Full wwPDB EM Validation Report ⓘ

Nov 6, 2023 – 12:12 PM JST

PDB ID	:	8IR1
EMDB ID	:	EMD-35672
Title	:	human nuclear pre-60S ribosomal particle - State A
Authors	:	Zhang, Y.; Gao, N.
Deposited on	:	2023-03-17
Resolution	:	3.30 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:

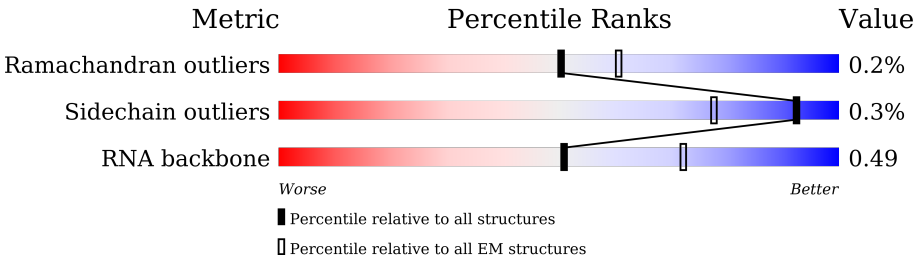
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.30 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	y	165	44% 98%
2	4	634	22% 95%
3	6	245	7% 98%
4	7	163	6% 83% 17%
5	B	403	5% 99%
6	D	427	83% 16%
7	E	115	83% 84% 15%
8	F	117	44% 93% 7%

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Mol	Chain	Length	Quality of chain
9	G	266	42% 80% 19%
10	H	123	98%
11	I	192	98%
12	K	105	21% 95%
13	L	148	75% 24%
14	M	97	6% 89% 11%
15	P	51	98%
16	Q	211	14% 95%
17	S	215	62% 37%
18	U	204	89% 11%
19	V	203	98%
20	X	92	62% 99%
21	Z	188	79% 20%
22	a	196	25% 75% 24%
23	b	176	100%
24	c	160	18% 72% 26%
25	e	140	93% 6%
26	h	145	92% 8%
27	i	136	96% 98%
28	l	137	91% 9%
29	m	257	61% 70% 30%
30	n	110	96%
31	o	288	13% 81% 18%
32	p	248	89% 9%
33	z	129	12% 51% 48%

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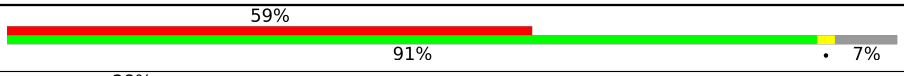
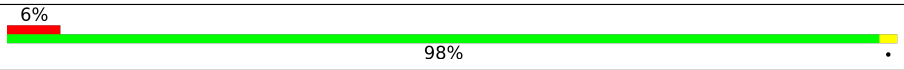
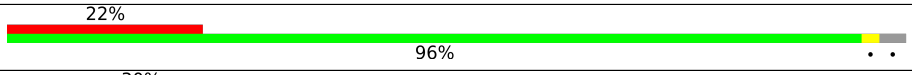
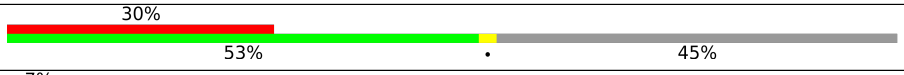
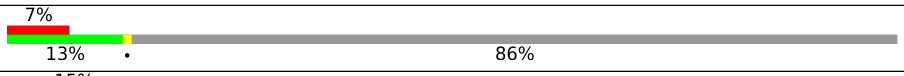
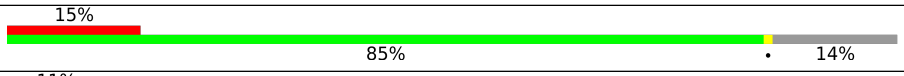
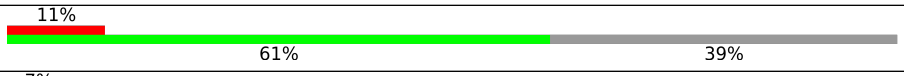
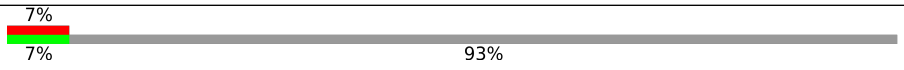
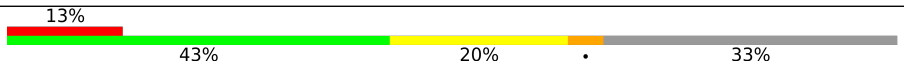
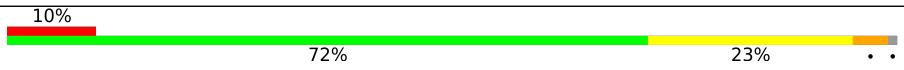
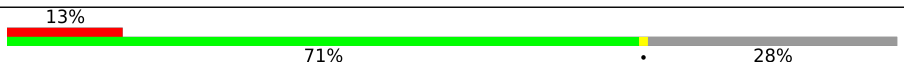
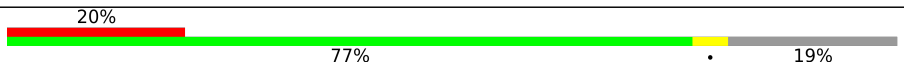
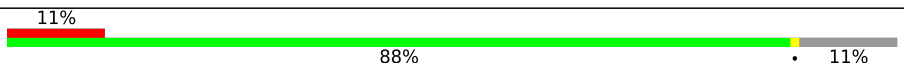
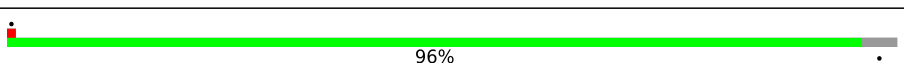
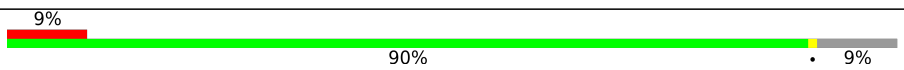
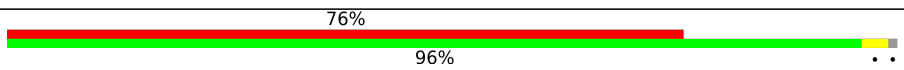
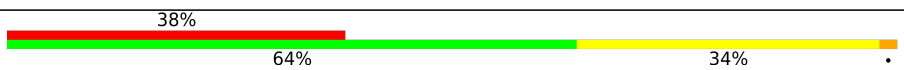
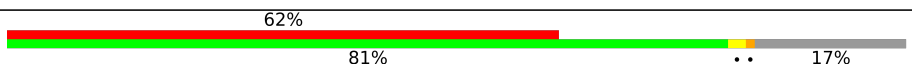
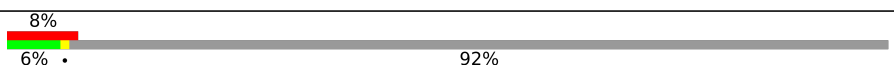
Mol	Chain	Length	Quality of chain
34	A	178	
35	C	297	
36	J	260	
37	N	485	
38	R	365	
39	u	549	
40	v	239	
41	w	731	
42	r	360	
43	2	5054	
44	8	156	
45	g	156	
46	d	128	
47	j	125	
48	k	135	
49	Y	184	
50	O	70	
51	W	120	
52	T	306	
53	9	847	

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 150033 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 60S ribosomal protein L12.

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

- Molecule 2 is a protein called GTP-binding protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	4	620	5093	3198	935	933	27	0	0

- Molecule 3 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	6	244	1852	1149	318	372	13	0	0

- Molecule 4 is a protein called Probable ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	7	135	1159	737	225	187	10	0	0

- Molecule 5 is a protein called 60S ribosomal protein L3.

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

- Molecule 6 is a protein called 60S ribosomal protein L4.

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

- Molecule 7 is a protein called 60S ribosomal protein L30.

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

- Molecule 8 is a protein called 60S ribosomal protein L34.

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

- Molecule 9 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	G	216	Total	C	N	O	S	1	0
			1729	1101	335	289	4		

- Molecule 10 is a protein called 60S ribosomal protein L35.

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

- Molecule 11 is a protein called 60S ribosomal protein L9.

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

- Molecule 12 is a protein called 60S ribosomal protein L36.

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

- Molecule 13 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	113	Total	C	N	O	S	0	0
			888	563	176	146	3		

- Molecule 14 is a protein called 60S ribosomal protein L37.

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

- Molecule 15 is a protein called 60S ribosomal protein L39.

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

- Molecule 16 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	203	Total	C	N	O	S	0	0
			1652	1036	341	272	3		

- Molecule 17 is a protein called 60S ribosomal protein L14.

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

- Molecule 18 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	U	182	Total	C	N	O	S	0	0
			1542	972	324	242	4		

- Molecule 19 is a protein called 60S ribosomal protein L13a.

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

- Molecule 20 is a protein called 60S ribosomal protein L37a.

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

- Molecule 21 is a protein called 60S ribosomal protein L18.

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

- Molecule 22 is a protein called 60S ribosomal protein L19.

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

- Molecule 23 is a protein called 60S ribosomal protein L18a.

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

- Molecule 24 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	c	119	Total	C	N	O	S	0	0
			975	619	189	164	3		

- Molecule 25 is a protein called 60S ribosomal protein L23.

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

- Molecule 26 is a protein called 60S ribosomal protein L26.

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

- Molecule 27 is a protein called 60S ribosomal protein L27.

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

- Molecule 28 is a protein called 60S ribosomal protein L28.

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

- Molecule 29 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	m	181	Total	C	N	O	S	0	0
			1397	885	273	234	5		

- Molecule 30 is a protein called 60S ribosomal protein L35a.

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

- Molecule 31 is a protein called 60S ribosomal protein L6.

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

- Molecule 32 is a protein called 60S ribosomal protein L7.

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

- Molecule 33 is a protein called Protein LLP homolog.

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

- Molecule 34 is a protein called 60S ribosomal protein L11.

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

- Molecule 35 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	C	248	Total	C	N	O	S	0	0
			2027	1289	370	354	14		

- Molecule 36 is a protein called Ribosome biogenesis protein NSA2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	J	259	Total	C	N	O	S	0	0
			2106	1339	399	359	9		

- Molecule 37 is a protein called Notchless protein homolog 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	N	472	Total	C	N	O	S	0	0
			3669	2307	660	690	12		

- Molecule 38 is a protein called Ribosome biogenesis regulatory protein homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	R	199	Total	C	N	O	S	0	0
			1636	1022	315	296	3		

- Molecule 39 is a protein called Guanine nucleotide-binding protein-like 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	u	75	Total	C	N	O	S	0	0
			639	400	138	98	3		

- Molecule 40 is a protein called mRNA turnover protein 4 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	v	205	Total	C	N	O	S	0	0
			1675	1069	292	303	11		

- Molecule 41 is a protein called G Protein Nucleolar 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	w	449	Total	C	N	O	S	0	0
			3623	2301	643	665	14		

- Molecule 42 is a protein called Coiled-coil domain-containing protein 86.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	r	24	Total	C	N	O	S	0	0
			217	134	45	37	1		

- Molecule 43 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	2	3369	Total	C	N	O	P	0	0
			72334	32257	13244	23465	3368		

- Molecule 44 is a RNA chain called 5.8S rRMA.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	8	155	Total	C	N	O	P	0	0
			3295	1472	583	1086	154		

- Molecule 45 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	g	112	Total	C	N	O	S	0	0
			919	588	171	159	1		

- Molecule 46 is a protein called 60S ribosomal protein L22.

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

- Molecule 47 is a protein called 60S ribosomal protein L31.

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

- 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 L17.

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

- Molecule 50 is a protein called 60S ribosomal protein L38.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
51	W	120	Total	C	N	O	P	0	0
			2558	1141	456	842	119		

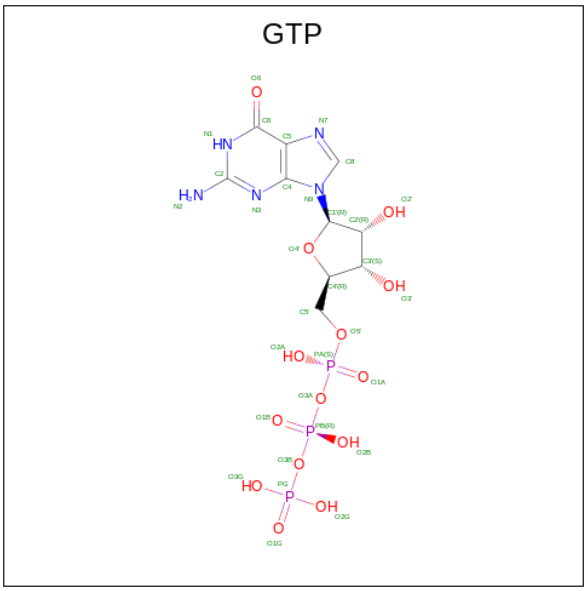
- Molecule 52 is a protein called Ribosome production factor 2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	T	255	Total	C	N	O	S	0	0
			2082	1336	364	371	11		

- Molecule 53 is a protein called pre-rRNA 2'-O-ribose RNA methyltransferase FTSJ3.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	9	65	Total	C	N	O	S	0	0
			538	334	103	98	3		

- 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).

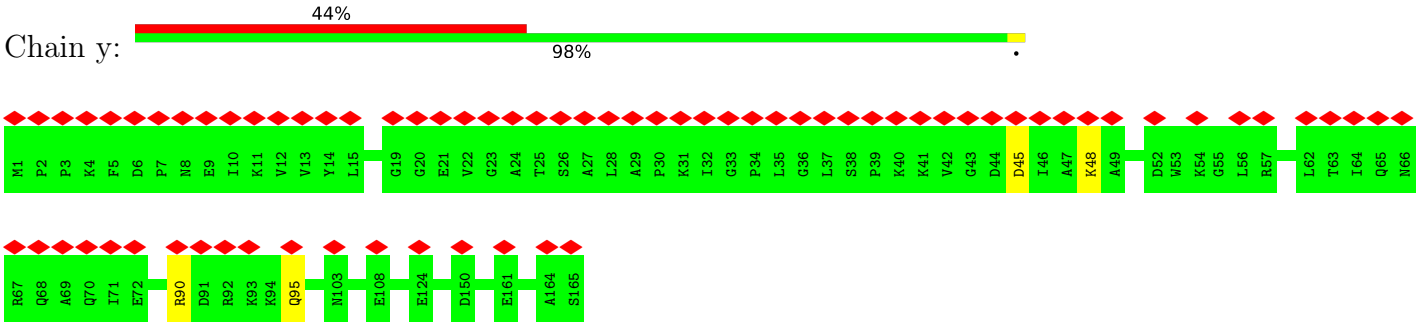
Mol	Chain	Residues	Atoms		AltConf
55	w	1	Total	Mg	0
			1	1	

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.

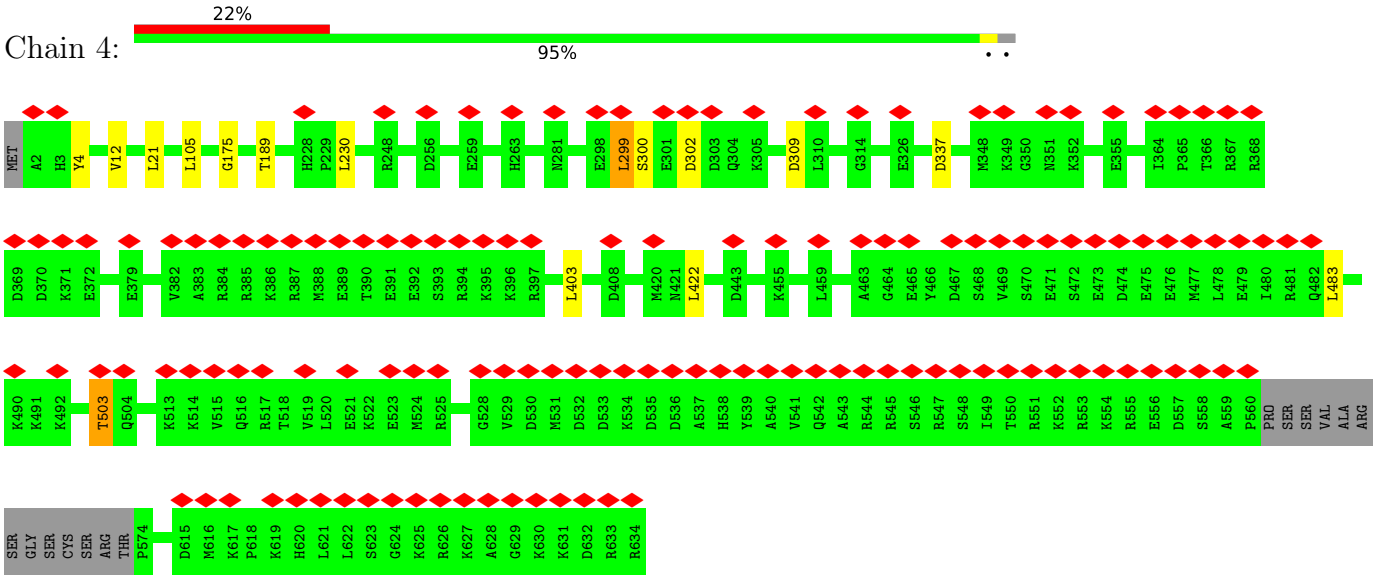
• Molecule 1: 60S ribosomal protein L12

Chain y:



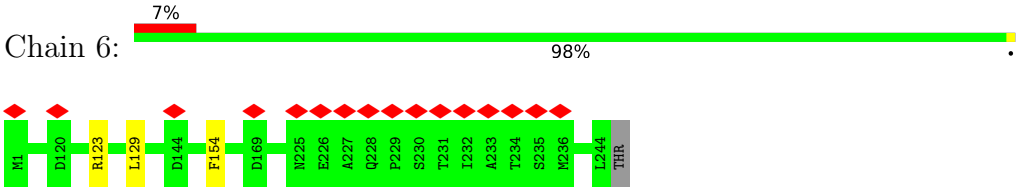
• Molecule 2: GTP-binding protein 4

Chain 4:



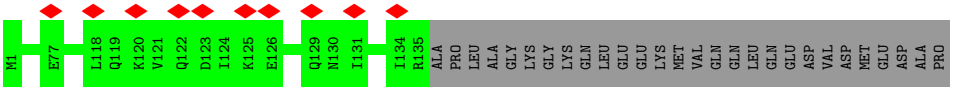
• Molecule 3: Eukaryotic translation initiation factor 6

Chain 6:



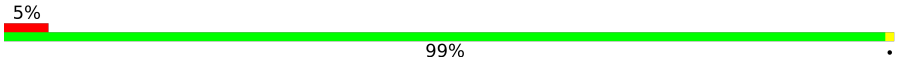
• Molecule 4: Probable ribosome biogenesis protein RLP24

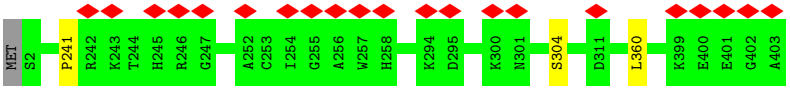
Chain 7:



• Molecule 5: 60S ribosomal protein L3

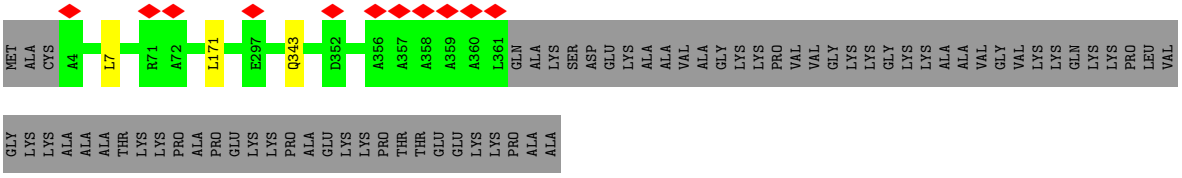
Chain B:





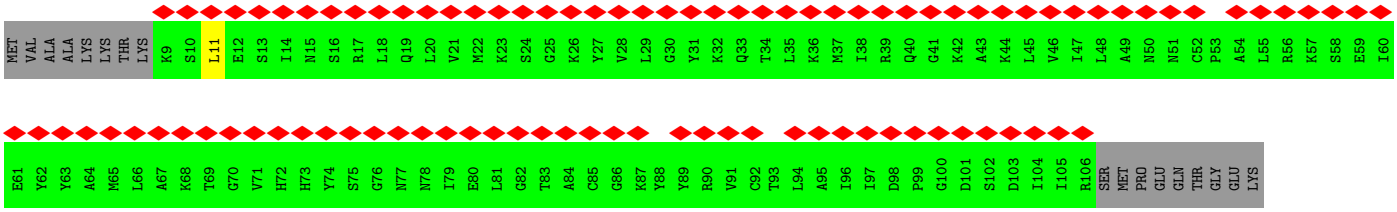
• Molecule 6: 60S ribosomal protein L4

Chain D:



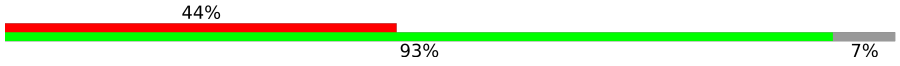
• Molecule 7: 60S ribosomal protein L30

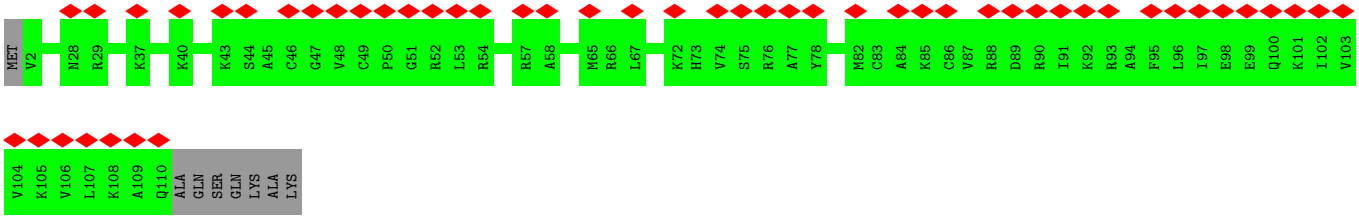
Chain E:



• Molecule 8: 60S ribosomal protein L34

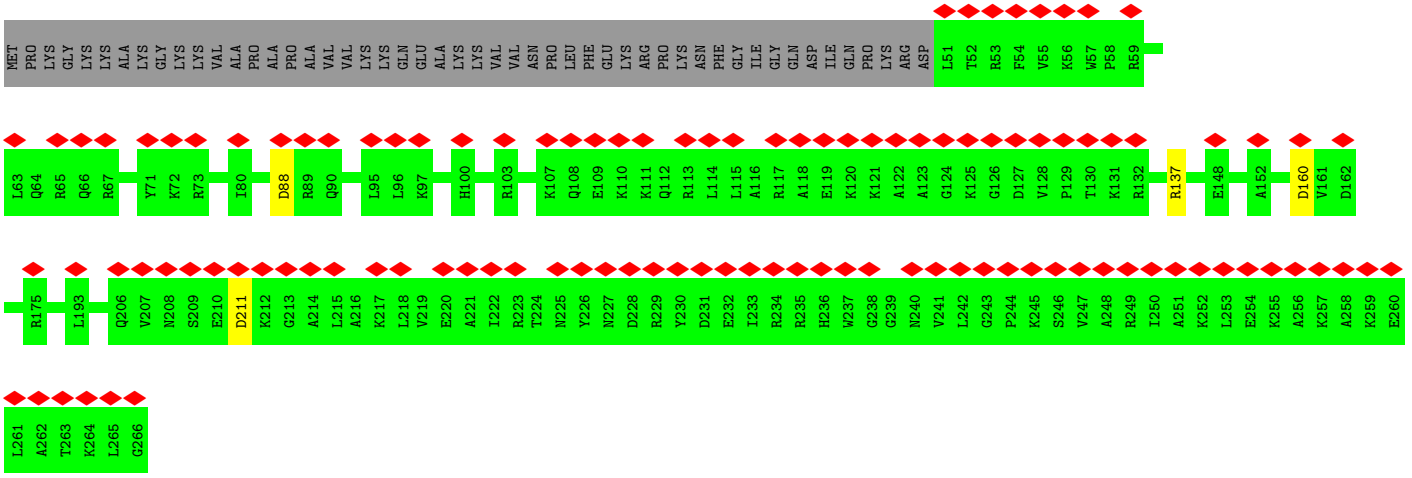
Chain F:



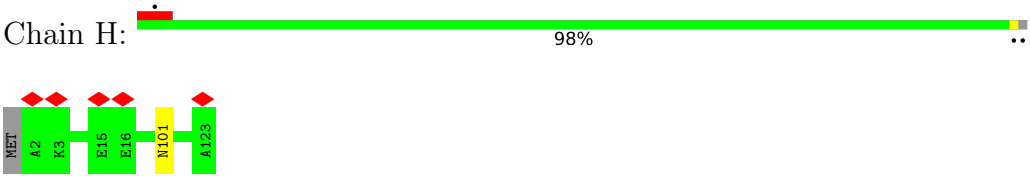


• Molecule 9: 60S ribosomal protein L7a

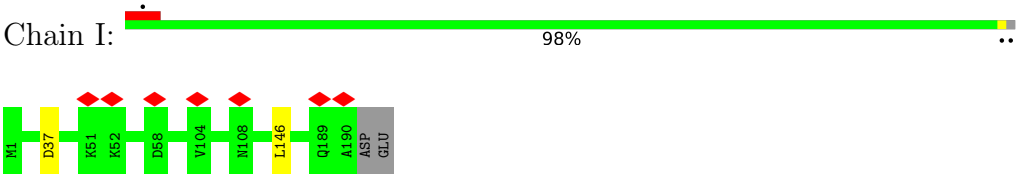
Chain G:



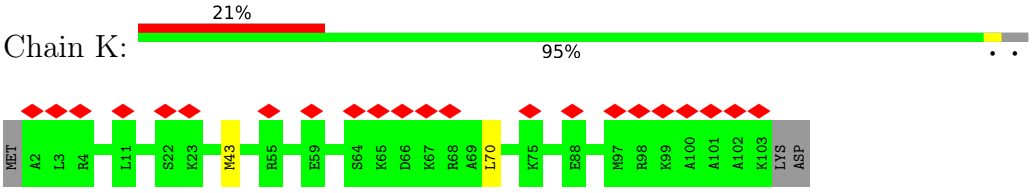
• Molecule 10: 60S ribosomal protein L35



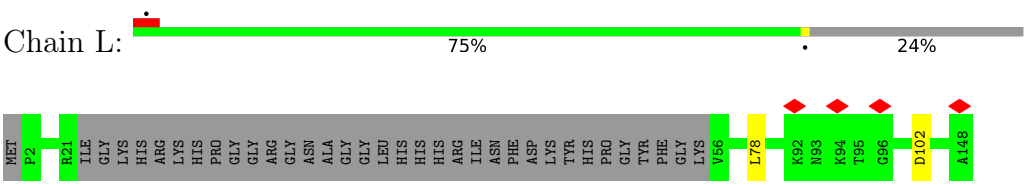
• Molecule 11: 60S ribosomal protein L9



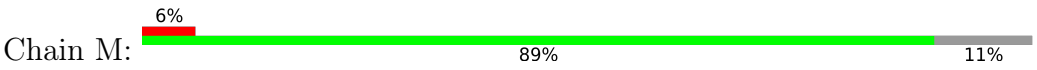
• Molecule 12: 60S ribosomal protein L36

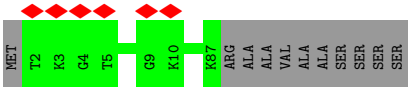


• Molecule 13: 60S ribosomal protein L27a



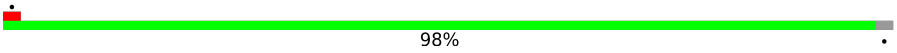
• Molecule 14: 60S ribosomal protein L37





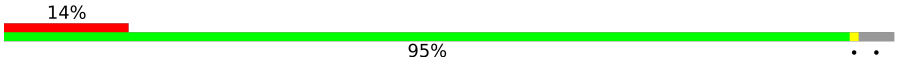
• Molecule 15: 60S ribosomal protein L39

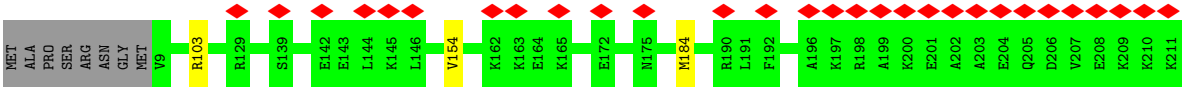
Chain P:



• Molecule 16: 60S ribosomal protein L13

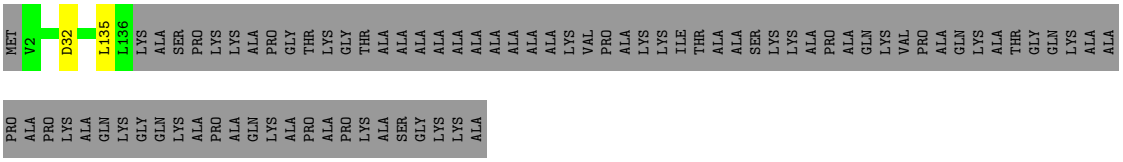
Chain Q:





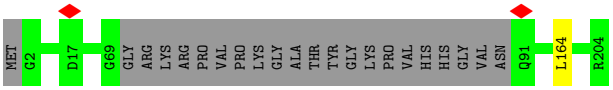
• Molecule 17: 60S ribosomal protein L14

Chain S:



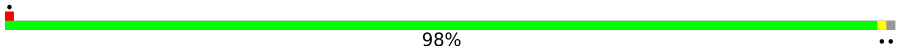
• Molecule 18: 60S ribosomal protein L15

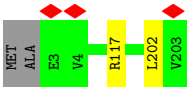
Chain U:



• Molecule 19: 60S ribosomal protein L13a

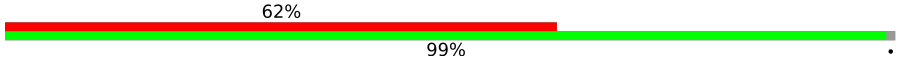
Chain V:

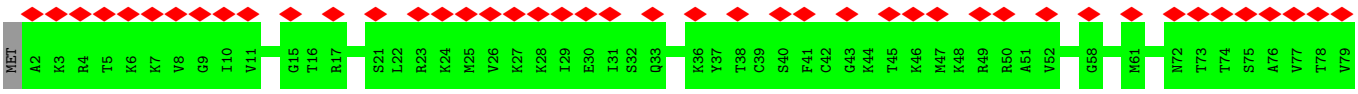


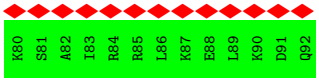


• Molecule 20: 60S ribosomal protein L37a

Chain X:





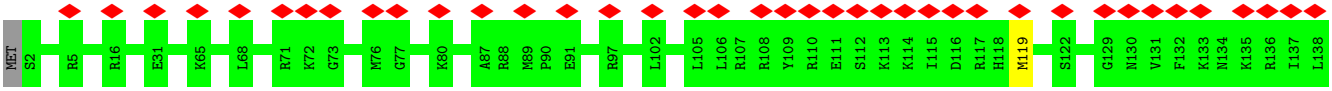


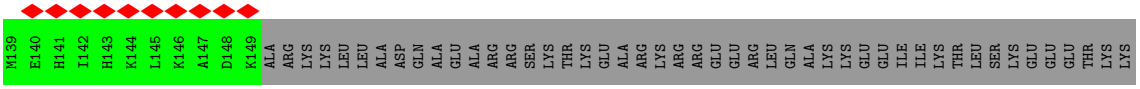
• Molecule 21: 60S ribosomal protein L18

Chain Z:

• Molecule 22: 60S ribosomal protein L19

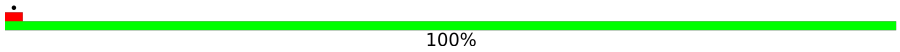
Chain a:

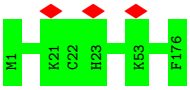




• Molecule 23: 60S ribosomal protein L18a

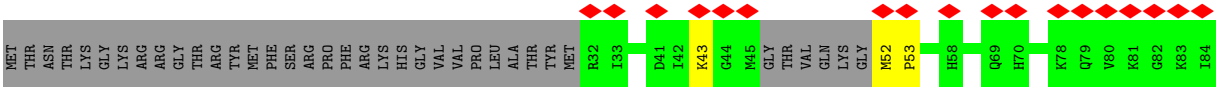
Chain b:

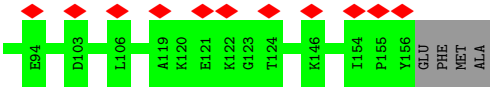




• Molecule 24: 60S ribosomal protein L21

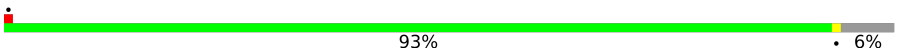
Chain c:

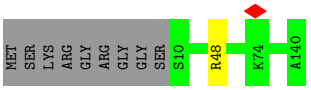




• Molecule 25: 60S ribosomal protein L23

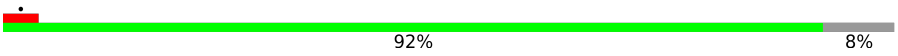
Chain e:

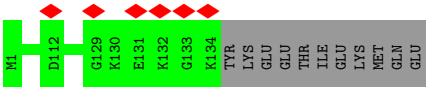




• Molecule 26: 60S ribosomal protein L26

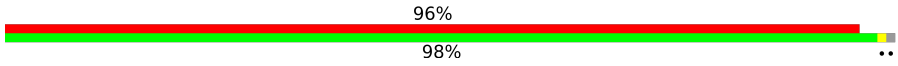
Chain h:

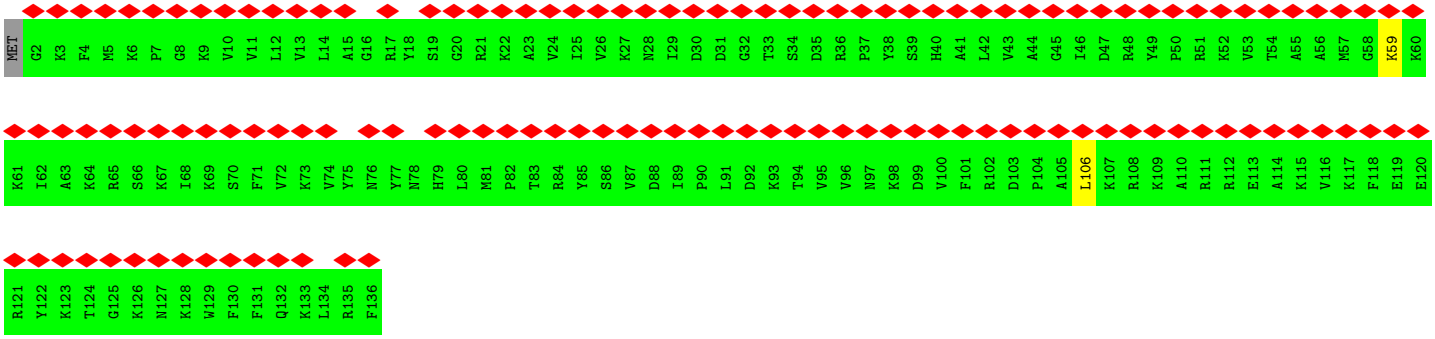




• Molecule 27: 60S ribosomal protein L27

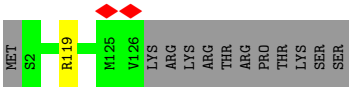
Chain i:





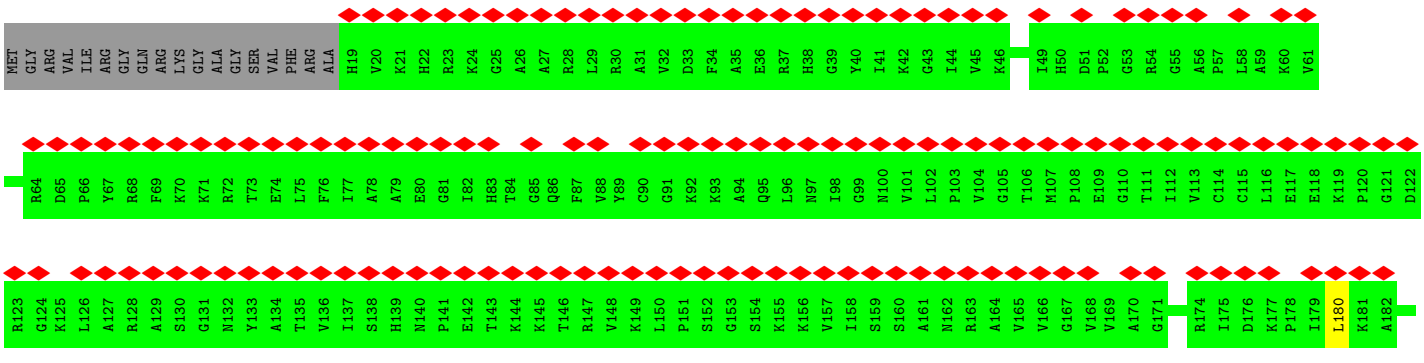
• Molecule 28: 60S ribosomal protein L28

Chain l:



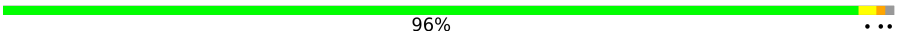
• Molecule 29: 60S ribosomal protein L8

Chain m:



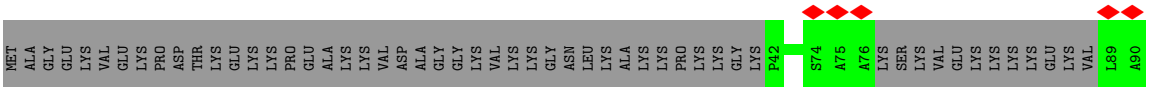
• Molecule 30: 60S ribosomal protein L35a

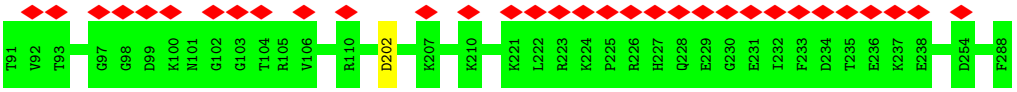
Chain n:



• Molecule 31: 60S ribosomal protein L6

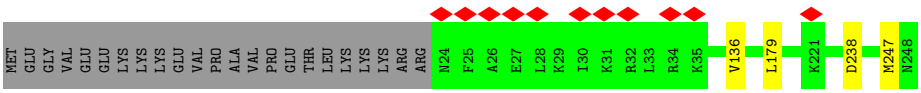
Chain o:





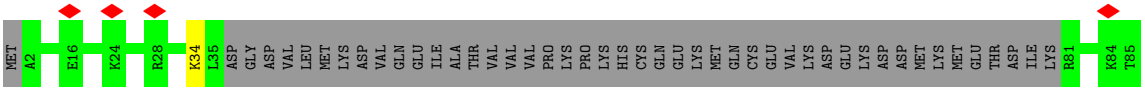
• Molecule 32: 60S ribosomal protein L7

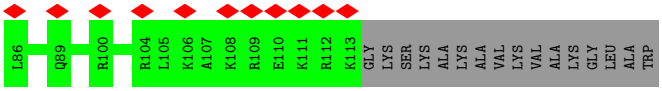
Chain p:



• Molecule 33: Protein LLP homolog

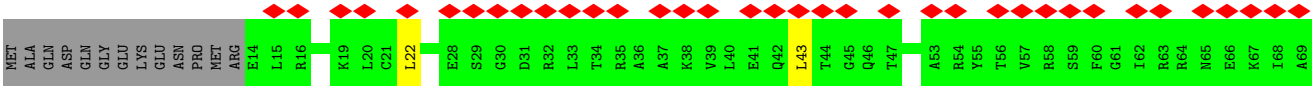
Chain z:

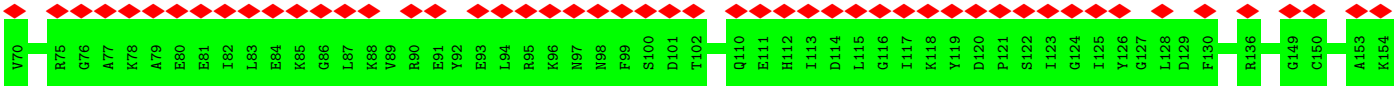


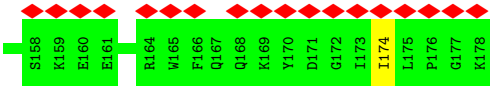


• Molecule 34: 60S ribosomal protein L11

Chain A:

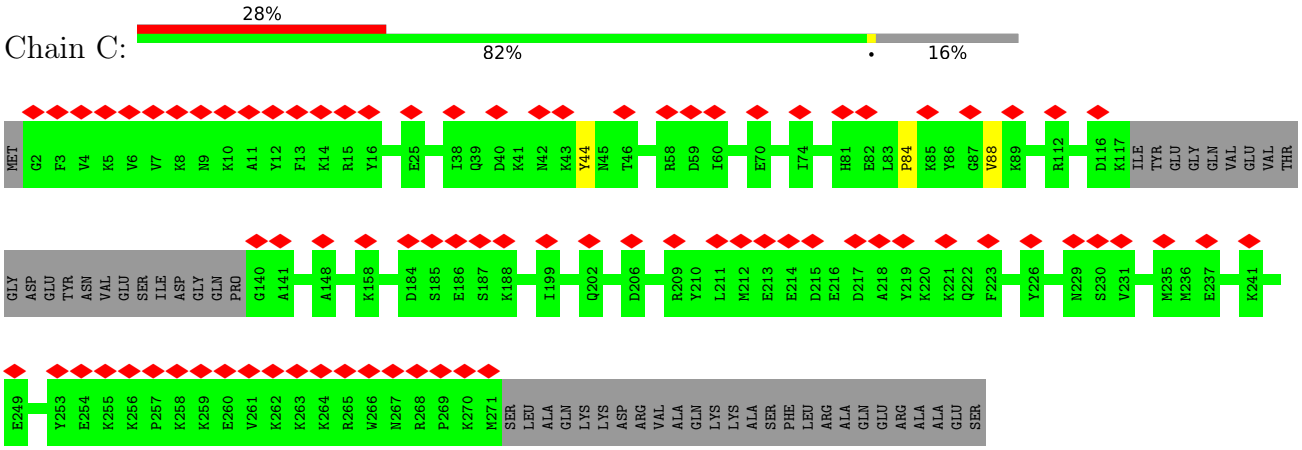






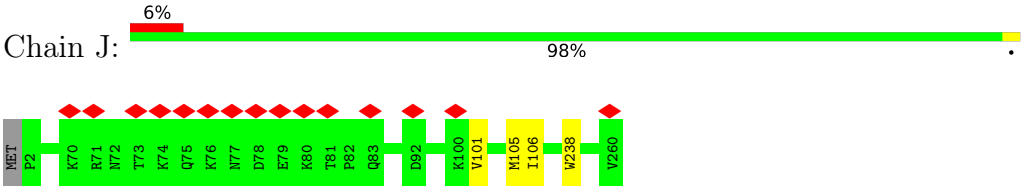
• Molecule 35: 60S ribosomal protein L5

Chain C:



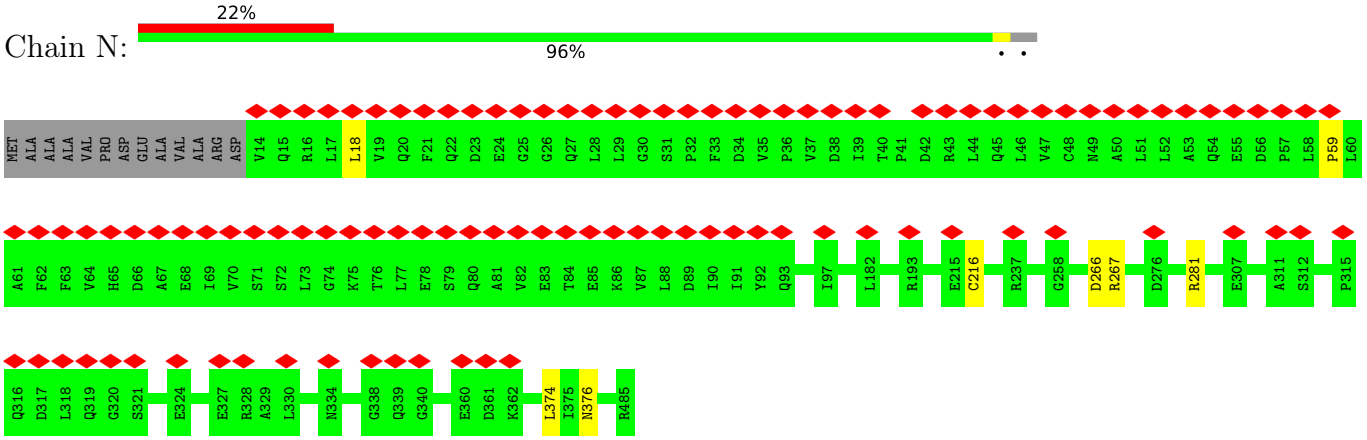
• Molecule 36: Ribosome biogenesis protein NSA2 homolog

Chain J:



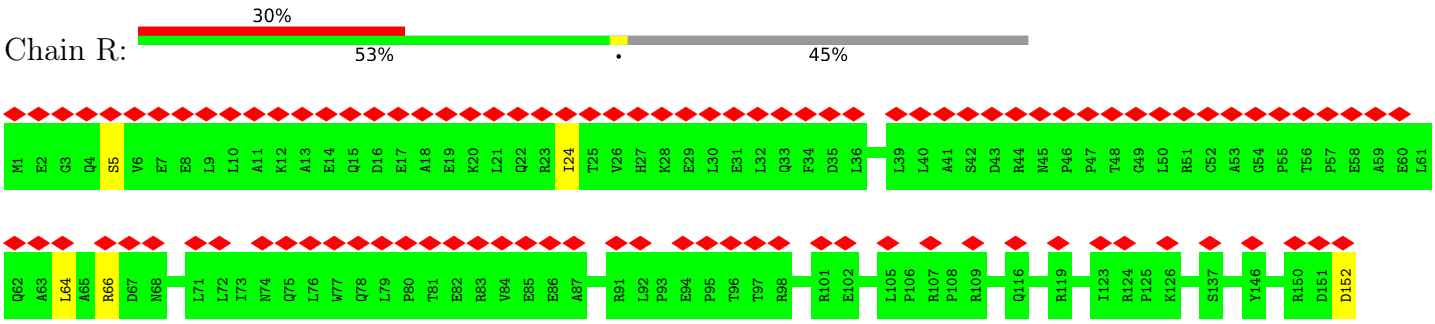
• Molecule 37: Notchless protein homolog 1

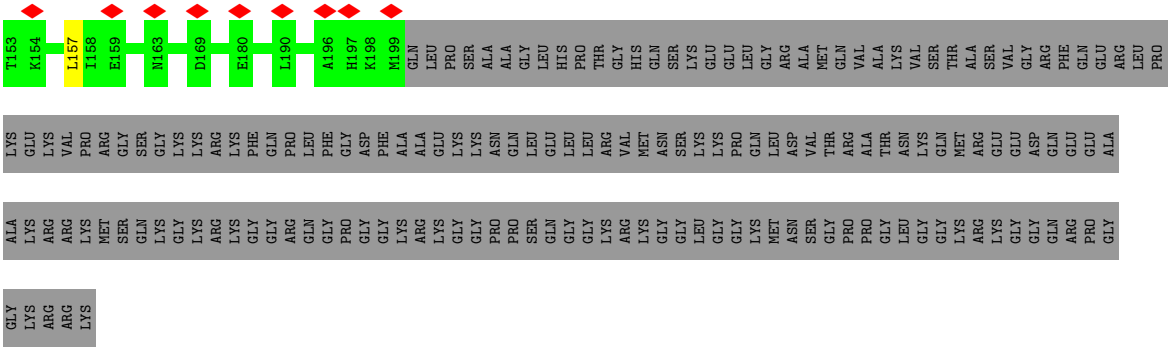
Chain N:



• Molecule 38: Ribosome biogenesis regulatory protein homolog

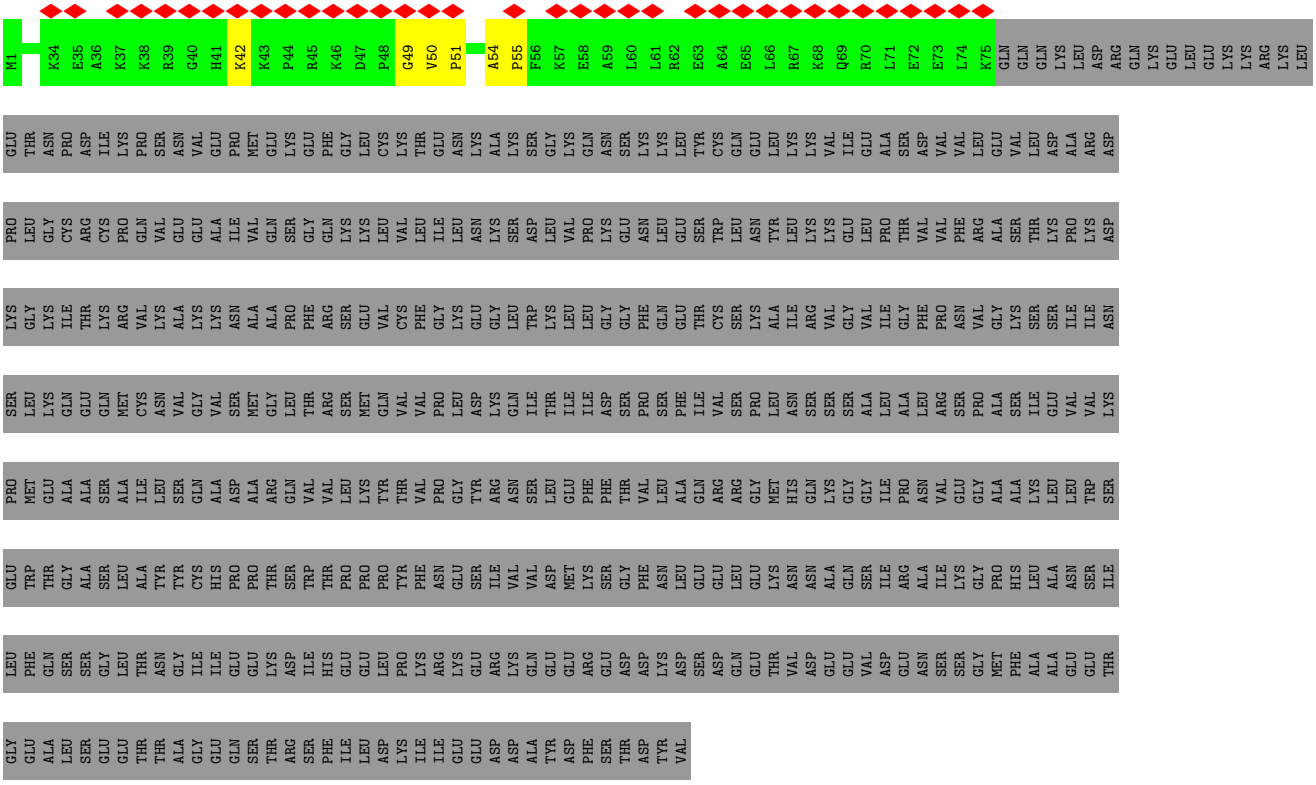
Chain R:





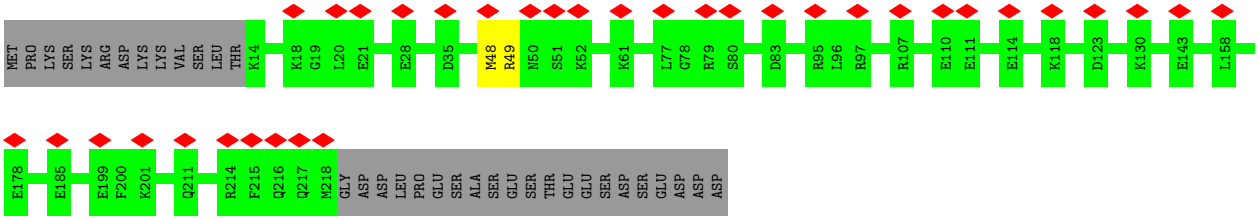
• Molecule 39: Guanine nucleotide-binding protein-like 3

Chain u:



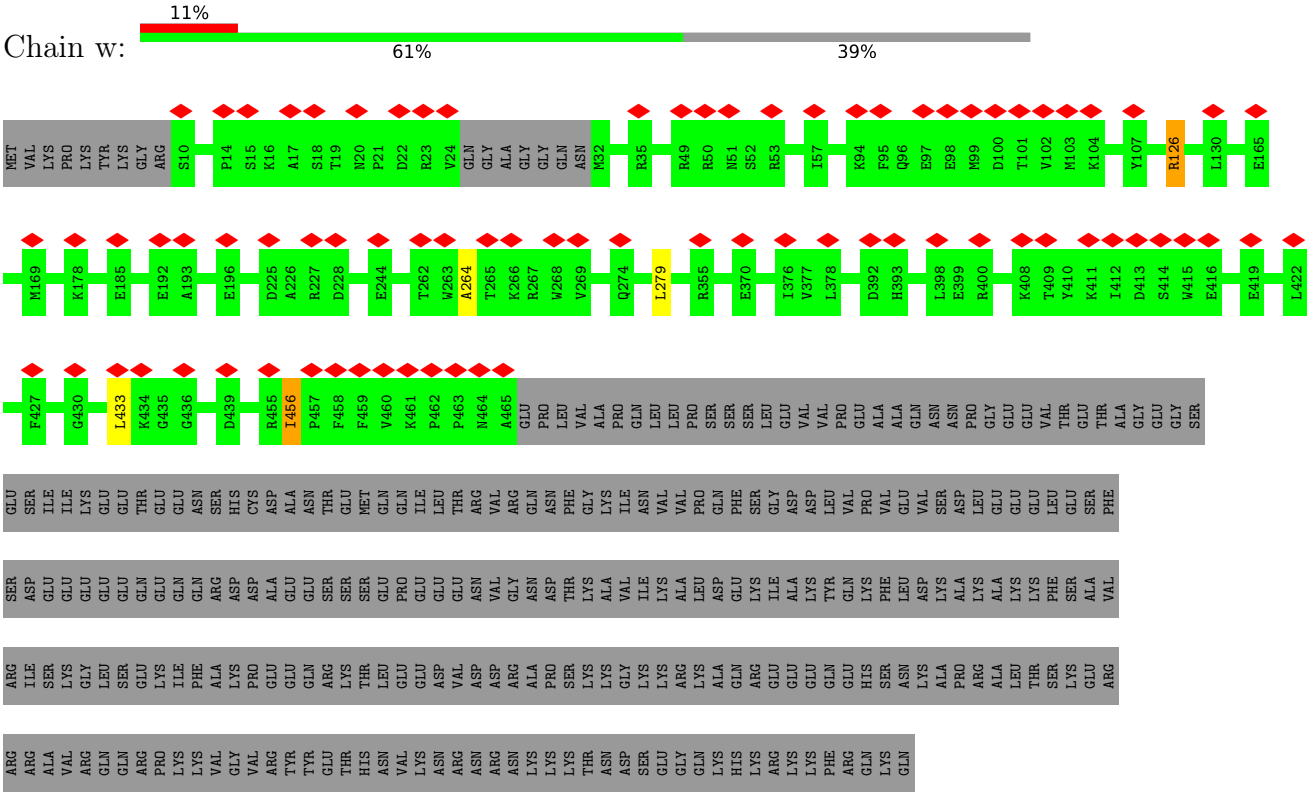
• Molecule 40: mRNA turnover protein 4 homolog

Chain v:



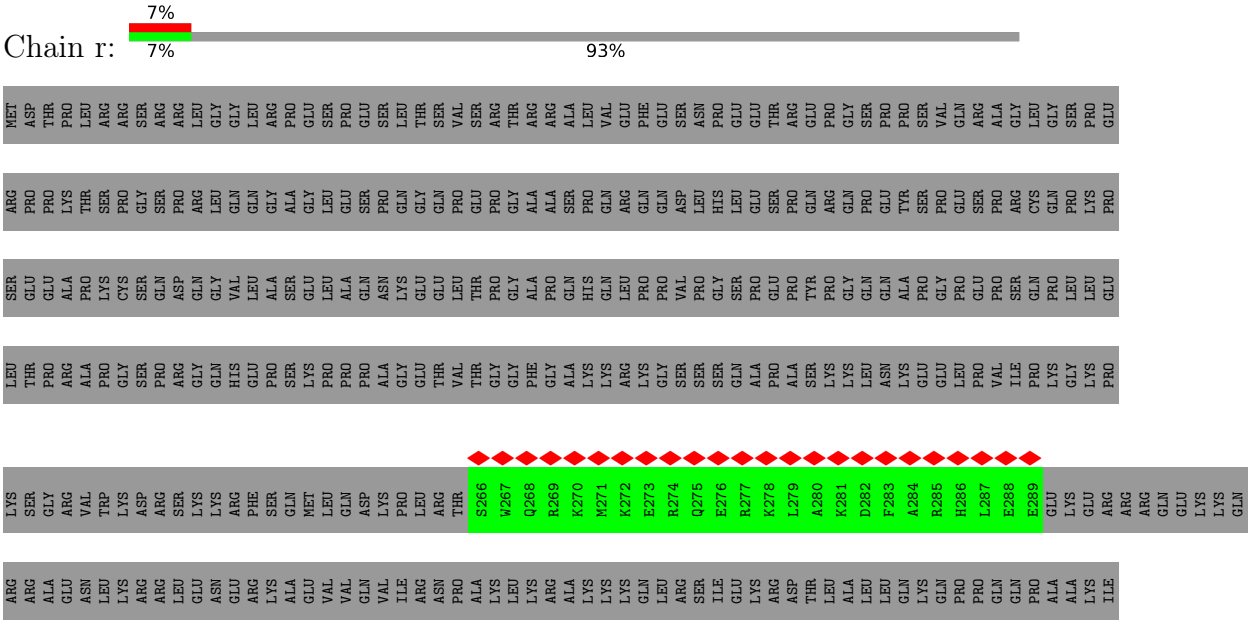
• Molecule 41: G Protein Nucleolar 2

Chain w:



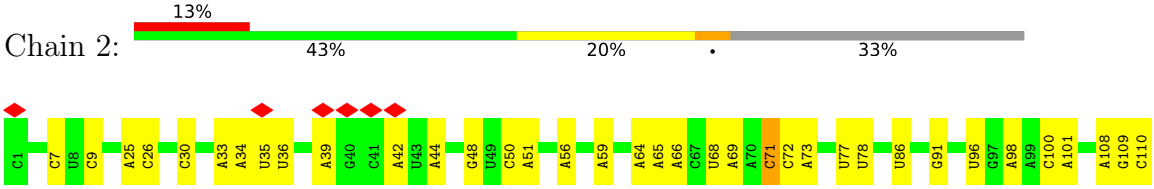
• Molecule 42: Coiled-coil domain-containing protein 86

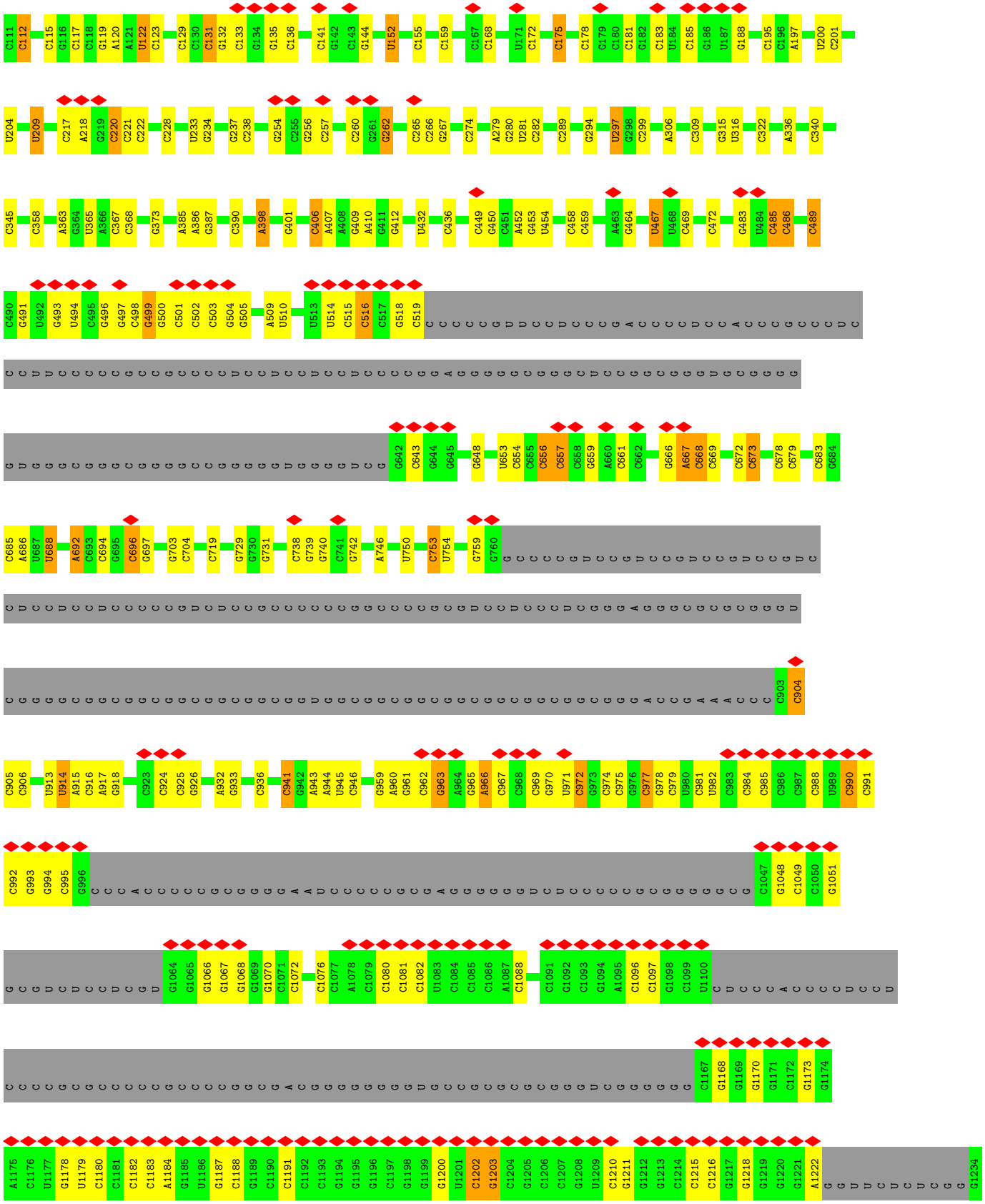
Chain r:

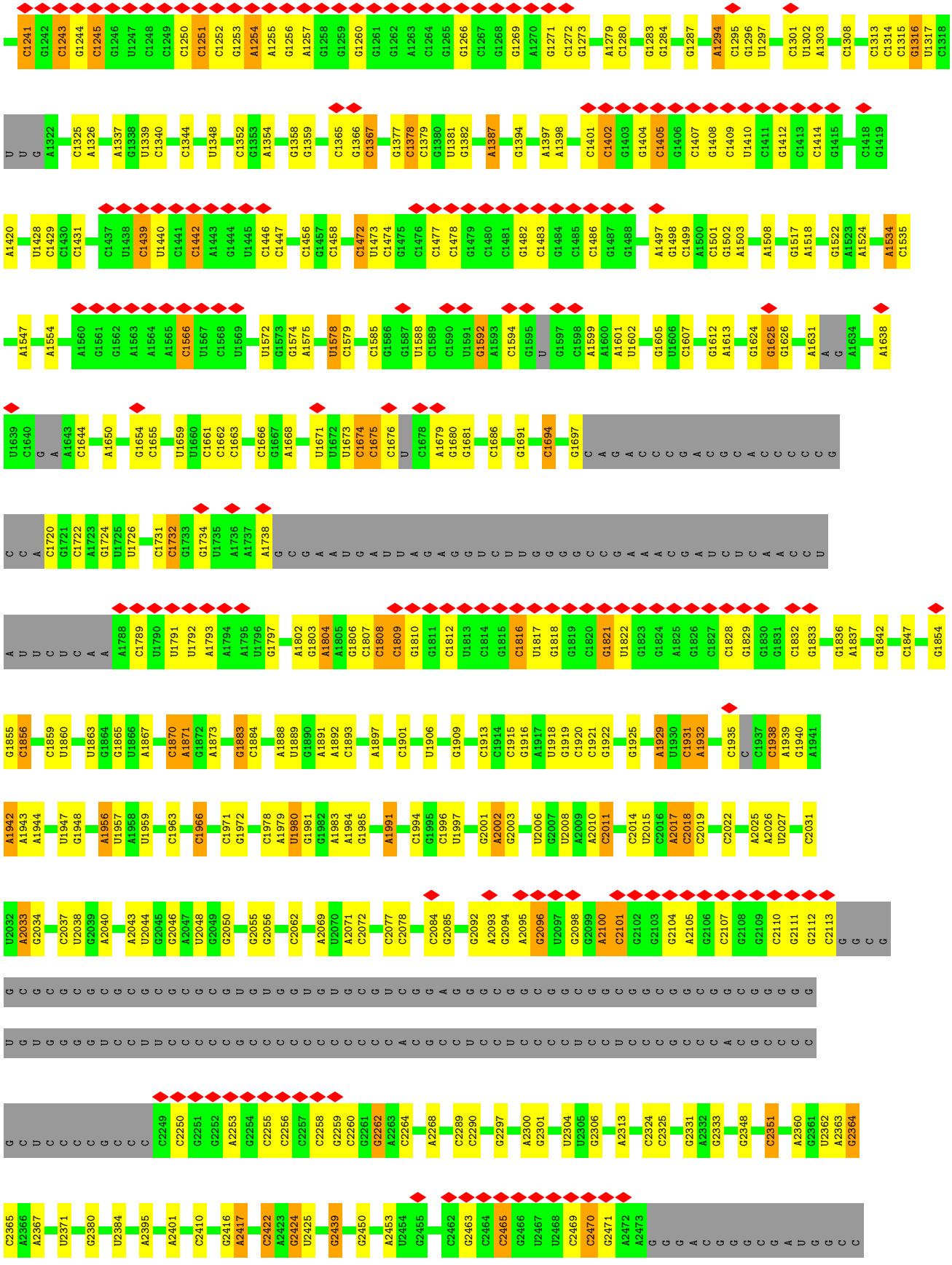


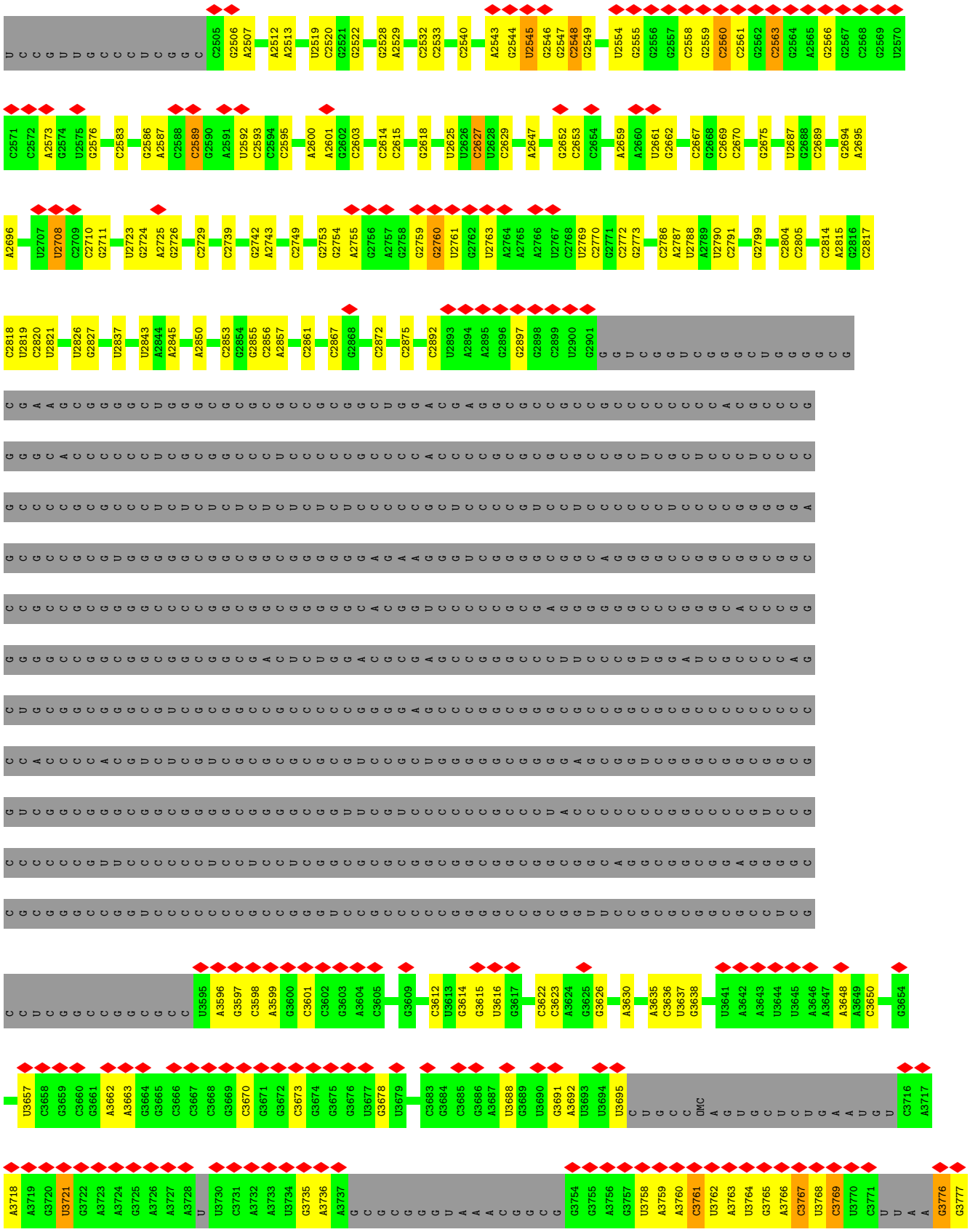
• Molecule 43: 28S rRNA

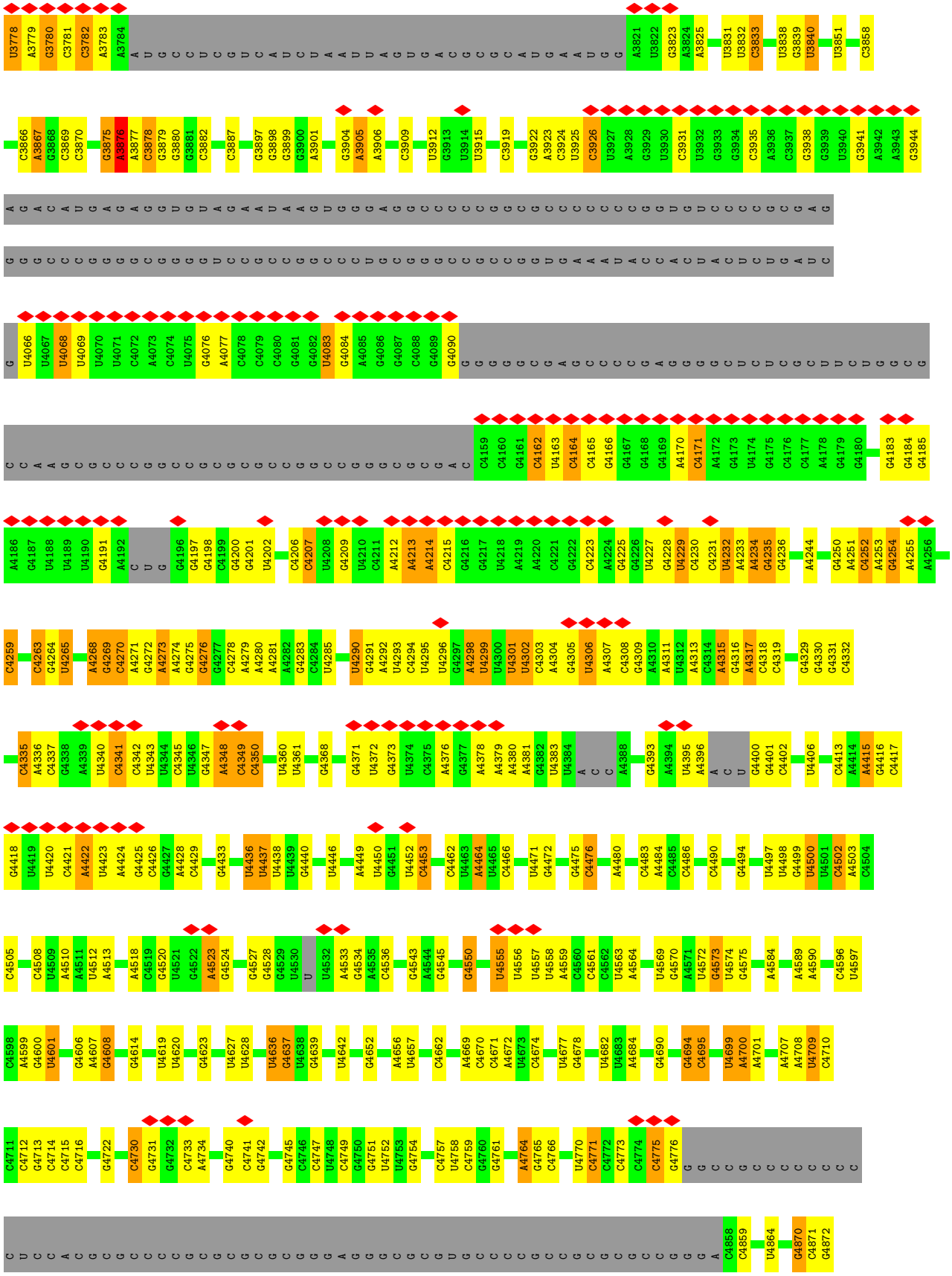
Chain 2:

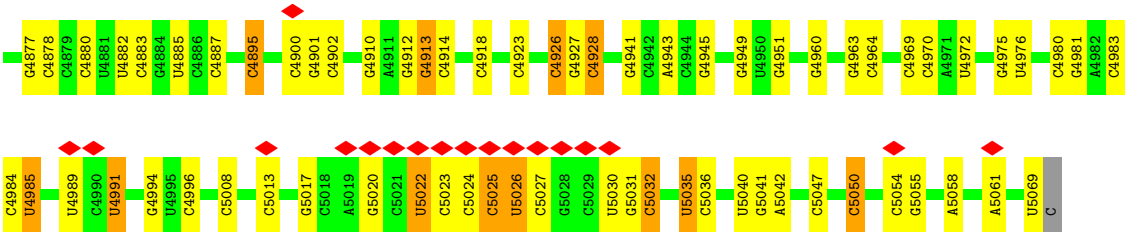




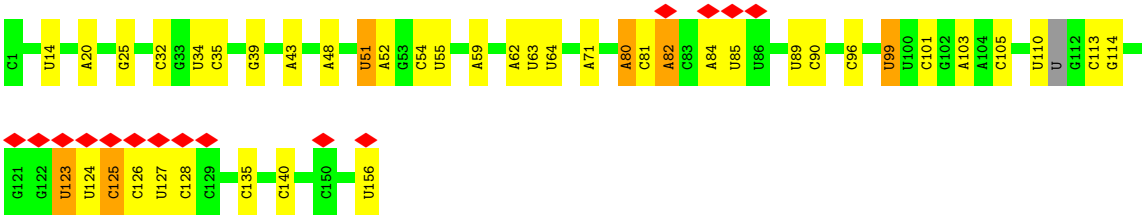




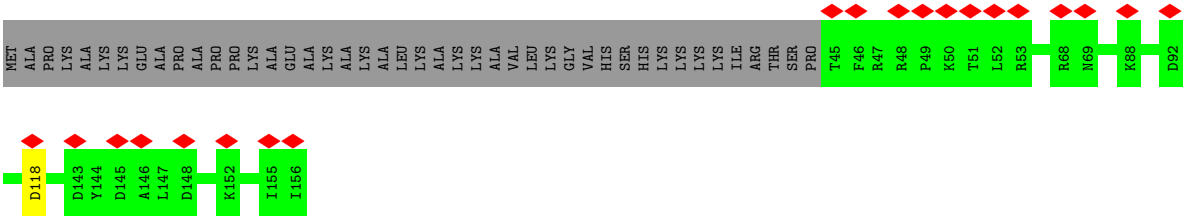




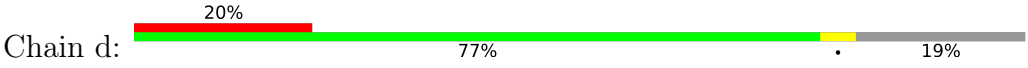
• Molecule 44: 5.8S rRMA

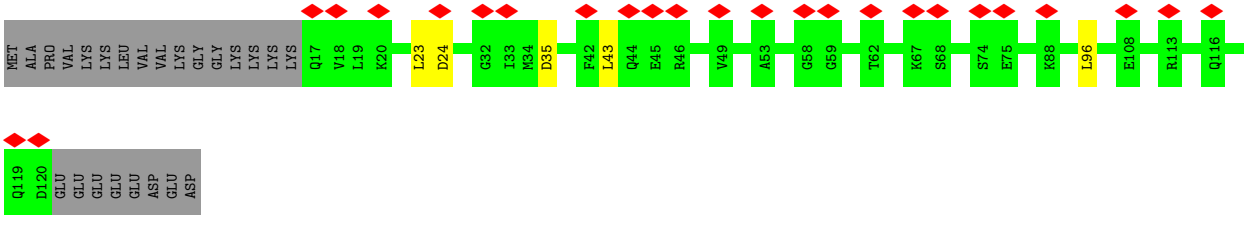


• Molecule 45: 60S ribosomal protein L23a

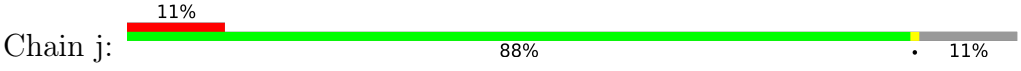


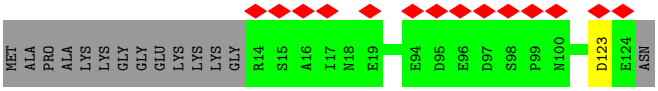
• Molecule 46: 60S ribosomal protein L22





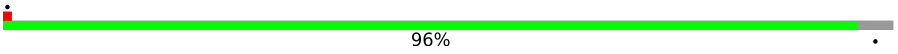
• Molecule 47: 60S ribosomal protein L31

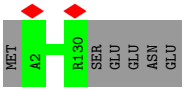




• Molecule 48: 60S ribosomal protein L32

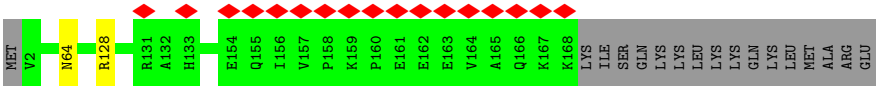
Chain k:





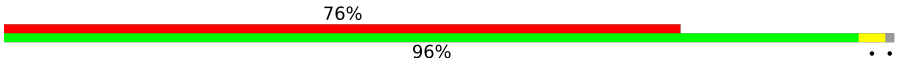
• Molecule 49: 60S ribosomal protein L17

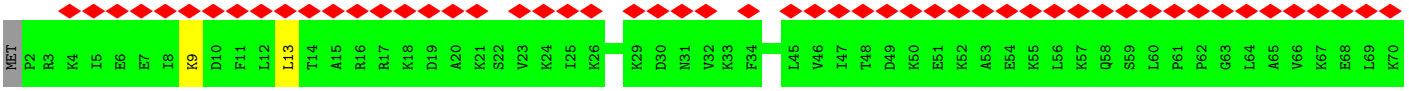
Chain Y:



• Molecule 50: 60S ribosomal protein L38

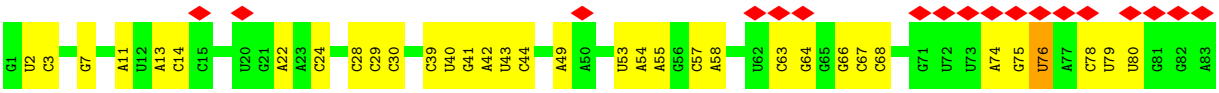
Chain O:

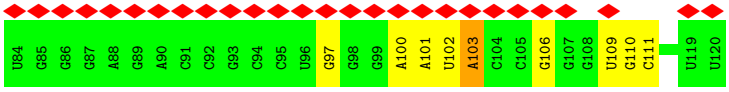




• Molecule 51: 5S RNA

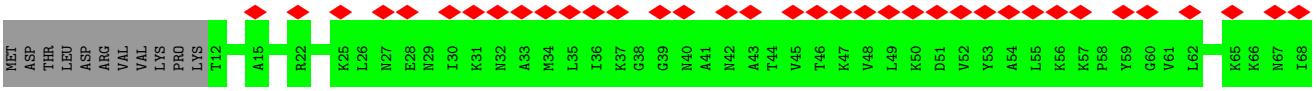
Chain W:

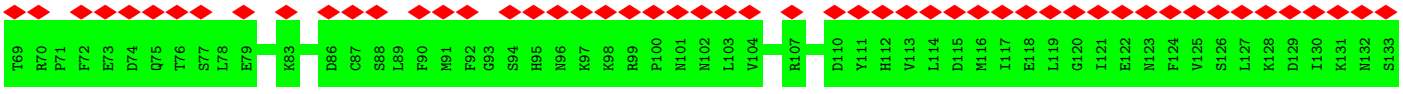


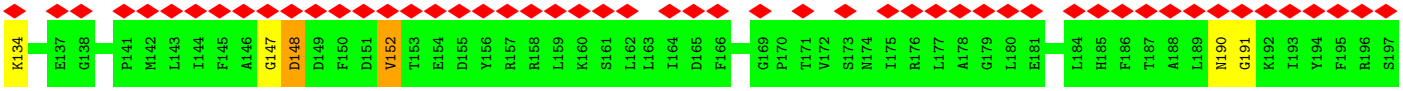


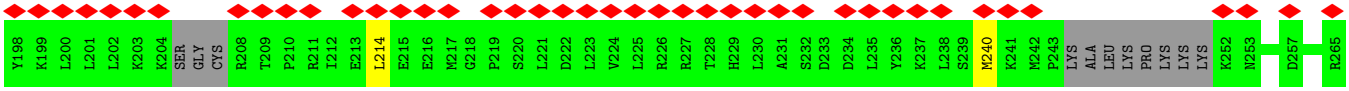
• Molecule 52: Ribosome production factor 2 homolog

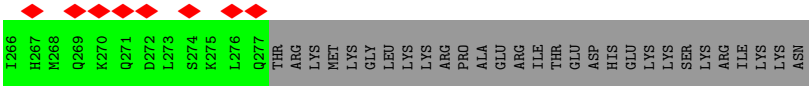
Chain T:





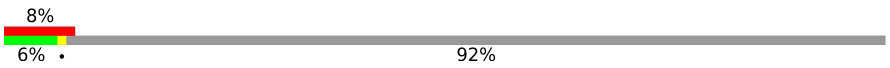


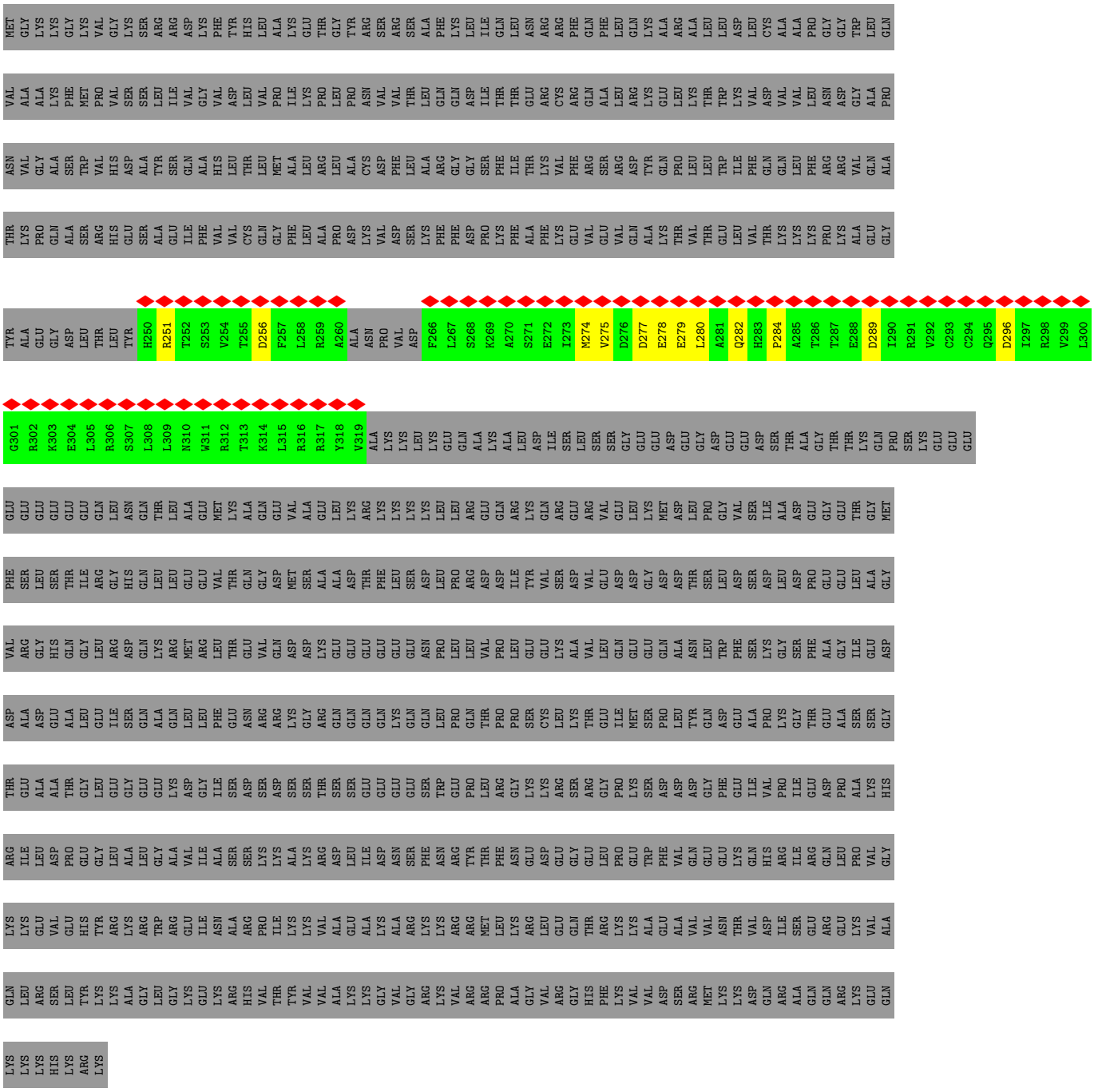




• Molecule 53: pre-rRNA 2'-O-ribose RNA methyltransferase FTSJ3

Chain 9:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	30311	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	0.173	Depositor
Minimum map value	-0.049	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.038	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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: OMC, A2M, P4U, MG, B8Q, OMU, BGH, P7G, M7A, B9H, 2MG, 5MU, I4U, GTP, B9B, B8W, E7G, 7MG, B8K, B8T, 1MA, UR3, OMG

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	y	0.33	0/1269	0.74	2/1712 (0.1%)
2	4	0.35	0/5177	0.80	14/6942 (0.2%)
3	6	0.32	0/1877	0.73	3/2554 (0.1%)
4	7	0.33	0/1181	0.63	0/1563
5	B	0.32	0/3315	0.67	1/4435 (0.0%)
6	D	0.31	0/2907	0.70	3/3905 (0.1%)
7	E	0.35	0/774	0.73	1/1038 (0.1%)
8	F	0.33	0/878	0.73	0/1170
9	G	0.36	0/1760	0.78	3/2368 (0.1%)
10	H	0.33	0/1023	0.65	0/1351
11	I	0.33	0/1537	0.76	2/2066 (0.1%)
12	K	0.34	0/843	0.86	2/1115 (0.2%)
13	L	0.32	0/904	0.74	2/1207 (0.2%)
14	M	0.30	0/720	0.69	0/952
15	P	0.29	0/454	0.65	0/599
16	Q	0.32	0/1682	0.70	1/2248 (0.0%)
17	S	0.35	0/1133	0.70	2/1516 (0.1%)
18	U	0.29	0/1580	0.66	1/2112 (0.0%)
19	V	0.32	0/1682	0.66	1/2250 (0.0%)
20	X	0.30	0/718	0.67	0/953
21	Z	0.30	0/1239	0.72	2/1658 (0.1%)
22	a	0.32	0/1255	0.74	1/1662 (0.1%)
23	b	0.31	0/1501	0.62	0/2013
24	c	0.36	0/994	0.71	0/1327
25	e	0.31	0/993	0.67	0/1332
26	h	0.34	0/1132	0.72	0/1504
27	i	0.37	0/1130	0.78	1/1507 (0.1%)
28	l	0.30	0/1017	0.67	0/1364
29	m	0.33	0/1426	0.73	1/1915 (0.1%)
30	n	0.32	0/895	0.74	1/1198 (0.1%)
31	o	0.32	0/1935	0.74	1/2596 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
32	p	0.36	0/1916	0.76	4/2553 (0.2%)
33	z	0.39	0/587	0.86	1/767 (0.1%)
34	A	0.37	0/1341	0.81	3/1793 (0.2%)
35	C	0.35	0/2068	0.70	2/2767 (0.1%)
36	J	0.30	0/2146	0.62	2/2865 (0.1%)
37	N	0.30	0/3756	0.68	4/5103 (0.1%)
38	R	0.32	0/1668	0.78	3/2255 (0.1%)
39	u	0.42	0/649	0.88	0/851
40	v	0.33	0/1709	0.67	3/2293 (0.1%)
41	w	0.32	0/3699	0.72	2/4992 (0.0%)
42	r	0.29	0/220	0.65	0/288
43	2	0.44	5/79277 (0.0%)	1.39	1180/123568 (1.0%)
44	8	0.41	0/3656	1.32	39/5694 (0.7%)
45	g	0.37	0/935	0.78	1/1257 (0.1%)
46	d	0.41	0/864	0.87	5/1160 (0.4%)
47	j	0.33	0/933	0.70	1/1256 (0.1%)
48	k	0.31	0/1082	0.67	0/1443
49	Y	0.30	0/1383	0.62	0/1856
50	O	0.39	0/575	0.84	1/761 (0.1%)
51	W	0.46	0/2858	1.42	60/4455 (1.3%)
52	T	0.36	0/2120	0.81	6/2837 (0.2%)
53	9	0.32	0/544	0.76	4/730 (0.5%)
All	All	0.39	5/158917 (0.0%)	1.16	1366/231676 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	4	0	4
5	B	0	2
16	Q	0	1
24	c	0	1
30	n	0	1
38	R	0	1
39	u	0	4
41	w	0	2
43	2	0	1
52	T	0	1
All	All	0	18

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2	3876	A	N9-C4	21.77	1.50	1.37
43	2	3876	A	N7-C5	-8.66	1.34	1.39
43	2	3876	A	N3-C4	5.88	1.38	1.34
43	2	3876	A	N9-C8	5.75	1.42	1.37
43	2	1929	A	N9-C4	5.65	1.41	1.37

All (1366) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	2	3876	A	C8-N9-C4	-51.59	85.17	105.80
43	2	3876	A	N7-C8-N9	34.63	131.12	113.80
43	2	3876	A	C2-N3-C4	23.44	122.32	110.60
43	2	3876	A	N3-C4-C5	-17.78	114.35	126.80
43	2	3876	A	C5-N7-C8	-15.87	95.97	103.90
43	2	3876	A	N9-C4-C5	15.45	111.98	105.80
43	2	2710	C	N1-C2-O2	13.04	126.73	118.90
43	2	4636	U	C2-N1-C1'	12.83	133.10	117.70
43	2	4636	U	N1-C2-O2	12.80	131.76	122.80
43	2	4926	C	N1-C2-O2	12.49	126.39	118.90
43	2	4636	U	N3-C2-O2	-12.23	113.64	122.20
43	2	1216	C	N1-C2-O2	12.16	126.20	118.90
43	2	2710	C	C6-N1-C2	-12.00	115.50	120.30
43	2	4926	C	C6-N1-C2	-11.98	115.51	120.30
43	2	753	C	N1-C2-O2	11.93	126.06	118.90
43	2	3761	C	N1-C2-O2	11.91	126.04	118.90
43	2	4302	U	C2-N1-C1'	11.87	131.94	117.70
43	2	1731	C	N1-C2-O2	11.78	125.97	118.90
43	2	2710	C	N3-C2-O2	-11.75	113.67	121.90
43	2	516	C	N1-C2-O2	11.51	125.81	118.90
43	2	1809	C	C6-N1-C2	-11.44	115.72	120.30
43	2	3876	A	C8-N9-C1'	11.44	148.29	127.70
43	2	4928	C	C6-N1-C2	-11.34	115.77	120.30
43	2	4306	U	N3-C2-O2	-11.23	114.34	122.20
43	2	1732	C	C6-N1-C2	-11.18	115.83	120.30
43	2	1994	C	C2-N1-C1'	11.01	130.91	118.80
43	2	100	C	C2-N1-C1'	10.99	130.89	118.80
43	2	4299	U	N1-C2-O2	10.94	130.46	122.80
43	2	4926	C	N3-C2-O2	-10.94	114.24	121.90
43	2	3761	C	C2-N1-C1'	10.91	130.80	118.80
43	2	2710	C	C2-N1-C1'	10.90	130.79	118.80
43	2	4306	U	N1-C2-O2	10.87	130.41	122.80
43	2	3778	U	N1-C2-O2	10.84	130.39	122.80
43	2	4302	U	N1-C2-O2	10.80	130.36	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	2	2018	C	C5-C6-N1	10.78	126.39	121.00
43	2	516	C	N3-C2-O2	-10.76	114.37	121.90
43	2	4299	U	N3-C2-O2	-10.74	114.68	122.20
43	2	2465	C	C5-C6-N1	10.72	126.36	121.00
43	2	4928	C	N1-C2-O2	10.70	125.32	118.90
43	2	753	C	C2-N1-C1'	10.70	130.57	118.80
43	2	1216	C	C2-N1-C1'	10.67	130.54	118.80
43	2	4207	C	N3-C2-O2	-10.66	114.44	121.90
43	2	4337	C	N1-C2-O2	10.64	125.28	118.90
43	2	100	C	N1-C2-O2	10.62	125.27	118.90
43	2	4229	U	N1-C2-O2	10.57	130.20	122.80
43	2	4420	U	N1-C2-O2	10.53	130.17	122.80
43	2	3778	U	N3-C2-O2	-10.52	114.83	122.20
43	2	1732	C	N1-C2-O2	10.51	125.21	118.90
43	2	4714	C	N1-C2-O2	10.48	125.19	118.90
43	2	4420	U	N3-C2-O2	-10.43	114.90	122.20
43	2	4302	U	N3-C2-O2	-10.35	114.95	122.20
43	2	2465	C	C6-N1-C2	-10.26	116.19	120.30
43	2	4337	C	C2-N1-C1'	10.26	130.08	118.80
43	2	1994	C	N1-C2-O2	10.12	124.97	118.90
43	2	3778	U	C2-N1-C1'	10.12	129.84	117.70
43	2	1731	C	C6-N1-C2	-9.94	116.33	120.30
43	2	1966	C	C6-N1-C2	-9.78	116.39	120.30
43	2	4229	U	N3-C2-O2	-9.71	115.40	122.20
43	2	1731	C	N3-C2-O2	-9.63	115.16	121.90
43	2	753	C	N3-C2-O2	-9.60	115.18	121.90
43	2	2022	C	N1-C2-O2	9.60	124.66	118.90
43	2	1732	C	N3-C2-O2	-9.56	115.21	121.90
43	2	2627	C	C6-N1-C2	-9.50	116.50	120.30
43	2	516	C	C6-N1-C2	-9.46	116.52	120.30
43	2	4880	C	N1-C2-O2	9.44	124.57	118.90
53	9	284	PRO	CA-N-CD	-9.40	98.34	111.50
43	2	3876	A	N9-C1'-C2'	9.39	126.21	114.00
43	2	3636	C	C6-N1-C2	-9.38	116.55	120.30
43	2	1809	C	C5-C6-N1	9.37	125.69	121.00
43	2	4417	C	N1-C2-O2	9.36	124.52	118.90
43	2	4928	C	N3-C2-O2	-9.36	115.35	121.90
43	2	4306	U	C2-N1-C1'	9.29	128.84	117.70
43	2	1216	C	N3-C2-O2	-9.28	115.41	121.90
43	2	1675	C	C6-N1-C2	-9.24	116.60	120.30
43	2	4758	U	C2-N1-C1'	9.23	128.78	117.70
43	2	4229	U	C2-N1-C1'	9.22	128.76	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	2	4306	U	C5-C6-N1	9.16	127.28	122.70
51	W	24	C	N1-C2-O2	9.14	124.38	118.90
43	2	4453	C	N1-C2-O2	9.12	124.37	118.90
43	2	2439	G	C4-N9-C1'	9.09	138.32	126.50
43	2	4682	U	N3-C2-O2	-9.08	115.85	122.20
43	2	4420	U	C2-N1-C1'	9.06	128.58	117.70
31	o	202	ASP	CB-CG-OD2	9.06	126.45	118.30
43	2	3761	C	N3-C2-O2	-9.06	115.56	121.90
43	2	77	U	N3-C2-O2	-9.05	115.86	122.20
43	2	4413	C	N1-C2-O2	8.98	124.29	118.90
43	2	4263	C	C2-N1-C1'	8.98	128.68	118.80
43	2	4299	U	C2-N1-C1'	8.95	128.44	117.70
43	2	4301	U	N1-C2-O2	8.95	129.06	122.80
43	2	1458	C	N1-C2-O2	8.93	124.26	118.90
43	2	3876	A	C5-C6-N1	8.93	122.16	117.70
43	2	467	U	N3-C2-O2	-8.89	115.97	122.20
44	8	64	U	N3-C2-O2	-8.89	115.98	122.20
43	2	4302	U	C5-C6-N1	8.88	127.14	122.70
43	2	4926	C	C2-N1-C1'	8.88	128.56	118.80
43	2	2018	C	C6-N1-C2	-8.86	116.76	120.30
43	2	499	G	N3-C4-N9	8.85	131.31	126.00
43	2	4301	U	C2-N1-C1'	8.85	128.32	117.70
43	2	4714	C	N3-C2-O2	-8.85	115.71	121.90
5	B	360	LEU	CA-CB-CG	8.83	135.62	115.30
43	2	485	C	C2-N1-C1'	8.81	128.49	118.80
43	2	467	U	N1-C2-O2	8.79	128.95	122.80
43	2	4926	C	C5-C6-N1	8.76	125.38	121.00
43	2	4215	C	N1-C2-O2	8.74	124.15	118.90
43	2	4887	C	N1-C2-O2	8.73	124.14	118.90
43	2	282	C	N1-C2-O2	8.73	124.14	118.90
43	2	112	C	C2-N1-C1'	8.72	128.40	118.80
43	2	4608	G	C8-N9-C4	-8.71	102.92	106.40
43	2	4682	U	N1-C2-O2	8.69	128.88	122.80
13	L	102	ASP	CB-CG-OD2	8.68	126.11	118.30
43	2	4758	U	N1-C2-O2	8.67	128.87	122.80
43	2	4714	C	C6-N1-C2	-8.65	116.84	120.30
43	2	2410	C	C6-N1-C2	-8.65	116.84	120.30
43	2	2015	U	N3-C2-O2	-8.65	116.15	122.20
43	2	100	C	N3-C2-O2	-8.63	115.86	121.90
43	2	2022	C	N3-C2-O2	-8.61	115.87	121.90
43	2	2627	C	C5-C6-N1	8.60	125.30	121.00
43	2	112	C	C6-N1-C2	-8.59	116.86	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	2	4306	U	C6-N1-C2	-8.59	115.85	121.00
43	2	1929	A	C2-N3-C4	8.57	114.89	110.60
43	2	4695	C	N1-C2-O2	8.57	124.04	118.90
43	2	4758	U	N3-C2-O2	-8.57	116.20	122.20
43	2	1994	C	N3-C2-O2	-8.56	115.91	121.90
2	4	175	GLY	C-N-CA	8.55	143.07	121.70
43	2	4636	U	C6-N1-C1'	-8.55	109.24	121.20
43	2	1816	C	C5-C6-N1	8.52	125.26	121.00
43	2	469	C	N1-C2-O2	8.46	123.97	118.90
43	2	4608	G	N7-C8-N9	8.43	117.32	113.10
43	2	3622	C	N1-C2-O2	8.43	123.96	118.90
43	2	96	U	N3-C2-O2	-8.39	116.33	122.20
43	2	4207	C	N1-C2-O2	8.38	123.93	118.90
43	2	4263	C	C6-N1-C2	-8.38	116.95	120.30
43	2	499	G	C4-N9-C1'	8.33	137.33	126.50
43	2	4335	C	N1-C2-O2	8.33	123.90	118.90
43	2	4928	C	C5-C6-N1	8.33	125.16	121.00
43	2	1966	C	C5-C6-N1	8.32	125.16	121.00
51	W	102	U	N3-C2-O2	-8.30	116.39	122.20
51	W	57	C	C6-N1-C2	-8.29	116.98	120.30
43	2	1966	C	C2-N1-C1'	8.28	127.91	118.80
38	R	152	ASP	CB-CG-OD1	8.26	125.74	118.30
51	W	29	C	C6-N1-C2	-8.24	117.00	120.30
43	2	1816	C	C6-N1-C2	-8.23	117.01	120.30
43	2	4337	C	N3-C2-O2	-8.22	116.15	121.90
43	2	2856	C	N1-C2-O2	8.22	123.83	118.90
43	2	4301	U	N3-C2-O2	-8.22	116.45	122.20
43	2	4066	U	N3-C2-O2	-8.19	116.46	122.20
43	2	1241	C	N1-C2-O2	8.17	123.80	118.90
43	2	3876	A	N1-C2-N3	-8.17	125.22	129.30
51	W	57	C	C5-C6-N1	8.16	125.08	121.00
43	2	2760	G	P-O3'-C3'	8.16	129.49	119.70
43	2	1675	C	N1-C2-O2	8.15	123.79	118.90
43	2	4928	C	C2-N1-C1'	8.15	127.76	118.80
43	2	1216	C	C6-N1-C2	-8.14	117.04	120.30
43	2	2101	C	C6-N1-C2	-8.11	117.05	120.30
43	2	2439	G	N3-C4-N9	8.11	130.87	126.00
51	W	102	U	N1-C2-O2	8.11	128.47	122.80
43	2	3778	U	C5-C6-N1	8.10	126.75	122.70
43	2	1921	C	C6-N1-C2	-8.10	117.06	120.30
43	2	4207	C	C6-N1-C2	-8.10	117.06	120.30
43	2	2410	C	C2-N1-C1'	8.09	127.70	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	2	4066	U	N1-C2-O2	8.09	128.46	122.80
43	2	1731	C	C2-N1-C1'	8.07	127.68	118.80
43	2	4864	U	N3-C2-O2	-8.06	116.55	122.20
43	2	2710	C	C5-C6-N1	8.06	125.03	121.00
43	2	4453	C	C2-N1-C1'	8.06	127.67	118.80
43	2	4864	U	N1-C2-O2	8.04	128.43	122.80
43	2	467	U	C2-N1-C1'	8.04	127.34	117.70
43	2	1402	C	N1-C2-O2	8.02	123.71	118.90
43	2	1720	C	N1-C2-O2	8.00	123.70	118.90
43	2	4573	G	N3-C4-C5	-8.00	124.60	128.60
43	2	3831	U	N3-C2-O2	-7.98	116.61	122.20
43	2	2563	C	N1-C2-O2	7.97	123.68	118.90
43	2	112	C	N1-C2-O2	7.94	123.67	118.90
43	2	1731	C	C5-C6-N1	7.94	124.97	121.00
43	2	5025	C	C6-N1-C2	-7.94	117.12	120.30
43	2	2850	A	C2-N3-C4	7.93	114.57	110.60
43	2	36	U	N3-C2-O2	-7.93	116.65	122.20
43	2	4215	C	C6-N1-C2	-7.92	117.13	120.30
43	2	672	C	N1-C2-O2	7.91	123.65	118.90
43	2	1732	C	C5-C6-N1	7.91	124.96	121.00
43	2	2439	G	C8-N9-C1'	-7.91	116.71	127.00
43	2	4265	U	N3-C2-O2	-7.90	116.67	122.20
43	2	4206	C	N1-C2-O2	7.88	123.63	118.90
43	2	914	U	P-O3'-C3'	7.87	129.14	119.70
43	2	485	C	C6-N1-C2	-7.85	117.16	120.30
43	2	2470	C	P-O3'-C3'	7.85	129.12	119.70
43	2	2015	U	N1-C2-O2	7.84	128.29	122.80
43	2	4235	G	P-O3'-C3'	7.83	129.10	119.70
43	2	1241	C	C2-N1-C1'	7.81	127.39	118.80
43	2	3833	C	C6-N1-C2	-7.81	117.17	120.30
43	2	4747	C	C6-N1-C2	-7.79	117.18	120.30
43	2	77	U	N1-C2-O2	7.79	128.25	122.80
43	2	2627	C	N1-C2-O2	7.78	123.57	118.90
43	2	4662	C	C6-N1-C2	-7.78	117.19	120.30
43	2	3762	U	N3-C2-O2	-7.78	116.76	122.20
43	2	36	U	N1-C2-O2	7.76	128.23	122.80
43	2	2439	G	N3-C4-C5	-7.75	124.72	128.60
43	2	4573	G	C4-N9-C1'	7.74	136.56	126.50
43	2	753	C	C6-N1-C2	-7.74	117.21	120.30
43	2	3926	C	N1-C2-O2	7.73	123.54	118.90
43	2	2627	C	C2-N1-C1'	7.73	127.30	118.80
43	2	2528	G	C4-N9-C1'	7.70	136.51	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	2	1978	C	N1-C2-O2	7.69	123.52	118.90
43	2	4232	U	N3-C2-O2	-7.69	116.81	122.20
43	2	4880	C	N3-C2-O2	-7.69	116.52	121.90
43	2	35	U	N3-C2-O2	-7.69	116.82	122.20
43	2	4766	C	C6-N1-C2	-7.68	117.23	120.30
43	2	3721	U	N3-C2-O2	-7.68	116.82	122.20
44	8	54	C	N1-C2-O2	7.67	123.50	118.90
43	2	469	C	C6-N1-C2	-7.66	117.23	120.30
43	2	499	G	N3-C4-C5	-7.66	124.77	128.60
43	2	4335	C	C6-N1-C2	-7.64	117.24	120.30
43	2	2548	C	N1-C2-O2	7.64	123.48	118.90
43	2	4985	U	N3-C2-O2	-7.64	116.85	122.20
43	2	1808	C	P-O3'-C3'	7.63	128.86	119.70
43	2	1978	C	C6-N1-C2	-7.63	117.25	120.30
44	8	123	U	C2-N1-C1'	7.61	126.83	117.70
51	W	30	C	C6-N1-C2	-7.60	117.26	120.30
43	2	1966	C	N1-C2-O2	7.60	123.46	118.90
43	2	1994	C	C6-N1-C1'	-7.59	111.69	120.80
43	2	2410	C	C5-C6-N1	7.59	124.80	121.00
43	2	2107	C	C6-N1-C2	-7.59	117.26	120.30
43	2	2410	C	N1-C2-O2	7.59	123.45	118.90
43	2	100	C	C6-N1-C1'	-7.58	111.70	120.80
43	2	472	C	C6-N1-C2	-7.57	117.27	120.30
43	2	2532	C	C6-N1-C2	-7.57	117.27	120.30
43	2	1401	C	C2-N1-C1'	7.56	127.12	118.80
43	2	1720	C	C6-N1-C2	-7.56	117.28	120.30
43	2	4232	U	N1-C2-O2	7.56	128.09	122.80
43	2	4413	C	N3-C2-O2	-7.55	116.61	121.90
43	2	2094	G	C4-N9-C1'	7.55	136.31	126.50
43	2	4229	U	P-O3'-C3'	7.55	128.76	119.70
46	d	24	ASP	CB-CG-OD1	7.55	125.09	118.30
43	2	2819	U	N3-C2-O2	-7.53	116.93	122.20
43	2	3761	C	C6-N1-C1'	-7.52	111.77	120.80
43	2	35	U	N1-C2-O2	7.51	128.06	122.80
43	2	1915	C	N1-C2-O2	7.50	123.40	118.90
43	2	282	C	N3-C2-O2	-7.50	116.65	121.90
43	2	3762	U	N1-C2-O2	7.49	128.04	122.80
43	2	4263	C	C5-C6-N1	7.49	124.75	121.00
43	2	1458	C	N3-C2-O2	-7.46	116.68	121.90
43	2	1938	C	N1-C2-O2	7.46	123.38	118.90
43	2	3622	C	C6-N1-C2	-7.45	117.32	120.30
43	2	4254	G	N3-C4-C5	-7.44	124.88	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	2	2033	A	P-O3'-C3'	7.40	128.58	119.70
43	2	974	C	N1-C2-O2	7.39	123.33	118.90
43	2	3721	U	N1-C2-O2	7.38	127.97	122.80
43	2	499	G	C8-N9-C1'	-7.37	117.41	127.00
43	2	2563	C	C6-N1-C2	-7.37	117.35	120.30
43	2	4402	C	N1-C2-O2	7.37	123.32	118.90
43	2	3831	U	N1-C2-O2	7.35	127.94	122.80
44	8	125	C	P-O3'-C3'	7.34	128.51	119.70
43	2	2002	A	C2-N3-C4	7.34	114.27	110.60
43	2	4453	C	N3-C2-O2	-7.31	116.78	121.90
43	2	485	C	N1-C2-O2	7.31	123.29	118.90
43	2	4360	U	N3-C2-O2	-7.31	117.08	122.20
43	2	4502	C	N1-C2-O2	7.31	123.28	118.90
43	2	4417	C	N3-C2-O2	-7.29	116.80	121.90
43	2	975	C	N1-C2-O2	7.28	123.27	118.90
43	2	1675	C	N3-C2-O2	-7.28	116.80	121.90
43	2	100	C	C6-N1-C2	-7.27	117.39	120.30
43	2	1732	C	C2-N1-C1'	7.26	126.79	118.80
43	2	4066	U	C2-N1-C1'	7.26	126.42	117.70
43	2	4775	C	C2-N1-C1'	7.26	126.79	118.80
43	2	1325	C	N1-C2-O2	7.26	123.26	118.90
43	2	5035	U	N3-C2-O2	-7.26	117.12	122.20
43	2	4426	C	C2-N1-C1'	7.25	126.78	118.80
43	2	4555	U	P-O3'-C3'	7.25	128.40	119.70
43	2	3761	C	C6-N1-C2	-7.25	117.40	120.30
41	w	433	LEU	CA-CB-CG	7.24	131.96	115.30
43	2	1994	C	C6-N1-C2	-7.24	117.41	120.30
43	2	112	C	C5-C6-N1	7.23	124.62	121.00
43	2	1367	C	C2-N1-C1'	7.21	126.73	118.80
43	2	4413	C	C6-N1-C2	-7.20	117.42	120.30
43	2	4302	U	C6-N1-C1'	-7.20	111.12	121.20
43	2	220	C	C6-N1-C2	-7.19	117.42	120.30
43	2	3637	U	N3-C2-O2	-7.18	117.17	122.20
32	p	238	ASP	CB-CG-OD2	7.18	124.76	118.30
43	2	1921	C	N1-C2-O2	7.17	123.20	118.90
43	2	4996	C	C6-N1-C2	-7.17	117.43	120.30
43	2	96	U	N1-C2-O2	7.17	127.82	122.80
43	2	3598	C	C6-N1-C2	-7.17	117.43	120.30
43	2	4887	C	N3-C2-O2	-7.17	116.88	121.90
43	2	1191	C	N3-C2-O2	-7.15	116.90	121.90
43	2	753	C	C6-N1-C1'	-7.14	112.23	120.80
43	2	4471	U	N3-C2-O2	-7.14	117.20	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	2	4360	U	N1-C2-O2	7.14	127.80	122.80
43	2	3926	C	C6-N1-C2	-7.13	117.45	120.30
43	2	4269	G	P-O3'-C3'	7.12	128.25	119.70
43	2	1405	C	N1-C2-O2	7.12	123.17	118.90
43	2	3935	C	C6-N1-C2	-7.11	117.45	120.30
43	2	1401	C	C6-N1-C2	-7.11	117.46	120.30
43	2	3905	A	P-O3'-C3'	7.11	128.23	119.70
43	2	4215	C	N3-C2-O2	-7.10	116.93	121.90
43	2	1980	U	P-O3'-C3'	7.10	128.22	119.70
43	2	4417	C	C6-N1-C2	-7.10	117.46	120.30
43	2	1402	C	C6-N1-C2	-7.10	117.46	120.30
43	2	4770	U	N3-C2-O2	-7.09	117.24	122.20
43	2	3833	C	C2-N1-C1'	7.08	126.59	118.80
43	2	115	C	C2-N1-C1'	7.08	126.59	118.80
43	2	2528	G	N3-C4-N9	7.07	130.24	126.00
44	8	64	U	N1-C2-O2	7.07	127.75	122.80
43	2	4476	C	C2-N1-C1'	7.06	126.57	118.80
43	2	2528	G	N3-C4-C5	-7.06	125.07	128.60
43	2	4747	C	C2-N1-C1'	7.06	126.56	118.80
43	2	4436	U	N3-C2-O2	-7.05	117.26	122.20
43	2	4302	U	C6-N1-C2	-7.04	116.78	121.00
43	2	4337	C	C6-N1-C1'	-7.04	112.35	120.80
43	2	1216	C	C5-C6-N1	7.04	124.52	121.00
43	2	1726	U	N3-C2-O2	-7.03	117.28	122.20
43	2	4985	U	N1-C2-O2	7.03	127.72	122.80
43	2	4627	U	N3-C2-O2	-7.03	117.28	122.20
43	2	282	C	C6-N1-C2	-7.03	117.49	120.30
43	2	3650	C	C6-N1-C2	-7.03	117.49	120.30
43	2	4573	G	N3-C4-N9	7.02	130.21	126.00
44	8	99	U	N3-C2-O2	-7.02	117.28	122.20
51	W	24	C	N3-C2-O2	-7.02	116.99	121.90
43	2	2532	C	C5-C6-N1	7.01	124.51	121.00
43	2	4254	G	N3-C4-N9	7.01	130.21	126.00
43	2	4972	U	N3-C2-O2	-7.01	117.29	122.20
43	2	3875	G	P-O3'-C3'	7.00	128.10	119.70
43	2	4895	C	N1-C2-O2	7.00	123.10	118.90
43	2	1245	C	C6-N1-C2	-7.00	117.50	120.30
43	2	1402	C	N3-C2-O2	-7.00	117.00	121.90
43	2	4695	C	N3-C2-O2	-7.00	117.00	121.90
43	2	1216	C	C6-N1-C1'	-6.99	112.41	120.80
43	2	1607	C	N1-C2-O2	6.99	123.09	118.90
43	2	5035	U	N1-C2-O2	6.99	127.69	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	2	1428	U	N3-C2-O2	-6.99	117.31	122.20
43	2	4773	C	C6-N1-C2	-6.98	117.51	120.30
43	2	209	U	N3-C2-O2	-6.98	117.32	122.20
43	2	469	C	N3-C2-O2	-6.96	117.03	121.90
43	2	972	C	C6-N1-C2	-6.96	117.52	120.30
43	2	4349	C	N1-C2-O2	6.95	123.07	118.90
43	2	2094	G	N3-C4-N9	6.94	130.17	126.00
43	2	972	C	N1-C2-O2	6.92	123.05	118.90
43	2	1367	C	N1-C2-O2	6.91	123.05	118.90
43	2	2362	U	N3-C2-O2	-6.91	117.36	122.20
43	2	4913	G	P-O3'-C3'	6.91	127.99	119.70
43	2	2107	C	C2-N1-C1'	6.91	126.40	118.80
44	8	101	C	C6-N1-C2	-6.90	117.54	120.30
51	W	43	U	N3-C2-O2	-6.90	117.37	122.20
43	2	2821	U	N3-C2-O2	-6.90	117.37	122.20
43	2	281	U	N3-C2-O2	-6.90	117.37	122.20
43	2	4413	C	C2-N1-C1'	6.90	126.39	118.80
43	2	4773	C	C5-C6-N1	6.90	124.45	121.00
43	2	1344	C	C6-N1-C2	-6.89	117.54	120.30
32	p	179	LEU	CA-CB-CG	6.89	131.15	115.30
43	2	2548	C	C2-N1-C1'	6.89	126.38	118.80
43	2	2560	C	C6-N1-C2	-6.88	117.55	120.30
43	2	2837	U	N3-C2-O2	-6.88	117.38	122.20
43	2	4162	C	N1-C2-O2	6.88	123.03	118.90
43	2	4335	C	N3-C2-O2	-6.87	117.09	121.90
43	2	472	C	N1-C2-O2	6.86	123.02	118.90
43	2	209	U	N1-C2-O2	6.86	127.60	122.80
43	2	2814	C	N1-C2-O2	6.85	123.01	118.90
43	2	86	U	N3-C2-O2	-6.84	117.41	122.20
43	2	974	C	C6-N1-C2	-6.84	117.56	120.30
9	G	211	ASP	CB-CG-OD1	6.84	124.45	118.30
43	2	4337	C	C6-N1-C2	-6.83	117.57	120.30
43	2	977	C	C6-N1-C2	-6.83	117.57	120.30
43	2	365	U	N3-C2-O2	-6.83	117.42	122.20
43	2	4436	U	N1-C2-O2	6.82	127.57	122.80
43	2	4290	U	N1-C2-O2	6.82	127.57	122.80
43	2	489	C	C6-N1-C2	-6.81	117.58	120.30
43	2	1315	C	C5-C6-N1	6.81	124.40	121.00
43	2	5035	U	P-O3'-C3'	6.81	127.87	119.70
43	2	2729	C	C6-N1-C2	-6.81	117.58	120.30
51	W	29	C	C2-N1-C1'	6.80	126.28	118.80
2	4	299	LEU	CA-CB-CG	6.80	130.94	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	2	2094	G	N3-C4-C5	-6.80	125.20	128.60
43	2	1315	C	C6-N1-C2	-6.80	117.58	120.30
43	2	3622	C	N3-C2-O2	-6.79	117.14	121.90
44	8	123	U	N1-C2-O2	6.79	127.56	122.80
51	W	43	U	N1-C2-O2	6.79	127.56	122.80
43	2	1816	C	C2-N1-C1'	6.78	126.26	118.80
43	2	4880	C	C6-N1-C2	-6.78	117.59	120.30
43	2	1088	C	C6-N1-C2	-6.78	117.59	120.30
43	2	4505	C	C6-N1-C2	-6.78	117.59	120.30
43	2	4573	G	C2-N3-C4	6.78	115.29	111.90
43	2	1929	A	C4-N9-C1'	6.77	138.48	126.30
43	2	4341	C	N1-C2-O2	6.77	122.96	118.90
43	2	4269	G	OP1-P-O3'	6.76	120.08	105.20
43	2	2856	C	C6-N1-C2	-6.76	117.60	120.30
43	2	4569	U	N3-C2-O2	-6.75	117.47	122.20
43	2	4426	C	N1-C2-O2	6.75	122.95	118.90
51	W	28	C	C6-N1-C2	-6.74	117.60	120.30
43	2	3688	U	N3-C2-O2	-6.74	117.48	122.20
29	m	180	LEU	CA-CB-CG	6.73	130.79	115.30
43	2	2362	U	N1-C2-O2	6.73	127.51	122.80
43	2	3636	C	N1-C2-O2	6.72	122.93	118.90
43	2	3776	G	C4-N9-C1'	6.72	135.23	126.50
43	2	4263	C	N1-C2-O2	6.72	122.93	118.90
43	2	4983	C	C6-N1-C2	-6.71	117.62	120.30
43	2	1251	C	C6-N1-C2	-6.71	117.62	120.30
43	2	4573	G	C8-N9-C1'	-6.71	118.28	127.00
51	W	29	C	C5-C6-N1	6.71	124.35	121.00
43	2	1720	C	N3-C2-O2	-6.70	117.21	121.90
27	i	106	LEU	CA-CB-CG	6.70	130.71	115.30
43	2	2008	U	C2-N1-C1'	6.70	125.74	117.70
43	2	2262	G	C4-N9-C1'	6.70	135.21	126.50
40	v	49	ARG	CG-CD-NE	6.69	125.85	111.80
43	2	2819	U	N1-C2-O2	6.69	127.48	122.80
43	2	904	C	N1-C2-O2	6.68	122.91	118.90
43	2	2667	C	N1-C2-O2	6.68	122.91	118.90
43	2	4417	C	C2-N1-C1'	6.68	126.14	118.80
43	2	4770	U	N1-C2-O2	6.68	127.47	122.80
43	2	2856	C	N3-C2-O2	-6.67	117.23	121.90
43	2	4508	C	N1-C2-O2	6.66	122.90	118.90
43	2	2465	C	C2-N1-C1'	6.65	126.11	118.80
43	2	2008	U	N3-C2-O2	-6.64	117.55	122.20
43	2	3637	U	N1-C2-O2	6.64	127.45	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	2	3833	C	C5-C6-N1	6.64	124.32	121.00
43	2	4269	G	N3-C4-N9	6.64	129.98	126.00
44	8	135	C	C2-N1-C1'	6.64	126.10	118.80
43	2	220	C	N1-C2-O2	6.63	122.88	118.90
43	2	472	C	C2-N1-C1'	6.63	126.09	118.80
43	2	485	C	C5-C6-N1	6.63	124.32	121.00
43	2	2821	U	N1-C2-O2	6.63	127.44	122.80
44	8	135	C	C6-N1-C2	-6.62	117.65	120.30
43	2	4476	C	N1-C2-O2	6.62	122.87	118.90
43	2	1245	C	C5-C6-N1	6.62	124.31	121.00
43	2	4880	C	C2-N1-C1'	6.62	126.08	118.80
44	8	123	U	N3-C2-O2	-6.62	117.57	122.20
44	8	54	C	C6-N1-C2	-6.62	117.65	120.30
43	2	2589	C	C6-N1-C2	-6.61	117.65	120.30
43	2	3636	C	C5-C6-N1	6.61	124.31	121.00
43	2	4627	U	N1-C2-O2	6.61	127.43	122.80
43	2	1607	C	N3-C2-O2	-6.61	117.28	121.90
43	2	1978	C	C2-N1-C1'	6.60	126.06	118.80
43	2	365	U	N1-C2-O2	6.59	127.41	122.80
43	2	4775	C	N1-C2-O2	6.59	122.85	118.90
43	2	4223	C	C6-N1-C2	-6.59	117.67	120.30
43	2	3670	C	N1-C2-O2	6.58	122.85	118.90
43	2	115	C	N1-C2-O2	6.58	122.85	118.90
43	2	1579	C	C6-N1-C2	-6.58	117.67	120.30
43	2	220	C	C5-C6-N1	6.57	124.29	121.00
51	W	3	C	C6-N1-C2	-6.57	117.67	120.30
43	2	2729	C	C2-N1-C1'	6.57	126.03	118.80
43	2	2062	C	C6-N1-C2	-6.57	117.67	120.30
43	2	2892	C	C2-N1-C1'	6.57	126.02	118.80
43	2	4350	C	C6-N1-C2	-6.57	117.67	120.30
43	2	155	C	N1-C2-O2	6.56	122.84	118.90
43	2	1686	C	C6-N1-C2	-6.56	117.68	120.30
43	2	4270	C	C6-N1-C2	-6.56	117.68	120.30
43	2	2528	G	C8-N9-C1'	-6.55	118.48	127.00
43	2	1816	C	N1-C2-O2	6.54	122.83	118.90
43	2	1675	C	C5-C6-N1	6.54	124.27	121.00
43	2	4766	C	C5-C6-N1	6.53	124.27	121.00
43	2	1809	C	N3-C4-N4	6.52	122.57	118.00
43	2	2262	G	N3-C4-C5	-6.52	125.34	128.60
43	2	367	C	C6-N1-C2	-6.52	117.69	120.30
43	2	3761	C	C5-C6-N1	6.51	124.26	121.00
51	W	78	C	C6-N1-C2	-6.51	117.70	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	2	4864	U	C2-N1-C1'	6.50	125.51	117.70
44	8	101	C	C2-N1-C1'	6.50	125.95	118.80
43	2	3776	G	N3-C4-N9	6.50	129.90	126.00
51	W	30	C	N1-C2-O2	6.50	122.80	118.90
51	W	44	C	N1-C2-O2	6.49	122.80	118.90
43	2	68	U	N3-C2-O2	-6.49	117.66	122.20
43	2	4505	C	C5-C6-N1	6.49	124.25	121.00
43	2	195	C	C6-N1-C2	-6.49	117.71	120.30
43	2	4747	C	C5-C6-N1	6.48	124.24	121.00
43	2	2667	C	C6-N1-C2	-6.48	117.71	120.30
43	2	4773	C	N1-C2-O2	6.48	122.79	118.90
36	J	105	MET	C-N-CA	6.47	137.89	121.70
43	2	1378	C	C2-N1-C1'	6.47	125.92	118.80
43	2	4497	U	N3-C2-O2	-6.47	117.67	122.20
43	2	3782	C	N1-C2-O2	6.47	122.78	118.90
51	W	68	C	C6-N1-C2	-6.46	117.71	120.30
43	2	1578	U	N3-C2-O2	-6.46	117.68	122.20
43	2	2563	C	N3-C2-O2	-6.46	117.38	121.90
43	2	178	C	C6-N1-C2	-6.45	117.72	120.30
43	2	2031	C	C6-N1-C2	-6.45	117.72	120.30
43	2	3876	A	C4-N9-C1'	-6.44	114.71	126.30
43	2	3876	A	N3-C4-N9	6.44	132.55	127.40
21	Z	129	ASP	CB-CG-OD1	6.44	124.09	118.30
43	2	122	U	N3-C2-O2	-6.43	117.70	122.20
43	2	4714	C	C2-N1-C1'	6.43	125.87	118.80
43	2	2262	G	N3-C4-N9	6.43	129.86	126.00
43	2	4215	C	C5-C6-N1	6.43	124.21	121.00
43	2	486	C	C6-N1-C2	-6.42	117.73	120.30
43	2	1477	C	C6-N1-C2	-6.42	117.73	120.30
43	2	4695	C	C6-N1-C2	-6.42	117.73	120.30
44	8	55	U	N3-C2-O2	-6.42	117.70	122.20
43	2	4232	U	C2-N1-C1'	6.42	125.40	117.70
43	2	4662	C	C5-C6-N1	6.42	124.21	121.00
43	2	4887	C	C2-N1-C1'	6.42	125.86	118.80
44	8	54	C	N3-C2-O2	-6.41	117.41	121.90
43	2	974	C	N3-C2-O2	-6.41	117.41	121.90
43	2	2094	G	C8-N9-C1'	-6.41	118.67	127.00
43	2	985	C	C6-N1-C2	-6.40	117.74	120.30
51	W	29	C	N1-C2-O2	6.40	122.74	118.90
43	2	4069	U	N1-C2-O2	6.40	127.28	122.80
43	2	406	C	P-O3'-C3'	6.39	127.37	119.70
43	2	4206	C	C2-N1-C1'	6.39	125.83	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	2	4887	C	C6-N1-C2	-6.39	117.74	120.30
43	2	4069	U	N3-C2-O2	-6.39	117.73	122.20
51	W	2	U	N3-C2-O2	-6.39	117.73	122.20
43	2	1401	C	N1-C2-O2	6.38	122.73	118.90
43	2	1978	C	N3-C2-O2	-6.38	117.43	121.90
43	2	4068	U	N3-C2-O2	-6.38	117.73	122.20
43	2	4268	A	O4'-C1'-N9	6.38	113.30	108.20
43	2	2351	C	C6-N1-C2	-6.38	117.75	120.30
43	2	2100	A	C2-N3-C4	6.37	113.78	110.60
43	2	3764	U	N3-C2-O2	-6.36	117.75	122.20
43	2	516	C	C5-C6-N1	6.36	124.18	121.00
3	6	129	LEU	CA-CB-CG	6.36	129.92	115.30
43	2	2837	U	N1-C2-O2	6.36	127.25	122.80
43	2	2820	C	N1-C2-O2	6.35	122.71	118.90
43	2	3866	C	C5-C6-N1	6.35	124.18	121.00
43	2	679	C	C6-N1-C2	-6.35	117.76	120.30
43	2	4234	A	C2-N3-C4	6.35	113.78	110.60
43	2	3833	C	N1-C2-O2	6.35	122.71	118.90
43	2	1938	C	C2-N1-C1'	6.34	125.78	118.80
43	2	2892	C	C6-N1-C2	-6.34	117.76	120.30
43	2	4766	C	C2-N1-C1'	6.34	125.77	118.80
43	2	1339	U	N3-C2-O2	-6.33	117.77	122.20
43	2	3935	C	C2-N1-C1'	6.33	125.76	118.80
43	2	753	C	C5-C6-N1	6.33	124.16	121.00
43	2	2614	C	N1-C2-O2	6.33	122.70	118.90
3	6	154	PHE	CB-CG-CD1	6.33	125.23	120.80
43	2	4265	U	C6-N1-C2	-6.33	117.20	121.00
43	2	3926	C	N3-C2-O2	-6.31	117.48	121.90
43	2	4747	C	N1-C2-O2	6.31	122.68	118.90
43	2	2008	U	N1-C2-O2	6.31	127.21	122.80
51	W	76	U	N1-C2-O2	6.30	127.21	122.80
43	2	516	C	C2-N1-C1'	6.30	125.73	118.80
43	2	1921	C	N3-C2-O2	-6.30	117.49	121.90
43	2	4561	C	C6-N1-C2	-6.30	117.78	120.30
43	2	4773	C	C2-N1-C1'	6.30	125.73	118.80
43	2	4709	U	N3-C2-O2	-6.29	117.80	122.20
43	2	672	C	N3-C2-O2	-6.29	117.50	121.90
43	2	4714	C	C5-C6-N1	6.29	124.14	121.00
43	2	2729	C	N1-C2-O2	6.28	122.67	118.90
43	2	3926	C	C5-C6-N1	6.28	124.14	121.00
51	W	76	U	N3-C2-O2	-6.28	117.81	122.20
43	2	155	C	N3-C2-O2	-6.28	117.51	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	W	14	C	C6-N1-C2	-6.28	117.79	120.30
43	2	3840	U	N3-C2-O2	-6.28	117.81	122.20
43	2	86	U	N1-C2-O2	6.27	127.19	122.80
43	2	2072	C	C6-N1-C2	-6.27	117.79	120.30
43	2	26	C	N1-C2-O2	6.27	122.66	118.90
43	2	3622	C	C5-C6-N1	6.27	124.14	121.00
44	8	99	U	N1-C2-O2	6.27	127.19	122.80
43	2	100	C	C5-C6-N1	6.27	124.13	121.00
43	2	1674	C	C2-N1-C1'	6.27	125.69	118.80
43	2	4406	U	N3-C2-O2	-6.27	117.81	122.20
43	2	2371	U	N3-C2-O2	-6.27	117.81	122.20
43	2	175	C	C6-N1-C2	-6.26	117.79	120.30
43	2	972	C	N3-C2-O2	-6.26	117.52	121.90
43	2	2558	C	C6-N1-C2	-6.26	117.80	120.30
43	2	4229	U	C6-N1-C1'	-6.26	112.44	121.20
43	2	1428	U	N1-C2-O2	6.26	127.18	122.80
43	2	4945	G	N3-C4-N9	6.25	129.75	126.00
43	2	5035	U	C2-N1-C1'	6.25	125.20	117.70
43	2	3866	C	C6-N1-C2	-6.25	117.80	120.30
43	2	3650	C	C5-C6-N1	6.25	124.12	121.00
43	2	1915	C	N3-C2-O2	-6.24	117.53	121.90
43	2	469	C	C5-C6-N1	6.24	124.12	121.00
43	2	5025	C	N1-C2-O2	6.24	122.64	118.90
52	T	240	MET	CA-CB-CG	6.24	123.91	113.30
43	2	3767	C	C6-N1-C2	-6.24	117.81	120.30
43	2	4970	C	N1-C2-O2	6.23	122.64	118.90
43	2	4420	U	C5-C6-N1	6.22	125.81	122.70
43	2	5035	U	C5-C6-N1	6.22	125.81	122.70
43	2	2548	C	C6-N1-C2	-6.22	117.81	120.30
44	8	90	C	C6-N1-C2	-6.22	117.81	120.30
43	2	3878	C	C6-N1-C2	-6.21	117.81	120.30
43	2	4563	U	N3-C2-O2	-6.21	117.85	122.20
43	2	2532	C	C2-N1-C1'	6.21	125.64	118.80
51	W	78	C	C5-C6-N1	6.21	124.11	121.00
43	2	673	C	C6-N1-C2	-6.21	117.82	120.30
43	2	2540	C	C5-C6-N1	6.20	124.10	121.00
43	2	4332	C	N3-C2-O2	-6.20	117.56	121.90
43	2	1674	C	C6-N1-C2	-6.20	117.82	120.30
43	2	4471	U	N1-C2-O2	6.20	127.14	122.80
43	2	36	U	C2-N1-C1'	6.20	125.14	117.70
43	2	2545	U	N1-C2-O2	6.19	127.13	122.80
43	2	3769	C	C5-C6-N1	6.19	124.09	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	8	32	C	N1-C2-O2	6.19	122.61	118.90
35	C	84	PRO	CA-N-CD	-6.19	102.84	111.50
43	2	672	C	C2-N1-C1'	6.19	125.61	118.80
43	2	4171	C	C6-N1-C2	-6.19	117.82	120.30
43	2	2101	C	C6-N1-C1'	6.19	128.23	120.80
43	2	3764	U	N1-C2-O2	6.19	127.13	122.80
43	2	4301	U	C6-N1-C1'	-6.19	112.54	121.20
43	2	4505	C	C2-N1-C1'	6.19	125.60	118.80
43	2	4254	G	C4-N9-C1'	6.18	134.54	126.50
43	2	4337	C	C5-C6-N1	6.18	124.09	121.00
43	2	472	C	C5-C6-N1	6.18	124.09	121.00
43	2	2592	U	N3-C2-O2	-6.18	117.88	122.20
43	2	297	U	N3-C2-O2	-6.18	117.88	122.20
43	2	3876	A	C4-C5-C6	6.18	120.09	117.00
43	2	4972	U	N1-C2-O2	6.17	127.12	122.80
43	2	750	U	N3-C2-O2	-6.17	117.88	122.20
43	2	2107	C	C5-C6-N1	6.17	124.08	121.00
43	2	26	C	C6-N1-C2	-6.17	117.83	120.30
43	2	2290	C	C6-N1-C2	-6.17	117.83	120.30
43	2	4996	C	C5-C6-N1	6.16	124.08	121.00
43	2	4984	C	N1-C2-O2	6.16	122.59	118.90
2	4	230	LEU	CA-CB-CG	6.16	129.46	115.30
43	2	30	C	C6-N1-C2	-6.16	117.84	120.30
43	2	1931	C	P-O3'-C3'	6.16	127.09	119.70
43	2	1938	C	N3-C2-O2	-6.16	117.59	121.90
43	2	1241	C	N3-C2-O2	-6.16	117.59	121.90
43	2	1921	C	C5-C6-N1	6.15	124.08	121.00
43	2	2729	C	C5-C6-N1	6.15	124.08	121.00
43	2	3688	U	N1-C2-O2	6.15	127.11	122.80
43	2	4406	U	C2-N1-C1'	6.15	125.08	117.70
51	W	28	C	N1-C2-O2	6.15	122.59	118.90
43	2	281	U	N1-C2-O2	6.14	127.10	122.80
43	2	4402	C	N3-C2-O2	-6.13	117.61	121.90
43	2	1666	C	C6-N1-C2	-6.13	117.85	120.30
43	2	2867	C	C6-N1-C2	-6.13	117.85	120.30
43	2	2038	U	N3-C2-O2	-6.13	117.91	122.20
43	2	4628	U	N3-C2-O2	-6.13	117.91	122.20
43	2	4269	G	N3-C4-C5	-6.13	125.54	128.60
40	v	48	MET	CA-CB-CG	6.12	123.71	113.30
43	2	4335	C	C5-C6-N1	6.12	124.06	121.00
43	2	4996	C	N1-C2-O2	6.12	122.57	118.90
43	2	4420	U	C6-N1-C2	-6.12	117.33	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	2	3598	C	C5-C6-N1	6.11	124.06	121.00
43	2	4969	C	C6-N1-C2	-6.11	117.86	120.30
52	T	147	GLY	C-N-CA	6.11	136.97	121.70
43	2	4068	U	N1-C2-O2	6.10	127.07	122.80
43	2	4923	C	N1-C2-O2	6.10	122.56	118.90
43	2	152	U	N3-C2-O2	-6.10	117.93	122.20
51	W	3	C	C5-C6-N1	6.09	124.05	121.00
43	2	4752	U	N3-C2-O2	-6.09	117.94	122.20
43	2	1352	C	C6-N1-C2	-6.09	117.86	120.30
43	2	4636	U	C5-C6-N1	6.09	125.74	122.70
43	2	1297	U	N3-C2-O2	-6.08	117.94	122.20
43	2	1963	C	N1-C2-O2	6.08	122.55	118.90
43	2	4561	C	N1-C2-O2	6.08	122.55	118.90
43	2	7	C	C5-C6-N1	6.08	124.04	121.00
43	2	1297	U	N1-C2-O2	6.08	127.05	122.80
43	2	100	C	O4'-C1'-N1	6.07	113.06	108.20
43	2	4171	C	N1-C2-O2	6.07	122.54	118.90
51	W	24	C	C6-N1-C2	-6.07	117.87	120.30
43	2	1325	C	N3-C2-O2	-6.07	117.65	121.90
43	2	4464	A	C2-N3-C4	6.07	113.64	110.60
43	2	5008	C	N1-C2-O2	6.07	122.54	118.90
35	C	88	VAL	CG1-CB-CG2	-6.07	101.19	110.90
51	W	68	C	C5-C6-N1	6.07	124.03	121.00
43	2	4674	C	C6-N1-C2	-6.07	117.87	120.30
43	2	4235	G	OP1-P-O3'	6.06	118.54	105.20
2	4	105	LEU	CB-CG-CD2	-6.06	100.70	111.00
43	2	1317	U	N1-C2-O2	6.06	127.04	122.80
43	2	2563	C	C5-C6-N1	6.06	124.03	121.00
43	2	988	C	C2-N1-C1'	6.05	125.46	118.80
43	2	2017	A	O4'-C1'-N9	6.05	113.04	108.20
45	g	118	ASP	CB-CG-OD1	6.05	123.74	118.30
43	2	2805	C	N1-C2-O2	6.05	122.53	118.90
43	2	4885	U	N3-C2-O2	-6.05	117.97	122.20
43	2	4229	U	OP1-P-O3'	6.04	118.50	105.20
9	G	160	ASP	CB-CG-OD2	6.04	123.74	118.30
43	2	390	C	C6-N1-C2	-6.04	117.88	120.30
43	2	2772	C	N3-C2-O2	-6.04	117.67	121.90
43	2	3778	U	C6-N1-C1'	-6.04	112.74	121.20
43	2	1076	C	C6-N1-C2	-6.04	117.88	120.30
43	2	4713	G	N3-C4-C5	-6.04	125.58	128.60
43	2	1856	C	C6-N1-C2	-6.04	117.89	120.30
43	2	975	C	N3-C2-O2	-6.04	117.67	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	2	988	C	N1-C2-O2	6.04	122.52	118.90
43	2	2710	C	C6-N1-C1'	-6.03	113.56	120.80
43	2	4206	C	N3-C2-O2	-6.03	117.68	121.90
43	2	1594	C	N1-C2-O2	6.02	122.52	118.90
51	W	2	U	N1-C2-O2	6.02	127.02	122.80
2	4	309	ASP	CB-CG-OD1	6.02	123.72	118.30
43	2	2019	C	N1-C2-O2	6.02	122.51	118.90
43	2	2867	C	C2-N1-C1'	6.01	125.42	118.80
43	2	2791	C	C6-N1-C2	-6.01	117.90	120.30
32	p	247	MET	CA-CB-CG	6.00	123.51	113.30
51	W	103	A	C2-N3-C4	6.00	113.60	110.60
43	2	4265	U	N1-C2-O2	6.00	127.00	122.80
43	2	204	U	N3-C2-O2	-6.00	118.00	122.20
43	2	2592	U	N1-C2-O2	6.00	127.00	122.80
43	2	981	C	C6-N1-C2	-6.00	117.90	120.30
43	2	4601	U	N3-C2-O2	-6.00	118.00	122.20
43	2	201	C	N1-C2-O2	5.99	122.50	118.90
43	2	1978	C	C5-C6-N1	5.99	124.00	121.00
43	2	3778	U	C6-N1-C2	-5.99	117.40	121.00
43	2	4758	U	C6-N1-C1'	-5.99	112.82	121.20
43	2	4293	U	N3-C2-O2	-5.99	118.01	122.20
43	2	1401	C	C5-C6-N1	5.98	123.99	121.00
43	2	4426	C	N3-C2-O2	-5.98	117.71	121.90
43	2	152	U	N1-C2-O2	5.98	126.98	122.80
43	2	1317	U	N3-C2-O2	-5.97	118.02	122.20
43	2	4561	C	C5-C6-N1	5.97	123.99	121.00
43	2	2465	C	N1-C2-O2	5.97	122.48	118.90
30	n	105	LEU	C-N-CA	5.97	136.63	121.70
43	2	4293	U	N1-C2-O2	5.97	126.98	122.80
43	2	977	C	C2-N1-C1'	5.96	125.36	118.80
43	2	2867	C	N1-C2-O2	5.96	122.48	118.90
43	2	4682	U	C2-N1-C1'	5.96	124.86	117.70
43	2	4402	C	C6-N1-C2	-5.96	117.92	120.30
43	2	1726	U	N1-C2-O2	5.96	126.97	122.80
43	2	2027	U	N3-C2-O2	-5.96	118.03	122.20
51	W	28	C	N3-C2-O2	-5.96	117.73	121.90
43	2	648	G	N3-C4-N9	5.95	129.57	126.00
43	2	3721	U	C2-N1-C1'	5.95	124.84	117.70
43	2	1663	C	C5-C6-N1	5.95	123.97	121.00
43	2	2022	C	C6-N1-C2	-5.95	117.92	120.30
43	2	2845	A	C2-N3-C4	5.95	113.58	110.60
43	2	3935	C	N1-C2-O2	5.94	122.47	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	2	1720	C	C5-C6-N1	5.93	123.97	121.00
43	2	1674	C	C5-C6-N1	5.93	123.97	121.00
43	2	4276	G	C5-C6-O6	-5.93	125.04	128.60
43	2	696	C	C6-N1-C2	-5.93	117.93	120.30
43	2	988	C	C6-N1-C2	-5.93	117.93	120.30
43	2	4699	U	OP1-P-O3'	5.93	118.24	105.20
51	W	57	C	N1-C2-O2	5.93	122.46	118.90
43	2	1592	G	N3-C4-N9	5.92	129.56	126.00
43	2	668	C	C6-N1-C2	-5.92	117.93	120.30
43	2	2031	C	N1-C2-O2	5.92	122.45	118.90
43	2	2625	U	N3-C2-O2	-5.92	118.06	122.20
43	2	1340	C	C6-N1-C2	-5.91	117.94	120.30
43	2	4662	C	N1-C2-O2	5.91	122.45	118.90
43	2	5032	C	C6-N1-C2	-5.91	117.94	120.30
43	2	1996	C	C6-N1-C2	-5.91	117.94	120.30
43	2	4996	C	C2-N1-C1'	5.91	125.30	118.80
43	2	3636	C	N3-C2-O2	-5.91	117.76	121.90
43	2	3782	C	C2-N1-C1'	5.91	125.30	118.80
43	2	1478	C	C6-N1-C2	-5.90	117.94	120.30
43	2	4596	C	N1-C2-O2	5.90	122.44	118.90
43	2	1856	C	C2-N1-C1'	5.90	125.29	118.80
43	2	78	U	N3-C2-O2	-5.90	118.07	122.20
43	2	1308	C	C6-N1-C2	-5.90	117.94	120.30
43	2	4349	C	C2-N1-C1'	5.90	125.29	118.80
46	d	43	LEU	CA-CB-CG	5.90	128.86	115.30
43	2	1566	C	C6-N1-C2	-5.89	117.94	120.30
43	2	1971	C	C6-N1-C2	-5.89	117.94	120.30
51	W	30	C	C5-C6-N1	5.89	123.95	121.00
43	2	2062	C	N1-C2-O2	5.89	122.44	118.90
43	2	654	C	C6-N1-C2	-5.88	117.95	120.30
43	2	1663	C	C6-N1-C2	-5.88	117.95	120.30
43	2	4476	C	N3-C2-O2	-5.88	117.78	121.90
43	2	4337	C	O4'-C1'-N1	5.88	112.90	108.20
32	p	136	VAL	CG1-CB-CG2	-5.88	101.50	110.90
43	2	1096	C	C5-C6-N1	5.87	123.94	121.00
43	2	4276	G	N3-C4-N9	5.87	129.52	126.00
43	2	1578	U	N1-C2-O2	5.87	126.91	122.80
43	2	1340	C	C5-C6-N1	5.87	123.93	121.00
43	2	4601	U	N1-C2-O2	5.87	126.91	122.80
43	2	1250	C	N1-C2-O2	5.86	122.42	118.90
43	2	4752	U	N1-C2-O2	5.86	126.90	122.80
44	8	90	C	C5-C6-N1	5.86	123.93	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	2	4508	C	C6-N1-C2	-5.86	117.96	120.30
43	2	2037	C	C6-N1-C2	-5.86	117.96	120.30
52	T	134	LYS	C-N-CA	5.86	136.34	121.70
52	T	214	LEU	CB-CG-CD1	5.86	120.95	111.00
43	2	3776	G	C6-C5-N7	-5.85	126.89	130.40
44	8	32	C	C6-N1-C2	-5.85	117.96	120.30
43	2	201	C	C6-N1-C2	-5.85	117.96	120.30
43	2	1906	U	N3-C2-O2	-5.85	118.10	122.20
43	2	1472	C	C6-N1-C2	-5.85	117.96	120.30
43	2	3622	C	C2-N1-C1'	5.84	125.23	118.80
43	2	4628	U	N1-C2-O2	5.84	126.89	122.80
43	2	4766	C	N1-C2-O2	5.84	122.41	118.90
43	2	297	U	N1-C2-O2	5.84	126.89	122.80
43	2	485	C	OP1-P-O3'	5.84	118.05	105.20
43	2	3767	C	P-O3'-C3'	5.84	126.71	119.70
43	2	1344	C	C5-C6-N1	5.84	123.92	121.00
43	2	5025	C	C5-C6-N1	5.84	123.92	121.00
43	2	2814	C	C2-N1-C1'	5.84	125.22	118.80
43	2	112	C	N3-C2-O2	-5.84	117.81	121.90
37	N	18	LEU	CA-CB-CG	5.83	128.71	115.30
43	2	4215	C	C2-N1-C1'	5.83	125.21	118.80
43	2	4563	U	N1-C2-O2	5.83	126.88	122.80
43	2	2548	C	N3-C2-O2	-5.83	117.82	121.90
43	2	4317	A	C2-N3-C4	5.82	113.51	110.60
43	2	4614	G	C5-C6-O6	5.82	132.09	128.60
43	2	1572	U	N3-C2-O2	-5.82	118.13	122.20
43	2	1325	C	C6-N1-C2	-5.82	117.97	120.30
43	2	1592	G	C4-N9-C1'	5.82	134.06	126.50
43	2	1644	C	C6-N1-C2	-5.82	117.97	120.30
43	2	2545	U	N3-C2-O2	-5.82	118.13	122.20
43	2	1931	C	O4'-C1'-N1	5.81	112.85	108.20
43	2	4090	G	N1-C6-O6	-5.81	116.41	119.90
43	2	4710	C	C6-N1-C2	-5.81	117.97	120.30
51	W	111	C	N1-C2-O2	5.81	122.39	118.90
43	2	71	C	C6-N1-C2	-5.80	117.98	120.30
43	2	1994	C	O4'-C1'-N1	5.80	112.84	108.20
43	2	345	C	C6-N1-C2	-5.80	117.98	120.30
43	2	5035	U	C6-N1-C2	-5.80	117.52	121.00
43	2	2892	C	C5-C6-N1	5.80	123.90	121.00
43	2	4730	C	C6-N1-C2	-5.79	117.98	120.30
43	2	1294	A	C2-N3-C4	5.79	113.49	110.60
43	2	2019	C	C6-N1-C2	-5.79	117.98	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	2	1694	C	C6-N1-C2	-5.78	117.99	120.30
43	2	719	C	C6-N1-C2	-5.78	117.99	120.30
43	2	2532	C	N1-C2-O2	5.78	122.37	118.90
44	8	80	A	C2-N3-C4	5.78	113.49	110.60
51	W	24	C	C2-N1-C1'	5.78	125.16	118.80
43	2	1378	C	C6-N1-C1'	-5.78	113.87	120.80
43	2	4502	C	N3-C2-O2	-5.78	117.86	121.90
43	2	4981	G	C4-N9-C1'	5.78	134.01	126.50
43	2	975	C	C6-N1-C2	-5.77	117.99	120.30
43	2	5025	C	N3-C2-O2	-5.77	117.86	121.90
43	2	4764	A	N1-C2-N3	-5.77	126.42	129.30
43	2	2371	U	N1-C2-O2	5.76	126.83	122.80
43	2	3780	G	C4-N9-C1'	5.76	133.99	126.50
43	2	2892	C	N1-C2-O2	5.76	122.36	118.90
43	2	4569	U	N1-C2-O2	5.76	126.83	122.80
43	2	368	C	N1-C2-O2	5.75	122.35	118.90
43	2	4712	C	N1-C2-O2	5.75	122.35	118.90
43	2	2589	C	C5-C6-N1	5.75	123.88	121.00
43	2	1889	U	N3-C2-O2	-5.75	118.18	122.20
43	2	1963	C	C6-N1-C2	-5.75	118.00	120.30
43	2	4771	C	C5-C6-N1	5.75	123.87	121.00
43	2	3870	C	C6-N1-C2	-5.75	118.00	120.30
43	2	4214	A	C2-N3-C4	5.74	113.47	110.60
43	2	657	C	N1-C2-O2	5.74	122.34	118.90
43	2	4201	G	N3-C4-N9	-5.74	122.56	126.00
1	y	45	ASP	CB-CG-OD2	5.74	123.46	118.30
43	2	2325	C	N1-C2-O2	5.74	122.34	118.90
43	2	1929	A	C8-N9-C1'	-5.73	117.38	127.70
43	2	1942	A	C2-N3-C4	5.73	113.47	110.60
43	2	3935	C	C5-C6-N1	5.73	123.86	121.00
43	2	3670	C	C6-N1-C2	-5.72	118.01	120.30
43	2	4235	G	O4'-C1'-N9	5.72	112.78	108.20
17	S	32	ASP	CB-CG-OD1	5.72	123.45	118.30
43	2	1081	C	N3-C2-O2	-5.72	117.90	121.90
43	2	204	U	N1-C2-O2	5.72	126.80	122.80
43	2	4695	C	C2-N1-C1'	5.71	125.08	118.80
43	2	4636	U	C6-N1-C2	-5.71	117.57	121.00
43	2	4162	C	C2-N1-C1'	5.71	125.08	118.80
43	2	299	C	C6-N1-C2	-5.71	118.02	120.30
43	2	390	C	C5-C6-N1	5.71	123.85	121.00
43	2	4985	U	C2-N1-C1'	5.70	124.54	117.70
22	a	119	MET	CA-CB-CG	5.70	122.99	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	2	178	C	C5-C6-N1	5.70	123.85	121.00
43	2	486	C	C5-C6-N1	5.70	123.85	121.00
44	8	55	U	N1-C2-O2	5.70	126.79	122.80
43	2	368	C	C6-N1-C2	-5.70	118.02	120.30
2	4	503	THR	C-N-CA	5.70	135.95	121.70
43	2	4895	C	C2-N1-C1'	5.70	125.07	118.80
43	2	4497	U	N1-C2-O2	5.70	126.79	122.80
43	2	4406	U	N1-C2-O2	5.70	126.79	122.80
43	2	1607	C	C6-N1-C2	-5.69	118.02	120.30
43	2	4393	G	C5-C6-O6	5.69	132.01	128.60
43	2	4417	C	C5-C6-N1	5.69	123.84	121.00
43	2	1929	A	N3-C4-N9	5.69	131.95	127.40
6	D	7	LEU	CA-CB-CG	5.69	128.38	115.30
43	2	358	C	N1-C2-O2	5.68	122.31	118.90
43	2	4561	C	C2-N1-C1'	5.68	125.05	118.80
43	2	4269	G	C4-N9-C1'	5.68	133.88	126.50
43	2	2667	C	N3-C2-O2	-5.68	117.93	121.90
43	2	4775	C	N3-C2-O2	-5.68	117.93	121.90
43	2	1722	C	C6-N1-C2	-5.67	118.03	120.30
43	2	122	U	N1-C2-O2	5.67	126.77	122.80
51	W	58	A	N1-C2-N3	-5.67	126.47	129.30
51	W	79	U	N3-C2-O2	-5.67	118.23	122.20
43	2	469	C	C2-N1-C1'	5.66	125.02	118.80
43	2	3763	A	C2-N3-C4	5.66	113.43	110.60
43	2	4341	C	C2-N1-C1'	5.66	125.02	118.80
43	2	386	A	C2-N3-C4	5.65	113.43	110.60
43	2	1096	C	C6-N1-C2	-5.65	118.04	120.30
43	2	4206	C	C6-N1-C2	-5.65	118.04	120.30
43	2	4290	U	N3-C2-O2	-5.65	118.25	122.20
40	v	49	ARG	CA-CB-CG	5.65	125.82	113.40
43	2	4984	C	C6-N1-C2	-5.65	118.04	120.30
43	2	131	C	C6-N1-C2	-5.65	118.04	120.30
43	2	3851	U	N3-C2-O2	-5.65	118.25	122.20
46	d	35	ASP	CB-CG-OD1	5.65	123.38	118.30
43	2	3636	C	C2-N1-C1'	5.64	125.01	118.80
43	2	4299	U	C6-N1-C1'	-5.64	113.30	121.20
43	2	1915	C	C2-N1-C1'	5.64	125.01	118.80
43	2	2772	C	N1-C2-O2	5.64	122.29	118.90
43	2	489	C	C5-C6-N1	5.64	123.82	121.00
43	2	1367	C	N3-C2-O2	-5.64	117.95	121.90
43	2	2593	C	N1-C2-O2	5.63	122.28	118.90
43	2	3905	A	OP2-P-O3'	5.63	117.60	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	2	1847	C	C6-N1-C2	-5.63	118.05	120.30
43	2	4709	U	N1-C2-O2	5.63	126.74	122.80
43	2	4770	U	C2-N1-C1'	5.63	124.45	117.70
43	2	4885	U	N1-C2-O2	5.63	126.74	122.80
43	2	988	C	C5-C6-N1	5.62	123.81	121.00
43	2	1243	C	C6-N1-C2	-5.62	118.05	120.30
43	2	2563	C	C2-N1-C1'	5.62	124.98	118.80
43	2	4502	C	C2-N1-C1'	5.61	124.97	118.80
43	2	459	C	C6-N1-C2	-5.61	118.06	120.30
43	2	26	C	C2-N1-C1'	5.61	124.97	118.80
43	2	4923	C	N3-C2-O2	-5.61	117.97	121.90
43	2	679	C	C5-C6-N1	5.61	123.80	121.00
43	2	1352	C	C5-C6-N1	5.60	123.80	121.00
43	2	2351	C	N1-C2-O2	5.60	122.26	118.90
43	2	2384	U	N3-C2-O2	-5.60	118.28	122.20
43	2	2689	C	C6-N1-C2	-5.60	118.06	120.30
43	2	643	C	N1-C2-O2	5.60	122.26	118.90
43	2	4254	G	C2-N3-C4	5.60	114.70	111.90
43	2	3764	U	C2-N1-C1'	5.60	124.42	117.70
43	2	1344	C	C2-N1-C1'	5.60	124.96	118.80
43	2	696	C	N1-C2-O2	5.59	122.25	118.90
43	2	485	C	C6-N1-C1'	-5.59	114.10	120.80
43	2	5042	A	C2-N3-C4	5.59	113.39	110.60
43	2	2872	C	C6-N1-C2	-5.58	118.07	120.30
43	2	4350	C	C5-C6-N1	5.58	123.79	121.00
43	2	1572	U	N1-C2-O2	5.58	126.70	122.80
43	2	4710	C	C5-C6-N1	5.58	123.79	121.00
43	2	2015	U	C2-N1-C1'	5.58	124.39	117.70
43	2	4878	C	C6-N1-C2	-5.58	118.07	120.30
2	4	21	LEU	CA-CB-CG	5.57	128.12	115.30
43	2	4466	C	C6-N1-C2	-5.57	118.07	120.30
3	6	154	PHE	CB-CG-CD2	-5.57	116.90	120.80
43	2	2072	C	C5-C6-N1	5.57	123.78	121.00
2	4	12	VAL	CA-CB-CG1	5.57	119.25	110.90
43	2	1203	G	N3-C4-C5	-5.57	125.82	128.60
37	N	216	CYS	CA-CB-SG	5.56	124.02	114.00
43	2	2850	A	C4-N9-C1'	5.56	136.31	126.30
38	R	64	LEU	CA-CB-CG	5.56	128.09	115.30
43	2	499	G	C2-N3-C4	5.56	114.68	111.90
43	2	3831	U	C2-N1-C1'	5.56	124.37	117.70
43	2	1828	C	C6-N1-C2	-5.56	118.08	120.30
43	2	1966	C	N3-C2-O2	-5.56	118.01	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	2	5022	U	P-O3'-C3'	5.56	126.37	119.70
43	2	238	C	C6-N1-C2	-5.56	118.08	120.30
43	2	257	C	C6-N1-C2	-5.56	118.08	120.30
43	2	1405	C	N3-C2-O2	-5.56	118.01	121.90
43	2	4453	C	C6-N1-C1'	-5.55	114.14	120.80
44	8	81	C	C6-N1-C2	-5.55	118.08	120.30
43	2	4263	C	C6-N1-C1'	-5.54	114.15	120.80
43	2	4713	G	N3-C4-N9	5.54	129.33	126.00
43	2	963	G	C4-N9-C1'	5.54	133.70	126.50
43	2	1081	C	C6-N1-C2	-5.54	118.08	120.30
44	8	89	U	N3-C2-O2	-5.54	118.33	122.20
43	2	3769	C	C6-N1-C2	-5.53	118.09	120.30
51	W	111	C	C6-N1-C2	-5.53	118.09	120.30
43	2	175	C	N3-C2-O2	-5.53	118.03	121.90
43	2	4462	C	C6-N1-C2	-5.53	118.09	120.30
43	2	2843	U	N3-C2-O2	-5.53	118.33	122.20
43	2	4771	C	C6-N1-C2	-5.53	118.09	120.30
43	2	1339	U	N1-C2-O2	5.52	126.67	122.80
43	2	1662	C	C6-N1-C2	-5.52	118.09	120.30
43	2	2540	C	C6-N1-C2	-5.52	118.09	120.30
43	2	4639	G	C4-N9-C1'	5.52	133.68	126.50
43	2	2006	U	N3-C2-O2	-5.52	118.34	122.20
43	2	1202	C	C6-N1-C2	-5.51	118.09	120.30
43	2	1251	C	N3-C2-O2	-5.51	118.04	121.90
43	2	1888	A	C2-N3-C4	5.51	113.36	110.60
43	2	2362	U	C2-N1-C1'	5.51	124.31	117.70
43	2	5008	C	C6-N1-C2	-5.51	118.10	120.30
43	2	1474	C	C6-N1-C2	-5.51	118.10	120.30
43	2	2627	C	N3-C2-O2	-5.51	118.05	121.90
43	2	4500	U	C2-N1-C1'	5.51	124.31	117.70
43	2	2262	G	C8-N9-C1'	-5.50	119.84	127.00
43	2	1458	C	C6-N1-C2	-5.50	118.10	120.30
43	2	3688	U	C2-N1-C1'	5.50	124.30	117.70
43	2	336	A	C2-N3-C4	5.50	113.35	110.60
43	2	2096	G	C4-N9-C1'	5.50	133.65	126.50
43	2	1414	C	C6-N1-C2	-5.50	118.10	120.30
43	2	4505	C	N1-C2-O2	5.50	122.20	118.90
43	2	4164	C	C6-N1-C2	-5.50	118.10	120.30
43	2	4213	A	C2-N3-C4	5.50	113.35	110.60
37	N	266	ASP	C-N-CA	5.49	135.43	121.70
43	2	260	C	C6-N1-C2	-5.49	118.10	120.30
43	2	1402	C	C5-C6-N1	5.49	123.75	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	2	1971	C	C2-N1-C1'	5.49	124.84	118.80
51	W	39	C	N1-C2-O2	5.49	122.19	118.90
43	2	979	C	C5-C6-N1	5.49	123.74	121.00
43	2	221	C	C6-N1-C2	-5.48	118.11	120.30
43	2	1884	C	C6-N1-C2	-5.48	118.11	120.30
43	2	977	C	C5-C6-N1	5.48	123.74	121.00
43	2	1429	C	C6-N1-C2	-5.48	118.11	120.30
44	8	113	C	C6-N1-C2	-5.48	118.11	120.30
43	2	168	C	C6-N1-C2	-5.48	118.11	120.30
43	2	2351	C	C5-C6-N1	5.48	123.74	121.00
43	2	1991	A	C2-N3-C4	5.48	113.34	110.60
43	2	2528	G	C2-N3-C4	5.48	114.64	111.90
43	2	30	C	C2-N1-C1'	5.47	124.82	118.80
43	2	661	C	C6-N1-C2	-5.47	118.11	120.30
43	2	274	C	N1-C2-O2	5.47	122.18	118.90
43	2	2708	U	N1-C2-O2	5.47	126.63	122.80
46	d	96	LEU	CA-CB-CG	5.47	127.88	115.30
43	2	485	C	P-O3'-C3'	5.47	126.26	119.70
44	8	54	C	C5-C6-N1	5.46	123.73	121.00
43	2	4206	C	C5-C6-N1	5.46	123.73	121.00
43	2	2410	C	N3-C2-O2	-5.46	118.08	121.90
43	2	2264	C	N1-C2-O2	5.46	122.17	118.90
43	2	3670	C	N3-C2-O2	-5.46	118.08	121.90
43	2	4319	C	C6-N1-C2	-5.46	118.12	120.30
43	2	1817	U	N3-C2-O2	-5.46	118.38	122.20
43	2	3851	U	N1-C2-O2	5.46	126.62	122.80
43	2	1241	C	C6-N1-C1'	-5.45	114.26	120.80
43	2	2856	C	C5-C6-N1	5.45	123.73	121.00
43	2	209	U	C2-N1-C1'	5.45	124.24	117.70
43	2	2325	C	C6-N1-C2	-5.45	118.12	120.30
43	2	703	G	C4-N9-C1'	5.44	133.57	126.50
43	2	51	A	C2-N3-C4	5.44	113.32	110.60
43	2	683	C	N1-C2-O2	5.44	122.16	118.90
43	2	294	G	C4-N9-C1'	5.43	133.56	126.50
43	2	4318	C	N1-C2-O2	5.43	122.16	118.90
43	2	4413	C	C5-C6-N1	5.43	123.72	121.00
50	O	13	LEU	CA-CB-CG	5.43	127.79	115.30
12	K	70	LEU	CA-CB-CG	5.43	127.79	115.30
43	2	5026	U	N1-C2-O2	5.43	126.60	122.80
43	2	117	C	N1-C2-O2	5.42	122.15	118.90
43	2	672	C	C6-N1-C2	-5.42	118.13	120.30
43	2	4991	U	N3-C2-O2	-5.42	118.41	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	A	22	LEU	CA-CB-CG	5.42	127.76	115.30
43	2	195	C	C5-C6-N1	5.42	123.71	121.00
43	2	4165	C	N1-C2-O2	5.42	122.15	118.90
51	W	14	C	C5-C6-N1	5.42	123.71	121.00
43	2	4775	C	C6-N1-C2	-5.41	118.14	120.30
51	W	24	C	C5-C6-N1	5.41	123.71	121.00
43	2	4880	C	C5-C6-N1	5.41	123.70	121.00
18	U	164	LEU	CA-CB-CG	5.41	127.74	115.30
43	2	750	U	N1-C2-O2	5.41	126.59	122.80
43	2	4771	C	N1-C2-O2	5.41	122.14	118.90
51	W	102	U	C2-N1-C1'	5.41	124.19	117.70
43	2	2011	C	C6-N1-C2	-5.41	118.14	120.30
43	2	30	C	N1-C2-O2	5.41	122.14	118.90
43	2	1216	C	C2-N3-C4	5.41	122.60	119.90
43	2	1812	C	C5-C6-N1	5.40	123.70	121.00
43	2	4662	C	N3-C2-O2	-5.40	118.12	121.90
43	2	3623	C	N1-C2-O2	5.40	122.14	118.90
43	2	4090	G	C5-C6-O6	5.40	131.84	128.60
43	2	2615	C	N1-C2-O2	5.40	122.14	118.90
43	2	1599	A	C2-N3-C4	5.39	113.30	110.60
43	2	1906	U	N1-C2-O2	5.39	126.57	122.80
43	2	4555	U	OP1-P-O3'	5.39	117.06	105.20
46	d	23	LEU	CA-CB-CG	5.39	127.70	115.30
44	8	135	C	C5-C6-N1	5.39	123.69	121.00
44	8	101	C	C5-C6-N1	5.39	123.69	121.00
43	2	472	C	N3-C2-O2	-5.38	118.13	121.90
43	2	1097	C	C5-C6-N1	5.38	123.69	121.00
44	8	101	C	N1-C2-O2	5.38	122.13	118.90
51	W	57	C	C2-N1-C1'	5.38	124.72	118.80
43	2	1535	C	C6-N1-C2	-5.37	118.15	120.30
43	2	2107	C	N1-C2-O2	5.37	122.12	118.90
43	2	985	C	C5-C6-N1	5.37	123.68	121.00
43	2	3695	U	N3-C2-O2	-5.37	118.44	122.20
43	2	489	C	C2-N1-C1'	5.37	124.70	118.80
44	8	82	A	C2-N3-C4	5.37	113.28	110.60
43	2	86	U	C2-N1-C1'	5.36	124.14	117.70
43	2	115	C	N3-C2-O2	-5.36	118.15	121.90
43	2	683	C	C6-N1-C2	-5.36	118.15	120.30
43	2	3858	C	C6-N1-C2	-5.36	118.16	120.30
43	2	4918	C	C6-N1-C2	-5.36	118.15	120.30
43	2	26	C	C5-C6-N1	5.36	123.68	121.00
43	2	1870	C	C6-N1-C2	-5.36	118.16	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	2	2014	C	C6-N1-C2	-5.36	118.16	120.30
43	2	4533	A	N1-C2-N3	-5.36	126.62	129.30
43	2	1477	C	C2-N1-C1'	5.36	124.69	118.80
43	2	4758	U	O4'-C1'-N1	5.36	112.48	108.20
9	G	88	ASP	CB-CG-OD1	5.35	123.12	118.30
21	Z	88	ASP	CB-CG-OD2	5.35	123.12	118.30
43	2	2062	C	C5-C6-N1	5.35	123.68	121.00
43	2	4639	G	N3-C4-C5	-5.35	125.92	128.60
43	2	9	C	C6-N1-C2	-5.35	118.16	120.30
43	2	3776	G	C8-N9-C1'	-5.35	120.05	127.00
43	2	1535	C	N1-C2-O2	5.35	122.11	118.90
43	2	4268	A	N1-C2-N3	-5.35	126.63	129.30
43	2	368	C	N3-C2-O2	-5.34	118.16	121.90
43	2	3776	G	N3-C4-C5	-5.34	125.93	128.60
43	2	3912	U	N3-C2-O2	-5.34	118.46	122.20
43	2	1344	C	N1-C2-O2	5.34	122.11	118.90
43	2	1963	C	N3-C2-O2	-5.34	118.16	121.90
43	2	2614	C	N3-C2-O2	-5.34	118.16	121.90
43	2	4400	G	C4-N9-C1'	5.34	133.44	126.50
43	2	262	G	N1-C2-N2	-5.34	111.39	116.20
43	2	2384	U	N1-C2-O2	5.34	126.54	122.80
44	8	51	U	N1-C2-O2	5.34	126.54	122.80
43	2	4259	C	N3-C2-O2	-5.33	118.17	121.90
2	4	337	ASP	CB-CG-OD1	5.33	123.10	118.30
43	2	68	U	N1-C2-O2	5.33	126.53	122.80
43	2	3919	C	N1-C2-O2	5.33	122.10	118.90
43	2	4716	C	C6-N1-C2	-5.33	118.17	120.30
43	2	7	C	C6-N1-C2	-5.33	118.17	120.30
43	2	436	C	C6-N1-C2	-5.32	118.17	120.30
43	2	2560	C	C5-C6-N1	5.32	123.66	121.00
43	2	4360	U	C2-N1-C1'	5.32	124.09	117.70
43	2	485	C	N3-C2-O2	-5.32	118.18	121.90
43	2	2548	C	C5-C6-N1	5.32	123.66	121.00
43	2	2856	C	C2-N1-C1'	5.32	124.65	118.80
43	2	486	C	OP1-P-OP2	-5.32	111.62	119.60
43	2	1994	C	C5-C6-N1	5.32	123.66	121.00
43	2	2561	C	C6-N1-C2	-5.31	118.17	120.30
43	2	3832	U	N3-C2-O2	-5.31	118.48	122.20
43	2	4345	C	C6-N1-C2	-5.31	118.17	120.30
43	2	494	U	N3-C2-O2	-5.31	118.48	122.20
43	2	1893	C	C6-N1-C2	-5.31	118.18	120.30
43	2	4268	A	C4-C5-C6	-5.31	114.35	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	8	51	U	N3-C2-O2	-5.31	118.49	122.20
43	2	4273	A	C2-N3-C4	5.30	113.25	110.60
43	2	1442	C	C6-N1-C2	-5.30	118.18	120.30
2	4	105	LEU	CB-CG-CD1	5.30	120.01	111.00
43	2	1913	C	C6-N1-C2	-5.30	118.18	120.30
43	2	4712	C	N3-C2-O2	-5.30	118.19	121.90
51	W	44	C	N3-C2-O2	-5.30	118.19	121.90
1	y	95	GLN	CA-CB-CG	5.29	125.05	113.40
43	2	123	C	C6-N1-C2	-5.29	118.18	120.30
43	2	1080	C	C6-N1-C2	-5.29	118.18	120.30
43	2	2533	C	C6-N1-C2	-5.29	118.18	120.30
43	2	3840	U	N1-C2-O2	5.29	126.50	122.80
43	2	4171	C	C5-C6-N1	5.29	123.65	121.00
43	2	4601	U	C2-N1-C1'	5.29	124.05	117.70
53	9	296	ASP	CB-CG-OD2	5.29	123.06	118.30
43	2	2614	C	C6-N1-C2	-5.28	118.19	120.30
43	2	4311	A	N1-C2-N3	-5.28	126.66	129.30
43	2	4453	C	C6-N1-C2	-5.28	118.19	120.30
43	2	2603	C	C6-N1-C2	-5.28	118.19	120.30
51	W	42	A	C2-N3-C4	5.28	113.24	110.60
43	2	905	C	C6-N1-C2	-5.28	118.19	120.30
43	2	3882	C	N1-C2-O2	5.28	122.07	118.90
43	2	4298	A	N1-C2-N3	-5.28	126.66	129.30
43	2	643	C	N3-C2-O2	-5.27	118.21	121.90
43	2	195	C	N1-C2-O2	5.27	122.06	118.90
43	2	4269	G	C6-C5-N7	-5.27	127.24	130.40
52	T	148	ASP	N-CA-C	5.27	125.23	111.00
43	2	1686	C	C5-C6-N1	5.27	123.64	121.00
43	2	1821	G	C4-N9-C1'	5.27	133.35	126.50
44	8	20	A	N1-C2-N3	-5.27	126.67	129.30
43	2	458	C	C6-N1-C2	-5.27	118.19	120.30
43	2	678	C	C6-N1-C2	-5.27	118.19	120.30
43	2	1644	C	C5-C6-N1	5.26	123.63	121.00
43	2	3876	A	C6-C5-N7	-5.26	128.62	132.30
43	2	4749	C	C6-N1-C2	-5.26	118.20	120.30
43	2	3762	U	C6-N1-C2	-5.26	117.85	121.00
43	2	1847	C	C5-C6-N1	5.25	123.63	121.00
43	2	5008	C	N3-C2-O2	-5.25	118.22	121.90
51	W	67	C	C6-N1-C2	-5.25	118.20	120.30
43	2	33	A	C2-N3-C4	5.25	113.23	110.60
43	2	1821	G	N3-C4-N9	5.25	129.15	126.00
43	2	2815	A	C2-N3-C4	5.25	113.22	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	2	2814	C	N3-C2-O2	-5.25	118.23	121.90
43	2	1402	C	C2-N1-C1'	5.25	124.57	118.80
2	4	483	LEU	CB-CG-CD1	5.25	119.92	111.00
43	2	1856	C	N1-C2-O2	5.25	122.05	118.90
43	2	2417	A	O4'-C1'-N9	5.25	112.40	108.20
43	2	4984	C	N3-C2-O2	-5.24	118.23	121.90
47	j	123	ASP	CB-CG-OD1	5.24	123.02	118.30
43	2	4527	G	N3-C4-N9	5.24	129.15	126.00
43	2	4712	C	C6-N1-C2	-5.24	118.20	120.30
43	2	133	C	C6-N1-C2	-5.24	118.20	120.30
43	2	2078	C	C6-N1-C2	-5.24	118.20	120.30
43	2	4165	C	N3-C2-O2	-5.24	118.23	121.90
43	2	1405	C	C6-N1-C2	-5.24	118.21	120.30
43	2	1817	U	N1-C2-O2	5.23	126.46	122.80
43	2	2002	A	N1-C2-N3	-5.23	126.68	129.30
43	2	3919	C	C6-N1-C2	-5.23	118.21	120.30
43	2	1808	C	OP1-P-O3'	5.23	116.71	105.20
43	2	4985	U	C6-N1-C2	-5.23	117.86	121.00
52	T	152	VAL	CA-CB-CG1	5.23	118.75	110.90
43	2	1081	C	N1-C2-O2	5.23	122.03	118.90
43	2	1191	C	N1-C2-O2	5.23	122.04	118.90
43	2	1579	C	C5-C6-N1	5.22	123.61	121.00
43	2	7	C	C2-N1-C1'	5.22	124.54	118.80
37	N	374	LEU	CA-CB-CG	5.22	127.30	115.30
43	2	673	C	C5-C6-N1	5.22	123.61	121.00
43	2	1566	C	C5-C6-N1	5.21	123.61	121.00
43	2	2749	C	C6-N1-C2	-5.21	118.21	120.30
43	2	4508	C	C5-C6-N1	5.21	123.61	121.00
43	2	4527	G	N3-C4-C5	-5.21	126.00	128.60
43	2	4642	U	N3-C2-O2	-5.21	118.55	122.20
43	2	3623	C	C6-N1-C2	-5.21	118.22	120.30
43	2	977	C	N1-C2-O2	5.21	122.03	118.90
11	I	37	ASP	CB-CG-OD1	5.21	122.99	118.30
43	2	4715	C	C6-N1-C2	-5.21	118.22	120.30
44	8	128	C	C6-N1-C2	-5.21	118.22	120.30
43	2	1957	U	N3-C2-O2	-5.21	118.56	122.20
43	2	2033	A	N1-C2-N3	-5.21	126.70	129.30
43	2	1439	C	C6-N1-C2	-5.20	118.22	120.30
43	2	1499	C	C6-N1-C2	-5.20	118.22	120.30
43	2	2439	G	C2-N3-C4	5.20	114.50	111.90
43	2	4669	A	N1-C2-N3	-5.19	126.70	129.30
43	2	1947	U	C2-N1-C1'	5.19	123.93	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	2	4508	C	N3-C2-O2	-5.19	118.27	121.90
43	2	4694	G	C4-N9-C1'	5.19	133.25	126.50
51	W	30	C	N3-C2-O2	-5.19	118.27	121.90
43	2	1429	C	C2-N1-C1'	5.19	124.51	118.80
43	2	112	C	C6-N1-C1'	-5.19	114.58	120.80
43	2	1429	C	N1-C2-O2	5.18	122.01	118.90
43	2	1431	C	C6-N1-C2	-5.18	118.23	120.30
43	2	1956	A	C2-N3-C4	5.18	113.19	110.60
43	2	4223	C	N1-C2-O2	5.18	122.01	118.90
43	2	4713	G	C4-N9-C1'	5.18	133.24	126.50
43	2	5050	C	N1-C2-O2	5.18	122.01	118.90
43	2	2520	C	C6-N1-C2	-5.18	118.23	120.30
43	2	656	C	C6-N1-C2	-5.18	118.23	120.30
53	9	256	ASP	CB-CG-OD2	5.18	122.96	118.30
43	2	131	C	C5-C6-N1	5.17	123.59	121.00
43	2	4164	C	C5-C6-N1	5.17	123.59	121.00
53	9	289	ASP	CB-CG-OD2	5.17	122.96	118.30
2	4	302	ASP	CB-CG-OD1	5.17	122.95	118.30
43	2	1188	C	C6-N1-C2	-5.17	118.23	120.30
43	2	1378	C	N1-C2-O2	5.17	122.00	118.90
43	2	2264	C	C6-N1-C2	-5.17	118.23	120.30
43	2	4420	U	C6-N1-C1'	-5.17	113.97	121.20
43	2	1722	C	C5-C6-N1	5.17	123.58	121.00
43	2	4348	A	C2-N3-C4	5.17	113.18	110.60
43	2	1594	C	C6-N1-C2	-5.16	118.23	120.30
43	2	2304	U	N1-C2-O2	5.16	126.42	122.80
43	2	4981	G	N3-C4-N9	5.16	129.10	126.00
44	8	135	C	N1-C2-O2	5.16	122.00	118.90
13	L	78	LEU	CA-CB-CG	5.16	127.17	115.30
19	V	202	LEU	CA-CB-CG	5.16	127.17	115.30
34	A	43	LEU	CA-CB-CG	5.16	127.17	115.30
43	2	4923	C	C6-N1-C2	-5.16	118.24	120.30
43	2	220	C	N3-C2-O2	-5.16	118.29	121.90
43	2	4699	U	P-O3'-C3'	5.16	125.89	119.70
43	2	4970	C	C6-N1-C2	-5.16	118.24	120.30
51	W	101	A	N1-C2-N3	-5.16	126.72	129.30
43	2	178	C	N1-C2-O2	5.15	121.99	118.90
43	2	1458	C	C2-N1-C1'	5.15	124.47	118.80
43	2	1662	C	C5-C6-N1	5.15	123.58	121.00
43	2	4695	C	C5-C6-N1	5.15	123.58	121.00
51	W	43	U	C2-N1-C1'	5.15	123.88	117.70
43	2	1250	C	N3-C2-O2	-5.15	118.30	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	2	1594	C	N3-C2-O2	-5.15	118.30	121.90
43	2	1592	G	C8-N9-C1'	-5.15	120.31	127.00
43	2	2867	C	C5-C6-N1	5.15	123.57	121.00
43	2	4975	G	O4'-C1'-N9	5.15	112.32	108.20
43	2	4486	C	N1-C2-O2	5.14	121.99	118.90
43	2	2629	C	N1-C2-O2	5.14	121.98	118.90
43	2	688	U	N3-C2-O2	-5.14	118.60	122.20
43	2	4066	U	C6-N1-C2	-5.14	117.92	121.00
43	2	4422	A	N1-C2-N3	-5.14	126.73	129.30
43	2	4970	C	C2-N1-C1'	5.14	124.45	118.80
43	2	101	A	C2-N3-C4	5.14	113.17	110.60
43	2	1097	C	C6-N1-C2	-5.14	118.25	120.30
43	2	4361	U	N3-C2-O2	-5.14	118.60	122.20
43	2	4722	G	C4-N9-C1'	5.14	133.18	126.50
51	W	80	U	N3-C2-O2	-5.14	118.60	122.20
43	2	222	C	C6-N1-C2	-5.13	118.25	120.30
43	2	1387	A	N1-C2-N3	-5.13	126.73	129.30
43	2	1668	A	C2-N3-C4	5.13	113.17	110.60
43	2	4490	C	C6-N1-C2	-5.13	118.25	120.30
43	2	1473	U	N3-C2-O2	-5.13	118.61	122.20
43	2	1602	U	N3-C2-O2	-5.13	118.61	122.20
43	2	2625	U	N1-C2-O2	5.13	126.39	122.80
6	D	343	GLN	CA-CB-CG	5.12	124.67	113.40
43	2	905	C	C2-N1-C1'	5.12	124.44	118.80
43	2	914	U	C5-C4-O4	-5.12	122.83	125.90
43	2	1947	U	N3-C2-O2	-5.12	118.61	122.20
44	8	32	C	N3-C2-O2	-5.12	118.32	121.90
43	2	2031	C	C5-C6-N1	5.12	123.56	121.00
43	2	4994	G	N3-C4-N9	5.12	129.07	126.00
43	2	34	A	N1-C2-N3	-5.12	126.74	129.30
43	2	201	C	C5-C6-N1	5.12	123.56	121.00
43	2	2820	C	N3-C2-O2	-5.12	118.32	121.90
43	2	4315	A	N1-C2-N3	-5.12	126.74	129.30
43	2	4945	G	C4-N9-C1'	5.12	133.15	126.50
43	2	406	C	C6-N1-C2	-5.11	118.25	120.30
43	2	1203	G	C4-N9-C1'	5.11	133.15	126.50
43	2	1477	C	C5-C6-N1	5.11	123.56	121.00
43	2	4165	C	C6-N1-C2	-5.11	118.25	120.30
43	2	50	C	C6-N1-C2	-5.11	118.25	120.30
43	2	694	C	N1-C2-O2	5.11	121.97	118.90
43	2	2017	A	N7-C8-N9	5.11	116.36	113.80
44	8	43	A	C2-N3-C4	5.11	113.16	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	A	174	ILE	CG1-CB-CG2	-5.11	100.16	111.40
43	2	499	G	O4'-C1'-N9	5.11	112.29	108.20
2	4	422	LEU	CA-CB-CG	5.11	127.04	115.30
43	2	1720	C	C2-N1-C1'	5.11	124.42	118.80
43	2	1807	C	N1-C2-O2	5.11	121.96	118.90
43	2	1892	A	O4'-C1'-N9	5.11	112.28	108.20
43	2	2689	C	C5-C6-N1	5.11	123.55	121.00
43	2	1088	C	C5-C6-N1	5.10	123.55	121.00
43	2	1585	C	C6-N1-C2	-5.10	118.26	120.30
43	2	2667	C	C5-C6-N1	5.10	123.55	121.00
43	2	4476	C	C6-N1-C2	-5.10	118.26	120.30
43	2	4527	G	C4-N9-C1'	5.10	133.13	126.50
43	2	1508	A	N1-C2-N3	-5.10	126.75	129.30
43	2	1804	A	N1-C6-N6	-5.10	115.54	118.60
43	2	966	A	C2-N3-C4	5.10	113.15	110.60
43	2	4902	C	C6-N1-C2	-5.10	118.26	120.30
43	2	4981	G	N3-C4-C5	-5.10	126.05	128.60
44	8	96	C	C6-N1-C2	-5.10	118.26	120.30
51	W	39	C	C6-N1-C2	-5.10	118.26	120.30
51	W	22	A	C2-N3-C4	5.10	113.15	110.60
43	2	228	C	C6-N1-C2	-5.09	118.26	120.30
51	W	55	A	C2-N3-C4	5.09	113.15	110.60
43	2	322	C	C6-N1-C2	-5.09	118.26	120.30
43	2	2533	C	N1-C2-O2	5.09	121.95	118.90
43	2	4701	A	N1-C2-N3	-5.09	126.75	129.30
43	2	4980	C	C6-N1-C2	-5.09	118.26	120.30
43	2	941	C	C6-N1-C2	-5.09	118.27	120.30
43	2	1655	C	C6-N1-C2	-5.09	118.27	120.30
43	2	2647	A	C2-N3-C4	5.09	113.14	110.60
43	2	1932	A	N1-C2-N3	-5.08	126.76	129.30
43	2	692	A	N1-C2-N3	-5.08	126.76	129.30
51	W	66	G	C4-N9-C1'	5.08	133.11	126.50
43	2	904	C	N3-C2-O2	-5.08	118.34	121.90
44	8	140	C	C6-N1-C2	-5.08	118.27	120.30
43	2	44	A	C2-N3-C4	5.08	113.14	110.60
43	2	4450	U	C2-N1-C1'	5.08	123.80	117.70
43	2	1929	A	N3-C4-C5	-5.08	123.25	126.80
43	2	2818	C	C6-N1-C2	-5.08	118.27	120.30
43	2	4528	G	C4-N9-C1'	5.08	133.10	126.50
51	W	80	U	N1-C2-O2	5.08	126.35	122.80
43	2	1254	A	N1-C2-N3	-5.07	126.76	129.30
43	2	282	C	C5-C6-N1	5.07	123.53	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	2	3601	C	C5-C6-N1	5.07	123.54	121.00
43	2	4619	U	N3-C2-O2	-5.07	118.65	122.20
43	2	289	C	C6-N1-C2	-5.07	118.27	120.30
2	4	403	LEU	CA-CB-CG	5.07	126.95	115.30
43	2	2324	C	C6-N1-C2	-5.07	118.27	120.30
43	2	2367	A	N1-C2-N3	-5.07	126.77	129.30
43	2	4983	C	C2-N1-C1'	5.07	124.37	118.80
43	2	1588	U	N3-C2-O2	-5.07	118.66	122.20
43	2	4994	G	C4-N9-C1'	5.07	133.09	126.50
38	R	157	LEU	CA-CB-CG	5.06	126.95	115.30
41	w	279	LEU	CA-CB-CG	5.06	126.95	115.30
43	2	2019	C	N3-C2-O2	-5.06	118.36	121.90
43	2	129	C	C5-C6-N1	5.06	123.53	121.00
43	2	3657	U	N3-C2-O2	-5.06	118.66	122.20
43	2	4639	G	N3-C4-N9	5.06	129.03	126.00
43	2	467	U	C6-N1-C2	-5.06	117.97	121.00
43	2	2853	C	N1-C2-O2	5.05	121.93	118.90
43	2	4700	A	N1-C2-N3	-5.05	126.77	129.30
43	2	1216	C	O4'-C1'-N1	5.05	112.24	108.20
43	2	4913	G	OP2-P-O3'	5.05	116.31	105.20
51	W	44	C	C6-N1-C2	-5.05	118.28	120.30
51	W	111	C	C5-C6-N1	5.05	123.53	121.00
43	2	367	C	C5-C6-N1	5.05	123.52	121.00
43	2	667	A	C2-N3-C4	5.05	113.12	110.60
43	2	4336	A	C2-N3-C4	5.05	113.12	110.60
16	Q	184	MET	CA-CB-CG	5.04	121.88	113.30
43	2	1929	A	N1-C2-N3	-5.04	126.78	129.30
43	2	4254	G	C8-N9-C1'	-5.04	120.44	127.00
43	2	4437	U	OP1-P-O3'	5.04	116.30	105.20
43	2	4450	U	N1-C2-O2	5.04	126.33	122.80
43	2	1821	G	N3-C4-C5	-5.04	126.08	128.60
43	2	345	C	C5-C6-N1	5.04	123.52	121.00
43	2	990	C	C6-N1-C2	-5.04	118.28	120.30
43	2	972	C	C5-C6-N1	5.04	123.52	121.00
43	2	979	C	C6-N1-C2	-5.04	118.28	120.30
43	2	1243	C	C2-N1-C1'	5.04	124.34	118.80
43	2	2614	C	C2-N1-C1'	5.04	124.34	118.80
43	2	1809	C	C2-N3-C4	5.04	122.42	119.90
43	2	4983	C	C5-C6-N1	5.04	123.52	121.00
43	2	2791	C	C2-N1-C1'	5.03	124.34	118.80
43	2	673	C	N1-C2-O2	5.03	121.92	118.90
36	J	238	TRP	CA-CB-CG	5.03	123.25	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	2	1889	U	N1-C2-O2	5.03	126.32	122.80
43	2	2595	C	C6-N1-C2	-5.03	118.29	120.30
11	I	146	LEU	CA-CB-CG	5.02	126.85	115.30
43	2	754	U	N3-C2-O2	-5.02	118.68	122.20
43	2	4963	G	N3-C4-C5	-5.02	126.09	128.60
6	D	171	LEU	CA-CB-CG	5.02	126.85	115.30
43	2	1812	C	C6-N1-C2	-5.02	118.29	120.30
43	2	2872	C	C5-C6-N1	5.02	123.51	121.00
51	W	42	A	N1-C2-N3	-5.02	126.79	129.30
43	2	2817	C	C6-N1-C2	-5.02	118.29	120.30
43	2	4162	C	N3-C2-O2	-5.02	118.39	121.90
17	S	135	LEU	CA-CB-CG	5.02	126.84	115.30
43	2	3612	C	C6-N1-C2	-5.02	118.29	120.30
43	2	1901	C	C6-N1-C2	-5.01	118.29	120.30
43	2	4450	U	N3-C2-O2	-5.01	118.69	122.20
43	2	4672	A	N1-C2-N3	-5.01	126.79	129.30
7	E	11	LEU	CA-CB-CG	5.01	126.83	115.30
33	z	34	LYS	CB-CG-CD	5.01	124.63	111.60
43	2	30	C	C5-C6-N1	5.01	123.50	121.00
12	K	43	MET	CB-CG-SD	5.01	127.43	112.40
43	2	1592	G	N3-C4-C5	-5.01	126.09	128.60
43	2	2708	U	N3-C2-O2	-5.01	118.69	122.20
43	2	4252	C	C6-N1-C2	-5.01	118.30	120.30
51	W	39	C	N3-C2-O2	-5.01	118.39	121.90
43	2	1873	A	N1-C2-N3	-5.00	126.80	129.30
43	2	2077	C	C6-N1-C2	-5.00	118.30	120.30
43	2	3870	C	C5-C6-N1	5.00	123.50	121.00
51	W	14	C	C2-N1-C1'	5.00	124.30	118.80
43	2	2384	U	C2-N1-C1'	5.00	123.70	117.70
43	2	2791	C	C5-C6-N1	5.00	123.50	121.00

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
43	2	3876	A	Sidechain
2	4	189	THR	Peptide
2	4	299	LEU	Peptide
2	4	300	SER	Peptide
2	4	503	THR	Peptide
5	B	241	PRO	Peptide
5	B	304	SER	Peptide

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Mol	Chain	Res	Type	Group
16	Q	154	VAL	Peptide
38	R	5	SER	Peptide
52	T	190	ASN	Peptide
24	c	52	MET	Peptide
30	n	106	TYR	Peptide
39	u	42	LYS	Peptide
39	u	49	GLY	Peptide
39	u	50	VAL	Peptide
39	u	54	ALA	Peptide
41	w	126	ARG	Peptide
41	w	456	ILE	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	y	163/165 (99%)	159 (98%)	4 (2%)	0	100	100
2	4	616/634 (97%)	555 (90%)	60 (10%)	1 (0%)	47	77
3	6	242/245 (99%)	226 (93%)	16 (7%)	0	100	100
4	7	133/163 (82%)	129 (97%)	4 (3%)	0	100	100
5	B	401/403 (100%)	380 (95%)	21 (5%)	0	100	100
6	D	356/427 (83%)	333 (94%)	23 (6%)	0	100	100
7	E	96/115 (84%)	92 (96%)	4 (4%)	0	100	100
8	F	107/117 (92%)	105 (98%)	2 (2%)	0	100	100
9	G	215/266 (81%)	204 (95%)	11 (5%)	0	100	100
10	H	120/123 (98%)	118 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	I	188/192 (98%)	178 (95%)	10 (5%)	0	100	100
12	K	100/105 (95%)	96 (96%)	4 (4%)	0	100	100
13	L	109/148 (74%)	102 (94%)	7 (6%)	0	100	100
14	M	84/97 (87%)	79 (94%)	5 (6%)	0	100	100
15	P	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
16	Q	201/211 (95%)	189 (94%)	12 (6%)	0	100	100
17	S	133/215 (62%)	127 (96%)	6 (4%)	0	100	100
18	U	178/204 (87%)	172 (97%)	6 (3%)	0	100	100
19	V	199/203 (98%)	193 (97%)	6 (3%)	0	100	100
20	X	89/92 (97%)	85 (96%)	4 (4%)	0	100	100
21	Z	149/188 (79%)	148 (99%)	1 (1%)	0	100	100
22	a	146/196 (74%)	141 (97%)	5 (3%)	0	100	100
23	b	174/176 (99%)	166 (95%)	8 (5%)	0	100	100
24	c	115/160 (72%)	104 (90%)	9 (8%)	2 (2%)	9	35
25	e	129/140 (92%)	117 (91%)	12 (9%)	0	100	100
26	h	132/145 (91%)	129 (98%)	3 (2%)	0	100	100
27	i	133/136 (98%)	125 (94%)	8 (6%)	0	100	100
28	l	123/137 (90%)	115 (94%)	8 (6%)	0	100	100
29	m	179/257 (70%)	163 (91%)	16 (9%)	0	100	100
30	n	107/110 (97%)	100 (94%)	5 (5%)	2 (2%)	8	34
31	o	231/288 (80%)	212 (92%)	19 (8%)	0	100	100
32	p	224/248 (90%)	209 (93%)	15 (7%)	0	100	100
33	z	63/129 (49%)	61 (97%)	2 (3%)	0	100	100
34	A	163/178 (92%)	152 (93%)	11 (7%)	0	100	100
35	C	244/297 (82%)	234 (96%)	9 (4%)	1 (0%)	34	66
36	J	257/260 (99%)	247 (96%)	8 (3%)	2 (1%)	19	51
37	N	470/485 (97%)	450 (96%)	18 (4%)	2 (0%)	34	66
38	R	197/365 (54%)	186 (94%)	10 (5%)	1 (0%)	29	61
39	u	73/549 (13%)	63 (86%)	8 (11%)	2 (3%)	5	26
40	v	203/239 (85%)	199 (98%)	4 (2%)	0	100	100
41	w	445/731 (61%)	414 (93%)	28 (6%)	3 (1%)	22	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	r	22/360 (6%)	21 (96%)	1 (4%)	0	100	100
45	g	110/156 (70%)	104 (94%)	6 (6%)	0	100	100
46	d	102/128 (80%)	96 (94%)	6 (6%)	0	100	100
47	j	109/125 (87%)	104 (95%)	5 (5%)	0	100	100
48	k	127/135 (94%)	120 (94%)	7 (6%)	0	100	100
49	Y	165/184 (90%)	158 (96%)	7 (4%)	0	100	100
50	O	67/70 (96%)	63 (94%)	4 (6%)	0	100	100
52	T	249/306 (81%)	224 (90%)	22 (9%)	3 (1%)	13	42
53	9	61/847 (7%)	52 (85%)	8 (13%)	1 (2%)	9	36
All	All	8747/11901 (74%)	8245 (94%)	482 (6%)	20 (0%)	50	77

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
24	c	53	PRO
36	J	106	ILE
37	N	59	PRO
37	N	267	ARG
39	u	51	PRO
39	u	55	PRO
41	w	126	ARG
41	w	264	ALA
52	T	148	ASP
52	T	152	VAL
53	9	282	GLN
35	C	44	TYR
36	J	101	VAL
52	T	191	GLY
24	c	43	LYS
41	w	456	ILE
2	4	4	TYR
30	n	107	PRO
30	n	106	TYR
38	R	24	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	y	137/137 (100%)	135 (98%)	2 (2%)	65 81
2	4	562/574 (98%)	562 (100%)	0	100 100
3	6	212/213 (100%)	211 (100%)	1 (0%)	88 93
4	7	126/149 (85%)	126 (100%)	0	100 100
5	B	349/349 (100%)	349 (100%)	0	100 100
6	D	298/348 (86%)	298 (100%)	0	100 100
7	E	83/97 (86%)	83 (100%)	0	100 100
8	F	94/100 (94%)	94 (100%)	0	100 100
9	G	181/223 (81%)	179 (99%)	2 (1%)	73 85
10	H	109/110 (99%)	108 (99%)	1 (1%)	78 87
11	I	169/171 (99%)	169 (100%)	0	100 100
12	K	86/89 (97%)	86 (100%)	0	100 100
13	L	95/121 (78%)	95 (100%)	0	100 100
14	M	73/80 (91%)	73 (100%)	0	100 100
15	P	47/48 (98%)	47 (100%)	0	100 100
16	Q	171/177 (97%)	170 (99%)	1 (1%)	86 91
17	S	115/161 (71%)	115 (100%)	0	100 100
18	U	155/172 (90%)	155 (100%)	0	100 100
19	V	173/174 (99%)	172 (99%)	1 (1%)	86 91
20	X	74/75 (99%)	74 (100%)	0	100 100
21	Z	136/165 (82%)	136 (100%)	0	100 100
22	a	133/175 (76%)	133 (100%)	0	100 100
23	b	157/157 (100%)	157 (100%)	0	100 100
24	c	106/140 (76%)	106 (100%)	0	100 100
25	e	101/107 (94%)	100 (99%)	1 (1%)	76 86
26	h	124/135 (92%)	124 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
27	i	117/118 (99%)	116 (99%)	1 (1%)	78 87
28	l	109/121 (90%)	108 (99%)	1 (1%)	78 87
29	m	143/199 (72%)	143 (100%)	0	100 100
30	n	88/89 (99%)	88 (100%)	0	100 100
31	o	208/252 (82%)	208 (100%)	0	100 100
32	p	195/215 (91%)	195 (100%)	0	100 100
33	z	61/115 (53%)	61 (100%)	0	100 100
34	A	138/149 (93%)	138 (100%)	0	100 100
35	C	209/250 (84%)	209 (100%)	0	100 100
36	J	227/228 (100%)	227 (100%)	0	100 100
37	N	396/404 (98%)	394 (100%)	2 (0%)	88 93
38	R	173/300 (58%)	172 (99%)	1 (1%)	86 91
39	u	68/485 (14%)	68 (100%)	0	100 100
40	v	182/214 (85%)	182 (100%)	0	100 100
41	w	405/654 (62%)	405 (100%)	0	100 100
42	r	22/312 (7%)	22 (100%)	0	100 100
45	g	100/133 (75%)	100 (100%)	0	100 100
46	d	94/115 (82%)	94 (100%)	0	100 100
47	j	101/110 (92%)	101 (100%)	0	100 100
48	k	115/121 (95%)	115 (100%)	0	100 100
49	Y	147/163 (90%)	145 (99%)	2 (1%)	67 82
50	O	64/65 (98%)	63 (98%)	1 (2%)	62 79
52	T	232/279 (83%)	232 (100%)	0	100 100
53	9	60/733 (8%)	53 (88%)	7 (12%)	5 21
All	All	7720/10271 (75%)	7696 (100%)	24 (0%)	92 96

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	y	48	LYS
1	y	90	ARG
3	6	123	ARG
9	G	137[A]	ARG
9	G	137[B]	ARG

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Mol	Chain	Res	Type
10	H	101	ASN
16	Q	103	ARG
19	V	117	ARG
25	e	48	ARG
27	i	59	LYS
28	l	119	ARG
37	N	281	ARG
37	N	376	ASN
38	R	66	ARG
49	Y	64	ASN
49	Y	128	ARG
50	O	9	LYS
53	9	251	ARG
53	9	274	MET
53	9	275	VAL
53	9	277	ASP
53	9	278	GLU
53	9	279	GLU
53	9	280	LEU

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

Mol	Chain	Res	Type
10	H	101	ASN
38	R	38	ASN
38	R	70	GLN
41	w	300	GLN
49	Y	64	ASN
53	9	282	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
43	2	3320/5054 (65%)	800 (24%)	26 (0%)
44	8	153/156 (98%)	26 (16%)	1 (0%)
51	W	119/120 (99%)	19 (15%)	0
All	All	3592/5330 (67%)	845 (23%)	27 (0%)

All (845) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
43	2	25	A
43	2	39	A
43	2	42	A
43	2	48	G
43	2	56	A
43	2	59	A
43	2	64	A
43	2	65	A
43	2	66	A
43	2	69	A
43	2	71	C
43	2	72	C
43	2	73	A
43	2	91	G
43	2	98	A
43	2	108	A
43	2	109	G
43	2	110	C
43	2	112	C
43	2	119	G
43	2	120	A
43	2	122	U
43	2	131	C
43	2	132	G
43	2	135	G
43	2	136	C
43	2	141	C
43	2	144	G
43	2	152	U
43	2	159	C
43	2	172	C
43	2	175	C
43	2	181	C
43	2	183	C
43	2	185	C
43	2	188	G
43	2	197	A
43	2	200	U
43	2	209	U
43	2	217	C
43	2	218	A
43	2	220	C
43	2	233	U

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Mol	Chain	Res	Type
43	2	234	G
43	2	254	G
43	2	256	G
43	2	262	G
43	2	265	C
43	2	266	C
43	2	267	G
43	2	279	A
43	2	280	G
43	2	297	U
43	2	306	A
43	2	309	C
43	2	315	G
43	2	316	U
43	2	340	C
43	2	363	A
43	2	385	A
43	2	387	G
43	2	398	A2M
43	2	401	G
43	2	406	C
43	2	407	A
43	2	409	G
43	2	410	A
43	2	412	G
43	2	432	U
43	2	449	C
43	2	450	G
43	2	452	A
43	2	453	G
43	2	454	U
43	2	464	G
43	2	467	U
43	2	483	G
43	2	485	C
43	2	486	C
43	2	489	C
43	2	491	G
43	2	493	G
43	2	496	G
43	2	497	G
43	2	498	C

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Mol	Chain	Res	Type
43	2	499	G
43	2	500	G
43	2	501	C
43	2	502	C
43	2	503	C
43	2	504	G
43	2	505	G
43	2	509	A
43	2	510	U
43	2	514	U
43	2	515	C
43	2	516	C
43	2	518	G
43	2	519	C
43	2	653	U
43	2	656	C
43	2	657	C
43	2	659	G
43	2	666	G
43	2	667	A
43	2	668	C
43	2	669	C
43	2	673	C
43	2	685	C
43	2	686	A
43	2	688	U
43	2	692	A
43	2	696	C
43	2	697	G
43	2	704	C
43	2	731	G
43	2	738	C
43	2	739	G
43	2	740	G
43	2	742	G
43	2	746	A
43	2	753	C
43	2	759	G
43	2	904	C
43	2	906	C
43	2	913	U
43	2	914	U

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Mol	Chain	Res	Type
43	2	915	A
43	2	916	C
43	2	917	A
43	2	918	G
43	2	924	C
43	2	925	C
43	2	926	G
43	2	932	A
43	2	933	G
43	2	936	C
43	2	941	C
43	2	943	A
43	2	944	A
43	2	945	U
43	2	946	C
43	2	959	G
43	2	960	A
43	2	961	G
43	2	962	C
43	2	963	G
43	2	965	G
43	2	966	A
43	2	967	C
43	2	969	C
43	2	970	G
43	2	971	U
43	2	972	C
43	2	977	C
43	2	982	U
43	2	984	C
43	2	990	C
43	2	991	C
43	2	992	C
43	2	993	G
43	2	994	G
43	2	995	C
43	2	1048	G
43	2	1049	C
43	2	1051	G
43	2	1066	G
43	2	1067	G
43	2	1068	G

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Mol	Chain	Res	Type
43	2	1070	G
43	2	1072	C
43	2	1082	C
43	2	1168	G
43	2	1170	G
43	2	1173	G
43	2	1178	G
43	2	1179	U
43	2	1180	C
43	2	1182	C
43	2	1183	C
43	2	1184	A
43	2	1187	G
43	2	1200	G
43	2	1202	C
43	2	1203	G
43	2	1210	C
43	2	1211	G
43	2	1215	C
43	2	1218	G
43	2	1222	A
43	2	1241	C
43	2	1243	C
43	2	1244	G
43	2	1245	C
43	2	1251	C
43	2	1252	C
43	2	1253	G
43	2	1254	A
43	2	1255	A
43	2	1256	G
43	2	1257	A
43	2	1260	G
43	2	1266	G
43	2	1269	G
43	2	1271	G
43	2	1272	C
43	2	1273	G
43	2	1279	A
43	2	1280	C
43	2	1283	G
43	2	1284	G

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Mol	Chain	Res	Type
43	2	1287	G
43	2	1294	A
43	2	1295	C
43	2	1296	G
43	2	1301	C
43	2	1302	U
43	2	1303	A
43	2	1313	C
43	2	1314	C
43	2	1316	OMG
43	2	1337	A
43	2	1354	A
43	2	1358	G
43	2	1359	G
43	2	1365	C
43	2	1366	G
43	2	1367	C
43	2	1377	G
43	2	1378	C
43	2	1379	C
43	2	1381	U
43	2	1382	G
43	2	1387	A
43	2	1394	G
43	2	1397	A
43	2	1398	A
43	2	1402	C
43	2	1404	G
43	2	1405	C
43	2	1407	C
43	2	1408	G
43	2	1409	C
43	2	1410	U
43	2	1412	G
43	2	1420	A
43	2	1439	C
43	2	1440	U
43	2	1442	C
43	2	1446	C
43	2	1447	C
43	2	1472	C
43	2	1482	G

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Mol	Chain	Res	Type
43	2	1483	C
43	2	1486	C
43	2	1497	A
43	2	1498	G
43	2	1501	C
43	2	1502	G
43	2	1503	A
43	2	1518	A
43	2	1534	A2M
43	2	1547	A
43	2	1554	A
43	2	1566	C
43	2	1575	A
43	2	1578	U
43	2	1592	G
43	2	1601	A
43	2	1612	G
43	2	1613	A
43	2	1624	G
43	2	1625	OMG
43	2	1626	G
43	2	1631	A
43	2	1638	A
43	2	1650	A
43	2	1654	G
43	2	1661	C
43	2	1671	U
43	2	1673	U
43	2	1674	C
43	2	1675	C
43	2	1676	C
43	2	1679	A
43	2	1680	G
43	2	1681	G
43	2	1691	G
43	2	1694	C
43	2	1697	G
43	2	1724	G
43	2	1732	C
43	2	1734	G
43	2	1738	A
43	2	1789	C

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Mol	Chain	Res	Type
43	2	1791	U
43	2	1792	U
43	2	1793	A
43	2	1802	A
43	2	1803	G
43	2	1804	A
43	2	1806	G
43	2	1809	C
43	2	1810	G
43	2	1816	C
43	2	1818	G
43	2	1821	G
43	2	1822	U
43	2	1829	G
43	2	1832	C
43	2	1833	G
43	2	1836	G
43	2	1837	A
43	2	1842	G
43	2	1854	G
43	2	1855	G
43	2	1856	C
43	2	1859	C
43	2	1860	U
43	2	1863	U
43	2	1865	G
43	2	1867	A
43	2	1870	C
43	2	1871	A2M
43	2	1883	OMG
43	2	1891	A
43	2	1897	A
43	2	1916	G
43	2	1918	U
43	2	1919	G
43	2	1920	C
43	2	1922	G
43	2	1925	G
43	2	1929	A
43	2	1931	C
43	2	1932	A
43	2	1935	C

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Mol	Chain	Res	Type
43	2	1938	C
43	2	1939	A
43	2	1940	G
43	2	1942	A
43	2	1943	A
43	2	1944	A
43	2	1948	G
43	2	1956	A
43	2	1959	U
43	2	1966	C
43	2	1972	G
43	2	1979	A
43	2	1980	U
43	2	1981	G
43	2	1983	A
43	2	1984	A
43	2	1985	G
43	2	1991	A
43	2	1997	U
43	2	2001	G
43	2	2002	A
43	2	2003	G
43	2	2010	A
43	2	2011	C
43	2	2017	A
43	2	2018	C
43	2	2025	A
43	2	2026	A
43	2	2033	A
43	2	2034	G
43	2	2040	A
43	2	2043	A
43	2	2044	U
43	2	2046	G
43	2	2048	U
43	2	2055	G
43	2	2056	G
43	2	2069	A
43	2	2071	A
43	2	2084	C
43	2	2085	G
43	2	2092	G

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Mol	Chain	Res	Type
43	2	2093	A
43	2	2095	A
43	2	2096	G
43	2	2098	G
43	2	2100	A
43	2	2101	C
43	2	2104	G
43	2	2105	A
43	2	2110	C
43	2	2111	G
43	2	2112	G
43	2	2113	C
43	2	2250	C
43	2	2253	A
43	2	2255	C
43	2	2256	C
43	2	2258	C
43	2	2259	G
43	2	2260	C
43	2	2262	G
43	2	2268	A
43	2	2289	C
43	2	2300	A
43	2	2301	G
43	2	2306	G
43	2	2313	A
43	2	2331	G
43	2	2333	G
43	2	2348	G
43	2	2351	C
43	2	2360	A
43	2	2364	OMG
43	2	2395	A
43	2	2416	G
43	2	2417	A
43	2	2422	OMC
43	2	2424	OMG
43	2	2425	U
43	2	2439	G
43	2	2450	G
43	2	2453	A
43	2	2463	G

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Mol	Chain	Res	Type
43	2	2465	C
43	2	2469	C
43	2	2470	C
43	2	2471	G
43	2	2506	G
43	2	2507	A
43	2	2512	A
43	2	2513	A
43	2	2519	U
43	2	2529	A
43	2	2543	A
43	2	2544	G
43	2	2545	U
43	2	2546	G
43	2	2547	G
43	2	2548	C
43	2	2549	G
43	2	2554	U
43	2	2555	G
43	2	2559	G
43	2	2560	C
43	2	2563	C
43	2	2566	G
43	2	2573	A
43	2	2576	G
43	2	2583	C
43	2	2586	G
43	2	2587	A
43	2	2589	C
43	2	2600	A
43	2	2601	A
43	2	2618	G
43	2	2627	C
43	2	2652	G
43	2	2653	C
43	2	2659	A
43	2	2661	U
43	2	2662	G
43	2	2669	C
43	2	2670	C
43	2	2675	G
43	2	2687	U

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Mol	Chain	Res	Type
43	2	2694	G
43	2	2695	A
43	2	2696	A
43	2	2708	U
43	2	2711	G
43	2	2723	U
43	2	2724	G
43	2	2725	A
43	2	2726	G
43	2	2739	C
43	2	2742	G
43	2	2743	A
43	2	2753	G
43	2	2755	A
43	2	2759	G
43	2	2761	U
43	2	2763	U
43	2	2769	U
43	2	2770	C
43	2	2787	A
43	2	2788	U
43	2	2790	U
43	2	2799	G
43	2	2826	U
43	2	2827	G
43	2	2855	G
43	2	2857	A
43	2	2875	C
43	2	2897	G
43	2	3596	A
43	2	3597	G
43	2	3599	A
43	2	3614	G
43	2	3615	G
43	2	3616	U
43	2	3626	G
43	2	3630	A
43	2	3635	A
43	2	3638	G
43	2	3648	A
43	2	3662	A
43	2	3663	A

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Mol	Chain	Res	Type
43	2	3673	C
43	2	3678	G
43	2	3691	G
43	2	3692	A
43	2	3718	A
43	2	3721	U
43	2	3735	G
43	2	3736	A
43	2	3758	U
43	2	3759	A
43	2	3760	A
43	2	3761	C
43	2	3765	G
43	2	3766	A
43	2	3767	C
43	2	3768	U
43	2	3769	C
43	2	3777	G
43	2	3778	U
43	2	3779	A
43	2	3780	G
43	2	3781	C
43	2	3782	C
43	2	3783	A
43	2	3823	G
43	2	3833	C
43	2	3838	U
43	2	3839	G
43	2	3840	U
43	2	3867	A2M
43	2	3875	G
43	2	3876	A
43	2	3877	A
43	2	3878	C
43	2	3879	G
43	2	3898	G
43	2	3901	A
43	2	3904	G
43	2	3905	A
43	2	3906	A
43	2	3915	U
43	2	3922	G

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Mol	Chain	Res	Type
43	2	3923	A
43	2	3924	C
43	2	3925	U
43	2	3926	C
43	2	3931	C
43	2	3938	G
43	2	3941	G
43	2	3944	G
43	2	4068	U
43	2	4076	G
43	2	4077	A
43	2	4083	5MU
43	2	4084	G
43	2	4162	C
43	2	4163	U
43	2	4164	C
43	2	4166	G
43	2	4170	A
43	2	4171	C
43	2	4183	G
43	2	4184	G
43	2	4191	G
43	2	4197	G
43	2	4198	G
43	2	4200	G
43	2	4202	U
43	2	4207	C
43	2	4209	G
43	2	4212	A
43	2	4213	A
43	2	4214	A
43	2	4225	G
43	2	4227	U
43	2	4228	G
43	2	4229	U
43	2	4230	C
43	2	4231	C
43	2	4232	U
43	2	4233	A
43	2	4234	A
43	2	4235	G
43	2	4236	G

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Mol	Chain	Res	Type
43	2	4244	A
43	2	4250	G
43	2	4251	A
43	2	4252	C
43	2	4253	A
43	2	4254	G
43	2	4255	A
43	2	4259	C
43	2	4263	C
43	2	4264	G
43	2	4265	U
43	2	4268	A
43	2	4269	G
43	2	4270	C
43	2	4271	A
43	2	4272	G
43	2	4273	A
43	2	4274	A
43	2	4275	G
43	2	4276	G
43	2	4278	C
43	2	4279	A
43	2	4280	A
43	2	4281	A
43	2	4283	G
43	2	4285	U
43	2	4290	U
43	2	4291	G
43	2	4292	A
43	2	4294	C
43	2	4295	U
43	2	4296	U
43	2	4298	A
43	2	4299	U
43	2	4301	U
43	2	4302	U
43	2	4303	C
43	2	4304	A
43	2	4305	G
43	2	4306	U
43	2	4307	A
43	2	4308	C

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Mol	Chain	Res	Type
43	2	4309	G
43	2	4313	A
43	2	4315	A
43	2	4316	G
43	2	4317	A
43	2	4329	G
43	2	4331	G
43	2	4335	C
43	2	4340	U
43	2	4341	C
43	2	4342	C
43	2	4343	U
43	2	4347	G
43	2	4348	A
43	2	4349	C
43	2	4350	C
43	2	4368	G
43	2	4371	G
43	2	4372	U
43	2	4373	G
43	2	4376	A
43	2	4378	A
43	2	4379	A
43	2	4380	A
43	2	4381	A
43	2	4383	U
43	2	4395	U
43	2	4396	A
43	2	4401	G
43	2	4415	1MA
43	2	4416	G
43	2	4418	G
43	2	4421	C
43	2	4422	A
43	2	4423	U
43	2	4424	A
43	2	4425	G
43	2	4428	A
43	2	4429	C
43	2	4433	G
43	2	4436	U
43	2	4437	U

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Mol	Chain	Res	Type
43	2	4438	U
43	2	4440	G
43	2	4446	U
43	2	4449	A
43	2	4452	U
43	2	4453	C
43	2	4464	A
43	2	4475	G
43	2	4476	C
43	2	4480	A
43	2	4484	A
43	2	4498	U
43	2	4499	G
43	2	4500	U
43	2	4502	C
43	2	4503	A
43	2	4510	A
43	2	4512	U
43	2	4513	A
43	2	4518	A
43	2	4520	G
43	2	4523	A2M
43	2	4524	G
43	2	4534	G
43	2	4536	C
43	2	4543	G
43	2	4545	G
43	2	4550	7MG
43	2	4555	U
43	2	4556	U
43	2	4557	U
43	2	4558	U
43	2	4559	A
43	2	4570	G
43	2	4573	G
43	2	4574	U
43	2	4575	G
43	2	4584	A
43	2	4589	A
43	2	4590	A
43	2	4599	A
43	2	4600	G

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Mol	Chain	Res	Type
43	2	4601	U
43	2	4606	G
43	2	4607	A
43	2	4608	G
43	2	4636	U
43	2	4637	OMG
43	2	4652	G
43	2	4656	A
43	2	4657	U
43	2	4670	C
43	2	4677	U
43	2	4678	G
43	2	4684	A
43	2	4694	G
43	2	4695	C
43	2	4700	A
43	2	4707	A
43	2	4708	A
43	2	4709	U
43	2	4730	C
43	2	4731	G
43	2	4733	C
43	2	4734	A
43	2	4740	G
43	2	4741	C
43	2	4742	G
43	2	4745	G
43	2	4751	G
43	2	4754	G
43	2	4757	C
43	2	4759	C
43	2	4761	G
43	2	4764	A
43	2	4765	G
43	2	4771	C
43	2	4775	C
43	2	4776	G
43	2	4859	C
43	2	4870	OMG
43	2	4871	C
43	2	4877	G
43	2	4882	U

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Mol	Chain	Res	Type
43	2	4883	C
43	2	4895	C
43	2	4900	C
43	2	4901	G
43	2	4910	G
43	2	4912	G
43	2	4914	C
43	2	4926	C
43	2	4927	G
43	2	4928	C
43	2	4941	G
43	2	4943	A
43	2	4949	G
43	2	4951	G
43	2	4960	G
43	2	4964	C
43	2	4976	U
43	2	4985	U
43	2	4989	U
43	2	4991	U
43	2	5013	C
43	2	5017	G
43	2	5020	G
43	2	5022	U
43	2	5023	C
43	2	5024	C
43	2	5025	C
43	2	5026	U
43	2	5027	C
43	2	5030	U
43	2	5031	G
43	2	5032	C
43	2	5035	U
43	2	5036	C
43	2	5040	U
43	2	5041	G
43	2	5047	C
43	2	5050	C
43	2	5054	C
43	2	5055	G
43	2	5058	A
43	2	5061	A

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Mol	Chain	Res	Type
43	2	5069	U
44	8	25	G
44	8	34	U
44	8	35	C
44	8	39	G
44	8	48	A
44	8	51	U
44	8	52	A
44	8	59	A
44	8	62	A
44	8	63	U
44	8	71	A
44	8	80	A
44	8	82	A
44	8	84	A
44	8	85	U
44	8	99	U
44	8	103	A
44	8	105	C
44	8	110	U
44	8	114	G
44	8	123	U
44	8	124	U
44	8	125	C
44	8	126	C
44	8	127	U
44	8	156	U
51	W	7	G
51	W	11	A
51	W	13	A
51	W	40	U
51	W	41	G
51	W	49	A
51	W	53	U
51	W	54	A
51	W	63	C
51	W	64	G
51	W	74	A
51	W	75	G
51	W	76	U
51	W	97	G
51	W	100	A

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Mol	Chain	Res	Type
51	W	103	A
51	W	106	G
51	W	109	U
51	W	110	G

All (27) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
43	2	406	C
43	2	914	U
43	2	1808	C
43	2	1931	C
43	2	1980	U
43	2	2033	A
43	2	2470	C
43	2	2546	G
43	2	2760	G
43	2	3596	A
43	2	3767	C
43	2	3776	G
43	2	3875	G
43	2	3905	A
43	2	4228	G
43	2	4229	U
43	2	4235	G
43	2	4269	G
43	2	4330	G
43	2	4555	U
43	2	4572	U
43	2	4636	U
43	2	4699	U
43	2	4913	G
43	2	5022	U
43	2	5035	U
44	8	125	C

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

62 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	$\#\|Z\| > 2$
43	2MG	2	729	43	18,26,27	2.68	6 (33%)	16,38,41	1.38	3 (18%)
43	OMC	2	2804	43	19,22,23	2.99	8 (42%)	26,31,34	0.70	0
44	OMU	8	14	44,43	19,22,23	2.99	8 (42%)	26,31,34	1.83	6 (23%)
43	A2M	2	1524	43	18,25,26	3.58	8 (44%)	18,36,39	3.45	4 (22%)
43	B8K	2	3897	43	24,28,29	3.47	11 (45%)	30,42,45	2.53	12 (40%)
43	B8K	2	4690	43	24,28,29	3.35	12 (50%)	30,42,45	2.59	12 (40%)
43	OMG	2	373	43	18,26,27	2.86	8 (44%)	19,38,41	1.56	5 (26%)
43	B8W	2	2380	43	18,26,27	2.10	2 (11%)	21,38,41	2.42	7 (33%)
43	7MG	2	4550	43	22,26,27	3.87	10 (45%)	29,39,42	1.99	9 (31%)
43	OMG	2	4623	43	18,26,27	2.84	8 (44%)	19,38,41	1.53	5 (26%)
43	OMC	2	2422	49,43	19,22,23	3.04	8 (42%)	26,31,34	1.01	2 (7%)
43	B8T	2	4483	43	19,22,23	3.61	8 (42%)	26,31,34	1.27	4 (15%)
43	OMG	2	1316	43	18,26,27	2.89	8 (44%)	19,38,41	1.53	5 (26%)
43	OMG	2	2424	43	18,26,27	2.90	8 (44%)	19,38,41	1.47	4 (21%)
43	OMU	2	4620	43	19,22,23	2.97	8 (42%)	26,31,34	1.69	4 (15%)
43	A2M	2	2401	43	18,25,26	3.60	8 (44%)	18,36,39	3.40	3 (16%)
43	M7A	2	4564	43	20,25,26	2.05	3 (15%)	28,37,40	3.91	8 (28%)
43	B8W	2	4185	43	18,26,27	2.12	2 (11%)	21,38,41	2.50	7 (33%)
43	P7G	2	1909	43	24,28,29	4.11	11 (45%)	27,41,44	1.56	3 (11%)
43	P7G	2	3880	43	24,28,29	4.05	11 (45%)	27,41,44	1.45	3 (11%)
43	OMC	2	3887	43	19,22,23	3.04	8 (42%)	26,31,34	1.03	1 (3%)
43	BGH	2	3899	43	25,29,30	4.62	17 (68%)	31,43,46	2.56	11 (35%)
43	B8Q	2	1456	43	17,22,23	2.99	4 (23%)	22,32,35	2.35	6 (27%)
43	2MG	2	978	43	18,26,27	2.75	6 (33%)	16,38,41	1.38	3 (18%)
43	I4U	2	1659	43	21,24,25	3.58	9 (42%)	27,34,37	1.19	2 (7%)
43	OMG	2	2773	43	18,26,27	2.92	8 (44%)	19,38,41	1.43	4 (21%)
43	A2M	2	3825	43	18,25,26	3.60	8 (44%)	18,36,39	3.41	4 (22%)
43	OMC	2	2861	43	19,22,23	3.09	8 (42%)	26,31,34	1.26	3 (11%)
43	A2M	2	2363	43	18,25,26	3.57	8 (44%)	18,36,39	3.42	4 (22%)
43	OMG	2	1522	43	18,26,27	2.88	8 (44%)	19,38,41	1.49	5 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
43	B9B	2	1574	43	21,28,29	2.02	3 (14%)	23,40,43	6.49	4 (17%)
43	A2M	2	3867	43	18,25,26	3.59	8 (44%)	18,36,39	3.47	4 (22%)
43	OMG	2	4870	43	18,26,27	2.91	8 (44%)	19,38,41	1.52	4 (21%)
43	B9B	2	237	43	21,28,29	2.00	3 (14%)	23,40,43	6.60	5 (21%)
43	OMC	2	2365	43	19,22,23	2.98	8 (42%)	26,31,34	0.71	0
43	OMG	2	2364	43	18,26,27	2.84	8 (44%)	19,38,41	1.46	4 (21%)
43	OMG	2	2050	43	18,26,27	2.82	8 (44%)	19,38,41	1.50	5 (26%)
43	B9H	2	2786	43	20,25,26	3.20	4 (20%)	22,35,38	1.69	4 (18%)
43	5MU	2	4083	43	19,22,23	7.26	8 (42%)	28,32,35	3.33	10 (35%)
43	7MG	2	1605	43	22,26,27	3.90	10 (45%)	29,39,42	1.96	9 (31%)
43	A2M	2	398	43	18,25,26	3.59	8 (44%)	18,36,39	3.44	3 (16%)
43	OMG	2	1625	43	18,26,27	2.95	8 (44%)	19,38,41	1.49	4 (21%)
43	OMC	2	3869	43	19,22,23	3.04	8 (42%)	26,31,34	0.99	1 (3%)
43	7MG	2	2522	43	22,26,27	3.85	10 (45%)	29,39,42	1.95	8 (27%)
43	OMC	2	3909	43	19,22,23	3.13	8 (42%)	26,31,34	1.86	7 (26%)
43	B9B	2	2754	43	21,28,29	2.02	3 (14%)	23,40,43	6.52	4 (17%)
43	B8W	2	4472	43	18,26,27	2.11	2 (11%)	21,38,41	2.49	7 (33%)
43	A2M	2	1326	43	18,25,26	3.60	8 (44%)	18,36,39	3.42	3 (16%)
43	P4U	2	1348	43	21,24,25	3.58	8 (38%)	27,33,36	1.07	1 (3%)
43	E7G	2	2297	43	24,27,28	4.02	11 (45%)	30,40,43	2.15	9 (30%)
43	2MG	2	1517	43	18,26,27	2.69	6 (33%)	16,38,41	1.43	3 (18%)
43	OMG	2	4494	43	18,26,27	2.90	8 (44%)	19,38,41	1.49	4 (21%)
43	1MA	2	4415	43	16,25,26	4.36	4 (25%)	18,37,40	1.75	3 (16%)
43	UR3	2	4597	43	19,22,23	2.83	7 (36%)	26,32,35	1.86	3 (11%)
43	A2M	2	1871	43	18,25,26	3.60	9 (50%)	18,36,39	3.43	3 (16%)
43	E7G	2	1797	43	24,27,28	4.11	11 (45%)	30,40,43	2.16	9 (30%)
43	B8T	2	4671	43	19,22,23	3.59	8 (42%)	26,31,34	0.92	1 (3%)
43	OMG	2	4637	43	18,26,27	2.85	8 (44%)	19,38,41	1.52	4 (21%)
43	A2M	2	1534	43	18,25,26	3.59	8 (44%)	18,36,39	3.54	3 (16%)
43	2MG	2	4872	43	18,26,27	2.62	6 (33%)	16,38,41	1.64	4 (25%)
43	A2M	2	4523	43	18,25,26	3.55	8 (44%)	18,36,39	3.56	5 (27%)
43	OMG	2	1883	43	18,26,27	2.91	8 (44%)	19,38,41	1.53	4 (21%)

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
43	2MG	2	729	43	-	2/5/27/28	0/3/3/3
43	OMC	2	2804	43	-	0/9/27/28	0/2/2/2
44	OMU	8	14	44,43	-	1/9/27/28	0/2/2/2
43	A2M	2	1524	43	-	0/5/27/28	0/3/3/3
43	B8K	2	3897	43	-	2/11/41/42	0/3/3/3
43	B8K	2	4690	43	-	0/11/41/42	0/3/3/3
43	OMG	2	373	43	-	1/5/27/28	0/3/3/3
43	B8W	2	2380	43	-	2/5/27/28	0/3/3/3
43	7MG	2	4550	43	-	2/7/37/38	0/3/3/3
43	OMG	2	4623	43	-	0/5/27/28	0/3/3/3
43	OMC	2	2422	49,43	-	1/9/27/28	0/2/2/2
43	B8T	2	4483	43	-	0/7/27/28	0/2/2/2
43	OMG	2	1316	43	-	2/5/27/28	0/3/3/3
43	OMG	2	2424	43	-	2/5/27/28	0/3/3/3
43	OMU	2	4620	43	-	0/9/27/28	0/2/2/2
43	A2M	2	2401	43	-	0/5/27/28	0/3/3/3
43	M7A	2	4564	43	-	0/7/37/38	0/3/3/3
43	B8W	2	4185	43	-	2/5/27/28	0/3/3/3
43	P7G	2	1909	43	-	4/10/40/41	0/3/3/3
43	P7G	2	3880	43	-	2/10/40/41	0/3/3/3
43	OMC	2	3887	43	-	1/9/27/28	0/2/2/2
43	BGH	2	3899	43	-	0/13/43/44	0/3/3/3
43	B8Q	2	1456	43	-	0/7/42/43	0/2/2/2
43	2MG	2	978	43	-	0/5/27/28	0/3/3/3
43	I4U	2	1659	43	-	2/9/29/30	0/2/2/2
43	OMG	2	2773	43	-	0/5/27/28	0/3/3/3
43	A2M	2	3825	43	-	0/5/27/28	0/3/3/3
43	OMC	2	2861	43	-	0/9/27/28	0/2/2/2
43	A2M	2	2363	43	-	0/5/27/28	0/3/3/3
43	OMG	2	1522	43	-	1/5/27/28	0/3/3/3
43	B9B	2	1574	43	-	5/7/29/30	0/3/3/3
43	A2M	2	3867	43	-	2/5/27/28	0/3/3/3
43	OMG	2	4870	43	-	3/5/27/28	0/3/3/3
43	B9B	2	237	43	-	4/7/29/30	0/3/3/3
43	OMC	2	2365	43	-	0/9/27/28	0/2/2/2
43	OMG	2	2364	43	-	2/5/27/28	0/3/3/3
43	OMG	2	2050	43	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	B9H	2	2786	43	-	0/12/47/48	0/2/2/2
43	5MU	2	4083	43	-	7/7/25/26	0/2/2/2
43	7MG	2	1605	43	-	0/7/37/38	0/3/3/3
43	A2M	2	398	43	-	2/5/27/28	0/3/3/3
43	OMG	2	1625	43	-	3/5/27/28	0/3/3/3
43	OMC	2	3869	43	-	1/9/27/28	0/2/2/2
43	7MG	2	2522	43	-	0/7/37/38	0/3/3/3
43	OMC	2	3909	43	-	1/9/27/28	0/2/2/2
43	B9B	2	2754	43	-	5/7/29/30	0/3/3/3
43	B8W	2	4472	43	-	2/5/27/28	0/3/3/3
43	A2M	2	1326	43	-	0/5/27/28	0/3/3/3
43	P4U	2	1348	43	-	1/10/29/30	0/2/2/2
43	E7G	2	2297	43	-	1/9/39/40	0/3/3/3
43	2MG	2	1517	43	-	2/5/27/28	0/3/3/3
43	OMG	2	4494	43	-	0/5/27/28	0/3/3/3
43	1MA	2	4415	43	-	1/3/25/26	0/3/3/3
43	UR3	2	4597	43	-	0/7/25/26	0/2/2/2
43	A2M	2	1871	43	-	2/5/27/28	0/3/3/3
43	E7G	2	1797	43	-	0/9/39/40	0/3/3/3
43	B8T	2	4671	43	-	0/7/27/28	0/2/2/2
43	OMG	2	4637	43	-	3/5/27/28	0/3/3/3
43	A2M	2	1534	43	-	2/5/27/28	0/3/3/3
43	2MG	2	4872	43	-	2/5/27/28	0/3/3/3
43	A2M	2	4523	43	-	2/5/27/28	0/3/3/3
43	OMG	2	1883	43	-	2/5/27/28	0/3/3/3

All (473) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2	4083	5MU	C4-C5	21.05	1.79	1.44
43	2	4415	1MA	C2-N3	16.13	1.48	1.29
43	2	4083	5MU	C6-N1	16.04	1.65	1.38
43	2	4083	5MU	C6-C5	-11.31	1.16	1.34
43	2	4083	5MU	C4-N3	-10.99	1.18	1.38
43	2	1659	I4U	C4-N3	10.68	1.45	1.31
43	2	1348	P4U	C4-N3	10.49	1.44	1.31
43	2	1797	E7G	C8-N9	9.97	1.51	1.46
43	2	2297	E7G	C5-N7	9.77	1.46	1.35
43	2	2786	B9H	C2-N3	9.58	1.49	1.37
43	2	1605	7MG	C8-N9	9.43	1.51	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2	3880	P7G	C5-N7	9.41	1.46	1.35
43	2	3897	B8K	C8-N9	9.33	1.51	1.46
43	2	1909	P7G	C5-N7	9.31	1.46	1.35
43	2	1797	E7G	C5-N7	9.30	1.46	1.35
43	2	1909	P7G	C8-N9	9.21	1.51	1.46
43	2	2522	7MG	C8-N9	9.18	1.51	1.46
43	2	4550	7MG	C8-N9	9.00	1.51	1.46
43	2	3880	P7G	C8-N9	8.97	1.51	1.46
43	2	1871	A2M	C3'-C4'	-8.97	1.30	1.53
43	2	4690	B8K	C8-N9	8.89	1.50	1.46
43	2	2297	E7G	C8-N9	8.88	1.50	1.46
43	2	3899	BGH	O4'-C1'	8.85	1.63	1.42
43	2	1605	7MG	C5-N7	8.83	1.45	1.35
43	2	1524	A2M	C3'-C4'	-8.82	1.30	1.53
43	2	398	A2M	C3'-C4'	-8.82	1.30	1.53
43	2	2522	7MG	C5-N7	8.80	1.45	1.35
43	2	4550	7MG	C5-N7	8.77	1.45	1.35
43	2	1326	A2M	C3'-C4'	-8.77	1.30	1.53
43	2	2363	A2M	C3'-C4'	-8.73	1.30	1.53
43	2	2401	A2M	C3'-C4'	-8.73	1.30	1.53
43	2	3899	BGH	C8-N9	8.73	1.50	1.46
43	2	1534	A2M	C3'-C4'	-8.73	1.30	1.53
43	2	3867	A2M	C3'-C4'	-8.72	1.30	1.53
43	2	3899	BGH	C2'-C1'	-8.72	1.30	1.53
43	2	3825	A2M	C3'-C4'	-8.71	1.30	1.53
43	2	1456	B8Q	C6-C5	8.32	1.52	1.33
43	2	4523	A2M	C3'-C4'	-8.24	1.31	1.53
43	2	4185	B8W	C2-N2	8.06	1.50	1.33
43	2	4472	B8W	C2-N2	7.98	1.49	1.33
43	2	2380	B8W	C2-N2	7.90	1.49	1.33
43	2	4523	A2M	O4'-C4'	7.80	1.62	1.45
43	2	2401	A2M	O4'-C4'	7.78	1.62	1.45
43	2	1534	A2M	O4'-C4'	7.74	1.62	1.45
43	2	1871	A2M	O4'-C4'	7.70	1.62	1.45
43	2	3825	A2M	O4'-C4'	7.69	1.62	1.45
43	2	398	A2M	O4'-C4'	7.65	1.62	1.45
43	2	1326	A2M	O4'-C4'	7.64	1.62	1.45
43	2	3899	BGH	O4'-C4'	-7.59	1.28	1.45
43	2	1524	A2M	O4'-C4'	7.58	1.61	1.45
43	2	2363	A2M	O4'-C4'	7.54	1.61	1.45
43	2	3867	A2M	O4'-C4'	7.43	1.61	1.45
43	2	4483	B8T	C2-N3	7.35	1.51	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2	3867	A2M	O4'-C1'	-7.29	1.30	1.41
43	2	4671	B8T	C2-N3	7.25	1.51	1.36
43	2	1326	A2M	O4'-C1'	-7.22	1.31	1.41
44	8	14	OMU	C2-N1	7.14	1.49	1.38
43	2	3825	A2M	O4'-C1'	-7.14	1.31	1.41
43	2	2786	B9H	C6-C5	7.12	1.49	1.33
43	2	4523	A2M	O4'-C1'	-7.10	1.31	1.41
43	2	4671	B8T	C4-N3	7.06	1.45	1.32
43	2	1524	A2M	O4'-C1'	-7.05	1.31	1.41
43	2	4483	B8T	C4-N3	7.03	1.45	1.32
43	2	4620	OMU	C2-N1	7.03	1.49	1.38
43	2	398	A2M	O4'-C1'	-7.02	1.31	1.41
43	2	2401	A2M	O4'-C1'	-7.00	1.31	1.41
43	2	2363	A2M	O4'-C1'	-6.98	1.31	1.41
43	2	1534	A2M	O4'-C1'	-6.97	1.31	1.41
43	2	978	2MG	C2-N2	6.90	1.48	1.33
43	2	4671	B8T	C6-C5	6.87	1.51	1.35
43	2	2786	B9H	C2-N1	6.86	1.48	1.38
43	2	4597	UR3	C6-C5	6.79	1.50	1.35
43	2	1456	B8Q	C2-N3	6.76	1.46	1.35
43	2	1517	2MG	C2-N2	6.75	1.48	1.33
43	2	4483	B8T	C6-C5	6.75	1.50	1.35
43	2	1871	A2M	O4'-C1'	-6.75	1.31	1.41
44	8	14	OMU	C2-N3	6.70	1.49	1.38
43	2	729	2MG	C2-N2	6.70	1.48	1.33
43	2	3909	OMC	C6-C5	6.64	1.50	1.35
43	2	3897	B8K	C2-N3	6.59	1.49	1.33
43	2	4690	B8K	C2-N3	6.58	1.49	1.33
43	2	1909	P7G	C4-N9	6.58	1.45	1.35
43	2	4620	OMU	C2-N3	6.53	1.49	1.38
43	2	2422	OMC	C2-N3	6.47	1.49	1.36
43	2	2861	OMC	C2-N3	6.45	1.49	1.36
43	2	4872	2MG	C2-N2	6.40	1.47	1.33
43	2	3869	OMC	C2-N3	6.37	1.49	1.36
43	2	3887	OMC	C2-N3	6.36	1.49	1.36
43	2	2804	OMC	C2-N3	6.35	1.49	1.36
43	2	4597	UR3	C2-N3	6.31	1.51	1.39
43	2	1625	OMG	C2-N3	6.31	1.48	1.33
43	2	1909	P7G	C4-N3	6.30	1.48	1.37
43	2	2297	E7G	C8-N7	6.29	1.51	1.45
43	2	4483	B8T	C4-N4	6.28	1.48	1.35
43	2	2754	B9B	O6-C6	6.27	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2	1797	E7G	C8-N7	6.27	1.51	1.45
43	2	2773	OMG	C2-N3	6.27	1.48	1.33
43	2	2424	OMG	C2-N3	6.26	1.48	1.33
43	2	1574	B9B	O6-C6	6.25	1.40	1.35
43	2	4671	B8T	C4-N4	6.25	1.48	1.35
43	2	2365	OMC	C2-N3	6.23	1.49	1.36
43	2	1883	OMG	C2-N3	6.21	1.48	1.33
43	2	3880	P7G	C4-N3	6.20	1.48	1.37
43	2	1659	I4U	C2-N3	6.19	1.48	1.36
43	2	4870	OMG	C2-N3	6.19	1.48	1.33
43	2	1348	P4U	C2-N3	6.16	1.48	1.36
43	2	1659	I4U	C6-C5	6.14	1.49	1.35
43	2	4597	UR3	C2-N1	6.13	1.47	1.38
43	2	2364	OMG	C2-N3	6.10	1.48	1.33
43	2	2773	OMG	C2-N2	6.10	1.48	1.34
43	2	4494	OMG	C2-N3	6.10	1.48	1.33
43	2	3880	P7G	C4-N9	6.09	1.44	1.35
43	2	237	B9B	O6-C6	6.09	1.40	1.35
43	2	1348	P4U	C6-C5	6.09	1.49	1.35
43	2	1625	OMG	C2-N2	6.09	1.48	1.34
43	2	1316	OMG	C2-N3	6.07	1.48	1.33
43	2	2424	OMG	C2-N2	6.06	1.48	1.34
43	2	4564	M7A	C4-N9	6.06	1.49	1.38
43	2	4870	OMG	C2-N2	6.05	1.48	1.34
43	2	3899	BGH	C4-N9	6.05	1.44	1.37
43	2	1883	OMG	C2-N2	6.05	1.48	1.34
43	2	4494	OMG	C2-N2	6.04	1.48	1.34
43	2	2861	OMC	C6-C5	6.04	1.49	1.35
43	2	2365	OMC	C6-C5	6.02	1.49	1.35
43	2	4637	OMG	C2-N3	6.01	1.47	1.33
43	2	1522	OMG	C2-N3	6.00	1.47	1.33
43	2	3880	P7G	C8-N7	5.99	1.51	1.45
43	2	1522	OMG	C2-N2	5.98	1.48	1.34
43	2	1316	OMG	C2-N2	5.97	1.48	1.34
43	2	3887	OMC	C6-C5	5.97	1.48	1.35
43	2	2422	OMC	C6-C5	5.97	1.48	1.35
43	2	2804	OMC	C6-C5	5.95	1.48	1.35
43	2	1909	P7G	C2-N2	5.94	1.48	1.34
43	2	4637	OMG	C2-N2	5.93	1.48	1.34
43	2	2364	OMG	C2-N2	5.92	1.48	1.34
43	2	3869	OMC	C6-C5	5.92	1.48	1.35
43	2	1909	P7G	C8-N7	5.92	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2	2050	OMG	C2-N3	5.90	1.47	1.33
43	2	4623	OMG	C2-N3	5.90	1.47	1.33
43	2	373	OMG	C2-N2	5.88	1.48	1.34
43	2	373	OMG	C2-N3	5.88	1.47	1.33
43	2	3880	P7G	C2-N2	5.87	1.48	1.34
43	2	1797	E7G	C2-N3	5.87	1.47	1.33
43	2	4623	OMG	C2-N2	5.83	1.48	1.34
43	2	2050	OMG	C2-N2	5.82	1.48	1.34
43	2	4550	7MG	C2-N3	5.82	1.47	1.33
43	2	2754	B9B	C2-N2	5.80	1.45	1.33
43	2	1797	E7G	C4-N9	5.80	1.44	1.37
43	2	1797	E7G	C4-N3	5.79	1.48	1.34
43	2	1574	B9B	C2-N2	5.78	1.45	1.33
43	2	2297	E7G	C4-N9	5.77	1.44	1.37
43	2	3897	B8K	C4-N9	5.77	1.44	1.37
43	2	237	B9B	C2-N2	5.75	1.45	1.33
43	2	3899	BGH	C2-N3	5.75	1.47	1.33
43	2	2297	E7G	C2-N3	5.74	1.47	1.33
43	2	1605	7MG	C2-N3	5.73	1.47	1.33
43	2	3899	BGH	C4-N3	5.73	1.47	1.34
43	2	2522	7MG	C2-N3	5.70	1.46	1.33
43	2	2297	E7G	C4-N3	5.68	1.47	1.34
43	2	3909	OMC	C2-N3	5.66	1.47	1.36
43	2	4550	7MG	C4-N3	5.63	1.47	1.34
43	2	4620	OMU	C6-C5	5.59	1.48	1.35
43	2	4550	7MG	C4-N9	5.57	1.44	1.37
43	2	2522	7MG	C4-N3	5.55	1.47	1.34
43	2	3909	OMC	C4-N4	5.54	1.47	1.33
43	2	1605	7MG	C4-N3	5.52	1.47	1.34
43	2	3909	OMC	C2-N1	5.43	1.51	1.40
43	2	1605	7MG	C4-N9	5.39	1.44	1.37
43	2	2522	7MG	C4-N9	5.35	1.43	1.37
44	8	14	OMU	C6-C5	5.32	1.47	1.35
43	2	729	2MG	C4-N3	5.32	1.50	1.37
43	2	3880	P7G	C2-N1	5.30	1.46	1.33
43	2	2861	OMC	C2-N1	5.26	1.51	1.40
43	2	1909	P7G	C2-N1	5.22	1.45	1.33
43	2	1797	E7G	C2-N2	5.22	1.46	1.34
43	2	978	2MG	C4-N3	5.19	1.50	1.37
43	2	2804	OMC	C4-N3	5.17	1.44	1.34
43	2	1517	2MG	C4-N3	5.16	1.49	1.37
43	2	2297	E7G	C2-N2	5.15	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2	4690	B8K	C4-N9	5.14	1.43	1.37
43	2	2365	OMC	C4-N3	5.11	1.44	1.34
43	2	2422	OMC	C4-N3	5.10	1.44	1.34
43	2	3869	OMC	C4-N3	5.08	1.44	1.34
43	2	2861	OMC	C4-N3	5.08	1.44	1.34
43	2	3887	OMC	C4-N3	5.03	1.44	1.34
43	2	3887	OMC	C2-N1	5.03	1.50	1.40
43	2	2861	OMC	C4-N4	4.98	1.45	1.33
43	2	1456	B8Q	C2-N1	4.96	1.45	1.38
43	2	2422	OMC	C2-N1	4.93	1.50	1.40
43	2	1625	OMG	C4-N3	4.93	1.49	1.37
43	2	3899	BGH	C2-N2	4.93	1.45	1.34
43	2	3869	OMC	C2-N1	4.90	1.50	1.40
43	2	3869	OMC	C4-N4	4.88	1.45	1.33
43	2	2804	OMC	C4-N4	4.88	1.45	1.33
43	2	1659	I4U	C5-C4	4.87	1.49	1.43
43	2	2365	OMC	C4-N4	4.87	1.45	1.33
43	2	1883	OMG	C4-N3	4.85	1.49	1.37
43	2	2424	OMG	C4-N3	4.85	1.49	1.37
43	2	2422	OMC	C4-N4	4.84	1.45	1.33
43	2	2773	OMG	C4-N3	4.84	1.49	1.37
43	2	1348	P4U	O4-C4	4.84	1.40	1.35
43	2	1605	7MG	C2-N2	4.83	1.45	1.34
43	2	4872	2MG	C4-N3	4.83	1.49	1.37
43	2	3887	OMC	C4-N4	4.83	1.45	1.33
43	2	4494	OMG	C4-N3	4.83	1.49	1.37
43	2	4483	B8T	C2-N1	4.82	1.50	1.40
43	2	4870	OMG	C4-N3	4.80	1.49	1.37
43	2	373	OMG	C6-N1	4.79	1.45	1.37
43	2	4550	7MG	C2-N2	4.79	1.45	1.34
43	2	2522	7MG	C2-N2	4.78	1.45	1.34
43	2	1316	OMG	C6-N1	4.72	1.44	1.37
43	2	2364	OMG	C4-N3	4.69	1.48	1.37
43	2	3899	BGH	C5-N7	4.69	1.47	1.39
43	2	4671	B8T	C2-N1	4.68	1.50	1.40
43	2	1522	OMG	C4-N3	4.67	1.48	1.37
43	2	1625	OMG	C6-N1	4.66	1.44	1.37
43	2	2773	OMG	C6-N1	4.66	1.44	1.37
43	2	1522	OMG	C6-N1	4.65	1.44	1.37
43	2	1316	OMG	C4-N3	4.65	1.48	1.37
43	2	4637	OMG	C4-N3	4.65	1.48	1.37
43	2	4083	5MU	C2-N3	4.63	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2	3909	OMC	C4-N3	4.61	1.43	1.34
43	2	4623	OMG	C6-N1	4.60	1.44	1.37
43	2	4494	OMG	C6-N1	4.55	1.44	1.37
43	2	2424	OMG	C6-N1	4.55	1.44	1.37
43	2	1883	OMG	C6-N1	4.54	1.44	1.37
43	2	2050	OMG	C6-N1	4.54	1.44	1.37
43	2	373	OMG	C4-N3	4.54	1.48	1.37
43	2	4623	OMG	C4-N3	4.51	1.48	1.37
43	2	2050	OMG	C4-N3	4.51	1.48	1.37
43	2	4870	OMG	C6-N1	4.51	1.44	1.37
43	2	4690	B8K	C4-N3	4.48	1.44	1.34
43	2	3897	B8K	C4-N3	4.46	1.44	1.34
43	2	4637	OMG	C6-N1	4.45	1.44	1.37
43	2	2364	OMG	C6-N1	4.42	1.44	1.37
43	2	3899	BGH	C5-C6	4.37	1.54	1.43
43	2	3897	B8K	C5-C6	4.34	1.54	1.43
43	2	978	2MG	C2-N1	4.34	1.43	1.36
43	2	4564	M7A	C6-N6	4.34	1.45	1.34
43	2	3897	B8K	C5-N7	4.33	1.47	1.39
43	2	2804	OMC	C2-N1	4.32	1.49	1.40
43	2	1659	I4U	C2-N1	4.32	1.49	1.40
43	2	1348	P4U	C2-N1	4.29	1.49	1.40
43	2	2365	OMC	C2-N1	4.29	1.49	1.40
43	2	4690	B8K	C5-N7	4.28	1.47	1.39
43	2	1348	P4U	C5-C4	4.28	1.48	1.43
43	2	1517	2MG	C2-N1	4.25	1.43	1.36
43	2	4872	2MG	C2-N1	4.20	1.43	1.36
43	2	729	2MG	C2-N1	4.14	1.43	1.36
44	8	14	OMU	C4-N3	4.08	1.45	1.38
43	2	4415	1MA	C4-N3	4.08	1.50	1.37
43	2	4690	B8K	C5-C6	4.07	1.54	1.43
43	2	4415	1MA	C2-N1	4.01	1.43	1.35
43	2	4620	OMU	C4-N3	3.98	1.45	1.38
43	2	4671	B8T	C5-C4	3.88	1.49	1.40
43	2	4564	M7A	C5-N7	3.88	1.48	1.39
43	2	4550	7MG	C5-C6	3.85	1.53	1.43
43	2	1909	P7G	C2-N3	3.83	1.47	1.37
43	2	1605	7MG	C5-C6	3.82	1.53	1.43
43	2	978	2MG	C6-N1	3.81	1.43	1.37
43	2	2297	E7G	C5-C6	3.79	1.53	1.43
43	2	4872	2MG	C6-N1	3.79	1.43	1.37
43	2	3897	B8K	C6-N1	3.78	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2	2522	7MG	C5-C6	3.78	1.53	1.43
43	2	1797	E7G	C5-C6	3.75	1.53	1.43
43	2	1605	7MG	C2-N1	3.73	1.46	1.37
43	2	3899	BGH	O2'-C2'	3.72	1.52	1.42
43	2	3880	P7G	C2-N3	3.70	1.46	1.37
43	2	4550	7MG	C2-N1	3.68	1.46	1.37
43	2	1517	2MG	C6-N1	3.67	1.43	1.37
43	2	1797	E7G	C2-N1	3.65	1.46	1.37
43	2	4083	5MU	C2-N1	3.65	1.44	1.38
43	2	2522	7MG	C2-N1	3.64	1.46	1.37
43	2	4872	2MG	C5-C6	3.64	1.54	1.47
43	2	3909	OMC	C6-N1	3.61	1.46	1.38
43	2	4483	B8T	C5-C4	3.61	1.48	1.40
43	2	4483	B8T	C6-N1	3.60	1.46	1.38
43	2	4690	B8K	C6-N1	3.60	1.45	1.38
43	2	3899	BGH	C71-N7	3.60	1.47	1.39
43	2	3897	B8K	C2-N2	3.59	1.42	1.34
43	2	4690	B8K	C71-N7	3.58	1.47	1.39
43	2	978	2MG	C5-C6	3.58	1.54	1.47
43	2	2297	E7G	C2-N1	3.57	1.46	1.37
43	2	3880	P7G	C6-N1	3.55	1.44	1.38
43	2	3899	BGH	C6-N1	3.55	1.45	1.38
43	2	729	2MG	C6-N1	3.54	1.43	1.37
43	2	4690	B8K	C2-N2	3.53	1.42	1.34
43	2	3897	B8K	C71-N7	3.53	1.47	1.39
43	2	1517	2MG	C5-C6	3.53	1.54	1.47
43	2	1909	P7G	C6-N1	3.48	1.44	1.38
43	2	1797	E7G	C6-N1	3.45	1.45	1.38
43	2	3897	B8K	C2-N1	3.45	1.46	1.37
43	2	729	2MG	C5-C6	3.44	1.54	1.47
43	2	3869	OMC	C6-N1	3.44	1.46	1.38
43	2	1909	P7G	C5-C4	3.44	1.44	1.37
43	2	1605	7MG	C6-N1	3.43	1.45	1.38
43	2	4550	7MG	C6-N1	3.39	1.45	1.38
43	2	1348	P4U	C6-N1	3.38	1.46	1.38
43	2	3899	BGH	C2-N1	3.37	1.46	1.37
43	2	2297	E7G	C6-N1	3.36	1.45	1.38
43	2	373	OMG	C5-C6	3.34	1.54	1.47
43	2	1316	OMG	C5-C6	3.33	1.54	1.47
43	2	4870	OMG	C5-C6	3.33	1.54	1.47
43	2	1625	OMG	C5-C6	3.31	1.54	1.47
43	2	2861	OMC	C6-N1	3.31	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2	4623	OMG	C5-C6	3.30	1.54	1.47
43	2	4637	OMG	C5-C6	3.30	1.54	1.47
43	2	2773	OMG	C5-C6	3.30	1.54	1.47
43	2	2522	7MG	C6-N1	3.29	1.44	1.38
43	2	3887	OMC	C6-N1	3.28	1.45	1.38
43	2	1522	OMG	C5-C6	3.27	1.54	1.47
43	2	3880	P7G	C5-C4	3.26	1.43	1.37
43	2	2365	OMC	C6-N1	3.26	1.45	1.38
43	2	4690	B8K	C2-N1	3.26	1.45	1.37
43	2	1659	I4U	C6-N1	3.25	1.45	1.38
43	2	4494	OMG	C5-C6	3.25	1.54	1.47
43	2	2422	OMC	C6-N1	3.24	1.45	1.38
43	2	2050	OMG	C5-C6	3.24	1.54	1.47
43	2	2804	OMC	C6-N1	3.22	1.45	1.38
43	2	2364	OMG	C5-C6	3.21	1.53	1.47
43	2	4523	A2M	O3'-C3'	3.21	1.50	1.43
43	2	1909	P7G	O6-C6	-3.20	1.18	1.23
43	2	4597	UR3	C6-N1	3.19	1.45	1.38
43	2	4523	A2M	C6-N6	3.17	1.45	1.34
43	2	3867	A2M	C6-N6	3.17	1.45	1.34
43	2	4671	B8T	C6-N1	3.17	1.45	1.38
43	2	1524	A2M	C6-N6	3.16	1.45	1.34
43	2	2401	A2M	C6-N6	3.15	1.45	1.34
43	2	1871	A2M	C6-N6	3.14	1.45	1.34
43	2	3825	A2M	C6-N6	3.14	1.45	1.34
43	2	1326	A2M	C6-N6	3.12	1.45	1.34
43	2	398	A2M	C6-N6	3.12	1.45	1.34
43	2	1534	A2M	C6-N6	3.12	1.45	1.34
43	2	2424	OMG	C5-C6	3.12	1.53	1.47
43	2	2363	A2M	C6-N6	3.11	1.45	1.34
43	2	3880	P7G	O6-C6	-3.10	1.18	1.23
43	2	1883	OMG	C5-C6	3.04	1.53	1.47
43	2	4620	OMU	O4-C4	-3.00	1.18	1.24
43	2	2401	A2M	O3'-C3'	2.99	1.50	1.43
43	2	3825	A2M	O3'-C3'	2.98	1.50	1.43
43	2	3899	BGH	O3'-C3'	-2.97	1.36	1.43
44	8	14	OMU	O4-C4	-2.95	1.18	1.24
43	2	3897	B8K	C5-C4	2.93	1.47	1.38
43	2	3867	A2M	O3'-C3'	2.91	1.49	1.43
43	2	1534	A2M	O3'-C3'	2.90	1.49	1.43
43	2	2363	A2M	O3'-C3'	2.89	1.49	1.43
43	2	398	A2M	O3'-C3'	2.85	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2	1659	I4U	O4-C4	2.84	1.41	1.35
43	2	1871	A2M	O3'-C3'	2.81	1.49	1.43
43	2	4872	2MG	C5-C4	-2.81	1.35	1.43
43	2	2050	OMG	O6-C6	-2.81	1.17	1.23
43	2	4671	B8T	O2-C2	-2.81	1.18	1.23
43	2	1883	OMG	O6-C6	-2.80	1.17	1.23
43	2	1524	A2M	O3'-C3'	2.80	1.49	1.43
43	2	4083	5MU	O4-C4	-2.80	1.18	1.23
43	2	4483	B8T	O2-C2	-2.78	1.18	1.23
43	2	4623	OMG	O6-C6	-2.78	1.17	1.23
43	2	978	2MG	C5-C4	-2.78	1.36	1.43
43	2	1326	A2M	O3'-C3'	2.78	1.49	1.43
43	2	1534	A2M	O2'-C2'	-2.78	1.35	1.42
43	2	1625	OMG	O6-C6	-2.77	1.17	1.23
43	2	4637	OMG	O6-C6	-2.76	1.17	1.23
43	2	237	B9B	C5-C4	-2.75	1.33	1.40
44	8	14	OMU	C6-N1	2.75	1.44	1.38
43	2	2364	OMG	O6-C6	-2.74	1.17	1.23
43	2	2424	OMG	O6-C6	-2.74	1.17	1.23
43	2	2804	OMC	O2-C2	-2.74	1.18	1.23
43	2	1522	OMG	O6-C6	-2.73	1.17	1.23
43	2	729	2MG	C5-C4	-2.73	1.36	1.43
43	2	1659	I4U	O2-C2	-2.73	1.18	1.23
43	2	1574	B9B	C5-C4	-2.73	1.33	1.40
43	2	4870	OMG	O6-C6	-2.72	1.17	1.23
43	2	4690	B8K	C5-C4	2.72	1.47	1.38
43	2	1517	2MG	C5-C4	-2.71	1.36	1.43
43	2	1316	OMG	O6-C6	-2.71	1.17	1.23
43	2	1659	I4U	O4-C41	-2.71	1.40	1.47
43	2	4494	OMG	O6-C6	-2.71	1.17	1.23
43	2	2365	OMC	O2-C2	-2.71	1.18	1.23
43	2	1348	P4U	O2-C2	-2.71	1.18	1.23
43	2	2380	B8W	C5-C4	-2.70	1.33	1.40
43	2	4620	OMU	C6-N1	2.70	1.44	1.38
43	2	2363	A2M	O2'-C2'	-2.66	1.35	1.42
43	2	4472	B8W	C5-C4	-2.66	1.33	1.40
43	2	1534	A2M	C5-C4	-2.65	1.33	1.40
43	2	373	OMG	O6-C6	-2.65	1.17	1.23
43	2	3899	BGH	O6-C6	-2.64	1.18	1.23
43	2	3909	OMC	C5-C4	2.64	1.49	1.42
43	2	2401	A2M	O2'-C2'	-2.63	1.35	1.42
43	2	1871	A2M	C5-C4	-2.63	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2	398	A2M	O2'-C2'	-2.62	1.35	1.42
43	2	2773	OMG	O6-C6	-2.62	1.18	1.23
43	2	4185	B8W	C5-C4	-2.61	1.34	1.40
43	2	3887	OMC	O2-C2	-2.61	1.18	1.23
43	2	3867	A2M	O2'-C2'	-2.60	1.36	1.42
43	2	2401	A2M	C5-C4	-2.60	1.34	1.40
43	2	3869	OMC	O2-C2	-2.59	1.18	1.23
43	2	1524	A2M	O2'-C2'	-2.59	1.36	1.42
43	2	2754	B9B	C5-C4	-2.59	1.34	1.40
43	2	1326	A2M	C5-C4	-2.58	1.34	1.40
43	2	373	OMG	C2-N1	2.58	1.44	1.37
43	2	2422	OMC	O2-C2	-2.57	1.18	1.23
43	2	3867	A2M	C2-N3	2.57	1.36	1.32
43	2	398	A2M	C5-C4	-2.57	1.34	1.40
43	2	1871	A2M	O2'-C2'	-2.56	1.36	1.42
43	2	1625	OMG	C2-N1	2.55	1.44	1.37
43	2	4083	5MU	O2-C2	-2.55	1.18	1.23
43	2	3825	A2M	C5-C4	-2.55	1.34	1.40
43	2	2363	A2M	C5-C4	-2.54	1.34	1.40
43	2	2861	OMC	O2-C2	-2.52	1.19	1.23
43	2	3867	A2M	C5-C4	-2.52	1.34	1.40
43	2	4523	A2M	C5-C4	-2.52	1.34	1.40
43	2	2773	OMG	C2-N1	2.52	1.43	1.37
43	2	3825	A2M	O2'-C2'	-2.51	1.36	1.42
43	2	1316	OMG	C2-N1	2.50	1.43	1.37
43	2	4550	7MG	O6-C6	-2.49	1.18	1.23
43	2	1522	OMG	C2-N1	2.48	1.43	1.37
43	2	4494	OMG	C2-N1	2.47	1.43	1.37
43	2	1456	B8Q	C6-N1	2.47	1.44	1.38
43	2	2522	7MG	O6-C6	-2.47	1.18	1.23
43	2	1524	A2M	C5-C4	-2.46	1.34	1.40
43	2	1326	A2M	O2'-C2'	-2.46	1.36	1.42
43	2	4623	OMG	C2-N1	2.46	1.43	1.37
43	2	1605	7MG	O6-C6	-2.45	1.18	1.23
43	2	2050	OMG	C2-N1	2.45	1.43	1.37
43	2	2424	OMG	C2-N1	2.45	1.43	1.37
44	8	14	OMU	O2-C2	-2.45	1.18	1.23
43	2	4870	OMG	C2-N1	2.45	1.43	1.37
43	2	2363	A2M	C2-N3	2.45	1.36	1.32
43	2	2297	E7G	O6-C6	-2.44	1.18	1.23
43	2	1883	OMG	C2-N1	2.44	1.43	1.37
43	2	2804	OMC	C5-C4	2.43	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2	2861	OMC	C5-C4	2.42	1.48	1.42
43	2	4523	A2M	O2'-C2'	-2.40	1.36	1.42
43	2	1797	E7G	O6-C6	-2.40	1.19	1.23
43	2	2422	OMC	C5-C4	2.40	1.48	1.42
43	2	4637	OMG	C2-N1	2.40	1.43	1.37
43	2	3887	OMC	C5-C4	2.39	1.48	1.42
43	2	2364	OMG	C2-N1	2.38	1.43	1.37
43	2	2365	OMC	C5-C4	2.37	1.48	1.42
43	2	4620	OMU	O2-C2	-2.35	1.18	1.23
43	2	373	OMG	C5-C4	-2.35	1.37	1.43
43	2	1883	OMG	C5-C4	-2.34	1.37	1.43
43	2	4623	OMG	C5-C4	-2.34	1.37	1.43
43	2	4415	1MA	C5-C4	-2.34	1.37	1.43
43	2	3825	A2M	C2-N3	2.34	1.35	1.32
43	2	4523	A2M	C2-N3	2.32	1.35	1.32
43	2	1534	A2M	C2-N3	2.31	1.35	1.32
43	2	1871	A2M	C2-N3	2.31	1.35	1.32
43	2	4620	OMU	C5-C4	2.30	1.48	1.43
43	2	3909	OMC	O2-C2	-2.29	1.19	1.23
43	2	1522	OMG	C5-C4	-2.27	1.37	1.43
43	2	1524	A2M	C2-N3	2.27	1.35	1.32
43	2	2050	OMG	C5-C4	-2.24	1.37	1.43
43	2	2401	A2M	C2-N3	2.24	1.35	1.32
43	2	1326	A2M	C2-N3	2.23	1.35	1.32
43	2	3869	OMC	C5-C4	2.23	1.48	1.42
43	2	398	A2M	C2-N3	2.23	1.35	1.32
43	2	2786	B9H	C31-N3	-2.23	1.43	1.46
43	2	4597	UR3	C5-C4	2.22	1.49	1.43
43	2	1316	OMG	C5-C4	-2.22	1.37	1.43
43	2	4637	OMG	C5-C4	-2.21	1.37	1.43
44	8	14	OMU	C5-C4	2.21	1.48	1.43
43	2	4870	OMG	C5-C4	-2.19	1.37	1.43
43	2	4494	OMG	C5-C4	-2.19	1.37	1.43
43	2	3899	BGH	C5-C4	2.17	1.45	1.38
43	2	2364	OMG	C5-C4	-2.16	1.37	1.43
43	2	2424	OMG	C5-C4	-2.15	1.37	1.43
43	2	4597	UR3	C4-N3	2.10	1.45	1.40
43	2	4690	B8K	O6-C6	-2.08	1.19	1.23
43	2	4597	UR3	O2-C2	-2.05	1.18	1.22
43	2	2773	OMG	C5-C4	-2.04	1.37	1.43
43	2	1625	OMG	C5-C4	-2.04	1.37	1.43
43	2	1871	A2M	O5'-C5'	-2.00	1.39	1.44

All (291) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	2	237	B9B	O6-C6-N1	-30.27	93.99	120.12
43	2	2754	B9B	O6-C6-N1	-29.85	94.36	120.12
43	2	1574	B9B	O6-C6-N1	-29.78	94.41	120.12
43	2	4564	M7A	C5-C6-N6	13.72	147.17	123.74
43	2	4564	M7A	N6-C6-N1	-11.68	92.76	118.35
43	2	1534	A2M	C5-C6-N6	10.75	136.68	120.35
43	2	4523	A2M	C5-C6-N6	10.52	136.34	120.35
43	2	398	A2M	C5-C6-N6	10.51	136.33	120.35
43	2	1326	A2M	C5-C6-N6	10.48	136.28	120.35
43	2	3867	A2M	C5-C6-N6	10.43	136.20	120.35
43	2	3825	A2M	C5-C6-N6	10.39	136.14	120.35
43	2	1524	A2M	C5-C6-N6	10.38	136.13	120.35
43	2	1871	A2M	C5-C6-N6	10.35	136.08	120.35
43	2	2401	A2M	C5-C6-N6	10.32	136.03	120.35
43	2	2363	A2M	C5-C6-N6	10.30	136.00	120.35
43	2	4083	5MU	C5-C4-N3	10.08	123.92	115.31
43	2	4083	5MU	C5-C6-N1	-7.88	115.23	123.34
43	2	1534	A2M	N6-C6-N1	-7.66	102.68	118.57
43	2	4597	UR3	C4-N3-C2	-7.42	117.58	124.56
43	2	3867	A2M	N6-C6-N1	-7.37	103.27	118.57
43	2	398	A2M	N6-C6-N1	-7.36	103.31	118.57
43	2	4523	A2M	N6-C6-N1	-7.34	103.34	118.57
43	2	1326	A2M	N6-C6-N1	-7.28	103.47	118.57
43	2	3825	A2M	N6-C6-N1	-7.24	103.55	118.57
43	2	2363	A2M	N6-C6-N1	-7.23	103.57	118.57
43	2	2401	A2M	N6-C6-N1	-7.23	103.57	118.57
43	2	1871	A2M	N6-C6-N1	-7.20	103.64	118.57
43	2	1524	A2M	N6-C6-N1	-7.16	103.70	118.57
43	2	4083	5MU	C4-N3-C2	-6.82	118.52	127.35
43	2	2401	A2M	N3-C2-N1	-6.42	118.64	128.68
43	2	1534	A2M	N3-C2-N1	-6.38	118.70	128.68
43	2	1871	A2M	N3-C2-N1	-6.33	118.78	128.68
43	2	4690	B8K	C72-C71-N7	6.33	128.38	118.86
43	2	3825	A2M	N3-C2-N1	-6.30	118.83	128.68
43	2	1326	A2M	N3-C2-N1	-6.29	118.85	128.68
43	2	398	A2M	N3-C2-N1	-6.27	118.88	128.68
43	2	4523	A2M	N3-C2-N1	-6.26	118.89	128.68
43	2	2363	A2M	N3-C2-N1	-6.20	118.99	128.68
43	2	3867	A2M	N3-C2-N1	-6.17	119.04	128.68
43	2	4690	B8K	C5-C6-N1	6.10	121.75	110.99
43	2	3897	B8K	C72-C71-N7	6.10	128.03	118.86
43	2	1524	A2M	N3-C2-N1	-6.08	119.18	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	2	4564	M7A	N3-C2-N1	-5.97	119.26	128.60
43	2	3899	BGH	C72-C71-N7	5.97	127.83	118.86
43	2	1456	B8Q	N3-C2-N1	5.91	124.07	117.13
43	2	4185	B8W	N2-C2-N3	5.87	127.35	117.79
43	2	2380	B8W	N2-C2-N3	5.83	127.30	117.79
43	2	4472	B8W	N2-C2-N3	5.76	127.18	117.79
43	2	3899	BGH	C5-C6-N1	5.76	121.14	110.99
43	2	3897	B8K	C5-C6-N1	5.64	120.92	110.99
43	2	4472	B8W	N3-C2-N1	-5.60	119.75	127.22
43	2	237	B9B	N3-C2-N1	-5.54	119.83	127.22
43	2	1574	B9B	N3-C2-N1	-5.48	119.92	127.22
43	2	3909	OMC	O2-C2-N3	-5.43	113.49	122.33
43	2	2754	B9B	N3-C2-N1	-5.40	120.02	127.22
43	2	4415	1MA	N1-C2-N3	-5.35	119.79	126.02
44	8	14	OMU	C4-N3-C2	-5.25	119.65	126.58
43	2	4185	B8W	N3-C2-N1	-5.24	120.23	127.22
43	2	1797	E7G	C5-C6-N1	5.22	120.20	110.99
43	2	2297	E7G	C5-C6-N1	5.16	120.08	110.99
43	2	2380	B8W	N3-C2-N1	-5.15	120.35	127.22
43	2	3880	P7G	C4-C5-N7	5.10	109.36	106.67
43	2	1909	P7G	C4-C5-N7	5.10	109.36	106.67
43	2	4620	OMU	C4-N3-C2	-5.09	119.86	126.58
43	2	4550	7MG	C5-C6-N1	5.05	119.90	110.99
43	2	4564	M7A	N3-C4-N9	5.02	133.21	126.87
43	2	3899	BGH	C2-N3-C4	5.01	121.23	112.30
43	2	1456	B8Q	O2-C2-N3	-4.98	115.64	122.95
43	2	2297	E7G	C4-C5-N7	4.96	109.32	104.91
43	2	3897	B8K	C2-N3-C4	4.91	121.04	112.30
43	2	1797	E7G	C4-C5-N7	4.90	109.27	104.91
43	2	1605	7MG	C5-C6-N1	4.89	119.62	110.99
43	2	4083	5MU	C5M-C5-C6	-4.89	116.32	122.85
43	2	1456	B8Q	C31-N3-C4	4.84	121.54	114.25
43	2	4690	B8K	C2-N3-C4	4.83	120.91	112.30
43	2	2522	7MG	C5-C6-N1	4.83	119.50	110.99
43	2	2754	B9B	C2-N3-C4	4.73	120.75	115.36
43	2	237	B9B	C2-N3-C4	4.72	120.75	115.36
43	2	4083	5MU	N3-C2-N1	4.66	121.07	114.89
43	2	2786	B9H	C31-N3-C2	4.63	123.00	117.21
43	2	2297	E7G	C2-N3-C4	4.55	120.41	112.30
43	2	1797	E7G	C2-N3-C4	4.51	120.33	112.30
43	2	4690	B8K	C4-C5-N7	4.48	108.89	104.91
43	2	2754	B9B	N2-C2-N3	4.47	125.08	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	2	1574	B9B	C2-N3-C4	4.46	120.45	115.36
43	2	237	B9B	N2-C2-N3	4.45	125.04	117.79
43	2	4550	7MG	C2-N3-C4	4.42	120.18	112.30
43	2	1456	B8Q	C6-N1-C2	-4.37	117.87	121.79
43	2	4472	B8W	C2-N3-C4	4.31	120.28	115.36
43	2	3897	B8K	C5-C4-N9	4.31	111.94	106.35
43	2	1605	7MG	C2-N3-C4	4.30	119.96	112.30
43	2	2522	7MG	C2-N3-C4	4.30	119.96	112.30
43	2	1574	B9B	N2-C2-N3	4.27	124.75	117.79
43	2	3899	BGH	C5-C4-N9	4.25	111.87	106.35
43	2	1659	I4U	C5-C4-N3	-4.21	118.51	124.91
43	2	2380	B8W	C2-N3-C4	4.14	120.08	115.36
43	2	3909	OMC	O2-C2-N1	4.10	127.36	118.89
43	2	2786	B9H	C6-N1-C2	-4.10	118.12	121.79
43	2	4185	B8W	O6-C6-N1	4.09	124.70	119.03
43	2	3899	BGH	N9-C8-N7	4.05	108.76	103.33
43	2	4185	B8W	C1'-N9-C4	-4.00	119.61	126.64
43	2	4415	1MA	C5-C6-N1	4.00	119.86	113.90
43	2	4083	5MU	C5M-C5-C4	3.97	123.14	118.77
43	2	4872	2MG	CM2-N2-C2	-3.97	115.08	123.86
43	2	3899	BGH	C4-C5-N7	3.95	108.42	104.91
43	2	4185	B8W	C2-N3-C4	3.94	119.86	115.36
43	2	2380	B8W	O6-C6-N1	3.93	124.48	119.03
43	2	3897	B8K	N9-C8-N7	3.84	108.49	103.33
43	2	4690	B8K	C5-C4-N9	3.82	111.30	106.35
43	2	3897	B8K	C4-C5-N7	3.82	108.31	104.91
43	2	2297	E7G	C5-C4-N3	-3.79	120.90	128.13
43	2	1797	E7G	C5-C4-N3	-3.77	120.94	128.13
43	2	4472	B8W	C1'-N9-C4	-3.73	120.08	126.64
43	2	4550	7MG	C5-C4-N3	-3.69	121.09	128.13
43	2	4620	OMU	N3-C2-N1	3.69	119.79	114.89
43	2	4083	5MU	O4-C4-C5	-3.67	120.64	124.90
43	2	1605	7MG	C5-C4-N9	3.67	111.11	106.35
43	2	1348	P4U	C5-C4-N3	-3.67	119.33	124.91
44	8	14	OMU	N3-C2-N1	3.66	119.75	114.89
43	2	1883	OMG	C5-C6-N1	3.61	120.32	113.95
43	2	4564	M7A	C2-N3-C4	3.60	120.27	111.75
43	2	1797	E7G	C5-C4-N9	3.60	111.02	106.35
43	2	2522	7MG	C5-C4-N9	3.58	111.00	106.35
43	2	1517	2MG	C5-C6-N1	3.57	120.25	113.95
43	2	2522	7MG	C5-C4-N3	-3.57	121.33	128.13
43	2	1605	7MG	C5-C4-N3	-3.56	121.34	128.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	2	978	2MG	C5-C6-N1	3.56	120.24	113.95
43	2	4690	B8K	N9-C8-N7	3.55	108.10	103.33
43	2	4870	OMG	C5-C6-N1	3.55	120.22	113.95
43	2	4637	OMG	C5-C6-N1	3.53	120.19	113.95
43	2	2424	OMG	C5-C6-N1	3.51	120.14	113.95
43	2	4550	7MG	C5-C4-N9	3.50	110.89	106.35
43	2	729	2MG	C5-C6-N1	3.48	120.10	113.95
43	2	4494	OMG	C5-C6-N1	3.47	120.07	113.95
43	2	2861	OMC	O2-C2-N3	-3.45	116.71	122.33
43	2	3899	BGH	C5-C4-N3	-3.45	121.55	128.13
43	2	2364	OMG	C5-C6-N1	3.45	120.04	113.95
43	2	1625	OMG	C5-C6-N1	3.43	120.01	113.95
43	2	4690	B8K	C6-C5-C4	-3.41	115.58	122.62
43	2	2050	OMG	C5-C6-N1	3.40	119.96	113.95
43	2	2297	E7G	C5-C4-N9	3.40	110.76	106.35
43	2	4872	2MG	C5-C6-N1	3.40	119.96	113.95
43	2	1316	OMG	C5-C6-N1	3.39	119.94	113.95
43	2	4623	OMG	C5-C6-N1	3.38	119.92	113.95
43	2	2773	OMG	C5-C6-N1	3.36	119.89	113.95
43	2	1522	OMG	C5-C6-N1	3.35	119.87	113.95
43	2	4620	OMU	C5-C4-N3	3.35	119.85	114.84
43	2	373	OMG	C5-C6-N1	3.34	119.84	113.95
43	2	1909	P7G	N9-C8-N7	3.32	108.12	103.38
44	8	14	OMU	C5-C4-N3	3.32	119.80	114.84
43	2	4637	OMG	C2-N1-C6	-3.27	119.08	125.10
43	2	2050	OMG	C2-N1-C6	-3.23	119.16	125.10
43	2	2380	B8W	C1'-N9-C4	-3.21	121.01	126.64
43	2	2364	OMG	C2-N1-C6	-3.20	119.21	125.10
43	2	3897	B8K	C6-C5-C4	-3.19	116.05	122.62
43	2	2380	B8W	N2-C2-N1	-3.15	112.35	117.25
43	2	3897	B8K	C5-C4-N3	-3.13	122.17	128.13
43	2	1883	OMG	C2-N1-C6	-3.11	119.37	125.10
43	2	4185	B8W	N2-C2-N1	-3.11	112.42	117.25
44	8	14	OMU	O4-C4-C5	-3.10	119.71	125.16
43	2	2861	OMC	C1'-N1-C2	3.10	125.33	118.42
43	2	4623	OMG	C2-N1-C6	-3.09	119.40	125.10
43	2	2424	OMG	C2-N1-C6	-3.08	119.42	125.10
43	2	4870	OMG	C2-N1-C6	-3.07	119.45	125.10
43	2	1316	OMG	C2-N1-C6	-3.07	119.45	125.10
43	2	4494	OMG	C2-N1-C6	-3.05	119.48	125.10
43	2	3867	A2M	C1'-N9-C4	3.05	132.00	126.64
43	2	373	OMG	C2-N1-C6	-3.04	119.50	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	2	3899	BGH	C6-C5-C4	-3.04	116.36	122.62
43	2	4690	B8K	C5-C4-N3	-3.01	122.40	128.13
43	2	4083	5MU	C6-C5-C4	3.00	120.54	118.03
43	2	3887	OMC	O2-C2-N3	-2.96	117.52	122.33
43	2	1625	OMG	C2-N1-C6	-2.95	119.66	125.10
43	2	2363	A2M	C1'-N9-C4	2.94	131.81	126.64
43	2	1522	OMG	C2-N1-C6	-2.94	119.69	125.10
43	2	4483	B8T	O3'-C3'-C2'	2.93	121.31	111.82
43	2	2773	OMG	C2-N1-C6	-2.92	119.72	125.10
43	2	4564	M7A	C4-N9-C1'	-2.89	119.73	126.60
43	2	4597	UR3	C6-N1-C2	-2.89	119.20	121.79
43	2	1605	7MG	N9-C8-N7	2.89	107.50	103.38
43	2	2522	7MG	N9-C8-N7	2.87	107.49	103.38
43	2	4597	UR3	C3U-N3-C2	2.85	122.31	117.31
43	2	4620	OMU	O4-C4-C5	-2.84	120.17	125.16
43	2	3909	OMC	C4-N3-C2	2.83	124.82	120.25
43	2	4472	B8W	C2-N1-C6	2.79	120.56	116.08
44	8	14	OMU	C1'-N1-C2	2.77	122.58	117.57
43	2	2522	7MG	C4-C5-N7	2.76	109.36	105.53
43	2	2422	OMC	O2-C2-N3	-2.74	117.87	122.33
43	2	3869	OMC	O2-C2-N3	-2.74	117.88	122.33
43	2	2297	E7G	N9-C8-N7	2.74	107.29	103.38
43	2	4472	B8W	O6-C6-N1	2.72	122.81	119.03
43	2	3899	BGH	O6-C6-N1	-2.72	114.91	120.12
43	2	4415	1MA	C8-N7-C5	2.70	108.13	102.99
43	2	4472	B8W	N2-C2-N1	-2.69	113.07	117.25
43	2	3909	OMC	C5-C4-N3	-2.68	116.77	121.33
43	2	1909	P7G	C71-N7-C5	2.68	130.87	124.52
43	2	4564	M7A	C5-C4-N3	-2.67	120.35	126.62
43	2	1797	E7G	N9-C8-N7	2.67	107.19	103.38
43	2	1605	7MG	C4-C5-N7	2.66	109.23	105.53
43	2	4872	2MG	C8-N7-C5	2.66	108.05	102.99
43	2	1456	B8Q	C31-N3-C2	2.62	121.59	117.79
43	2	3909	OMC	C5-C4-N4	2.61	124.69	120.57
43	2	4690	B8K	C2-N1-C6	-2.61	120.33	125.10
43	2	4550	7MG	C4-C5-N7	2.61	109.15	105.53
43	2	1797	E7G	C2-N1-C6	-2.60	120.36	125.10
43	2	4671	B8T	C6-C5-C4	2.60	120.14	116.96
43	2	1524	A2M	C1'-N9-C4	2.59	131.20	126.64
43	2	978	2MG	C8-N7-C5	2.58	107.90	102.99
43	2	2297	E7G	C2-N1-C6	-2.56	120.42	125.10
43	2	1883	OMG	O6-C6-C5	-2.56	119.37	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	2	3880	P7G	N9-C8-N7	2.55	107.03	103.38
43	2	4550	7MG	N9-C8-N7	2.53	107.00	103.38
43	2	4550	7MG	C2-N1-C6	-2.53	120.48	125.10
43	2	4523	A2M	C2'-C3'-C4'	2.52	107.47	101.99
43	2	729	2MG	C8-N7-C5	2.51	107.78	102.99
43	2	3897	B8K	O6-C6-N1	-2.51	115.31	120.12
43	2	1517	2MG	C8-N7-C5	2.49	107.74	102.99
44	8	14	OMU	CM2-O2'-C2'	2.49	121.05	114.52
43	2	1456	B8Q	C1'-N1-C2	2.48	121.18	116.99
43	2	1605	7MG	C2-N1-C6	-2.45	120.63	125.10
43	2	4083	5MU	O4-C4-N3	-2.44	115.44	120.12
43	2	1625	OMG	C8-N7-C5	2.44	107.63	102.99
43	2	4483	B8T	O3'-C3'-C4'	2.43	118.08	111.05
43	2	3899	BGH	C2-N1-C6	-2.42	120.68	125.10
43	2	1316	OMG	C8-N7-C5	2.42	107.59	102.99
43	2	373	OMG	C8-N7-C5	2.38	107.52	102.99
43	2	4870	OMG	C8-N7-C5	2.38	107.52	102.99
43	2	4623	OMG	C8-N7-C5	2.36	107.49	102.99
43	2	3897	B8K	C2-N1-C6	-2.35	120.81	125.10
43	2	373	OMG	N2-C2-N1	2.35	121.71	116.71
43	2	2424	OMG	O6-C6-C5	-2.34	119.81	124.37
43	2	4690	B8K	O6-C6-N1	-2.34	115.64	120.12
43	2	4185	B8W	C2-N1-C6	2.34	119.83	116.08
43	2	4637	OMG	C8-N7-C5	2.33	107.43	102.99
43	2	3897	B8K	N1-C2-N3	-2.32	119.00	123.32
43	2	978	2MG	O6-C6-C5	-2.31	119.85	124.37
43	2	4690	B8K	N1-C2-N3	-2.30	119.03	123.32
43	2	3899	BGH	N1-C2-N3	-2.30	119.03	123.32
43	2	4083	5MU	O2-C2-N1	-2.29	119.74	122.79
43	2	2522	7MG	C2-N1-C6	-2.29	120.92	125.10
43	2	2861	OMC	O2-C2-N1	2.29	123.61	118.89
43	2	1625	OMG	O6-C6-C5	-2.26	119.96	124.37
43	2	2364	OMG	O6-C6-C5	-2.25	119.97	124.37
43	2	1522	OMG	C8-N7-C5	2.25	107.28	102.99
43	2	2786	B9H	O2-C2-N1	-2.23	117.49	122.72
43	2	1797	E7G	O6-C6-C5	-2.23	122.06	127.54
43	2	3909	OMC	C6-N1-C2	-2.23	116.63	120.49
43	2	4494	OMG	C8-N7-C5	2.23	107.23	102.99
43	2	4623	OMG	N2-C2-N1	2.22	121.45	116.71
43	2	2773	OMG	O6-C6-C5	-2.22	120.04	124.37
43	2	4483	B8T	C6-C5-C4	2.21	119.67	116.96
43	2	1517	2MG	O6-C6-C5	-2.21	120.06	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	2	4872	2MG	O6-C6-C5	-2.20	120.07	124.37
43	2	1659	I4U	O2-C2-N3	-2.19	118.77	122.33
43	2	3880	P7G	C71-N7-C5	2.19	129.70	124.52
43	2	1883	OMG	C8-N7-C5	2.18	107.15	102.99
43	2	4870	OMG	O6-C6-C5	-2.18	120.11	124.37
43	2	2786	B9H	O3'-C3'-C4'	2.18	117.35	111.05
43	2	1522	OMG	O6-C6-C5	-2.17	120.13	124.37
43	2	729	2MG	O6-C6-C5	-2.17	120.13	124.37
43	2	4637	OMG	O6-C6-C5	-2.16	120.14	124.37
43	2	373	OMG	O6-C6-C5	-2.16	120.15	124.37
43	2	2050	OMG	O6-C6-C5	-2.16	120.15	124.37
43	2	2050	OMG	C8-N7-C5	2.16	107.10	102.99
43	2	2050	OMG	N2-C2-N1	2.15	121.28	116.71
43	2	2380	B8W	C2-N1-C6	2.15	119.53	116.08
43	2	1316	OMG	N2-C2-N1	2.14	121.26	116.71
43	2	2773	OMG	C8-N7-C5	2.13	107.04	102.99
43	2	2422	OMC	C1'-N1-C2	2.13	123.17	118.42
43	2	3909	OMC	C1'-N1-C2	2.12	123.16	118.42
43	2	4494	OMG	O6-C6-C5	-2.12	120.23	124.37
43	2	2297	E7G	O6-C6-C5	-2.12	122.33	127.54
43	2	4523	A2M	C3'-C2'-C1'	2.10	106.84	102.89
43	2	2364	OMG	C8-N7-C5	2.09	106.97	102.99
43	2	1316	OMG	O6-C6-C5	-2.08	120.32	124.37
43	2	3825	A2M	C1'-N9-C4	2.07	130.28	126.64
43	2	4623	OMG	O6-C6-C5	-2.07	120.33	124.37
43	2	2297	E7G	C6-C5-C4	-2.05	118.40	122.62
43	2	1797	E7G	C6-C5-C4	-2.04	118.42	122.62
43	2	237	B9B	C61-O6-C6	-2.03	113.71	117.51
43	2	4564	M7A	C71-N7-C5	-2.03	116.21	124.01
43	2	4550	7MG	O6-C6-C5	-2.03	122.56	127.54
43	2	2424	OMG	C8-N7-C5	2.02	106.84	102.99
43	2	4550	7MG	C6-C5-C4	-2.02	118.46	122.62
43	2	2522	7MG	C6-C5-C4	-2.02	118.46	122.62
43	2	1605	7MG	C6-C5-C4	-2.02	118.46	122.62
43	2	3897	B8K	N2-C2-N1	2.02	121.01	116.71
43	2	4483	B8T	O2-C2-N3	-2.01	119.06	122.33
43	2	1522	OMG	N2-C2-N1	2.01	121.00	116.71
43	2	1605	7MG	O6-C6-C5	-2.01	122.61	127.54
43	2	4690	B8K	O6-C6-C5	-2.01	122.61	127.54

There are no chirality outliers.

All (82) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
44	8	14	OMU	C1'-C2'-O2'-CM2
43	2	237	B9B	C5-C6-O6-C61
43	2	237	B9B	N1-C6-O6-C61
43	2	237	B9B	C3'-C4'-C5'-O5'
43	2	237	B9B	O4'-C4'-C5'-O5'
43	2	398	A2M	O4'-C4'-C5'-O5'
43	2	1316	OMG	O4'-C4'-C5'-O5'
43	2	1316	OMG	C3'-C4'-C5'-O5'
43	2	1348	P4U	N3-C4-O4-C41
43	2	1574	B9B	C5-C6-O6-C61
43	2	1574	B9B	N1-C6-O6-C61
43	2	1625	OMG	C3'-C4'-C5'-O5'
43	2	1871	A2M	O4'-C4'-C5'-O5'
43	2	1871	A2M	C3'-C4'-C5'-O5'
43	2	1883	OMG	O4'-C4'-C5'-O5'
43	2	1883	OMG	C3'-C4'-C5'-O5'
43	2	2364	OMG	O4'-C4'-C5'-O5'
43	2	2380	B8W	C5-C6-O6-C61
43	2	2424	OMG	O4'-C4'-C5'-O5'
43	2	2424	OMG	C3'-C4'-C5'-O5'
43	2	2754	B9B	C5-C6-O6-C61
43	2	2754	B9B	N1-C6-O6-C61
43	2	4083	5MU	O4'-C4'-C5'-O5'
43	2	4185	B8W	C5-C6-O6-C61
43	2	4472	B8W	C5-C6-O6-C61
43	2	4472	B8W	N1-C6-O6-C61
43	2	4550	7MG	O4'-C4'-C5'-O5'
43	2	4550	7MG	C3'-C4'-C5'-O5'
43	2	4637	OMG	O4'-C4'-C5'-O5'
43	2	4637	OMG	C1'-C2'-O2'-CM2
43	2	4870	OMG	C3'-C4'-C5'-O5'
43	2	729	2MG	O4'-C4'-C5'-O5'
43	2	2364	OMG	C3'-C4'-C5'-O5'
43	2	4083	5MU	C3'-C4'-C5'-O5'
43	2	4523	A2M	O4'-C4'-C5'-O5'
43	2	4637	OMG	C3'-C4'-C5'-O5'
43	2	4870	OMG	O4'-C4'-C5'-O5'
43	2	2380	B8W	N1-C6-O6-C61
43	2	398	A2M	C3'-C4'-C5'-O5'
43	2	1625	OMG	O4'-C4'-C5'-O5'
43	2	3897	B8K	O4'-C4'-C5'-O5'
43	2	4872	2MG	O4'-C4'-C5'-O5'
43	2	4872	2MG	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
43	2	4083	5MU	C2'-C1'-N1-C6
43	2	3897	B8K	C3'-C4'-C5'-O5'
43	2	729	2MG	C3'-C4'-C5'-O5'
43	2	4523	A2M	C3'-C4'-C5'-O5'
43	2	1625	OMG	C4'-C5'-O5'-P
43	2	4083	5MU	O4'-C1'-N1-C6
43	2	2297	E7G	C72-C71-N7-C8
43	2	1517	2MG	C4'-C5'-O5'-P
43	2	4083	5MU	C4'-C5'-O5'-P
43	2	4083	5MU	C2'-C1'-N1-C2
43	2	3869	OMC	C3'-C2'-O2'-CM2
43	2	1909	P7G	O4'-C4'-C5'-O5'
43	2	3867	A2M	C3'-C4'-C5'-O5'
43	2	3867	A2M	C4'-C5'-O5'-P
43	2	4870	OMG	C4'-C5'-O5'-P
43	2	1574	B9B	O4'-C4'-C5'-O5'
43	2	4185	B8W	N1-C6-O6-C61
43	2	1909	P7G	C72-C71-N7-C8
43	2	4083	5MU	O4'-C1'-N1-C2
43	2	1534	A2M	C4'-C5'-O5'-P
43	2	373	OMG	C4'-C5'-O5'-P
43	2	2754	B9B	O6-C61-C62-C63
43	2	3887	OMC	C4'-C5'-O5'-P
43	2	1659	I4U	C42-C41-O4-C4
43	2	1659	I4U	C43-C41-O4-C4
43	2	1574	B9B	C62-C61-O6-C6
43	2	2422	OMC	O4'-C4'-C5'-O5'
43	2	2754	B9B	C4'-C5'-O5'-P
43	2	1522	OMG	O4'-C4'-C5'-O5'
43	2	3880	P7G	O4'-C4'-C5'-O5'
43	2	1574	B9B	C3'-C4'-C5'-O5'
43	2	1517	2MG	O4'-C4'-C5'-O5'
43	2	3880	P7G	C3'-C4'-C5'-O5'
43	2	3909	OMC	C2'-C1'-N1-C2
43	2	2754	B9B	C62-C61-O6-C6
43	2	1534	A2M	O4'-C4'-C5'-O5'
43	2	1909	P7G	C3'-C4'-C5'-O5'
43	2	1909	P7G	N7-C71-C72-C73
43	2	4415	1MA	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	0.98	2 (7%)	32,54,54	0.82	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	-	3/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	w	801	GTP	C5-C6	-2.70	1.41	1.47
54	w	801	GTP	C8-N7	-2.12	1.31	1.35

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

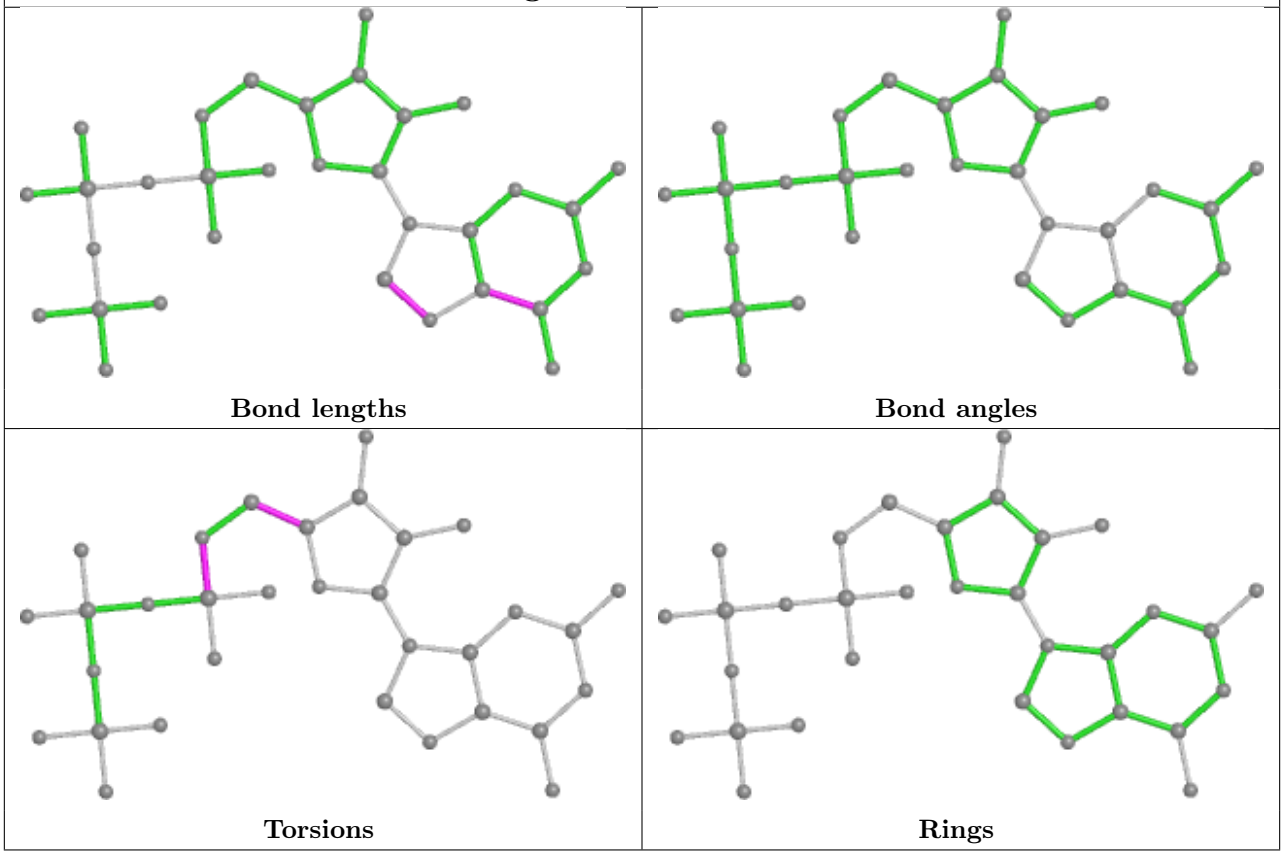
Mol	Chain	Res	Type	Atoms
54	w	801	GTP	C3'-C4'-C5'-O5'
54	w	801	GTP	O4'-C4'-C5'-O5'
54	w	801	GTP	C5'-O5'-PA-O1A

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.

Ligand GTP w 801



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.

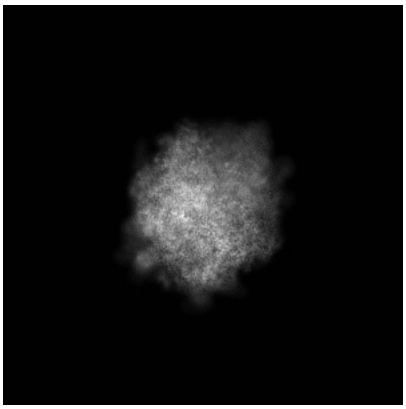
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-35672. These allow visual inspection of the internal detail of the map and identification of artifacts.

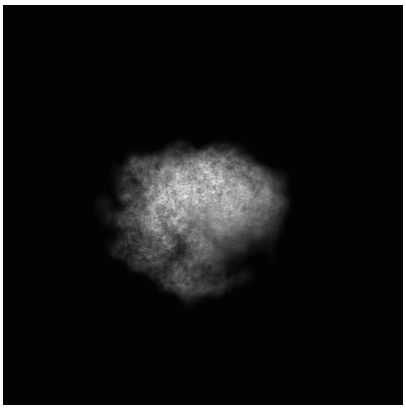
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

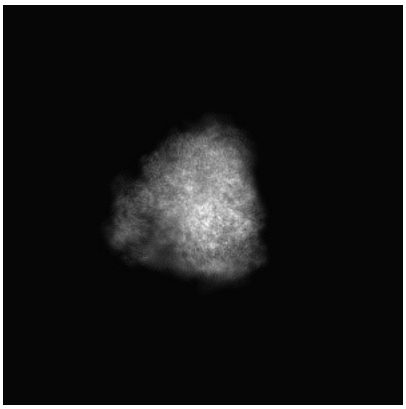
6.1.1 Primary map



X

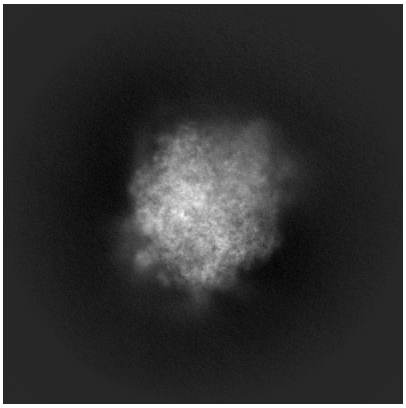


Y

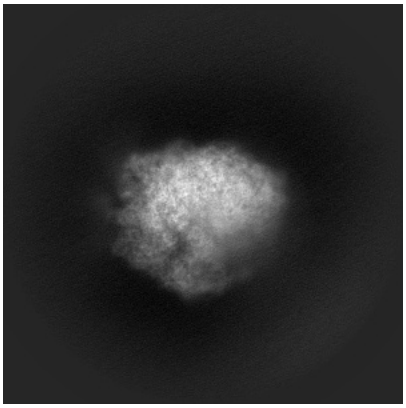


Z

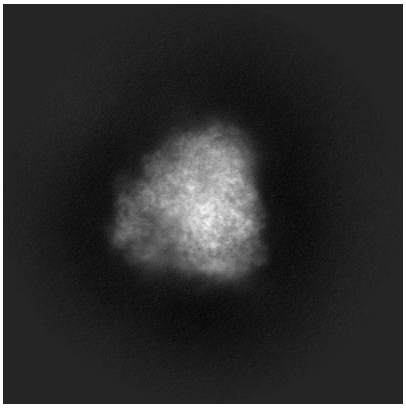
6.1.2 Raw map



X



Y

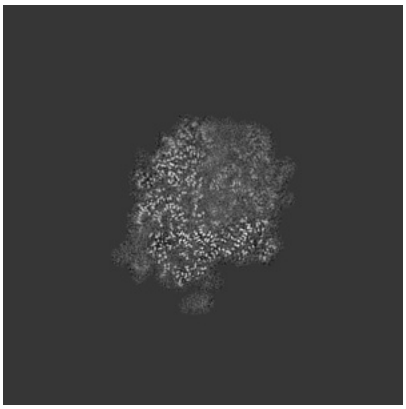


Z

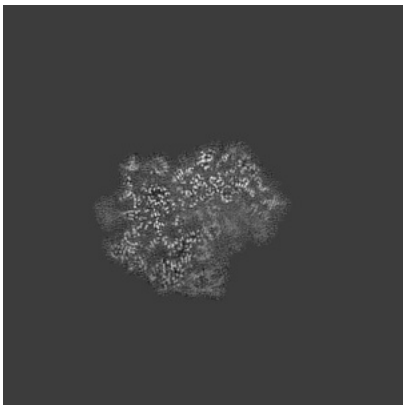
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

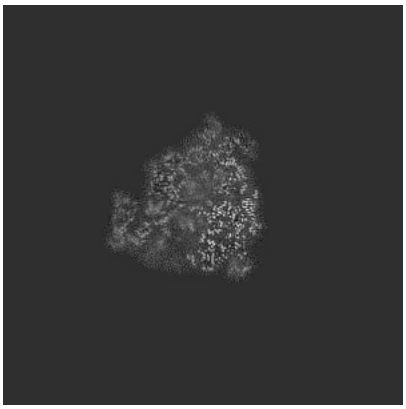
6.2.1 Primary map



X Index: 200

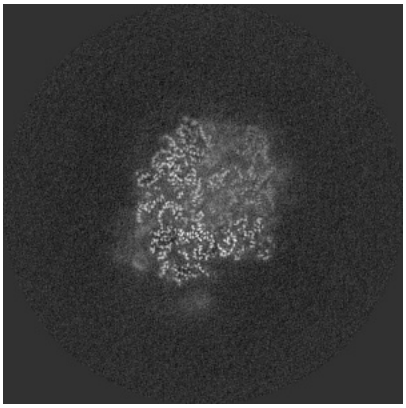


Y Index: 200

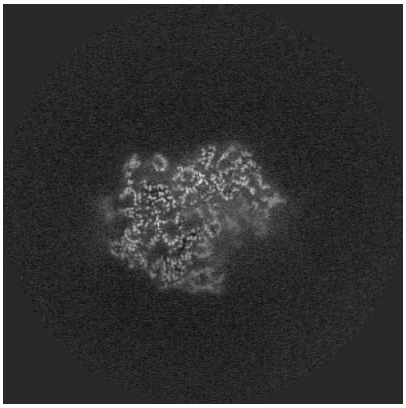


Z Index: 200

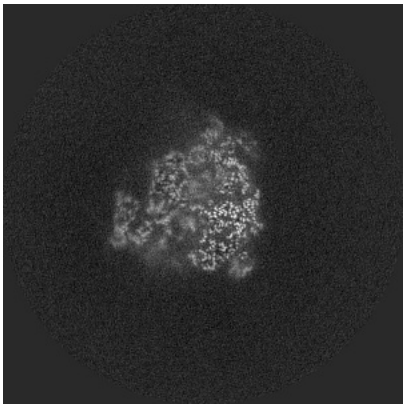
6.2.2 Raw map



X Index: 200



Y Index: 200

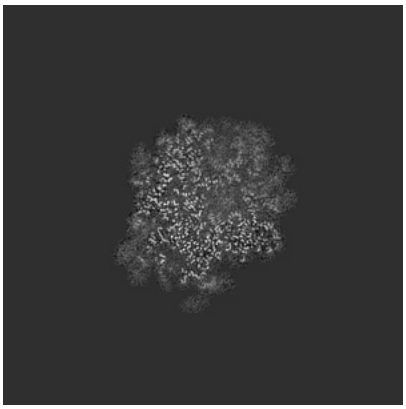


Z Index: 200

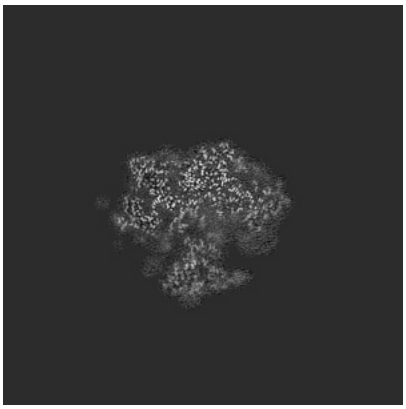
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

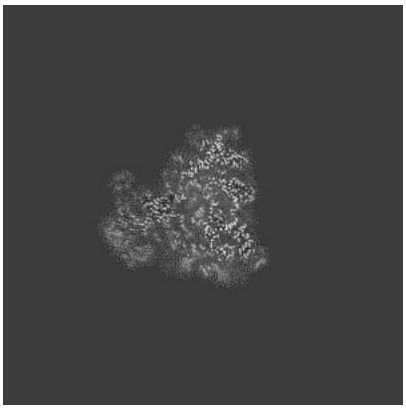
6.3.1 Primary map



X Index: 206

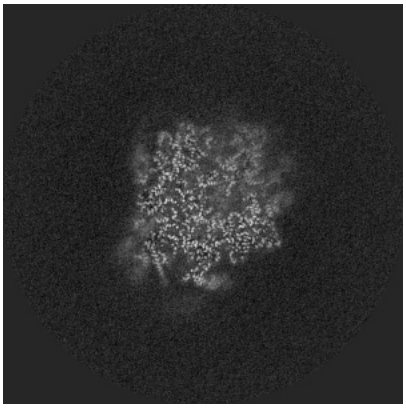


Y Index: 180

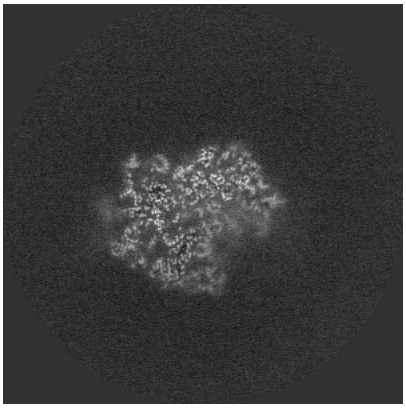


Z Index: 183

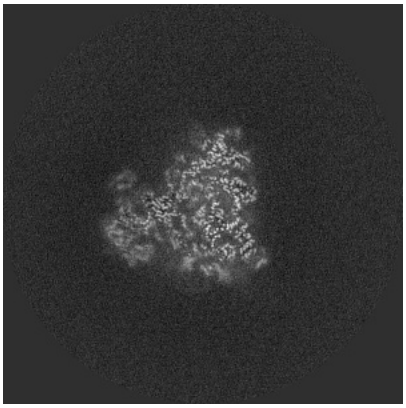
6.3.2 Raw map



X Index: 210



Y Index: 199

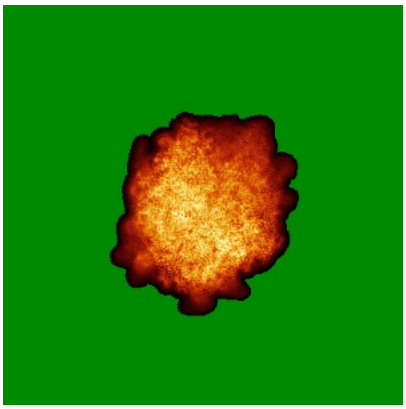


Z Index: 184

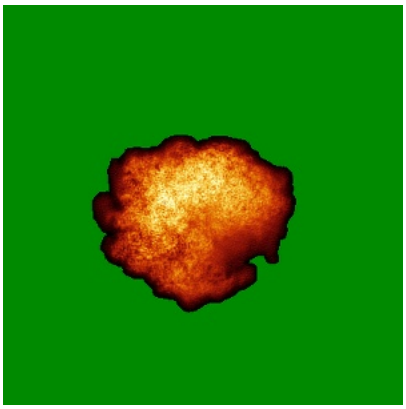
The images above show the largest variance slices of the map in three orthogonal directions.

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

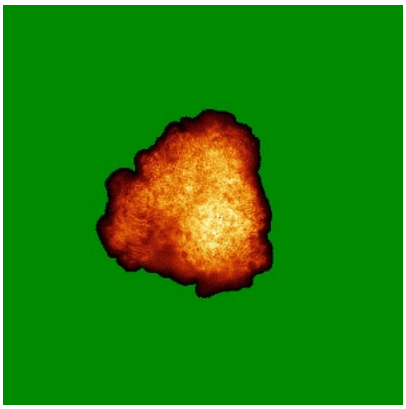
6.4.1 Primary map



X

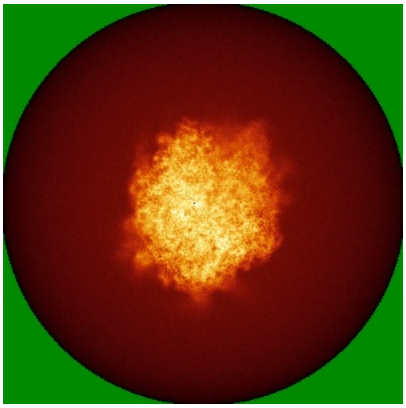


Y

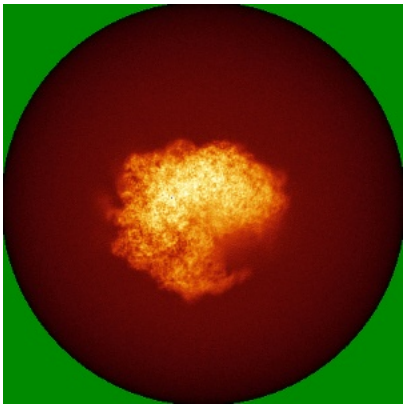


Z

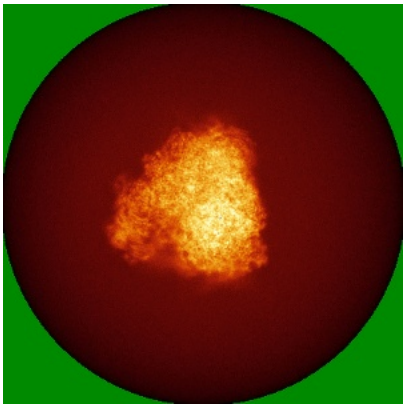
6.4.2 Raw map



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 0.038. 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.

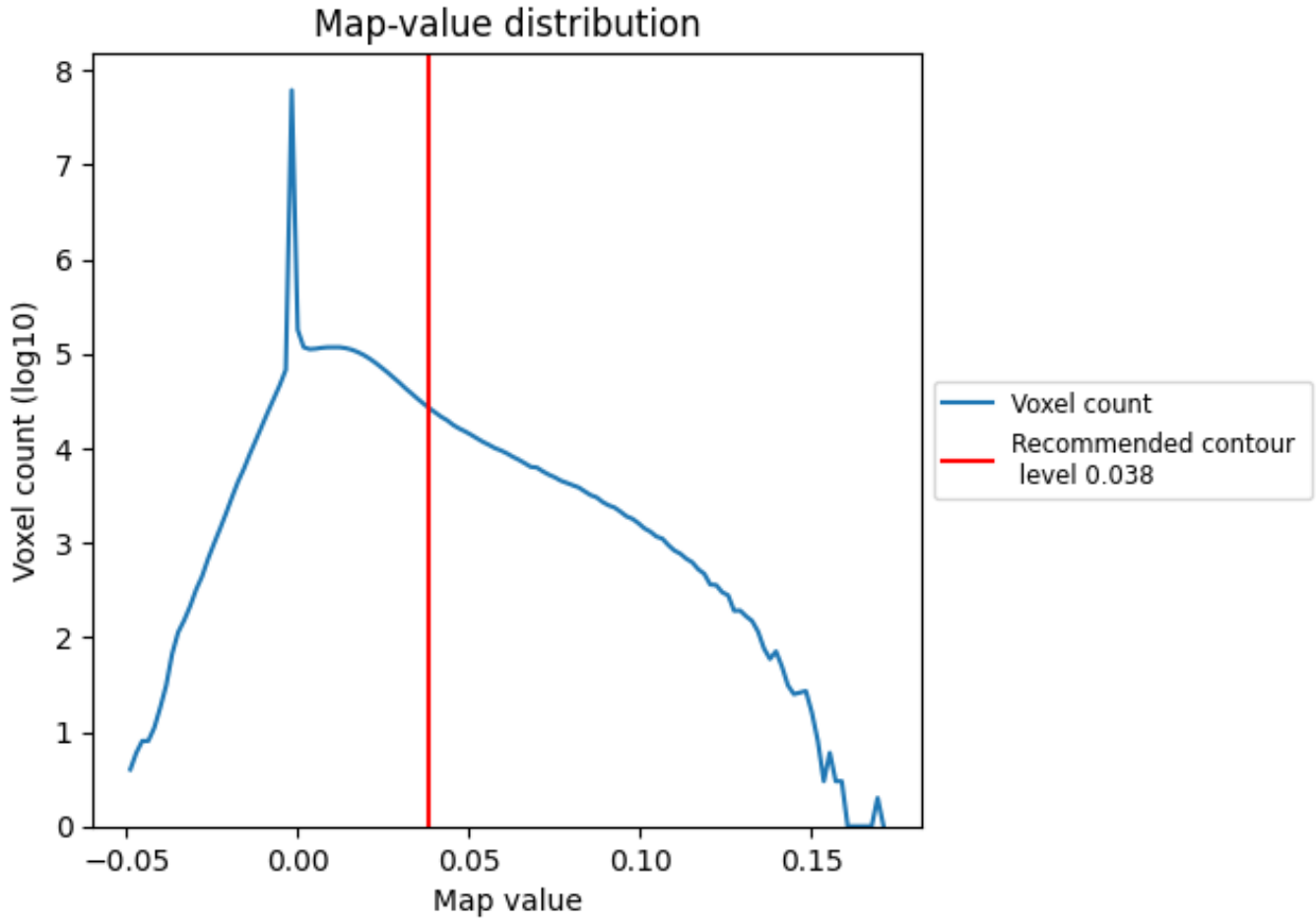
6.6 Mask visualisation (i)

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

7 Map analysis

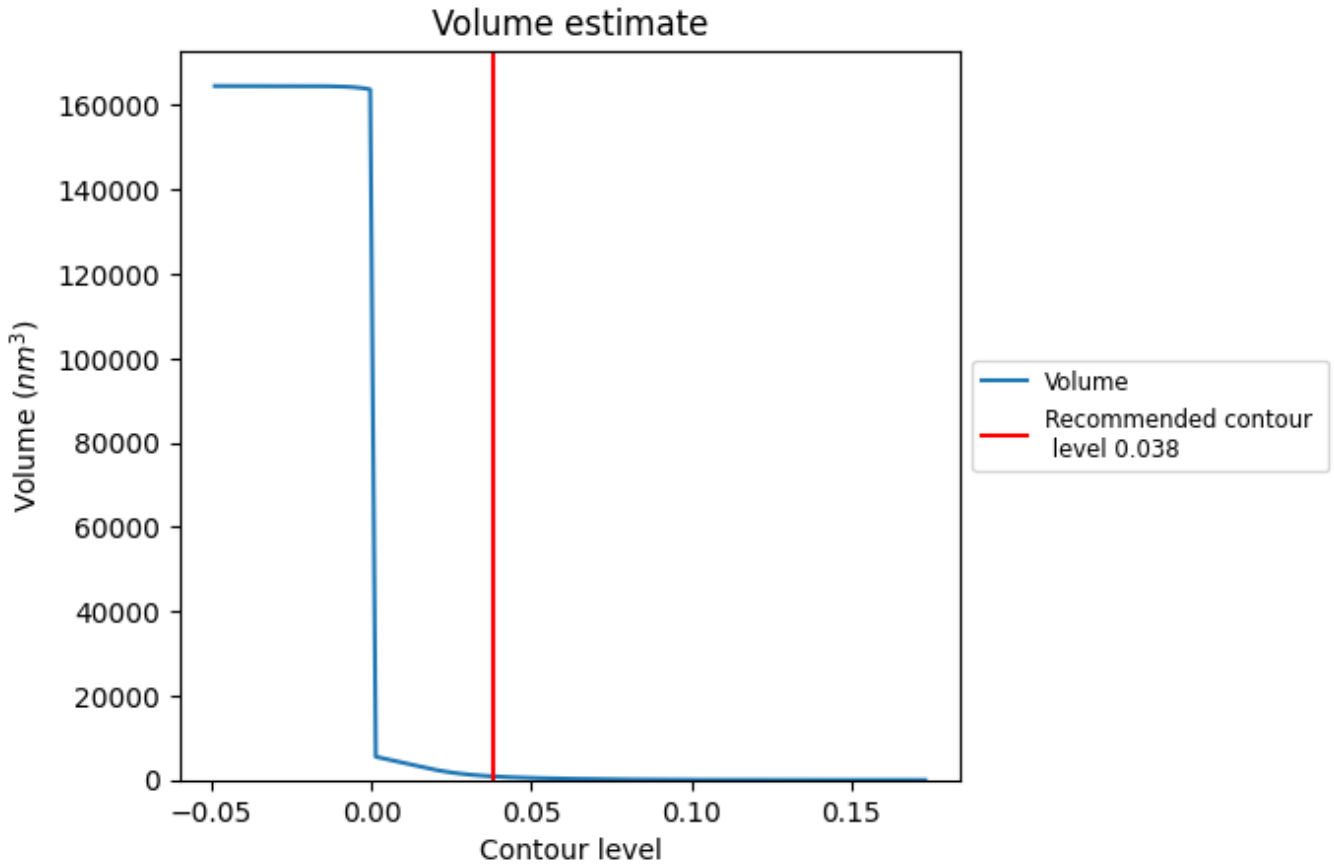
This section contains the results of statistical analysis of the map.

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.

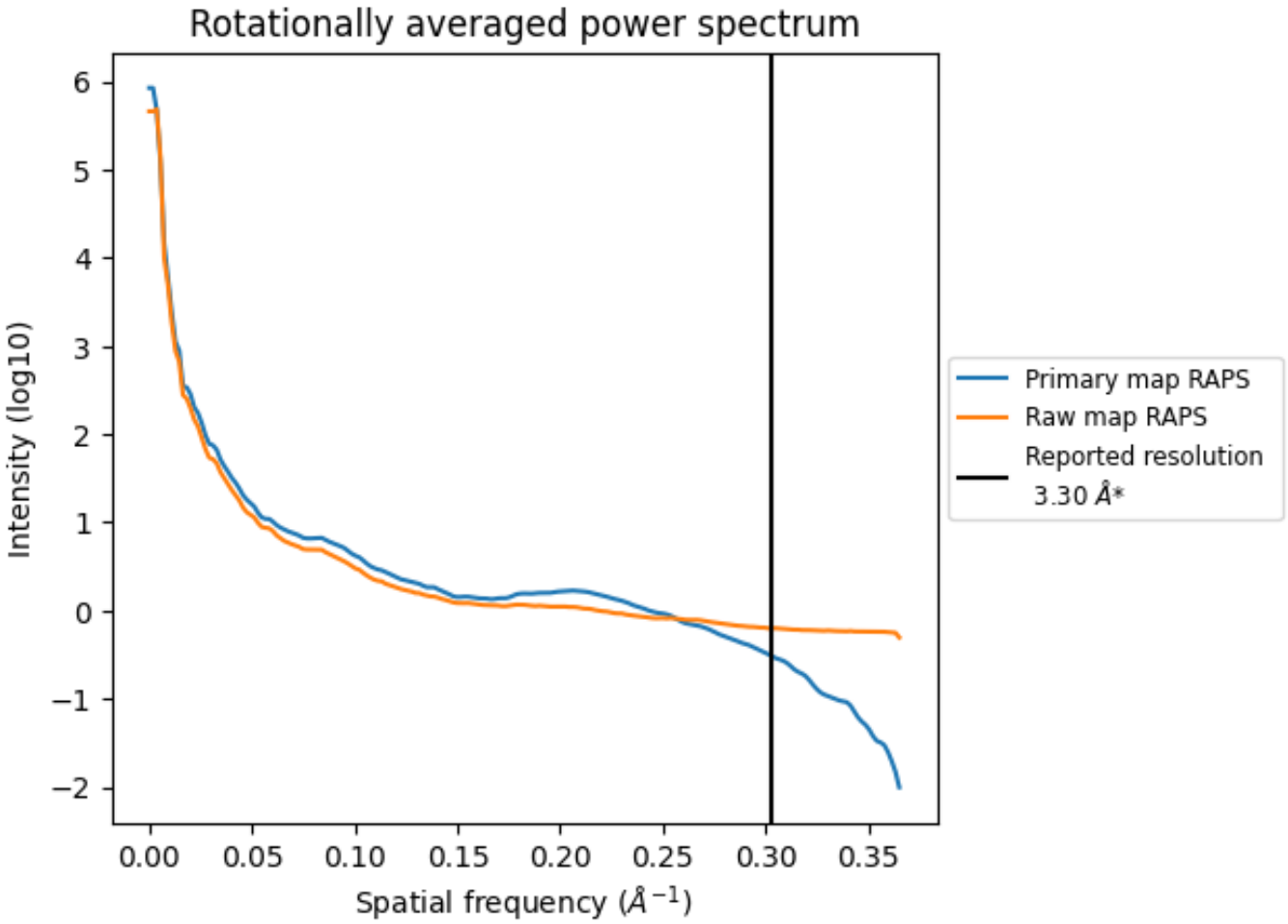
7.2 Volume estimate



The volume at the recommended contour level is 851 nm^3; this corresponds to an approximate mass of 769 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)

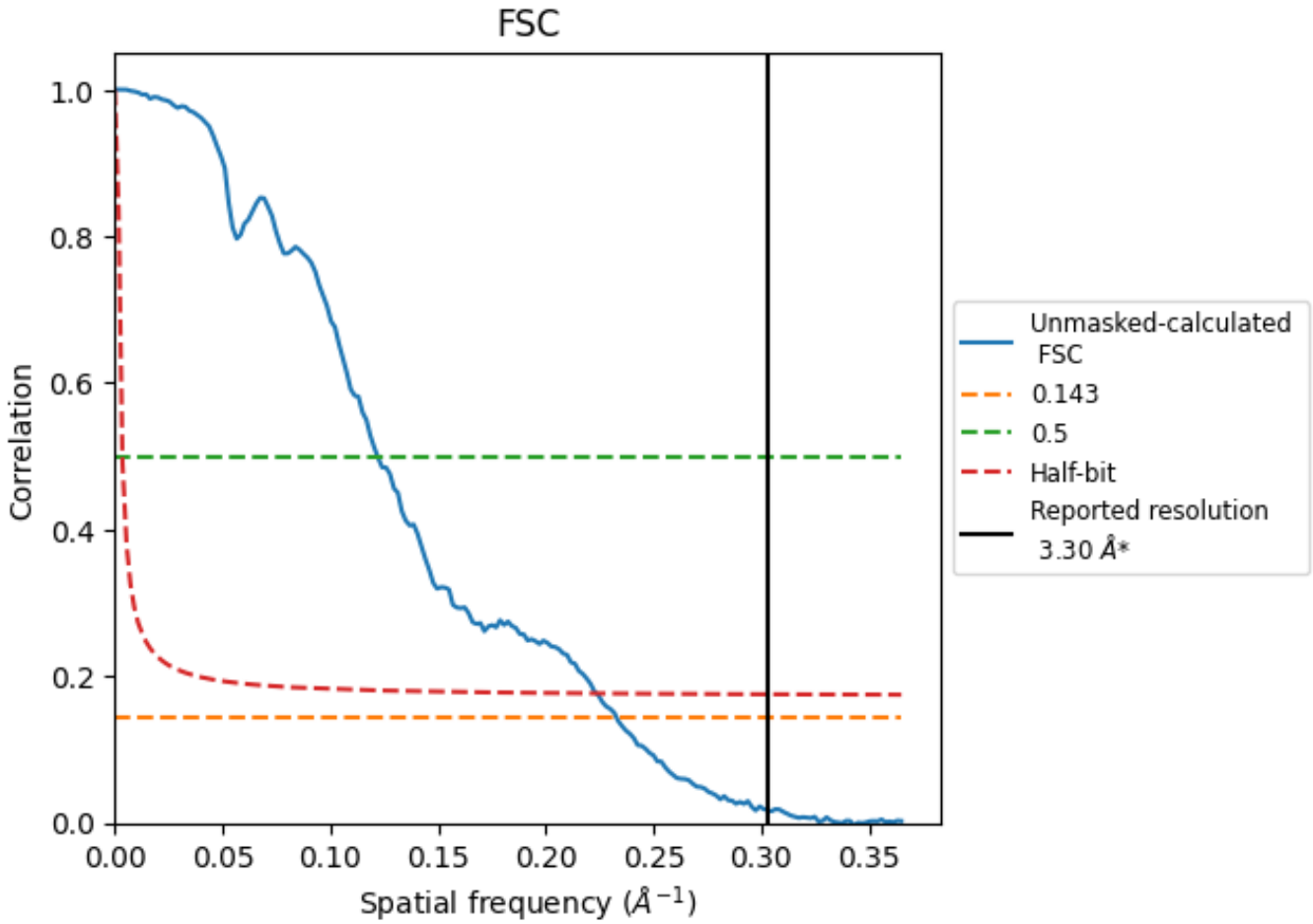


*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

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 0.303 Å^{-1}

8.2 Resolution estimates (i)

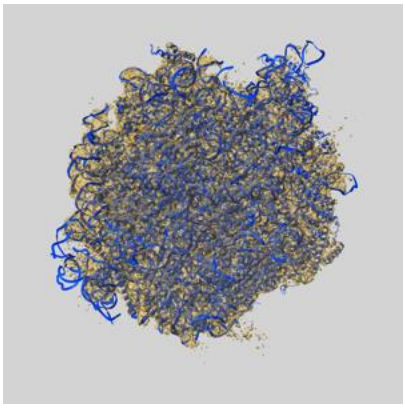
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.29	8.20	4.47

*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 4.29 differs from the reported value 3.3 by more than 10 %

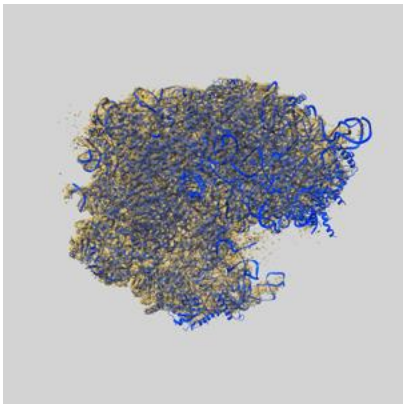
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-35672 and PDB model 8IR1. Per-residue inclusion information can be found in section 3 on page 14.

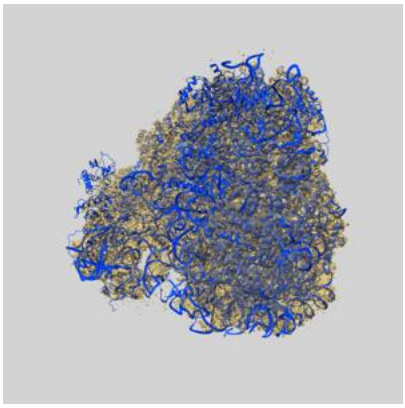
9.1 Map-model overlay



X



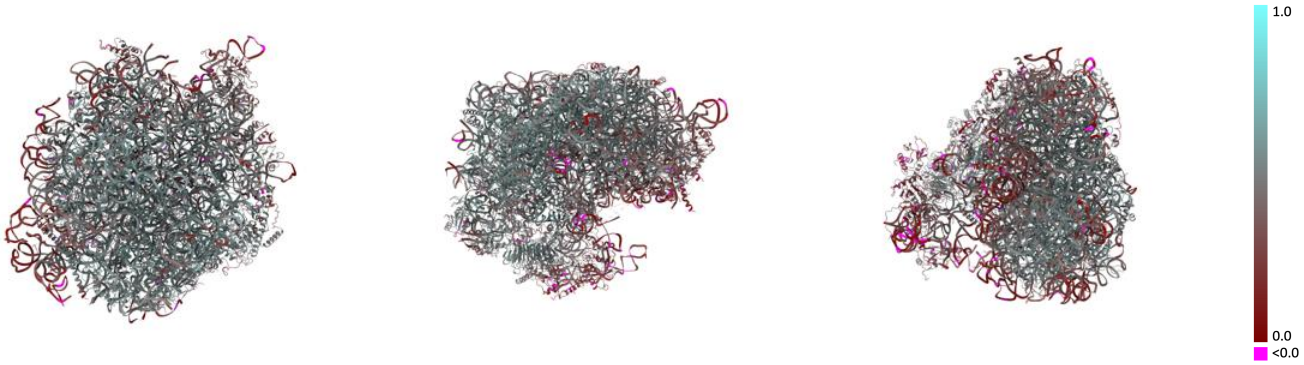
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.038 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.

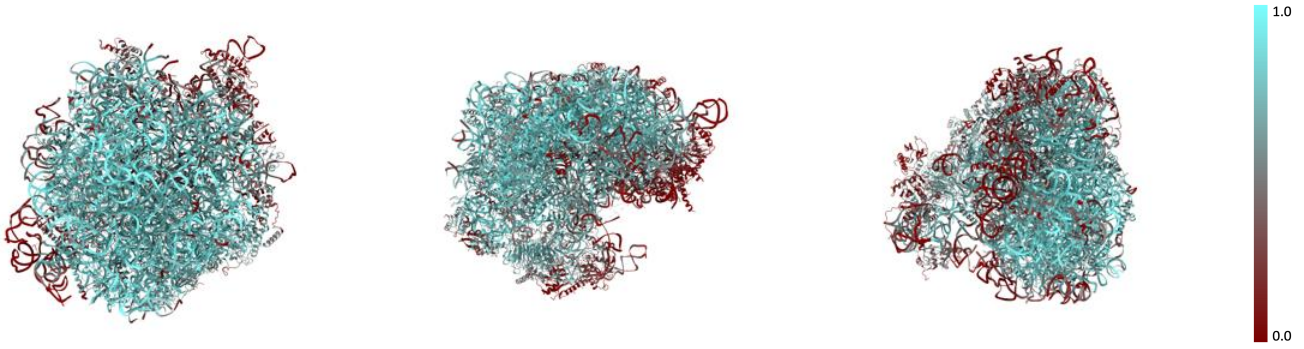
9.2 Q-score mapped to coordinate model



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.

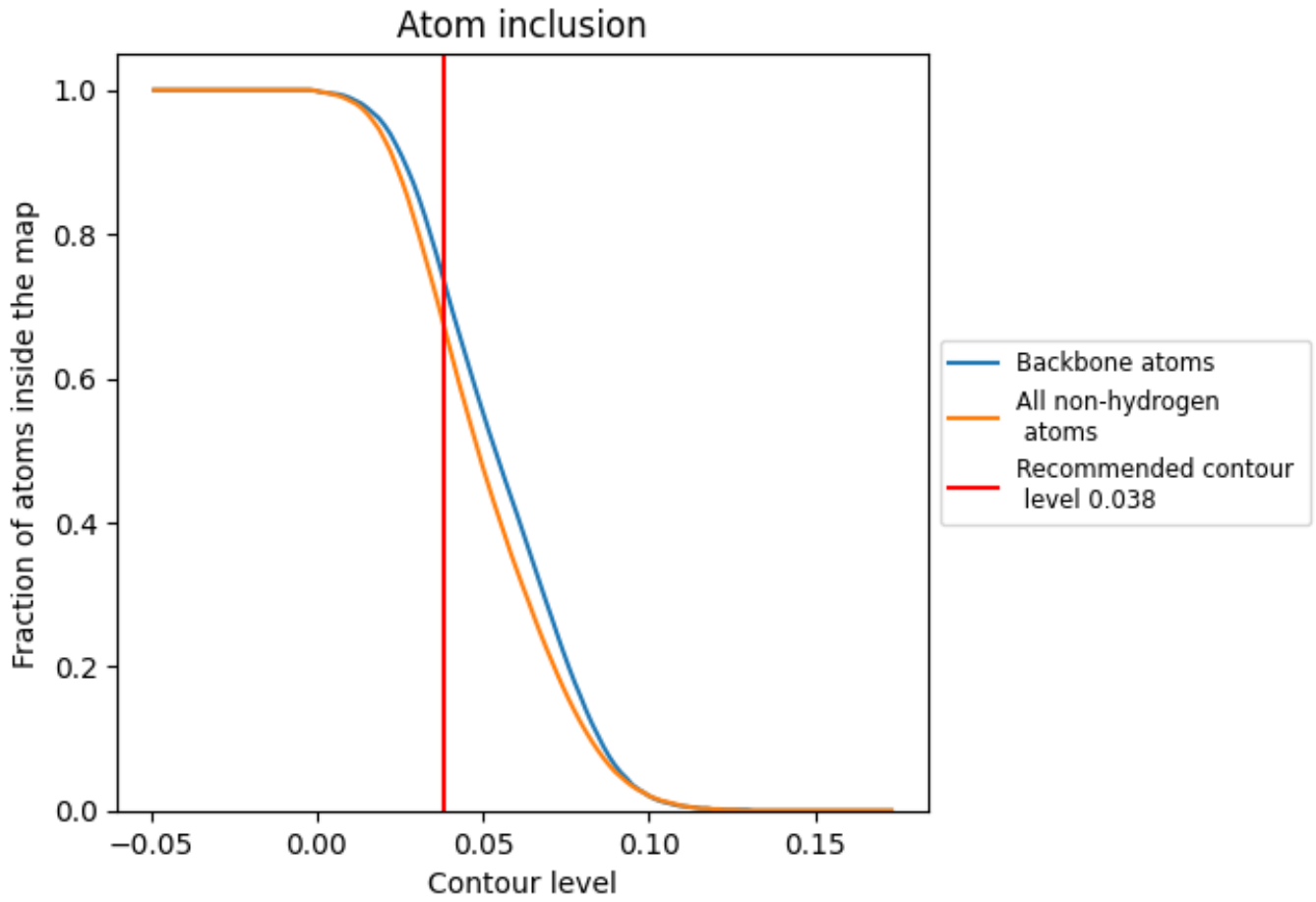
9.3 Atom inclusion mapped to coordinate model



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 (0.038).

9.4 Atom inclusion (i)



At the recommended contour level, 74% of all backbone atoms, 68% 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 (0.038) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6780	0.4490
2	0.7250	0.4370
4	0.6150	0.4570
6	0.7140	0.5030
7	0.7440	0.5220
8	0.8450	0.4840
9	0.0100	0.0940
A	0.3290	0.3340
B	0.8130	0.5420
C	0.4970	0.3990
D	0.8510	0.5470
E	0.0990	0.3640
F	0.4620	0.4560
G	0.3790	0.3730
H	0.7110	0.4960
I	0.7560	0.5350
J	0.7560	0.5240
K	0.5990	0.4350
L	0.7900	0.5260
M	0.8200	0.5270
N	0.5820	0.4550
O	0.2320	0.4160
P	0.8200	0.5460
Q	0.7030	0.4790
R	0.3680	0.3490
S	0.8080	0.5390
T	0.2760	0.2420
U	0.8460	0.5370
V	0.8480	0.5480
W	0.4800	0.2340
X	0.3120	0.3960
Y	0.7740	0.5230
Z	0.8520	0.5500
a	0.5480	0.4660
b	0.8200	0.5470

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Chain	Atom inclusion	Q-score
c	0.5630	0.4190
d	0.5690	0.4810
e	0.8310	0.5360
g	0.6150	0.4880
h	0.7980	0.5370
i	0.0770	0.3350
j	0.7600	0.5190
k	0.8770	0.5590
l	0.8600	0.5530
m	0.1920	0.3490
n	0.8820	0.5640
o	0.6720	0.4860
p	0.8000	0.5240
r	0.0380	0.2700
u	0.4680	0.3770
v	0.6160	0.4850
w	0.6200	0.4320
y	0.4340	0.3930
z	0.5940	0.4560