'	6.48	125.92	118.80
53	2	201	C	C2-N1-C1'	6.47	125.92	118.80
53	2	3739	C	C6-N1-C2	-6.47	117.71	120.30
25	Z	83	VAL	CG1-CB-CG2	-6.47	100.55	110.90
53	2	1325	C	C6-N1-C2	-6.46	117.71	120.30
53	2	5030	U	C5-C6-N1	6.46	125.93	122.70
53	2	3618	C	C6-N1-C2	-6.46	117.72	120.30
53	2	2783	A	N1-C2-N3	-6.46	126.07	129.30
4	8	54	C	C6-N1-C2	-6.46	117.72	120.30
53	2	3769	C	N1-C2-O2	6.46	122.77	118.90
1	N	354	LEU	CA-CB-CG	-6.45	100.46	115.30
51	3	29	C	C5-C6-N1	6.45	124.22	121.00
53	2	1081	C	C6-N1-C2	-6.45	117.72	120.30
53	2	515	C	C2-N1-C1'	6.44	125.89	118.80
53	2	2303	C	C6-N1-C2	-6.43	117.73	120.30
53	2	2498	C	C6-N1-C2	-6.43	117.73	120.30
53	2	1309	C	C5-C6-N1	6.43	124.21	121.00
53	2	3657	U	N1-C2-O2	6.42	127.30	122.80
53	2	1702	C	N1-C2-O2	6.42	122.75	118.90
53	2	485	C	P-O3'-C3'	6.42	127.40	119.70
53	2	386	A	C2-N3-C4	6.42	113.81	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	2	322	C	C2-N1-C1'	6.42	125.86	118.80
53	2	322	C	C5-C6-N1	6.42	124.21	121.00
53	2	4969	C	C6-N1-C2	-6.41	117.73	120.30
53	2	28	C	C6-N1-C2	-6.41	117.73	120.30
53	2	2561	C	N1-C2-O2	6.41	122.75	118.90
53	2	4747	C	N1-C2-O2	6.41	122.74	118.90
53	2	4243	C	C6-N1-C2	-6.40	117.74	120.30
53	2	4078	C	C6-N1-C2	-6.40	117.74	120.30
53	2	2035	C	C5-C6-N1	6.40	124.20	121.00
53	2	2019	C	N1-C2-O2	6.39	122.73	118.90
53	2	3636	C	C5-C6-N1	6.39	124.19	121.00
53	2	694	C	C2-N1-C1'	6.39	125.83	118.80
53	2	469	C	N3-C2-O2	-6.38	117.43	121.90
53	2	195	C	C5-C6-N1	6.38	124.19	121.00
16	L	117	LEU	CA-CB-CG	6.38	129.97	115.30
53	2	4662	C	C5-C6-N1	6.38	124.19	121.00
53	2	281	U	N1-C2-O2	6.37	127.26	122.80
53	2	1808	C	C6-N1-C2	-6.37	117.75	120.30
53	2	390	C	C5-C6-N1	6.37	124.19	121.00
53	2	4256	A	C2-N3-C4	6.37	113.78	110.60
53	2	1472	C	N1-C2-O2	6.37	122.72	118.90
53	2	1344	C	C5-C6-N1	6.36	124.18	121.00
53	2	1978	C	C5-C6-N1	6.35	124.18	121.00
53	2	4308	C	C6-N1-C2	-6.35	117.76	120.30
53	2	668	C	N3-C2-O2	-6.35	117.45	121.90
53	2	3876	A	N1-C6-N6	-6.35	114.79	118.60
53	2	1732	C	N3-C2-O2	-6.35	117.46	121.90
53	2	4880	C	C5-C6-N1	6.35	124.17	121.00
53	2	4880	C	C2-N1-C1'	6.34	125.78	118.80
53	2	2337	C	N3-C2-O2	-6.34	117.46	121.90
53	2	1683	U	N3-C2-O2	-6.34	117.76	122.20
53	2	3915	U	N1-C2-O2	6.34	127.23	122.80
53	2	4703	U	N3-C2-O2	-6.33	117.77	122.20
53	2	9	C	C5-C6-N1	6.33	124.17	121.00
53	2	661	C	C6-N1-C2	-6.33	117.77	120.30
53	2	4714	C	C2-N1-C1'	6.33	125.76	118.80
53	2	115	C	C6-N1-C1'	-6.33	113.21	120.80
53	2	1472	C	C5-C6-N1	6.32	124.16	121.00
53	2	4674	C	C5-C6-N1	6.32	124.16	121.00
53	2	2819	U	N3-C2-O2	-6.32	117.78	122.20
53	2	1656	U	N1-C2-O2	6.31	127.22	122.80
53	2	3637	U	N1-C2-O2	6.31	127.22	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	2	100	C	O4'-C1'-N1	6.31	113.25	108.20
53	2	1720	C	C6-N1-C2	-6.31	117.78	120.30
53	2	4972	U	N1-C2-O2	6.31	127.22	122.80
44	W	283	LEU	CA-CB-CG	6.30	129.80	115.30
53	2	672	C	N3-C2-O2	-6.30	117.49	121.90
53	2	4683	U	N3-C2-O2	-6.29	117.80	122.20
53	2	515	C	C5-C6-N1	6.29	124.15	121.00
53	2	3932	U	N3-C2-O2	-6.29	117.80	122.20
4	8	32	C	N1-C2-O2	6.29	122.67	118.90
53	2	1243	C	N3-C2-O2	-6.29	117.50	121.90
53	2	2351	C	N1-C2-O2	6.28	122.67	118.90
53	2	79	C	C6-N1-C2	-6.28	117.79	120.30
53	2	3670	C	N1-C2-O2	6.28	122.67	118.90
53	2	4712	C	N1-C2-O2	6.28	122.67	118.90
53	2	2445	C	C5-C6-N1	6.28	124.14	121.00
4	8	32	C	C6-N1-C2	-6.28	117.79	120.30
53	2	4270	C	C6-N1-C2	-6.27	117.79	120.30
51	3	72	U	OP1-P-OP2	-6.27	110.19	119.60
53	2	1088	C	C6-N1-C2	-6.27	117.79	120.30
53	2	4601	U	N3-C2-O2	-6.27	117.81	122.20
53	2	1467	C	C6-N1-C2	-6.27	117.79	120.30
53	2	469	C	C6-N1-C2	-6.26	117.80	120.30
53	2	1996	C	C5-C6-N1	6.26	124.13	121.00
53	2	50	C	N3-C2-O2	-6.25	117.52	121.90
53	2	322	C	N1-C2-O2	6.25	122.65	118.90
51	3	92	C	C6-N1-C2	-6.24	117.80	120.30
53	2	1938	C	C2-N1-C1'	6.24	125.67	118.80
53	2	977	C	C2-N1-C1'	6.24	125.67	118.80
53	2	2403	A	C2-N3-C4	6.24	113.72	110.60
53	2	3606	U	C2-N1-C1'	6.24	125.19	117.70
53	2	1505	C	C6-N1-C2	-6.24	117.81	120.30
53	2	3882	C	C2-N1-C1'	6.24	125.66	118.80
53	2	1405	C	C6-N1-C2	-6.23	117.81	120.30
53	2	209	U	N3-C2-O2	-6.23	117.84	122.20
53	2	2290	C	C5-C6-N1	6.23	124.11	121.00
53	2	2094	G	C4-N9-C1'	6.22	134.59	126.50
53	2	4112	C	C5-C6-N1	6.22	124.11	121.00
53	2	4771	C	C5-C6-N1	6.22	124.11	121.00
53	2	2791	C	C5-C6-N1	6.22	124.11	121.00
53	2	1655	C	N3-C2-O2	-6.22	117.55	121.90
51	3	72	U	P-O3'-C3'	6.21	127.16	119.70
53	2	2497	C	C5-C6-N1	6.21	124.11	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	2	440	U	N3-C2-O2	-6.21	117.85	122.20
53	2	4695	C	N3-C2-O2	-6.21	117.56	121.90
51	3	3	C	C6-N1-C2	-6.20	117.82	120.30
53	2	2689	C	C6-N1-C2	-6.20	117.82	120.30
53	2	1429	C	C6-N1-C2	-6.20	117.82	120.30
53	2	4481	U	N1-C2-O2	6.20	127.14	122.80
53	2	4614	G	C5-C6-O6	6.20	132.32	128.60
53	2	516	C	C5-C6-N1	6.20	124.10	121.00
53	2	2072	C	C5-C6-N1	6.20	124.10	121.00
4	8	55	U	N3-C2-O2	-6.19	117.87	122.20
53	2	1203	G	N3-C4-N9	6.18	129.71	126.00
53	2	1966	C	N1-C2-O2	6.18	122.61	118.90
53	2	4758	U	C6-N1-C2	-6.18	117.29	121.00
53	2	1405	C	C2-N1-C1'	6.18	125.60	118.80
53	2	2035	C	C6-N1-C2	-6.18	117.83	120.30
51	3	72	U	O5'-P-OP1	6.17	118.11	110.70
53	2	2892	C	C2-N1-C1'	6.17	125.59	118.80
53	2	3866	C	C6-N1-C2	-6.17	117.83	120.30
53	2	3926	C	N3-C2-O2	-6.17	117.58	121.90
53	2	1678	C	C2-N1-C1'	6.17	125.58	118.80
53	2	1202	C	C6-N1-C2	-6.17	117.83	120.30
53	2	209	U	N1-C2-O2	6.16	127.11	122.80
53	2	201	C	N1-C2-O2	6.16	122.60	118.90
53	2	1477	C	C5-C6-N1	6.16	124.08	121.00
53	2	2362	U	C2-N1-C1'	6.16	125.09	117.70
53	2	4130	C	C5-C6-N1	6.16	124.08	121.00
53	2	4522	G	C8-N9-C1'	-6.16	119.00	127.00
53	2	1216	C	C6-N1-C1'	-6.16	113.41	120.80
53	2	259	C	C2-N1-C1'	6.16	125.57	118.80
53	2	988	C	N1-C2-O2	6.16	122.59	118.90
53	2	4653	C	C5-C6-N1	6.16	124.08	121.00
53	2	2892	C	N1-C2-O2	6.14	122.58	118.90
53	2	282	C	C6-N1-C2	-6.14	117.84	120.30
53	2	1971	C	N1-C2-O2	6.13	122.58	118.90
53	2	1386	C	C6-N1-C2	-6.13	117.85	120.30
53	2	2653	C	C6-N1-C2	-6.13	117.85	120.30
53	2	4555	U	P-O3'-C3'	6.13	127.06	119.70
53	2	2614	C	N1-C2-O2	6.13	122.58	118.90
53	2	68	U	N3-C2-O2	-6.13	117.91	122.20
53	2	220	C	C2-N1-C1'	6.12	125.54	118.80
53	2	977	C	N1-C2-O2	6.12	122.57	118.90
53	2	4237	C	C6-N1-C2	-6.12	117.85	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	2	1402	C	C5-C6-N1	6.12	124.06	121.00
53	2	26	C	N1-C2-O2	6.12	122.57	118.90
53	2	1963	C	C2-N1-C1'	6.12	125.53	118.80
53	2	2632	U	N3-C2-O2	-6.12	117.92	122.20
37	r	310	LEU	CA-CB-CG	6.11	129.36	115.30
53	2	260	C	C6-N1-C2	-6.11	117.86	120.30
4	8	135	C	C6-N1-C2	-6.10	117.86	120.30
4	8	111	U	C2-N1-C1'	6.10	125.02	117.70
53	2	2856	C	C6-N1-C2	-6.10	117.86	120.30
53	2	4361	U	N3-C2-O2	-6.09	117.94	122.20
53	2	201	C	C5-C6-N1	6.09	124.05	121.00
53	2	1808	C	P-O3'-C3'	6.09	127.00	119.70
53	2	4694	G	C8-N9-C4	-6.09	103.97	106.40
53	2	485	C	OP1-P-O3'	6.08	118.59	105.20
53	2	2011	C	N3-C2-O2	-6.08	117.64	121.90
53	2	1957	U	N3-C2-O2	-6.08	117.94	122.20
53	2	4171	C	C5-C6-N1	6.08	124.04	121.00
53	2	750	U	N3-C2-O2	-6.08	117.94	122.20
53	2	1686	C	C6-N1-C2	-6.08	117.87	120.30
53	2	2791	C	C2-N1-C1'	6.07	125.48	118.80
53	2	3767	C	N1-C2-O2	6.07	122.54	118.90
50	d	56	LEU	CA-CB-CG	6.07	129.26	115.30
53	2	4710	C	C6-N1-C2	-6.07	117.87	120.30
53	2	668	C	C6-N1-C2	-6.07	117.87	120.30
53	2	3882	C	N1-C2-O2	6.07	122.54	118.90
53	2	257	C	C6-N1-C2	-6.07	117.87	120.30
53	2	2337	C	C6-N1-C2	-6.07	117.87	120.30
53	2	4294	C	C6-N1-C2	-6.07	117.87	120.30
4	8	54	C	N3-C2-O2	-6.06	117.66	121.90
43	R	208	MET	CG-SD-CE	6.06	109.90	100.20
53	2	2821	U	N3-C2-O2	-6.06	117.96	122.20
53	2	4162	C	C2-N1-C1'	6.06	125.46	118.80
53	2	961	G	C2-N3-C4	6.05	114.93	111.90
53	2	1678	C	N1-C2-O2	6.05	122.53	118.90
51	3	84	U	C6-N1-C1'	-6.05	112.73	121.20
53	2	4314	C	N1-C2-O2	6.05	122.53	118.90
53	2	4402	C	C6-N1-C2	-6.04	117.88	120.30
53	2	3622	C	C2-N1-C1'	6.04	125.45	118.80
53	2	1203	G	C8-N9-C1'	-6.04	119.15	127.00
53	2	3858	C	C6-N1-C2	-6.04	117.88	120.30
53	2	4764	A	C6-N1-C2	6.04	122.22	118.60
53	2	1538	U	N3-C2-O2	-6.04	117.97	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	2	4387	C	C2-N1-C1'	6.03	125.44	118.80
53	2	204	U	N1-C2-O2	6.03	127.02	122.80
53	2	4406	U	N3-C2-O2	-6.03	117.98	122.20
53	2	1447	C	C5-C6-N1	6.02	124.01	121.00
53	2	4237	C	C5-C6-N1	6.02	124.01	121.00
53	2	3882	C	C6-N1-C2	-6.01	117.90	120.30
53	2	4887	C	N1-C2-O2	6.01	122.51	118.90
51	3	71	G	OP1-P-O3'	6.01	118.42	105.20
53	2	2505	C	N1-C2-O2	6.01	122.51	118.90
53	2	2667	C	N3-C2-O2	-6.01	117.69	121.90
53	2	14	C	N1-C2-O2	6.01	122.50	118.90
53	2	4132	C	C5-C6-N1	6.00	124.00	121.00
51	3	29	C	N1-C2-O2	6.00	122.50	118.90
53	2	486	C	C5-C6-N1	6.00	124.00	121.00
53	2	486	C	O5'-P-OP2	-6.00	100.30	105.70
53	2	5050	C	C6-N1-C2	-6.00	117.90	120.30
53	2	257	C	C5-C6-N1	5.99	124.00	121.00
53	2	1966	C	C2-N1-C1'	5.99	125.39	118.80
4	8	101	C	N1-C2-O2	5.99	122.49	118.90
53	2	2017	A	O4'-C1'-N9	5.99	112.99	108.20
53	2	3870	C	C5-C6-N1	5.99	123.99	121.00
21	S	81	ASP	CB-CG-OD2	5.98	123.68	118.30
53	2	4471	U	C2-N1-C1'	5.98	124.87	117.70
53	2	78	U	N1-C2-O2	5.97	126.98	122.80
53	2	4469	U	N3-C2-O2	-5.97	118.02	122.20
53	2	26	C	C2-N1-C1'	5.97	125.36	118.80
53	2	345	C	C6-N1-C2	-5.97	117.91	120.30
53	2	2867	C	N1-C2-O2	5.97	122.48	118.90
53	2	3622	C	C5-C6-N1	5.97	123.98	121.00
53	2	4918	C	C6-N1-C2	-5.96	117.91	120.30
53	2	175	C	N3-C2-O2	-5.96	117.73	121.90
53	2	14	C	C6-N1-C2	-5.96	117.92	120.30
53	2	294	G	C4-N9-C1'	5.96	134.25	126.50
53	2	4923	C	N1-C2-O2	5.96	122.47	118.90
53	2	1978	C	N3-C2-O2	-5.95	117.73	121.90
53	2	2107	C	C2-N1-C1'	5.95	125.34	118.80
51	3	17	C	N1-C2-O2	5.95	122.47	118.90
51	3	57	C	C5-C6-N1	5.94	123.97	121.00
53	2	4206	C	C6-N1-C2	-5.94	117.92	120.30
53	2	694	C	N1-C2-O2	5.94	122.47	118.90
53	2	4601	U	N1-C2-O2	5.94	126.96	122.80
53	2	4206	C	N3-C2-O2	-5.93	117.75	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	2	4350	C	N1-C2-O2	5.93	122.46	118.90
53	2	1893	C	C5-C6-N1	5.93	123.97	121.00
53	2	2615	C	N1-C2-O2	5.93	122.46	118.90
53	2	4709	U	C6-N1-C2	-5.93	117.44	121.00
53	2	86	U	N1-C2-O2	5.93	126.95	122.80
53	2	1401	C	C2-N1-C1'	5.93	125.32	118.80
53	2	1428	U	N3-C2-O2	-5.93	118.05	122.20
53	2	498	C	C6-N1-C2	-5.92	117.93	120.30
53	2	1884	C	C6-N1-C2	-5.92	117.93	120.30
30	h	119	LEU	CA-CB-CG	5.92	128.91	115.30
53	2	1447	C	C6-N1-C2	-5.92	117.93	120.30
53	2	122	U	N1-C2-O2	5.92	126.94	122.80
53	2	489	C	C6-N1-C2	-5.92	117.93	120.30
53	2	654	C	C5-C6-N1	5.92	123.96	121.00
37	r	287	LEU	CA-CB-CG	5.91	128.90	115.30
53	2	1893	C	C2-N1-C1'	5.91	125.30	118.80
53	2	3631	U	N1-C2-O2	5.91	126.93	122.80
53	2	5008	C	C6-N1-C2	-5.91	117.94	120.30
53	2	4537	C	C6-N1-C2	-5.90	117.94	120.30
53	2	4771	C	C2-N1-C1'	5.89	125.28	118.80
53	2	643	C	N3-C2-O2	-5.89	117.78	121.90
53	2	4502	C	C2-N1-C1'	5.89	125.28	118.80
53	2	4914	C	C5-C6-N1	5.89	123.95	121.00
53	2	3598	C	C6-N1-C2	-5.89	117.95	120.30
53	2	4612	C	N1-C2-O2	5.89	122.43	118.90
21	S	32	ASP	CB-CG-OD1	5.88	123.60	118.30
53	2	988	C	C6-N1-C2	-5.88	117.95	120.30
53	2	2560	C	C5-C6-N1	5.88	123.94	121.00
53	2	3598	C	N1-C2-O2	5.88	122.43	118.90
53	2	1241	C	C6-N1-C1'	-5.88	113.74	120.80
53	2	1310	C	C5-C6-N1	5.88	123.94	121.00
53	2	4596	C	N1-C2-O2	5.88	122.43	118.90
53	2	984	C	C2-N1-C1'	5.88	125.27	118.80
53	2	4683	U	N1-C2-O2	5.88	126.92	122.80
53	2	115	C	C6-N1-C2	-5.88	117.95	120.30
53	2	2845	A	C2-N3-C4	5.88	113.54	110.60
53	2	2410	C	N3-C2-O2	-5.87	117.79	121.90
53	2	4712	C	N3-C2-O2	-5.87	117.79	121.90
53	2	4308	C	N3-C2-O2	-5.87	117.79	121.90
53	2	4945	G	N3-C4-N9	5.87	129.52	126.00
53	2	2792	C	C6-N1-C2	-5.87	117.95	120.30
53	2	3650	C	C5-C6-N1	5.86	123.93	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	2	2009	A	N1-C2-N3	-5.86	126.37	129.30
53	2	2081	C	C6-N1-C2	-5.86	117.96	120.30
53	2	654	C	C6-N1-C2	-5.86	117.96	120.30
4	8	135	C	C2-N1-C1'	5.85	125.24	118.80
53	2	289	C	C6-N1-C2	-5.85	117.96	120.30
53	2	4500	U	C2-N1-C1'	5.85	124.72	117.70
53	2	5010	U	N3-C2-O2	-5.85	118.11	122.20
53	2	1378	C	C6-N1-C1'	-5.85	113.78	120.80
53	2	2002	A	C2-N3-C4	5.84	113.52	110.60
53	2	4461	C	C6-N1-C2	-5.84	117.96	120.30
53	2	3926	C	C5-C6-N1	5.84	123.92	121.00
53	2	4885	U	C2-N1-C1'	5.84	124.71	117.70
53	2	365	U	C2-N1-C1'	5.84	124.70	117.70
53	2	1401	C	C6-N1-C2	-5.83	117.97	120.30
53	2	3653	A	N7-C8-N9	5.83	116.72	113.80
53	2	4772	C	C6-N1-C2	-5.83	117.97	120.30
53	2	653	U	N3-C2-O2	-5.83	118.12	122.20
53	2	4266	G	C2-N3-C4	5.83	114.81	111.90
53	2	1816	C	C5-C6-N1	5.83	123.91	121.00
53	2	1879	C	C6-N1-C2	-5.82	117.97	120.30
53	2	436	C	N1-C2-O2	5.82	122.39	118.90
53	2	4752	U	N3-C2-O2	-5.81	118.13	122.20
53	2	1250	C	N3-C2-O2	-5.81	117.83	121.90
53	2	1367	C	N3-C2-O2	-5.81	117.83	121.90
53	2	2814	C	N3-C2-O2	-5.81	117.83	121.90
53	2	3587	C	N3-C2-O2	-5.81	117.83	121.90
53	2	4464	A	C2-N3-C4	5.81	113.50	110.60
53	2	4349	C	C2-N1-C1'	5.80	125.18	118.80
53	2	1993	C	C2-N1-C1'	5.80	125.18	118.80
53	2	3866	C	C5-C6-N1	5.80	123.90	121.00
53	2	4775	C	C5-C6-N1	5.80	123.90	121.00
53	2	4996	C	C5-C6-N1	5.80	123.90	121.00
53	2	657	C	C6-N1-C2	-5.80	117.98	120.30
53	2	2671	C	C6-N1-C2	-5.79	117.98	120.30
53	2	30	C	C2-N1-C1'	5.79	125.17	118.80
53	2	2053	C	C5-C6-N1	5.79	123.90	121.00
53	2	2684	C	C6-N1-C2	-5.79	117.98	120.30
39	w	425	LEU	CB-CG-CD2	5.79	120.84	111.00
53	2	688	U	N3-C2-O2	-5.79	118.15	122.20
51	3	26	C	C6-N1-C2	-5.79	117.98	120.30
53	2	683	C	N1-C2-O2	5.79	122.37	118.90
53	2	985	C	C5-C6-N1	5.79	123.89	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	2	5032	C	C6-N1-C2	-5.79	117.99	120.30
53	2	1315	C	C5-C6-N1	5.78	123.89	121.00
53	2	30	C	C5-C6-N1	5.78	123.89	121.00
53	2	2351	C	C5-C6-N1	5.78	123.89	121.00
53	2	904	C	C6-N1-C2	-5.78	117.99	120.30
53	2	1428	U	N1-C2-O2	5.78	126.84	122.80
53	2	1450	C	C6-N1-C2	-5.78	117.99	120.30
53	2	1592	G	N3-C4-N9	5.78	129.47	126.00
53	2	1894	C	C6-N1-C2	-5.78	117.99	120.30
53	2	2373	C	C6-N1-C2	-5.78	117.99	120.30
53	2	4639	G	N3-C4-C5	-5.77	125.71	128.60
53	2	1592	G	C8-N9-C1'	-5.77	119.50	127.00
53	2	3844	U	N3-C2-O2	-5.77	118.16	122.20
53	2	4231	C	C2-N1-C1'	5.77	125.14	118.80
53	2	3848	U	N1-C2-O2	5.76	126.83	122.80
53	2	4562	C	N3-C2-O2	-5.76	117.86	121.90
53	2	1395	U	N3-C2-O2	-5.76	118.17	122.20
53	2	1731	C	N1-C2-O2	5.76	122.36	118.90
53	2	5004	C	C6-N1-C2	-5.76	118.00	120.30
53	2	1458	C	C6-N1-C2	-5.76	118.00	120.30
51	3	17	C	C6-N1-C2	-5.76	118.00	120.30
53	2	1694	C	C6-N1-C2	-5.76	118.00	120.30
53	2	3739	C	N1-C2-O2	5.76	122.35	118.90
51	3	35	U	N3-C2-O2	-5.75	118.17	122.20
53	2	4983	C	C6-N1-C2	-5.75	118.00	120.30
53	2	4070	U	N1-C2-O2	5.75	126.82	122.80
53	2	4123	C	N1-C2-O2	5.75	122.35	118.90
53	2	5025	C	C6-N1-C2	-5.75	118.00	120.30
53	2	643	C	N1-C2-O2	5.74	122.35	118.90
53	2	4406	U	N1-C2-O2	5.74	126.82	122.80
53	2	4608	G	C5-N7-C8	-5.74	101.43	104.30
53	2	228	C	C6-N1-C2	-5.74	118.00	120.30
53	2	657	C	N3-C2-O2	-5.74	117.88	121.90
53	2	4069	U	N3-C2-O2	-5.74	118.18	122.20
53	2	4341	C	C2-N1-C1'	5.74	125.11	118.80
53	2	4486	C	N1-C2-O2	5.74	122.34	118.90
6	A	116	LEU	CA-CB-CG	5.73	128.49	115.30
53	2	4722	G	C4-N9-C1'	5.73	133.94	126.50
53	2	271	C	C5-C6-N1	5.72	123.86	121.00
53	2	2037	C	C6-N1-C2	-5.72	118.01	120.30
53	2	692	A	N1-C2-N3	-5.72	126.44	129.30
53	2	4991	U	C2-N1-C1'	5.72	124.57	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	2	1085	C	C6-N1-C2	-5.72	118.01	120.30
53	2	1884	C	N1-C2-O2	5.72	122.33	118.90
53	2	1915	C	C2-N1-C1'	5.72	125.09	118.80
53	2	50	C	C5-C6-N1	5.72	123.86	121.00
53	2	1216	C	C6-N1-C2	-5.72	118.01	120.30
53	2	4460	U	N3-C2-O2	-5.72	118.20	122.20
53	2	2689	C	C5-C6-N1	5.71	123.86	121.00
53	2	4608	G	C6-C5-N7	-5.71	126.97	130.40
53	2	2351	C	N3-C2-O2	-5.70	117.91	121.90
53	2	3636	C	C2-N1-C1'	5.70	125.08	118.80
53	2	2018	C	C6-N1-C2	-5.70	118.02	120.30
53	2	2528	G	C2-N3-C4	5.70	114.75	111.90
53	2	2670	C	C5-C6-N1	5.70	123.85	121.00
53	2	2708	U	N1-C2-O2	5.70	126.79	122.80
53	2	2821	U	N1-C2-O2	5.70	126.79	122.80
53	2	30	C	N1-C2-O2	5.70	122.32	118.90
53	2	2053	C	C6-N1-C2	-5.69	118.02	120.30
53	2	1585	C	C6-N1-C2	-5.69	118.02	120.30
53	2	1607	C	C2-N1-C1'	5.69	125.06	118.80
53	2	4263	C	C6-N1-C2	-5.69	118.02	120.30
53	2	3851	U	N1-C2-O2	5.69	126.78	122.80
53	2	2015	U	N3-C2-O2	-5.69	118.22	122.20
53	2	2100	A	C2-N3-C4	5.69	113.44	110.60
53	2	1566	C	C6-N1-C2	-5.68	118.03	120.30
53	2	4682	U	C2-N1-C1'	5.68	124.52	117.70
53	2	713	C	C6-N1-C2	-5.68	118.03	120.30
4	8	55	U	N1-C2-O2	5.68	126.78	122.80
53	2	2843	U	N3-C2-O2	-5.68	118.22	122.20
53	2	2683	C	C6-N1-C2	-5.68	118.03	120.30
53	2	1066	G	C4-N9-C1'	5.67	133.88	126.50
53	2	3878	C	C2-N1-C1'	5.67	125.04	118.80
53	2	658	C	C6-N1-C2	-5.67	118.03	120.30
53	2	1856	C	C6-N1-C2	-5.67	118.03	120.30
53	2	2372	U	N1-C2-O2	5.67	126.77	122.80
51	3	67	C	C5-C6-N1	5.67	123.83	121.00
53	2	1703	C	C2-N1-C1'	5.67	125.03	118.80
21	S	24	LEU	CA-CB-CG	5.66	128.32	115.30
53	2	516	C	C2-N1-C1'	5.66	125.03	118.80
53	2	5008	C	N1-C2-O2	5.66	122.30	118.90
51	3	18	C	C5-C6-N1	5.66	123.83	121.00
53	2	4206	C	C2-N1-C1'	5.66	125.03	118.80
46	4	459	LEU	CA-CB-CG	5.65	128.30	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	2	4772	C	C5-C6-N1	5.65	123.83	121.00
53	2	3670	C	C6-N1-C2	-5.65	118.04	120.30
53	2	4070	U	N3-C2-O2	-5.65	118.25	122.20
53	2	977	C	C5-C6-N1	5.64	123.82	121.00
53	2	1703	C	N3-C2-O2	-5.64	117.95	121.90
53	2	2497	C	N3-C2-O2	-5.64	117.95	121.90
53	2	4442	U	N3-C2-O2	-5.64	118.25	122.20
53	2	2018	C	C5-C6-N1	5.64	123.82	121.00
53	2	1929	A	N3-C4-N9	5.64	131.91	127.40
53	2	4153	C	C6-N1-C2	-5.64	118.05	120.30
53	2	4878	C	N1-C2-O2	5.63	122.28	118.90
53	2	3930	U	N3-C2-O2	-5.63	118.26	122.20
53	2	2250	C	C6-N1-C2	-5.63	118.05	120.30
53	2	2074	C	C6-N1-C2	-5.62	118.05	120.30
53	2	2325	C	N3-C2-O2	-5.62	117.96	121.90
53	2	2616	C	C6-N1-C2	-5.62	118.05	120.30
53	2	3847	C	C6-N1-C2	-5.62	118.05	120.30
53	2	4069	U	N1-C2-O2	5.62	126.73	122.80
53	2	1720	C	N3-C2-O2	-5.62	117.97	121.90
53	2	297	U	N3-C2-O2	-5.62	118.27	122.20
53	2	2505	C	C5-C6-N1	5.62	123.81	121.00
53	2	4747	C	C5-C6-N1	5.62	123.81	121.00
53	2	2014	C	C6-N1-C2	-5.61	118.06	120.30
53	2	4709	U	C5-C6-N1	5.61	125.51	122.70
53	2	489	C	C2-N1-C1'	5.61	124.97	118.80
53	2	2595	C	C6-N1-C2	-5.61	118.06	120.30
53	2	4502	C	N3-C2-O2	-5.61	117.97	121.90
46	4	12	VAL	CA-CB-CG1	5.61	119.31	110.90
53	2	1315	C	N1-C2-O2	5.61	122.27	118.90
53	2	3851	U	N3-C2-O2	-5.61	118.27	122.20
53	2	4361	U	N1-C2-O2	5.61	126.72	122.80
51	3	6	C	C6-N1-C2	-5.61	118.06	120.30
53	2	2625	U	N3-C2-O2	-5.61	118.28	122.20
33	m	102	LEU	CA-CB-CG	5.60	128.19	115.30
51	3	57	C	C6-N1-C2	-5.60	118.06	120.30
53	2	972	C	C2-N1-C1'	5.60	124.96	118.80
53	2	2303	C	N1-C2-O2	5.60	122.26	118.90
53	2	1592	G	N3-C4-C5	-5.60	125.80	128.60
53	2	4752	U	N1-C2-O2	5.60	126.72	122.80
53	2	2367	A	N1-C2-N3	-5.60	126.50	129.30
53	2	350	C	C6-N1-C2	-5.59	118.06	120.30
53	2	3901	A	C2-N3-C4	5.59	113.40	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	8	99	U	N3-C2-O2	-5.59	118.28	122.20
53	2	4402	C	N3-C2-O2	-5.59	117.99	121.90
53	2	2371	U	N3-C2-O2	-5.58	118.29	122.20
53	2	2867	C	C5-C6-N1	5.58	123.79	121.00
53	2	4878	C	C6-N1-C2	-5.58	118.07	120.30
53	2	1929	A	C8-N9-C1'	-5.58	117.65	127.70
53	2	2019	C	C2-N1-C1'	5.58	124.94	118.80
53	2	4469	U	N1-C2-O2	5.58	126.71	122.80
53	2	141	C	N1-C2-O2	5.58	122.25	118.90
53	2	673	C	N1-C2-O2	5.58	122.25	118.90
53	2	1332	C	C6-N1-C2	-5.58	118.07	120.30
53	2	2281	U	C2-N1-C1'	5.58	124.39	117.70
53	2	4358	U	N3-C2-O2	-5.58	118.30	122.20
53	2	260	C	N1-C2-O2	5.57	122.24	118.90
53	2	1994	C	O4'-C1'-N1	5.57	112.65	108.20
53	2	4207	C	C5-C6-N1	5.57	123.78	121.00
40	y	62	LEU	CA-CB-CG	5.57	128.10	115.30
53	2	4506	C	N1-C2-O2	5.57	122.24	118.90
53	2	390	C	C2-N1-C1'	5.56	124.92	118.80
53	2	486	C	OP1-P-OP2	-5.56	111.26	119.60
53	2	661	C	N1-C2-O2	5.56	122.24	118.90
53	2	1577	G	N3-C2-N2	-5.56	116.01	119.90
53	2	4895	C	C2-N1-C1'	5.56	124.92	118.80
53	2	2571	C	C6-N1-C2	-5.56	118.08	120.30
53	2	3939	G	N3-C4-N9	5.56	129.34	126.00
53	2	4701	A	N1-C2-N3	-5.55	126.52	129.30
4	8	54	C	C5-C6-N1	5.55	123.78	121.00
53	2	4601	U	C2-N1-C1'	5.55	124.36	117.70
53	2	988	C	C5-C6-N1	5.55	123.77	121.00
53	2	3858	C	N1-C2-O2	5.55	122.23	118.90
53	2	4895	C	N3-C2-O2	-5.55	118.02	121.90
53	2	2290	C	C2-N1-C1'	5.55	124.90	118.80
53	2	2729	C	C6-N1-C2	-5.54	118.08	120.30
53	2	4970	C	C6-N1-C2	-5.54	118.08	120.30
53	2	1620	U	N3-C2-O2	-5.54	118.32	122.20
53	2	2556	G	N3-C4-N9	5.54	129.33	126.00
53	2	3696	C	N1-C2-O2	5.54	122.23	118.90
53	2	4068	U	N3-C2-O2	-5.54	118.32	122.20
53	2	683	C	C6-N1-C2	-5.54	118.08	120.30
53	2	1655	C	C5-C6-N1	5.54	123.77	121.00
53	2	1889	U	C2-N1-C1'	5.54	124.35	117.70
53	2	1731	C	C2-N1-C1'	5.54	124.89	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	2	4442	U	N1-C2-O2	5.54	126.68	122.80
53	2	67	C	C6-N1-C2	-5.54	118.08	120.30
53	2	1096	C	C5-C6-N1	5.54	123.77	121.00
53	2	4506	C	C6-N1-C2	-5.54	118.08	120.30
53	2	385	A	N1-C2-N3	-5.54	126.53	129.30
53	2	1074	G	N3-C4-N9	5.54	129.32	126.00
53	2	1572	U	N1-C2-O2	5.53	126.67	122.80
53	2	2508	U	N3-C2-O2	-5.53	118.33	122.20
53	2	4413	C	C6-N1-C2	-5.53	118.09	120.30
51	3	71	G	P-O3'-C3'	5.53	126.34	119.70
53	2	469	C	C5-C6-N1	5.53	123.77	121.00
53	2	2563	C	C6-N1-C2	-5.53	118.09	120.30
53	2	1467	C	C2-N1-C1'	5.53	124.89	118.80
53	2	3623	C	C6-N1-C2	-5.53	118.09	120.30
53	2	2632	U	N1-C2-O2	5.53	126.67	122.80
53	2	3905	A	OP2-P-O3'	5.53	117.36	105.20
53	2	4453	C	N3-C2-O2	-5.53	118.03	121.90
53	2	221	C	C6-N1-C2	-5.53	118.09	120.30
53	2	1847	C	C6-N1-C2	-5.53	118.09	120.30
53	2	1901	C	C6-N1-C2	-5.52	118.09	120.30
53	2	2107	C	C5-C6-N1	5.52	123.76	121.00
4	8	111	U	N1-C2-O2	5.52	126.66	122.80
53	2	1633	G	P-O3'-C3'	5.52	126.32	119.70
46	4	503	THR	C-N-CA	5.51	135.49	121.70
53	2	4594	U	N3-C2-O2	-5.51	118.34	122.20
53	2	1938	C	N1-C2-O2	5.51	122.21	118.90
53	2	1812	C	C2-N1-C1'	5.51	124.86	118.80
53	2	4703	U	N1-C2-O2	5.51	126.66	122.80
53	2	180	C	C6-N1-C2	-5.51	118.10	120.30
53	2	2403	A	N1-C2-N3	-5.51	126.55	129.30
53	2	3587	C	C5-C6-N1	5.51	123.75	121.00
53	2	1725	U	N3-C2-O2	-5.50	118.35	122.20
53	2	1812	C	N1-C2-O2	5.50	122.20	118.90
53	2	4619	U	N3-C2-O2	-5.50	118.35	122.20
53	2	27	C	C6-N1-C2	-5.50	118.10	120.30
53	2	2101	C	C6-N1-C2	-5.50	118.10	120.30
53	2	2002	A	N1-C6-N6	-5.50	115.30	118.60
53	2	4162	C	N3-C2-O2	-5.50	118.05	121.90
53	2	1957	U	N1-C2-O2	5.49	126.64	122.80
53	2	2072	C	N1-C2-O2	5.49	122.19	118.90
53	2	657	C	C2-N1-C1'	5.48	124.83	118.80
53	2	2844	A	N1-C2-N3	-5.48	126.56	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	2	673	C	C5-C6-N1	5.48	123.74	121.00
53	2	2603	C	C5-C6-N1	5.48	123.74	121.00
53	2	1540	C	C6-N1-C2	-5.48	118.11	120.30
53	2	1251	C	N3-C2-O2	-5.47	118.07	121.90
53	2	1807	C	C6-N1-C2	-5.47	118.11	120.30
53	2	3858	C	N3-C2-O2	-5.47	118.07	121.90
53	2	274	C	N1-C2-O2	5.47	122.18	118.90
53	2	3840	U	N3-C2-O2	-5.47	118.37	122.20
4	8	80	A	C2-N3-C4	5.47	113.33	110.60
53	2	914	U	C5-C4-O4	-5.47	122.62	125.90
53	2	1468	C	N1-C2-O2	5.47	122.18	118.90
4	8	128	C	C6-N1-C2	-5.47	118.11	120.30
53	2	196	C	C6-N1-C2	-5.46	118.11	120.30
53	2	274	C	C6-N1-C2	-5.46	118.11	120.30
53	2	3700	C	C6-N1-C2	-5.46	118.11	120.30
53	2	1963	C	N1-C2-O2	5.46	122.18	118.90
53	2	1971	C	N3-C2-O2	-5.46	118.08	121.90
53	2	2498	C	C5-C6-N1	5.46	123.73	121.00
51	3	49	A	N1-C2-N3	-5.46	126.57	129.30
53	2	1308	C	C6-N1-C2	-5.46	118.12	120.30
53	2	3882	C	C5-C6-N1	5.46	123.73	121.00
26	a	38	ARG	C-N-CA	5.45	135.33	121.70
46	4	406	GLY	C-N-CA	5.45	135.34	121.70
53	2	489	C	C5-C6-N1	5.45	123.73	121.00
53	2	905	C	C5-C6-N1	5.45	123.73	121.00
44	W	266	ASP	C-N-CA	5.45	135.32	121.70
53	2	2853	C	N1-C2-O2	5.45	122.17	118.90
53	2	4387	C	C5-C6-N1	5.45	123.72	121.00
53	2	467	U	C6-N1-C2	-5.45	117.73	121.00
53	2	688	U	N1-C2-O2	5.45	126.61	122.80
53	2	4294	C	N1-C2-O2	5.45	122.17	118.90
53	2	2727	C	C5-C6-N1	5.45	123.72	121.00
51	3	81	G	C6-C5-N7	-5.44	127.13	130.40
53	2	2850	A	C4-N9-C1'	5.44	136.10	126.30
53	2	4360	U	C6-N1-C2	-5.44	117.74	121.00
44	W	374	LEU	CA-CB-CG	5.44	127.81	115.30
53	2	195	C	C2-N1-C1'	5.44	124.78	118.80
53	2	1683	U	N1-C2-O2	5.44	126.61	122.80
53	2	4229	U	C2-N1-C1'	5.44	124.22	117.70
4	8	51	U	N1-C2-O2	5.43	126.60	122.80
53	2	124	C	C6-N1-C2	-5.43	118.13	120.30
53	2	2670	C	C2-N1-C1'	5.43	124.78	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	2	2264	C	N1-C2-O2	5.43	122.16	118.90
51	3	2	U	N3-C2-O2	-5.42	118.40	122.20
53	2	4294	C	C5-C6-N1	5.42	123.71	121.00
53	2	712	C	C6-N1-C2	-5.42	118.13	120.30
53	2	3668	C	C6-N1-C2	-5.42	118.13	120.30
13	I	111	LEU	CA-CB-CG	5.42	127.77	115.30
53	2	4155	C	N1-C2-O2	5.42	122.15	118.90
53	2	4689	U	C5-C6-N1	5.42	125.41	122.70
53	2	4453	C	C6-N1-C1'	-5.42	114.30	120.80
53	2	4639	G	C4-N9-C1'	5.42	133.54	126.50
53	2	4639	G	N3-C4-N9	5.42	129.25	126.00
53	2	368	C	C6-N1-C2	-5.42	118.13	120.30
53	2	691	C	C5-C6-N1	5.42	123.71	121.00
53	2	1294	A	O4'-C1'-N9	5.42	112.53	108.20
53	2	3931	C	C6-N1-C2	-5.42	118.13	120.30
53	2	2820	C	C5-C6-N1	5.41	123.71	121.00
51	3	26	C	N1-C2-O2	5.41	122.15	118.90
4	8	111	U	N3-C2-O2	-5.41	118.41	122.20
53	2	4068	U	N1-C2-O2	5.41	126.59	122.80
51	3	104	C	N1-C2-O2	5.41	122.14	118.90
53	2	4864	U	C6-N1-C2	-5.41	117.76	121.00
53	2	1678	C	OP2-P-O3'	5.40	117.09	105.20
53	2	1875	C	N3-C2-O2	-5.40	118.12	121.90
53	2	2593	C	N1-C2-O2	5.40	122.14	118.90
51	3	2	U	N1-C2-O2	5.40	126.58	122.80
53	2	297	U	N1-C2-O2	5.40	126.58	122.80
53	2	1344	C	N1-C2-O2	5.40	122.14	118.90
53	2	2508	U	N1-C2-O2	5.40	126.58	122.80
53	2	1847	C	C5-C6-N1	5.40	123.70	121.00
53	2	1350	C	C6-N1-C2	-5.40	118.14	120.30
53	2	1494	U	C6-N1-C2	-5.40	117.76	121.00
53	2	2603	C	C6-N1-C2	-5.39	118.14	120.30
53	2	2670	C	N1-C2-O2	5.39	122.14	118.90
53	2	2856	C	C2-N1-C1'	5.39	124.73	118.80
53	2	1323	A	N1-C2-N3	-5.39	126.60	129.30
53	2	2817	C	C6-N1-C2	-5.39	118.14	120.30
46	4	403	LEU	CA-CB-CG	5.39	127.69	115.30
53	2	112	C	N3-C2-O2	-5.39	118.13	121.90
53	2	5002	U	C2-N1-C1'	5.39	124.16	117.70
53	2	1430	C	C6-N1-C2	-5.38	118.15	120.30
51	3	35	U	N1-C2-O2	5.38	126.57	122.80
53	2	974	C	N1-C2-O2	5.38	122.13	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	2	1679	A	N1-C2-N3	-5.38	126.61	129.30
53	2	1679	A	C2-N3-C4	5.38	113.29	110.60
53	2	1991	A	N1-C2-N3	-5.38	126.61	129.30
35	o	106	VAL	CG1-CB-CG2	-5.38	102.30	110.90
4	8	107	C	C6-N1-C2	-5.38	118.15	120.30
53	2	2036	C	C6-N1-C2	-5.37	118.15	120.30
53	2	4229	U	N1-C2-O2	5.37	126.56	122.80
53	2	1720	C	C5-C6-N1	5.37	123.69	121.00
53	2	2264	C	C6-N1-C2	-5.37	118.15	120.30
53	2	653	U	N1-C2-O2	5.37	126.56	122.80
53	2	4710	C	C2-N1-C1'	5.37	124.70	118.80
53	2	1203	G	C2-N3-C4	5.37	114.58	111.90
53	2	2015	U	N1-C2-O2	5.37	126.56	122.80
53	2	4687	A	C2-N3-C4	5.37	113.28	110.60
53	2	436	C	C6-N1-C2	-5.37	118.15	120.30
53	2	1191	C	C6-N1-C2	-5.37	118.15	120.30
53	2	3692	A	C2-N3-C4	5.37	113.28	110.60
51	3	36	C	N1-C2-O2	5.36	122.12	118.90
53	2	26	C	C5-C6-N1	5.36	123.68	121.00
53	2	274	C	C2-N1-C1'	5.36	124.70	118.80
53	2	1458	C	C2-N1-C1'	5.36	124.70	118.80
53	2	2727	C	C6-N1-C2	-5.36	118.16	120.30
44	W	298	ASP	CB-CG-OD1	5.36	123.12	118.30
53	2	2505	C	N3-C2-O2	-5.36	118.15	121.90
53	2	3587	C	C2-N1-C1'	5.36	124.69	118.80
53	2	3912	U	N3-C2-O2	-5.36	118.45	122.20
53	2	472	C	N3-C2-O2	-5.35	118.15	121.90
53	2	4341	C	N3-C2-O2	-5.35	118.15	121.90
53	2	4699	U	OP1-P-O3'	5.35	116.98	105.20
53	2	408	A	N1-C2-N3	-5.35	126.62	129.30
53	2	1567	U	N3-C2-O2	-5.35	118.45	122.20
53	2	2617	G	C4-N9-C1'	5.35	133.46	126.50
53	2	4440	G	N3-C4-N9	5.35	129.21	126.00
46	4	520	LEU	CA-CB-CG	5.35	127.60	115.30
53	2	3835	C	C6-N1-C2	-5.35	118.16	120.30
53	2	719	C	C5-C6-N1	5.34	123.67	121.00
4	8	135	C	N1-C2-O2	5.34	122.11	118.90
53	2	3766	A	C2-N3-C4	5.34	113.27	110.60
53	2	4508	C	N3-C2-O2	-5.34	118.16	121.90
53	2	4891	G	N3-C4-N9	5.34	129.21	126.00
53	2	2683	C	C5-C6-N1	5.34	123.67	121.00
51	3	68	C	C6-N1-C2	-5.34	118.16	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	2	1315	C	C2-N1-C1'	5.34	124.67	118.80
53	2	4773	C	N1-C2-O2	5.34	122.10	118.90
53	2	3767	C	C6-N1-C2	-5.34	118.17	120.30
46	4	41	HIS	C-N-CA	5.34	135.04	121.70
51	3	103	A	C2-N3-C4	5.34	113.27	110.60
53	2	4859	C	C6-N1-C2	-5.34	118.17	120.30
53	2	4902	C	C6-N1-C2	-5.34	118.17	120.30
53	2	1478	C	C6-N1-C2	-5.33	118.17	120.30
53	2	1632	A	N1-C2-N3	-5.33	126.63	129.30
53	2	3598	C	N3-C2-O2	-5.33	118.17	121.90
53	2	2325	C	N1-C2-O2	5.33	122.10	118.90
53	2	3910	C	C6-N1-C2	-5.33	118.17	120.30
53	2	4308	C	C5-C6-N1	5.33	123.67	121.00
53	2	5007	A	N1-C2-N3	-5.33	126.63	129.30
53	2	1832	C	N3-C2-O2	-5.33	118.17	121.90
53	2	1848	C	C6-N1-C2	-5.33	118.17	120.30
53	2	332	C	N1-C2-O2	5.33	122.10	118.90
53	2	4710	C	C5-C6-N1	5.33	123.66	121.00
51	3	44	C	C6-N1-C2	-5.33	118.17	120.30
53	2	467	U	C6-N1-C1'	-5.33	113.74	121.20
53	2	1081	C	N1-C2-O2	5.32	122.09	118.90
53	2	2011	C	C5-C6-N1	5.32	123.66	121.00
4	8	32	C	N3-C2-O2	-5.32	118.17	121.90
53	2	262	G	N1-C6-O6	-5.32	116.71	119.90
53	2	672	C	C2-N1-C1'	5.32	124.65	118.80
53	2	1267	C	N3-C2-O2	-5.32	118.18	121.90
53	2	2704	C	N1-C2-O2	5.32	122.09	118.90
51	3	96	U	N3-C2-O2	-5.32	118.48	122.20
53	2	417	G	O4'-C1'-N9	5.32	112.45	108.20
53	2	1442	C	C5-C6-N1	5.32	123.66	121.00
53	2	1906	U	N3-C2-O2	-5.32	118.48	122.20
53	2	4758	U	O4'-C1'-N1	5.32	112.45	108.20
53	2	2081	C	C5-C6-N1	5.32	123.66	121.00
53	2	2445	C	N1-C2-O2	5.32	122.09	118.90
53	2	2667	C	C5-C6-N1	5.32	123.66	121.00
53	2	4891	G	N3-C4-C5	-5.32	125.94	128.60
53	2	948	C	C6-N1-C2	-5.31	118.17	120.30
53	2	1732	C	C5-C6-N1	5.31	123.66	121.00
53	2	5048	A	N1-C2-N3	-5.31	126.64	129.30
53	2	2019	C	C5-C6-N1	5.31	123.65	121.00
46	4	21	LEU	CA-CB-CG	5.31	127.50	115.30
53	2	2281	U	C5-C6-N1	5.31	125.35	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	R	103	LEU	CA-CB-CG	5.30	127.50	115.30
51	3	78	C	C6-N1-C1'	-5.30	114.44	120.80
53	2	914	U	OP2-P-O3'	5.30	116.87	105.20
53	2	367	C	C6-N1-C2	-5.30	118.18	120.30
53	2	3668	C	N1-C2-O2	5.30	122.08	118.90
53	2	4120	U	N1-C2-O2	5.30	126.51	122.80
53	2	1588	U	N3-C2-O2	-5.30	118.49	122.20
53	2	3915	U	C2-N1-C1'	5.30	124.06	117.70
53	2	436	C	N3-C2-O2	-5.30	118.19	121.90
53	2	4206	C	C5-C6-N1	5.30	123.65	121.00
53	2	4612	C	N3-C2-O2	-5.30	118.19	121.90
53	2	4940	C	N1-C2-O2	5.30	122.08	118.90
53	2	4981	G	C4-N9-C1'	5.30	133.39	126.50
53	2	1066	G	C8-N9-C1'	-5.29	120.12	127.00
53	2	2078	C	C6-N1-C2	-5.29	118.18	120.30
43	R	235	MET	CA-CB-CG	5.29	122.30	113.30
53	2	3720	G	C4-N9-C1'	5.29	133.38	126.50
53	2	4662	C	N3-C2-O2	-5.29	118.20	121.90
4	8	96	C	C6-N1-C2	-5.29	118.19	120.30
53	2	296	A	N1-C2-N3	-5.29	126.66	129.30
53	2	984	C	C5-C6-N1	5.29	123.64	121.00
53	2	4313	A	N1-C2-N3	-5.29	126.66	129.30
53	2	4700	A	C2-N3-C4	5.29	113.24	110.60
53	2	4923	C	C6-N1-C2	-5.29	118.19	120.30
53	2	467	U	C5-C6-N1	5.29	125.34	122.70
53	2	4758	U	C5-C6-N1	5.29	125.34	122.70
53	2	100	C	C5-C6-N1	5.28	123.64	121.00
53	2	1599	A	C2-N3-C4	5.28	113.24	110.60
53	2	2533	C	C6-N1-C2	-5.28	118.19	120.30
53	2	3706	C	C6-N1-C2	-5.28	118.19	120.30
53	2	1294	A	C2-N3-C4	5.28	113.24	110.60
53	2	2094	G	C8-N9-C1'	-5.28	120.14	127.00
53	2	1467	C	N1-C2-O2	5.27	122.06	118.90
53	2	4730	C	C6-N1-C2	-5.27	118.19	120.30
53	2	4945	G	C4-N9-C1'	5.27	133.36	126.50
43	R	109	LEU	CA-CB-CG	5.27	127.43	115.30
53	2	703	G	C4-N9-C1'	5.27	133.35	126.50
53	2	1448	G	C4-N9-C1'	5.27	133.35	126.50
51	3	95	C	O4'-C1'-N1	5.27	112.42	108.20
53	2	1661	C	C6-N1-C2	-5.27	118.19	120.30
53	2	2019	C	N3-C2-O2	-5.27	118.21	121.90
53	2	2704	C	C5-C6-N1	5.27	123.64	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	2	928	C	C6-N1-C2	-5.27	118.19	120.30
53	2	1664	U	N3-C2-O2	-5.27	118.51	122.20
53	2	4317	A	C2-N3-C4	5.27	113.23	110.60
53	2	4436	U	C2-N1-C1'	5.27	124.02	117.70
53	2	1682	A	N1-C2-N3	-5.27	126.67	129.30
53	2	4231	C	N3-C2-O2	-5.27	118.21	121.90
53	2	1468	C	C6-N1-C2	-5.26	118.19	120.30
53	2	1666	C	C5-C6-N1	5.26	123.63	121.00
53	2	1848	C	C5-C6-N1	5.26	123.63	121.00
53	2	2325	C	C6-N1-C2	-5.26	118.19	120.30
53	2	4466	C	C6-N1-C2	-5.26	118.19	120.30
4	8	99	U	N1-C2-O2	5.26	126.48	122.80
53	2	1074	G	C4-N9-C1'	5.26	133.34	126.50
53	2	691	C	C6-N1-C2	-5.26	118.20	120.30
53	2	1893	C	N1-C2-O2	5.26	122.06	118.90
53	2	2853	C	C6-N1-C2	-5.26	118.20	120.30
53	2	2006	U	N3-C2-O2	-5.26	118.52	122.20
53	2	1947	U	N1-C2-O2	5.25	126.48	122.80
53	2	1924	C	C6-N1-C2	-5.25	118.20	120.30
53	2	2002	A	N1-C2-N3	-5.25	126.67	129.30
53	2	56	A	N1-C2-N3	-5.25	126.68	129.30
53	2	1726	U	C2-N1-C1'	5.25	124.00	117.70
53	2	3844	U	N1-C2-O2	5.25	126.47	122.80
53	2	4417	C	C5-C6-N1	5.25	123.62	121.00
53	2	2482	C	C6-N1-C2	-5.25	118.20	120.30
53	2	4387	C	N3-C2-O2	-5.25	118.23	121.90
53	2	4562	C	C6-N1-C2	-5.25	118.20	120.30
53	2	1809	C	C6-N1-C2	-5.24	118.20	120.30
51	3	17	C	N3-C2-O2	-5.24	118.23	121.90
53	2	1931	C	C5-C6-N1	5.24	123.62	121.00
53	2	2892	C	C6-N1-C2	-5.24	118.20	120.30
53	2	3930	U	N1-C2-O2	5.24	126.47	122.80
53	2	4588	U	N3-C2-O2	-5.24	118.53	122.20
53	2	4685	U	N3-C2-O2	-5.24	118.53	122.20
53	2	4426	C	C5-C6-N1	5.23	123.62	121.00
53	2	1634	A	N1-C2-N3	-5.23	126.69	129.30
53	2	2032	U	N3-C2-O2	-5.23	118.54	122.20
53	2	2078	C	C2-N1-C1'	5.23	124.55	118.80
53	2	110	C	C6-N1-C2	-5.22	118.21	120.30
53	2	966	A	C2-N3-C4	5.22	113.21	110.60
53	2	1607	C	C5-C6-N1	5.22	123.61	121.00
53	2	4349	C	N3-C2-O2	-5.22	118.24	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	2	221	C	C5-C6-N1	5.22	123.61	121.00
53	2	972	C	C5-C6-N1	5.22	123.61	121.00
53	2	4385	A	N1-C2-N3	-5.22	126.69	129.30
53	2	195	C	N1-C2-O2	5.22	122.03	118.90
53	2	2684	C	C5-C6-N1	5.22	123.61	121.00
53	2	3607	U	N3-C2-O2	-5.22	118.55	122.20
53	2	4662	C	N1-C2-O2	5.22	122.03	118.90
53	2	158	A	N1-C2-N3	-5.21	126.69	129.30
53	2	1572	U	N3-C2-O2	-5.21	118.55	122.20
53	2	2302	C	C6-N1-C2	-5.21	118.22	120.30
51	3	18	C	C6-N1-C2	-5.21	118.22	120.30
53	2	485	C	C6-N1-C2	-5.21	118.22	120.30
53	2	1628	C	C6-N1-C2	-5.21	118.22	120.30
53	2	1602	U	N3-C2-O2	-5.21	118.55	122.20
53	2	2303	C	N3-C2-O2	-5.21	118.25	121.90
53	2	259	C	N3-C2-O2	-5.21	118.25	121.90
53	2	4345	C	N1-C2-O2	5.21	122.03	118.90
53	2	26	C	N3-C2-O2	-5.21	118.25	121.90
53	2	115	C	C5-C6-N1	5.21	123.60	121.00
53	2	1963	C	N3-C2-O2	-5.21	118.26	121.90
53	2	2392	C	C6-N1-C2	-5.20	118.22	120.30
53	2	4522	G	N7-C8-N9	5.20	115.70	113.10
53	2	474	C	C6-N1-C2	-5.20	118.22	120.30
53	2	4891	G	C4-N9-C1'	5.20	133.25	126.50
53	2	2073	C	C6-N1-C2	-5.19	118.22	120.30
53	2	174	C	N1-C2-O2	5.19	122.02	118.90
53	2	1662	C	C6-N1-C2	-5.19	118.22	120.30
53	2	1858	A	N1-C2-N3	-5.19	126.70	129.30
51	3	55	A	N1-C2-N3	-5.19	126.70	129.30
44	W	448	LEU	CA-CB-CG	5.19	127.23	115.30
53	2	2499	C	C6-N1-C1'	-5.19	114.57	120.80
53	2	709	C	C6-N1-C2	-5.19	118.23	120.30
53	2	1418	C	C6-N1-C2	-5.19	118.23	120.30
53	2	178	C	N3-C2-O2	-5.18	118.27	121.90
53	2	260	C	C2-N1-C1'	5.18	124.50	118.80
53	2	294	G	N3-C4-N9	5.18	129.11	126.00
53	2	3749	C	C6-N1-C2	-5.18	118.23	120.30
4	8	101	C	C2-N1-C1'	5.18	124.50	118.80
53	2	5050	C	C2-N1-C1'	5.18	124.50	118.80
44	W	157	HIS	CB-CA-C	5.18	120.76	110.40
53	2	130	C	C6-N1-C2	-5.18	118.23	120.30
53	2	4319	C	C5-C6-N1	5.18	123.59	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	2	4628	U	N3-C2-O2	-5.18	118.58	122.20
53	2	1081	C	C5-C6-N1	5.18	123.59	121.00
53	2	2274	C	C6-N1-C2	-5.18	118.23	120.30
53	2	89	C	C6-N1-C2	-5.17	118.23	120.30
53	2	2290	C	N1-C2-O2	5.17	122.00	118.90
53	2	1267	C	N1-C2-O2	5.17	122.00	118.90
53	2	4088	C	C6-N1-C2	-5.17	118.23	120.30
53	2	1520	C	C6-N1-C2	-5.17	118.23	120.30
53	2	1566	C	N1-C2-O2	5.17	122.00	118.90
53	2	2835	A	N1-C2-N3	-5.17	126.72	129.30
53	2	750	U	N1-C2-O2	5.17	126.42	122.80
53	2	2729	C	C2-N1-C1'	5.16	124.48	118.80
53	2	1503	A	N1-C2-N3	-5.16	126.72	129.30
53	2	1494	U	C5-C6-N1	5.16	125.28	122.70
53	2	238	C	C6-N1-C2	-5.15	118.24	120.30
53	2	2533	C	N1-C2-O2	5.15	121.99	118.90
53	2	440	U	N1-C2-O2	5.15	126.41	122.80
53	2	4977	A	N1-C2-N3	-5.15	126.72	129.30
53	2	1442	C	N1-C2-O2	5.15	121.99	118.90
53	2	2708	U	N3-C2-O2	-5.15	118.59	122.20
53	2	1702	C	C6-N1-C1'	-5.15	114.62	120.80
53	2	2667	C	C2-N1-C1'	5.15	124.46	118.80
53	2	4774	C	N1-C2-O2	5.15	121.99	118.90
53	2	4975	G	O4'-C1'-N9	5.15	112.32	108.20
53	2	1508	A	N1-C2-N3	-5.14	126.73	129.30
53	2	1994	C	C5-C6-N1	5.14	123.57	121.00
53	2	4535	A	N1-C2-N3	-5.14	126.73	129.30
53	2	4923	C	N3-C2-O2	-5.14	118.30	121.90
53	2	2892	C	C5-C6-N1	5.14	123.57	121.00
53	2	3599	A	N1-C2-N3	-5.14	126.73	129.30
53	2	4072	C	C6-N1-C2	-5.14	118.24	120.30
53	2	4120	U	C2-N1-C1'	5.14	123.87	117.70
53	2	4628	U	N1-C2-O2	5.14	126.40	122.80
53	2	47	A	N1-C2-N3	-5.14	126.73	129.30
53	2	1993	C	C5-C6-N1	5.14	123.57	121.00
53	2	1940	G	O4'-C1'-N9	5.14	112.31	108.20
53	2	148	C	C6-N1-C2	-5.14	118.25	120.30
53	2	1577	G	C2-N3-C4	5.14	114.47	111.90
53	2	4687	A	N1-C2-N3	-5.14	126.73	129.30
53	2	4878	C	C5-C6-N1	5.14	123.57	121.00
53	2	5030	U	C6-N1-C2	-5.14	117.92	121.00
4	8	81	C	C6-N1-C2	-5.13	118.25	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	W	288	HIS	CB-CA-C	5.13	120.67	110.40
53	2	162	A	N1-C2-N3	-5.13	126.73	129.30
53	2	4996	C	C2-N1-C1'	5.13	124.45	118.80
39	w	304	LEU	CA-CB-CG	5.13	127.11	115.30
53	2	956	A	N1-C2-N3	-5.13	126.73	129.30
53	2	360	A	N1-C2-N3	-5.13	126.73	129.30
53	2	1523	A	N1-C2-N3	-5.13	126.73	129.30
53	2	4607	A	O4'-C1'-N9	5.13	112.31	108.20
45	T	113	ASP	CB-CG-OD1	5.13	122.92	118.30
53	2	1371	A	N1-C2-N3	-5.13	126.73	129.30
53	2	1879	C	C5-C6-N1	5.13	123.56	121.00
53	2	910	G	C4-N9-C1'	5.13	133.16	126.50
53	2	2262	G	N7-C8-N9	5.13	115.66	113.10
53	2	4093	G	C4-N9-C1'	5.13	133.16	126.50
53	2	2029	A	N1-C2-N3	-5.12	126.74	129.30
53	2	4883	C	C6-N1-C2	-5.12	118.25	120.30
53	2	5004	C	C5-C6-N1	5.12	123.56	121.00
53	2	2410	C	C6-N1-C1'	-5.12	114.66	120.80
53	2	4636	U	C2-N1-C1'	5.12	123.85	117.70
53	2	4711	C	C5-C6-N1	5.12	123.56	121.00
53	2	1373	A	N1-C2-N3	-5.12	126.74	129.30
53	2	4886	C	N1-C2-O2	5.12	121.97	118.90
53	2	4527	G	O4'-C1'-N9	5.12	112.29	108.20
53	2	4165	C	C6-N1-C2	-5.12	118.25	120.30
53	2	2317	C	C6-N1-C2	-5.11	118.25	120.30
53	2	5019	A	N1-C2-N3	-5.11	126.74	129.30
53	2	2307	A	N1-C2-N3	-5.11	126.74	129.30
53	2	4984	C	C6-N1-C2	-5.11	118.25	120.30
51	3	92	C	N1-C2-O2	5.11	121.96	118.90
53	2	163	A	N1-C2-N3	-5.11	126.75	129.30
53	2	1637	A	N1-C2-N3	-5.11	126.75	129.30
53	2	2384	U	N3-C2-O2	-5.11	118.62	122.20
53	2	5042	A	N1-C2-N3	-5.11	126.75	129.30
53	2	1795	A	N1-C2-N3	-5.11	126.75	129.30
53	2	2373	C	C5-C6-N1	5.11	123.55	121.00
53	2	5032	C	C5-C6-N1	5.11	123.55	121.00
53	2	474	C	C5-C6-N1	5.10	123.55	121.00
53	2	406	C	P-O3'-C3'	5.10	125.82	119.70
53	2	975	C	C6-N1-C2	-5.10	118.26	120.30
53	2	4130	C	C6-N1-C2	-5.10	118.26	120.30
53	2	5042	A	C2-N3-C4	5.10	113.15	110.60
53	2	271	C	C6-N1-C2	-5.10	118.26	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	2	1913	C	C6-N1-C2	-5.10	118.26	120.30
53	2	2094	G	N3-C4-N9	5.10	129.06	126.00
24	X	79	VAL	CG1-CB-CG2	-5.10	102.75	110.90
53	2	77	U	C2-N1-C1'	5.10	123.82	117.70
53	2	2304	U	C2-N1-C1'	5.10	123.82	117.70
53	2	2882	A	N1-C2-N3	-5.10	126.75	129.30
53	2	4962	C	C6-N1-C2	-5.10	118.26	120.30
53	2	2803	U	N1-C2-O2	5.09	126.37	122.80
53	2	3939	G	C4-N9-C1'	5.09	133.12	126.50
53	2	3893	C	C6-N1-C2	-5.09	118.26	120.30
53	2	2572	C	C6-N1-C2	-5.09	118.26	120.30
53	2	4471	U	C6-N1-C2	-5.09	117.94	121.00
53	2	1449	C	C6-N1-C2	-5.09	118.26	120.30
53	2	1729	A	N1-C2-N3	-5.09	126.75	129.30
53	2	7	C	C5-C6-N1	5.09	123.54	121.00
53	2	486	C	O5'-P-OP1	5.09	116.81	110.70
53	2	4120	U	N3-C2-O2	-5.09	118.64	122.20
53	2	4684	A	N1-C2-N3	-5.09	126.76	129.30
53	2	155	C	C6-N1-C2	-5.09	118.27	120.30
53	2	657	C	C5-C6-N1	5.09	123.54	121.00
53	2	1929	A	N1-C2-N3	-5.09	126.76	129.30
53	2	2570	U	N3-C2-O2	-5.08	118.64	122.20
53	2	2779	C	C6-N1-C2	-5.08	118.27	120.30
53	2	4766	C	N3-C2-O2	-5.08	118.34	121.90
53	2	712	C	C5-C6-N1	5.08	123.54	121.00
53	2	2262	G	C8-N9-C4	-5.08	104.37	106.40
53	2	4667	C	C6-N1-C2	-5.08	118.27	120.30
51	3	104	C	C2-N1-C1'	5.08	124.39	118.80
53	2	910	G	N3-C4-N9	5.08	129.05	126.00
53	2	2472	A	N1-C2-N3	-5.08	126.76	129.30
53	2	2616	C	C5-C6-N1	5.08	123.54	121.00
51	3	3	C	N1-C2-O2	5.08	121.95	118.90
51	3	4	U	N1-C2-O2	5.08	126.36	122.80
53	2	2716	C	C6-N1-C2	-5.08	118.27	120.30
53	2	350	C	C2-N1-C1'	5.08	124.39	118.80
53	2	1387	A	N1-C2-N3	-5.08	126.76	129.30
53	2	2695	A	N1-C2-N3	-5.08	126.76	129.30
53	2	4774	C	N3-C2-O2	-5.08	118.34	121.90
53	2	2498	C	N1-C2-O2	5.08	121.95	118.90
53	2	3872	A	N1-C2-N3	-5.08	126.76	129.30
53	2	4887	C	C6-N1-C2	-5.07	118.27	120.30
51	3	78	C	O4'-C1'-N1	5.07	112.26	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	2	67	C	C5-C6-N1	5.07	123.54	121.00
53	2	661	C	N3-C2-O2	-5.07	118.35	121.90
53	2	1632	A	C4-N9-C1'	5.07	135.43	126.30
53	2	3685	C	C5-C6-N1	5.07	123.53	121.00
53	2	4561	C	N1-C2-O2	5.07	121.94	118.90
53	2	294	G	C8-N9-C1'	-5.07	120.41	127.00
53	2	2520	C	C6-N1-C2	-5.07	118.27	120.30
53	2	1535	C	N1-C2-O2	5.07	121.94	118.90
53	2	4940	C	C6-N1-C2	-5.07	118.27	120.30
53	2	981	C	C6-N1-C2	-5.06	118.27	120.30
53	2	1401	C	N1-C2-O2	5.06	121.94	118.90
53	2	4467	A	N1-C2-N3	-5.06	126.77	129.30
53	2	1093	C	C6-N1-C2	-5.06	118.28	120.30
53	2	4476	C	O4'-C1'-N1	5.06	112.25	108.20
53	2	4681	A	N1-C2-N3	-5.06	126.77	129.30
4	8	32	C	C2-N1-C1'	5.05	124.36	118.80
53	2	3752	C	P-O3'-C3'	5.05	125.77	119.70
53	2	4700	A	N1-C2-N3	-5.05	126.77	129.30
22	U	17	ASP	CB-CG-OD1	5.05	122.85	118.30
50	d	54	GLY	C-N-CA	5.05	134.32	121.70
53	2	2040	A	N1-C2-N3	-5.05	126.78	129.30
4	8	20	A	N1-C2-N3	-5.05	126.78	129.30
53	2	1431	C	C6-N1-C2	-5.05	118.28	120.30
53	2	2379	A	N1-C2-N3	-5.05	126.78	129.30
53	2	1535	C	C6-N1-C2	-5.04	118.28	120.30
4	8	82	A	C2-N3-C4	5.04	113.12	110.60
53	2	1671	U	C6-N1-C1'	-5.04	114.14	121.20
53	2	2560	C	N3-C2-O2	-5.04	118.37	121.90
53	2	2614	C	C6-N1-C2	-5.04	118.28	120.30
53	2	2729	C	C5-C6-N1	5.04	123.52	121.00
53	2	4276	G	N3-C4-N9	5.04	129.03	126.00
53	2	76	A	N1-C2-N3	-5.04	126.78	129.30
53	2	227	A	N1-C2-N3	-5.04	126.78	129.30
53	2	694	C	C5-C6-N1	5.04	123.52	121.00
53	2	1085	C	C5-C6-N1	5.04	123.52	121.00
51	3	79	U	N3-C2-O2	-5.04	118.67	122.20
53	2	2787	A	N1-C2-N3	-5.04	126.78	129.30
53	2	468	U	C6-N1-C2	-5.04	117.98	121.00
53	2	2465	C	C6-N1-C2	-5.04	118.28	120.30
53	2	4146	G	N3-C4-N9	5.04	129.02	126.00
53	2	363	A	N1-C2-N3	-5.04	126.78	129.30
5	9	35	LEU	CA-CB-CG	5.04	126.88	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	E	11	LEU	CA-CB-CG	5.04	126.88	115.30
53	2	1345	A	N1-C2-N3	-5.04	126.78	129.30
53	2	2593	C	C6-N1-C2	-5.04	118.29	120.30
53	2	4887	C	N3-C2-O2	-5.04	118.38	121.90
53	2	5043	A	N1-C2-N3	-5.04	126.78	129.30
4	8	76	C	C6-N1-C2	-5.03	118.29	120.30
53	2	147	A	C2-N3-C4	5.03	113.12	110.60
53	2	1814	C	C6-N1-C2	-5.03	118.29	120.30
53	2	4237	C	N1-C2-O2	5.03	121.92	118.90
53	2	4694	G	C4-N9-C1'	5.03	133.04	126.50
53	2	1856	C	C2-N1-C1'	5.03	124.33	118.80
53	2	2465	C	C2-N1-C1'	5.03	124.33	118.80
53	2	736	C	C6-N1-C2	-5.03	118.29	120.30
53	2	4696	C	C6-N1-C2	-5.03	118.29	120.30
51	3	71	G	C4-N9-C1'	5.03	133.04	126.50
53	2	2041	A	N1-C2-N3	-5.03	126.79	129.30
53	2	1367	C	C6-N1-C1'	-5.03	114.77	120.80
53	2	1405	C	C5-C6-N1	5.03	123.51	121.00
51	3	81	G	C4-C5-N7	5.03	112.81	110.80
53	2	51	A	N1-C2-N3	-5.03	126.79	129.30
53	2	2023	C	N1-C2-O2	5.03	121.92	118.90
53	2	2729	C	N1-C2-O2	5.03	121.92	118.90
53	2	4177	C	C6-N1-C2	-5.03	118.29	120.30
53	2	4455	G	N3-C4-N9	5.02	129.01	126.00
53	2	4500	U	N3-C2-O2	-5.02	118.68	122.20
53	2	1644	C	C6-N1-C2	-5.02	118.29	120.30
53	2	1875	C	C6-N1-C2	-5.02	118.29	120.30
53	2	2802	C	C6-N1-C2	-5.02	118.29	120.30
53	2	4715	C	C6-N1-C2	-5.02	118.29	120.30
46	4	391	GLU	C-N-CA	5.02	134.25	121.70
53	2	313	U	N3-C2-O2	-5.02	118.69	122.20
53	2	683	C	N3-C2-O2	-5.02	118.39	121.90
53	2	1558	A	N1-C2-N3	-5.02	126.79	129.30
51	3	88	A	N1-C2-N3	-5.02	126.79	129.30
53	2	1947	U	C2-N1-C1'	5.02	123.72	117.70
53	2	4315	A	C2-N3-C4	5.02	113.11	110.60
53	2	2818	C	C6-N1-C2	-5.02	118.29	120.30
53	2	3720	G	N3-C4-N9	5.02	129.01	126.00
53	2	4345	C	N3-C2-O2	-5.02	118.39	121.90
53	2	4990	C	C6-N1-C2	-5.02	118.29	120.30
53	2	353	A	N1-C2-N3	-5.02	126.79	129.30
53	2	4722	G	C8-N9-C1'	-5.02	120.48	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	2	87	A	N1-C2-N3	-5.01	126.79	129.30
53	2	2264	C	C5-C6-N1	5.01	123.51	121.00
53	2	2671	C	C2-N1-C1'	5.01	124.31	118.80
53	2	4500	U	N1-C2-O2	5.01	126.31	122.80
53	2	662	C	C6-N1-C2	-5.01	118.30	120.30
53	2	53	C	C6-N1-C2	-5.01	118.30	120.30
53	2	2094	G	N3-C4-C5	-5.01	126.09	128.60
4	8	9	A	N1-C2-N3	-5.01	126.80	129.30
38	u	54	ALA	CB-CA-C	5.01	117.61	110.10
53	2	3756	A	N1-C2-N3	-5.01	126.80	129.30
53	2	963	G	N7-C8-N9	5.01	115.60	113.10
53	2	1368	A	N1-C2-N3	-5.01	126.80	129.30
53	2	1692	C	C6-N1-C2	-5.01	118.30	120.30
53	2	1706	A	N1-C2-N3	-5.01	126.80	129.30
53	2	4983	C	N1-C2-O2	5.01	121.91	118.90
53	2	5008	C	N3-C2-O2	-5.01	118.39	121.90
51	3	22	A	C2-N3-C4	5.01	113.10	110.60
53	2	115	C	O4'-C1'-N1	5.01	112.20	108.20
53	2	1397	A	N1-C2-N3	-5.01	126.80	129.30
53	2	4969	C	C5-C6-N1	5.01	123.50	121.00
53	2	2814	C	C6-N1-C1'	-5.00	114.79	120.80
53	2	3668	C	C2-N1-C1'	5.00	124.31	118.80
4	8	128	C	C5-C6-N1	5.00	123.50	121.00
51	3	51	G	C2'-C3'-O3'	5.00	121.70	113.70
53	2	294	G	N3-C4-C5	-5.00	126.10	128.60
53	2	2583	C	C6-N1-C2	-5.00	118.30	120.30
53	2	2803	U	N3-C2-O2	-5.00	118.70	122.20
53	2	338	A	N1-C2-N3	-5.00	126.80	129.30

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
53	2	3876	A	Sidechain
46	4	503	THR	Peptide
8	D	231	ASN	Peptide
1	N	380	ASN	Peptide
43	R	196	ARG	Sidechain
43	R	43	LYS	Peptide
45	T	63	ARG	Sidechain
34	n	106	TYR	Peptide
38	u	54	ALA	Peptide

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Mol	Chain	Res	Type	Group
40	y	55	GLY	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	324/687 (47%)	313 (97%)	11 (3%)	0	100	100
2	6	242/245 (99%)	227 (94%)	15 (6%)	0	100	100
3	7	133/163 (82%)	130 (98%)	3 (2%)	0	100	100
5	9	82/134 (61%)	75 (92%)	7 (8%)	0	100	100
6	A	41/159 (26%)	41 (100%)	0	0	100	100
7	B	401/403 (100%)	384 (96%)	17 (4%)	0	100	100
8	D	356/427 (83%)	335 (94%)	21 (6%)	0	100	100
9	E	96/115 (84%)	93 (97%)	3 (3%)	0	100	100
10	F	107/117 (92%)	105 (98%)	2 (2%)	0	100	100
11	G	239/266 (90%)	231 (97%)	8 (3%)	0	100	100
12	H	120/123 (98%)	118 (98%)	2 (2%)	0	100	100
13	I	188/192 (98%)	181 (96%)	7 (4%)	0	100	100
14	J	213/260 (82%)	208 (98%)	5 (2%)	0	100	100
15	K	100/105 (95%)	97 (97%)	3 (3%)	0	100	100
16	L	108/148 (73%)	101 (94%)	7 (6%)	0	100	100
17	M	84/97 (87%)	79 (94%)	5 (6%)	0	100	100
18	O	67/70 (96%)	64 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	P	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
20	Q	208/211 (99%)	198 (95%)	10 (5%)	0	100	100
21	S	133/215 (62%)	126 (95%)	7 (5%)	0	100	100
22	U	201/204 (98%)	190 (94%)	10 (5%)	1 (0%)	29	67
23	V	199/203 (98%)	191 (96%)	8 (4%)	0	100	100
24	X	89/92 (97%)	86 (97%)	3 (3%)	0	100	100
25	Z	149/188 (79%)	147 (99%)	2 (1%)	0	100	100
26	a	146/196 (74%)	143 (98%)	3 (2%)	0	100	100
27	b	174/176 (99%)	167 (96%)	7 (4%)	0	100	100
28	e	129/140 (92%)	120 (93%)	9 (7%)	0	100	100
29	g	115/156 (74%)	111 (96%)	4 (4%)	0	100	100
30	h	132/145 (91%)	129 (98%)	3 (2%)	0	100	100
31	i	133/136 (98%)	128 (96%)	4 (3%)	1 (1%)	19	58
32	l	123/137 (90%)	117 (95%)	6 (5%)	0	100	100
33	m	246/257 (96%)	224 (91%)	22 (9%)	0	100	100
34	n	107/110 (97%)	103 (96%)	4 (4%)	0	100	100
35	o	231/288 (80%)	217 (94%)	14 (6%)	0	100	100
36	p	224/248 (90%)	217 (97%)	7 (3%)	0	100	100
37	r	80/360 (22%)	76 (95%)	4 (5%)	0	100	100
38	u	64/549 (12%)	57 (89%)	5 (8%)	2 (3%)	4	26
39	w	427/731 (58%)	411 (96%)	13 (3%)	3 (1%)	22	61
40	y	163/165 (99%)	156 (96%)	7 (4%)	0	100	100
41	z	63/129 (49%)	63 (100%)	0	0	100	100
42	C	163/178 (92%)	152 (93%)	11 (7%)	0	100	100
43	R	291/297 (98%)	271 (93%)	17 (6%)	3 (1%)	15	54
44	W	386/485 (80%)	369 (96%)	16 (4%)	1 (0%)	41	74
45	T	120/160 (75%)	109 (91%)	11 (9%)	0	100	100
46	4	607/634 (96%)	558 (92%)	46 (8%)	3 (0%)	29	67
47	Y	165/184 (90%)	156 (94%)	9 (6%)	0	100	100
48	k	127/135 (94%)	121 (95%)	6 (5%)	0	100	100
49	j	109/125 (87%)	104 (95%)	5 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
50	d	102/128 (80%)	92 (90%)	10 (10%)	0	100 100
52	v	215/239 (90%)	204 (95%)	11 (5%)	0	100 100
All	All	8770/11363 (77%)	8341 (95%)	415 (5%)	14 (0%)	50 79

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
38	u	55	PRO
44	W	267	ARG
38	u	14	THR
39	w	27	ALA
46	4	88	ASP
43	R	44	TYR
22	U	147	ASP
31	i	31	ASP
39	w	323	LYS
43	R	269	PRO
39	w	132	VAL
43	R	270	LYS
46	4	366	THR
46	4	427	ASP

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
1	N	308/629 (49%)	306 (99%)	2 (1%)	86 94
2	6	212/213 (100%)	211 (100%)	1 (0%)	88 95
3	7	126/149 (85%)	126 (100%)	0	100 100
5	9	74/114 (65%)	74 (100%)	0	100 100
6	A	34/126 (27%)	34 (100%)	0	100 100
7	B	349/349 (100%)	348 (100%)	1 (0%)	92 96
8	D	298/348 (86%)	297 (100%)	1 (0%)	92 96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	E	83/97 (86%)	83 (100%)	0	100	100
10	F	94/100 (94%)	94 (100%)	0	100	100
11	G	203/223 (91%)	203 (100%)	0	100	100
12	H	109/110 (99%)	109 (100%)	0	100	100
13	I	169/171 (99%)	169 (100%)	0	100	100
14	J	191/228 (84%)	190 (100%)	1 (0%)	88	95
15	K	86/89 (97%)	86 (100%)	0	100	100
16	L	94/121 (78%)	94 (100%)	0	100	100
17	M	73/80 (91%)	73 (100%)	0	100	100
18	O	64/65 (98%)	64 (100%)	0	100	100
19	P	47/48 (98%)	47 (100%)	0	100	100
20	Q	176/177 (99%)	175 (99%)	1 (1%)	86	94
21	S	115/161 (71%)	115 (100%)	0	100	100
22	U	171/172 (99%)	171 (100%)	0	100	100
23	V	173/174 (99%)	173 (100%)	0	100	100
24	X	74/75 (99%)	74 (100%)	0	100	100
25	Z	136/165 (82%)	136 (100%)	0	100	100
26	a	133/175 (76%)	133 (100%)	0	100	100
27	b	157/157 (100%)	156 (99%)	1 (1%)	86	94
28	e	101/107 (94%)	101 (100%)	0	100	100
29	g	105/133 (79%)	105 (100%)	0	100	100
30	h	124/135 (92%)	124 (100%)	0	100	100
31	i	117/118 (99%)	117 (100%)	0	100	100
32	l	109/121 (90%)	109 (100%)	0	100	100
33	m	190/199 (96%)	190 (100%)	0	100	100
34	n	88/89 (99%)	88 (100%)	0	100	100
35	o	208/252 (82%)	207 (100%)	1 (0%)	88	95
36	p	195/215 (91%)	195 (100%)	0	100	100
37	r	76/312 (24%)	76 (100%)	0	100	100
38	u	62/485 (13%)	62 (100%)	0	100	100
39	w	385/654 (59%)	385 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
40	y	137/137 (100%)	136 (99%)	1 (1%)	84 94
41	z	61/115 (53%)	60 (98%)	1 (2%)	62 84
42	C	138/149 (93%)	138 (100%)	0	100 100
43	R	246/250 (98%)	244 (99%)	2 (1%)	81 93
44	W	322/404 (80%)	322 (100%)	0	100 100
45	T	109/140 (78%)	108 (99%)	1 (1%)	78 91
46	4	554/574 (96%)	553 (100%)	1 (0%)	93 98
47	Y	147/163 (90%)	147 (100%)	0	100 100
48	k	115/121 (95%)	115 (100%)	0	100 100
49	j	101/110 (92%)	101 (100%)	0	100 100
50	d	94/115 (82%)	94 (100%)	0	100 100
52	v	194/214 (91%)	193 (100%)	1 (0%)	88 95
All	All	7727/9828 (79%)	7711 (100%)	16 (0%)	93 98

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

Mol	Chain	Res	Type
1	N	108	ARG
1	N	341	ARG
2	6	237	ARG
7	B	300	LYS
8	D	75	ARG
14	J	141	ARG
20	Q	103	ARG
27	b	77	ASN
35	o	56	ARG
40	y	61	LYS
41	z	100	ARG
43	R	270	LYS
43	R	284	LYS
45	T	54	HIS
46	4	385	ARG
52	v	216	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
11	G	43	GLN
30	h	14	ASN
37	r	256	GLN
42	C	97	ASN
46	4	5	ASN
52	v	58	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	8	155/156 (99%)	30 (19%)	0
51	3	113/120 (94%)	25 (22%)	2 (1%)
53	2	3451/5054 (68%)	864 (25%)	19 (0%)
All	All	3719/5330 (69%)	919 (24%)	21 (0%)

All (919) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	8	25	G
4	8	34	U
4	8	35	C
4	8	39	G
4	8	48	A
4	8	51	U
4	8	52	A
4	8	59	A
4	8	62	A
4	8	63	U
4	8	71	A
4	8	80	A
4	8	82	A
4	8	84	A
4	8	85	U
4	8	86	U
4	8	88	A
4	8	103	A
4	8	104	A
4	8	105	C
4	8	110	U
4	8	114	G
4	8	123	U
4	8	124	U

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Mol	Chain	Res	Type
4	8	126	C
4	8	127	U
4	8	128	C
4	8	147	G
4	8	150	C
4	8	151	G
51	3	7	G
51	3	10	C
51	3	11	A
51	3	22	A
51	3	41	G
51	3	48	G
51	3	49	A
51	3	51	G
51	3	52	C
51	3	53	U
51	3	54	A
51	3	56	G
51	3	60	G
51	3	62	U
51	3	63	C
51	3	64	G
51	3	72	U
51	3	73	U
51	3	74	A
51	3	75	G
51	3	83	A
51	3	84	U
51	3	85	G
51	3	100	A
51	3	110	G
53	2	39	A
53	2	42	A
53	2	44	A
53	2	48	G
53	2	56	A
53	2	59	A
53	2	64	A
53	2	65	A
53	2	69	A
53	2	72	C
53	2	73	A

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Mol	Chain	Res	Type
53	2	84	A
53	2	91	G
53	2	98	A
53	2	108	A
53	2	109	G
53	2	110	C
53	2	112	C
53	2	119	G
53	2	120	A
53	2	131	C
53	2	132	G
53	2	134	G
53	2	135	G
53	2	136	C
53	2	144	G
53	2	145	G
53	2	152	U
53	2	158	A
53	2	159	C
53	2	183	C
53	2	185	C
53	2	186	G
53	2	188	G
53	2	197	A
53	2	200	U
53	2	209	U
53	2	216	C
53	2	217	C
53	2	218	A
53	2	220	C
53	2	234	G
53	2	254	G
53	2	255	C
53	2	256	G
53	2	265	C
53	2	266	C
53	2	267	G
53	2	279	A
53	2	280	G
53	2	297	U
53	2	306	A
53	2	315	G

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Mol	Chain	Res	Type
53	2	316	U
53	2	340	C
53	2	347	A
53	2	363	A
53	2	387	G
53	2	398	A2M
53	2	407	A
53	2	408	A
53	2	409	G
53	2	410	A
53	2	412	G
53	2	432	U
53	2	433	A
53	2	440	U
53	2	449	C
53	2	450	G
53	2	452	A
53	2	453	G
53	2	454	U
53	2	461	G
53	2	464	G
53	2	465	G
53	2	467	U
53	2	484	U
53	2	485	C
53	2	486	C
53	2	489	C
53	2	491	G
53	2	492	U
53	2	493	G
53	2	497	G
53	2	498	C
53	2	499	G
53	2	500	G
53	2	501	C
53	2	502	C
53	2	503	C
53	2	504	G
53	2	505	G
53	2	509	A
53	2	510	U
53	2	512	U

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Mol	Chain	Res	Type
53	2	513	U
53	2	514	U
53	2	515	C
53	2	516	C
53	2	517	C
53	2	518	G
53	2	519	C
53	2	648	G
53	2	653	U
53	2	654	C
53	2	656	C
53	2	657	C
53	2	659	G
53	2	666	G
53	2	667	A
53	2	668	C
53	2	673	C
53	2	685	C
53	2	686	A
53	2	696	C
53	2	703	G
53	2	704	C
53	2	731	G
53	2	738	C
53	2	739	G
53	2	740	G
53	2	742	G
53	2	753	C
53	2	759	G
53	2	904	C
53	2	905	C
53	2	913	U
53	2	914	U
53	2	915	A
53	2	916	C
53	2	917	A
53	2	918	G
53	2	924	C
53	2	925	C
53	2	926	G
53	2	932	A
53	2	933	G

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Mol	Chain	Res	Type
53	2	935	A
53	2	936	C
53	2	937	U
53	2	941	C
53	2	943	A
53	2	944	A
53	2	945	U
53	2	946	C
53	2	956	A
53	2	959	G
53	2	960	A
53	2	961	G
53	2	962	C
53	2	965	G
53	2	966	A
53	2	967	C
53	2	969	C
53	2	970	G
53	2	971	U
53	2	972	C
53	2	977	C
53	2	982	U
53	2	984	C
53	2	990	C
53	2	991	C
53	2	992	C
53	2	993	G
53	2	994	G
53	2	995	C
53	2	1048	G
53	2	1049	C
53	2	1051	G
53	2	1066	G
53	2	1067	G
53	2	1068	G
53	2	1070	G
53	2	1072	C
53	2	1082	C
53	2	1100	U
53	2	1168	G
53	2	1173	G
53	2	1178	G

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Mol	Chain	Res	Type
53	2	1179	U
53	2	1180	C
53	2	1182	C
53	2	1186	U
53	2	1189	G
53	2	1195	G
53	2	1198	G
53	2	1200	G
53	2	1202	C
53	2	1203	G
53	2	1204	C
53	2	1210	C
53	2	1211	G
53	2	1215	C
53	2	1216	C
53	2	1218	G
53	2	1222	A
53	2	1240	G
53	2	1241	C
53	2	1243	C
53	2	1244	G
53	2	1245	C
53	2	1253	G
53	2	1254	A
53	2	1255	A
53	2	1256	G
53	2	1260	G
53	2	1266	G
53	2	1268	G
53	2	1271	G
53	2	1272	C
53	2	1273	G
53	2	1275	G
53	2	1280	C
53	2	1283	G
53	2	1284	G
53	2	1285	U
53	2	1287	G
53	2	1294	A
53	2	1295	C
53	2	1296	G
53	2	1302	U

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Mol	Chain	Res	Type
53	2	1303	A
53	2	1313	C
53	2	1314	C
53	2	1315	C
53	2	1320	U
53	2	1321	G
53	2	1337	A
53	2	1354	A
53	2	1358	G
53	2	1359	G
53	2	1365	C
53	2	1366	G
53	2	1367	C
53	2	1372	A
53	2	1377	G
53	2	1378	C
53	2	1379	C
53	2	1382	G
53	2	1387	A
53	2	1394	G
53	2	1397	A
53	2	1398	A
53	2	1399	G
53	2	1402	C
53	2	1407	C
53	2	1409	C
53	2	1410	U
53	2	1412	G
53	2	1419	G
53	2	1420	A
53	2	1425	G
53	2	1438	U
53	2	1439	C
53	2	1442	C
53	2	1444	G
53	2	1446	C
53	2	1447	C
53	2	1449	C
53	2	1465	G
53	2	1482	G
53	2	1483	C
53	2	1497	A

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Mol	Chain	Res	Type
53	2	1498	G
53	2	1503	A
53	2	1518	A
53	2	1523	A
53	2	1534	A2M
53	2	1547	A
53	2	1560	A
53	2	1562	G
53	2	1564	A
53	2	1566	C
53	2	1578	U
53	2	1592	G
53	2	1595	G
53	2	1596	U
53	2	1597	G
53	2	1613	A
53	2	1624	G
53	2	1625	OMG
53	2	1626	G
53	2	1631	A
53	2	1633	G
53	2	1634	A
53	2	1637	A
53	2	1638	A
53	2	1641	G
53	2	1649	U
53	2	1650	A
53	2	1654	G
53	2	1661	C
53	2	1670	G
53	2	1672	U
53	2	1673	U
53	2	1674	C
53	2	1675	C
53	2	1676	C
53	2	1677	U
53	2	1679	A
53	2	1680	G
53	2	1691	G
53	2	1697	G
53	2	1699	A
53	2	1700	G

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Mol	Chain	Res	Type
53	2	1701	A
53	2	1703	C
53	2	1704	C
53	2	1705	G
53	2	1707	C
53	2	1708	G
53	2	1709	C
53	2	1715	C
53	2	1716	G
53	2	1718	C
53	2	1719	A
53	2	1721	G
53	2	1724	G
53	2	1726	U
53	2	1729	A
53	2	1796	U
53	2	1798	G
53	2	1803	G
53	2	1804	A
53	2	1806	G
53	2	1809	C
53	2	1810	G
53	2	1813	U
53	2	1815	G
53	2	1816	C
53	2	1817	U
53	2	1820	C
53	2	1823	G
53	2	1824	G
53	2	1829	G
53	2	1832	C
53	2	1833	G
53	2	1834	U
53	2	1836	G
53	2	1837	A
53	2	1842	G
53	2	1854	G
53	2	1855	G
53	2	1856	C
53	2	1861	U
53	2	1865	G
53	2	1866	U

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Mol	Chain	Res	Type
53	2	1870	C
53	2	1871	A2M
53	2	1882	U
53	2	1883	OMG
53	2	1891	A
53	2	1897	A
53	2	1900	C
53	2	1918	U
53	2	1919	G
53	2	1920	C
53	2	1921	C
53	2	1922	G
53	2	1925	G
53	2	1931	C
53	2	1932	A
53	2	1935	C
53	2	1939	A
53	2	1940	G
53	2	1942	A
53	2	1943	A
53	2	1944	A
53	2	1948	G
53	2	1952	G
53	2	1956	A
53	2	1959	U
53	2	1966	C
53	2	1972	G
53	2	1974	U
53	2	1975	G
53	2	1980	U
53	2	1981	G
53	2	1984	A
53	2	1985	G
53	2	1990	A
53	2	1997	U
53	2	2001	G
53	2	2002	A
53	2	2003	G
53	2	2004	U
53	2	2007	G
53	2	2008	U
53	2	2011	C

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Mol	Chain	Res	Type
53	2	2017	A
53	2	2018	C
53	2	2025	A
53	2	2026	A
53	2	2033	A
53	2	2034	G
53	2	2040	A
53	2	2044	U
53	2	2046	G
53	2	2048	U
53	2	2055	G
53	2	2056	G
53	2	2069	A
53	2	2084	C
53	2	2085	G
53	2	2090	U
53	2	2091	C
53	2	2092	G
53	2	2093	A
53	2	2094	G
53	2	2095	A
53	2	2096	G
53	2	2097	U
53	2	2098	G
53	2	2101	C
53	2	2102	G
53	2	2104	G
53	2	2105	A
53	2	2106	G
53	2	2110	C
53	2	2111	G
53	2	2112	G
53	2	2250	C
53	2	2251	G
53	2	2253	A
53	2	2254	G
53	2	2255	C
53	2	2256	C
53	2	2258	C
53	2	2259	G
53	2	2260	C
53	2	2269	C

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Mol	Chain	Res	Type
53	2	2289	C
53	2	2300	A
53	2	2301	G
53	2	2306	G
53	2	2313	A
53	2	2314	G
53	2	2316	G
53	2	2333	G
53	2	2346	C
53	2	2348	G
53	2	2351	C
53	2	2360	A
53	2	2395	A
53	2	2410	C
53	2	2416	G
53	2	2417	A
53	2	2422	OMC
53	2	2425	U
53	2	2441	C
53	2	2450	G
53	2	2463	G
53	2	2464	C
53	2	2465	C
53	2	2471	G
53	2	2474	G
53	2	2475	G
53	2	2478	C
53	2	2484	A
53	2	2486	G
53	2	2487	G
53	2	2488	C
53	2	2489	C
53	2	2490	U
53	2	2491	C
53	2	2493	G
53	2	2494	U
53	2	2495	U
53	2	2496	G
53	2	2497	C
53	2	2498	C
53	2	2502	G
53	2	2503	G

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Mol	Chain	Res	Type
53	2	2504	C
53	2	2505	C
53	2	2506	G
53	2	2507	A
53	2	2511	A
53	2	2512	A
53	2	2513	A
53	2	2519	U
53	2	2529	A
53	2	2537	A
53	2	2543	A
53	2	2544	G
53	2	2545	U
53	2	2546	G
53	2	2547	G
53	2	2554	U
53	2	2555	G
53	2	2559	G
53	2	2560	C
53	2	2563	C
53	2	2566	G
53	2	2567	G
53	2	2573	A
53	2	2583	C
53	2	2587	A
53	2	2589	C
53	2	2600	A
53	2	2601	A
53	2	2618	G
53	2	2627	C
53	2	2643	G
53	2	2653	C
53	2	2661	U
53	2	2662	G
53	2	2669	C
53	2	2670	C
53	2	2674	A
53	2	2675	G
53	2	2687	U
53	2	2694	G
53	2	2695	A
53	2	2696	A

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Mol	Chain	Res	Type
53	2	2707	U
53	2	2708	U
53	2	2710	C
53	2	2711	G
53	2	2719	C
53	2	2721	G
53	2	2723	U
53	2	2724	G
53	2	2726	G
53	2	2739	C
53	2	2742	G
53	2	2743	A
53	2	2746	A
53	2	2753	G
53	2	2756	G
53	2	2759	G
53	2	2761	U
53	2	2762	G
53	2	2763	U
53	2	2769	U
53	2	2770	C
53	2	2787	A
53	2	2788	U
53	2	2790	U
53	2	2815	A
53	2	2826	U
53	2	2827	G
53	2	2828	U
53	2	2842	G
53	2	2846	G
53	2	2882	A
53	2	2897	G
53	2	2901	G
53	2	2902	G
53	2	2904	U
53	2	2905	C
53	2	2906	G
53	2	2908	U
53	2	2910	G
53	2	3585	G
53	2	3588	C
53	2	3591	C

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Mol	Chain	Res	Type
53	2	3593	C
53	2	3595	U
53	2	3596	A
53	2	3597	G
53	2	3599	A
53	2	3605	C
53	2	3615	G
53	2	3616	U
53	2	3618	C
53	2	3626	G
53	2	3630	A
53	2	3635	A
53	2	3638	G
53	2	3644	U
53	2	3662	A
53	2	3673	C
53	2	3679	U
53	2	3680	U
53	2	3682	A
53	2	3691	G
53	2	3692	A
53	2	3696	C
53	2	3710	G
53	2	3711	A
53	2	3712	A
53	2	3713	U
53	2	3714	G
53	2	3729	U
53	2	3735	G
53	2	3736	A
53	2	3748	A
53	2	3750	G
53	2	3753	G
53	2	3771	C
53	2	3772	U
53	2	3773	U
53	2	3774	A
53	2	3775	A
53	2	3776	G
53	2	3833	C
53	2	3838	U
53	2	3839	G

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Mol	Chain	Res	Type
53	2	3840	U
53	2	3867	A2M
53	2	3875	G
53	2	3876	A
53	2	3877	A
53	2	3878	C
53	2	3879	G
53	2	3898	G
53	2	3903	A
53	2	3904	G
53	2	3905	A
53	2	3906	A
53	2	3914	U
53	2	3915	U
53	2	3922	G
53	2	3938	G
53	2	3939	G
53	2	4068	U
53	2	4076	G
53	2	4077	A
53	2	4084	G
53	2	4095	G
53	2	4097	G
53	2	4099	G
53	2	4100	C
53	2	4101	C
53	2	4102	C
53	2	4103	C
53	2	4104	G
53	2	4105	A
53	2	4107	G
53	2	4108	G
53	2	4111	U
53	2	4113	U
53	2	4114	C
53	2	4115	G
53	2	4116	C
53	2	4117	U
53	2	4119	C
53	2	4130	C
53	2	4131	G
53	2	4135	G

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Mol	Chain	Res	Type
53	2	4139	G
53	2	4140	C
53	2	4142	C
53	2	4143	G
53	2	4145	C
53	2	4146	G
53	2	4149	C
53	2	4154	G
53	2	4162	C
53	2	4163	U
53	2	4168	G
53	2	4170	A
53	2	4179	G
53	2	4183	G
53	2	4184	G
53	2	4190	U
53	2	4207	C
53	2	4208	U
53	2	4210	U
53	2	4211	C
53	2	4223	C
53	2	4228	G
53	2	4229	U
53	2	4230	C
53	2	4231	C
53	2	4234	A
53	2	4235	G
53	2	4236	G
53	2	4243	C
53	2	4251	A
53	2	4254	G
53	2	4255	A
53	2	4258	C
53	2	4265	U
53	2	4266	G
53	2	4267	G
53	2	4271	A
53	2	4273	A
53	2	4274	A
53	2	4275	G
53	2	4279	A
53	2	4280	A

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Mol	Chain	Res	Type
53	2	4281	A
53	2	4282	A
53	2	4283	G
53	2	4286	C
53	2	4288	C
53	2	4289	U
53	2	4290	U
53	2	4291	G
53	2	4292	A
53	2	4297	G
53	2	4302	U
53	2	4313	A
53	2	4315	A
53	2	4319	C
53	2	4326	G
53	2	4329	G
53	2	4330	G
53	2	4332	C
53	2	4341	C
53	2	4342	C
53	2	4343	U
53	2	4347	G
53	2	4348	A
53	2	4349	C
53	2	4350	C
53	2	4354	U
53	2	4355	G
53	2	4368	G
53	2	4371	G
53	2	4372	U
53	2	4381	A
53	2	4387	C
53	2	4395	U
53	2	4396	A
53	2	4401	G
53	2	4413	C
53	2	4414	A
53	2	4415	A
53	2	4416	G
53	2	4417	C
53	2	4418	G
53	2	4419	U

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Mol	Chain	Res	Type
53	2	4420	U
53	2	4421	C
53	2	4422	A
53	2	4423	U
53	2	4424	A
53	2	4425	G
53	2	4427	G
53	2	4428	A
53	2	4429	C
53	2	4433	G
53	2	4437	U
53	2	4440	G
53	2	4446	U
53	2	4447	C
53	2	4448	G
53	2	4449	A
53	2	4450	U
53	2	4451	G
53	2	4452	U
53	2	4453	C
53	2	4455	G
53	2	4464	A
53	2	4465	U
53	2	4466	C
53	2	4475	G
53	2	4476	C
53	2	4484	A
53	2	4498	U
53	2	4499	G
53	2	4500	U
53	2	4503	A
53	2	4510	A
53	2	4512	U
53	2	4513	A
53	2	4518	A
53	2	4519	C
53	2	4524	G
53	2	4530	UR3
53	2	4531	U
53	2	4538	G
53	2	4545	G
53	2	4548	A

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Mol	Chain	Res	Type
53	2	4550	7MG
53	2	4555	U
53	2	4556	U
53	2	4557	U
53	2	4558	U
53	2	4560	C
53	2	4584	A
53	2	4589	A
53	2	4590	A
53	2	4600	G
53	2	4601	U
53	2	4606	G
53	2	4607	A
53	2	4608	G
53	2	4627	U
53	2	4635	A
53	2	4636	U
53	2	4637	OMG
53	2	4656	A
53	2	4670	C
53	2	4677	U
53	2	4678	G
53	2	4684	A
53	2	4694	G
53	2	4695	C
53	2	4703	U
53	2	4707	A
53	2	4708	A
53	2	4709	U
53	2	4720	C
53	2	4730	C
53	2	4731	G
53	2	4733	C
53	2	4734	A
53	2	4740	G
53	2	4741	C
53	2	4742	G
53	2	4745	G
53	2	4751	G
53	2	4754	G
53	2	4757	C
53	2	4759	C

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Mol	Chain	Res	Type
53	2	4761	G
53	2	4764	A
53	2	4765	G
53	2	4771	C
53	2	4773	C
53	2	4775	C
53	2	4776	G
53	2	4859	C
53	2	4870	OMG
53	2	4871	C
53	2	4872	2MG
53	2	4874	A
53	2	4875	G
53	2	4877	G
53	2	4882	U
53	2	4883	C
53	2	4887	C
53	2	4889	G
53	2	4895	C
53	2	4900	C
53	2	4901	G
53	2	4910	G
53	2	4912	G
53	2	4914	C
53	2	4915	G
53	2	4916	G
53	2	4927	G
53	2	4928	C
53	2	4934	A
53	2	4940	C
53	2	4941	G
53	2	4943	A
53	2	4949	G
53	2	4975	G
53	2	4976	U
53	2	4988	U
53	2	4989	U
53	2	4991	U
53	2	5014	A
53	2	5017	G
53	2	5022	U
53	2	5024	C

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Mol	Chain	Res	Type
53	2	5026	U
53	2	5027	C
53	2	5028	G
53	2	5030	U
53	2	5031	G
53	2	5034	A
53	2	5041	G
53	2	5047	C
53	2	5050	C
53	2	5054	C
53	2	5055	G
53	2	5061	A
53	2	5069	U

All (21) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
51	3	51	G
51	3	72	U
53	2	914	U
53	2	1633	G
53	2	1678	C
53	2	1808	C
53	2	1931	C
53	2	1980	U
53	2	2017	A
53	2	2033	A
53	2	2760	G
53	2	3596	A
53	2	3752	C
53	2	3774	A
53	2	3905	A
53	2	4235	G
53	2	4415	A
53	2	4555	U
53	2	4636	U
53	2	4707	A
53	2	4913	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
53	OMC	2	3909	53	19,22,23	3.13	8 (42%)	26,31,34	1.95	7 (26%)
53	OMC	2	2365	53	19,22,23	2.90	8 (42%)	26,31,34	0.81	0
53	OMG	2	4494	53	18,26,27	2.90	8 (44%)	19,38,41	1.50	4 (21%)
53	M7A	2	4564	53	20,25,26	1.99	3 (15%)	28,37,40	3.91	7 (25%)
53	E7G	2	2297	53	24,27,28	3.89	11 (45%)	30,40,43	2.10	7 (23%)
53	A2M	2	398	53	18,25,26	3.62	8 (44%)	18,36,39	3.48	3 (16%)
53	B8T	2	4671	53	19,22,23	3.57	8 (42%)	26,31,34	0.94	1 (3%)
53	2MG	2	4872	53	18,26,27	2.53	6 (33%)	16,38,41	1.72	4 (25%)
53	A2M	2	2363	53	18,25,26	3.61	8 (44%)	18,36,39	3.39	4 (22%)
53	OMG	2	1883	53	18,26,27	2.85	8 (44%)	19,38,41	1.52	4 (21%)
53	OMC	2	3887	53	19,22,23	3.04	8 (42%)	26,31,34	1.06	2 (7%)
53	OMG	2	2364	53	18,26,27	2.76	8 (44%)	19,38,41	1.48	3 (15%)
53	UR3	2	4530	53	19,22,23	2.83	7 (36%)	26,32,35	1.33	3 (11%)
53	OMG	2	2424	53	18,26,27	2.81	8 (44%)	19,38,41	1.48	3 (15%)
53	B8Q	2	1456	53	17,22,23	2.91	5 (29%)	22,32,35	2.24	6 (27%)
53	2MG	2	978	53	18,26,27	2.72	6 (33%)	16,38,41	1.47	4 (25%)
53	P7G	2	3880	53	24,28,29	4.01	11 (45%)	27,41,44	1.45	3 (11%)
53	A2M	2	1534	53	18,25,26	3.61	8 (44%)	18,36,39	3.57	5 (27%)
53	B8K	2	3897	53	24,28,29	3.44	11 (45%)	30,42,45	2.55	11 (36%)
53	BGH	2	3899	53	25,29,30	4.52	17 (68%)	31,43,46	2.59	11 (35%)
53	B8K	2	4690	53	24,28,29	3.27	11 (45%)	30,42,45	2.57	11 (36%)
53	7MG	2	1605	53	22,26,27	3.73	10 (45%)	29,39,42	2.01	10 (34%)
53	5MU	2	4083	53	19,22,23	7.24	8 (42%)	28,32,35	3.38	10 (35%)
53	OMG	2	1625	53	18,26,27	2.89	8 (44%)	19,38,41	1.41	4 (21%)
53	OMC	2	4536	53	19,22,23	3.00	8 (42%)	26,31,34	1.08	2 (7%)
53	A2M	2	3723	53	18,25,26	3.54	8 (44%)	18,36,39	3.38	4 (22%)
53	A2M	2	4571	53	18,25,26	3.60	8 (44%)	18,36,39	3.42	4 (22%)
53	OMC	2	2861	53	19,22,23	3.04	8 (42%)	26,31,34	1.18	3 (11%)
53	2MG	2	729	53	18,26,27	2.64	6 (33%)	16,38,41	1.43	3 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
53	A2M	2	3825	53	18,25,26	3.59	8 (44%)	18,36,39	3.47	4 (22%)
4	OMU	8	14	4,53	19,22,23	3.04	8 (42%)	26,31,34	1.74	5 (19%)
53	B9B	2	237	53	21,28,29	1.97	3 (14%)	23,40,43	6.42	5 (21%)
53	A2M	2	3867	53	18,25,26	3.61	8 (44%)	18,36,39	3.47	4 (22%)
53	OMC	2	2422	47,53	19,22,23	2.99	8 (42%)	26,31,34	1.18	3 (11%)
53	P4U	2	1348	53	21,24,25	3.48	8 (38%)	27,33,36	1.14	2 (7%)
53	A2M	2	2401	53	18,25,26	3.60	8 (44%)	18,36,39	3.37	3 (16%)
53	7MG	2	4550	53	22,26,27	3.85	10 (45%)	29,39,42	1.99	9 (31%)
53	I4U	2	1659	53	21,24,25	3.51	9 (42%)	27,34,37	1.15	2 (7%)
53	A2M	2	1326	53	18,25,26	3.62	8 (44%)	18,36,39	3.49	4 (22%)
53	B8W	2	4185	53	18,26,27	2.12	2 (11%)	21,38,41	2.47	6 (28%)
53	A2M	2	4523	53	18,25,26	3.59	8 (44%)	18,36,39	3.46	3 (16%)
53	B8W	2	4472	53	18,26,27	2.12	2 (11%)	21,38,41	2.42	7 (33%)
53	OMG	2	4623	53	18,26,27	2.78	8 (44%)	19,38,41	1.56	4 (21%)
53	OMG	2	1522	53	18,26,27	2.80	8 (44%)	19,38,41	1.47	5 (26%)
53	OMG	2	373	53	18,26,27	2.85	8 (44%)	19,38,41	1.59	5 (26%)
53	P7G	2	1909	53	24,28,29	4.05	11 (45%)	27,41,44	1.50	3 (11%)
53	OMG	2	2050	53	18,26,27	2.79	8 (44%)	19,38,41	1.48	4 (21%)
53	OMC	2	2804	53	19,22,23	2.96	8 (42%)	26,31,34	0.76	0
53	OMG	2	1316	53	18,26,27	2.82	8 (44%)	19,38,41	1.55	4 (21%)
53	B9B	2	2754	53	21,28,29	2.03	3 (14%)	23,40,43	6.55	5 (21%)
53	OMU	2	4620	53	19,22,23	2.92	8 (42%)	26,31,34	1.70	5 (19%)
53	OMG	2	4637	53	18,26,27	2.84	8 (44%)	19,38,41	1.55	4 (21%)
53	A2M	2	1871	53	18,25,26	3.58	9 (50%)	18,36,39	3.53	5 (27%)
53	OMG	2	2773	53	18,26,27	2.91	8 (44%)	19,38,41	1.50	4 (21%)
53	B9B	2	1574	53	21,28,29	1.94	3 (14%)	23,40,43	6.41	5 (21%)
53	7MG	2	2522	53	22,26,27	3.73	10 (45%)	29,39,42	1.99	8 (27%)
53	B8T	2	4483	53	19,22,23	3.61	8 (42%)	26,31,34	1.45	5 (19%)
53	B8W	2	4129	53	18,26,27	2.14	2 (11%)	21,38,41	2.48	5 (23%)
53	B8W	2	4529	53	18,26,27	2.13	2 (11%)	21,38,41	2.46	7 (33%)
53	A2M	2	3718	53	18,25,26	3.62	8 (44%)	18,36,39	3.34	4 (22%)
53	B8W	2	2380	53	18,26,27	2.06	2 (11%)	21,38,41	2.40	7 (33%)
53	UR3	2	4597	53	19,22,23	2.75	7 (36%)	26,32,35	1.91	4 (15%)
53	OMC	2	3869	53	19,22,23	2.96	8 (42%)	26,31,34	0.93	1 (3%)
53	A2M	2	1524	53	18,25,26	3.60	8 (44%)	18,36,39	3.42	4 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
53	OMG	2	4870	53	18,26,27	2.89	8 (44%)	19,38,41	1.53	4 (21%)
53	2MG	2	1517	53	18,26,27	2.66	6 (33%)	16,38,41	1.53	4 (25%)
53	B9H	2	2786	53	20,25,26	3.27	3 (15%)	22,35,38	2.36	6 (27%)
53	OMC	2	3701	53	19,22,23	3.02	8 (42%)	26,31,34	0.75	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	OMC	2	3909	53	-	3/9/27/28	0/2/2/2
53	OMC	2	2365	53	-	1/9/27/28	0/2/2/2
53	OMG	2	4494	53	-	0/5/27/28	0/3/3/3
53	M7A	2	4564	53	-	0/7/37/38	0/3/3/3
53	E7G	2	2297	53	-	1/9/39/40	0/3/3/3
53	A2M	2	398	53	-	2/5/27/28	0/3/3/3
53	B8T	2	4671	53	-	0/7/27/28	0/2/2/2
53	2MG	2	4872	53	-	2/5/27/28	0/3/3/3
53	A2M	2	2363	53	-	0/5/27/28	0/3/3/3
53	OMG	2	1883	53	-	2/5/27/28	0/3/3/3
53	OMC	2	3887	53	-	1/9/27/28	0/2/2/2
53	OMG	2	2364	53	-	2/5/27/28	0/3/3/3
53	UR3	2	4530	53	-	0/7/25/26	0/2/2/2
53	OMG	2	2424	53	-	2/5/27/28	0/3/3/3
53	B8Q	2	1456	53	-	0/7/42/43	0/2/2/2
53	2MG	2	978	53	-	0/5/27/28	0/3/3/3
53	P7G	2	3880	53	-	4/10/40/41	0/3/3/3
53	A2M	2	1534	53	-	2/5/27/28	0/3/3/3
53	B8K	2	3897	53	-	3/11/41/42	0/3/3/3
53	BGH	2	3899	53	-	1/13/43/44	0/3/3/3
53	B8K	2	4690	53	-	0/11/41/42	0/3/3/3
53	7MG	2	1605	53	-	0/7/37/38	0/3/3/3
53	5MU	2	4083	53	-	0/7/25/26	0/2/2/2
53	OMG	2	1625	53	-	2/5/27/28	0/3/3/3
53	OMC	2	4536	53	-	0/9/27/28	0/2/2/2
53	A2M	2	3723	53	-	1/5/27/28	0/3/3/3
53	A2M	2	4571	53	-	0/5/27/28	0/3/3/3
53	OMC	2	2861	53	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	2MG	2	729	53	-	2/5/27/28	0/3/3/3
53	A2M	2	3825	53	-	0/5/27/28	0/3/3/3
4	OMU	8	14	4,53	-	1/9/27/28	0/2/2/2
53	B9B	2	237	53	-	4/7/29/30	0/3/3/3
53	A2M	2	3867	53	-	3/5/27/28	0/3/3/3
53	OMC	2	2422	47,53	-	1/9/27/28	0/2/2/2
53	P4U	2	1348	53	-	1/10/29/30	0/2/2/2
53	A2M	2	2401	53	-	0/5/27/28	0/3/3/3
53	7MG	2	4550	53	-	2/7/37/38	0/3/3/3
53	I4U	2	1659	53	-	2/9/29/30	0/2/2/2
53	A2M	2	1326	53	-	0/5/27/28	0/3/3/3
53	B8W	2	4185	53	-	0/5/27/28	0/3/3/3
53	A2M	2	4523	53	-	1/5/27/28	0/3/3/3
53	B8W	2	4472	53	-	2/5/27/28	0/3/3/3
53	OMG	2	4623	53	-	0/5/27/28	0/3/3/3
53	OMG	2	1522	53	-	0/5/27/28	0/3/3/3
53	OMG	2	373	53	-	1/5/27/28	0/3/3/3
53	P7G	2	1909	53	-	2/10/40/41	0/3/3/3
53	OMG	2	2050	53	-	0/5/27/28	0/3/3/3
53	OMC	2	2804	53	-	0/9/27/28	0/2/2/2
53	OMG	2	1316	53	-	0/5/27/28	0/3/3/3
53	B9B	2	2754	53	-	3/7/29/30	0/3/3/3
53	OMU	2	4620	53	-	0/9/27/28	0/2/2/2
53	OMG	2	4637	53	-	4/5/27/28	0/3/3/3
53	A2M	2	1871	53	-	2/5/27/28	0/3/3/3
53	OMG	2	2773	53	-	1/5/27/28	0/3/3/3
53	B9B	2	1574	53	-	4/7/29/30	0/3/3/3
53	7MG	2	2522	53	-	0/7/37/38	0/3/3/3
53	B8T	2	4483	53	-	0/7/27/28	0/2/2/2
53	B8W	2	4129	53	-	4/5/27/28	0/3/3/3
53	B8W	2	4529	53	-	4/5/27/28	0/3/3/3
53	A2M	2	3718	53	-	0/5/27/28	0/3/3/3
53	B8W	2	2380	53	-	3/5/27/28	0/3/3/3
53	UR3	2	4597	53	-	0/7/25/26	0/2/2/2
53	OMC	2	3869	53	-	2/9/27/28	0/2/2/2
53	A2M	2	1524	53	-	1/5/27/28	0/3/3/3
53	OMG	2	4870	53	-	2/5/27/28	0/3/3/3
53	2MG	2	1517	53	-	3/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	B9H	2	2786	53	-	2/12/47/48	0/2/2/2
53	OMC	2	3701	53	-	2/9/27/28	0/2/2/2

All (508) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	2	4083	5MU	C4-C5	20.77	1.79	1.44
53	2	4083	5MU	C6-N1	16.04	1.65	1.38
53	2	4083	5MU	C6-C5	-11.52	1.15	1.34
53	2	4083	5MU	C4-N3	-11.04	1.18	1.38
53	2	1659	I4U	C4-N3	10.62	1.45	1.31
53	2	2786	B9H	C2-N3	10.24	1.50	1.37
53	2	1348	P4U	C4-N3	10.13	1.44	1.31
53	2	3880	P7G	C5-N7	9.48	1.46	1.35
53	2	1909	P7G	C8-N9	9.38	1.51	1.46
53	2	2297	E7G	C5-N7	9.26	1.46	1.35
53	2	1909	P7G	C5-N7	9.24	1.45	1.35
53	2	4550	7MG	C8-N9	9.20	1.51	1.46
53	2	3897	B8K	C8-N9	9.07	1.51	1.46
53	2	1871	A2M	C3'-C4'	-9.01	1.30	1.53
53	2	3899	BGH	C2'-C1'	-9.00	1.29	1.53
53	2	1326	A2M	C3'-C4'	-8.97	1.30	1.53
53	2	398	A2M	C3'-C4'	-8.96	1.30	1.53
53	2	3899	BGH	O4'-C1'	8.94	1.63	1.42
53	2	4523	A2M	C3'-C4'	-8.92	1.30	1.53
53	2	4571	A2M	C3'-C4'	-8.90	1.30	1.53
53	2	3718	A2M	C3'-C4'	-8.86	1.30	1.53
53	2	2401	A2M	C3'-C4'	-8.85	1.30	1.53
53	2	1524	A2M	C3'-C4'	-8.83	1.30	1.53
53	2	4550	7MG	C5-N7	8.83	1.45	1.35
53	2	2363	A2M	C3'-C4'	-8.81	1.30	1.53
53	2	3825	A2M	C3'-C4'	-8.72	1.30	1.53
53	2	1534	A2M	C3'-C4'	-8.71	1.30	1.53
53	2	3723	A2M	C3'-C4'	-8.69	1.30	1.53
53	2	3880	P7G	C8-N9	8.68	1.50	1.46
53	2	3867	A2M	C3'-C4'	-8.66	1.30	1.53
53	2	2297	E7G	C8-N9	8.57	1.50	1.46
53	2	1605	7MG	C5-N7	8.56	1.45	1.35
53	2	2522	7MG	C5-N7	8.56	1.45	1.35
53	2	4690	B8K	C8-N9	8.54	1.50	1.46
53	2	1605	7MG	C8-N9	8.50	1.50	1.46
53	2	2522	7MG	C8-N9	8.46	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	2	1456	B8Q	C6-C5	8.30	1.52	1.33
53	2	4529	B8W	C2-N2	8.01	1.49	1.33
53	2	4185	B8W	C2-N2	7.97	1.49	1.33
53	2	4129	B8W	C2-N2	7.96	1.49	1.33
53	2	4472	B8W	C2-N2	7.93	1.49	1.33
53	2	3718	A2M	O4'-C4'	7.77	1.62	1.45
53	2	2380	B8W	C2-N2	7.74	1.49	1.33
53	2	3899	BGH	C8-N9	7.67	1.50	1.46
53	2	3867	A2M	O4'-C1'	-7.62	1.30	1.41
53	2	1871	A2M	O4'-C4'	7.61	1.62	1.45
53	2	3825	A2M	O4'-C4'	7.61	1.62	1.45
53	2	1534	A2M	O4'-C4'	7.58	1.61	1.45
53	2	2401	A2M	O4'-C4'	7.57	1.61	1.45
53	2	398	A2M	O4'-C4'	7.56	1.61	1.45
53	2	3899	BGH	O4'-C4'	-7.56	1.28	1.45
53	2	3723	A2M	O4'-C4'	7.53	1.61	1.45
53	2	4571	A2M	O4'-C4'	7.52	1.61	1.45
53	2	1326	A2M	O4'-C4'	7.50	1.61	1.45
53	2	2363	A2M	O4'-C4'	7.45	1.61	1.45
53	2	4523	A2M	O4'-C4'	7.42	1.61	1.45
53	2	3867	A2M	O4'-C4'	7.40	1.61	1.45
53	2	4483	B8T	C2-N3	7.38	1.51	1.36
53	2	1524	A2M	O4'-C4'	7.33	1.61	1.45
53	2	1326	A2M	O4'-C1'	-7.27	1.30	1.41
53	2	1524	A2M	O4'-C1'	-7.27	1.30	1.41
53	2	4671	B8T	C2-N3	7.26	1.51	1.36
4	8	14	OMU	C2-N1	7.24	1.50	1.38
53	2	1534	A2M	O4'-C1'	-7.21	1.31	1.41
53	2	2363	A2M	O4'-C1'	-7.21	1.31	1.41
53	2	398	A2M	O4'-C1'	-7.16	1.31	1.41
53	2	4523	A2M	O4'-C1'	-7.14	1.31	1.41
53	2	3825	A2M	O4'-C1'	-7.10	1.31	1.41
53	2	2786	B9H	C2-N1	7.09	1.48	1.38
53	2	2401	A2M	O4'-C1'	-7.08	1.31	1.41
53	2	4571	A2M	O4'-C1'	-7.05	1.31	1.41
53	2	3718	A2M	O4'-C1'	-7.01	1.31	1.41
53	2	4671	B8T	C4-N3	6.97	1.44	1.32
53	2	3723	A2M	O4'-C1'	-6.96	1.31	1.41
53	2	4671	B8T	C6-C5	6.91	1.51	1.35
53	2	4483	B8T	C4-N3	6.88	1.44	1.32
53	2	4620	OMU	C2-N1	6.86	1.49	1.38
53	2	978	2MG	C2-N2	6.81	1.48	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	8	14	OMU	C2-N3	6.77	1.50	1.38
53	2	2786	B9H	C6-C5	6.73	1.48	1.33
53	2	3909	OMC	C6-C5	6.70	1.50	1.35
53	2	4483	B8T	C6-C5	6.70	1.50	1.35
53	2	3897	B8K	C2-N3	6.68	1.49	1.33
53	2	4597	UR3	C6-C5	6.66	1.50	1.35
53	2	4530	UR3	C6-C5	6.66	1.50	1.35
53	2	1517	2MG	C2-N2	6.63	1.48	1.33
53	2	1871	A2M	O4'-C1'	-6.61	1.31	1.41
53	2	729	2MG	C2-N2	6.61	1.48	1.33
53	2	4690	B8K	C2-N3	6.59	1.49	1.33
53	2	4530	UR3	C2-N1	6.57	1.48	1.38
53	2	3887	OMC	C2-N3	6.45	1.49	1.36
53	2	1456	B8Q	C2-N3	6.44	1.46	1.35
53	2	4620	OMU	C2-N3	6.42	1.49	1.38
53	2	3701	OMC	C2-N3	6.39	1.49	1.36
53	2	2861	OMC	C2-N3	6.34	1.49	1.36
53	2	4494	OMG	C2-N3	6.33	1.48	1.33
53	2	4671	B8T	C4-N4	6.33	1.48	1.35
53	2	2422	OMC	C2-N3	6.33	1.49	1.36
53	2	4483	B8T	C4-N4	6.32	1.48	1.35
53	2	2297	E7G	C8-N7	6.31	1.51	1.45
53	2	3869	OMC	C2-N3	6.27	1.49	1.36
53	2	4536	OMC	C2-N3	6.26	1.49	1.36
53	2	2754	B9B	O6-C6	6.26	1.40	1.35
53	2	1625	OMG	C2-N3	6.25	1.48	1.33
53	2	4870	OMG	C2-N3	6.21	1.48	1.33
53	2	4872	2MG	C2-N2	6.21	1.47	1.33
53	2	2773	OMG	C2-N3	6.19	1.48	1.33
53	2	1909	P7G	C4-N9	6.18	1.44	1.35
53	2	2804	OMC	C2-N3	6.17	1.48	1.36
53	2	1909	P7G	C4-N3	6.17	1.48	1.37
53	2	3880	P7G	C4-N9	6.15	1.44	1.35
53	2	4597	UR3	C2-N3	6.14	1.50	1.39
53	2	1659	I4U	C2-N3	6.14	1.48	1.36
53	2	3880	P7G	C4-N3	6.13	1.48	1.37
53	2	3899	BGH	C4-N9	6.11	1.44	1.37
53	2	1625	OMG	C2-N2	6.11	1.48	1.34
53	2	3701	OMC	C6-C5	6.06	1.49	1.35
53	2	2773	OMG	C2-N2	6.05	1.48	1.34
53	2	1883	OMG	C2-N3	6.05	1.47	1.33
53	2	4637	OMG	C2-N3	6.04	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	2	4870	OMG	C2-N2	6.02	1.48	1.34
53	2	1348	P4U	C2-N3	6.01	1.48	1.36
53	2	1348	P4U	C6-C5	6.01	1.49	1.35
53	2	3897	B8K	C4-N9	6.01	1.44	1.37
53	2	237	B9B	O6-C6	6.01	1.40	1.35
53	2	2365	OMC	C2-N3	6.00	1.48	1.36
53	2	1316	OMG	C2-N3	5.99	1.47	1.33
53	2	373	OMG	C2-N2	5.99	1.48	1.34
53	2	1883	OMG	C2-N2	5.97	1.48	1.34
53	2	4494	OMG	C2-N2	5.96	1.48	1.34
53	2	2424	OMG	C2-N2	5.96	1.48	1.34
53	2	2424	OMG	C2-N3	5.96	1.47	1.33
53	2	2861	OMC	C6-C5	5.96	1.48	1.35
53	2	4536	OMC	C6-C5	5.93	1.48	1.35
53	2	1659	I4U	C6-C5	5.92	1.48	1.35
53	2	1316	OMG	C2-N2	5.92	1.48	1.34
53	2	2365	OMC	C6-C5	5.89	1.48	1.35
53	2	2364	OMG	C2-N3	5.88	1.47	1.33
53	2	373	OMG	C2-N3	5.88	1.47	1.33
53	2	4637	OMG	C2-N2	5.88	1.48	1.34
53	2	4564	M7A	C4-N9	5.87	1.49	1.38
53	2	1574	B9B	O6-C6	5.87	1.40	1.35
53	2	2804	OMC	C6-C5	5.87	1.48	1.35
53	2	1909	P7G	C2-N2	5.86	1.48	1.34
53	2	2050	OMG	C2-N2	5.85	1.48	1.34
53	2	1522	OMG	C2-N2	5.84	1.48	1.34
53	2	4597	UR3	C2-N1	5.83	1.46	1.38
53	2	3880	P7G	C2-N2	5.83	1.48	1.34
53	2	2050	OMG	C2-N3	5.82	1.47	1.33
53	2	1522	OMG	C2-N3	5.81	1.47	1.33
53	2	3880	P7G	C8-N7	5.80	1.51	1.45
53	2	2754	B9B	C2-N2	5.79	1.45	1.33
53	2	3887	OMC	C6-C5	5.79	1.48	1.35
53	2	3869	OMC	C6-C5	5.78	1.48	1.35
53	2	4550	7MG	C2-N3	5.77	1.47	1.33
53	2	2364	OMG	C2-N2	5.74	1.47	1.34
53	2	2422	OMC	C6-C5	5.74	1.48	1.35
53	2	4623	OMG	C2-N2	5.71	1.47	1.34
53	2	3909	OMC	C4-N4	5.71	1.47	1.33
53	2	4530	UR3	C2-N3	5.68	1.50	1.39
53	2	2522	7MG	C2-N3	5.64	1.46	1.33
53	2	2297	E7G	C4-N9	5.62	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	2	1605	7MG	C2-N3	5.62	1.46	1.33
53	2	3899	BGH	C4-N3	5.60	1.47	1.34
53	2	237	B9B	C2-N2	5.60	1.45	1.33
53	2	2297	E7G	C2-N3	5.60	1.46	1.33
53	2	3899	BGH	C2-N3	5.59	1.46	1.33
53	2	1574	B9B	C2-N2	5.57	1.45	1.33
4	8	14	OMU	C6-C5	5.55	1.47	1.35
53	2	4550	7MG	C4-N3	5.54	1.47	1.34
53	2	4623	OMG	C2-N3	5.54	1.46	1.33
53	2	2297	E7G	C4-N3	5.52	1.47	1.34
53	2	2522	7MG	C4-N3	5.52	1.47	1.34
53	2	4620	OMU	C6-C5	5.50	1.47	1.35
53	2	1909	P7G	C8-N7	5.48	1.51	1.45
53	2	1605	7MG	C4-N3	5.46	1.47	1.34
53	2	3909	OMC	C2-N1	5.46	1.51	1.40
53	2	3909	OMC	C2-N3	5.43	1.47	1.36
53	2	729	2MG	C4-N3	5.36	1.50	1.37
53	2	2522	7MG	C4-N9	5.34	1.43	1.37
53	2	3880	P7G	C2-N1	5.28	1.45	1.33
53	2	3701	OMC	C4-N3	5.27	1.45	1.34
53	2	1909	P7G	C2-N1	5.21	1.45	1.33
53	2	4550	7MG	C4-N9	5.20	1.43	1.37
53	2	4483	B8T	C2-N1	5.16	1.51	1.40
53	2	1605	7MG	C4-N9	5.16	1.43	1.37
53	2	2422	OMC	C2-N1	5.14	1.51	1.40
53	2	2861	OMC	C2-N1	5.13	1.51	1.40
53	2	3887	OMC	C4-N3	5.10	1.44	1.34
53	2	2861	OMC	C4-N3	5.06	1.44	1.34
53	2	978	2MG	C4-N3	5.06	1.49	1.37
53	2	1517	2MG	C4-N3	5.05	1.49	1.37
53	2	2804	OMC	C4-N3	5.05	1.44	1.34
53	2	2297	E7G	C2-N2	5.04	1.46	1.34
53	2	3887	OMC	C2-N1	5.03	1.50	1.40
53	2	3869	OMC	C4-N3	5.01	1.44	1.34
53	2	4690	B8K	C4-N9	5.00	1.43	1.37
53	2	4536	OMC	C2-N1	4.98	1.50	1.40
53	2	4536	OMC	C4-N3	4.96	1.44	1.34
53	2	4494	OMG	C4-N3	4.95	1.49	1.37
53	2	2422	OMC	C4-N3	4.95	1.44	1.34
53	2	3899	BGH	C2-N2	4.88	1.45	1.34
53	2	3701	OMC	C4-N4	4.87	1.45	1.33
53	2	3887	OMC	C4-N4	4.86	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	2	2861	OMC	C4-N4	4.86	1.45	1.33
53	2	1625	OMG	C4-N3	4.85	1.49	1.37
53	2	2365	OMC	C4-N4	4.83	1.45	1.33
53	2	4550	7MG	C2-N2	4.81	1.45	1.34
53	2	2804	OMC	C4-N4	4.80	1.45	1.33
53	2	4536	OMC	C4-N4	4.79	1.45	1.33
53	2	1605	7MG	C2-N2	4.79	1.45	1.34
53	2	4870	OMG	C4-N3	4.77	1.48	1.37
53	2	2422	OMC	C4-N4	4.77	1.45	1.33
53	2	3869	OMC	C4-N4	4.76	1.45	1.33
53	2	2365	OMC	C4-N3	4.74	1.44	1.34
53	2	2522	7MG	C2-N2	4.74	1.45	1.34
53	2	2773	OMG	C4-N3	4.70	1.48	1.37
53	2	4637	OMG	C4-N3	4.66	1.48	1.37
53	2	4872	2MG	C4-N3	4.66	1.48	1.37
53	2	1456	B8Q	C2-N1	4.66	1.45	1.38
53	2	2773	OMG	C6-N1	4.63	1.44	1.37
53	2	1316	OMG	C4-N3	4.62	1.48	1.37
53	2	373	OMG	C6-N1	4.61	1.44	1.37
53	2	1883	OMG	C4-N3	4.60	1.48	1.37
53	2	3869	OMC	C2-N1	4.59	1.49	1.40
53	2	4623	OMG	C6-N1	4.56	1.44	1.37
53	2	2424	OMG	C4-N3	4.56	1.48	1.37
53	2	3897	B8K	C4-N3	4.55	1.45	1.34
53	2	2050	OMG	C4-N3	4.54	1.48	1.37
53	2	373	OMG	C4-N3	4.52	1.48	1.37
53	2	3909	OMC	C4-N3	4.49	1.43	1.34
53	2	1348	P4U	C2-N1	4.49	1.49	1.40
53	2	4083	5MU	C2-N3	4.49	1.46	1.38
53	2	3701	OMC	C2-N1	4.48	1.49	1.40
53	2	1522	OMG	C4-N3	4.48	1.48	1.37
53	2	4671	B8T	C2-N1	4.47	1.49	1.40
53	2	2364	OMG	C4-N3	4.46	1.48	1.37
53	2	4870	OMG	C6-N1	4.45	1.44	1.37
53	2	3899	BGH	C5-N7	4.44	1.47	1.39
53	2	2804	OMC	C2-N1	4.43	1.49	1.40
53	2	2424	OMG	C6-N1	4.41	1.44	1.37
53	2	1316	OMG	C6-N1	4.40	1.44	1.37
53	2	1659	I4U	C5-C4	4.39	1.48	1.43
53	2	1522	OMG	C6-N1	4.38	1.44	1.37
53	2	1883	OMG	C6-N1	4.38	1.44	1.37
53	2	4690	B8K	C4-N3	4.38	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	2	4494	OMG	C6-N1	4.37	1.44	1.37
53	2	1348	P4U	O4-C4	4.37	1.40	1.35
53	2	1625	OMG	C6-N1	4.33	1.44	1.37
53	2	4637	OMG	C6-N1	4.33	1.44	1.37
53	2	2050	OMG	C6-N1	4.31	1.44	1.37
53	2	4564	M7A	C6-N6	4.29	1.44	1.34
53	2	3897	B8K	C5-N7	4.29	1.47	1.39
53	2	2364	OMG	C6-N1	4.29	1.44	1.37
53	2	4623	OMG	C4-N3	4.27	1.47	1.37
53	2	3897	B8K	C5-C6	4.25	1.54	1.43
53	2	978	2MG	C2-N1	4.24	1.43	1.36
4	8	14	OMU	C4-N3	4.24	1.46	1.38
53	2	1659	I4U	C2-N1	4.20	1.49	1.40
53	2	1517	2MG	C2-N1	4.20	1.43	1.36
53	2	4690	B8K	C5-N7	4.18	1.46	1.39
53	2	3899	BGH	C5-C6	4.17	1.54	1.43
53	2	2365	OMC	C2-N1	4.15	1.49	1.40
53	2	1348	P4U	C5-C4	4.13	1.48	1.43
53	2	4690	B8K	C5-C6	4.05	1.54	1.43
53	2	4872	2MG	C2-N1	4.03	1.43	1.36
53	2	729	2MG	C2-N1	3.84	1.42	1.36
53	2	4620	OMU	C4-N3	3.83	1.45	1.38
53	2	4550	7MG	C5-C6	3.82	1.53	1.43
53	2	978	2MG	C6-N1	3.79	1.43	1.37
53	2	1517	2MG	C6-N1	3.73	1.43	1.37
53	2	1909	P7G	C2-N3	3.73	1.46	1.37
53	2	4671	B8T	C5-C4	3.68	1.48	1.40
53	2	1605	7MG	C2-N1	3.68	1.46	1.37
53	2	2522	7MG	C5-C6	3.65	1.53	1.43
53	2	3897	B8K	C71-N7	3.64	1.47	1.39
53	2	1605	7MG	C5-C6	3.63	1.52	1.43
53	2	2297	E7G	C5-C6	3.63	1.52	1.43
53	2	3880	P7G	C2-N3	3.62	1.46	1.37
53	2	3909	OMC	C6-N1	3.61	1.46	1.38
53	2	1909	P7G	C6-N1	3.60	1.44	1.38
53	2	4564	M7A	C5-N7	3.59	1.48	1.39
53	2	3880	P7G	C6-N1	3.57	1.44	1.38
53	2	3899	BGH	C71-N7	3.55	1.47	1.39
53	2	4483	B8T	C6-N1	3.55	1.46	1.38
53	2	4550	7MG	C2-N1	3.54	1.46	1.37
53	2	3899	BGH	O2'-C2'	3.54	1.51	1.42
53	2	4690	B8K	C6-N1	3.54	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	2	2522	7MG	C2-N1	3.52	1.46	1.37
53	2	4483	B8T	C5-C4	3.50	1.48	1.40
53	2	3897	B8K	C2-N2	3.50	1.42	1.34
53	2	4690	B8K	C2-N2	3.50	1.42	1.34
53	2	4690	B8K	C71-N7	3.49	1.47	1.39
53	2	4083	5MU	C2-N1	3.47	1.44	1.38
53	2	3897	B8K	C6-N1	3.47	1.45	1.38
53	2	729	2MG	C5-C6	3.44	1.54	1.47
53	2	978	2MG	C5-C6	3.44	1.54	1.47
53	2	4872	2MG	C5-C6	3.41	1.54	1.47
53	2	4623	OMG	C5-C6	3.41	1.54	1.47
53	2	4530	UR3	C6-N1	3.39	1.46	1.38
53	2	1605	7MG	C6-N1	3.39	1.45	1.38
53	2	729	2MG	C6-N1	3.38	1.42	1.37
53	2	4872	2MG	C6-N1	3.38	1.42	1.37
53	2	3887	OMC	C6-N1	3.35	1.46	1.38
53	2	1909	P7G	C5-C4	3.31	1.43	1.37
53	2	2297	E7G	C2-N1	3.31	1.45	1.37
53	2	1517	2MG	C5-C6	3.29	1.54	1.47
53	2	3880	P7G	O6-C6	-3.28	1.18	1.23
53	2	4550	7MG	C6-N1	3.27	1.44	1.38
53	2	2773	OMG	C5-C6	3.26	1.54	1.47
53	2	1348	P4U	C6-N1	3.26	1.45	1.38
53	2	2522	7MG	C6-N1	3.25	1.44	1.38
53	2	4870	OMG	C5-C6	3.24	1.54	1.47
53	2	2861	OMC	C6-N1	3.23	1.45	1.38
53	2	3899	BGH	C2-N1	3.22	1.45	1.37
53	2	2422	OMC	C6-N1	3.22	1.45	1.38
53	2	2365	OMC	C6-N1	3.21	1.45	1.38
53	2	3869	OMC	C6-N1	3.21	1.45	1.38
53	2	1659	I4U	C6-N1	3.21	1.45	1.38
53	2	4494	OMG	C5-C6	3.20	1.53	1.47
53	2	3899	BGH	C6-N1	3.18	1.44	1.38
53	2	1909	P7G	O6-C6	-3.18	1.18	1.23
53	2	4690	B8K	C2-N1	3.16	1.45	1.37
53	2	3897	B8K	C2-N1	3.16	1.45	1.37
53	2	1534	A2M	C6-N6	3.16	1.45	1.34
53	2	3825	A2M	C6-N6	3.16	1.45	1.34
53	2	3718	A2M	C6-N6	3.16	1.45	1.34
53	2	1522	OMG	C5-C6	3.16	1.53	1.47
53	2	1524	A2M	C6-N6	3.16	1.45	1.34
53	2	4637	OMG	C5-C6	3.15	1.53	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	2	1871	A2M	C6-N6	3.14	1.45	1.34
53	2	4523	A2M	C6-N6	3.13	1.45	1.34
53	2	2804	OMC	C6-N1	3.13	1.45	1.38
53	2	3723	A2M	C6-N6	3.13	1.45	1.34
53	2	3880	P7G	C5-C4	3.12	1.43	1.37
53	2	2401	A2M	C6-N6	3.12	1.45	1.34
53	2	4671	B8T	C6-N1	3.12	1.45	1.38
53	2	4536	OMC	C6-N1	3.11	1.45	1.38
53	2	1326	A2M	C6-N6	3.11	1.45	1.34
53	2	398	A2M	C6-N6	3.10	1.45	1.34
53	2	4571	A2M	C6-N6	3.10	1.45	1.34
53	2	4620	OMU	O4-C4	-3.08	1.18	1.24
53	2	3867	A2M	C6-N6	3.08	1.45	1.34
53	2	3701	OMC	C6-N1	3.06	1.45	1.38
53	2	2297	E7G	C6-N1	3.05	1.44	1.38
53	2	373	OMG	C5-C6	3.04	1.53	1.47
53	2	2364	OMG	C5-C6	3.04	1.53	1.47
53	2	1316	OMG	C5-C6	3.04	1.53	1.47
53	2	2363	A2M	C6-N6	3.03	1.45	1.34
53	2	2050	OMG	C5-C6	3.03	1.53	1.47
53	2	1625	OMG	C5-C6	3.02	1.53	1.47
53	2	4597	UR3	C6-N1	3.00	1.45	1.38
53	2	3899	BGH	O3'-C3'	-2.99	1.35	1.43
53	2	3897	B8K	C5-C4	2.97	1.47	1.38
53	2	1534	A2M	O3'-C3'	2.97	1.50	1.43
53	2	1883	OMG	O6-C6	-2.94	1.17	1.23
53	2	4083	5MU	O4-C4	-2.93	1.18	1.23
53	2	3825	A2M	O3'-C3'	2.92	1.49	1.43
53	2	2050	OMG	O6-C6	-2.91	1.17	1.23
53	2	1524	A2M	O3'-C3'	2.90	1.49	1.43
53	2	4872	2MG	C5-C4	-2.89	1.35	1.43
53	2	3718	A2M	O3'-C3'	2.89	1.49	1.43
53	2	978	2MG	C5-C4	-2.89	1.35	1.43
53	2	3867	A2M	O3'-C3'	2.88	1.49	1.43
53	2	2380	B8W	C5-C4	-2.88	1.33	1.40
53	2	2363	A2M	O3'-C3'	2.87	1.49	1.43
53	2	1517	2MG	C5-C4	-2.87	1.35	1.43
53	2	1883	OMG	C5-C6	2.86	1.53	1.47
53	2	4637	OMG	O6-C6	-2.86	1.17	1.23
53	2	2401	A2M	O3'-C3'	2.85	1.49	1.43
53	2	1522	OMG	O6-C6	-2.85	1.17	1.23
53	2	4185	B8W	C5-C4	-2.85	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	8	14	OMU	O4-C4	-2.84	1.19	1.24
53	2	398	A2M	O3'-C3'	2.84	1.49	1.43
53	2	4083	5MU	O2-C2	-2.84	1.17	1.23
53	2	2365	OMC	O2-C2	-2.84	1.18	1.23
53	2	2363	A2M	O2'-C2'	-2.83	1.35	1.42
53	2	2424	OMG	C5-C6	2.82	1.53	1.47
53	2	1326	A2M	O3'-C3'	2.80	1.49	1.43
53	2	2364	OMG	O6-C6	-2.80	1.17	1.23
4	8	14	OMU	C6-N1	2.80	1.44	1.38
53	2	1316	OMG	O6-C6	-2.80	1.17	1.23
53	2	4623	OMG	O6-C6	-2.80	1.17	1.23
53	2	2754	B9B	C5-C4	-2.80	1.33	1.40
53	2	4671	B8T	O2-C2	-2.79	1.18	1.23
53	2	2804	OMC	O2-C2	-2.79	1.18	1.23
53	2	1659	I4U	O2-C2	-2.78	1.18	1.23
53	2	1659	I4U	O4-C4	2.78	1.40	1.35
53	2	1348	P4U	O2-C2	-2.78	1.18	1.23
53	2	4870	OMG	O6-C6	-2.77	1.17	1.23
53	2	4494	OMG	O6-C6	-2.76	1.17	1.23
53	2	4571	A2M	C5-C4	-2.76	1.33	1.40
53	2	3869	OMC	O2-C2	-2.76	1.18	1.23
53	2	1524	A2M	O2'-C2'	-2.76	1.35	1.42
53	2	3899	BGH	O6-C6	-2.75	1.18	1.23
53	2	237	B9B	C5-C4	-2.75	1.33	1.40
53	2	4472	B8W	C5-C4	-2.75	1.33	1.40
53	2	2424	OMG	O6-C6	-2.75	1.17	1.23
53	2	1871	A2M	O3'-C3'	2.74	1.49	1.43
53	2	2363	A2M	C5-C4	-2.74	1.33	1.40
53	2	4571	A2M	O3'-C3'	2.74	1.49	1.43
53	2	1574	B9B	C5-C4	-2.74	1.33	1.40
53	2	4571	A2M	O2'-C2'	-2.74	1.35	1.42
53	2	3723	A2M	O3'-C3'	2.73	1.49	1.43
53	2	4483	B8T	O2-C2	-2.73	1.18	1.23
53	2	373	OMG	O6-C6	-2.73	1.17	1.23
53	2	2773	OMG	O6-C6	-2.72	1.17	1.23
53	2	729	2MG	C5-C4	-2.71	1.36	1.43
53	2	398	A2M	C5-C4	-2.71	1.33	1.40
53	2	3909	OMC	C5-C4	2.70	1.49	1.42
53	2	3867	A2M	C5-C4	-2.69	1.33	1.40
53	2	2401	A2M	O2'-C2'	-2.69	1.35	1.42
53	2	1659	I4U	O4-C41	-2.68	1.40	1.47
53	2	4523	A2M	O3'-C3'	2.68	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	2	1326	A2M	C5-C4	-2.68	1.33	1.40
53	2	1534	A2M	O2'-C2'	-2.67	1.35	1.42
53	2	1625	OMG	O6-C6	-2.67	1.17	1.23
53	2	4536	OMC	O2-C2	-2.67	1.18	1.23
53	2	1534	A2M	C5-C4	-2.66	1.33	1.40
53	2	2401	A2M	C5-C4	-2.66	1.33	1.40
53	2	3718	A2M	O2'-C2'	-2.66	1.35	1.42
53	2	4690	B8K	C5-C4	2.65	1.46	1.38
53	2	3825	A2M	C5-C4	-2.63	1.34	1.40
53	2	4523	A2M	C5-C4	-2.62	1.34	1.40
53	2	1605	7MG	O6-C6	-2.61	1.18	1.23
53	2	3825	A2M	O2'-C2'	-2.60	1.35	1.42
53	2	4529	B8W	C5-C4	-2.60	1.34	1.40
53	2	3723	A2M	C5-C4	-2.60	1.34	1.40
53	2	3718	A2M	C5-C4	-2.59	1.34	1.40
53	2	4523	A2M	O2'-C2'	-2.59	1.36	1.42
53	2	2773	OMG	C2-N1	2.59	1.44	1.37
53	2	2522	7MG	O6-C6	-2.58	1.18	1.23
53	2	1871	A2M	C5-C4	-2.57	1.34	1.40
53	2	3701	OMC	O2-C2	-2.56	1.19	1.23
53	2	398	A2M	O2'-C2'	-2.56	1.36	1.42
53	2	3701	OMC	C5-C4	2.55	1.48	1.42
53	2	3887	OMC	O2-C2	-2.55	1.19	1.23
53	2	373	OMG	C2-N1	2.55	1.44	1.37
53	2	2422	OMC	O2-C2	-2.55	1.19	1.23
53	2	1871	A2M	O2'-C2'	-2.54	1.36	1.42
53	2	2861	OMC	O2-C2	-2.54	1.19	1.23
53	2	4620	OMU	C6-N1	2.53	1.44	1.38
53	2	2297	E7G	O6-C6	-2.52	1.18	1.23
53	2	1524	A2M	C5-C4	-2.52	1.34	1.40
53	2	4530	UR3	C4-N3	2.52	1.46	1.40
53	2	4623	OMG	C5-C4	-2.51	1.36	1.43
53	2	4620	OMU	O2-C2	-2.51	1.18	1.23
53	2	373	OMG	C5-C4	-2.51	1.36	1.43
53	2	1326	A2M	O2'-C2'	-2.50	1.36	1.42
53	2	3867	A2M	C2-N3	2.49	1.36	1.32
53	2	1883	OMG	C5-C4	-2.49	1.36	1.43
53	2	4129	B8W	C5-C4	-2.48	1.34	1.40
53	2	4550	7MG	O6-C6	-2.48	1.18	1.23
53	2	3723	A2M	O2'-C2'	-2.48	1.36	1.42
53	2	1522	OMG	C2-N1	2.46	1.43	1.37
53	2	4870	OMG	C2-N1	2.45	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	2	1534	A2M	C2-N3	2.42	1.36	1.32
53	2	2804	OMC	C5-C4	2.41	1.48	1.42
53	2	2861	OMC	C5-C4	2.41	1.48	1.42
53	2	1316	OMG	C5-C4	-2.41	1.36	1.43
53	2	3867	A2M	O2'-C2'	-2.41	1.36	1.42
53	2	1625	OMG	C2-N1	2.40	1.43	1.37
53	2	1883	OMG	C2-N1	2.40	1.43	1.37
4	8	14	OMU	C5-C4	2.40	1.48	1.43
53	2	4637	OMG	C2-N1	2.40	1.43	1.37
53	2	2050	OMG	C2-N1	2.39	1.43	1.37
53	2	2364	OMG	C2-N1	2.39	1.43	1.37
53	2	1871	A2M	C2-N3	2.39	1.35	1.32
53	2	1316	OMG	C2-N1	2.38	1.43	1.37
53	2	4623	OMG	C2-N1	2.37	1.43	1.37
53	2	2424	OMG	C2-N1	2.36	1.43	1.37
53	2	1522	OMG	C5-C4	-2.36	1.37	1.43
53	2	4494	OMG	C2-N1	2.35	1.43	1.37
53	2	4523	A2M	C2-N3	2.35	1.35	1.32
53	2	2050	OMG	C5-C4	-2.35	1.37	1.43
53	2	1524	A2M	C2-N3	2.35	1.35	1.32
53	2	2424	OMG	C5-C4	-2.35	1.37	1.43
53	2	3825	A2M	C2-N3	2.32	1.35	1.32
53	2	1326	A2M	C2-N3	2.32	1.35	1.32
53	2	4870	OMG	C5-C4	-2.32	1.37	1.43
53	2	3723	A2M	C2-N3	2.31	1.35	1.32
4	8	14	OMU	O2-C2	-2.30	1.18	1.23
53	2	3909	OMC	O2-C2	-2.30	1.19	1.23
53	2	1456	B8Q	C6-N1	2.30	1.43	1.38
53	2	2364	OMG	C5-C4	-2.29	1.37	1.43
53	2	3887	OMC	C5-C4	2.28	1.48	1.42
53	2	4637	OMG	C5-C4	-2.25	1.37	1.43
53	2	4536	OMC	C5-C4	2.24	1.48	1.42
53	2	2365	OMC	C5-C4	2.24	1.48	1.42
53	2	2401	A2M	C2-N3	2.23	1.35	1.32
53	2	398	A2M	C2-N3	2.20	1.35	1.32
53	2	4597	UR3	C5-C4	2.19	1.49	1.43
53	2	2363	A2M	C2-N3	2.18	1.35	1.32
53	2	2773	OMG	C5-C4	-2.17	1.37	1.43
53	2	4571	A2M	C2-N3	2.15	1.35	1.32
53	2	4494	OMG	C5-C4	-2.14	1.37	1.43
53	2	1625	OMG	C5-C4	-2.14	1.37	1.43
53	2	4620	OMU	C5-C4	2.14	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	2	3718	A2M	C2-N3	2.13	1.35	1.32
53	2	1871	A2M	O5'-C5'	-2.12	1.39	1.44
53	2	4530	UR3	C5-C4	2.11	1.49	1.43
53	2	4597	UR3	C4-N3	2.11	1.45	1.40
53	2	4597	UR3	O2-C2	-2.10	1.18	1.22
53	2	3869	OMC	C5-C4	2.10	1.47	1.42
53	2	2422	OMC	C5-C4	2.07	1.47	1.42
53	2	3899	BGH	C5-C4	2.05	1.44	1.38
53	2	1456	B8Q	O2-C2	-2.01	1.18	1.22
53	2	4530	UR3	O2-C2	-2.00	1.18	1.22

All (312) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	2	2754	B9B	O6-C6-N1	-29.96	94.26	120.12
53	2	237	B9B	O6-C6-N1	-29.36	94.78	120.12
53	2	1574	B9B	O6-C6-N1	-29.34	94.80	120.12
53	2	4564	M7A	C5-C6-N6	13.75	147.23	123.74
53	2	4564	M7A	N6-C6-N1	-11.72	92.67	118.35
53	2	1326	A2M	C5-C6-N6	10.64	136.52	120.35
53	2	398	A2M	C5-C6-N6	10.61	136.48	120.35
53	2	1534	A2M	C5-C6-N6	10.57	136.41	120.35
53	2	3825	A2M	C5-C6-N6	10.53	136.36	120.35
53	2	4523	A2M	C5-C6-N6	10.52	136.35	120.35
53	2	1871	A2M	C5-C6-N6	10.50	136.31	120.35
53	2	2401	A2M	C5-C6-N6	10.32	136.04	120.35
53	2	3723	A2M	C5-C6-N6	10.29	135.98	120.35
53	2	3718	A2M	C5-C6-N6	10.26	135.94	120.35
53	2	3867	A2M	C5-C6-N6	10.26	135.94	120.35
53	2	4571	A2M	C5-C6-N6	10.25	135.93	120.35
53	2	1524	A2M	C5-C6-N6	10.19	135.84	120.35
53	2	2363	A2M	C5-C6-N6	10.11	135.72	120.35
53	2	4083	5MU	C5-C4-N3	10.06	123.89	115.31
53	2	4083	5MU	C5-C6-N1	-7.88	115.23	123.34
53	2	4597	UR3	C4-N3-C2	-7.64	117.37	124.56
53	2	1534	A2M	N6-C6-N1	-7.53	102.93	118.57
53	2	1326	A2M	N6-C6-N1	-7.51	102.98	118.57
53	2	3825	A2M	N6-C6-N1	-7.46	103.10	118.57
53	2	4523	A2M	N6-C6-N1	-7.45	103.10	118.57
53	2	398	A2M	N6-C6-N1	-7.44	103.13	118.57
53	2	1871	A2M	N6-C6-N1	-7.31	103.39	118.57
53	2	3867	A2M	N6-C6-N1	-7.23	103.56	118.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	2	3723	A2M	N6-C6-N1	-7.22	103.58	118.57
53	2	4571	A2M	N6-C6-N1	-7.17	103.70	118.57
53	2	2363	A2M	N6-C6-N1	-7.15	103.73	118.57
53	2	1524	A2M	N6-C6-N1	-7.10	103.84	118.57
53	2	2401	A2M	N6-C6-N1	-7.08	103.88	118.57
53	2	4083	5MU	C4-N3-C2	-7.02	118.26	127.35
53	2	3718	A2M	N6-C6-N1	-6.95	104.15	118.57
53	2	2786	B9H	C31-N3-C2	6.81	125.72	117.21
53	2	4571	A2M	N3-C2-N1	-6.49	118.54	128.68
53	2	3897	B8K	C72-C71-N7	6.37	128.44	118.86
53	2	4690	B8K	C72-C71-N7	6.35	128.41	118.86
53	2	1871	A2M	N3-C2-N1	-6.35	118.76	128.68
53	2	3867	A2M	N3-C2-N1	-6.34	118.77	128.68
53	2	3825	A2M	N3-C2-N1	-6.34	118.78	128.68
53	2	398	A2M	N3-C2-N1	-6.32	118.80	128.68
53	2	2363	A2M	N3-C2-N1	-6.29	118.85	128.68
53	2	1326	A2M	N3-C2-N1	-6.28	118.86	128.68
53	2	2401	A2M	N3-C2-N1	-6.28	118.86	128.68
53	2	1524	A2M	N3-C2-N1	-6.25	118.91	128.68
53	2	4523	A2M	N3-C2-N1	-6.25	118.91	128.68
53	2	1534	A2M	N3-C2-N1	-6.23	118.94	128.68
53	2	3899	BGH	C72-C71-N7	6.18	128.16	118.86
53	2	3723	A2M	N3-C2-N1	-6.18	119.02	128.68
53	2	4129	B8W	C2-N3-C4	6.12	122.35	115.36
53	2	4564	M7A	N3-C2-N1	-6.06	119.11	128.60
53	2	3718	A2M	N3-C2-N1	-6.05	119.22	128.68
53	2	4690	B8K	C5-C6-N1	6.05	121.65	110.99
53	2	3899	BGH	C5-C6-N1	5.77	121.16	110.99
53	2	4472	B8W	N3-C2-N1	-5.70	119.61	127.22
53	2	4185	B8W	N2-C2-N3	5.69	127.07	117.79
53	2	2380	B8W	N2-C2-N3	5.67	127.04	117.79
53	2	3897	B8K	C5-C6-N1	5.65	120.96	110.99
53	2	4129	B8W	N2-C2-N3	5.64	126.98	117.79
53	2	4529	B8W	N2-C2-N3	5.63	126.96	117.79
53	2	3909	OMC	O2-C2-N3	-5.63	113.18	122.33
53	2	2754	B9B	N3-C2-N1	-5.57	119.79	127.22
53	2	4129	B8W	N3-C2-N1	-5.57	119.79	127.22
53	2	1456	B8Q	N3-C2-N1	5.51	123.60	117.13
53	2	4472	B8W	N2-C2-N3	5.41	126.60	117.79
53	2	4185	B8W	N3-C2-N1	-5.41	120.01	127.22
53	2	2786	B9H	C6-N1-C2	-5.33	117.01	121.79
53	2	2380	B8W	N3-C2-N1	-5.27	120.19	127.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	2	1574	B9B	N3-C2-N1	-5.25	120.21	127.22
53	2	237	B9B	N3-C2-N1	-5.25	120.22	127.22
53	2	3899	BGH	C2-N3-C4	5.19	121.55	112.30
53	2	4529	B8W	N3-C2-N1	-5.12	120.39	127.22
4	8	14	OMU	C4-N3-C2	-5.11	119.84	126.58
53	2	4620	OMU	C4-N3-C2	-5.09	119.86	126.58
53	2	1909	P7G	C4-C5-N7	5.04	109.33	106.67
53	2	3880	P7G	C4-C5-N7	5.02	109.32	106.67
53	2	2522	7MG	C5-C6-N1	5.01	119.82	110.99
53	2	4083	5MU	N3-C2-N1	5.00	121.53	114.89
53	2	2297	E7G	C5-C6-N1	5.00	119.80	110.99
53	2	1456	B8Q	C31-N3-C4	5.00	121.78	114.25
53	2	4564	M7A	N3-C4-N9	4.98	133.16	126.87
53	2	4550	7MG	C5-C6-N1	4.97	119.75	110.99
53	2	1605	7MG	C5-C6-N1	4.97	119.74	110.99
53	2	4529	B8W	O6-C6-N1	4.92	125.85	119.03
53	2	4083	5MU	C5M-C5-C6	-4.90	116.31	122.85
53	2	2297	E7G	C4-C5-N7	4.89	109.26	104.91
53	2	1456	B8Q	O2-C2-N3	-4.83	115.86	122.95
53	2	3897	B8K	C2-N3-C4	4.82	120.88	112.30
53	2	4690	B8K	C2-N3-C4	4.78	120.81	112.30
53	2	2754	B9B	C2-N3-C4	4.76	120.80	115.36
53	2	4185	B8W	C2-N3-C4	4.73	120.76	115.36
53	2	4530	UR3	C4-N3-C2	-4.67	120.17	124.56
53	2	237	B9B	C2-N3-C4	4.65	120.67	115.36
53	2	4472	B8W	C2-N3-C4	4.54	120.54	115.36
53	2	4550	7MG	C2-N3-C4	4.44	120.22	112.30
53	2	2754	B9B	N2-C2-N3	4.44	125.03	117.79
53	2	1605	7MG	C2-N3-C4	4.43	120.20	112.30
53	2	2297	E7G	C2-N3-C4	4.40	120.15	112.30
53	2	237	B9B	N2-C2-N3	4.37	124.91	117.79
53	2	1574	B9B	C2-N3-C4	4.35	120.32	115.36
53	2	4690	B8K	C4-C5-N7	4.33	108.76	104.91
53	2	2522	7MG	C2-N3-C4	4.33	120.01	112.30
53	2	2786	B9H	C21-O2'-C2'	4.31	125.83	114.52
53	2	4185	B8W	O6-C6-N1	4.30	124.99	119.03
53	2	4872	2MG	CM2-N2-C2	-4.30	114.36	123.86
53	2	3897	B8K	C4-C5-N7	4.26	108.70	104.91
53	2	1574	B9B	N2-C2-N3	4.24	124.70	117.79
53	2	3909	OMC	O2-C2-N1	4.24	127.64	118.89
53	2	4529	B8W	C2-N3-C4	4.21	120.17	115.36
53	2	3899	BGH	C5-C4-N9	4.10	111.67	106.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	2	1659	I4U	C5-C4-N3	-4.08	118.71	124.91
53	2	3899	BGH	C4-C5-N7	3.98	108.45	104.91
53	2	2380	B8W	C2-N3-C4	3.98	119.90	115.36
53	2	3899	BGH	N9-C8-N7	3.96	108.65	103.33
53	2	4083	5MU	O4-C4-C5	-3.93	120.35	124.90
53	2	3897	B8K	N9-C8-N7	3.88	108.54	103.33
53	2	4690	B8K	C5-C4-N9	3.87	111.36	106.35
53	2	3897	B8K	C5-C4-N9	3.86	111.36	106.35
53	2	2297	E7G	C5-C4-N3	-3.79	120.91	128.13
53	2	4083	5MU	C5M-C5-C4	3.78	122.93	118.77
53	2	1456	B8Q	C6-N1-C2	-3.75	118.43	121.79
53	2	4620	OMU	N3-C2-N1	3.71	119.81	114.89
53	2	2380	B8W	C1'-N9-C4	-3.69	120.15	126.64
53	2	3899	BGH	C5-C4-N3	-3.68	121.12	128.13
53	2	729	2MG	C5-C6-N1	3.65	120.40	113.95
53	2	4872	2MG	C5-C6-N1	3.64	120.39	113.95
53	2	1517	2MG	C5-C6-N1	3.62	120.34	113.95
53	2	4550	7MG	C5-C4-N3	-3.62	121.24	128.13
53	2	1605	7MG	C5-C4-N9	3.62	111.04	106.35
53	2	2522	7MG	C5-C4-N3	-3.61	121.25	128.13
53	2	978	2MG	C5-C6-N1	3.61	120.33	113.95
53	2	4494	OMG	C5-C6-N1	3.60	120.30	113.95
53	2	4637	OMG	C5-C6-N1	3.58	120.28	113.95
53	2	4550	7MG	C5-C4-N9	3.57	110.98	106.35
53	2	4564	M7A	C2-N3-C4	3.55	120.14	111.75
53	2	1883	OMG	C5-C6-N1	3.55	120.21	113.95
4	8	14	OMU	N3-C2-N1	3.53	119.58	114.89
53	2	1605	7MG	C5-C4-N3	-3.53	121.41	128.13
53	2	2424	OMG	C5-C6-N1	3.52	120.16	113.95
53	2	4870	OMG	C5-C6-N1	3.51	120.16	113.95
53	2	2297	E7G	C5-C4-N9	3.51	110.90	106.35
53	2	2522	7MG	C5-C4-N9	3.50	110.89	106.35
53	2	1316	OMG	C5-C6-N1	3.47	120.08	113.95
53	2	2773	OMG	C5-C6-N1	3.46	120.07	113.95
53	2	1348	P4U	C5-C4-N3	-3.46	119.65	124.91
53	2	2380	B8W	O6-C6-N1	3.43	123.79	119.03
4	8	14	OMU	C5-C4-N3	3.40	119.93	114.84
53	2	4620	OMU	C5-C4-N3	3.40	119.92	114.84
53	2	2364	OMG	C5-C6-N1	3.39	119.94	113.95
53	2	4690	B8K	C6-C5-C4	-3.39	115.63	122.62
53	2	2050	OMG	C5-C6-N1	3.38	119.92	113.95
53	2	3897	B8K	C5-C4-N3	-3.37	121.71	128.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	2	4690	B8K	N9-C8-N7	3.37	107.85	103.33
53	2	1625	OMG	C5-C6-N1	3.33	119.84	113.95
53	2	373	OMG	C5-C6-N1	3.33	119.83	113.95
53	2	1522	OMG	C5-C6-N1	3.33	119.83	113.95
53	2	4472	B8W	C1'-N9-C4	-3.32	120.82	126.64
53	2	2422	OMC	O2-C2-N3	-3.31	116.94	122.33
53	2	2364	OMG	C2-N1-C6	-3.31	119.00	125.10
53	2	1909	P7G	N9-C8-N7	3.30	108.10	103.38
53	2	4637	OMG	C2-N1-C6	-3.27	119.07	125.10
53	2	4083	5MU	C6-C5-C4	3.27	120.76	118.03
53	2	4623	OMG	C5-C6-N1	3.26	119.71	113.95
53	2	4494	OMG	C2-N1-C6	-3.24	119.14	125.10
53	2	2861	OMC	O2-C2-N3	-3.23	117.07	122.33
53	2	4483	B8T	O2-C2-N3	-3.23	117.08	122.33
53	2	1316	OMG	C2-N1-C6	-3.17	119.25	125.10
53	2	3909	OMC	C5-C4-N4	3.16	125.54	120.57
53	2	2363	A2M	C1'-N9-C4	3.14	132.15	126.64
53	2	2050	OMG	C2-N1-C6	-3.13	119.34	125.10
53	2	3909	OMC	C4-N3-C2	3.10	125.27	120.25
53	2	1883	OMG	C2-N1-C6	-3.08	119.43	125.10
53	2	4870	OMG	C2-N1-C6	-3.05	119.48	125.10
53	2	3897	B8K	C6-C5-C4	-3.05	116.34	122.62
53	2	2773	OMG	C2-N1-C6	-3.04	119.50	125.10
53	2	1625	OMG	C2-N1-C6	-3.03	119.51	125.10
53	2	2424	OMG	C2-N1-C6	-3.01	119.56	125.10
53	2	4536	OMC	O2-C2-N3	-3.01	117.44	122.33
53	2	4623	OMG	C2-N1-C6	-3.00	119.57	125.10
53	2	4129	B8W	O6-C6-N1	3.00	123.18	119.03
53	2	1605	7MG	N9-C8-N7	2.98	107.65	103.38
53	2	4690	B8K	C5-C4-N3	-2.98	122.46	128.13
53	2	3887	OMC	O2-C2-N3	-2.97	117.50	122.33
53	2	373	OMG	C2-N1-C6	-2.97	119.63	125.10
53	2	4529	B8W	N2-C2-N1	-2.96	112.65	117.25
53	2	2786	B9H	O2'-C2'-C1'	2.95	114.83	109.08
53	2	4564	M7A	C4-N9-C1'	-2.94	119.61	126.60
53	2	4483	B8T	O3'-C3'-C2'	2.94	121.32	111.82
53	2	1522	OMG	C2-N1-C6	-2.93	119.69	125.10
53	2	3899	BGH	C6-C5-C4	-2.92	116.60	122.62
4	8	14	OMU	O4-C4-C5	-2.92	120.03	125.16
53	2	4620	OMU	O4-C4-C5	-2.91	120.04	125.16
53	2	2522	7MG	N9-C8-N7	2.89	107.51	103.38
53	2	2380	B8W	N2-C2-N1	-2.88	112.77	117.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	2	3899	BGH	O6-C6-N1	-2.88	114.60	120.12
53	2	237	B9B	C61-O6-C6	-2.86	112.17	117.51
53	2	1574	B9B	C61-O6-C6	-2.85	112.19	117.51
53	2	2861	OMC	C1'-N1-C2	2.84	124.75	118.42
53	2	3909	OMC	C5-C4-N3	-2.82	116.53	121.33
53	2	2522	7MG	C4-C5-N7	2.80	109.42	105.53
53	2	4185	B8W	N2-C2-N1	-2.79	112.92	117.25
53	2	4597	UR3	C3U-N3-C2	2.78	122.18	117.31
53	2	1605	7MG	C4-C5-N7	2.74	109.34	105.53
53	2	4623	OMG	N2-C2-N1	2.73	122.53	116.71
53	2	4185	B8W	C1'-N9-C4	-2.73	121.84	126.64
53	2	3897	B8K	O6-C6-N1	-2.73	114.89	120.12
53	2	4597	UR3	C6-N1-C2	-2.70	119.37	121.79
53	2	1348	P4U	O2-C2-N3	-2.70	117.95	122.33
53	2	4472	B8W	C2-N1-C6	2.69	120.41	116.08
53	2	3867	A2M	C1'-N9-C4	2.67	131.32	126.64
53	2	4671	B8T	C6-C5-C4	2.65	120.20	116.96
53	2	2786	B9H	O2-C2-N1	-2.64	116.53	122.72
53	2	4550	7MG	C4-C5-N7	2.64	109.20	105.53
53	2	4472	B8W	O6-C6-N1	2.62	122.66	119.03
53	2	1524	A2M	C1'-N9-C4	2.61	131.23	126.64
53	2	4690	B8K	C2-N1-C6	-2.60	120.35	125.10
53	2	4550	7MG	N9-C8-N7	2.60	107.09	103.38
53	2	4530	UR3	C6-N1-C2	-2.59	119.47	121.79
53	2	4129	B8W	N2-C2-N1	-2.59	113.23	117.25
53	2	1456	B8Q	C1'-N1-C2	2.59	121.36	116.99
53	2	729	2MG	C8-N7-C5	2.58	107.91	102.99
53	2	1316	OMG	C8-N7-C5	2.58	107.91	102.99
53	2	4083	5MU	O2-C2-N1	-2.58	119.36	122.79
53	2	2297	E7G	N9-C8-N7	2.58	107.07	103.38
53	2	4872	2MG	C8-N7-C5	2.58	107.90	102.99
53	2	1909	P7G	C71-N7-C5	2.57	130.60	124.52
53	2	4564	M7A	C5-C4-N3	-2.56	120.61	126.62
53	2	4483	B8T	O3'-C3'-C4'	2.56	118.46	111.05
53	2	1883	OMG	O6-C6-C5	-2.55	119.38	124.37
53	2	1534	A2M	C1'-N9-C4	2.55	131.12	126.64
53	2	978	2MG	CM2-N2-C2	-2.54	118.25	123.86
4	8	14	OMU	C1'-N1-C2	2.54	122.16	117.57
53	2	4690	B8K	O6-C6-N1	-2.53	115.26	120.12
53	2	3825	A2M	C1'-N9-C4	2.53	131.09	126.64
53	2	978	2MG	C8-N7-C5	2.51	107.78	102.99
53	2	3880	P7G	N9-C8-N7	2.51	106.97	103.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	2	2422	OMC	C1'-N1-C2	2.49	123.99	118.42
53	2	2522	7MG	C2-N1-C6	-2.48	120.58	125.10
53	2	3718	A2M	C1'-N9-C4	2.47	130.99	126.64
53	2	2297	E7G	C2-N1-C6	-2.46	120.62	125.10
53	2	4870	OMG	C8-N7-C5	2.45	107.66	102.99
53	2	3909	OMC	C6-N1-C2	-2.45	116.25	120.49
53	2	2754	B9B	C61-O6-C6	-2.43	112.97	117.51
53	2	1517	2MG	C8-N7-C5	2.42	107.60	102.99
53	2	1517	2MG	O6-C6-C5	-2.41	119.66	124.37
53	2	4623	OMG	C8-N7-C5	2.41	107.58	102.99
53	2	3899	BGH	N1-C2-N3	-2.41	118.83	123.32
53	2	1517	2MG	CM2-N2-C2	-2.40	118.57	123.86
53	2	1871	A2M	C1'-N9-C4	2.39	130.84	126.64
53	2	3899	BGH	C2-N1-C6	-2.39	120.75	125.10
53	2	2050	OMG	O6-C6-C5	-2.38	119.72	124.37
53	2	1456	B8Q	C31-N3-C2	2.38	121.25	117.79
53	2	1534	A2M	O4'-C1'-C2'	-2.38	102.46	106.59
53	2	1605	7MG	C2-N1-C6	-2.38	120.77	125.10
53	2	1871	A2M	O4'-C4'-C3'	-2.37	100.42	105.11
53	2	373	OMG	C8-N7-C5	2.35	107.47	102.99
53	2	3897	B8K	C2-N1-C6	-2.35	120.81	125.10
53	2	2424	OMG	O6-C6-C5	-2.34	119.79	124.37
53	2	978	2MG	O6-C6-C5	-2.34	119.80	124.37
53	2	4550	7MG	C2-N1-C6	-2.34	120.83	125.10
53	2	2380	B8W	C2-N1-C6	2.33	119.83	116.08
53	2	2364	OMG	O6-C6-C5	-2.33	119.83	124.37
53	2	373	OMG	O6-C6-C5	-2.32	119.84	124.37
53	2	4637	OMG	C8-N7-C5	2.32	107.41	102.99
53	2	3869	OMC	O2-C2-N3	-2.32	118.56	122.33
53	2	2773	OMG	O6-C6-C5	-2.30	119.88	124.37
53	2	2773	OMG	C8-N7-C5	2.30	107.37	102.99
53	2	1625	OMG	O6-C6-C5	-2.29	119.90	124.37
53	2	3723	A2M	C1'-N9-C4	2.29	130.66	126.64
53	2	4571	A2M	C1'-N9-C4	2.28	130.64	126.64
53	2	4083	5MU	O4-C4-N3	-2.28	115.75	120.12
53	2	4690	B8K	N1-C2-N3	-2.27	119.09	123.32
53	2	3880	P7G	C71-N7-C5	2.26	129.88	124.52
53	2	3909	OMC	C1'-N1-C2	2.26	123.46	118.42
53	2	4494	OMG	O6-C6-C5	-2.25	119.97	124.37
53	2	1316	OMG	O6-C6-C5	-2.25	119.98	124.37
53	2	4472	B8W	N2-C2-N1	-2.23	113.78	117.25
53	2	1883	OMG	C8-N7-C5	2.22	107.22	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	2	1326	A2M	C1'-N9-C4	2.21	130.53	126.64
53	2	4870	OMG	O6-C6-C5	-2.21	120.06	124.37
53	2	373	OMG	N2-C2-N1	2.20	121.39	116.71
53	2	729	2MG	O6-C6-C5	-2.19	120.09	124.37
53	2	1522	OMG	C8-N7-C5	2.18	107.14	102.99
53	2	4536	OMC	C1'-N1-C2	2.17	123.27	118.42
53	2	4529	B8W	C1'-N9-C4	-2.17	122.82	126.64
53	2	4637	OMG	O6-C6-C5	-2.17	120.13	124.37
53	2	4530	UR3	C3U-N3-C4	2.16	120.98	117.89
53	2	3897	B8K	N1-C2-N3	-2.16	119.30	123.32
53	2	1625	OMG	C8-N7-C5	2.15	107.09	102.99
53	2	1605	7MG	O6-C6-C5	-2.15	122.27	127.54
53	2	2050	OMG	C8-N7-C5	2.15	107.08	102.99
53	2	4494	OMG	C8-N7-C5	2.15	107.08	102.99
53	2	2861	OMC	O2-C2-N1	2.14	123.31	118.89
53	2	1522	OMG	N2-C2-N1	2.14	121.26	116.71
53	2	4872	2MG	O6-C6-C5	-2.13	120.21	124.37
53	2	4550	7MG	O6-C6-C5	-2.13	122.32	127.54
53	2	4483	B8T	C6-N1-C2	-2.11	116.83	120.49
53	2	1605	7MG	C6-C5-C4	-2.10	118.30	122.62
53	2	4597	UR3	O2-C2-N3	-2.08	118.40	121.34
53	2	4550	7MG	C6-C5-C4	-2.08	118.33	122.62
53	2	2422	OMC	O2-C2-N1	2.08	123.19	118.89
53	2	4483	B8T	C6-C5-C4	2.06	119.49	116.96
53	2	2786	B9H	C32-C31-N3	2.05	116.75	112.47
53	2	2522	7MG	C6-C5-C4	-2.04	118.41	122.62
53	2	1522	OMG	O6-C6-C5	-2.04	120.39	124.37
53	2	4529	B8W	C2-N1-C6	2.02	119.32	116.08
53	2	4620	OMU	O2-C2-N1	-2.01	120.12	122.79
53	2	3887	OMC	C1'-N1-C2	2.01	122.90	118.42
53	2	1605	7MG	N1-C2-N3	-2.00	119.58	123.32
53	2	1659	I4U	O2-C2-N3	-2.00	119.07	122.33

There are no chirality outliers.

All (88) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	8	14	OMU	C1'-C2'-O2'-CM2
53	2	237	B9B	C5-C6-O6-C61
53	2	237	B9B	N1-C6-O6-C61
53	2	237	B9B	C3'-C4'-C5'-O5'
53	2	237	B9B	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
53	2	398	A2M	O4'-C4'-C5'-O5'
53	2	1348	P4U	N3-C4-O4-C41
53	2	1574	B9B	C5-C6-O6-C61
53	2	1574	B9B	N1-C6-O6-C61
53	2	1625	OMG	C3'-C4'-C5'-O5'
53	2	1871	A2M	O4'-C4'-C5'-O5'
53	2	1871	A2M	C3'-C4'-C5'-O5'
53	2	1883	OMG	O4'-C4'-C5'-O5'
53	2	1883	OMG	C3'-C4'-C5'-O5'
53	2	2380	B8W	C5-C6-O6-C61
53	2	2380	B8W	N1-C6-O6-C61
53	2	2424	OMG	C3'-C4'-C5'-O5'
53	2	2754	B9B	C5-C6-O6-C61
53	2	2754	B9B	N1-C6-O6-C61
53	2	2786	B9H	C1'-C2'-O2'-C21
53	2	4129	B8W	C5-C6-O6-C61
53	2	4129	B8W	N1-C6-O6-C61
53	2	4129	B8W	C3'-C4'-C5'-O5'
53	2	4472	B8W	C5-C6-O6-C61
53	2	4472	B8W	N1-C6-O6-C61
53	2	4529	B8W	C5-C6-O6-C61
53	2	4529	B8W	C3'-C4'-C5'-O5'
53	2	4529	B8W	O4'-C4'-C5'-O5'
53	2	4550	7MG	O4'-C4'-C5'-O5'
53	2	4550	7MG	C3'-C4'-C5'-O5'
53	2	4637	OMG	O4'-C4'-C5'-O5'
53	2	4637	OMG	C3'-C4'-C5'-O5'
53	2	4637	OMG	C1'-C2'-O2'-CM2
53	2	4870	OMG	O4'-C4'-C5'-O5'
53	2	4870	OMG	C3'-C4'-C5'-O5'
53	2	398	A2M	C3'-C4'-C5'-O5'
53	2	1625	OMG	O4'-C4'-C5'-O5'
53	2	2424	OMG	O4'-C4'-C5'-O5'
53	2	3897	B8K	O4'-C4'-C5'-O5'
53	2	4129	B8W	O4'-C4'-C5'-O5'
53	2	4872	2MG	O4'-C4'-C5'-O5'
53	2	729	2MG	O4'-C4'-C5'-O5'
53	2	2364	OMG	O4'-C4'-C5'-O5'
53	2	3880	P7G	C3'-C4'-C5'-O5'
53	2	3880	P7G	O4'-C4'-C5'-O5'
53	2	3897	B8K	C3'-C4'-C5'-O5'
53	2	4872	2MG	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
53	2	1517	2MG	O4'-C4'-C5'-O5'
53	2	1909	P7G	O4'-C4'-C5'-O5'
53	2	3909	OMC	O4'-C4'-C5'-O5'
53	2	1574	B9B	C62-C61-O6-C6
53	2	729	2MG	C3'-C4'-C5'-O5'
53	2	3701	OMC	O4'-C4'-C5'-O5'
53	2	1517	2MG	C3'-C4'-C5'-O5'
53	2	2364	OMG	C3'-C4'-C5'-O5'
53	2	3867	A2M	C3'-C4'-C5'-O5'
53	2	3880	P7G	N7-C71-C72-C73
53	2	3701	OMC	C3'-C4'-C5'-O5'
53	2	3867	A2M	C4'-C5'-O5'-P
53	2	1534	A2M	O4'-C4'-C5'-O5'
53	2	2786	B9H	C3'-C2'-O2'-C21
53	2	3723	A2M	O4'-C4'-C5'-O5'
53	2	3867	A2M	O4'-C4'-C5'-O5'
53	2	3899	BGH	O4'-C4'-C5'-O5'
53	2	4529	B8W	N1-C6-O6-C61
53	2	3887	OMC	C4'-C5'-O5'-P
53	2	2365	OMC	C3'-C2'-O2'-CM2
53	2	1574	B9B	O6-C61-C62-C63
53	2	1517	2MG	C4'-C5'-O5'-P
53	2	3897	B8K	C4'-C5'-O5'-P
53	2	2297	E7G	C72-C71-N7-C8
53	2	373	OMG	C4'-C5'-O5'-P
53	2	4637	OMG	C4'-C5'-O5'-P
53	2	3909	OMC	C3'-C4'-C5'-O5'
53	2	1524	A2M	C3'-C2'-O2'-CM'
53	2	3869	OMC	C3'-C2'-O2'-CM2
53	2	4523	A2M	C3'-C2'-O2'-CM'
53	2	2422	OMC	O4'-C4'-C5'-O5'
53	2	1909	P7G	C3'-C4'-C5'-O5'
53	2	2773	OMG	C3'-C4'-C5'-O5'
53	2	3869	OMC	C1'-C2'-O2'-CM2
53	2	3909	OMC	C2'-C1'-N1-C2
53	2	1534	A2M	C3'-C4'-C5'-O5'
53	2	2380	B8W	O4'-C4'-C5'-O5'
53	2	1659	I4U	C42-C41-O4-C4
53	2	1659	I4U	C43-C41-O4-C4
53	2	2754	B9B	C62-C61-O6-C6
53	2	3880	P7G	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
54	GTP	w	801	55	26,34,34	0.99	3 (11%)	32,54,54	0.84	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	GTP	w	801	55	-	1/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	w	801	GTP	C5-C6	-2.69	1.42	1.47
54	w	801	GTP	C8-N7	-2.11	1.31	1.35
54	w	801	GTP	C5-C4	-2.06	1.37	1.43

There are no bond angle outliers.

There are no chirality outliers.

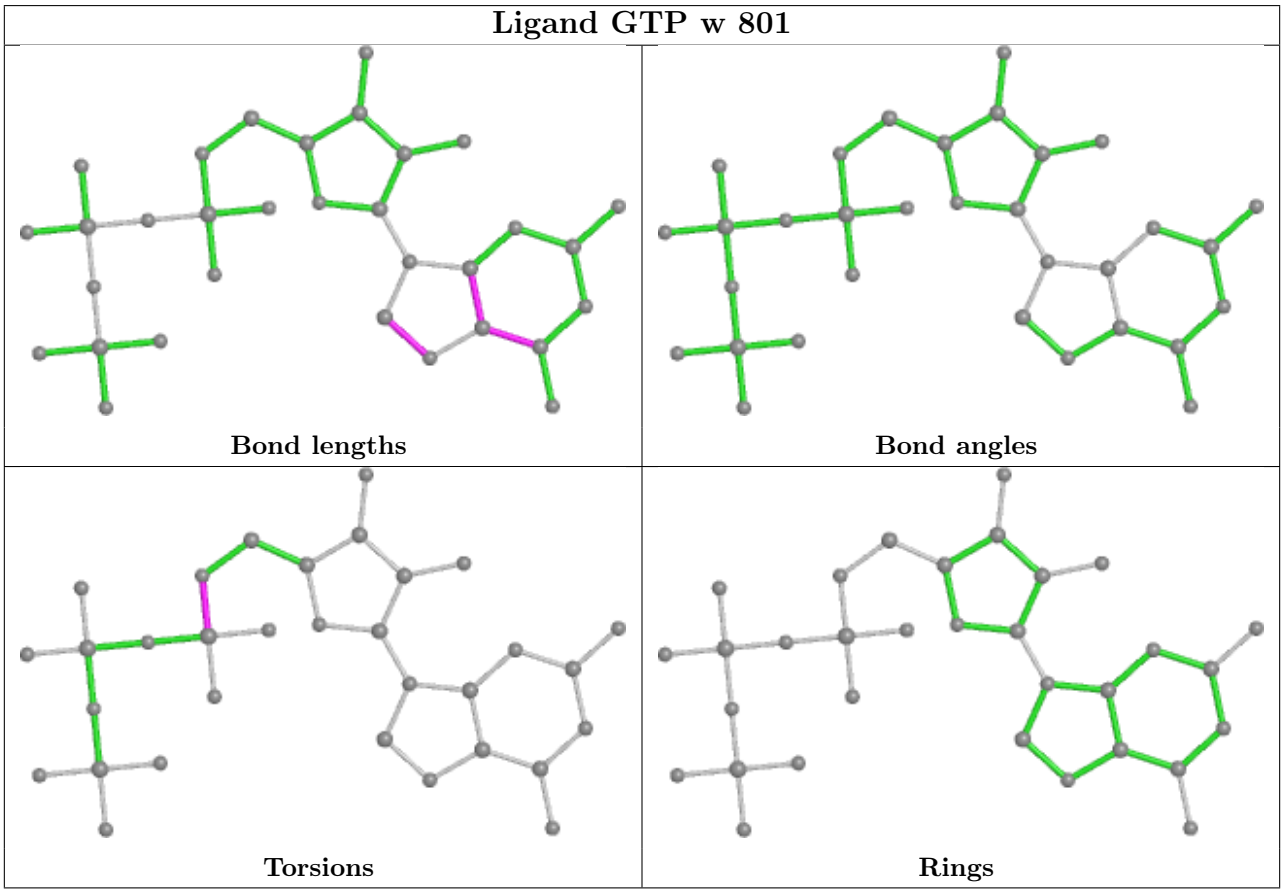
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	w	801	GTP	C5'-O5'-PA-O1A

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

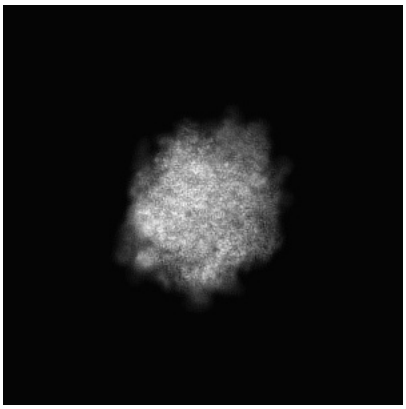
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-35599. These allow visual inspection of the internal detail of the map and identification of artifacts.

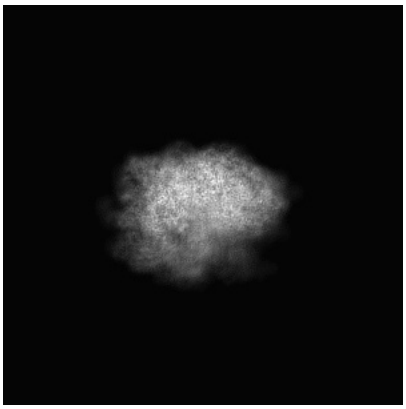
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

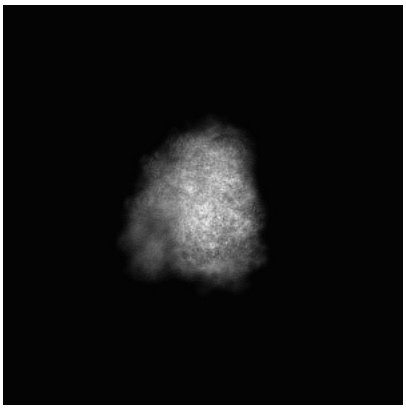
6.1.1 Primary map



X

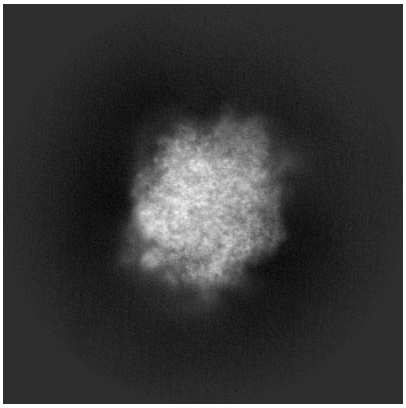


Y

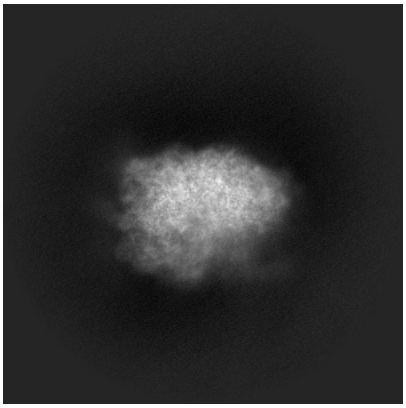


Z

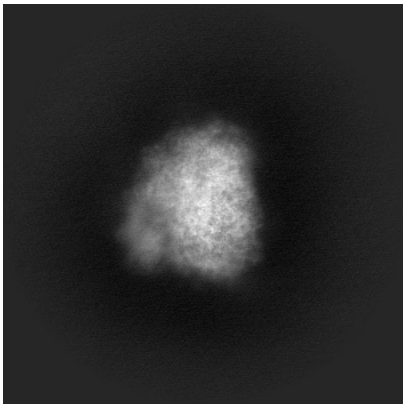
6.1.2 Raw map



X



Y

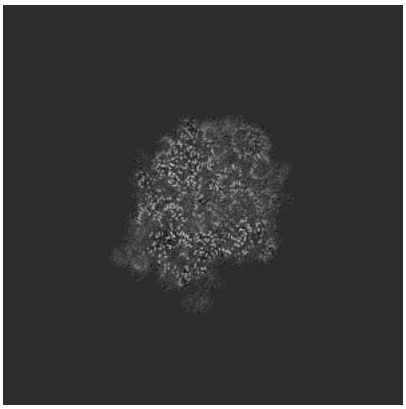


Z

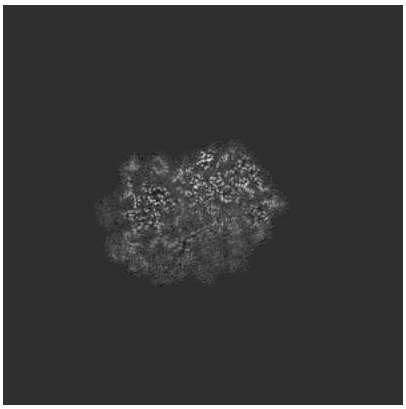
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

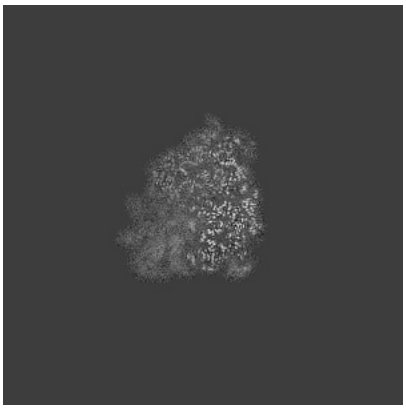
6.2.1 Primary map



X Index: 200

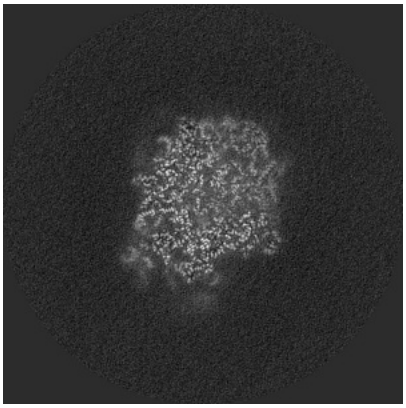


Y Index: 200

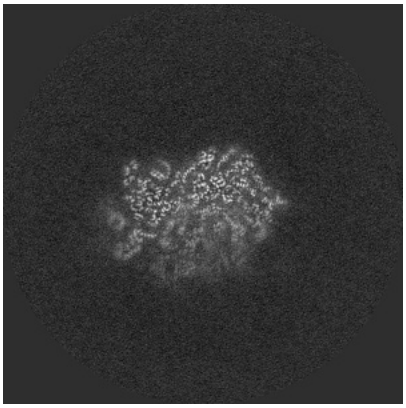


Z Index: 200

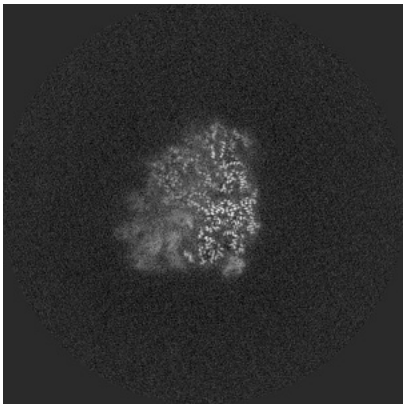
6.2.2 Raw map



X Index: 200



Y Index: 200

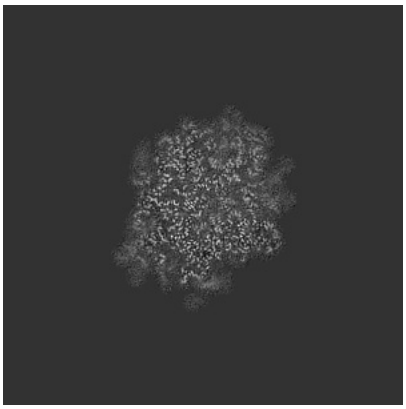


Z Index: 200

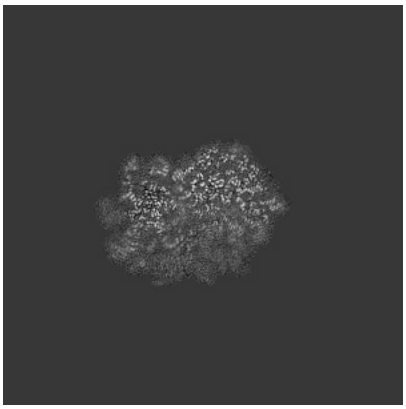
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

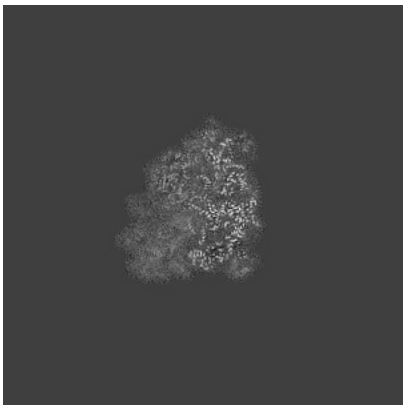
6.3.1 Primary map



X Index: 206

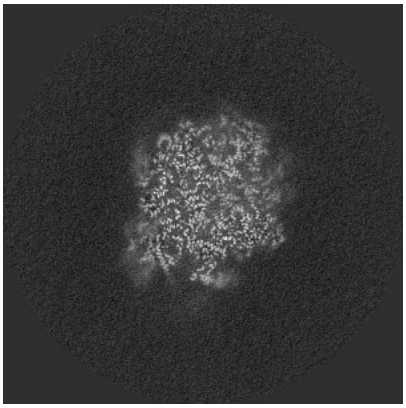


Y Index: 199

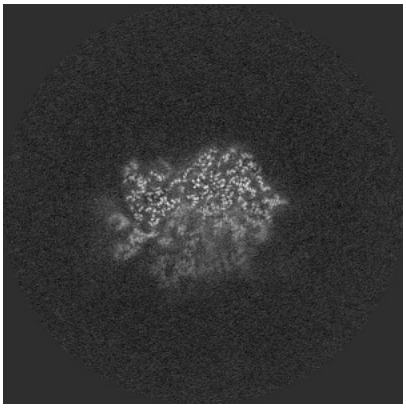


Z Index: 198

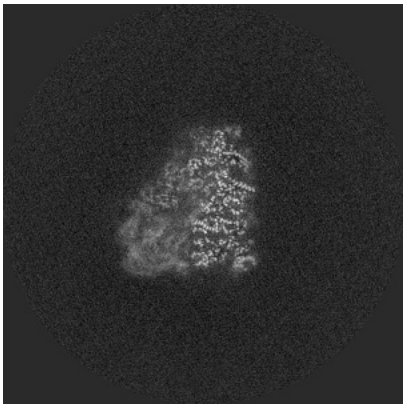
6.3.2 Raw map



X Index: 206



Y Index: 199

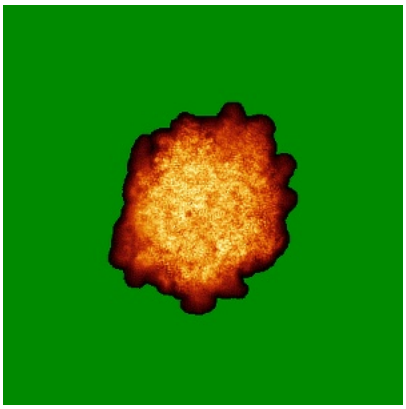


Z Index: 190

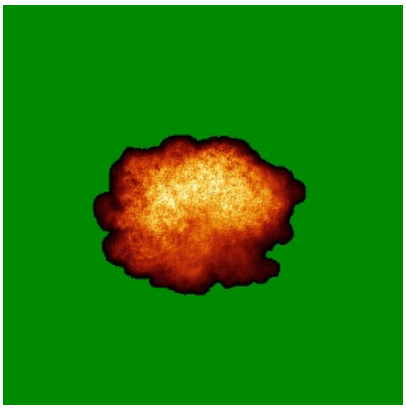
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

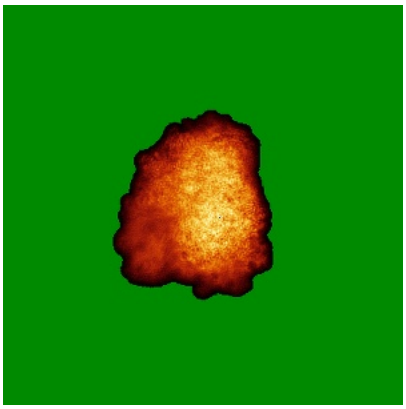
6.4.1 Primary map



X

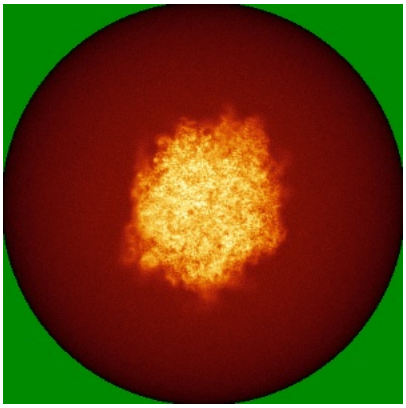


Y

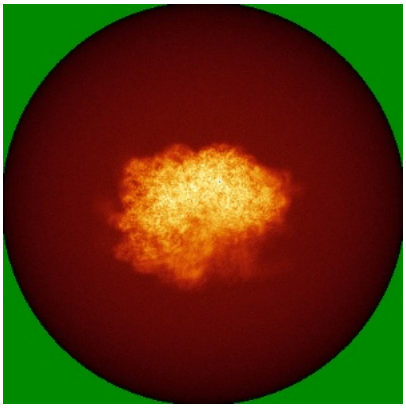


Z

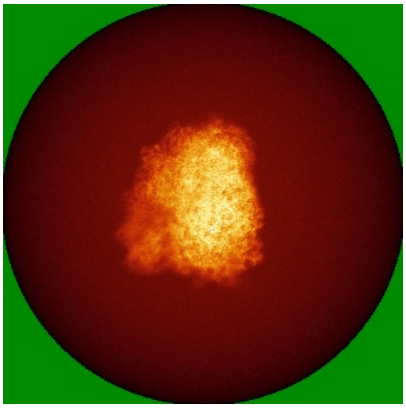
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.031. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

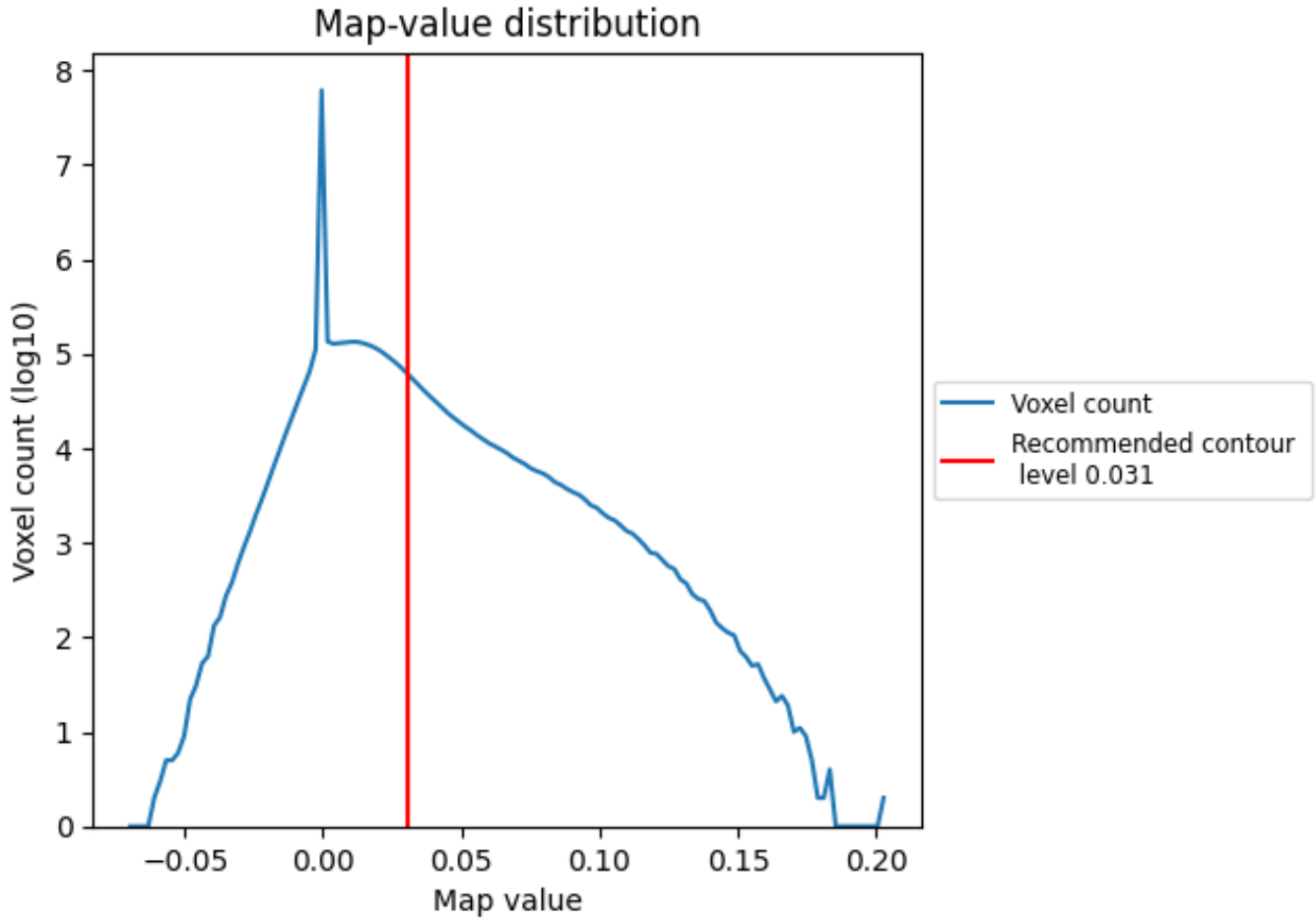
6.6 Mask visualisation (i)

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

7 Map analysis

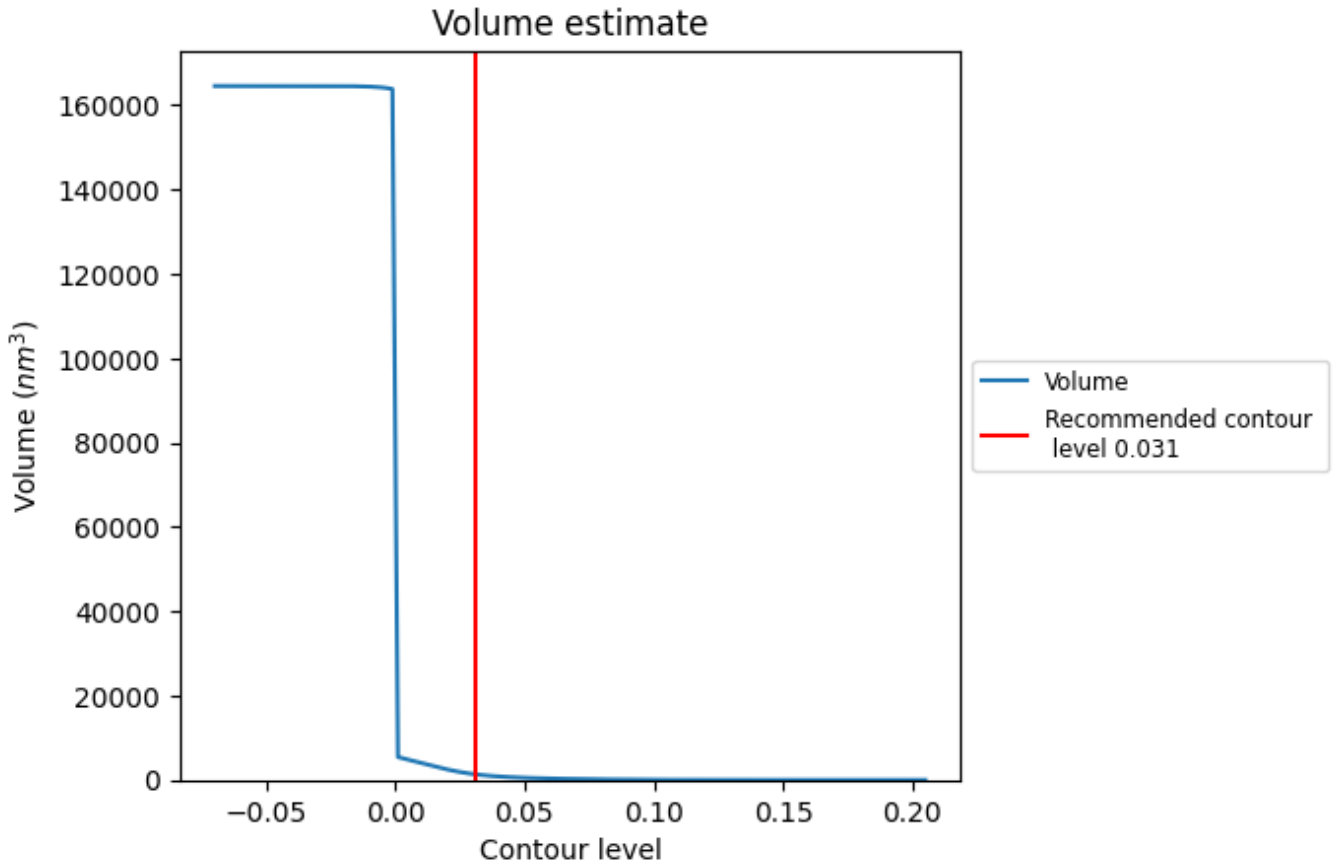
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

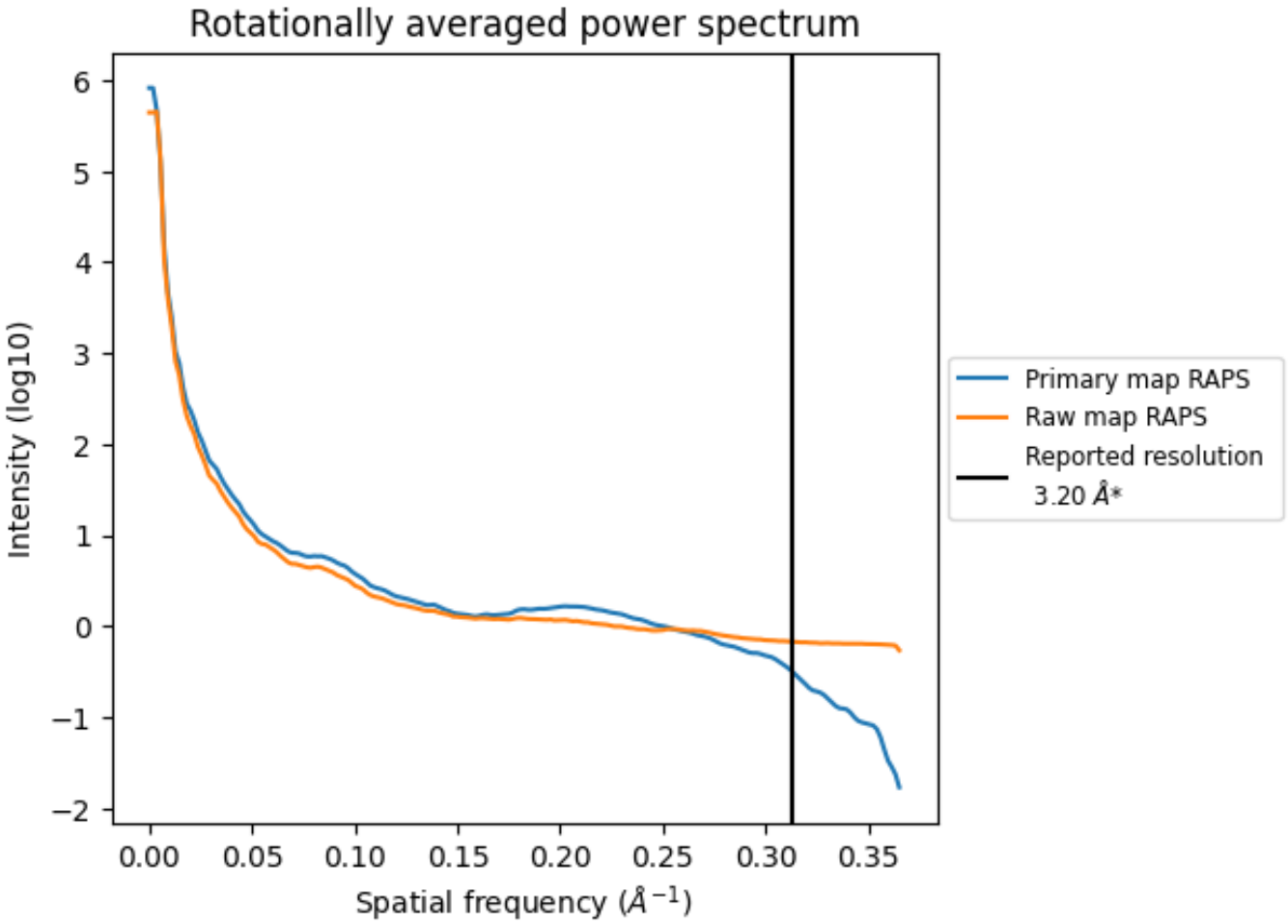
7.2 Volume estimate



The volume at the recommended contour level is 1338 nm^3; this corresponds to an approximate mass of 1209 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)

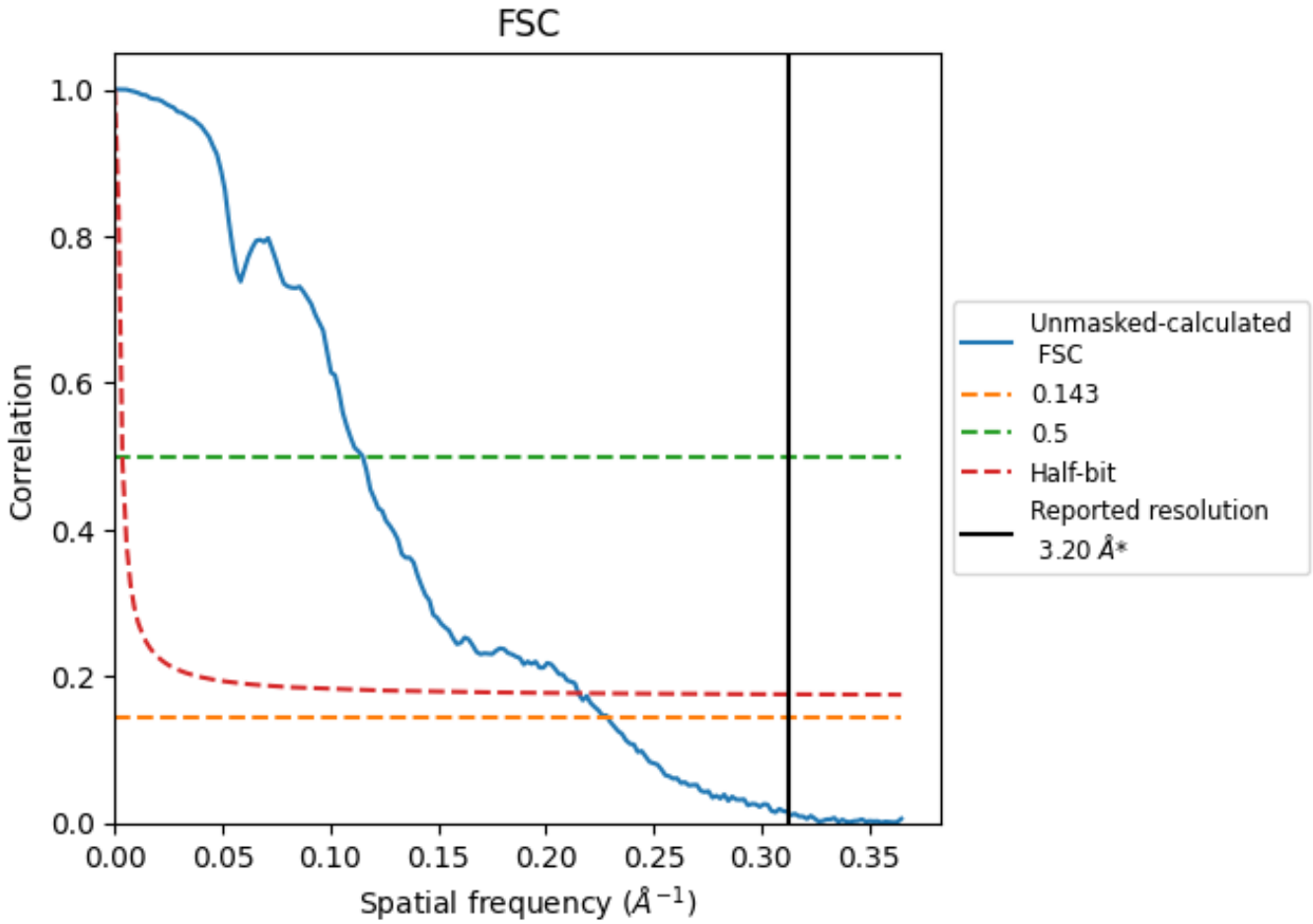


*Reported resolution corresponds to spatial frequency of 0.312 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8.2 Resolution estimates (i)

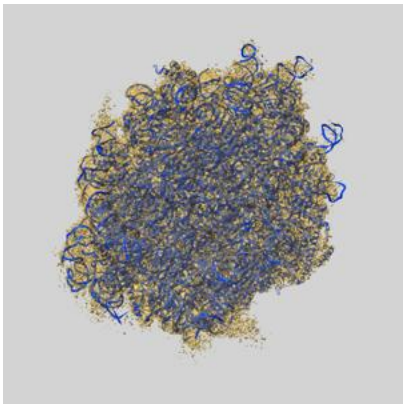
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.37	8.70	4.65

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.37 differs from the reported value 3.2 by more than 10 %

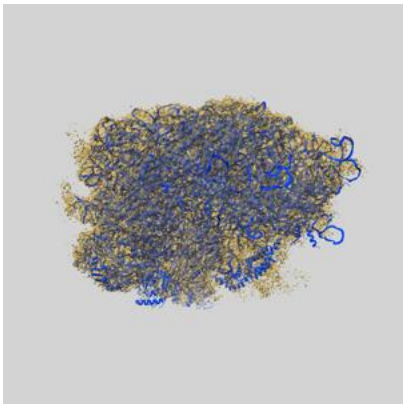
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-35599 and PDB model 8INK. Per-residue inclusion information can be found in section 3 on page 14.

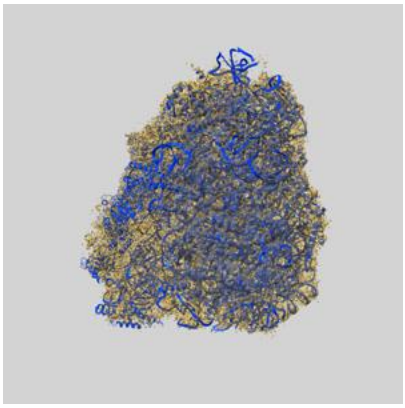
9.1 Map-model overlay



X



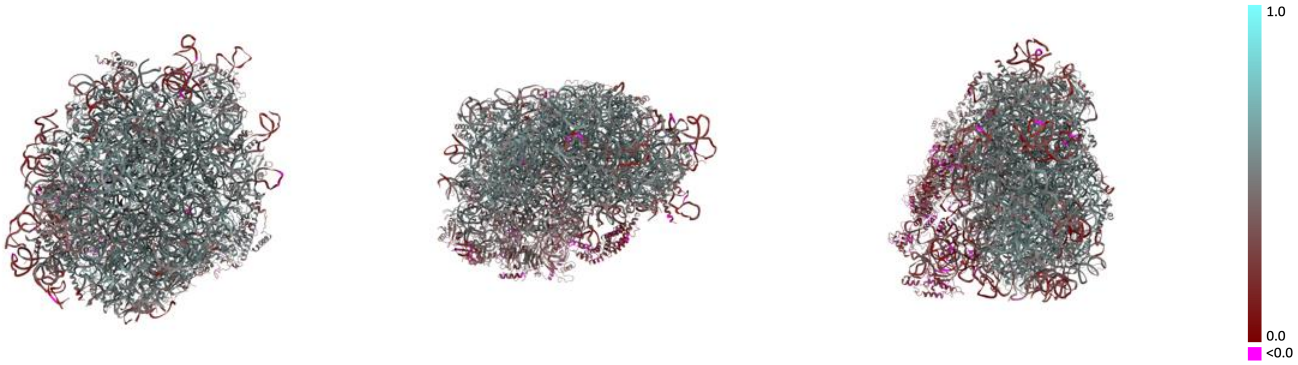
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.031 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.

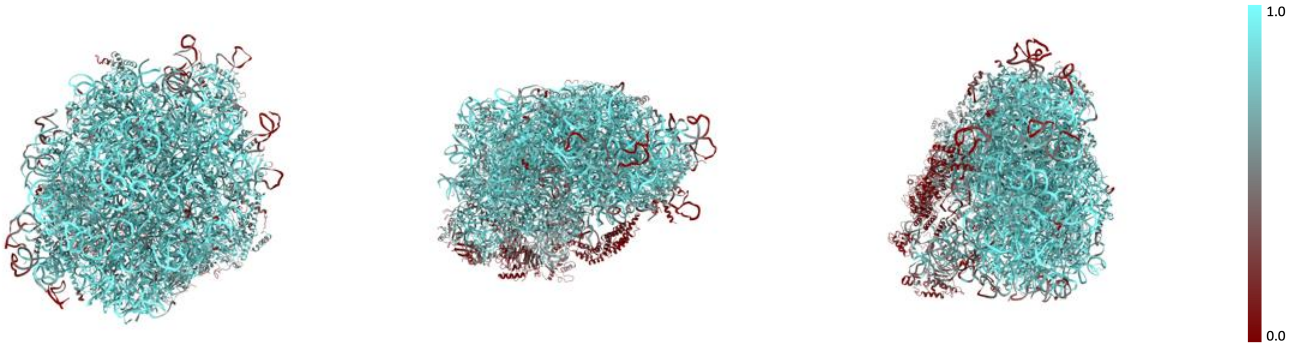
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

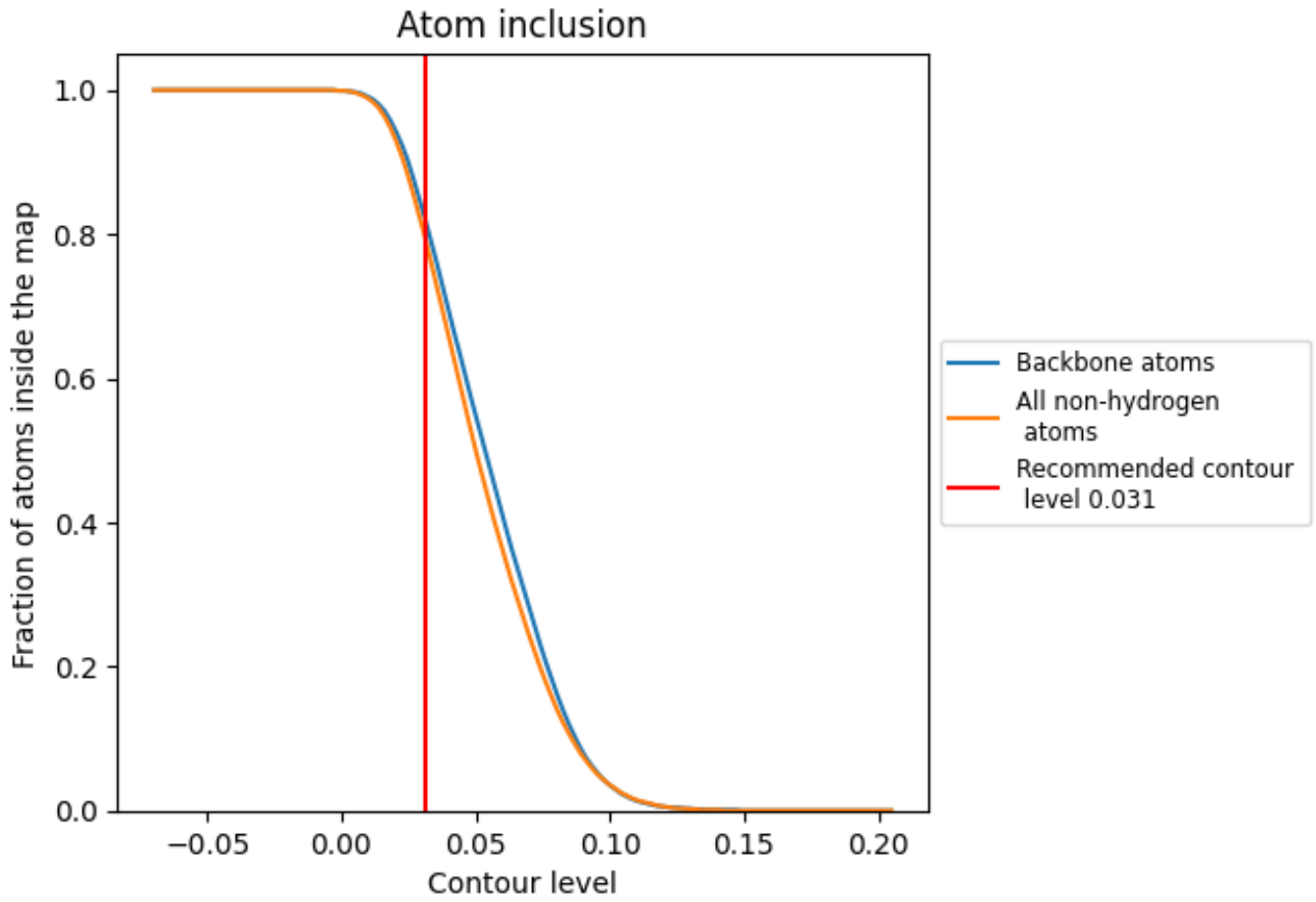
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.031).

9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 80% 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 (0.031) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7980	0.4550
2	0.8700	0.4640
3	0.7720	0.3080
4	0.6970	0.4290
6	0.7670	0.4760
7	0.8480	0.5120
8	0.9440	0.5160
9	0.3710	0.3610
A	0.5840	0.3760
B	0.9010	0.5380
C	0.2590	0.2110
D	0.9200	0.5410
E	0.6010	0.4300
F	0.8510	0.5030
G	0.6830	0.4300
H	0.8720	0.5090
I	0.8350	0.5060
J	0.7950	0.4750
K	0.8060	0.4710
L	0.9230	0.5400
M	0.9520	0.5520
N	0.1090	0.1830
O	0.6970	0.4580
P	0.9720	0.5530
Q	0.8090	0.4860
R	0.2770	0.1820
S	0.8970	0.5280
T	0.5790	0.2680
U	0.9180	0.5240
V	0.9050	0.5400
W	0.1950	0.3230
X	0.7600	0.4670
Y	0.8670	0.5310
Z	0.9220	0.5470
a	0.8270	0.4890

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Chain	Atom inclusion	Q-score
b	0.9200	0.5510
d	0.7800	0.4870
e	0.8760	0.5210
g	0.8830	0.5220
h	0.8790	0.5250
i	0.7230	0.4490
j	0.8400	0.5090
k	0.9470	0.5640
l	0.9160	0.5490
m	0.8320	0.4900
n	0.9510	0.5700
o	0.7960	0.4720
p	0.9010	0.5320
r	0.3640	0.3220
u	0.5260	0.3660
v	0.6020	0.4230
w	0.7010	0.4360
y	0.3620	0.2770
z	0.6650	0.4280