Full wwPDB EM Validation Report ⓘ

Nov 6, 2023 – 11:05 AM JST

PDB ID	:	8INE
EMDB ID	:	EMD-35596
Title	:	human nuclear pre-60S ribosomal particle - State G'
Authors	:	Zhang, Y.; Gao, N.
Deposited on	:	2023-03-09
Resolution	:	3.20 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

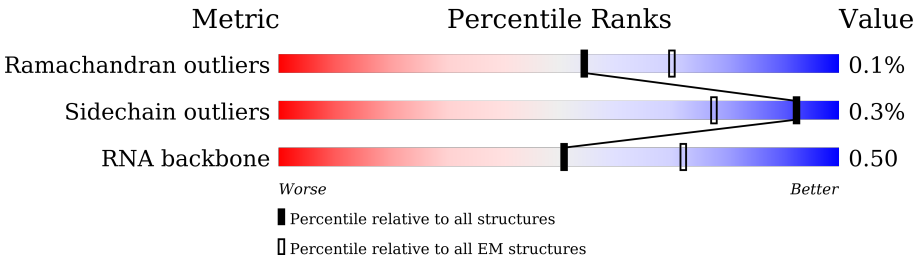
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.20 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	u	490	49% 49% 51%
2	t	293	35% 37% 62%
3	3	255	69% 88% 10%
4	2	5054	5% 44% 22% 30%
5	4	634	16% 93%
6	5	120	68% 30%
7	6	245	6% 99%
8	7	163	83% 15%

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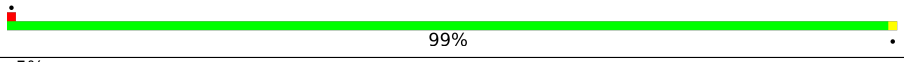
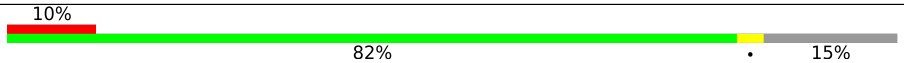
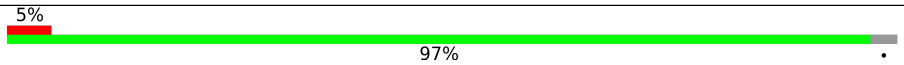
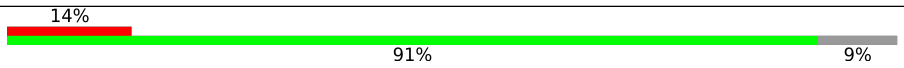
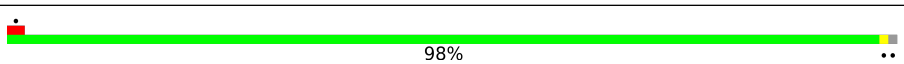
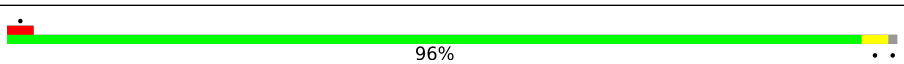
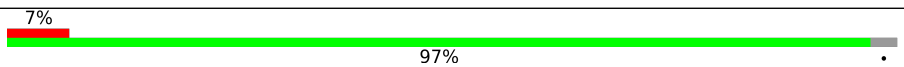
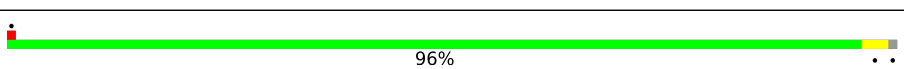
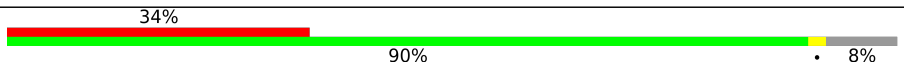
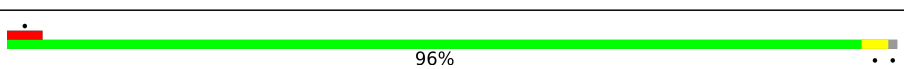
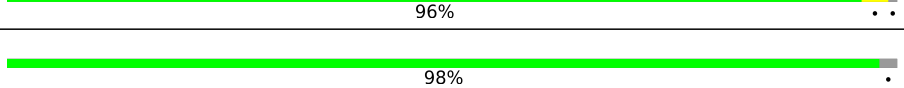
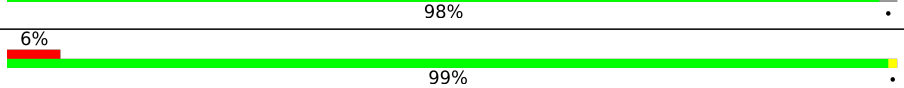
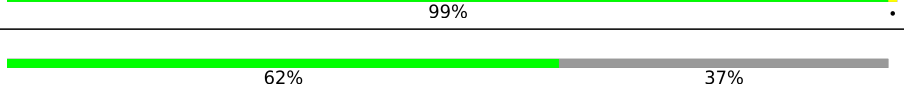
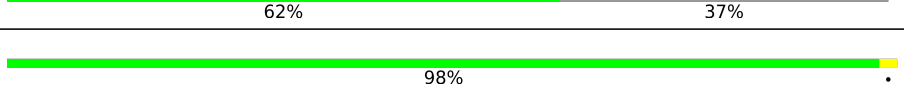
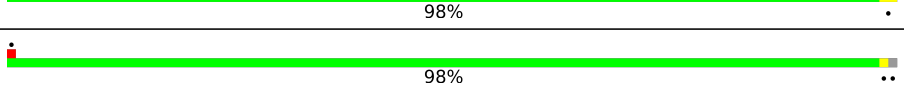
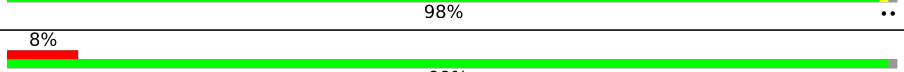
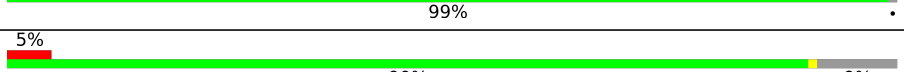
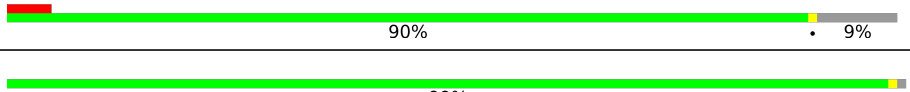
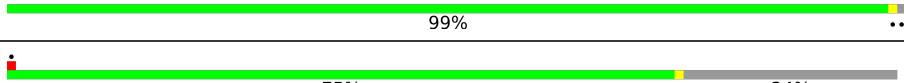
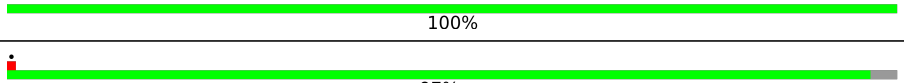
Mol	Chain	Length	Quality of chain
9	9	134	
10	B	403	
11	C	159	
12	D	427	
13	E	115	
14	F	117	
15	G	266	
16	H	123	
17	I	192	
18	K	105	
19	L	148	
20	M	97	
21	N	178	
22	O	70	
23	P	51	
24	Q	211	
25	S	215	
26	U	204	
27	V	203	
28	X	92	
29	Y	184	
30	Z	188	
31	a	196	
32	b	176	
33	c	160	

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Mol	Chain	Length	Quality of chain
34	d	128	78% 19%
35	e	140	92% 6%
36	g	156	7% 88% 8%
37	h	145	91% 8%
38	i	136	99%
39	j	125	6% 88% 11%
40	k	135	95%
41	l	137	91% 9%
42	m	257	96%
43	n	110	96%
44	o	288	8% 81% 18%
45	p	248	90% 9%
46	r	297	26% 95%
47	z	129	12% 50% 48%
48	A	731	10% 45% 54%
49	R	203	47% 74% 25%
50	J	239	82% 91% 7%
51	y	165	84% 98%
52	v	588	36% 68% 31%
53	8	156	69% 25% 5%
54	W	106	20% 94% 5%
55	T	99	6% 51% 49%
56	s	260	10% 13% 87%
57	w	478	28% 53% 46%
58	x	60	95% 95% 5%

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 159473 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 Ribosomal L1 domain-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	u	239	1924	1232	338	348	6	0	0

- Molecule 2 is a protein called MKI67 FHA domain-interacting nucleolar phosphoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	t	111	928	601	157	167	3	0	0

- Molecule 3 is a protein called 60S ribosomal protein L7-like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	3	230	1901	1229	358	310	4	0	0

- Molecule 4 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	2	3537	75949	33873	13891	24649	3536	0	0

- Molecule 5 is a protein called GTP-binding protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4	611	5016	3151	918	920	27	0	0

- Molecule 6 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	5	120	2558	1141	456	842	119	0	0

- Molecule 7 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	244	Total	C	N	O	S	0	0
			1852	1149	318	372	13		

- Molecule 8 is a protein called Probable ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	139	Total	C	N	O	S	0	0
			1184	754	229	191	10		

- Molecule 9 is a protein called Zinc finger protein 593.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	9	97	Total	C	N	O	S	0	0
			787	481	168	134	4		

- Molecule 10 is a protein called 60S ribosomal protein L3.

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

- Molecule 11 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	C	93	Total	C	N	O	S	0	0
			764	476	167	117	4		

- Molecule 12 is a protein called 60S ribosomal protein L4.

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

- Molecule 13 is a protein called 60S ribosomal protein L30.

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

- Molecule 14 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	F	113	Total	C	N	O	S	0	0
			897	560	185	146	6		

- Molecule 15 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	G	241	Total	C	N	O	S	1	0
			1935	1233	374	324	4		

- Molecule 16 is a protein called 60S ribosomal protein L35.

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

- Molecule 17 is a protein called 60S ribosomal protein L9.

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

- Molecule 18 is a protein called 60S ribosomal protein L36.

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

- Molecule 19 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	L	147	Total	C	N	O	S	0	0
			1162	736	237	186	3		

- Molecule 20 is a protein called 60S ribosomal protein L37.

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

- Molecule 21 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	N	164	Total	C	N	O	S	0	0
			1310	830	243	232	5		

- Molecule 22 is a protein called 60S ribosomal protein L38.

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

- Molecule 23 is a protein called 60S ribosomal protein L39.

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

- Molecule 24 is a protein called 60S ribosomal protein L13.

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

- Molecule 25 is a protein called 60S ribosomal protein L14.

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

- Molecule 26 is a protein called 60S ribosomal protein L15.

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

- Molecule 27 is a protein called 60S ribosomal protein L13a.

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

- Molecule 28 is a protein called 60S ribosomal protein L37a.

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

- Molecule 29 is a protein called 60S ribosomal protein L17.

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

- Molecule 30 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Z	187	Total	C	N	O	S	0	0
			1513	944	314	250	5		

- Molecule 31 is a protein called 60S ribosomal protein L19.

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

- Molecule 32 is a protein called 60S ribosomal protein L18a.

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

- Molecule 33 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	c	155	Total	C	N	O	S	0	0
			1264	801	248	210	5		

- Molecule 34 is a protein called 60S ribosomal protein L22.

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

- Molecule 35 is a protein called 60S ribosomal protein L23.

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

- Molecule 36 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	g	143	Total	C	N	O	S	0	0
			1156	740	220	195	1		

- Molecule 37 is a protein called 60S ribosomal protein L26.

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

- Molecule 38 is a protein called 60S ribosomal protein L27.

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

- Molecule 39 is a protein called 60S ribosomal protein L31.

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

- Molecule 40 is a protein called 60S ribosomal protein L32.

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

- Molecule 41 is a protein called 60S ribosomal protein L28.

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

- Molecule 42 is a protein called 60S ribosomal protein L8.

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

- Molecule 43 is a protein called 60S ribosomal protein L35a.

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

- Molecule 44 is a protein called 60S ribosomal protein L6.

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

- Molecule 45 is a protein called 60S ribosomal protein L7.

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

- Molecule 46 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	r	284	Total	C	N	O	S	0	0
			2312	1463	420	415	14		

- Molecule 47 is a protein called Protein LLP homolog.

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

- Molecule 48 is a protein called G Protein Nucleolar 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	A	333	Total	C	N	O	S	0	0
			2672	1710	457	497	8		

- Molecule 49 is a protein called Translation machinery-associated protein 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	R	153	Total	C	N	O	S	0	0
			1296	810	248	233	5		

- Molecule 50 is a protein called mRNA turnover protein 4 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	J	223	Total	C	N	O	S	0	0
			1809	1140	309	349	11		

- Molecule 51 is a protein called 60S ribosomal protein L12.

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

- Molecule 52 is a protein called Pescadillo homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	v	404	Total	C	N	O	S	0	0
			3317	2140	582	582	13		

- Molecule 53 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	8	155	Total	C	N	O	P	0	0
			3295	1472	583	1086	154		

- Molecule 54 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	W	101	Total	C	N	O	S	0	0
			827	517	170	134	6		

- Molecule 55 is a protein called Leydig cell tumor 10 kDa protein homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	T	50	Total	C	N	O	S	0	0
			393	247	82	63	1		

- Molecule 56 is a protein called Ribosome biogenesis protein NSA2 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
56	s	35	Total	C	N	O	0	0
			316	196	68	52		

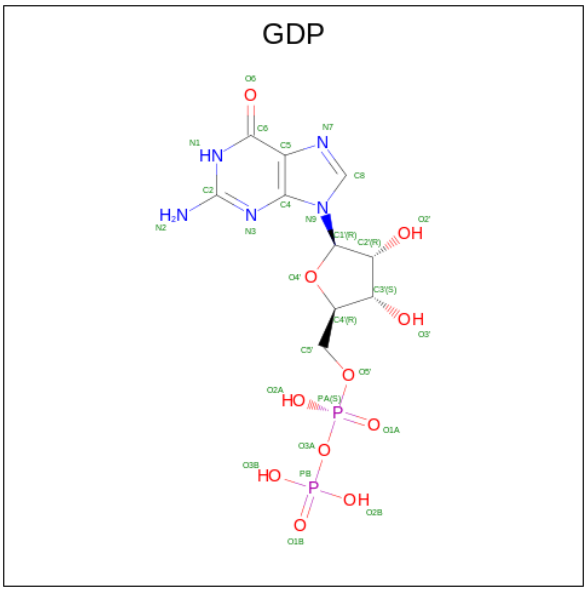
- Molecule 57 is a protein called Ribosome biogenesis protein NOP53.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	w	258	Total	C	N	O	S	0	0
			2137	1326	427	382	2		

- Molecule 58 is a RNA chain called Internal Transcribed Spacer 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	x	57	Total	C	N	O	P	0	0
			684	285	1	341	57		

- Molecule 59 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					AltConf
59	A	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 60 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
60	A	1	Total	Mg	0
			1	1	

- Molecule 61 is POTASSIUM ION (three-letter code: K) (formula: K).

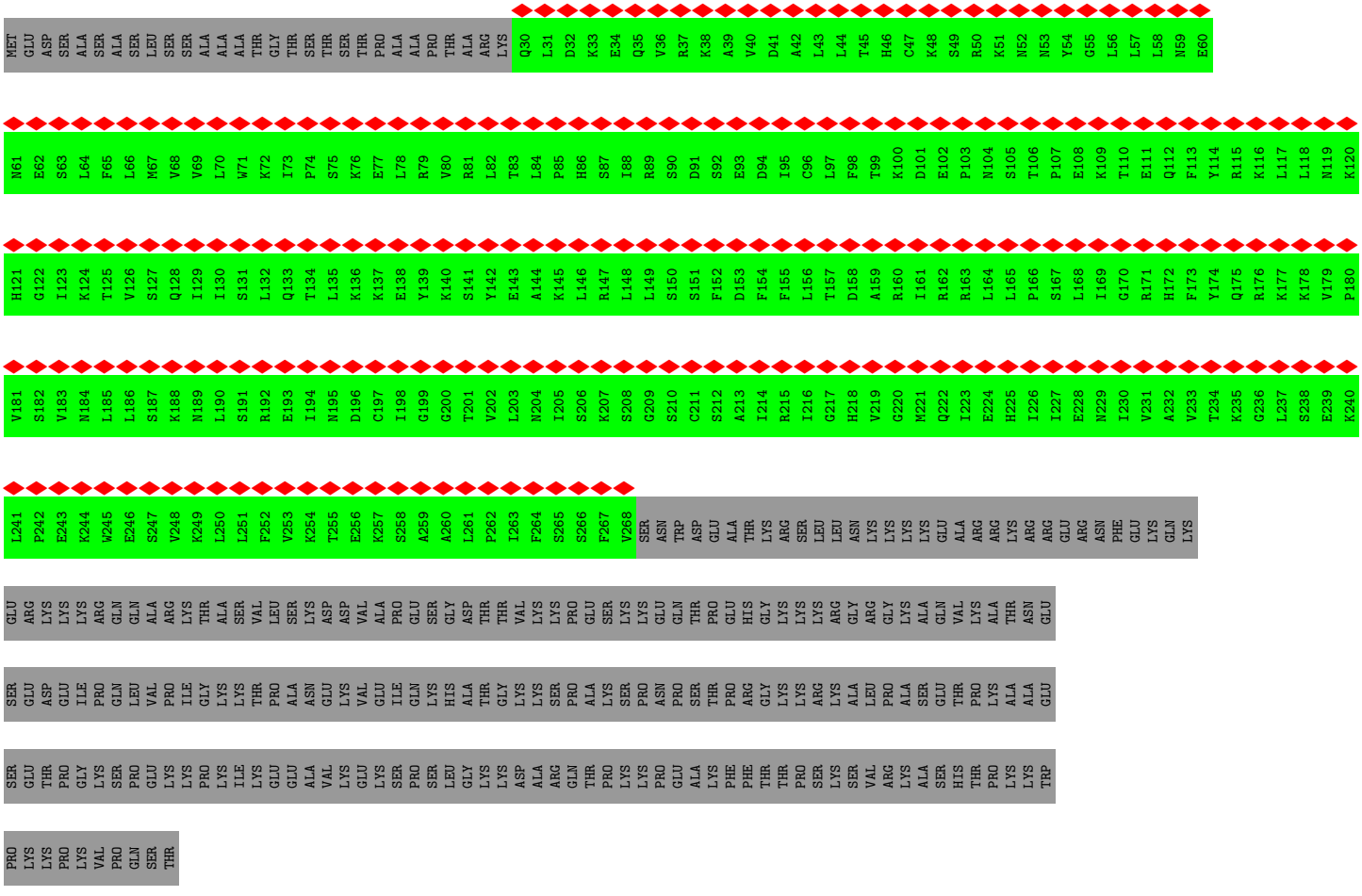
Mol	Chain	Residues	Atoms		AltConf
			Total	K	
61	A	1	1	1	0

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.

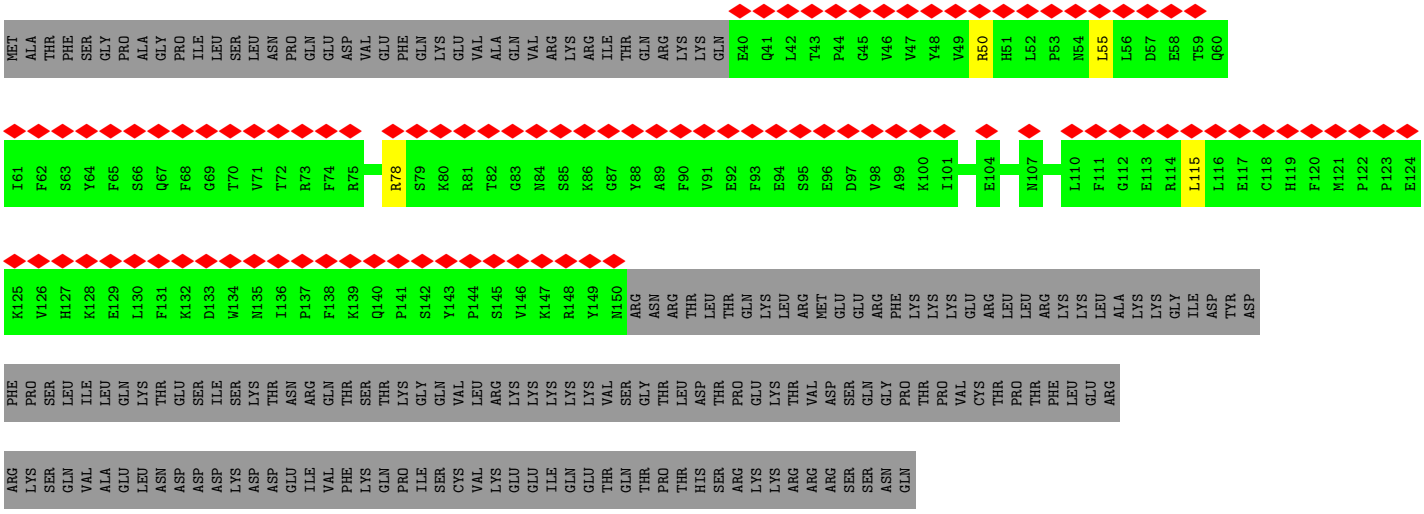
• Molecule 1: Ribosomal L1 domain-containing protein 1

Chain u:



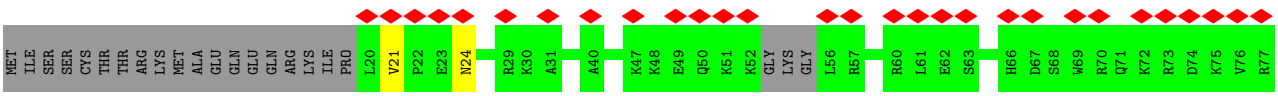
• Molecule 2: MKI67 FHA domain-interacting nucleolar phosphoprotein

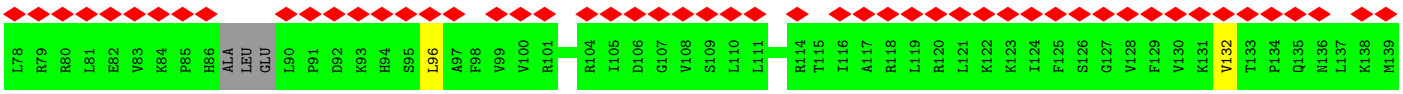
Chain t:

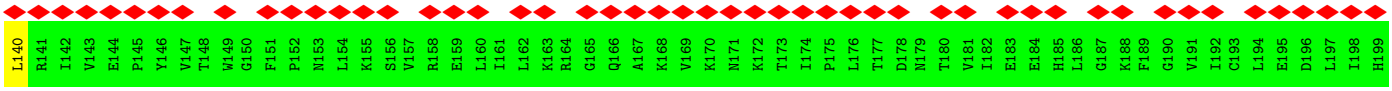


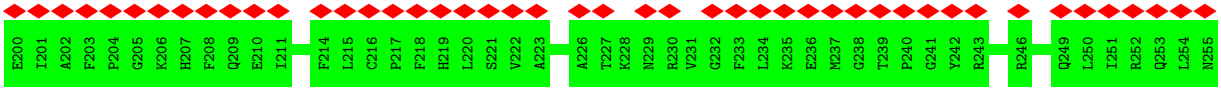
• Molecule 3: 60S ribosomal protein L7-like 1

Chain 3:



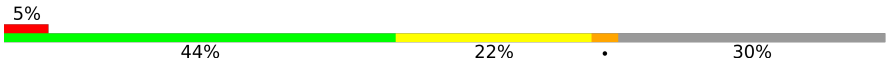


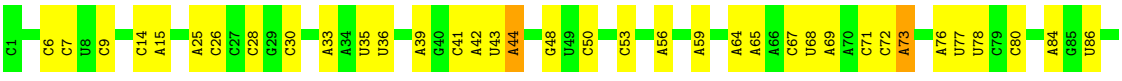


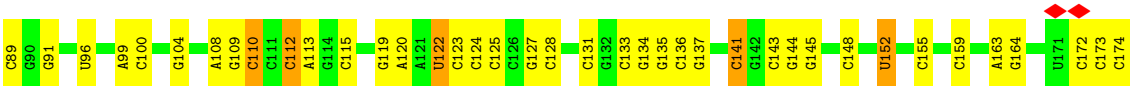


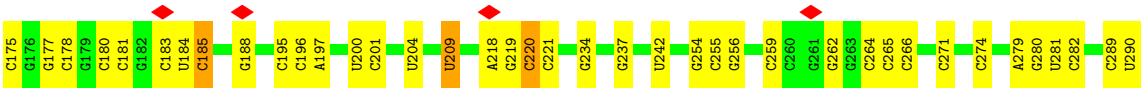
• Molecule 4: 28S rRNA

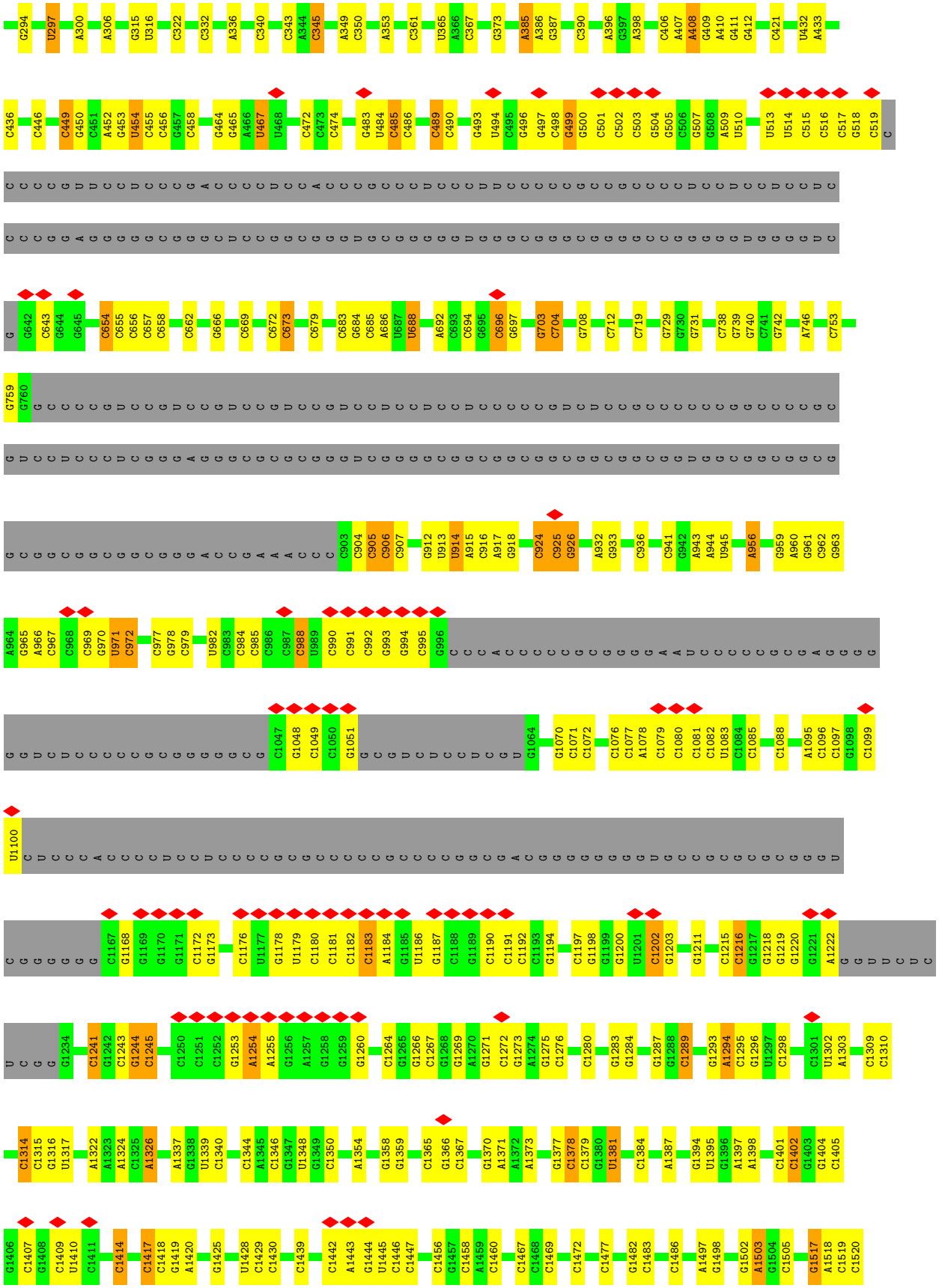
Chain 2:

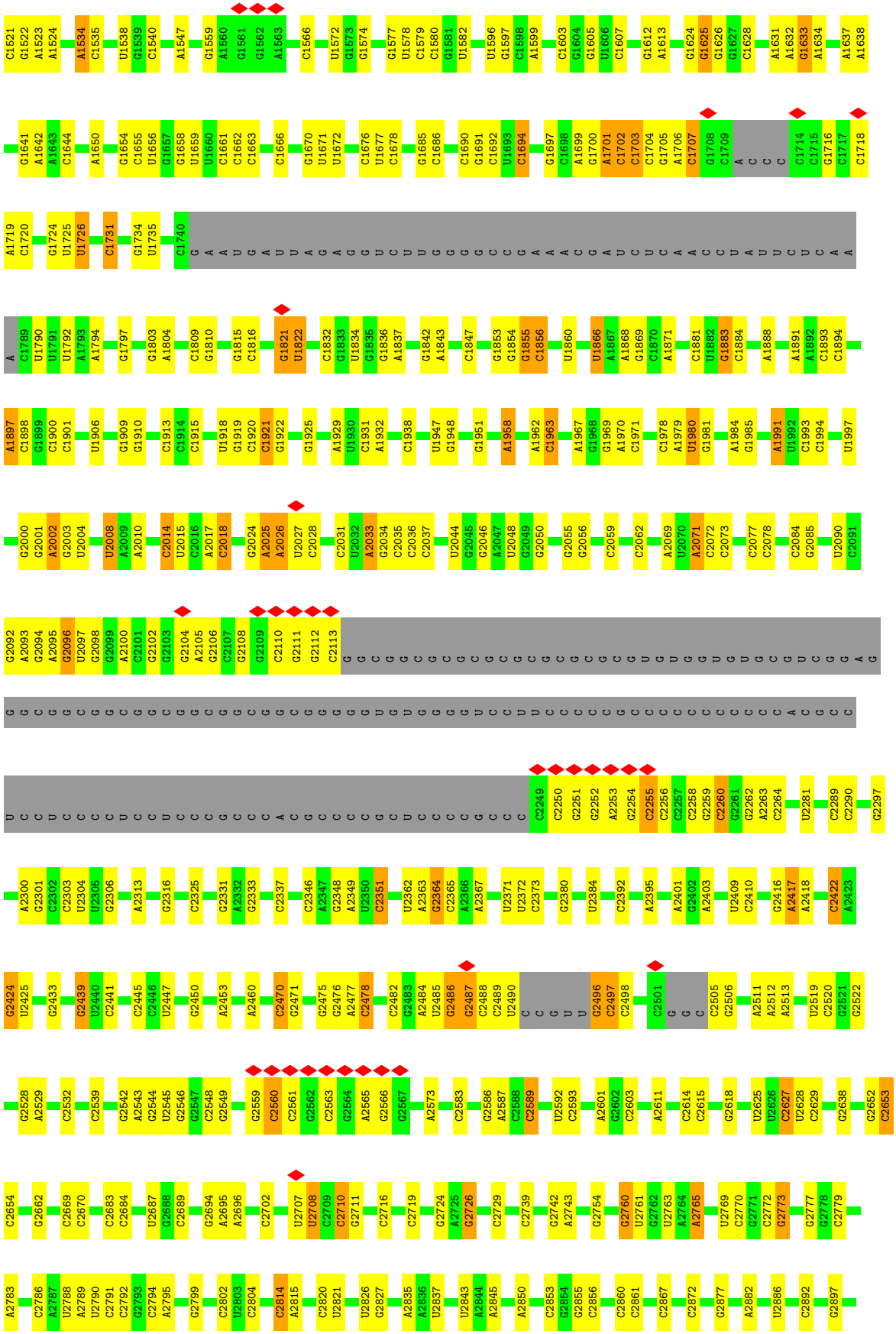


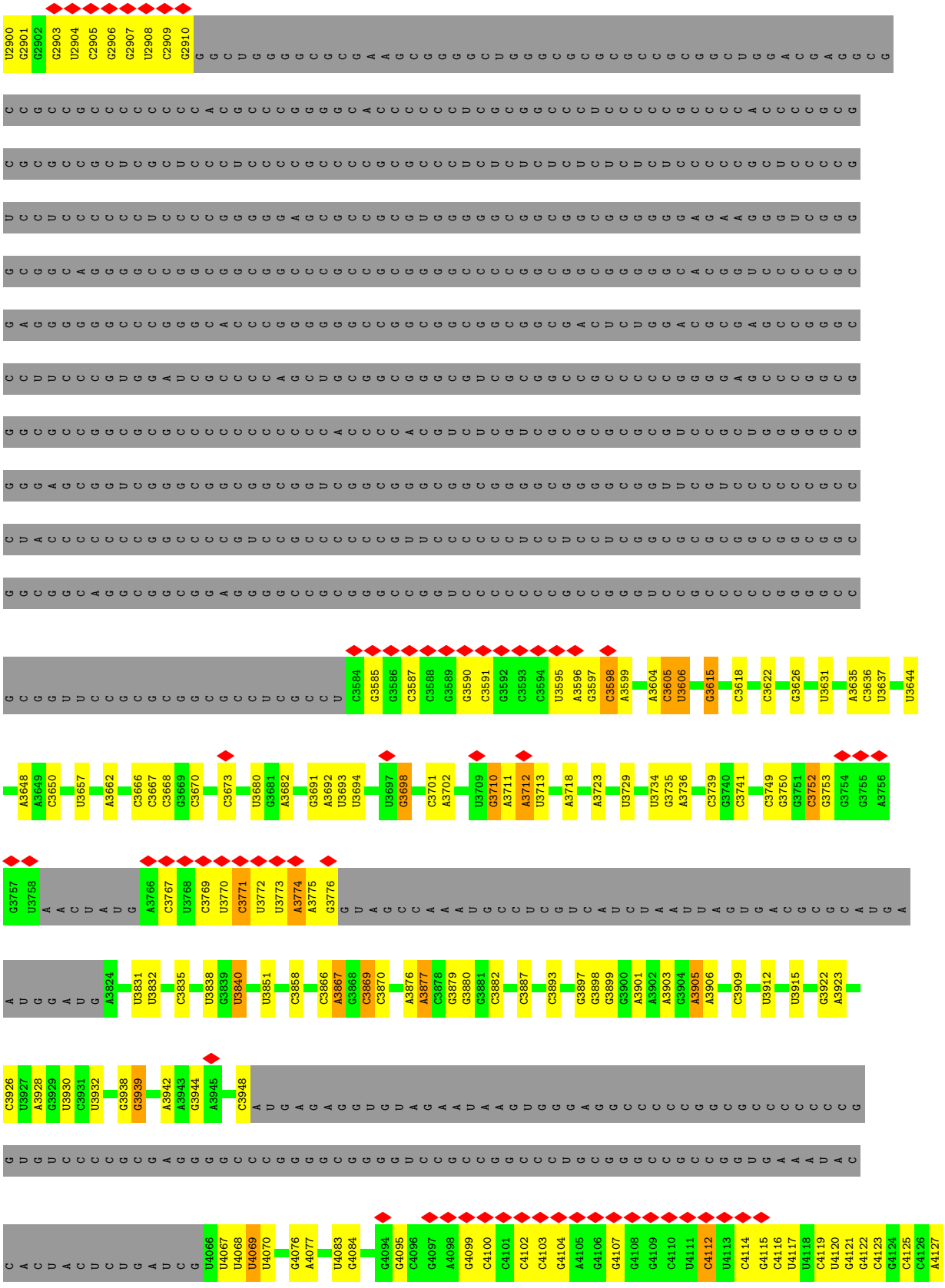


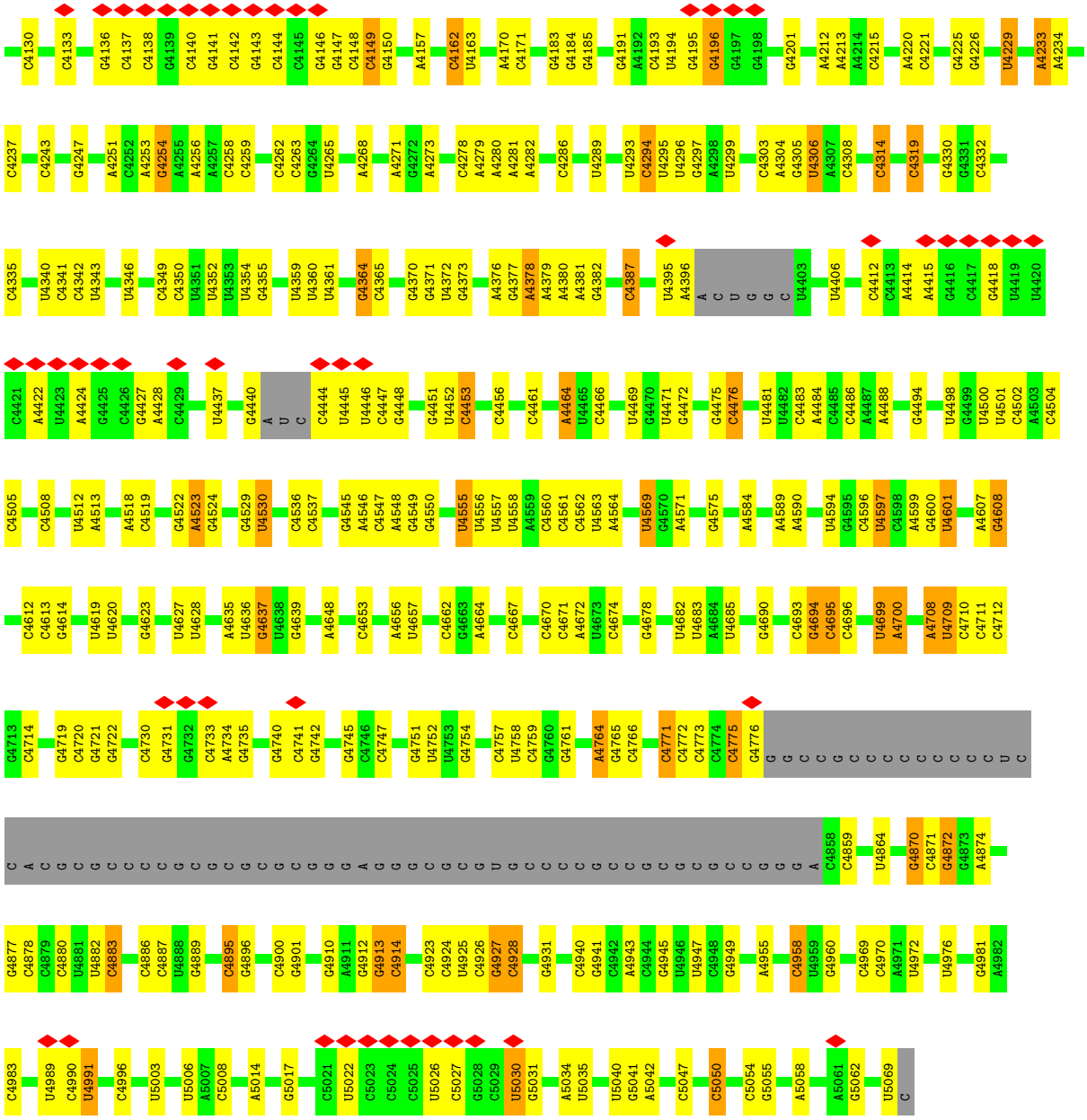






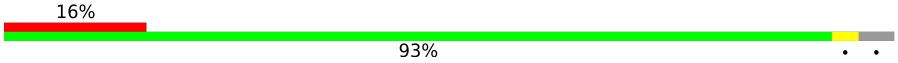


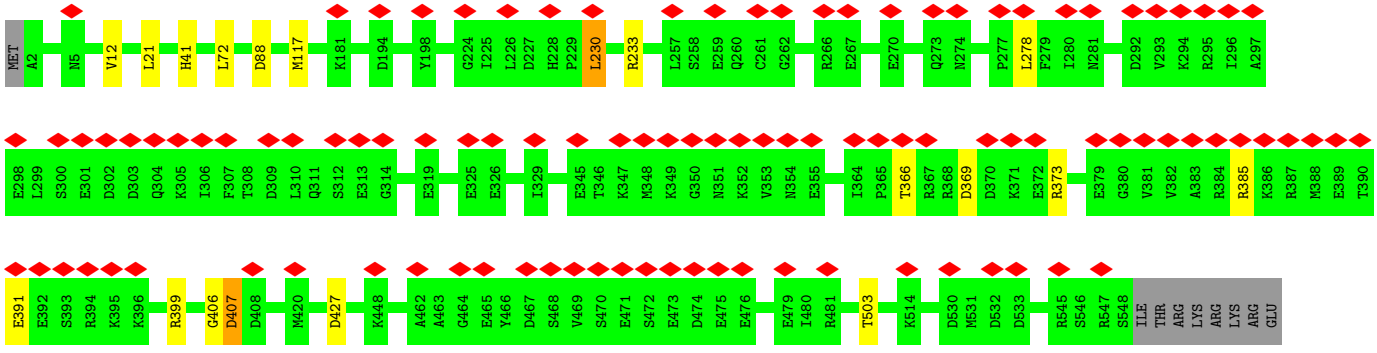


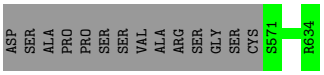


• Molecule 5: GTP-binding protein 4

Chain 4:

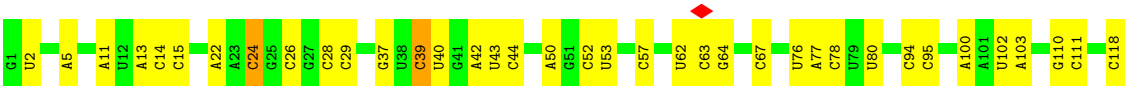






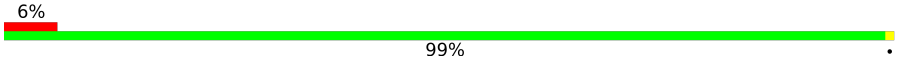
• Molecule 6: 5S rRNA

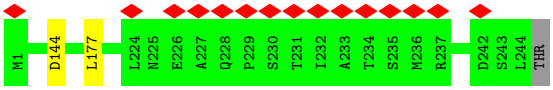
Chain 5:



• Molecule 7: Eukaryotic translation initiation factor 6

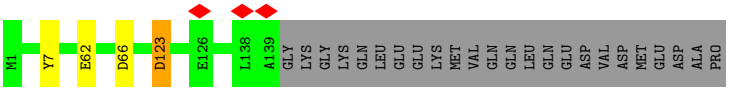
Chain 6:





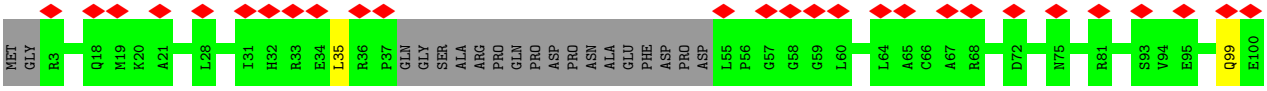
• Molecule 8: Probable ribosome biogenesis protein RLP24

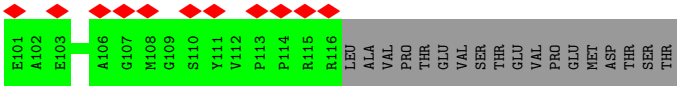
Chain 7:



• Molecule 9: Zinc finger protein 593

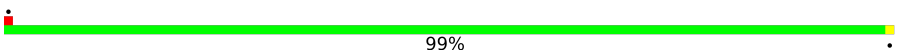
Chain 9:

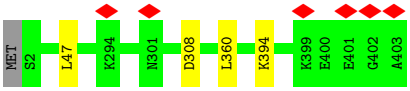




• Molecule 10: 60S ribosomal protein L3

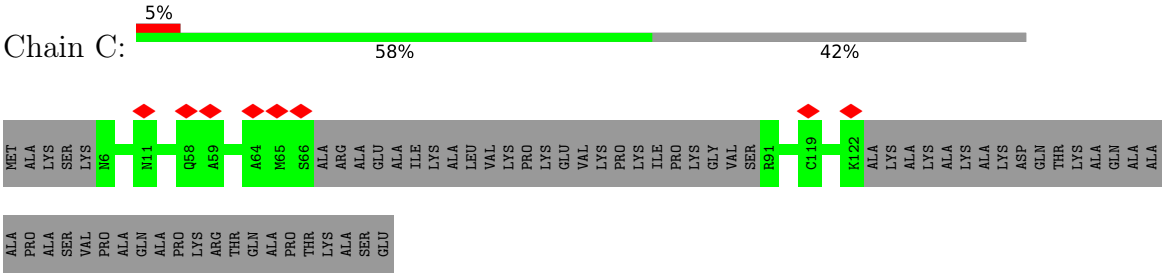
Chain B:





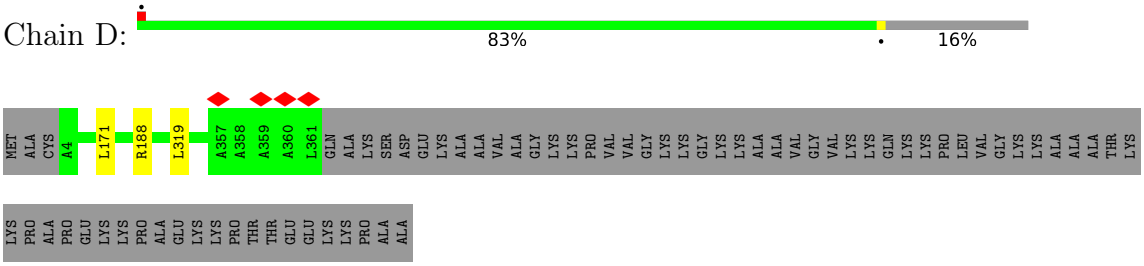
• Molecule 11: 60S ribosomal protein L29

Chain C:



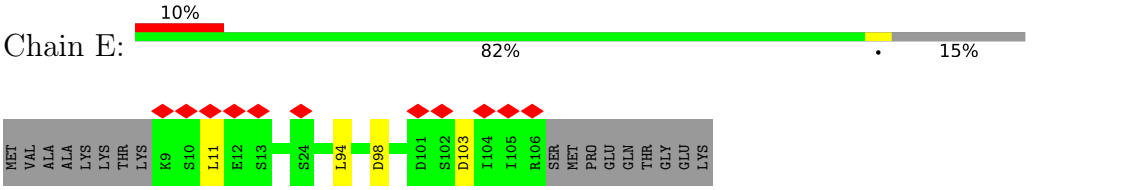
• Molecule 12: 60S ribosomal protein L4

Chain D:



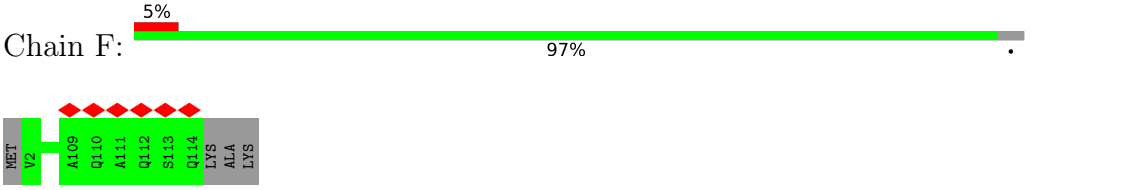
• Molecule 13: 60S ribosomal protein L30

Chain E:



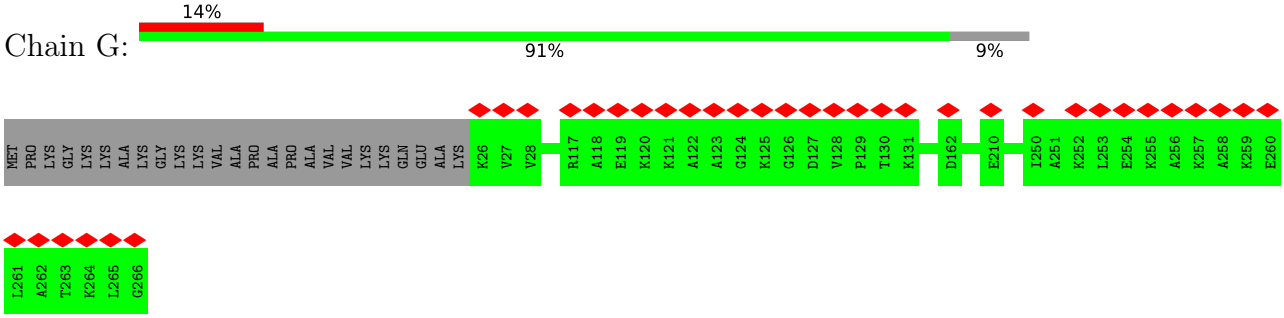
• Molecule 14: 60S ribosomal protein L34

Chain F:



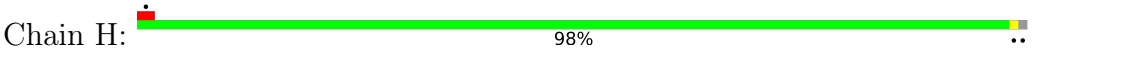
• Molecule 15: 60S ribosomal protein L7a

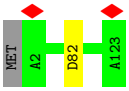
Chain G:



• Molecule 16: 60S ribosomal protein L35

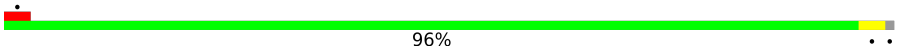
Chain H:

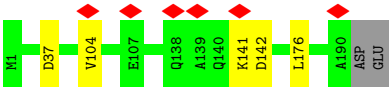




• Molecule 17: 60S ribosomal protein L9

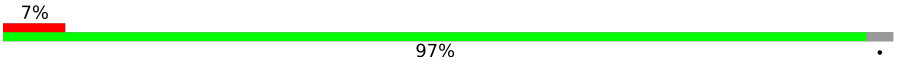
Chain I:

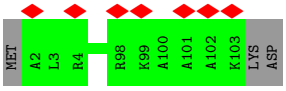




• Molecule 18: 60S ribosomal protein L36

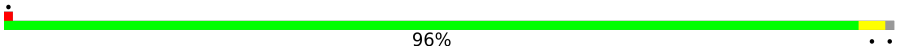
Chain K:

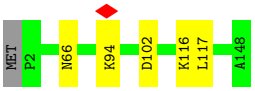




• Molecule 19: 60S ribosomal protein L27a

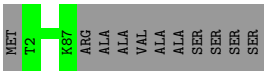
Chain L:





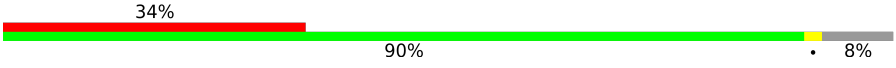
• Molecule 20: 60S ribosomal protein L37

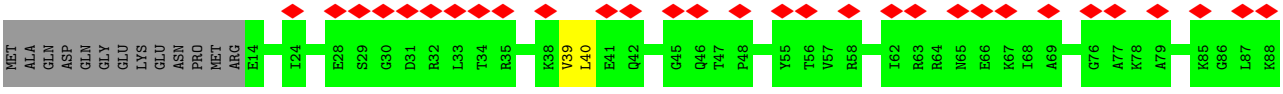
Chain M:

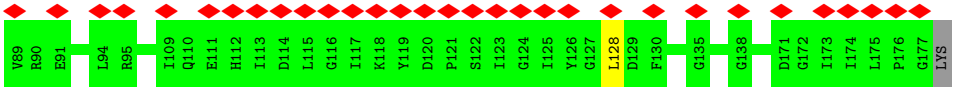


• Molecule 21: 60S ribosomal protein L11

Chain N:

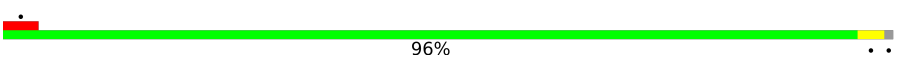


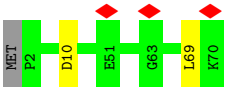




• Molecule 22: 60S ribosomal protein L38

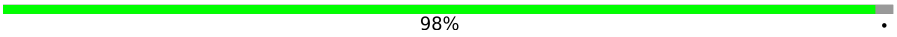
Chain O:





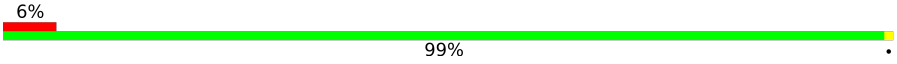
• Molecule 23: 60S ribosomal protein L39

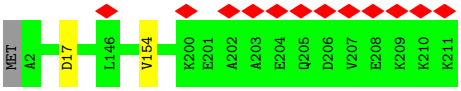
Chain P:



• Molecule 24: 60S ribosomal protein L13

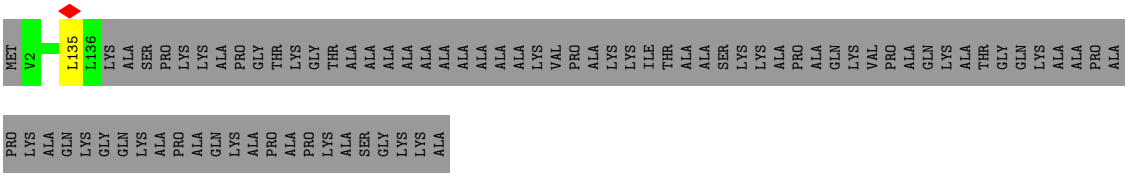
Chain Q:





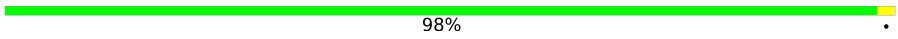
• Molecule 25: 60S ribosomal protein L14

Chain S:



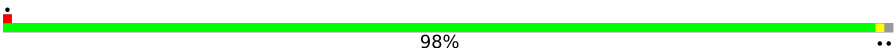
• Molecule 26: 60S ribosomal protein L15

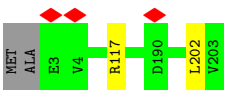
Chain U:



• Molecule 27: 60S ribosomal protein L13a

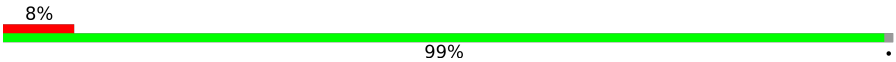
Chain V:

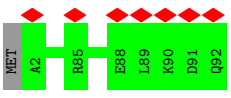




• Molecule 28: 60S ribosomal protein L37a

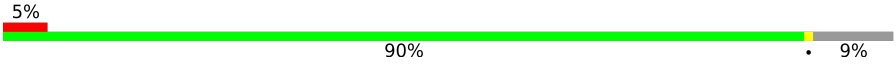
Chain X:

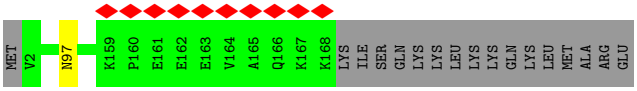




• Molecule 29: 60S ribosomal protein L17

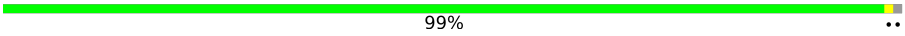
Chain Y:





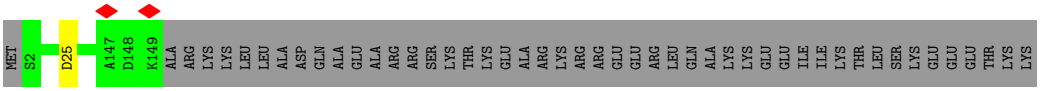
• Molecule 30: 60S ribosomal protein L18

Chain Z:



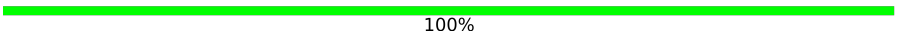
• Molecule 31: 60S ribosomal protein L19

Chain a:



• Molecule 32: 60S ribosomal protein L18a

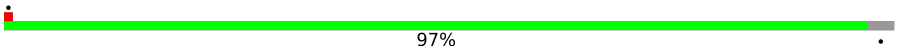
Chain b:

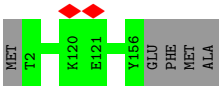


There are no outlier residues recorded for this chain.

• Molecule 33: 60S ribosomal protein L21

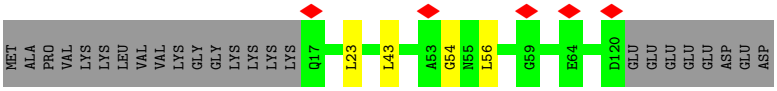
Chain c:





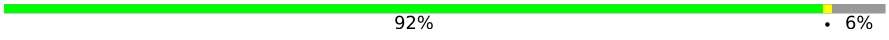
• Molecule 34: 60S ribosomal protein L22

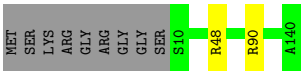
Chain d:



• Molecule 35: 60S ribosomal protein L23

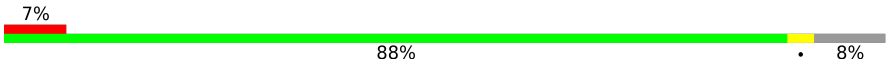
Chain e:

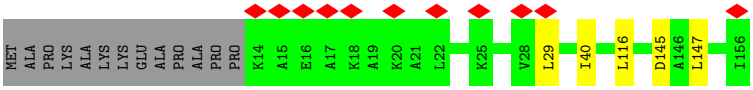




• Molecule 36: 60S ribosomal protein L23a

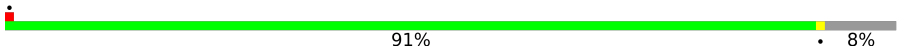
Chain g:

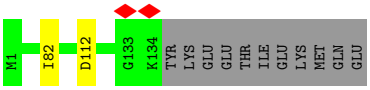




• Molecule 37: 60S ribosomal protein L26

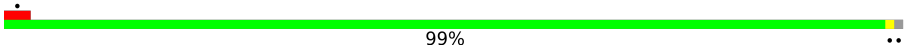
Chain h:

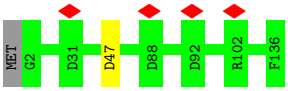




• Molecule 38: 60S ribosomal protein L27

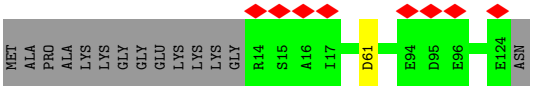
Chain i:





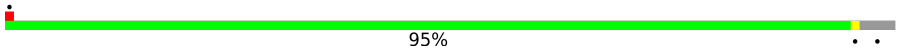
• Molecule 39: 60S ribosomal protein L31

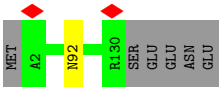
Chain j:



• Molecule 40: 60S ribosomal protein L32

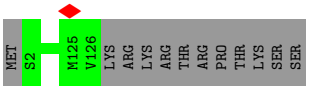
Chain k:





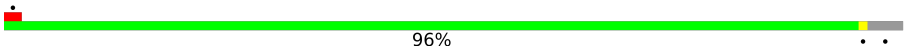
• Molecule 41: 60S ribosomal protein L28

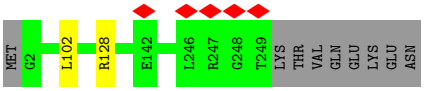
Chain l:



• Molecule 42: 60S ribosomal protein L8

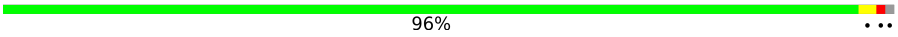
Chain m:

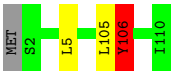




• Molecule 43: 60S ribosomal protein L35a

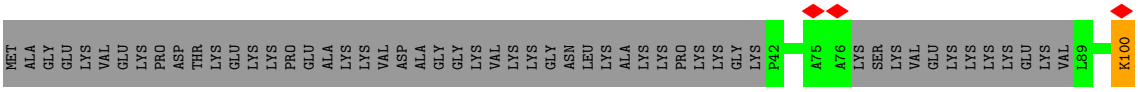
Chain n:

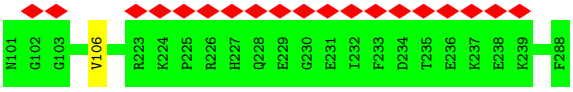




• Molecule 44: 60S ribosomal protein L6

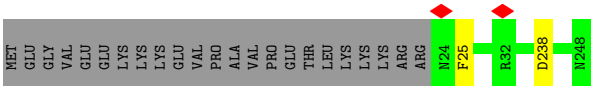
Chain o:





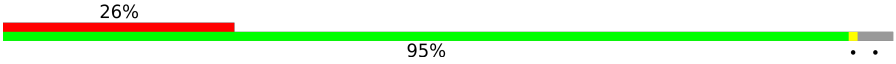
• Molecule 45: 60S ribosomal protein L7

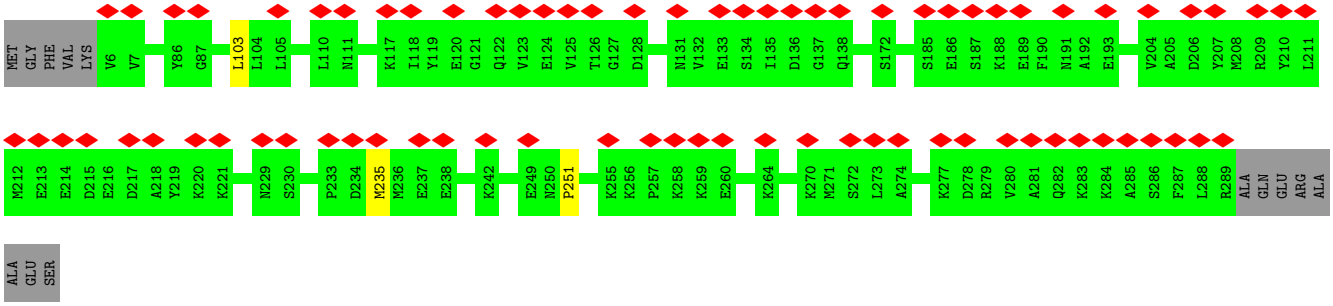
Chain p:



• Molecule 46: 60S ribosomal protein L5

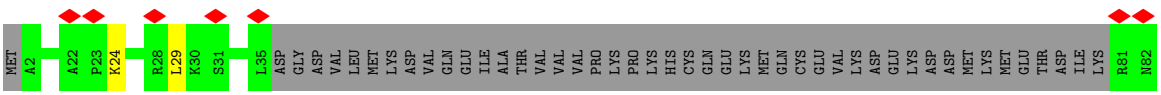
Chain r:

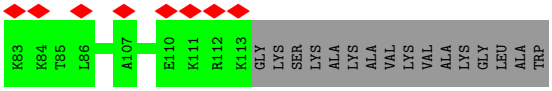




• Molecule 47: Protein LLP homolog

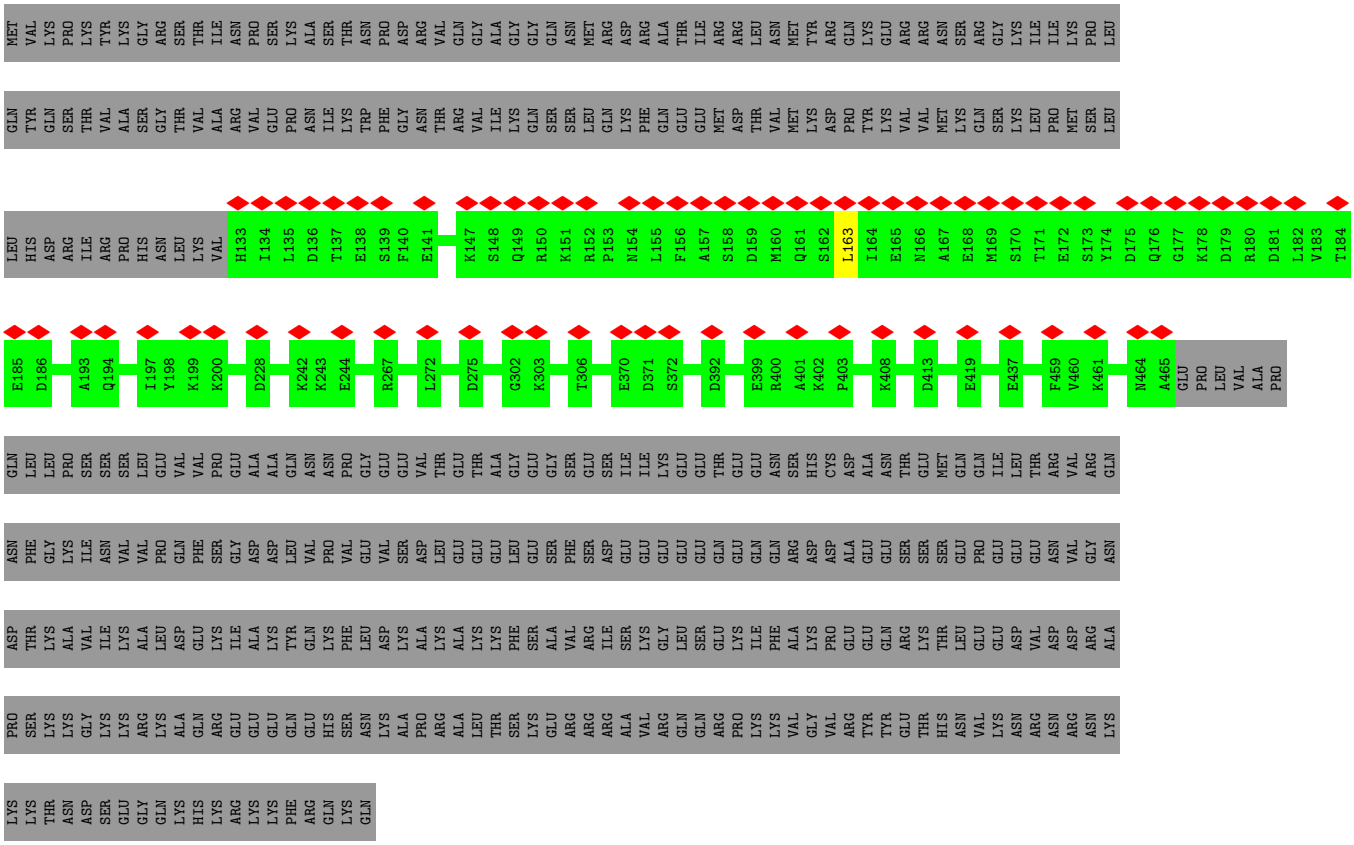
Chain z:





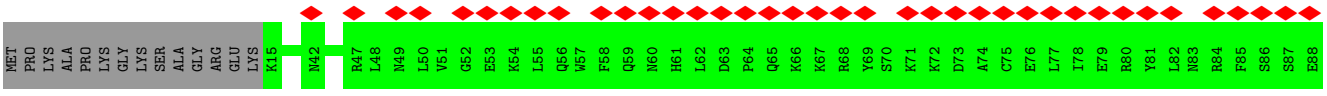
• Molecule 48: G Protein Nucleolar 2

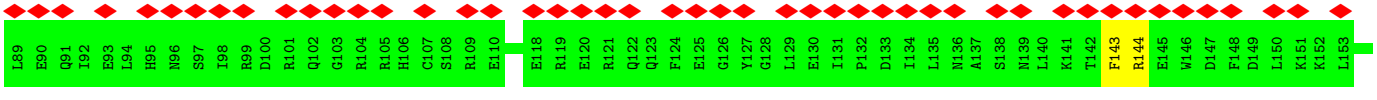
Chain A:

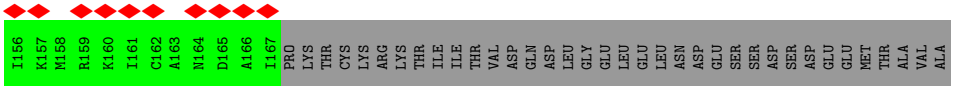


• Molecule 49: Translation machinery-associated protein 16

Chain R:

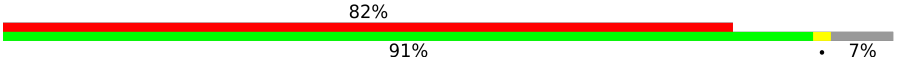


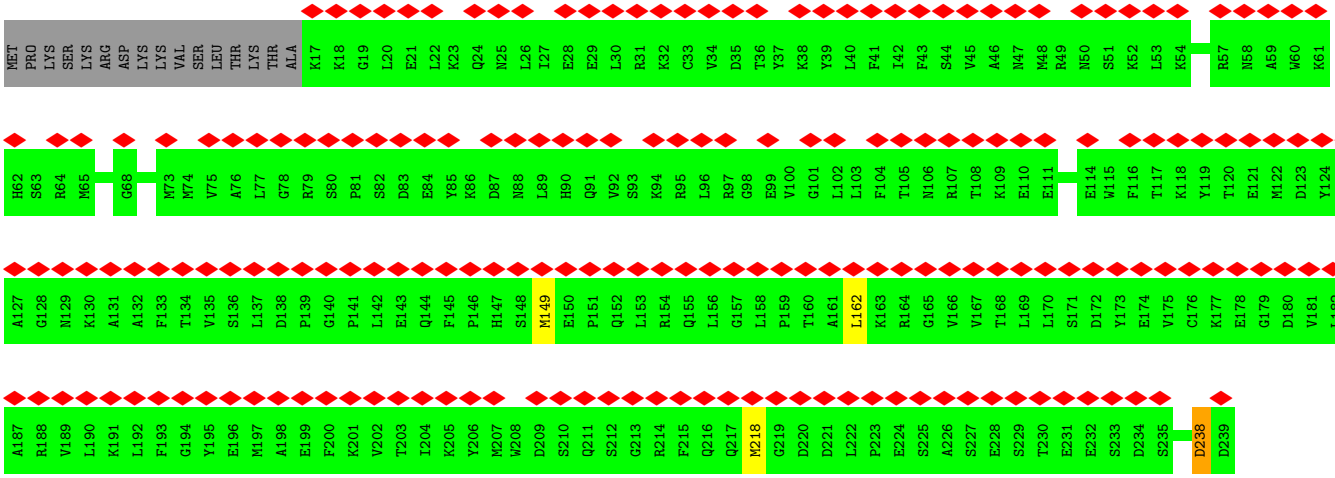




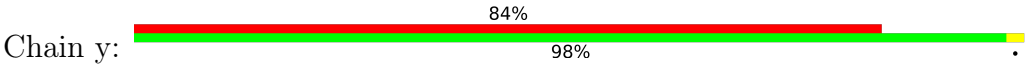
• Molecule 50: mRNA turnover protein 4 homolog

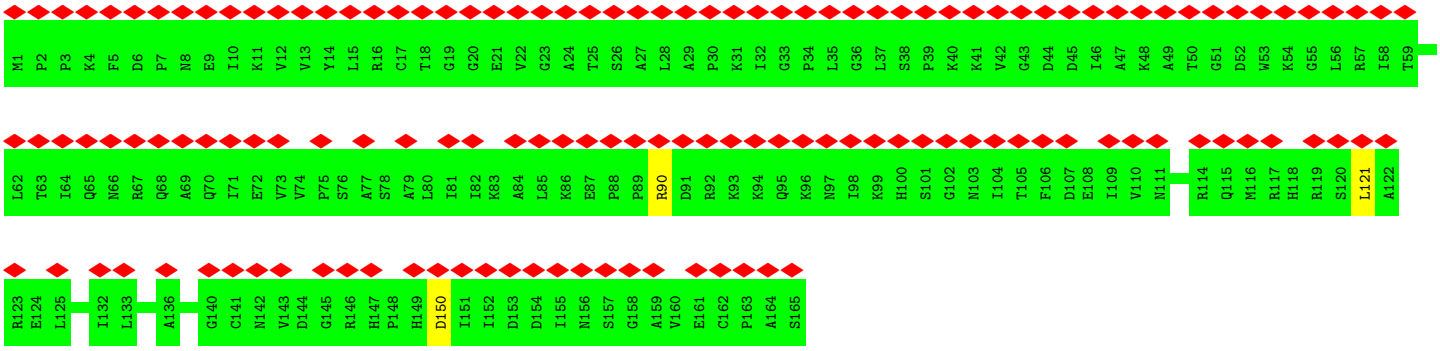
Chain J:



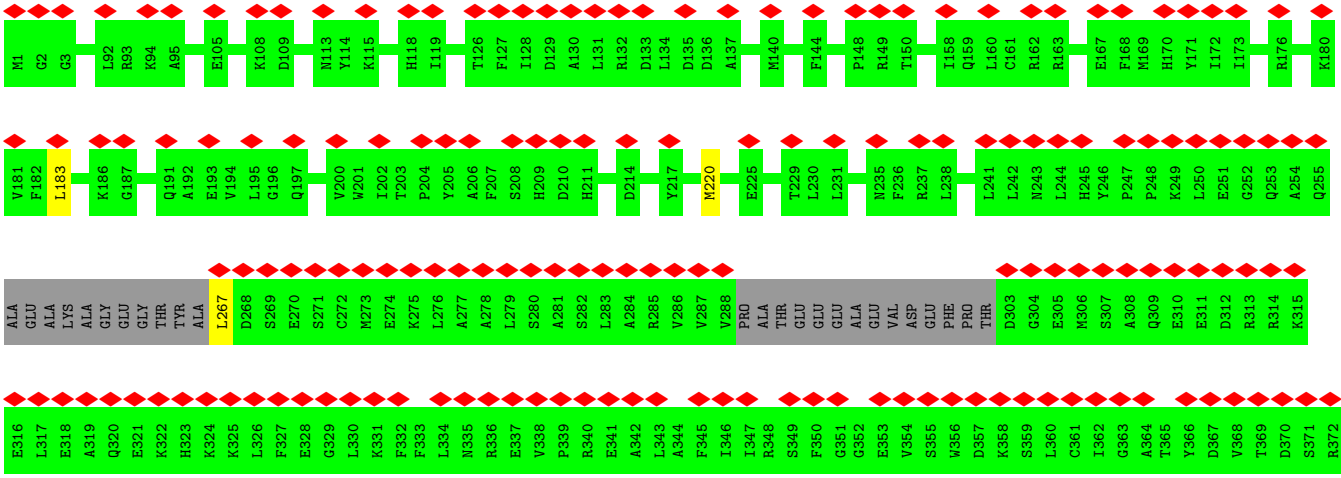


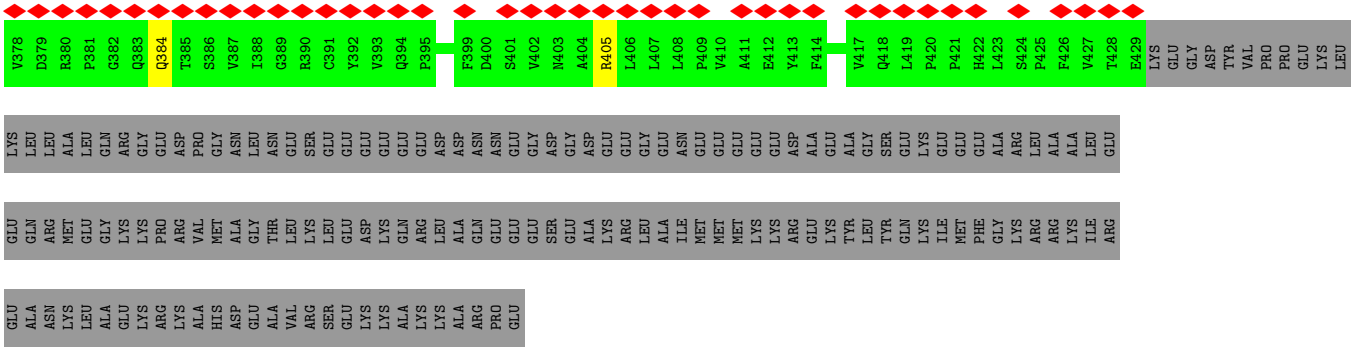
• Molecule 51: 60S ribosomal protein L12





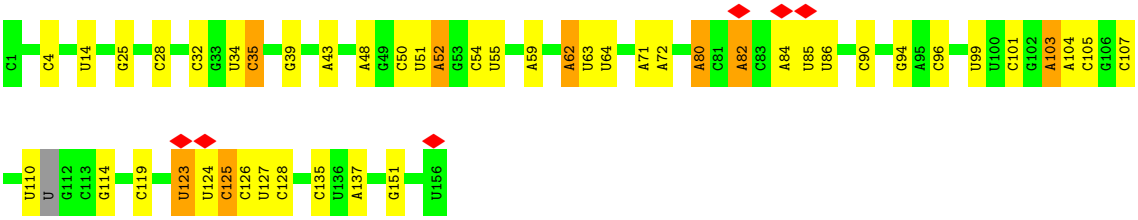
• Molecule 52: Pescadillo homolog





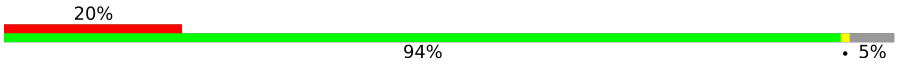
• Molecule 53: 5.8S rRNA

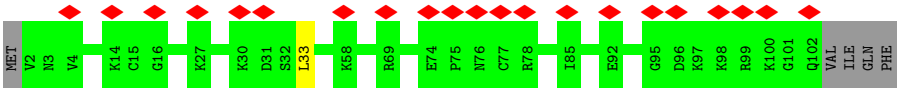
Chain 8:



• Molecule 54: 60S ribosomal protein L36a

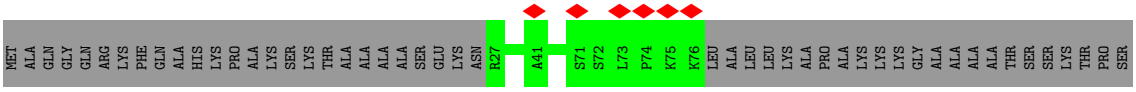
Chain W:





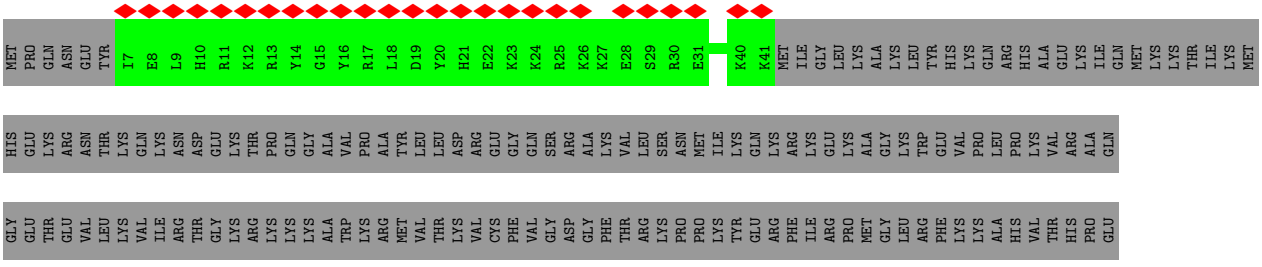
• Molecule 55: Leydig cell tumor 10 kDa protein homolog

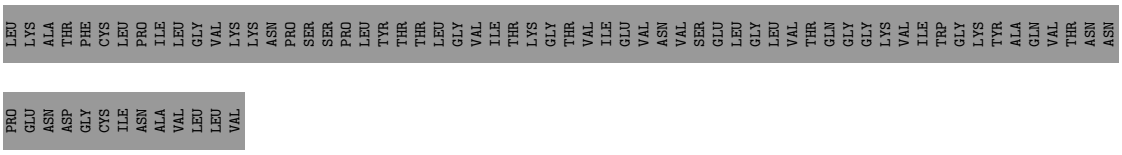
Chain T:



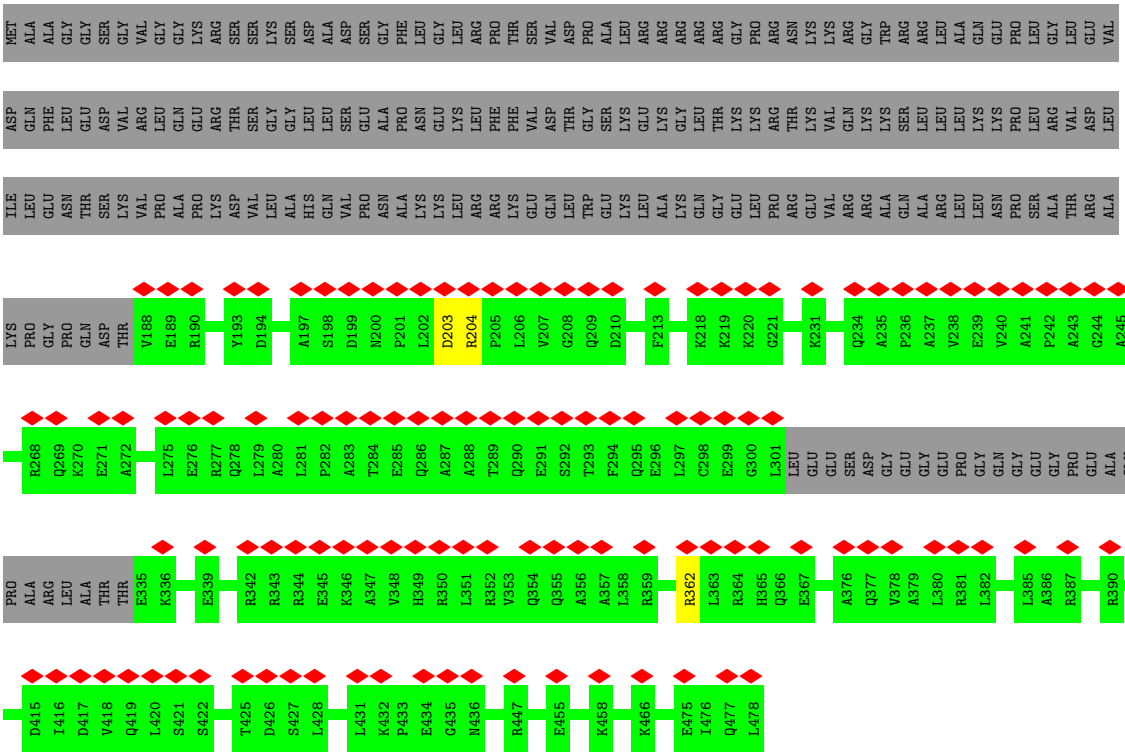
• Molecule 56: Ribosome biogenesis protein NSA2 homolog

Chain s:

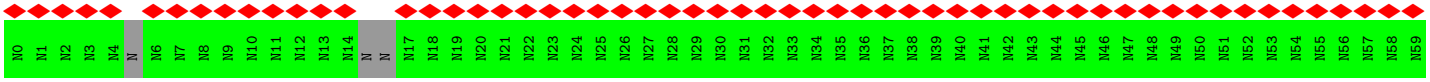




• Molecule 57: Ribosome biogenesis protein NOP53



• Molecule 58: Internal Transcribed Spacer 2



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	25102	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	0.206	Depositor
Minimum map value	-0.070	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.032	Depositor
Map size (Å)	548.0, 548.0, 548.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.37, 1.37, 1.37	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OMU, K, MG, OMG, E6G, B8H, P4U, A2M, P7G, M7A, 2MG, B9H, 7MG, B8Q, UR3, B9B, 5MC, E7G, 6MZ, 5MU, I4U, 1MA, BGH, OMC, B8K, MHG, GDP, B8T, B8W

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	u	0.31	0/1956	0.59	0/2631
2	t	0.38	0/955	0.78	2/1290 (0.2%)
3	3	0.37	0/1937	0.76	4/2595 (0.2%)
4	2	1.70	11/82935 (0.0%)	1.39	1267/129293 (1.0%)
5	4	0.34	0/5099	0.76	12/6840 (0.2%)
6	5	0.46	0/2858	1.39	50/4455 (1.1%)
7	6	0.33	0/1877	0.71	2/2554 (0.1%)
8	7	0.37	0/1207	0.75	3/1600 (0.2%)
9	9	0.32	0/802	0.81	1/1069 (0.1%)
10	B	0.33	0/3315	0.70	3/4435 (0.1%)
11	C	0.32	0/777	0.69	0/1026
12	D	0.32	0/2907	0.75	2/3905 (0.1%)
13	E	0.31	0/774	0.78	4/1038 (0.4%)
14	F	0.29	0/907	0.70	0/1209
15	G	0.34	0/1971	0.71	0/2651
16	H	0.33	0/1023	0.73	2/1351 (0.1%)
17	I	0.36	0/1537	0.85	4/2066 (0.2%)
18	K	0.31	0/843	0.69	0/1115
19	L	0.30	0/1191	0.68	2/1591 (0.1%)
20	M	0.31	0/720	0.70	0/952
21	N	0.35	0/1332	0.84	3/1782 (0.2%)
22	O	0.36	0/575	0.80	2/761 (0.3%)
23	P	0.31	0/454	0.66	0/599
24	Q	0.34	0/1732	0.74	1/2315 (0.0%)
25	S	0.35	0/1133	0.71	1/1516 (0.1%)
26	U	0.31	0/1746	0.73	4/2338 (0.2%)
27	V	0.34	0/1682	0.69	1/2250 (0.0%)
28	X	0.31	0/718	0.64	0/953
29	Y	0.30	0/1383	0.61	0/1856
30	Z	0.32	0/1537	0.70	0/2052
31	a	0.32	0/1255	0.77	1/1662 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	b	0.32	0/1501	0.65	0/2013
33	c	0.33	0/1291	0.67	0/1725
34	d	0.42	0/864	0.92	4/1160 (0.3%)
35	e	0.31	0/993	0.69	1/1332 (0.1%)
36	g	0.31	0/1175	0.72	4/1572 (0.3%)
37	h	0.34	0/1132	0.74	2/1504 (0.1%)
38	i	0.35	0/1130	0.73	1/1507 (0.1%)
39	j	0.33	0/933	0.72	1/1256 (0.1%)
40	k	0.32	0/1082	0.67	0/1443
41	l	0.30	0/1017	0.66	0/1364
42	m	0.32	0/1936	0.71	1/2596 (0.0%)
43	n	0.35	0/895	0.81	3/1198 (0.3%)
44	o	0.34	0/1935	0.75	2/2596 (0.1%)
45	p	0.36	0/1916	0.74	2/2553 (0.1%)
46	r	0.33	0/2357	0.74	3/3158 (0.1%)
47	z	0.37	0/587	0.81	2/767 (0.3%)
48	A	0.32	0/2733	0.59	1/3697 (0.0%)
49	R	0.39	0/1317	0.78	2/1757 (0.1%)
50	J	1.07	2/1844 (0.1%)	0.91	8/2476 (0.3%)
51	y	0.31	0/1269	0.69	2/1712 (0.1%)
52	v	0.32	0/3395	0.66	3/4578 (0.1%)
53	8	0.47	0/3656	1.34	49/5694 (0.9%)
54	W	0.32	0/840	0.69	1/1107 (0.1%)
55	T	0.30	0/396	0.78	0/522
56	s	0.26	0/321	0.54	0/418
57	w	0.31	0/2169	0.71	0/2902
All	All	1.23	13/167822 (0.0%)	1.15	1463/244357 (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
8	7	0	1
24	Q	0	1
43	n	0	1
50	J	0	1
57	w	0	1
All	All	0	5

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	2	1958	A	N3-C4	250.97	2.85	1.34
4	2	1958	A	C6-N1	215.25	2.86	1.35
4	2	1958	A	C5-C4	189.12	2.71	1.38
4	2	1958	A	C2-N3	163.66	2.80	1.33
4	2	1958	A	N1-C2	161.07	2.79	1.34
4	2	1958	A	C5-C6	160.22	2.85	1.41
50	J	238	ASP	CA-CB	42.23	2.46	1.53
4	2	1958	A	C8-N7	13.23	1.40	1.31
4	2	1958	A	N9-C8	10.90	1.46	1.37
50	J	238	ASP	CB-CG	9.94	1.72	1.51
4	2	4444	C	C1'-N1	5.30	1.56	1.48
4	2	1929	A	N9-C4	5.29	1.41	1.37
4	2	4445	U	C1'-N1	5.23	1.56	1.48

All (1463) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	2	1958	A	N7-C8-N9	48.21	137.91	113.80
4	2	1958	A	C4-C5-N7	-47.96	86.72	110.70
4	2	1958	A	N9-C4-C5	-34.64	91.94	105.80
4	2	1958	A	N1-C2-N3	-31.60	113.50	129.30
4	2	1958	A	C2-N3-C4	29.08	125.14	110.60
4	2	1958	A	C6-C5-N7	28.46	152.22	132.30
4	2	1958	A	N3-C4-N9	27.77	149.61	127.40
4	2	1958	A	C5-N7-C8	19.46	113.63	103.90
50	J	238	ASP	CB-CG-OD1	16.91	133.52	118.30
4	2	485	C	C2-N1-C1'	14.95	135.24	118.80
4	2	516	C	N1-C2-O2	14.88	127.83	118.90
4	2	485	C	N1-C2-O2	13.58	127.05	118.90
4	2	4502	C	N1-C2-O2	13.03	126.72	118.90
4	2	516	C	N3-C2-O2	-12.50	113.15	121.90
50	J	238	ASP	CB-CA-C	12.39	135.18	110.40
4	2	4502	C	N3-C2-O2	-12.25	113.33	121.90
4	2	753	C	N1-C2-O2	12.16	126.20	118.90
4	2	4926	C	N1-C2-O2	12.07	126.14	118.90
4	2	1958	A	N3-C4-C5	-12.04	118.38	126.80
4	2	467	U	N1-C2-O2	11.98	131.19	122.80
4	2	1216	C	N1-C2-O2	11.74	125.94	118.90
4	2	753	C	C6-N1-C2	-11.71	115.61	120.30
4	2	516	C	C6-N1-C2	-11.65	115.64	120.30
26	U	147	ASP	CB-CG-OD1	11.58	128.72	118.30
4	2	753	C	N3-C2-O2	-11.36	113.95	121.90
4	2	467	U	N3-C2-O2	-11.31	114.28	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	2	467	U	C2-N1-C1'	11.20	131.14	117.70
50	J	238	ASP	CA-CB-CG	11.17	137.98	113.40
4	2	2627	C	N1-C2-O2	11.15	125.59	118.90
4	2	485	C	C6-N1-C2	-11.06	115.87	120.30
4	2	100	C	N1-C2-O2	11.05	125.53	118.90
4	2	2820	C	N1-C2-O2	11.04	125.53	118.90
4	2	1994	C	C2-N1-C1'	11.02	130.92	118.80
4	2	4502	C	C6-N1-C2	-10.99	115.91	120.30
4	2	516	C	C2-N1-C1'	10.95	130.84	118.80
16	H	82	ASP	CB-CG-OD2	10.91	128.12	118.30
4	2	1216	C	C2-N1-C1'	10.77	130.65	118.80
4	2	100	C	C2-N1-C1'	10.76	130.63	118.80
4	2	1994	C	N1-C2-O2	10.51	125.21	118.90
4	2	4138	C	N3-C2-O2	-10.51	114.54	121.90
4	2	4926	C	C2-N1-C1'	10.48	130.33	118.80
4	2	485	C	N3-C2-O2	-10.42	114.61	121.90
12	D	171	LEU	CA-CB-CG	10.41	139.25	115.30
4	2	4613	C	N1-C2-O2	10.29	125.08	118.90
34	d	43	LEU	CA-CB-CG	10.19	138.74	115.30
4	2	4149	C	N3-C2-O2	-10.10	114.83	121.90
4	2	3636	C	C6-N1-C2	-10.03	116.29	120.30
4	2	485	C	C6-N1-C1'	-10.00	108.80	120.80
4	2	1958	A	C8-N9-C4	9.97	109.79	105.80
4	2	1671	U	N3-C2-O2	-9.95	115.23	122.20
4	2	4709	U	N3-C2-O2	-9.94	115.24	122.20
4	2	1241	C	N1-C2-O2	9.91	124.84	118.90
4	2	1216	C	N3-C2-O2	-9.90	114.97	121.90
4	2	1958	A	C6-N1-C2	9.87	124.52	118.60
4	2	4682	U	N3-C2-O2	-9.84	115.31	122.20
4	2	2627	C	N3-C2-O2	-9.83	115.02	121.90
4	2	2860	C	N1-C2-O2	9.69	124.71	118.90
4	2	4505	C	C6-N1-C2	-9.60	116.46	120.30
4	2	4612	C	N1-C2-O2	9.59	124.65	118.90
4	2	4926	C	N3-C2-O2	-9.51	115.25	121.90
4	2	4682	U	N1-C2-O2	9.51	129.45	122.80
4	2	4758	U	C2-N1-C1'	9.50	129.09	117.70
4	2	485	C	C5-C6-N1	9.45	125.72	121.00
4	2	220	C	N1-C2-O2	9.43	124.56	118.90
4	2	4709	U	N1-C2-O2	9.42	129.39	122.80
4	2	753	C	C2-N1-C1'	9.37	129.10	118.80
4	2	4505	C	C2-N1-C1'	9.35	129.09	118.80
4	2	4453	C	N1-C2-O2	9.34	124.51	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	2	643	C	N1-C2-O2	9.28	124.47	118.90
4	2	2505	C	N1-C2-O2	9.22	124.43	118.90
4	2	2260	C	N1-C2-O2	9.21	124.43	118.90
4	2	1726	U	N3-C2-O2	-9.20	115.76	122.20
4	2	2262	G	C4-N9-C1'	9.19	138.44	126.50
4	2	2860	C	C6-N1-C2	-9.17	116.63	120.30
4	2	77	U	N3-C2-O2	-9.16	115.78	122.20
4	2	1079	C	N1-C2-O2	9.13	124.38	118.90
4	2	1183	C	N1-C2-O2	9.09	124.35	118.90
5	4	230	LEU	CA-CB-CG	9.08	136.18	115.30
4	2	3772	U	N3-C2-O2	-9.07	115.85	122.20
4	2	1216	C	C6-N1-C2	-9.06	116.67	120.30
4	2	2820	C	N3-C2-O2	-9.05	115.57	121.90
4	2	2439	G	C4-N9-C1'	9.02	138.23	126.50
4	2	100	C	N3-C2-O2	-9.01	115.59	121.90
10	B	360	LEU	CA-CB-CG	8.97	135.93	115.30
4	2	1963	C	C6-N1-C2	-8.96	116.72	120.30
19	L	102	ASP	CB-CG-OD1	8.96	126.36	118.30
17	I	37	ASP	CB-CG-OD1	8.95	126.36	118.30
4	2	2351	C	C6-N1-C2	-8.91	116.73	120.30
4	2	4887	C	N1-C2-O2	8.89	124.23	118.90
4	2	2439	G	C8-N9-C1'	-8.88	115.45	127.00
4	2	4504	C	N1-C2-O2	8.86	124.21	118.90
4	2	4758	U	N1-C2-O2	8.85	128.99	122.80
53	8	64	U	N3-C2-O2	-8.81	116.03	122.20
4	2	4215	C	N1-C2-O2	8.81	124.19	118.90
4	2	1929	A	C2-N3-C4	8.79	115.00	110.60
4	2	2592	U	N3-C2-O2	-8.74	116.08	122.20
43	n	5	LEU	CA-CB-CG	8.72	135.36	115.30
4	2	2410	C	C6-N1-C2	-8.70	116.82	120.30
12	D	319	LEU	CA-CB-CG	8.70	135.30	115.30
4	2	282	C	N1-C2-O2	8.69	124.12	118.90
4	2	2505	C	C2-N1-C1'	8.69	128.36	118.80
4	2	1994	C	N3-C2-O2	-8.63	115.86	121.90
4	2	1079	C	C5-C6-N1	8.61	125.30	121.00
4	2	516	C	C5-C6-N1	8.57	125.28	121.00
4	2	4314	C	N1-C2-O2	8.56	124.04	118.90
4	2	1921	C	N1-C2-O2	8.53	124.02	118.90
4	2	4613	C	N3-C2-O2	-8.52	115.94	121.90
17	I	142	ASP	CB-CG-OD2	8.52	125.96	118.30
4	2	1241	C	C2-N1-C1'	8.51	128.16	118.80
4	2	4880	C	N1-C2-O2	8.50	124.00	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	2	2592	U	N1-C2-O2	8.48	128.74	122.80
4	2	4758	U	N3-C2-O2	-8.48	116.26	122.20
4	2	1176	C	N1-C2-O2	8.46	123.98	118.90
4	2	4171	C	N1-C2-O2	8.45	123.97	118.90
4	2	1921	C	C6-N1-C2	-8.40	116.94	120.30
4	2	112	C	C6-N1-C2	-8.35	116.96	120.30
31	a	25	ASP	CB-CG-OD1	8.34	125.81	118.30
4	2	2262	G	N3-C4-C5	-8.33	124.44	128.60
4	2	1726	U	N1-C2-O2	8.32	128.62	122.80
4	2	3615	G	C4-N9-C1'	8.32	137.32	126.50
5	4	407	ASP	CB-CG-OD1	8.31	125.78	118.30
4	2	4360	U	N3-C2-O2	-8.29	116.40	122.20
4	2	3587	C	N1-C2-O2	8.28	123.87	118.90
4	2	2532	C	C6-N1-C2	-8.28	116.99	120.30
4	2	4453	C	C2-N1-C1'	8.28	127.91	118.80
6	5	76	U	N3-C2-O2	-8.27	116.41	122.20
4	2	985	C	C6-N1-C2	-8.25	117.00	120.30
4	2	1241	C	N3-C2-O2	-8.25	116.12	121.90
4	2	1655	C	N1-C2-O2	8.25	123.85	118.90
4	2	4502	C	C2-N1-C1'	8.25	127.88	118.80
4	2	2498	C	N1-C2-O2	8.25	123.85	118.90
4	2	112	C	C2-N1-C1'	8.24	127.86	118.80
4	2	1458	C	N1-C2-O2	8.23	123.84	118.90
4	2	2860	C	N3-C2-O2	-8.23	116.14	121.90
4	2	4138	C	C6-N1-C2	-8.23	117.01	120.30
4	2	1856	C	C6-N1-C2	-8.22	117.01	120.30
4	2	242	U	N3-C2-O2	-8.21	116.45	122.20
6	5	76	U	N1-C2-O2	8.20	128.54	122.80
17	I	176	LEU	CA-CB-CG	8.20	134.16	115.30
4	2	2262	G	N3-C4-N9	8.20	130.92	126.00
4	2	2410	C	C2-N1-C1'	8.19	127.81	118.80
4	2	4505	C	N1-C2-O2	8.19	123.81	118.90
4	2	1655	C	C6-N1-C2	-8.19	117.03	120.30
4	2	1191	C	N3-C2-O2	-8.16	116.19	121.90
4	2	2528	G	C4-N9-C1'	8.15	137.09	126.50
4	2	4505	C	C5-C6-N1	8.12	125.06	121.00
4	2	1958	A	C4-C5-C6	8.12	121.06	117.00
4	2	50	C	N1-C2-O2	8.11	123.77	118.90
4	2	924	C	C6-N1-C2	-8.11	117.06	120.30
4	2	4747	C	C6-N1-C2	-8.08	117.07	120.30
4	2	1079	C	C6-N1-C2	-8.07	117.07	120.30
4	2	3670	C	N1-C2-O2	8.07	123.74	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	2	1822	U	N3-C2-O2	-8.06	116.56	122.20
4	2	1632	A	C2-N3-C4	8.02	114.61	110.60
4	2	1671	U	N1-C2-O2	8.02	128.42	122.80
6	5	43	U	N1-C2-O2	8.00	128.40	122.80
7	6	144	ASP	CB-CG-OD1	7.99	125.49	118.30
4	2	2026	A	O4'-C1'-N9	7.97	114.57	108.20
4	2	2820	C	C6-N1-C2	-7.94	117.12	120.30
4	2	914	U	P-O3'-C3'	7.91	129.19	119.70
4	2	499	G	N3-C4-N9	7.90	130.74	126.00
4	2	2351	C	C5-C6-N1	7.90	124.95	121.00
53	8	125	C	P-O3'-C3'	7.90	129.18	119.70
4	2	1822	U	N1-C2-O2	7.89	128.32	122.80
4	2	2362	U	N3-C2-O2	-7.88	116.68	122.20
4	2	1472	C	C6-N1-C2	-7.88	117.15	120.30
4	2	2528	G	N3-C4-C5	-7.85	124.67	128.60
4	2	4340	U	N3-C2-O2	-7.85	116.70	122.20
4	2	2710	C	N1-C2-O2	7.84	123.61	118.90
4	2	3741	C	N1-C2-O2	7.84	123.60	118.90
4	2	2470	C	P-O3'-C3'	7.83	129.09	119.70
4	2	365	U	N3-C2-O2	-7.82	116.72	122.20
4	2	1702	C	N1-C2-O2	7.82	123.59	118.90
4	2	3769	C	C6-N1-C2	-7.82	117.17	120.30
4	2	499	G	C4-N9-C1'	7.82	136.66	126.50
4	2	2856	C	N1-C2-O2	7.80	123.58	118.90
4	2	643	C	N3-C2-O2	-7.80	116.44	121.90
4	2	3637	U	N3-C2-O2	-7.79	116.74	122.20
4	2	4608	G	C8-N9-C4	-7.79	103.28	106.40
4	2	1079	C	C2-N1-C1'	7.78	127.36	118.80
4	2	1191	C	N1-C2-O2	7.78	123.57	118.90
4	2	6	C	N1-C2-O2	7.77	123.56	118.90
4	2	1720	C	C6-N1-C2	-7.76	117.20	120.30
4	2	449	C	N1-C2-O2	7.75	123.55	118.90
4	2	1994	C	C6-N1-C1'	-7.74	111.51	120.80
4	2	4263	C	N1-C2-O2	7.74	123.54	118.90
4	2	4453	C	N3-C2-O2	-7.74	116.48	121.90
4	2	77	U	N1-C2-O2	7.74	128.22	122.80
4	2	2532	C	C5-C6-N1	7.74	124.87	121.00
4	2	322	C	N1-C2-O2	7.74	123.54	118.90
4	2	220	C	C6-N1-C2	-7.73	117.21	120.30
4	2	2563	C	N1-C2-O2	7.73	123.54	118.90
4	2	1607	C	N1-C2-O2	7.73	123.54	118.90
4	2	3636	C	N1-C2-O2	7.72	123.53	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	2	1963	C	C5-C6-N1	7.72	124.86	121.00
4	2	4612	C	N3-C2-O2	-7.71	116.50	121.90
4	2	3769	C	C5-C6-N1	7.71	124.86	121.00
50	J	238	ASP	CB-CG-OD2	-7.71	111.36	118.30
4	2	2262	G	C8-N9-C1'	-7.70	116.99	127.00
4	2	3622	C	N1-C2-O2	7.70	123.52	118.90
4	2	3636	C	N3-C2-O2	-7.69	116.52	121.90
6	5	14	C	C6-N1-C2	-7.69	117.22	120.30
4	2	1703	C	N1-C2-O2	7.67	123.50	118.90
4	2	4747	C	N1-C2-O2	7.67	123.50	118.90
4	2	2814	C	N1-C2-O2	7.67	123.50	118.90
4	2	4149	C	N1-C2-O2	7.67	123.50	118.90
4	2	2627	C	C6-N1-C2	-7.66	117.24	120.30
4	2	1414	C	C6-N1-C2	-7.66	117.24	120.30
4	2	2528	G	N3-C4-N9	7.65	130.59	126.00
4	2	4928	C	C2-N1-C1'	7.64	127.21	118.80
4	2	4229	U	N3-C2-O2	-7.64	116.85	122.20
4	2	96	U	N3-C2-O2	-7.64	116.85	122.20
4	2	1915	C	N1-C2-O2	7.64	123.48	118.90
43	n	105	LEU	C-N-CA	7.62	140.75	121.70
4	2	2486	G	P-O3'-C3'	7.61	128.84	119.70
53	8	54	C	N1-C2-O2	7.61	123.47	118.90
4	2	2410	C	N1-C2-O2	7.61	123.47	118.90
4	2	4766	C	C6-N1-C2	-7.60	117.26	120.30
4	2	3615	G	N3-C4-N9	7.59	130.56	126.00
4	2	3774	A	P-O3'-C3'	7.59	128.81	119.70
4	2	115	C	N1-C2-O2	7.59	123.45	118.90
4	2	1402	C	N1-C2-O2	7.59	123.45	118.90
4	2	2760	G	P-O3'-C3'	7.58	128.79	119.70
4	2	1405	C	N1-C2-O2	7.58	123.44	118.90
4	2	972	C	N1-C2-O2	7.57	123.44	118.90
4	2	4887	C	N3-C2-O2	-7.56	116.61	121.90
4	2	4771	C	C6-N1-C2	-7.55	117.28	120.30
4	2	2482	C	N1-C2-O2	7.55	123.43	118.90
4	2	30	C	C6-N1-C2	-7.55	117.28	120.30
4	2	4360	U	N1-C2-O2	7.54	128.08	122.80
4	2	4340	U	N1-C2-O2	7.54	128.08	122.80
4	2	2710	C	C2-N1-C1'	7.54	127.09	118.80
4	2	2281	U	N1-C2-O2	7.53	128.07	122.80
4	2	1097	C	C5-C6-N1	7.53	124.76	121.00
6	5	24	C	C6-N1-C2	-7.52	117.29	120.30
4	2	100	C	C6-N1-C1'	-7.50	111.80	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	2	6	C	N3-C2-O2	-7.50	116.65	121.90
4	2	3598	C	N1-C2-O2	7.50	123.40	118.90
4	2	4342	C	N1-C2-O2	7.49	123.39	118.90
4	2	1607	C	N3-C2-O2	-7.47	116.67	121.90
4	2	4215	C	C6-N1-C2	-7.47	117.31	120.30
6	5	43	U	N3-C2-O2	-7.47	116.97	122.20
6	5	15	C	N1-C2-O2	7.46	123.38	118.90
4	2	467	U	C6-N1-C1'	-7.46	110.76	121.20
4	2	4864	U	N1-C2-O2	7.46	128.02	122.80
4	2	4747	C	C2-N1-C1'	7.46	127.00	118.80
4	2	1702	C	C2-N1-C1'	7.45	126.99	118.80
4	2	2445	C	N1-C2-O2	7.45	123.37	118.90
4	2	4138	C	N1-C2-O2	7.43	123.36	118.90
4	2	4714	C	C6-N1-C2	-7.42	117.33	120.30
4	2	2351	C	C2-N1-C1'	7.41	126.95	118.80
4	2	4229	U	N1-C2-O2	7.41	127.98	122.80
4	2	2505	C	N3-C2-O2	-7.40	116.72	121.90
4	2	2362	U	N1-C2-O2	7.40	127.98	122.80
4	2	3926	C	N1-C2-O2	7.40	123.34	118.90
4	2	2260	C	C2-N1-C1'	7.39	126.93	118.80
4	2	2548	C	N1-C2-O2	7.39	123.33	118.90
4	2	4771	C	C5-C6-N1	7.39	124.69	121.00
4	2	4614	G	C5-C6-O6	7.39	133.03	128.60
36	g	116	LEU	CA-CB-CG	7.38	132.28	115.30
4	2	1472	C	C2-N1-C1'	7.38	126.92	118.80
4	2	365	U	N1-C2-O2	7.37	127.96	122.80
4	2	4171	C	C6-N1-C2	-7.37	117.35	120.30
4	2	175	C	C6-N1-C2	-7.37	117.35	120.30
4	2	282	C	N3-C2-O2	-7.36	116.75	121.90
4	2	4215	C	N3-C2-O2	-7.36	116.75	121.90
4	2	985	C	C2-N1-C1'	7.36	126.89	118.80
4	2	925	C	C6-N1-C2	-7.35	117.36	120.30
6	5	39	C	N1-C2-O2	7.35	123.31	118.90
4	2	2482	C	N3-C2-O2	-7.35	116.75	121.90
4	2	4308	C	N1-C2-O2	7.35	123.31	118.90
4	2	977	C	C6-N1-C2	-7.35	117.36	120.30
4	2	1655	C	N3-C2-O2	-7.34	116.76	121.90
4	2	2033	A	P-O3'-C3'	7.33	128.49	119.70
4	2	2281	U	N3-C2-O2	-7.31	117.08	122.20
4	2	2410	C	C5-C6-N1	7.31	124.66	121.00
39	j	61	ASP	CB-CG-OD2	7.31	124.88	118.30
53	8	99	U	N3-C2-O2	-7.31	117.08	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	2	2072	C	C6-N1-C2	-7.30	117.38	120.30
4	2	4972	U	N3-C2-O2	-7.28	117.10	122.20
6	5	24	C	N1-C2-O2	7.28	123.27	118.90
4	2	4476	C	C2-N1-C1'	7.28	126.81	118.80
4	2	4864	U	N3-C2-O2	-7.28	117.11	122.20
4	2	112	C	N1-C2-O2	7.27	123.26	118.90
4	2	1993	C	C6-N1-C2	-7.27	117.39	120.30
4	2	4926	C	C6-N1-C2	-7.26	117.40	120.30
4	2	4895	C	N1-C2-O2	7.25	123.25	118.90
4	2	489	C	N1-C2-O2	7.25	123.25	118.90
4	2	3650	C	C6-N1-C2	-7.25	117.40	120.30
4	2	499	G	C8-N9-C1'	-7.24	117.58	127.00
4	2	1183	C	N3-C2-O2	-7.24	116.83	121.90
4	2	4608	G	N7-C8-N9	7.24	116.72	113.10
4	2	3631	U	N3-C2-O2	-7.24	117.14	122.20
8	7	66	ASP	CB-CG-OD1	7.23	124.81	118.30
4	2	2560	C	C6-N1-C2	-7.22	117.41	120.30
4	2	3615	G	N3-C4-C5	-7.22	124.99	128.60
4	2	2860	C	C5-C6-N1	7.22	124.61	121.00
4	2	220	C	C5-C6-N1	7.21	124.60	121.00
4	2	972	C	C6-N1-C2	-7.21	117.42	120.30
4	2	2853	C	N1-C2-O2	7.20	123.22	118.90
4	2	3598	C	N3-C2-O2	-7.20	116.86	121.90
4	2	4969	C	C6-N1-C2	-7.20	117.42	120.30
4	2	1980	U	P-O3'-C3'	7.20	128.33	119.70
4	2	2589	C	C6-N1-C2	-7.19	117.42	120.30
45	p	238	ASP	CB-CG-OD1	7.19	124.77	118.30
53	8	135	C	C6-N1-C2	-7.18	117.43	120.30
4	2	4914	C	C6-N1-C2	-7.18	117.43	120.30
4	2	3637	U	N1-C2-O2	7.17	127.82	122.80
4	2	4714	C	N1-C2-O2	7.17	123.20	118.90
36	g	145	ASP	CB-CG-OD2	7.16	124.75	118.30
4	2	2892	C	C2-N1-C1'	7.16	126.68	118.80
4	2	1243	C	C6-N1-C2	-7.15	117.44	120.30
4	2	3926	C	C6-N1-C2	-7.14	117.44	120.30
7	6	177	LEU	CA-CB-CG	7.13	131.71	115.30
4	2	112	C	C5-C6-N1	7.12	124.56	121.00
4	2	3615	G	C8-N9-C1'	-7.12	117.74	127.00
4	2	26	C	C6-N1-C2	-7.12	117.45	120.30
4	2	4926	C	C6-N1-C1'	-7.12	112.25	120.80
4	2	1458	C	N3-C2-O2	-7.12	116.92	121.90
4	2	1216	C	C5-C6-N1	7.11	124.55	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	2	489	C	C6-N1-C2	-7.10	117.46	120.30
4	2	4262	C	N1-C2-O2	7.09	123.16	118.90
4	2	4913	G	P-O3'-C3'	7.09	128.21	119.70
4	2	3772	U	N1-C2-O2	7.09	127.76	122.80
6	5	14	C	C5-C6-N1	7.09	124.54	121.00
4	2	753	C	C5-C6-N1	7.08	124.54	121.00
4	2	3905	A	P-O3'-C3'	7.08	128.19	119.70
4	2	4476	C	N1-C2-O2	7.07	123.14	118.90
4	2	220	C	N3-C2-O2	-7.07	116.95	121.90
52	v	183	LEU	CA-CB-CG	7.06	131.55	115.30
4	2	1414	C	C5-C6-N1	7.06	124.53	121.00
4	2	2059	C	C6-N1-C2	-7.06	117.47	120.30
4	2	1921	C	N3-C2-O2	-7.06	116.96	121.90
4	2	1097	C	C6-N1-C2	-7.05	117.48	120.30
4	2	2260	C	N3-C2-O2	-7.05	116.96	121.90
38	i	47	ASP	CB-CG-OD2	7.05	124.64	118.30
4	2	4712	C	C6-N1-C2	-7.04	117.48	120.30
4	2	4504	C	N3-C2-O2	-7.04	116.98	121.90
4	2	367	C	C6-N1-C2	-7.03	117.49	120.30
4	2	489	C	C2-N1-C1'	7.03	126.54	118.80
4	2	4137	C	N1-C2-O2	7.03	123.12	118.90
4	2	155	C	N1-C2-O2	7.03	123.12	118.90
4	2	5035	U	N3-C2-O2	-7.02	117.28	122.20
4	2	924	C	C5-C6-N1	7.02	124.51	121.00
4	2	1582	U	N3-C2-O2	-7.01	117.29	122.20
4	2	4880	C	N3-C2-O2	-7.01	116.99	121.90
53	8	64	U	N1-C2-O2	7.01	127.71	122.80
4	2	115	C	C2-N1-C1'	7.01	126.51	118.80
4	2	2445	C	C6-N1-C2	-7.00	117.50	120.30
4	2	50	C	C6-N1-C2	-7.00	117.50	120.30
4	2	1088	C	C6-N1-C2	-7.00	117.50	120.30
4	2	4314	C	N3-C2-O2	-6.99	117.01	121.90
6	5	28	C	N1-C2-O2	6.98	123.09	118.90
4	2	1921	C	C5-C6-N1	6.98	124.49	121.00
4	2	4880	C	C6-N1-C2	-6.97	117.51	120.30
4	2	26	C	N1-C2-O2	6.97	123.08	118.90
4	2	1731	C	C6-N1-C2	-6.96	117.52	120.30
4	2	988	C	C6-N1-C2	-6.96	117.52	120.30
4	2	2532	C	C2-N1-C1'	6.96	126.45	118.80
4	2	2563	C	C6-N1-C2	-6.96	117.52	120.30
4	2	1176	C	N3-C2-O2	-6.95	117.04	121.90
4	2	4149	C	C6-N1-C2	-6.95	117.52	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	2	4481	U	N3-C2-O2	-6.95	117.34	122.20
4	2	4123	C	N1-C2-O2	6.93	123.06	118.90
6	5	28	C	C6-N1-C2	-6.93	117.53	120.30
4	2	1822	U	C2-N1-C1'	6.92	126.01	117.70
51	y	121	LEU	CA-CB-CG	6.92	131.22	115.30
4	2	654	C	C6-N1-C2	-6.91	117.54	120.30
4	2	4314	C	C6-N1-C2	-6.89	117.54	120.30
4	2	672	C	N1-C2-O2	6.88	123.03	118.90
4	2	100	C	C6-N1-C2	-6.88	117.55	120.30
4	2	2371	U	N3-C2-O2	-6.88	117.39	122.20
4	2	175	C	N3-C2-O2	-6.87	117.09	121.90
4	2	322	C	C6-N1-C2	-6.87	117.55	120.30
4	2	4709	U	C2-N1-C1'	6.87	125.94	117.70
22	O	10	ASP	CB-CG-OD1	6.86	124.48	118.30
4	2	1656	U	N3-C2-O2	-6.86	117.40	122.20
6	5	15	C	N3-C2-O2	-6.86	117.10	121.90
4	2	472	C	C6-N1-C2	-6.86	117.56	120.30
4	2	9	C	C6-N1-C2	-6.84	117.56	120.30
4	2	1994	C	C6-N1-C2	-6.84	117.56	120.30
4	2	4130	C	C6-N1-C2	-6.84	117.56	120.30
4	2	3712	A	C2-N3-C4	6.83	114.02	110.60
4	2	281	U	N3-C2-O2	-6.83	117.42	122.20
53	8	99	U	N1-C2-O2	6.83	127.58	122.80
4	2	1856	C	C5-C6-N1	6.83	124.41	121.00
4	2	4303	C	C2-N1-C1'	6.83	126.31	118.80
4	2	971	U	C2-N1-C1'	6.82	125.89	117.70
4	2	2528	G	C8-N9-C1'	-6.82	118.13	127.00
4	2	1929	A	C4-N9-C1'	6.82	138.57	126.30
4	2	2548	C	C6-N1-C2	-6.82	117.57	120.30
4	2	673	C	C6-N1-C2	-6.82	117.57	120.30
4	2	3774	A	OP1-P-O3'	6.82	120.19	105.20
4	2	1731	C	N1-C2-O2	6.81	122.99	118.90
4	2	4162	C	N1-C2-O2	6.81	122.99	118.90
4	2	1402	C	N3-C2-O2	-6.81	117.13	121.90
4	2	1183	C	C6-N1-C2	-6.81	117.58	120.30
4	2	3587	C	N3-C2-O2	-6.81	117.14	121.90
4	2	1472	C	N1-C2-O2	6.80	122.98	118.90
4	2	4243	C	C6-N1-C2	-6.80	117.58	120.30
4	2	924	C	N1-C2-O2	6.79	122.98	118.90
4	2	4171	C	N3-C2-O2	-6.79	117.15	121.90
4	2	977	C	C2-N1-C1'	6.79	126.26	118.80
4	2	4341	C	N1-C2-O2	6.79	122.97	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	2	1216	C	C6-N1-C1'	-6.78	112.66	120.80
4	2	2837	U	N3-C2-O2	-6.78	117.45	122.20
53	8	55	U	N3-C2-O2	-6.78	117.45	122.20
4	2	472	C	N1-C2-O2	6.78	122.97	118.90
4	2	195	C	C6-N1-C2	-6.77	117.59	120.30
4	2	2031	C	C6-N1-C2	-6.77	117.59	120.30
4	2	1367	C	C2-N1-C1'	6.77	126.25	118.80
4	2	1731	C	C5-C6-N1	6.74	124.37	121.00
4	2	3752	C	P-O3'-C3'	6.74	127.78	119.70
4	2	1241	C	C6-N1-C2	-6.74	117.61	120.30
4	2	2498	C	N3-C2-O2	-6.74	117.19	121.90
53	8	54	C	C6-N1-C2	-6.74	117.61	120.30
4	2	1978	C	C6-N1-C2	-6.73	117.61	120.30
4	2	719	C	C6-N1-C2	-6.73	117.61	120.30
4	2	4502	C	C5-C6-N1	6.72	124.36	121.00
4	2	1289	C	N1-C2-O2	6.72	122.93	118.90
4	2	1607	C	C6-N1-C2	-6.72	117.61	120.30
4	2	654	C	C5-C6-N1	6.72	124.36	121.00
4	2	2014	C	N3-C2-O2	-6.72	117.20	121.90
53	8	32	C	C6-N1-C2	-6.71	117.61	120.30
4	2	155	C	N3-C2-O2	-6.71	117.20	121.90
4	2	4887	C	C6-N1-C2	-6.71	117.62	120.30
4	2	115	C	N3-C2-O2	-6.70	117.21	121.90
4	2	1243	C	C2-N1-C1'	6.70	126.17	118.80
4	2	1340	C	C5-C6-N1	6.70	124.35	121.00
4	2	96	U	N1-C2-O2	6.70	127.49	122.80
4	2	4775	C	C2-N1-C1'	6.70	126.17	118.80
4	2	643	C	C6-N1-C2	-6.69	117.62	120.30
4	2	4612	C	C6-N1-C2	-6.69	117.62	120.30
4	2	4747	C	C5-C6-N1	6.69	124.35	121.00
4	2	2627	C	C2-N1-C1'	6.69	126.16	118.80
4	2	454	U	N1-C2-O2	6.69	127.48	122.80
4	2	1856	C	O5'-P-OP1	6.69	118.73	110.70
4	2	2439	G	N3-C4-N9	6.69	130.01	126.00
4	2	3769	C	N1-C2-O2	6.68	122.91	118.90
4	2	4766	C	C5-C6-N1	6.67	124.33	121.00
4	2	2563	C	N3-C2-O2	-6.66	117.24	121.90
4	2	1978	C	N1-C2-O2	6.66	122.89	118.90
4	2	1176	C	C6-N1-C2	-6.64	117.64	120.30
4	2	4613	C	C6-N1-C2	-6.64	117.64	120.30
4	2	1096	C	C6-N1-C2	-6.63	117.65	120.30
4	2	3739	C	C6-N1-C2	-6.63	117.65	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	2	201	C	C6-N1-C2	-6.62	117.65	120.30
4	2	4342	C	C6-N1-C2	-6.62	117.65	120.30
4	2	4481	U	N1-C2-O2	6.62	127.44	122.80
4	2	242	U	N1-C2-O2	6.62	127.43	122.80
4	2	5008	C	C6-N1-C2	-6.61	117.66	120.30
4	2	4148	C	N1-C2-O2	6.61	122.87	118.90
4	2	1915	C	N3-C2-O2	-6.61	117.28	121.90
4	2	4508	C	N1-C2-O2	6.60	122.86	118.90
4	2	1254	A	C2-N3-C4	6.60	113.90	110.60
4	2	4486	C	N1-C2-O2	6.59	122.86	118.90
4	2	1340	C	C6-N1-C2	-6.59	117.67	120.30
4	2	3882	C	C6-N1-C2	-6.59	117.67	120.30
4	2	1656	U	N1-C2-O2	6.58	127.40	122.80
4	2	2482	C	C6-N1-C2	-6.58	117.67	120.30
4	2	2892	C	C6-N1-C2	-6.57	117.67	120.30
4	2	3587	C	C6-N1-C2	-6.56	117.67	120.30
4	2	50	C	N3-C2-O2	-6.56	117.31	121.90
4	2	274	C	C6-N1-C2	-6.56	117.67	120.30
4	2	4773	C	C6-N1-C2	-6.56	117.68	120.30
4	2	274	C	C2-N1-C1'	6.55	126.01	118.80
4	2	2017	A	C2-N3-C4	6.55	113.88	110.60
4	2	4928	C	N1-C2-O2	6.55	122.83	118.90
4	2	704	C	N1-C2-O2	6.54	122.83	118.90
4	2	3670	C	N3-C2-O2	-6.54	117.32	121.90
4	2	2264	C	N1-C2-O2	6.53	122.82	118.90
4	2	2710	C	N3-C2-O2	-6.52	117.33	121.90
6	5	102	U	N1-C2-O2	6.52	127.37	122.80
4	2	454	U	N3-C2-O2	-6.51	117.64	122.20
4	2	1472	C	C5-C6-N1	6.51	124.26	121.00
4	2	2548	C	C2-N1-C1'	6.51	125.96	118.80
4	2	1855	G	P-O3'-C3'	6.50	127.50	119.70
6	5	67	C	C6-N1-C2	-6.49	117.70	120.30
21	N	128	LEU	CA-CB-CG	6.49	130.24	115.30
4	2	322	C	N3-C2-O2	-6.49	117.36	121.90
4	2	1414	C	C2-N1-C1'	6.49	125.94	118.80
4	2	4263	C	N3-C2-O2	-6.48	117.36	121.90
53	8	54	C	N3-C2-O2	-6.48	117.36	121.90
4	2	4752	U	N3-C2-O2	-6.48	117.67	122.20
4	2	3741	C	C6-N1-C2	-6.48	117.71	120.30
4	2	2653	C	C6-N1-C2	-6.48	117.71	120.30
4	2	2856	C	C6-N1-C2	-6.47	117.71	120.30
4	2	2860	C	C2-N1-C1'	6.47	125.92	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	2	489	C	C5-C6-N1	6.47	124.23	121.00
4	2	4471	U	N3-C2-O2	-6.47	117.67	122.20
4	2	2094	G	C4-N9-C1'	6.47	134.91	126.50
4	2	985	C	C5-C6-N1	6.46	124.23	121.00
4	2	4972	U	N1-C2-O2	6.46	127.32	122.80
4	2	1582	U	N1-C2-O2	6.46	127.32	122.80
4	2	2792	C	C6-N1-C2	-6.45	117.72	120.30
4	2	4766	C	N1-C2-O2	6.45	122.77	118.90
4	2	972	C	N3-C2-O2	-6.44	117.39	121.90
4	2	1267	C	N1-C2-O2	6.43	122.76	118.90
4	2	4627	U	N3-C2-O2	-6.43	117.70	122.20
4	2	2371	U	N1-C2-O2	6.43	127.30	122.80
4	2	44	A	C2-N3-C4	6.42	113.81	110.60
4	2	4237	C	C6-N1-C2	-6.42	117.73	120.30
4	2	1720	C	C5-C6-N1	6.42	124.21	121.00
4	2	1378	C	C2-N1-C1'	6.42	125.86	118.80
4	2	2031	C	N1-C2-O2	6.41	122.75	118.90
4	2	1315	C	C6-N1-C2	-6.41	117.74	120.30
4	2	4752	U	N1-C2-O2	6.41	127.28	122.80
4	2	3741	C	N3-C2-O2	-6.40	117.42	121.90
6	5	78	C	C6-N1-C2	-6.40	117.74	120.30
6	5	15	C	C6-N1-C2	-6.40	117.74	120.30
4	2	924	C	N3-C2-O2	-6.39	117.43	121.90
4	2	26	C	N3-C2-O2	-6.38	117.43	121.90
4	2	4766	C	C2-N1-C1'	6.38	125.81	118.80
4	2	2072	C	C5-C6-N1	6.37	124.19	121.00
4	2	4342	C	N3-C2-O2	-6.37	117.44	121.90
4	2	4522	G	C4-N9-C1'	6.37	134.78	126.50
4	2	2478	C	C2-N1-C1'	6.37	125.81	118.80
4	2	985	C	N1-C2-O2	6.37	122.72	118.90
4	2	4945	G	N3-C4-N9	6.37	129.82	126.00
13	E	103	ASP	CB-CG-OD2	6.37	124.03	118.30
4	2	2867	C	C6-N1-C2	-6.36	117.75	120.30
4	2	4171	C	C5-C6-N1	6.35	124.18	121.00
4	2	4601	U	N1-C2-O2	6.35	127.25	122.80
4	2	3636	C	C5-C6-N1	6.35	124.17	121.00
6	5	102	U	N3-C2-O2	-6.35	117.76	122.20
4	2	209	U	N3-C2-O2	-6.35	117.76	122.20
4	2	173	C	N1-C2-O2	6.34	122.71	118.90
4	2	2362	U	C2-N1-C1'	6.34	125.31	117.70
4	2	4361	U	N3-C2-O2	-6.33	117.77	122.20
4	2	963	G	C4-N9-C1'	6.33	134.73	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	2	3622	C	N3-C2-O2	-6.33	117.47	121.90
4	2	86	U	N3-C2-O2	-6.33	117.77	122.20
4	2	2532	C	N1-C2-O2	6.33	122.69	118.90
4	2	1469	C	C6-N1-C2	-6.32	117.77	120.30
4	2	2560	C	C2-N1-C1'	6.32	125.75	118.80
4	2	3711	A	C2-N3-C4	6.32	113.76	110.60
47	z	29	LEU	CB-CG-CD1	6.32	121.74	111.00
4	2	2856	C	N3-C2-O2	-6.31	117.48	121.90
4	2	4469	U	N3-C2-O2	-6.31	117.78	122.20
4	2	242	U	C6-N1-C2	-6.30	117.22	121.00
4	2	4352	U	N3-C2-O2	-6.30	117.79	122.20
4	2	4341	C	C6-N1-C2	-6.30	117.78	120.30
4	2	1702	C	N3-C2-O2	-6.29	117.50	121.90
4	2	4887	C	C2-N1-C1'	6.29	125.72	118.80
4	2	679	C	C6-N1-C2	-6.29	117.78	120.30
4	2	977	C	N1-C2-O2	6.29	122.67	118.90
4	2	3698	G	C4-N9-C1'	6.29	134.67	126.50
4	2	2325	C	N3-C2-O2	-6.28	117.50	121.90
4	2	4758	U	C6-N1-C1'	-6.28	112.40	121.20
4	2	28	C	C6-N1-C2	-6.28	117.79	120.30
4	2	3851	U	N3-C2-O2	-6.28	117.80	122.20
4	2	4308	C	C6-N1-C2	-6.28	117.79	120.30
4	2	1405	C	N3-C2-O2	-6.28	117.50	121.90
4	2	4147	G	N1-C6-O6	-6.28	116.13	119.90
4	2	4162	C	C2-N1-C1'	6.28	125.70	118.80
4	2	2845	A	C2-N3-C4	6.28	113.74	110.60
6	5	28	C	N3-C2-O2	-6.28	117.51	121.90
4	2	271	C	C6-N1-C2	-6.27	117.79	120.30
4	2	3631	U	N1-C2-O2	6.27	127.19	122.80
4	2	4601	U	N3-C2-O2	-6.27	117.81	122.20
4	2	3698	G	N3-C4-N9	6.26	129.76	126.00
4	2	1672	U	N3-C2-O2	-6.26	117.82	122.20
6	5	24	C	N3-C2-O2	-6.26	117.52	121.90
4	2	4996	C	C6-N1-C2	-6.26	117.80	120.30
4	2	4308	C	N3-C2-O2	-6.25	117.52	121.90
4	2	131	C	C6-N1-C2	-6.25	117.80	120.30
4	2	1901	C	C6-N1-C2	-6.25	117.80	120.30
4	2	174	C	N1-C2-O2	6.25	122.65	118.90
4	2	4714	C	C5-C6-N1	6.25	124.12	121.00
4	2	1315	C	C5-C6-N1	6.24	124.12	121.00
4	2	1856	C	O5'-P-OP2	-6.24	100.09	105.70
4	2	3657	U	N3-C2-O2	-6.24	117.84	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	2	1884	C	C6-N1-C2	-6.23	117.81	120.30
53	8	80	A	C2-N3-C4	6.22	113.71	110.60
4	2	180	C	C6-N1-C2	-6.22	117.81	120.30
4	2	1577	G	C2-N3-C4	6.22	115.01	111.90
4	2	1655	C	C5-C6-N1	6.22	124.11	121.00
4	2	3767	C	N1-C2-O2	6.22	122.63	118.90
4	2	4694	G	N3-C4-C5	-6.21	125.49	128.60
4	2	2445	C	N3-C2-O2	-6.21	117.55	121.90
4	2	3926	C	N3-C2-O2	-6.21	117.55	121.90
4	2	1809	C	C6-N1-C2	-6.21	117.82	120.30
4	2	1577	G	N3-C2-N2	-6.20	115.56	119.90
4	2	274	C	N1-C2-O2	6.19	122.61	118.90
4	2	4970	C	C6-N1-C2	-6.19	117.83	120.30
4	2	4130	C	C5-C6-N1	6.18	124.09	121.00
4	2	2615	C	N1-C2-O2	6.18	122.61	118.90
4	2	1096	C	C5-C6-N1	6.18	124.09	121.00
4	2	4880	C	C2-N1-C1'	6.18	125.59	118.80
6	5	44	C	N1-C2-O2	6.18	122.61	118.90
4	2	4682	U	C2-N1-C1'	6.17	125.11	117.70
4	2	4710	C	C6-N1-C2	-6.17	117.83	120.30
4	2	4069	U	N3-C2-O2	-6.16	117.89	122.20
4	2	5008	C	N1-C2-O2	6.16	122.60	118.90
4	2	1477	C	C6-N1-C2	-6.16	117.84	120.30
4	2	30	C	C2-N1-C1'	6.15	125.57	118.80
4	2	516	C	C6-N1-C1'	-6.15	113.42	120.80
4	2	4561	C	C6-N1-C2	-6.15	117.84	120.30
4	2	2837	U	N1-C2-O2	6.14	127.10	122.80
53	8	28	C	C6-N1-C2	-6.14	117.84	120.30
4	2	282	C	C6-N1-C2	-6.14	117.84	120.30
4	2	926	G	N3-C4-N9	6.14	129.68	126.00
4	2	2850	A	C2-N3-C4	6.14	113.67	110.60
19	L	117	LEU	CA-CB-CG	6.14	129.42	115.30
4	2	449	C	N3-C2-O2	-6.14	117.60	121.90
4	2	4555	U	P-O3'-C3'	6.13	127.06	119.70
4	2	643	C	C5-C6-N1	6.13	124.06	121.00
4	2	2539	C	N1-C2-O2	6.13	122.58	118.90
4	2	3882	C	C2-N1-C1'	6.12	125.54	118.80
53	8	101	C	N1-C2-O2	6.12	122.57	118.90
4	2	2548	C	C5-C6-N1	6.12	124.06	121.00
53	8	101	C	C6-N1-C2	-6.12	117.85	120.30
4	2	2820	C	C2-N1-C1'	6.12	125.53	118.80
4	2	3851	U	N1-C2-O2	6.12	127.08	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	2	173	C	N3-C2-O2	-6.11	117.62	121.90
4	2	4709	U	C6-N1-C2	-6.11	117.33	121.00
4	2	68	U	N3-C2-O2	-6.11	117.92	122.20
4	2	2791	C	C6-N1-C2	-6.11	117.86	120.30
4	2	1726	U	C2-N1-C1'	6.10	125.02	117.70
4	2	3650	C	C5-C6-N1	6.10	124.05	121.00
4	2	1081	C	N1-C2-O2	6.10	122.56	118.90
54	W	33	LEU	CA-CB-CG	6.09	129.31	115.30
4	2	204	U	N3-C2-O2	-6.09	117.94	122.20
4	2	2486	G	OP1-P-O3'	6.09	118.60	105.20
4	2	4387	C	N1-C2-O2	6.09	122.55	118.90
17	I	104	VAL	CG1-CB-CG2	-6.09	101.16	110.90
4	2	1429	C	C6-N1-C2	-6.08	117.87	120.30
4	2	4926	C	C5-C6-N1	6.08	124.04	121.00
4	2	1816	C	C6-N1-C2	-6.08	117.87	120.30
4	2	3698	G	N3-C4-C5	-6.08	125.56	128.60
4	2	386	A	C2-N3-C4	6.08	113.64	110.60
4	2	1099	C	C6-N1-C2	-6.08	117.87	120.30
4	2	3670	C	C6-N1-C2	-6.08	117.87	120.30
4	2	4773	C	C5-C6-N1	6.07	124.03	121.00
4	2	1644	C	C6-N1-C2	-6.07	117.87	120.30
4	2	3831	U	N3-C2-O2	-6.07	117.95	122.20
4	2	1672	U	N1-C2-O2	6.06	127.05	122.80
4	2	2351	C	N1-C2-O2	6.06	122.54	118.90
4	2	3693	U	N1-C2-O2	6.06	127.05	122.80
4	2	220	C	C2-N1-C1'	6.06	125.47	118.80
4	2	1993	C	C2-N1-C1'	6.05	125.46	118.80
4	2	2843	U	N3-C2-O2	-6.05	117.96	122.20
4	2	2418	A	N7-C8-N9	6.05	116.83	113.80
4	2	712	C	C6-N1-C2	-6.05	117.88	120.30
4	2	3693	U	N3-C2-O2	-6.05	117.97	122.20
4	2	4710	C	C5-C6-N1	6.05	124.02	121.00
53	8	32	C	N1-C2-O2	6.05	122.53	118.90
4	2	4773	C	N1-C2-O2	6.04	122.53	118.90
4	2	1197	C	C6-N1-C2	-6.04	117.88	120.30
4	2	2560	C	N1-C2-O2	6.04	122.52	118.90
4	2	2589	C	C5-C6-N1	6.04	124.02	121.00
4	2	4596	C	N1-C2-O2	6.03	122.52	118.90
2	t	115	LEU	CA-CB-CG	6.03	129.17	115.30
4	2	3840	U	N3-C2-O2	-6.03	117.98	122.20
53	8	55	U	N1-C2-O2	6.03	127.02	122.80
4	2	2560	C	C5-C6-N1	6.02	124.01	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	5	24	C	C5-C6-N1	6.02	124.01	121.00
4	2	3702	A	C2-N3-C4	6.02	113.61	110.60
4	2	209	U	N1-C2-O2	6.01	127.01	122.80
4	2	1289	C	N3-C2-O2	-6.01	117.69	121.90
4	2	390	C	C6-N1-C2	-6.01	117.90	120.30
4	2	1662	C	C6-N1-C2	-6.00	117.90	120.30
4	2	4504	C	C6-N1-C2	-6.00	117.90	120.30
4	2	281	U	N1-C2-O2	6.00	127.00	122.80
4	2	365	U	C2-N1-C1'	6.00	124.90	117.70
4	2	2281	U	C2-N1-C1'	6.00	124.89	117.70
4	2	672	C	N3-C2-O2	-5.99	117.70	121.90
4	2	455	C	C6-N1-C2	-5.99	117.90	120.30
4	2	26	C	C2-N1-C1'	5.99	125.39	118.80
4	2	472	C	C5-C6-N1	5.99	124.00	121.00
4	2	977	C	C5-C6-N1	5.99	124.00	121.00
4	2	3618	C	C6-N1-C2	-5.99	117.91	120.30
4	2	3749	C	C6-N1-C2	-5.99	117.91	120.30
4	2	4469	U	N1-C2-O2	5.99	126.99	122.80
4	2	4505	C	N3-C2-O2	-5.99	117.71	121.90
4	2	4695	C	N1-C2-O2	5.99	122.49	118.90
4	2	2505	C	C6-N1-C1'	-5.98	113.62	120.80
34	d	56	LEU	CA-CB-CG	5.98	129.06	115.30
4	2	3772	U	C2-N1-C1'	5.98	124.88	117.70
4	2	4627	U	N1-C2-O2	5.98	126.99	122.80
4	2	4878	C	C6-N1-C2	-5.98	117.91	120.30
4	2	4299	U	N3-C2-O2	-5.98	118.02	122.20
46	r	103	LEU	CA-CB-CG	5.97	129.04	115.30
4	2	1809	C	C2-N1-C1'	5.97	125.37	118.80
4	2	4714	C	N3-C2-O2	-5.97	117.72	121.90
4	2	2337	C	C6-N1-C2	-5.96	117.91	120.30
4	2	4147	G	C5-C6-O6	5.96	132.18	128.60
53	8	101	C	C2-N1-C1'	5.96	125.36	118.80
4	2	3870	C	C6-N1-C2	-5.96	117.92	120.30
4	2	2062	C	C6-N1-C2	-5.96	117.92	120.30
4	2	4471	U	N1-C2-O2	5.96	126.97	122.80
4	2	3926	C	C5-C6-N1	5.95	123.98	121.00
4	2	472	C	C2-N1-C1'	5.95	125.34	118.80
4	2	907	C	N1-C2-O2	5.95	122.47	118.90
4	2	2820	C	C5-C6-N1	5.95	123.97	121.00
47	z	29	LEU	CA-CB-CG	5.95	128.98	115.30
5	4	503	THR	C-N-CA	5.95	136.57	121.70
4	2	4136	G	N1-C6-O6	-5.95	116.33	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	2	4700	A	C2-N3-C4	5.95	113.57	110.60
4	2	1264	C	C6-N1-C2	-5.94	117.92	120.30
4	2	1978	C	C2-N1-C1'	5.94	125.33	118.80
4	2	4694	G	C2-N3-C4	5.94	114.87	111.90
4	2	2000	G	C4-N9-C1'	5.94	134.22	126.50
4	2	2625	U	N3-C2-O2	-5.94	118.04	122.20
4	2	4350	C	C6-N1-C2	-5.94	117.92	120.30
4	2	4289	U	N1-C2-O2	5.93	126.95	122.80
4	2	4453	C	C6-N1-C1'	-5.92	113.69	120.80
4	2	4561	C	C2-N1-C1'	5.92	125.31	118.80
44	o	106	VAL	CG1-CB-CG2	-5.92	101.43	110.90
4	2	516	C	C2-N3-C4	5.91	122.85	119.90
4	2	3831	U	N1-C2-O2	5.91	126.94	122.80
4	2	1633	G	P-O3'-C3'	5.91	126.79	119.70
5	4	72	LEU	CA-CB-CG	5.91	128.88	115.30
4	2	1978	C	C5-C6-N1	5.90	123.95	121.00
4	2	2777	G	N3-C4-C5	-5.90	125.65	128.60
35	e	90	ARG	C-N-CA	5.90	136.45	121.70
4	2	704	C	C2-N1-C1'	5.90	125.29	118.80
4	2	696	C	C6-N1-C2	-5.90	117.94	120.30
4	2	1243	C	N1-C2-O2	5.90	122.44	118.90
4	2	1428	U	N3-C2-O2	-5.89	118.07	122.20
4	2	1963	C	N1-C2-O2	5.89	122.44	118.90
4	2	907	C	C2-N1-C1'	5.89	125.28	118.80
4	2	4508	C	C6-N1-C2	-5.89	117.94	120.30
4	2	1267	C	N3-C2-O2	-5.89	117.78	121.90
4	2	4365	C	C6-N1-C2	-5.89	117.94	120.30
4	2	1994	C	O4'-C1'-N1	5.88	112.91	108.20
4	2	1671	U	C6-N1-C2	-5.88	117.47	121.00
4	2	274	C	C5-C6-N1	5.88	123.94	121.00
4	2	3622	C	C6-N1-C2	-5.88	117.95	120.30
4	2	2014	C	N1-C2-O2	5.88	122.43	118.90
4	2	2033	A	N1-C2-N3	-5.88	126.36	129.30
6	5	29	C	N1-C2-O2	5.88	122.43	118.90
4	2	712	C	C5-C6-N1	5.88	123.94	121.00
4	2	2373	C	C6-N1-C2	-5.87	117.95	120.30
4	2	2886	U	N3-C2-O2	-5.87	118.09	122.20
4	2	421	C	C6-N1-C2	-5.87	117.95	120.30
4	2	2372	U	N3-C2-O2	-5.86	118.09	122.20
4	2	907	C	C6-N1-C2	-5.86	117.95	120.30
4	2	2853	C	N3-C2-O2	-5.86	117.80	121.90
4	2	4764	A	N1-C2-N3	-5.86	126.37	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	2	289	C	C6-N1-C2	-5.86	117.96	120.30
6	5	44	C	C6-N1-C2	-5.86	117.96	120.30
4	2	1577	G	C8-N9-C4	-5.85	104.06	106.40
4	2	2498	C	C6-N1-C2	-5.85	117.96	120.30
4	2	2002	A	C2-N3-C4	5.85	113.53	110.60
6	5	103	A	C2-N3-C4	5.85	113.53	110.60
4	2	1243	C	C5-C6-N1	5.85	123.92	121.00
4	2	1663	C	C5-C6-N1	5.85	123.92	121.00
4	2	3932	U	N3-C2-O2	-5.85	118.11	122.20
4	2	242	U	C2-N1-C1'	5.85	124.72	117.70
4	2	1720	C	N1-C2-O2	5.85	122.41	118.90
4	2	4303	C	N1-C2-O2	5.85	122.41	118.90
4	2	4771	C	N1-C2-O2	5.85	122.41	118.90
5	4	12	VAL	CA-CB-CG1	5.85	119.67	110.90
4	2	4476	C	N3-C2-O2	-5.84	117.81	121.90
4	2	2729	C	C6-N1-C2	-5.84	117.96	120.30
4	2	2821	U	N3-C2-O2	-5.84	118.11	122.20
4	2	4878	C	C5-C6-N1	5.84	123.92	121.00
4	2	1344	C	C6-N1-C2	-5.84	117.97	120.30
4	2	1540	C	C6-N1-C2	-5.84	117.97	120.30
4	2	2403	A	C2-N3-C4	5.84	113.52	110.60
4	2	71	C	C6-N1-C2	-5.83	117.97	120.30
4	2	148	C	C6-N1-C2	-5.83	117.97	120.30
4	2	2496	G	P-O3'-C3'	5.83	126.70	119.70
4	2	4262	C	N3-C2-O2	-5.83	117.82	121.90
4	2	971	U	N1-C2-O2	5.83	126.88	122.80
4	2	50	C	C5-C6-N1	5.82	123.91	121.00
4	2	446	C	C6-N1-C2	-5.82	117.97	120.30
4	2	204	U	N1-C2-O2	5.82	126.88	122.80
4	2	4215	C	C5-C6-N1	5.82	123.91	121.00
4	2	4699	U	OP1-P-O3'	5.82	118.01	105.20
4	2	1809	C	N1-C2-O2	5.82	122.39	118.90
4	2	3866	C	C6-N1-C2	-5.82	117.97	120.30
4	2	3893	C	C6-N1-C2	-5.81	117.97	120.30
4	2	180	C	C5-C6-N1	5.81	123.91	121.00
4	2	4773	C	C2-N1-C1'	5.81	125.19	118.80
4	2	963	G	N3-C4-C5	-5.81	125.70	128.60
5	4	369	ASP	CB-CG-OD1	5.81	123.53	118.30
49	R	143	PHE	CB-CG-CD1	5.80	124.86	120.80
4	2	1894	C	C6-N1-C2	-5.80	117.98	120.30
4	2	1963	C	C2-N1-C1'	5.79	125.17	118.80
4	2	4350	C	N1-C2-O2	5.79	122.38	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	2	988	C	C5-C6-N1	5.79	123.90	121.00
4	2	3866	C	C5-C6-N1	5.79	123.89	121.00
4	2	4069	U	N1-C2-O2	5.79	126.85	122.80
4	2	1703	C	C2-N1-C1'	5.79	125.17	118.80
4	2	2008	U	C2-N1-C1'	5.79	124.65	117.70
4	2	4613	C	C2-N1-C1'	5.79	125.17	118.80
4	2	100	C	O4'-C1'-N1	5.79	112.83	108.20
4	2	2410	C	N3-C2-O2	-5.79	117.85	121.90
24	Q	17	ASP	CB-CG-OD2	5.79	123.51	118.30
4	2	1637	A	N1-C2-N3	-5.78	126.41	129.30
4	2	963	G	N3-C4-N9	5.78	129.47	126.00
4	2	2325	C	N1-C2-O2	5.78	122.36	118.90
4	2	1893	C	N1-C2-O2	5.77	122.36	118.90
4	2	1913	C	C6-N1-C2	-5.77	117.99	120.30
4	2	688	U	N1-C2-O2	5.77	126.84	122.80
4	2	2593	C	C6-N1-C2	-5.77	117.99	120.30
53	8	123	U	C2-N1-C1'	5.77	124.62	117.70
4	2	1929	A	C8-N9-C1'	-5.77	117.32	127.70
6	5	52	C	C6-N1-C2	-5.76	117.99	120.30
4	2	1467	C	C6-N1-C2	-5.76	118.00	120.30
4	2	271	C	C5-C6-N1	5.76	123.88	121.00
4	2	4864	U	C2-N1-C1'	5.76	124.61	117.70
4	2	2497	C	C6-N1-C2	-5.75	118.00	120.30
4	2	1395	U	N3-C2-O2	-5.75	118.17	122.20
4	2	5035	U	N1-C2-O2	5.75	126.83	122.80
4	2	4364	G	N3-C4-C5	-5.75	125.72	128.60
4	2	1469	C	C5-C6-N1	5.75	123.87	121.00
4	2	4708	A	C2-N3-C4	5.75	113.47	110.60
4	2	2528	G	C2-N3-C4	5.74	114.77	111.90
4	2	4123	C	N3-C2-O2	-5.74	117.88	121.90
4	2	4758	U	O4'-C1'-N1	5.74	112.79	108.20
4	2	4289	U	N3-C2-O2	-5.74	118.18	122.20
4	2	2505	C	C6-N1-C2	-5.74	118.00	120.30
4	2	4969	C	C5-C6-N1	5.74	123.87	121.00
4	2	1906	U	N3-C2-O2	-5.74	118.19	122.20
4	2	4319	C	C6-N1-C2	-5.74	118.01	120.30
6	5	80	U	N3-C2-O2	-5.74	118.19	122.20
4	2	124	C	C6-N1-C2	-5.73	118.01	120.30
4	2	499	G	N3-C4-C5	-5.73	125.73	128.60
4	2	972	C	C5-C6-N1	5.73	123.87	121.00
4	2	2096	G	N3-C4-N9	5.73	129.44	126.00
4	2	4303	C	N3-C2-O2	-5.73	117.89	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	8	32	C	N3-C2-O2	-5.73	117.89	121.90
4	2	1381	U	N3-C2-O2	-5.73	118.19	122.20
26	U	164	LEU	CA-CB-CG	5.73	128.47	115.30
4	2	4352	U	N1-C2-O2	5.72	126.81	122.80
4	2	14	C	C6-N1-C2	-5.72	118.01	120.30
4	2	1447	C	C6-N1-C2	-5.72	118.01	120.30
4	2	1632	A	N1-C2-N3	-5.72	126.44	129.30
4	2	2814	C	N3-C2-O2	-5.72	117.89	121.90
53	8	51	U	N3-C2-O2	-5.72	118.19	122.20
4	2	1628	C	C6-N1-C2	-5.72	118.01	120.30
4	2	2094	G	N3-C4-C5	-5.72	125.74	128.60
4	2	1579	C	C6-N1-C2	-5.72	118.01	120.30
4	2	4747	C	N3-C2-O2	-5.72	117.90	121.90
10	B	308	ASP	CB-CG-OD1	5.72	123.44	118.30
6	5	2	U	N3-C2-O2	-5.71	118.20	122.20
4	2	345	C	C6-N1-C2	-5.71	118.02	120.30
4	2	1644	C	C5-C6-N1	5.71	123.86	121.00
4	2	2892	C	N1-C2-O2	5.71	122.33	118.90
53	8	43	A	C2-N3-C4	5.71	113.45	110.60
4	2	4341	C	N3-C2-O2	-5.71	117.90	121.90
50	J	162	LEU	CA-CB-CG	5.71	128.43	115.30
4	2	1183	C	C2-N1-C1'	5.71	125.08	118.80
4	2	4981	G	N3-C4-N9	5.70	129.42	126.00
4	2	1921	C	C2-N1-C1'	5.70	125.07	118.80
4	2	4508	C	C5-C6-N1	5.70	123.85	121.00
4	2	4562	C	C6-N1-C2	-5.70	118.02	120.30
4	2	3939	G	N3-C4-C5	-5.70	125.75	128.60
4	2	2814	C	C2-N1-C1'	5.69	125.06	118.80
4	2	1731	C	C2-N1-C1'	5.69	125.06	118.80
4	2	467	U	C5-C6-N1	5.69	125.55	122.70
4	2	4406	U	C2-N1-C1'	5.69	124.52	117.70
4	2	86	U	N1-C2-O2	5.68	126.78	122.80
4	2	2281	U	C5-C6-N1	5.68	125.54	122.70
4	2	2684	C	C6-N1-C2	-5.68	118.03	120.30
4	2	1244	G	C4-N9-C1'	5.68	133.88	126.50
4	2	4136	G	C5-C6-O6	5.68	132.01	128.60
4	2	4771	C	C2-N1-C1'	5.68	125.04	118.80
4	2	36	U	N3-C2-O2	-5.67	118.23	122.20
4	2	1190	C	N1-C2-O2	5.67	122.31	118.90
4	2	4662	C	C6-N1-C2	-5.67	118.03	120.30
5	4	21	LEU	CA-CB-CG	5.67	128.35	115.30
53	8	125	C	OP1-P-O3'	5.67	117.68	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	2	3831	U	C2-N1-C1'	5.67	124.51	117.70
4	2	1703	C	N3-C2-O2	-5.67	117.93	121.90
4	2	2892	C	C5-C6-N1	5.67	123.83	121.00
4	2	1458	C	C6-N1-C2	-5.67	118.03	120.30
4	2	2726	G	N3-C4-C5	-5.67	125.77	128.60
4	2	78	U	N3-C2-O2	-5.66	118.24	122.20
4	2	1245	C	C5-C6-N1	5.66	123.83	121.00
4	2	719	C	C5-C6-N1	5.66	123.83	121.00
4	2	4229	U	C2-N1-C1'	5.66	124.49	117.70
4	2	4945	G	C4-N9-C1'	5.66	133.85	126.50
4	2	4233	A	C2-N3-C4	5.66	113.43	110.60
4	2	201	C	N1-C2-O2	5.66	122.29	118.90
4	2	322	C	C5-C6-N1	5.66	123.83	121.00
4	2	1077	C	C6-N1-C2	-5.66	118.04	120.30
53	8	82	A	C2-N3-C4	5.66	113.43	110.60
4	2	4928	C	C6-N1-C1'	-5.65	114.02	120.80
34	d	23	LEU	CA-CB-CG	5.65	128.30	115.30
4	2	654	C	C2-N1-C1'	5.65	125.02	118.80
4	2	925	C	C5-C6-N1	5.65	123.83	121.00
4	2	1663	C	C6-N1-C2	-5.65	118.04	120.30
4	2	201	C	C5-C6-N1	5.65	123.82	121.00
4	2	926	G	N3-C4-C5	-5.65	125.78	128.60
53	8	107	C	C6-N1-C2	-5.65	118.04	120.30
4	2	2478	C	N1-C2-O2	5.64	122.29	118.90
4	2	3882	C	C5-C6-N1	5.64	123.82	121.00
4	2	1915	C	C2-N1-C1'	5.64	125.00	118.80
4	2	4712	C	C5-C6-N1	5.64	123.82	121.00
4	2	221	C	C6-N1-C2	-5.63	118.05	120.30
4	2	4522	G	N3-C4-N9	5.63	129.38	126.00
4	2	2031	C	C5-C6-N1	5.63	123.81	121.00
53	8	135	C	C2-N1-C1'	5.63	124.99	118.80
4	2	100	C	C5-C6-N1	5.63	123.81	121.00
4	2	5030	U	C5-C6-N1	5.63	125.51	122.70
4	2	152	U	N3-C2-O2	-5.63	118.26	122.20
4	2	30	C	N1-C2-O2	5.62	122.27	118.90
4	2	4303	C	C6-N1-C2	-5.62	118.05	120.30
4	2	4343	U	N3-C2-O2	-5.62	118.27	122.20
4	2	4628	U	N3-C2-O2	-5.62	118.27	122.20
4	2	688	U	N3-C2-O2	-5.62	118.27	122.20
4	2	4709	U	C5-C6-N1	5.62	125.51	122.70
4	2	1429	C	N1-C2-O2	5.61	122.27	118.90
4	2	673	C	C5-C6-N1	5.61	123.81	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	2	1572	U	N3-C2-O2	-5.61	118.28	122.20
4	2	4346	U	N3-C2-O2	-5.61	118.27	122.20
4	2	4137	C	N3-C2-O2	-5.61	117.98	121.90
4	2	3749	C	C5-C6-N1	5.60	123.80	121.00
4	2	4522	G	N3-C4-C5	-5.60	125.80	128.60
4	2	110	C	C6-N1-C2	-5.60	118.06	120.30
4	2	1856	C	OP1-P-OP2	-5.60	111.20	119.60
4	2	2337	C	N1-C2-O2	5.60	122.26	118.90
4	2	2439	G	C4-C5-N7	5.60	113.04	110.80
4	2	1809	C	C5-C6-N1	5.60	123.80	121.00
4	2	4639	G	N3-C4-C5	-5.60	125.80	128.60
4	2	2031	C	C2-N1-C1'	5.59	124.95	118.80
4	2	1183	C	C5-C6-N1	5.59	123.80	121.00
4	2	3770	U	N1-C2-O2	5.59	126.71	122.80
53	8	135	C	C5-C6-N1	5.59	123.80	121.00
4	2	2783	A	N1-C2-N3	-5.59	126.50	129.30
4	2	4895	C	C2-N1-C1'	5.58	124.94	118.80
4	2	703	G	C4-N9-C1'	5.58	133.76	126.50
4	2	4886	C	N1-C2-O2	5.58	122.25	118.90
5	4	278	LEU	CA-CB-CG	5.58	128.14	115.30
4	2	2077	C	C6-N1-C2	-5.58	118.07	120.30
4	2	2627	C	C5-C6-N1	5.58	123.79	121.00
4	2	4314	C	C5-C6-N1	5.58	123.79	121.00
53	8	99	U	C2-N1-C1'	5.58	124.39	117.70
4	2	2264	C	C6-N1-C2	-5.57	118.07	120.30
4	2	4294	C	C5-C6-N1	5.57	123.79	121.00
6	5	39	C	N3-C2-O2	-5.57	118.00	121.90
53	8	54	C	C5-C6-N1	5.57	123.79	121.00
4	2	4683	U	N1-C2-O2	5.57	126.70	122.80
4	2	1405	C	C6-N1-C2	-5.57	118.07	120.30
4	2	1666	C	C6-N1-C2	-5.57	118.07	120.30
4	2	2094	G	N3-C4-N9	5.57	129.34	126.00
4	2	914	U	C5-C4-O4	-5.57	122.56	125.90
6	5	14	C	N1-C2-O2	5.57	122.24	118.90
4	2	4991	U	N3-C2-O2	-5.57	118.30	122.20
26	U	134	LEU	CA-CB-CG	5.57	128.11	115.30
4	2	1418	C	C6-N1-C2	-5.56	118.07	120.30
4	2	5008	C	C5-C6-N1	5.56	123.78	121.00
4	2	2689	C	C6-N1-C2	-5.56	118.08	120.30
4	2	1079	C	N3-C2-O2	-5.56	118.01	121.90
4	2	1381	U	N1-C2-O2	5.56	126.69	122.80
4	2	1929	A	N3-C4-N9	5.56	131.85	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	2	385	A	N1-C2-N3	-5.56	126.52	129.30
4	2	3636	C	C2-N1-C1'	5.56	124.91	118.80
4	2	4387	C	N3-C2-O2	-5.56	118.01	121.90
4	2	1572	U	N1-C2-O2	5.56	126.69	122.80
4	2	2625	U	N1-C2-O2	5.56	126.69	122.80
4	2	4628	U	N1-C2-O2	5.55	126.69	122.80
50	J	238	ASP	N-CA-C	-5.55	96.00	111.00
53	8	51	U	N1-C2-O2	5.55	126.69	122.80
6	5	2	U	N1-C2-O2	5.55	126.69	122.80
4	2	3668	C	C2-N1-C1'	5.55	124.91	118.80
4	2	9	C	C5-C6-N1	5.55	123.77	121.00
4	2	2439	G	N9-C4-C5	-5.54	103.18	105.40
53	8	128	C	C6-N1-C2	-5.54	118.08	120.30
4	2	1245	C	C6-N1-C2	-5.54	118.08	120.30
4	2	2096	G	N3-C4-C5	-5.54	125.83	128.60
4	2	2290	C	C6-N1-C2	-5.54	118.08	120.30
4	2	2303	C	C6-N1-C2	-5.54	118.08	120.30
4	2	4361	U	N1-C2-O2	5.54	126.68	122.80
4	2	4456	C	N1-C2-O2	5.54	122.22	118.90
4	2	2821	U	N1-C2-O2	5.54	126.67	122.80
4	2	67	C	C6-N1-C2	-5.53	118.09	120.30
4	2	1735	U	N3-C2-O2	-5.52	118.34	122.20
4	2	1078	A	C2-N3-C4	5.52	113.36	110.60
4	2	4683	U	N3-C2-O2	-5.52	118.34	122.20
4	2	4958	C	N3-C2-O2	-5.52	118.04	121.90
3	3	132	VAL	C-N-CA	5.51	135.49	121.70
48	A	163	LEU	CA-CB-CG	5.51	127.98	115.30
4	2	14	C	N1-C2-O2	5.51	122.21	118.90
4	2	141	C	N1-C2-O2	5.51	122.21	118.90
4	2	2548	C	N3-C2-O2	-5.51	118.04	121.90
4	2	1367	C	N1-C2-O2	5.51	122.21	118.90
50	J	149	MET	CA-CB-CG	5.51	122.67	113.30
4	2	694	C	C6-N1-C2	-5.50	118.10	120.30
4	2	1298	C	C6-N1-C2	-5.50	118.10	120.30
4	2	1293	G	C4-N9-C1'	5.50	133.65	126.50
4	2	122	U	N3-C2-O2	-5.50	118.35	122.20
4	2	2856	C	C5-C6-N1	5.50	123.75	121.00
4	2	3905	A	OP2-P-O3'	5.50	117.29	105.20
4	2	4923	C	N1-C2-O2	5.49	122.20	118.90
4	2	4880	C	C5-C6-N1	5.49	123.75	121.00
4	2	30	C	C5-C6-N1	5.49	123.74	121.00
4	2	2872	C	C6-N1-C2	-5.49	118.11	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	2	173	C	C6-N1-C2	-5.49	118.11	120.30
4	2	971	U	N3-C2-O2	-5.49	118.36	122.20
4	2	3587	C	C2-N1-C1'	5.49	124.83	118.80
4	2	4561	C	N1-C2-O2	5.49	122.19	118.90
4	2	2702	C	C6-N1-C2	-5.48	118.11	120.30
5	4	406	GLY	C-N-CA	5.48	135.41	121.70
2	t	55	LEU	CA-CB-CG	5.48	127.91	115.30
4	2	1993	C	C5-C6-N1	5.48	123.74	121.00
4	2	4596	C	N3-C2-O2	-5.48	118.06	121.90
4	2	1428	U	N1-C2-O2	5.48	126.64	122.80
4	2	2867	C	C2-N1-C1'	5.48	124.83	118.80
4	2	4619	U	N3-C2-O2	-5.48	118.36	122.20
4	2	185	C	C6-N1-C2	-5.47	118.11	120.30
4	2	1241	C	C6-N1-C1'	-5.47	114.23	120.80
4	2	4461	C	C6-N1-C2	-5.47	118.11	120.30
6	5	14	C	C2-N1-C1'	5.47	124.81	118.80
4	2	365	U	C6-N1-C2	-5.46	117.72	121.00
4	2	2403	A	N1-C2-N3	-5.46	126.57	129.30
4	2	4569	U	N3-C2-O2	-5.46	118.38	122.20
4	2	1197	C	C5-C6-N1	5.46	123.73	121.00
4	2	5042	A	C2-N3-C4	5.46	113.33	110.60
4	2	196	C	C6-N1-C2	-5.46	118.12	120.30
4	2	498	C	C6-N1-C2	-5.46	118.12	120.30
4	2	4619	U	N1-C2-O2	5.46	126.62	122.80
4	2	1176	C	C5-C6-N1	5.46	123.73	121.00
4	2	4233	A	N1-C2-N3	-5.46	126.57	129.30
6	5	26	C	N1-C2-O2	5.46	122.17	118.90
4	2	123	C	C6-N1-C2	-5.45	118.12	120.30
6	5	42	A	C2-N3-C4	5.45	113.33	110.60
4	2	68	U	N1-C2-O2	5.45	126.61	122.80
4	2	4299	U	N1-C2-O2	5.45	126.61	122.80
4	2	115	C	C6-N1-C2	-5.45	118.12	120.30
4	2	1339	U	N3-C2-O2	-5.45	118.39	122.20
4	2	2073	C	C6-N1-C2	-5.44	118.12	120.30
4	2	4612	C	C5-C6-N1	5.44	123.72	121.00
4	2	2304	U	N1-C2-O2	5.44	126.61	122.80
36	g	147	LEU	CA-CB-CG	5.44	127.81	115.30
4	2	1310	C	C6-N1-C2	-5.44	118.12	120.30
4	2	4775	C	N1-C2-O2	5.44	122.16	118.90
4	2	449	C	C2-N1-C1'	5.44	124.78	118.80
4	2	4712	C	N1-C2-O2	5.44	122.16	118.90
4	2	2886	U	N1-C2-O2	5.43	126.60	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	2	3606	U	N3-C2-O2	-5.43	118.40	122.20
4	2	4594	U	N3-C2-O2	-5.43	118.40	122.20
4	2	2445	C	C5-C6-N1	5.43	123.72	121.00
8	7	123	ASP	CB-CG-OD1	5.43	123.19	118.30
4	2	390	C	C5-C6-N1	5.42	123.71	121.00
4	2	3604	A	C2-N3-C4	5.42	113.31	110.60
4	2	4958	C	N1-C2-O2	5.42	122.15	118.90
4	2	4928	C	N3-C2-O2	-5.42	118.11	121.90
5	4	391	GLU	C-N-CA	5.42	135.25	121.70
53	8	123	U	N1-C2-O2	5.42	126.59	122.80
4	2	4259	C	C6-N1-C2	-5.42	118.13	120.30
27	V	202	LEU	CA-CB-CG	5.42	127.76	115.30
4	2	2561	C	N1-C2-O2	5.42	122.15	118.90
4	2	979	C	C6-N1-C2	-5.41	118.14	120.30
4	2	2886	U	C2-N1-C1'	5.41	124.20	117.70
4	2	1821	G	N3-C4-C5	-5.41	125.90	128.60
4	2	4674	C	C6-N1-C2	-5.41	118.14	120.30
4	2	43	U	N3-C2-O2	-5.41	118.42	122.20
4	2	1402	C	C6-N1-C2	-5.41	118.14	120.30
4	2	2304	U	N3-C2-O2	-5.41	118.42	122.20
4	2	4505	C	C6-N1-C1'	-5.40	114.32	120.80
4	2	367	C	C5-C6-N1	5.40	123.70	121.00
4	2	2867	C	C5-C6-N1	5.40	123.70	121.00
4	2	3670	C	C2-N1-C1'	5.40	124.74	118.80
4	2	3739	C	N1-C2-O2	5.40	122.14	118.90
4	2	1081	C	N3-C2-O2	-5.40	118.12	121.90
4	2	1414	C	N1-C2-O2	5.40	122.14	118.90
4	2	2325	C	C6-N1-C2	-5.40	118.14	120.30
4	2	4412	C	C6-N1-C2	-5.40	118.14	120.30
4	2	7	C	C6-N1-C2	-5.40	118.14	120.30
4	2	2264	C	N3-C2-O2	-5.39	118.12	121.90
4	2	4120	U	N3-C2-O2	-5.39	118.42	122.20
4	2	131	C	C5-C6-N1	5.39	123.70	121.00
4	2	1686	C	C6-N1-C2	-5.39	118.14	120.30
4	2	2792	C	C5-C6-N1	5.39	123.70	121.00
4	2	4639	G	C4-N9-C1'	5.39	133.51	126.50
4	2	4213	A	N1-C2-N3	-5.39	126.60	129.30
4	2	1081	C	C6-N1-C2	-5.39	118.14	120.30
4	2	36	U	N1-C2-O2	5.38	126.57	122.80
4	2	1460	C	C6-N1-C2	-5.38	118.15	120.30
4	2	1991	A	C2-N3-C4	5.38	113.29	110.60
6	5	76	U	C2-N1-C1'	5.38	124.16	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	2	294	G	C4-N9-C1'	5.38	133.50	126.50
4	2	1276	C	C6-N1-C2	-5.38	118.15	120.30
4	2	2290	C	N1-C2-O2	5.38	122.13	118.90
4	2	1694	C	C6-N1-C2	-5.38	118.15	120.30
4	2	4319	C	C2-N1-C1'	5.38	124.71	118.80
4	2	3870	C	C5-C6-N1	5.37	123.69	121.00
4	2	4667	C	C6-N1-C2	-5.37	118.15	120.30
4	2	2096	G	C4-N9-C1'	5.37	133.48	126.50
4	2	655	C	C5-C6-N1	5.37	123.69	121.00
4	2	696	C	N1-C2-O2	5.37	122.12	118.90
4	2	4685	U	N3-C2-O2	-5.37	118.44	122.20
45	p	25	PHE	CB-CG-CD1	5.37	124.56	120.80
4	2	3590	G	N3-C4-N9	5.37	129.22	126.00
4	2	3694	U	N1-C2-O2	5.37	126.56	122.80
4	2	4682	U	C5-C6-N1	5.37	125.38	122.70
4	2	2036	C	C6-N1-C2	-5.36	118.15	120.30
4	2	3590	G	N3-C4-C5	-5.36	125.92	128.60
4	2	1906	U	N1-C2-O2	5.36	126.55	122.80
4	2	3882	C	N1-C2-O2	5.36	122.11	118.90
4	2	4120	U	C2-N1-C1'	5.36	124.13	117.70
4	2	3739	C	C2-N1-C1'	5.35	124.69	118.80
4	2	4981	G	C4-N9-C1'	5.35	133.46	126.50
4	2	906	C	C2-N1-C1'	5.35	124.69	118.80
16	H	82	ASP	CB-CG-OD1	-5.35	113.48	118.30
4	2	467	U	C6-N1-C2	-5.35	117.79	121.00
4	2	1202	C	C6-N1-C2	-5.35	118.16	120.30
4	2	2520	C	C6-N1-C2	-5.35	118.16	120.30
4	2	4639	G	N3-C4-N9	5.35	129.21	126.00
4	2	1538	U	N3-C2-O2	-5.34	118.46	122.20
4	2	4254	G	C4-N9-C1'	5.34	133.44	126.50
4	2	4563	U	N3-C2-O2	-5.34	118.46	122.20
4	2	679	C	C5-C6-N1	5.34	123.67	121.00
53	8	50	C	C6-N1-C2	-5.34	118.17	120.30
4	2	2094	G	C8-N9-C1'	-5.33	120.07	127.00
4	2	3698	G	C8-N9-C1'	-5.33	120.07	127.00
4	2	4710	C	C2-N1-C1'	5.33	124.67	118.80
4	2	2777	G	N3-C4-N9	5.33	129.20	126.00
4	2	125	C	C6-N1-C2	-5.33	118.17	120.30
4	2	694	C	N1-C2-O2	5.33	122.10	118.90
4	2	4504	C	C2-N1-C1'	5.33	124.66	118.80
4	2	2373	C	C5-C6-N1	5.33	123.66	121.00
4	2	1477	C	C2-N1-C1'	5.32	124.65	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	3	21	VAL	CA-CB-CG1	5.32	118.88	110.90
4	2	3877	A	N1-C2-N3	-5.32	126.64	129.30
4	2	4476	C	C6-N1-C2	-5.32	118.17	120.30
4	2	2392	C	C6-N1-C2	-5.32	118.17	120.30
4	2	3835	C	C5-C6-N1	5.32	123.66	121.00
4	2	1821	G	N3-C4-N9	5.32	129.19	126.00
4	2	2078	C	C6-N1-C2	-5.32	118.17	120.30
4	2	4112	C	C6-N1-C2	-5.32	118.17	120.30
4	2	4682	U	C6-N1-C2	-5.32	117.81	121.00
4	2	490	C	C6-N1-C2	-5.31	118.17	120.30
4	2	3692	A	C2-N3-C4	5.31	113.26	110.60
4	2	3770	U	N3-C2-O2	-5.31	118.48	122.20
4	2	673	C	N1-C2-O2	5.31	122.09	118.90
4	2	436	C	N1-C2-O2	5.31	122.09	118.90
4	2	1429	C	C2-N1-C1'	5.31	124.64	118.80
4	2	2615	C	N3-C2-O2	-5.30	118.19	121.90
4	2	3939	G	N3-C4-N9	5.30	129.18	126.00
53	8	4	C	C6-N1-C2	-5.30	118.18	120.30
4	2	1832	C	N1-C2-O2	5.30	122.08	118.90
44	o	100	LYS	CA-CB-CG	5.30	125.06	113.40
4	2	112	C	N3-C2-O2	-5.30	118.19	121.90
4	2	185	C	N1-C2-O2	5.30	122.08	118.90
4	2	2487	G	P-O3'-C3'	5.29	126.05	119.70
6	5	57	C	C6-N1-C2	-5.29	118.18	120.30
4	2	2096	G	C2-N3-C4	5.29	114.55	111.90
6	5	80	U	N1-C2-O2	5.29	126.50	122.80
4	2	456	C	C6-N1-C2	-5.29	118.18	120.30
4	2	1350	C	C6-N1-C2	-5.29	118.18	120.30
4	2	2653	C	C5-C6-N1	5.29	123.64	121.00
4	2	2026	A	N1-C6-N6	-5.29	115.43	118.60
4	2	1577	G	N1-C6-O6	-5.28	116.73	119.90
4	2	3668	C	N1-C2-O2	5.28	122.07	118.90
4	2	4653	C	C6-N1-C2	-5.28	118.19	120.30
4	2	1430	C	C6-N1-C2	-5.28	118.19	120.30
43	n	106	TYR	N-CA-C	5.28	125.25	111.00
4	2	2561	C	C6-N1-C2	-5.28	118.19	120.30
4	2	3605	C	C2-N1-C1'	5.27	124.60	118.80
4	2	1309	C	C5-C6-N1	5.27	123.64	121.00
6	5	111	C	C6-N1-C2	-5.27	118.19	120.30
4	2	332	C	N1-C2-O2	5.26	122.06	118.90
4	2	1725	U	N3-C2-O2	-5.26	118.52	122.20
4	2	1176	C	C2-N1-C1'	5.26	124.59	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	2	336	A	C2-N3-C4	5.26	113.23	110.60
4	2	1520	C	C6-N1-C2	-5.26	118.20	120.30
4	2	1580	C	C6-N1-C2	-5.26	118.20	120.30
4	2	2031	C	N3-C2-O2	-5.26	118.22	121.90
53	8	62	A	N1-C2-N3	-5.26	126.67	129.30
4	2	1947	U	C2-N1-C1'	5.25	124.01	117.70
4	2	2614	C	C6-N1-C2	-5.25	118.20	120.30
4	2	1429	C	C5-C6-N1	5.25	123.63	121.00
4	2	1690	C	C6-N1-C2	-5.25	118.20	120.30
4	2	2603	C	C6-N1-C2	-5.25	118.20	120.30
4	2	4561	C	C5-C6-N1	5.25	123.63	121.00
10	B	47	LEU	CA-CB-CG	5.25	127.38	115.30
25	S	135	LEU	CA-CB-CG	5.25	127.38	115.30
4	2	446	C	C2-N1-C1'	5.25	124.57	118.80
4	2	1794	A	C2-N3-C4	5.25	113.22	110.60
4	2	3835	C	C6-N1-C2	-5.25	118.20	120.30
4	2	4722	G	C4-N9-C1'	5.25	133.32	126.50
3	3	140	LEU	CA-CB-CG	5.25	127.36	115.30
4	2	436	C	C6-N1-C2	-5.24	118.20	120.30
4	2	4613	C	C5-C6-N1	5.24	123.62	121.00
37	h	82	ILE	CG1-CB-CG2	-5.24	99.87	111.40
4	2	35	U	N3-C2-O2	-5.24	118.53	122.20
4	2	1958	A	C4-N9-C1'	-5.24	116.87	126.30
4	2	4278	C	C6-N1-C2	-5.24	118.20	120.30
46	r	235	MET	CA-CB-CG	5.24	122.21	113.30
4	2	365	U	C5-C6-N1	5.24	125.32	122.70
4	2	2684	C	C5-C6-N1	5.24	123.62	121.00
4	2	2802	C	C6-N1-C2	-5.24	118.20	120.30
4	2	3858	C	C6-N1-C2	-5.24	118.20	120.30
4	2	53	C	C6-N1-C2	-5.24	118.20	120.30
4	2	4983	C	N3-C2-O2	-5.24	118.23	121.90
4	2	489	C	N3-C2-O2	-5.24	118.23	121.90
4	2	4923	C	C6-N1-C2	-5.24	118.21	120.30
37	h	112	ASP	CB-CG-OD1	5.24	123.01	118.30
4	2	41	C	C6-N1-C2	-5.23	118.21	120.30
6	5	78	C	C5-C6-N1	5.23	123.62	121.00
4	2	454	U	C2-N1-C1'	5.23	123.98	117.70
4	2	4711	C	C6-N1-C2	-5.23	118.21	120.30
6	5	118	C	C6-N1-C2	-5.23	118.21	120.30
4	2	1794	A	N1-C2-N3	-5.23	126.69	129.30
4	2	2262	G	C2-N3-C4	5.23	114.51	111.90
4	2	1099	C	C5-C6-N1	5.23	123.61	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	2	1979	A	C2-N3-C4	5.23	113.21	110.60
13	E	98	ASP	CB-CG-OD1	5.23	123.00	118.30
4	2	499	G	C6-C5-N7	-5.22	127.27	130.40
4	2	4614	G	N1-C6-O6	-5.22	116.77	119.90
4	2	1289	C	C6-N1-C2	-5.22	118.21	120.30
4	2	2367	A	N1-C2-N3	-5.22	126.69	129.30
4	2	2498	C	C2-N1-C1'	5.22	124.54	118.80
4	2	408	A	N1-C2-N3	-5.22	126.69	129.30
4	2	1662	C	C5-C6-N1	5.22	123.61	121.00
6	5	95	C	N1-C2-O2	5.22	122.03	118.90
4	2	1847	C	C6-N1-C2	-5.21	118.22	120.30
4	2	4996	C	C5-C6-N1	5.21	123.61	121.00
4	2	2689	C	C5-C6-N1	5.21	123.61	121.00
4	2	282	C	C2-N1-C1'	5.21	124.53	118.80
4	2	4927	G	N3-C4-C5	-5.21	126.00	128.60
4	2	1314	C	O5'-P-OP2	-5.21	101.02	105.70
4	2	1505	C	C6-N1-C2	-5.21	118.22	120.30
4	2	2592	U	C6-N1-C2	-5.21	117.88	121.00
53	8	96	C	N1-C2-O2	5.20	122.02	118.90
6	5	94	C	N1-C2-O2	5.20	122.02	118.90
4	2	683	C	N1-C2-O2	5.20	122.02	118.90
4	2	4486	C	N3-C2-O2	-5.20	118.26	121.90
50	J	218	MET	CA-CB-CG	5.20	122.14	113.30
4	2	2779	C	C6-N1-C2	-5.20	118.22	120.30
4	2	3926	C	C2-N1-C1'	5.20	124.52	118.80
4	2	1192	C	N1-C2-O2	5.19	122.02	118.90
4	2	4878	C	N1-C2-O2	5.19	122.02	118.90
4	2	2062	C	N1-C2-O2	5.19	122.01	118.90
4	2	2478	C	N3-C2-O2	-5.19	118.27	121.90
4	2	3668	C	C6-N1-C2	-5.19	118.22	120.30
3	3	96	LEU	CB-CG-CD2	5.19	119.82	111.00
4	2	1417	C	C6-N1-C2	-5.19	118.22	120.30
53	8	35	C	C6-N1-C2	-5.19	118.22	120.30
4	2	4883	C	C6-N1-C2	-5.18	118.23	120.30
4	2	2255	C	C6-N1-C2	-5.18	118.23	120.30
4	2	3741	C	C5-C6-N1	5.18	123.59	121.00
4	2	4464	A	C2-N3-C4	5.18	113.19	110.60
4	2	3901	A	C2-N3-C4	5.18	113.19	110.60
4	2	1707	C	C6-N1-C2	-5.18	118.23	120.30
4	2	4546	A	N1-C2-N3	-5.17	126.71	129.30
5	4	117	MET	CA-CB-CG	5.17	122.10	113.30
4	2	163	A	N1-C2-N3	-5.17	126.71	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	2	3694	U	N3-C2-O2	-5.17	118.58	122.20
4	2	1294	A	O4'-C1'-N9	5.17	112.34	108.20
4	2	2629	C	N1-C2-O2	5.17	122.00	118.90
4	2	113	A	N1-C2-N3	-5.17	126.72	129.30
4	2	3587	C	C5-C6-N1	5.17	123.58	121.00
4	2	4562	C	N1-C2-O2	5.17	122.00	118.90
4	2	683	C	C6-N1-C2	-5.16	118.23	120.30
4	2	2018	C	N1-C2-O2	5.16	122.00	118.90
4	2	4319	C	C5-C6-N1	5.16	123.58	121.00
4	2	4710	C	N1-C2-O2	5.16	122.00	118.90
4	2	1190	C	C6-N1-C2	-5.16	118.23	120.30
6	5	77	A	N1-C2-N3	-5.16	126.72	129.30
4	2	131	C	C2-N1-C1'	5.16	124.48	118.80
4	2	1445	U	N1-C2-O2	5.16	126.41	122.80
4	2	1519	C	C6-N1-C2	-5.16	118.24	120.30
4	2	2710	C	C6-N1-C1'	-5.16	114.61	120.80
53	8	4	C	C5-C6-N1	5.16	123.58	121.00
53	8	90	C	C6-N1-C2	-5.16	118.24	120.30
4	2	1373	A	N1-C2-N3	-5.16	126.72	129.30
4	2	5050	C	C6-N1-C2	-5.16	118.24	120.30
4	2	2439	G	C6-C5-N7	-5.16	127.31	130.40
4	2	2260	C	C6-N1-C1'	-5.15	114.62	120.80
4	2	2654	C	C6-N1-C2	-5.15	118.24	120.30
4	2	3710	G	N3-C4-N9	5.15	129.09	126.00
4	2	4970	C	C2-N1-C1'	5.15	124.47	118.80
4	2	5008	C	N3-C2-O2	-5.15	118.29	121.90
4	2	76	A	N1-C2-N3	-5.15	126.72	129.30
4	2	963	G	C8-N9-C1'	-5.15	120.31	127.00
4	2	472	C	N3-C2-O2	-5.14	118.30	121.90
4	2	1085	C	C6-N1-C2	-5.14	118.24	120.30
4	2	1384	C	C6-N1-C2	-5.14	118.24	120.30
4	2	1599	A	C2-N3-C4	5.14	113.17	110.60
4	2	1702	C	C6-N1-C1'	-5.14	114.63	120.80
4	2	1994	C	C5-C6-N1	5.14	123.57	121.00
4	2	2563	C	C5-C6-N1	5.14	123.57	121.00
4	2	4914	C	C5-C6-N1	5.14	123.57	121.00
4	2	2037	C	C6-N1-C2	-5.14	118.24	120.30
4	2	2470	C	OP2-P-O3'	5.14	116.51	105.20
4	2	2765	A	N1-C2-N3	-5.14	126.73	129.30
53	8	101	C	C5-C6-N1	5.14	123.57	121.00
53	8	103	A	N1-C2-N3	-5.14	126.73	129.30
4	2	1071	C	C6-N1-C2	-5.14	118.25	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	2	1080	C	C6-N1-C2	-5.14	118.25	120.30
4	2	290	U	N3-C2-O2	-5.13	118.61	122.20
9	9	35	LEU	CA-CB-CG	5.13	127.11	115.30
4	2	446	C	C5-C6-N1	5.13	123.57	121.00
4	2	1216	C	O4'-C1'-N1	5.13	112.31	108.20
4	2	1445	U	C2-N1-C1'	5.13	123.86	117.70
4	2	1632	A	C4-N9-C1'	5.13	135.54	126.30
4	2	4259	C	C5-C6-N1	5.13	123.56	121.00
4	2	1293	G	N3-C4-N9	5.13	129.08	126.00
4	2	2729	C	C2-N1-C1'	5.13	124.44	118.80
4	2	2791	C	C5-C6-N1	5.13	123.56	121.00
4	2	4648	A	N1-C2-N3	-5.13	126.74	129.30
13	E	94	LEU	CA-CB-CG	5.13	127.09	115.30
21	N	40	LEU	CA-CB-CG	5.13	127.09	115.30
4	2	300	A	N1-C2-N3	-5.12	126.74	129.30
4	2	1346	C	C6-N1-C2	-5.12	118.25	120.30
4	2	1535	C	C6-N1-C2	-5.12	118.25	120.30
4	2	4522	G	C8-N9-C1'	-5.12	120.34	127.00
6	5	94	C	C6-N1-C2	-5.12	118.25	120.30
46	r	251	PRO	CA-N-CD	-5.12	104.33	111.50
4	2	15	A	N1-C2-N3	-5.12	126.74	129.30
4	2	345	C	C5-C6-N1	5.12	123.56	121.00
4	2	4694	G	C4-N9-C1'	5.12	133.16	126.50
4	2	4263	C	C6-N1-C2	-5.12	118.25	120.30
4	2	5042	A	N1-C2-N3	-5.12	126.74	129.30
4	2	41	C	C5-C6-N1	5.12	123.56	121.00
4	2	221	C	C5-C6-N1	5.12	123.56	121.00
4	2	406	C	P-O3'-C3'	5.12	125.84	119.70
4	2	1978	C	N3-C2-O2	-5.12	118.32	121.90
4	2	1077	C	C5-C6-N1	5.11	123.56	121.00
13	E	11	LEU	CA-CB-CG	5.11	127.06	115.30
4	2	89	C	C6-N1-C2	-5.11	118.26	120.30
4	2	1477	C	C5-C6-N1	5.11	123.56	121.00
4	2	1521	C	N1-C2-O2	5.11	121.97	118.90
4	2	3710	G	C4-N9-C1'	5.11	133.14	126.50
4	2	80	C	C6-N1-C2	-5.11	118.26	120.30
4	2	1822	U	C6-N1-C2	-5.11	117.94	121.00
4	2	2835	A	N1-C2-N3	-5.11	126.75	129.30
4	2	4343	U	N1-C2-O2	5.11	126.37	122.80
4	2	4772	C	C6-N1-C2	-5.11	118.26	120.30
4	2	3912	U	N3-C2-O2	-5.10	118.63	122.20
4	2	454	U	C5-C6-N1	5.10	125.25	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	2	1293	G	N3-C4-C5	-5.10	126.05	128.60
4	2	4537	C	C6-N1-C2	-5.10	118.26	120.30
4	2	1378	C	C6-N1-C1'	-5.10	114.68	120.80
5	4	41	HIS	C-N-CA	5.10	134.45	121.70
4	2	2384	U	N3-C2-O2	-5.10	118.63	122.20
4	2	4500	U	N3-C2-O2	-5.10	118.63	122.20
4	2	4664	A	N1-C2-N3	-5.10	126.75	129.30
4	2	4700	A	N1-C2-N3	-5.10	126.75	129.30
4	2	4162	C	N3-C2-O2	-5.10	118.33	121.90
26	U	147	ASP	CB-CG-OD2	-5.10	113.71	118.30
4	2	3622	C	C2-N1-C1'	5.09	124.40	118.80
4	2	985	C	N3-C2-O2	-5.09	118.33	121.90
4	2	1910	G	N3-C4-C5	-5.09	126.05	128.60
4	2	2708	U	C2-N1-C1'	5.09	123.81	117.70
4	2	474	C	C6-N1-C2	-5.09	118.26	120.30
6	5	67	C	C5-C6-N1	5.09	123.55	121.00
4	2	956	A	N1-C2-N3	-5.09	126.75	129.30
4	2	1897	A	N1-C2-N3	-5.09	126.76	129.30
4	2	905	C	C5-C6-N1	5.09	123.54	121.00
4	2	1603	C	C6-N1-C2	-5.09	118.27	120.30
4	2	4342	C	C5-C6-N1	5.09	123.54	121.00
34	d	54	GLY	C-N-CA	5.09	134.42	121.70
4	2	2035	C	C6-N1-C2	-5.08	118.27	120.30
8	7	7	TYR	C-N-CA	5.08	134.41	121.70
4	2	297	U	N3-C2-O2	-5.08	118.64	122.20
4	2	1692	C	N1-C2-O2	5.08	121.95	118.90
4	2	2008	U	N3-C2-O2	-5.08	118.64	122.20
4	2	2716	C	C6-N1-C2	-5.08	118.27	120.30
4	2	3615	G	C2-N3-C4	5.08	114.44	111.90
4	2	4501	U	N3-C2-O2	-5.08	118.64	122.20
4	2	4913	G	OP2-P-O3'	5.08	116.38	105.20
6	5	44	C	C5-C6-N1	5.08	123.54	121.00
52	v	220	MET	CB-CG-SD	5.08	127.64	112.40
4	2	1294	A	C2-N3-C4	5.08	113.14	110.60
4	2	1929	A	N1-C2-N3	-5.08	126.76	129.30
4	2	2683	C	C6-N1-C2	-5.08	118.27	120.30
4	2	4378	A	N1-C2-N3	-5.08	126.76	129.30
4	2	124	C	C5-C6-N1	5.08	123.54	121.00
4	2	353	A	N1-C2-N3	-5.08	126.76	129.30
4	2	4926	C	O4'-C1'-N1	5.08	112.26	108.20
51	y	150	ASP	CB-CG-OD1	5.08	122.87	118.30
4	2	2654	C	N1-C2-O2	5.07	121.94	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	2	1317	U	N1-C2-O2	5.07	126.35	122.80
4	2	926	G	C4-N9-C1'	5.07	133.09	126.50
4	2	3769	C	N3-C2-O2	-5.07	118.35	121.90
4	2	242	U	C5-C6-N1	5.07	125.23	122.70
4	2	3771	C	N1-C2-O2	5.07	121.94	118.90
4	2	4289	U	C2-N1-C1'	5.07	123.78	117.70
4	2	4364	G	C4-N9-C1'	5.07	133.09	126.50
21	N	39	VAL	CG1-CB-CG2	-5.07	102.79	110.90
4	2	33	A	N1-C2-N3	-5.06	126.77	129.30
4	2	350	C	C2-N1-C1'	5.06	124.37	118.80
4	2	2025	A	N1-C2-N3	-5.06	126.77	129.30
4	2	2760	G	OP2-P-O3'	5.06	116.34	105.20
4	2	3598	C	C6-N1-C2	-5.06	118.28	120.30
4	2	3667	C	C6-N1-C2	-5.06	118.28	120.30
4	2	3923	A	N1-C2-N3	-5.06	126.77	129.30
4	2	4359	U	N3-C2-O2	-5.06	118.66	122.20
53	8	51	U	C2-N1-C1'	5.06	123.77	117.70
53	8	28	C	C5-C6-N1	5.06	123.53	121.00
4	2	1191	C	C6-N1-C2	-5.06	118.28	120.30
4	2	2028	C	N3-C2-O2	-5.06	118.36	121.90
53	8	80	A	N1-C2-N3	-5.06	126.77	129.30
36	g	29	LEU	CA-CB-CG	5.06	126.93	115.30
42	m	102	LEU	CA-CB-CG	5.06	126.93	115.30
4	2	3650	C	N1-C2-O2	5.06	121.93	118.90
4	2	294	G	N3-C4-N9	5.05	129.03	126.00
4	2	490	C	C5-C6-N1	5.05	123.53	121.00
49	R	143	PHE	CB-CG-CD2	-5.05	117.26	120.80
4	2	1076	C	C6-N1-C2	-5.05	118.28	120.30
4	2	1967	A	N1-C2-N3	-5.05	126.78	129.30
4	2	2417	A	O4'-C1'-N9	5.05	112.24	108.20
4	2	905	C	C6-N1-C2	-5.05	118.28	120.30
4	2	1720	C	N3-C2-O2	-5.05	118.36	121.90
4	2	2628	U	N3-C2-O2	-5.05	118.67	122.20
4	2	4601	U	C2-N1-C1'	5.05	123.76	117.70
4	2	4945	G	C8-N9-C1'	-5.05	120.44	127.00
4	2	2071	A	C2-N3-C4	5.05	113.12	110.60
4	2	3930	U	N3-C2-O2	-5.05	118.67	122.20
4	2	4286	C	C6-N1-C2	-5.05	118.28	120.30
4	2	5050	C	N1-C2-O2	5.05	121.93	118.90
4	2	2349	A	N1-C2-N3	-5.04	126.78	129.30
4	2	4215	C	C2-N1-C1'	5.04	124.35	118.80
6	5	5	A	N1-C2-N3	-5.04	126.78	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	v	267	LEU	CA-CB-CG	5.04	126.91	115.30
4	2	86	U	C2-N1-C1'	5.04	123.75	117.70
4	2	99	A	N1-C2-N3	-5.04	126.78	129.30
4	2	5003	U	N3-C2-O2	-5.04	118.67	122.20
53	8	52	A	N1-C2-N3	-5.04	126.78	129.30
22	O	69	LEU	CA-CB-CG	5.04	126.89	115.30
4	2	1317	U	N3-C2-O2	-5.04	118.67	122.20
4	2	4237	C	C5-C6-N1	5.04	123.52	121.00
4	2	4341	C	C5-C6-N1	5.04	123.52	121.00
4	2	977	C	N3-C2-O2	-5.04	118.38	121.90
4	2	3666	C	C6-N1-C2	-5.04	118.29	120.30
4	2	3942	A	C2-N3-C4	5.04	113.12	110.60
4	2	1503	A	N1-C2-N3	-5.03	126.78	129.30
4	2	1701	A	N1-C2-N3	-5.03	126.78	129.30
4	2	4981	G	N3-C4-C5	-5.03	126.08	128.60
53	8	119	C	C6-N1-C2	-5.03	118.29	120.30
4	2	2815	A	C2-N3-C4	5.03	113.12	110.60
4	2	73	A	N1-C2-N3	-5.03	126.79	129.30
4	2	2729	C	N1-C2-O2	5.03	121.92	118.90
53	8	72	A	N1-C2-N3	-5.03	126.79	129.30
4	2	3752	C	C2'-C3'-O3'	5.03	121.74	113.70
4	2	3939	G	C4-N9-C1'	5.03	133.03	126.50
6	5	28	C	C5-C6-N1	5.03	123.51	121.00
4	2	1706	A	C2-N3-C4	5.02	113.11	110.60
4	2	4193	C	C2-N1-C1'	5.02	124.33	118.80
4	2	2802	C	C5-C6-N1	5.02	123.51	121.00
4	2	26	C	C5-C6-N1	5.02	123.51	121.00
4	2	1792	U	N3-C2-O2	-5.02	118.69	122.20
6	5	44	C	N3-C2-O2	-5.02	118.39	121.90
4	2	128	C	N1-C2-O2	5.02	121.91	118.90
4	2	1254	A	N1-C2-N3	-5.02	126.79	129.30
4	2	2611	A	N1-C2-N3	-5.01	126.79	129.30
4	2	3928	A	N1-C2-N3	-5.01	126.79	129.30
53	8	123	U	N3-C2-O2	-5.01	118.69	122.20
4	2	458	C	C6-N1-C2	-5.01	118.30	120.30
4	2	4254	G	N3-C4-N9	5.01	129.01	126.00
6	5	94	C	C2-N1-C1'	5.01	124.31	118.80
4	2	1078	A	N1-C2-N3	-5.01	126.80	129.30
4	2	350	C	N1-C2-O2	5.01	121.91	118.90
4	2	4365	C	N1-C2-O2	5.01	121.91	118.90
4	2	4672	A	N1-C2-N3	-5.01	126.80	129.30
4	2	343	C	C6-N1-C2	-5.01	118.30	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	2	2593	C	N1-C2-O2	5.01	121.90	118.90
4	2	2710	C	C6-N1-C2	-5.01	118.30	120.30
4	2	4243	C	C5-C6-N1	5.01	123.50	121.00
4	2	4352	U	C2-N1-C1'	5.01	123.71	117.70
4	2	662	C	C6-N1-C2	-5.00	118.30	120.30
53	8	137	A	N1-C2-N3	-5.00	126.80	129.30
4	2	4696	C	N1-C2-O2	5.00	121.90	118.90
4	2	1888	A	N1-C2-N3	-5.00	126.80	129.30
4	2	2853	C	C6-N1-C2	-5.00	118.30	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	7	123	ASP	Peptide
50	J	238	ASP	Peptide
24	Q	154	VAL	Peptide
43	n	106	TYR	Peptide
57	w	204	ARG	Peptide

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	u	237/490 (48%)	232 (98%)	5 (2%)	0	100	100
2	t	109/293 (37%)	103 (94%)	6 (6%)	0	100	100
3	3	224/255 (88%)	215 (96%)	8 (4%)	1 (0%)	34	69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	4	607/634 (96%)	556 (92%)	46 (8%)	5 (1%)	19	58
7	6	242/245 (99%)	226 (93%)	16 (7%)	0	100	100
8	7	137/163 (84%)	133 (97%)	3 (2%)	1 (1%)	22	61
9	9	93/134 (69%)	79 (85%)	13 (14%)	1 (1%)	14	51
10	B	401/403 (100%)	374 (93%)	27 (7%)	0	100	100
11	C	89/159 (56%)	85 (96%)	4 (4%)	0	100	100
12	D	356/427 (83%)	331 (93%)	25 (7%)	0	100	100
13	E	96/115 (84%)	91 (95%)	5 (5%)	0	100	100
14	F	111/117 (95%)	108 (97%)	3 (3%)	0	100	100
15	G	240/266 (90%)	230 (96%)	10 (4%)	0	100	100
16	H	120/123 (98%)	115 (96%)	5 (4%)	0	100	100
17	I	188/192 (98%)	181 (96%)	7 (4%)	0	100	100
18	K	100/105 (95%)	95 (95%)	5 (5%)	0	100	100
19	L	145/148 (98%)	136 (94%)	9 (6%)	0	100	100
20	M	84/97 (87%)	78 (93%)	6 (7%)	0	100	100
21	N	162/178 (91%)	139 (86%)	23 (14%)	0	100	100
22	O	67/70 (96%)	61 (91%)	6 (9%)	0	100	100
23	P	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
24	Q	208/211 (99%)	191 (92%)	17 (8%)	0	100	100
25	S	133/215 (62%)	127 (96%)	6 (4%)	0	100	100
26	U	201/204 (98%)	192 (96%)	9 (4%)	0	100	100
27	V	199/203 (98%)	189 (95%)	10 (5%)	0	100	100
28	X	89/92 (97%)	87 (98%)	2 (2%)	0	100	100
29	Y	165/184 (90%)	155 (94%)	10 (6%)	0	100	100
30	Z	185/188 (98%)	177 (96%)	8 (4%)	0	100	100
31	a	146/196 (74%)	142 (97%)	4 (3%)	0	100	100
32	b	174/176 (99%)	169 (97%)	5 (3%)	0	100	100
33	c	153/160 (96%)	146 (95%)	7 (5%)	0	100	100
34	d	102/128 (80%)	94 (92%)	8 (8%)	0	100	100
35	e	129/140 (92%)	117 (91%)	12 (9%)	0	100	100
36	g	141/156 (90%)	136 (96%)	4 (3%)	1 (1%)	22	61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	h	132/145 (91%)	129 (98%)	3 (2%)	0	100	100
38	i	133/136 (98%)	126 (95%)	7 (5%)	0	100	100
39	j	109/125 (87%)	104 (95%)	5 (5%)	0	100	100
40	k	127/135 (94%)	122 (96%)	5 (4%)	0	100	100
41	l	123/137 (90%)	112 (91%)	11 (9%)	0	100	100
42	m	246/257 (96%)	226 (92%)	20 (8%)	0	100	100
43	n	107/110 (97%)	99 (92%)	7 (6%)	1 (1%)	17	56
44	o	231/288 (80%)	216 (94%)	15 (6%)	0	100	100
45	p	224/248 (90%)	214 (96%)	10 (4%)	0	100	100
46	r	282/297 (95%)	261 (93%)	21 (7%)	0	100	100
47	z	63/129 (49%)	60 (95%)	2 (3%)	1 (2%)	9	43
48	A	331/731 (45%)	324 (98%)	7 (2%)	0	100	100
49	R	151/203 (74%)	141 (93%)	10 (7%)	0	100	100
50	J	221/239 (92%)	209 (95%)	12 (5%)	0	100	100
51	y	163/165 (99%)	159 (98%)	4 (2%)	0	100	100
52	v	398/588 (68%)	386 (97%)	12 (3%)	0	100	100
54	W	99/106 (93%)	94 (95%)	5 (5%)	0	100	100
55	T	48/99 (48%)	46 (96%)	2 (4%)	0	100	100
56	s	33/260 (13%)	33 (100%)	0	0	100	100
57	w	254/478 (53%)	242 (95%)	11 (4%)	1 (0%)	34	69
All	All	9356/11794 (79%)	8840 (94%)	504 (5%)	12 (0%)	54	83

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
43	n	106	TYR
57	w	203	ASP
3	3	24	ASN
5	4	88	ASP
47	z	24	LYS
5	4	230	LEU
8	7	62	GLU
9	9	99	GLN
5	4	427	ASP
5	4	407	ASP

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Mol	Chain	Res	Type
5	4	366	THR
36	g	40	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	u	222/437 (51%)	222 (100%)	0	100	100
2	t	103/274 (38%)	101 (98%)	2 (2%)	57	81
3	3	207/228 (91%)	207 (100%)	0	100	100
5	4	554/574 (96%)	550 (99%)	4 (1%)	84	94
7	6	212/213 (100%)	212 (100%)	0	100	100
8	7	128/149 (86%)	128 (100%)	0	100	100
9	9	81/114 (71%)	81 (100%)	0	100	100
10	B	349/349 (100%)	348 (100%)	1 (0%)	92	96
11	C	78/126 (62%)	78 (100%)	0	100	100
12	D	298/348 (86%)	297 (100%)	1 (0%)	92	96
13	E	83/97 (86%)	83 (100%)	0	100	100
14	F	97/100 (97%)	97 (100%)	0	100	100
15	G	204/223 (92%)	204 (100%)	0	100	100
16	H	109/110 (99%)	109 (100%)	0	100	100
17	I	169/171 (99%)	168 (99%)	1 (1%)	86	94
18	K	86/89 (97%)	86 (100%)	0	100	100
19	L	120/121 (99%)	117 (98%)	3 (2%)	47	77
20	M	73/80 (91%)	73 (100%)	0	100	100
21	N	137/149 (92%)	137 (100%)	0	100	100
22	O	64/65 (98%)	64 (100%)	0	100	100
23	P	47/48 (98%)	47 (100%)	0	100	100
24	Q	176/177 (99%)	176 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	S	115/161 (71%)	115 (100%)	0	100	100
26	U	171/172 (99%)	170 (99%)	1 (1%)	86	94
27	V	173/174 (99%)	172 (99%)	1 (1%)	86	94
28	X	74/75 (99%)	74 (100%)	0	100	100
29	Y	147/163 (90%)	146 (99%)	1 (1%)	84	94
30	Z	164/165 (99%)	163 (99%)	1 (1%)	86	94
31	a	133/175 (76%)	133 (100%)	0	100	100
32	b	157/157 (100%)	157 (100%)	0	100	100
33	c	136/140 (97%)	136 (100%)	0	100	100
34	d	94/115 (82%)	94 (100%)	0	100	100
35	e	101/107 (94%)	100 (99%)	1 (1%)	76	90
36	g	124/133 (93%)	124 (100%)	0	100	100
37	h	124/135 (92%)	124 (100%)	0	100	100
38	i	117/118 (99%)	117 (100%)	0	100	100
39	j	101/110 (92%)	101 (100%)	0	100	100
40	k	115/121 (95%)	114 (99%)	1 (1%)	78	91
41	l	109/121 (90%)	109 (100%)	0	100	100
42	m	190/199 (96%)	189 (100%)	1 (0%)	88	95
43	n	88/89 (99%)	88 (100%)	0	100	100
44	o	208/252 (82%)	207 (100%)	1 (0%)	88	95
45	p	195/215 (91%)	195 (100%)	0	100	100
46	r	240/250 (96%)	240 (100%)	0	100	100
47	z	61/115 (53%)	61 (100%)	0	100	100
48	A	296/654 (45%)	296 (100%)	0	100	100
49	R	141/184 (77%)	140 (99%)	1 (1%)	84	94
50	J	199/214 (93%)	198 (100%)	1 (0%)	88	95
51	y	137/137 (100%)	136 (99%)	1 (1%)	84	94
52	v	359/509 (70%)	357 (99%)	2 (1%)	86	94
54	W	89/94 (95%)	89 (100%)	0	100	100
55	T	43/76 (57%)	43 (100%)	0	100	100
56	s	32/228 (14%)	32 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
57	w	222/402 (55%)	221 (100%)	1 (0%)	88 95
All	All	8252/10202 (81%)	8226 (100%)	26 (0%)	92 96

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	t	50	ARG
2	t	78	ARG
5	4	233	ARG
5	4	373	ARG
5	4	385	ARG
5	4	399	ARG
10	B	394	LYS
12	D	188	ARG
17	I	141	LYS
19	L	66	ASN
19	L	94	LYS
19	L	116	LYS
26	U	204	ARG
27	V	117	ARG
29	Y	97	ASN
30	Z	150	ARG
35	e	48	ARG
40	k	92	ASN
42	m	128	ARG
44	o	100	LYS
49	R	144	ARG
50	J	126	ARG
51	y	90	ARG
52	v	384	GLN
52	v	405	ARG
57	w	362	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
29	Y	64	ASN
32	b	77	ASN
42	m	215	ASN
52	v	209	HIS
56	s	10	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	2	3493/5054 (69%)	815 (23%)	21 (0%)
53	8	153/156 (98%)	27 (17%)	2 (1%)
58	x	0/60	-	-
6	5	119/120 (99%)	15 (12%)	0
All	All	3765/5390 (69%)	857 (22%)	23 (0%)

All (857) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	2	25	A
4	2	39	A
4	2	42	A
4	2	44	A
4	2	48	G
4	2	56	A
4	2	59	A
4	2	64	A
4	2	65	A
4	2	69	A
4	2	72	C
4	2	73	A
4	2	84	A
4	2	91	G
4	2	104	G
4	2	108	A
4	2	109	G
4	2	110	C
4	2	112	C
4	2	119	G
4	2	120	A
4	2	122	U
4	2	127	G
4	2	133	C
4	2	134	G
4	2	135	G
4	2	136	C
4	2	137	G
4	2	141	C
4	2	143	C
4	2	144	G
4	2	145	G

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Mol	Chain	Res	Type
4	2	152	U
4	2	159	C
4	2	164	G
4	2	172	C
4	2	177	G
4	2	178	C
4	2	181	C
4	2	183	C
4	2	184	U
4	2	185	C
4	2	188	G
4	2	197	A
4	2	200	U
4	2	209	U
4	2	218	A
4	2	219	G
4	2	220	C
4	2	234	G
4	2	254	G
4	2	255	C
4	2	256	G
4	2	259	C
4	2	262	G
4	2	264	C
4	2	265	C
4	2	266	C
4	2	279	A
4	2	280	G
4	2	297	U
4	2	306	A
4	2	315	G
4	2	316	U
4	2	340	C
4	2	345	C
4	2	349	A
4	2	361	C
4	2	385	A
4	2	387	G
4	2	396	A
4	2	407	A
4	2	408	A
4	2	409	G

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Mol	Chain	Res	Type
4	2	410	A
4	2	411	G
4	2	412	G
4	2	432	U
4	2	433	A
4	2	449	C
4	2	450	G
4	2	452	A
4	2	453	G
4	2	454	U
4	2	464	G
4	2	465	G
4	2	467	U
4	2	483	G
4	2	484	U
4	2	485	C
4	2	486	C
4	2	489	C
4	2	493	G
4	2	494	U
4	2	496	G
4	2	497	G
4	2	499	G
4	2	500	G
4	2	501	C
4	2	502	C
4	2	503	C
4	2	504	G
4	2	505	G
4	2	507	G
4	2	509	A
4	2	510	U
4	2	513	U
4	2	514	U
4	2	515	C
4	2	517	C
4	2	518	G
4	2	519	C
4	2	654	C
4	2	656	C
4	2	657	C
4	2	658	C

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Mol	Chain	Res	Type
4	2	666	G
4	2	669	C
4	2	673	C
4	2	684	G
4	2	685	C
4	2	686	A
4	2	688	U
4	2	692	A
4	2	696	C
4	2	697	G
4	2	703	G
4	2	704	C
4	2	708	G
4	2	731	G
4	2	738	C
4	2	739	G
4	2	740	G
4	2	742	G
4	2	746	A
4	2	759	G
4	2	904	C
4	2	905	C
4	2	906	C
4	2	912	G
4	2	913	U
4	2	914	U
4	2	915	A
4	2	916	C
4	2	917	A
4	2	918	G
4	2	924	C
4	2	925	C
4	2	926	G
4	2	932	A
4	2	933	G
4	2	936	C
4	2	941	C
4	2	943	A
4	2	944	A
4	2	945	U
4	2	956	A
4	2	959	G

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Mol	Chain	Res	Type
4	2	960	A
4	2	961	G
4	2	962	C
4	2	965	G
4	2	966	A
4	2	967	C
4	2	969	C
4	2	970	G
4	2	971	U
4	2	972	C
4	2	982	U
4	2	984	C
4	2	988	C
4	2	990	C
4	2	991	C
4	2	992	C
4	2	993	G
4	2	994	G
4	2	995	C
4	2	1048	G
4	2	1049	C
4	2	1051	G
4	2	1070	G
4	2	1072	C
4	2	1082	C
4	2	1083	U
4	2	1095	A
4	2	1100	U
4	2	1168	G
4	2	1172	C
4	2	1173	G
4	2	1178	G
4	2	1179	U
4	2	1180	C
4	2	1181	C
4	2	1182	C
4	2	1183	C
4	2	1184	A
4	2	1186	U
4	2	1187	G
4	2	1194	G
4	2	1198	G

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Mol	Chain	Res	Type
4	2	1200	G
4	2	1202	C
4	2	1203	G
4	2	1211	G
4	2	1215	C
4	2	1216	C
4	2	1218	G
4	2	1219	G
4	2	1220	G
4	2	1222	A
4	2	1241	C
4	2	1244	G
4	2	1245	C
4	2	1253	G
4	2	1254	A
4	2	1255	A
4	2	1260	G
4	2	1266	G
4	2	1269	G
4	2	1271	G
4	2	1272	C
4	2	1273	G
4	2	1275	G
4	2	1280	C
4	2	1283	G
4	2	1284	G
4	2	1287	G
4	2	1289	C
4	2	1294	A
4	2	1295	C
4	2	1296	G
4	2	1302	U
4	2	1303	A
4	2	1314	C
4	2	1324	A
4	2	1326	A2M
4	2	1337	A
4	2	1354	A
4	2	1358	G
4	2	1359	G
4	2	1365	C
4	2	1366	G

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Mol	Chain	Res	Type
4	2	1370	G
4	2	1371	A
4	2	1377	G
4	2	1378	C
4	2	1379	C
4	2	1381	U
4	2	1387	A
4	2	1394	G
4	2	1397	A
4	2	1398	A
4	2	1401	C
4	2	1402	C
4	2	1404	G
4	2	1407	C
4	2	1409	C
4	2	1410	U
4	2	1414	C
4	2	1417	C
4	2	1419	G
4	2	1420	A
4	2	1425	G
4	2	1439	C
4	2	1442	C
4	2	1443	A
4	2	1444	G
4	2	1446	C
4	2	1482	G
4	2	1483	C
4	2	1486	C
4	2	1497	A
4	2	1498	G
4	2	1502	G
4	2	1503	A
4	2	1517	2MG
4	2	1518	A
4	2	1523	A
4	2	1534	A2M
4	2	1547	A
4	2	1559	G
4	2	1566	C
4	2	1578	U
4	2	1596	U

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Mol	Chain	Res	Type
4	2	1597	G
4	2	1612	G
4	2	1613	A
4	2	1624	G
4	2	1625	OMG
4	2	1626	G
4	2	1631	A
4	2	1633	G
4	2	1634	A
4	2	1638	A
4	2	1641	G
4	2	1642	A
4	2	1650	A
4	2	1654	G
4	2	1658	G
4	2	1661	C
4	2	1670	G
4	2	1676	C
4	2	1677	U
4	2	1678	C
4	2	1685	G
4	2	1691	G
4	2	1694	C
4	2	1697	G
4	2	1699	A
4	2	1700	G
4	2	1701	A
4	2	1702	C
4	2	1703	C
4	2	1704	C
4	2	1705	G
4	2	1707	C
4	2	1716	G
4	2	1718	C
4	2	1719	A
4	2	1724	G
4	2	1726	U
4	2	1731	C
4	2	1734	G
4	2	1790	U
4	2	1803	G
4	2	1804	A

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Mol	Chain	Res	Type
4	2	1810	G
4	2	1815	G
4	2	1821	G
4	2	1822	U
4	2	1834	U
4	2	1836	G
4	2	1837	A
4	2	1842	G
4	2	1843	A
4	2	1853	G
4	2	1854	G
4	2	1855	G
4	2	1856	C
4	2	1866	UR3
4	2	1868	A
4	2	1869	G
4	2	1881	C
4	2	1883	OMG
4	2	1891	A
4	2	1897	A
4	2	1898	C
4	2	1900	C
4	2	1918	U
4	2	1919	G
4	2	1920	C
4	2	1921	C
4	2	1922	G
4	2	1925	G
4	2	1931	C
4	2	1932	A
4	2	1938	C
4	2	1948	G
4	2	1951	G
4	2	1958	A
4	2	1962	A
4	2	1963	C
4	2	1969	G
4	2	1970	A
4	2	1971	C
4	2	1980	U
4	2	1981	G
4	2	1984	A

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Mol	Chain	Res	Type
4	2	1985	G
4	2	1991	A
4	2	1997	U
4	2	2001	G
4	2	2002	A
4	2	2003	G
4	2	2004	U
4	2	2008	U
4	2	2010	A
4	2	2015	U
4	2	2018	C
4	2	2024	G
4	2	2025	A
4	2	2026	A
4	2	2027	U
4	2	2033	A
4	2	2034	G
4	2	2044	U
4	2	2046	G
4	2	2048	U
4	2	2055	G
4	2	2056	G
4	2	2069	A
4	2	2071	A
4	2	2084	C
4	2	2085	G
4	2	2090	U
4	2	2092	G
4	2	2093	A
4	2	2095	A
4	2	2096	G
4	2	2097	U
4	2	2098	G
4	2	2100	A
4	2	2102	G
4	2	2104	G
4	2	2105	A
4	2	2106	G
4	2	2108	G
4	2	2110	C
4	2	2111	G
4	2	2112	G

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Mol	Chain	Res	Type
4	2	2113	C
4	2	2250	C
4	2	2251	G
4	2	2252	G
4	2	2253	A
4	2	2254	G
4	2	2255	C
4	2	2256	C
4	2	2258	C
4	2	2259	G
4	2	2260	C
4	2	2263	A
4	2	2289	C
4	2	2300	A
4	2	2301	G
4	2	2306	G
4	2	2313	A
4	2	2316	G
4	2	2331	G
4	2	2333	G
4	2	2346	C
4	2	2348	G
4	2	2351	C
4	2	2364	OMG
4	2	2395	A
4	2	2409	U
4	2	2416	G
4	2	2417	A
4	2	2422	OMC
4	2	2424	OMG
4	2	2425	U
4	2	2433	G
4	2	2439	G
4	2	2441	C
4	2	2447	U
4	2	2450	G
4	2	2453	A
4	2	2460	A
4	2	2470	C
4	2	2471	G
4	2	2475	G
4	2	2476	G

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Mol	Chain	Res	Type
4	2	2477	A
4	2	2478	C
4	2	2484	A
4	2	2485	U
4	2	2486	G
4	2	2487	G
4	2	2488	C
4	2	2489	C
4	2	2490	U
4	2	2497	C
4	2	2506	G
4	2	2511	A
4	2	2512	A
4	2	2513	A
4	2	2519	U
4	2	2529	A
4	2	2542	G
4	2	2543	A
4	2	2544	G
4	2	2545	U
4	2	2546	G
4	2	2549	G
4	2	2559	G
4	2	2560	C
4	2	2565	A
4	2	2566	G
4	2	2573	A
4	2	2583	C
4	2	2586	G
4	2	2587	A
4	2	2589	C
4	2	2601	A
4	2	2618	G
4	2	2627	C
4	2	2638	G
4	2	2652	G
4	2	2653	C
4	2	2662	G
4	2	2669	C
4	2	2670	C
4	2	2687	U
4	2	2694	G

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Mol	Chain	Res	Type
4	2	2695	A
4	2	2696	A
4	2	2707	U
4	2	2708	U
4	2	2710	C
4	2	2711	G
4	2	2719	C
4	2	2724	G
4	2	2726	G
4	2	2739	C
4	2	2742	G
4	2	2743	A
4	2	2761	U
4	2	2763	U
4	2	2765	A
4	2	2769	U
4	2	2770	C
4	2	2772	C
4	2	2773	OMG
4	2	2788	U
4	2	2789	A
4	2	2790	U
4	2	2794	C
4	2	2795	A
4	2	2799	G
4	2	2814	C
4	2	2826	U
4	2	2827	G
4	2	2855	G
4	2	2877	G
4	2	2882	A
4	2	2897	G
4	2	2900	U
4	2	2901	G
4	2	2903	G
4	2	2904	U
4	2	2905	C
4	2	2906	G
4	2	2907	G
4	2	2908	U
4	2	2909	C
4	2	2910	G

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Mol	Chain	Res	Type
4	2	3585	G
4	2	3591	C
4	2	3595	U
4	2	3596	A
4	2	3597	G
4	2	3598	C
4	2	3599	A
4	2	3605	C
4	2	3606	U
4	2	3615	G
4	2	3626	G
4	2	3635	A
4	2	3644	U
4	2	3648	A
4	2	3662	A
4	2	3673	C
4	2	3680	U
4	2	3682	A
4	2	3691	G
4	2	3698	G
4	2	3710	G
4	2	3712	A
4	2	3713	U
4	2	3729	U
4	2	3734	U
4	2	3735	G
4	2	3736	A
4	2	3750	G
4	2	3753	G
4	2	3771	C
4	2	3773	U
4	2	3774	A
4	2	3775	A
4	2	3776	G
4	2	3832	U
4	2	3838	U
4	2	3840	U
4	2	3867	A2M
4	2	3869	OMC
4	2	3876	A
4	2	3877	A
4	2	3879	G

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Mol	Chain	Res	Type
4	2	3898	G
4	2	3903	A
4	2	3905	A
4	2	3906	A
4	2	3909	C
4	2	3915	U
4	2	3922	G
4	2	3938	G
4	2	3939	G
4	2	3944	G
4	2	3948	C
4	2	4067	U
4	2	4068	U
4	2	4069	U
4	2	4070	U
4	2	4076	G
4	2	4077	A
4	2	4084	G
4	2	4095	G
4	2	4099	G
4	2	4100	C
4	2	4102	C
4	2	4103	C
4	2	4104	G
4	2	4107	G
4	2	4112	C
4	2	4114	C
4	2	4115	G
4	2	4116	C
4	2	4117	U
4	2	4119	C
4	2	4121	G
4	2	4122	G
4	2	4125	C
4	2	4127	A
4	2	4133	C
4	2	4140	C
4	2	4141	G
4	2	4142	C
4	2	4143	G
4	2	4144	C
4	2	4146	G

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Mol	Chain	Res	Type
4	2	4149	C
4	2	4150	G
4	2	4157	A
4	2	4162	C
4	2	4163	U
4	2	4170	A
4	2	4183	G
4	2	4184	G
4	2	4191	G
4	2	4194	U
4	2	4195	G
4	2	4196	OMG
4	2	4201	G
4	2	4212	A
4	2	4221	C
4	2	4225	G
4	2	4226	G
4	2	4229	U
4	2	4233	A
4	2	4234	A
4	2	4247	G
4	2	4251	A
4	2	4253	A
4	2	4254	G
4	2	4256	A
4	2	4258	C
4	2	4265	U
4	2	4268	A
4	2	4271	A
4	2	4273	A
4	2	4279	A
4	2	4280	A
4	2	4281	A
4	2	4282	A
4	2	4293	U
4	2	4294	C
4	2	4295	U
4	2	4297	G
4	2	4304	A
4	2	4305	G
4	2	4306	OMU
4	2	4314	C

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Mol	Chain	Res	Type
4	2	4319	C
4	2	4330	G
4	2	4332	C
4	2	4349	C
4	2	4354	U
4	2	4364	G
4	2	4372	U
4	2	4373	G
4	2	4376	A
4	2	4377	G
4	2	4378	A
4	2	4379	A
4	2	4380	A
4	2	4381	A
4	2	4382	G
4	2	4387	C
4	2	4395	U
4	2	4396	A
4	2	4414	A
4	2	4415	A
4	2	4418	G
4	2	4422	A
4	2	4424	A
4	2	4427	G
4	2	4428	A
4	2	4437	U
4	2	4440	G
4	2	4446	U
4	2	4447	C
4	2	4448	G
4	2	4451	G
4	2	4452	U
4	2	4453	C
4	2	4464	A
4	2	4466	C
4	2	4475	G
4	2	4476	C
4	2	4484	A
4	2	4488	A
4	2	4498	U
4	2	4512	U
4	2	4513	A

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Mol	Chain	Res	Type
4	2	4518	A
4	2	4519	C
4	2	4523	A2M
4	2	4524	G
4	2	4530	UR3
4	2	4545	G
4	2	4547	C
4	2	4548	A
4	2	4549	G
4	2	4555	U
4	2	4556	U
4	2	4557	U
4	2	4558	U
4	2	4560	C
4	2	4569	U
4	2	4575	G
4	2	4584	A
4	2	4589	A
4	2	4590	A
4	2	4597	UR3
4	2	4599	A
4	2	4600	G
4	2	4601	U
4	2	4607	A
4	2	4608	G
4	2	4635	A
4	2	4636	U
4	2	4637	OMG
4	2	4656	A
4	2	4657	U
4	2	4670	C
4	2	4678	G
4	2	4693	C
4	2	4694	G
4	2	4695	C
4	2	4700	A
4	2	4708	A
4	2	4709	U
4	2	4719	G
4	2	4720	C
4	2	4721	G
4	2	4730	C

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Mol	Chain	Res	Type
4	2	4731	G
4	2	4733	C
4	2	4734	A
4	2	4735	G
4	2	4740	G
4	2	4741	C
4	2	4742	G
4	2	4745	G
4	2	4751	G
4	2	4754	G
4	2	4757	C
4	2	4759	C
4	2	4761	G
4	2	4764	A
4	2	4765	G
4	2	4771	C
4	2	4775	C
4	2	4776	G
4	2	4859	C
4	2	4870	OMG
4	2	4871	C
4	2	4872	2MG
4	2	4874	A
4	2	4877	G
4	2	4882	U
4	2	4883	C
4	2	4889	G
4	2	4895	C
4	2	4896	G
4	2	4900	C
4	2	4901	G
4	2	4910	G
4	2	4912	G
4	2	4914	C
4	2	4924	C
4	2	4925	U
4	2	4927	G
4	2	4928	C
4	2	4931	G
4	2	4940	C
4	2	4941	G
4	2	4943	A

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Mol	Chain	Res	Type
4	2	4947	U
4	2	4949	G
4	2	4955	A
4	2	4958	C
4	2	4960	G
4	2	4976	U
4	2	4989	U
4	2	4990	C
4	2	4991	U
4	2	5006	U
4	2	5014	A
4	2	5017	G
4	2	5022	U
4	2	5026	U
4	2	5027	C
4	2	5030	U
4	2	5031	G
4	2	5034	A
4	2	5040	U
4	2	5041	G
4	2	5047	C
4	2	5050	C
4	2	5054	C
4	2	5055	G
4	2	5058	A
4	2	5062	G
4	2	5069	U
6	5	11	A
6	5	13	A
6	5	22	A
6	5	24	C
6	5	37	G
6	5	39	C
6	5	40	U
6	5	50	A
6	5	53	U
6	5	62	U
6	5	63	C
6	5	64	G
6	5	100	A
6	5	110	G
6	5	120	U

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Mol	Chain	Res	Type
53	8	25	G
53	8	34	U
53	8	35	C
53	8	39	G
53	8	48	A
53	8	52	A
53	8	59	A
53	8	62	A
53	8	63	U
53	8	71	A
53	8	80	A
53	8	82	A
53	8	84	A
53	8	85	U
53	8	86	U
53	8	94	G
53	8	103	A
53	8	104	A
53	8	105	C
53	8	110	U
53	8	114	G
53	8	123	U
53	8	124	U
53	8	125	C
53	8	126	C
53	8	127	U
53	8	151	G

All (23) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	2	914	U
4	2	1625	OMG
4	2	1633	G
4	2	1980	U
4	2	2014	C
4	2	2033	A
4	2	2470	C
4	2	2486	G
4	2	2487	G
4	2	2496	G
4	2	2760	G

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Mol	Chain	Res	Type
4	2	3596	A
4	2	3752	C
4	2	3773	U
4	2	3774	A
4	2	3905	A
4	2	4380	A
4	2	4547	C
4	2	4555	U
4	2	4699	U
4	2	4913	G
53	8	124	U
53	8	125	C

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

77 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	$\#\|Z\| > 2$
4	OMG	2	1316	4	18,26,27	2.86	8 (44%)	19,38,41	1.57	5 (26%)
4	A2M	2	4571	4	18,25,26	3.54	8 (44%)	18,36,39	3.41	4 (22%)
4	OMG	2	1883	4	18,26,27	2.89	8 (44%)	19,38,41	1.56	4 (21%)
4	B8W	2	4185	4	18,26,27	2.10	2 (11%)	21,38,41	2.40	6 (28%)
4	2MG	2	1517	4	18,26,27	2.68	6 (33%)	16,38,41	1.52	4 (25%)
4	B9B	2	237	4	21,28,29	2.02	3 (14%)	23,40,43	6.39	5 (21%)
4	7MG	2	2522	4	22,26,27	3.71	10 (45%)	29,39,42	1.99	9 (31%)
4	A2M	2	2363	4	18,25,26	3.60	8 (44%)	18,36,39	3.44	4 (22%)
4	UR3	2	4597	4	19,22,23	2.77	7 (36%)	26,32,35	2.03	5 (19%)
4	A2M	2	4523	4	18,25,26	3.57	8 (44%)	18,36,39	3.35	4 (22%)
4	OMC	2	3869	4	19,22,23	3.01	8 (42%)	26,31,34	0.90	2 (7%)
4	OMG	2	1522	4	18,26,27	2.82	8 (44%)	19,38,41	1.56	5 (26%)
4	OMG	2	2773	4	18,26,27	2.87	8 (44%)	19,38,41	1.45	3 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	2MG	2	4872	4	18,26,27	2.53	6 (33%)	16,38,41	1.74	4 (25%)
4	A2M	2	398	4	18,25,26	3.61	8 (44%)	18,36,39	3.42	3 (16%)
4	OMG	2	373	4	18,26,27	2.85	8 (44%)	19,38,41	1.62	5 (26%)
4	2MG	2	978	4	18,26,27	2.72	6 (33%)	16,38,41	1.40	3 (18%)
4	B8T	2	4671	4	19,22,23	3.60	8 (42%)	26,31,34	0.88	1 (3%)
4	B8W	2	4529	4	18,26,27	2.12	2 (11%)	21,38,41	2.62	7 (33%)
4	OMC	2	3887	4	19,22,23	3.05	8 (42%)	26,31,34	0.95	1 (3%)
4	A2M	2	3867	4	18,25,26	3.59	8 (44%)	18,36,39	3.47	4 (22%)
4	B8T	2	4483	4	19,22,23	3.65	8 (42%)	26,31,34	1.37	4 (15%)
4	5MU	2	4083	4	19,22,23	7.28	8 (42%)	28,32,35	3.27	11 (39%)
4	B8H	2	4296	4	20,22,23	6.62	6 (30%)	21,32,35	2.35	5 (23%)
4	A2M	2	3723	4	18,25,26	3.59	9 (50%)	18,36,39	3.30	4 (22%)
4	A2M	2	1524	4	18,25,26	3.62	8 (44%)	18,36,39	3.45	4 (22%)
4	OMG	2	2364	4	18,26,27	2.82	8 (44%)	19,38,41	1.53	5 (26%)
4	OMC	2	2861	4	19,22,23	3.02	8 (42%)	26,31,34	1.18	3 (11%)
4	5MC	2	4335	4	18,22,23	3.58	7 (38%)	26,32,35	1.09	2 (7%)
4	7MG	2	4550	4	22,26,27	3.87	10 (45%)	29,39,42	1.98	9 (31%)
4	A2M	2	1534	4	18,25,26	3.61	8 (44%)	18,36,39	3.60	4 (22%)
4	OMG	2	4196	4	18,26,27	2.96	7 (38%)	19,38,41	1.65	6 (31%)
4	OMG	2	4494	4	18,26,27	2.87	8 (44%)	19,38,41	1.46	3 (15%)
4	OMG	2	2424	4	18,26,27	2.86	8 (44%)	19,38,41	1.52	3 (15%)
4	OMC	2	2365	4	19,22,23	2.94	8 (42%)	26,31,34	0.75	0
4	E7G	2	2297	4	24,27,28	3.95	11 (45%)	30,40,43	2.14	7 (23%)
4	A2M	2	1871	4	18,25,26	3.58	8 (44%)	18,36,39	3.46	4 (22%)
4	OMU	2	4306	4	19,22,23	3.00	8 (42%)	26,31,34	1.70	5 (19%)
4	OMC	2	4536	4	19,22,23	3.01	8 (42%)	26,31,34	1.13	3 (11%)
4	OMG	2	4870	4	18,26,27	2.92	8 (44%)	19,38,41	1.61	5 (26%)
4	BGH	2	3899	4	25,29,30	4.60	17 (68%)	31,43,46	2.58	11 (35%)
4	OMC	2	3701	4	19,22,23	3.01	8 (42%)	26,31,34	0.77	0
4	A2M	2	1326	4	18,25,26	3.53	8 (44%)	18,36,39	3.42	3 (16%)
4	1MA	2	1322	4	16,25,26	4.39	5 (31%)	18,37,40	1.71	3 (16%)
4	B8H	2	1860	4	20,22,23	6.60	6 (30%)	21,32,35	2.32	5 (23%)
4	B9B	2	1574	4	21,28,29	1.97	3 (14%)	23,40,43	6.61	4 (17%)
4	UR3	2	1866	4	19,22,23	2.94	6 (31%)	26,32,35	1.31	2 (7%)
4	I4U	2	1659	4	21,24,25	3.57	9 (42%)	27,34,37	1.18	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	OMG	2	4637	4	18,26,27	2.86	8 (44%)	19,38,41	1.54	4 (21%)
4	A2M	2	3718	4	18,25,26	3.59	8 (44%)	18,36,39	3.38	4 (22%)
4	B8K	2	4690	4	24,28,29	3.37	11 (45%)	30,42,45	2.59	11 (36%)
4	B8Q	2	1456	4	17,22,23	2.97	5 (29%)	22,32,35	2.32	6 (27%)
4	OMG	2	4623	4	18,26,27	2.81	8 (44%)	19,38,41	1.52	5 (26%)
4	7MG	2	1605	4	22,26,27	3.83	10 (45%)	29,39,42	1.98	7 (24%)
53	OMU	8	14	53,4	19,22,23	2.90	8 (42%)	26,31,34	1.86	5 (19%)
4	A2M	2	2401	4	18,25,26	3.62	8 (44%)	18,36,39	3.41	3 (16%)
4	P4U	2	1348	4	21,24,25	3.55	8 (38%)	27,33,36	1.04	1 (3%)
4	B8W	2	2380	4	18,26,27	2.09	2 (11%)	21,38,41	2.45	7 (33%)
4	B8W	2	4472	4	18,26,27	2.10	2 (11%)	21,38,41	2.47	6 (28%)
4	2MG	2	729	4	18,26,27	2.61	6 (33%)	16,38,41	1.44	3 (18%)
4	OMG	2	2050	4	18,26,27	2.74	8 (44%)	19,38,41	1.52	5 (26%)
4	E7G	2	1797	4	24,27,28	4.07	11 (45%)	30,40,43	2.26	9 (30%)
4	P7G	2	1909	4	24,28,29	4.01	11 (45%)	27,41,44	1.60	3 (11%)
4	6MZ	2	4220	4	18,25,26	1.87	3 (16%)	16,36,39	3.68	3 (18%)
4	UR3	2	4530	4	19,22,23	2.90	6 (31%)	26,32,35	1.33	2 (7%)
4	OMG	2	4370	4	18,26,27	2.86	8 (44%)	19,38,41	1.46	4 (21%)
4	B9B	2	2754	4	21,28,29	1.95	3 (14%)	23,40,43	6.49	5 (21%)
4	P7G	2	3880	4	24,28,29	4.11	11 (45%)	27,41,44	1.42	3 (11%)
4	E6G	2	4355	4	20,27,28	2.77	3 (15%)	22,39,42	3.21	7 (31%)
4	B9H	2	2786	4	20,25,26	3.22	5 (25%)	22,35,38	2.22	7 (31%)
4	OMC	2	2422	4,29	19,22,23	3.01	8 (42%)	26,31,34	1.06	2 (7%)
4	MHG	2	4371	4	29,32,33	3.92	11 (37%)	34,46,49	2.35	13 (38%)
4	OMU	2	4620	4	19,22,23	2.93	8 (42%)	26,31,34	1.65	4 (15%)
4	M7A	2	4564	4	20,25,26	2.00	3 (15%)	28,37,40	3.91	6 (21%)
4	OMG	2	1625	4	18,26,27	2.90	8 (44%)	19,38,41	1.45	3 (15%)
4	B8K	2	3897	4	24,28,29	3.35	11 (45%)	30,42,45	2.48	11 (36%)
4	OMC	2	2804	4	19,22,23	2.96	8 (42%)	26,31,34	1.33	3 (11%)

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
4	OMG	2	1316	4	-	0/5/27/28	0/3/3/3
4	A2M	2	4571	4	-	0/5/27/28	0/3/3/3
4	OMG	2	1883	4	-	2/5/27/28	0/3/3/3
4	B8W	2	4185	4	-	2/5/27/28	0/3/3/3
4	2MG	2	1517	4	-	3/5/27/28	0/3/3/3
4	B9B	2	237	4	-	6/7/29/30	0/3/3/3
4	7MG	2	2522	4	-	0/7/37/38	0/3/3/3
4	A2M	2	2363	4	-	0/5/27/28	0/3/3/3
4	UR3	2	4597	4	-	2/7/25/26	0/2/2/2
4	A2M	2	4523	4	-	5/5/27/28	0/3/3/3
4	OMC	2	3869	4	-	7/9/27/28	0/2/2/2
4	OMG	2	1522	4	-	0/5/27/28	0/3/3/3
4	OMG	2	2773	4	-	2/5/27/28	0/3/3/3
4	2MG	2	4872	4	-	2/5/27/28	0/3/3/3
4	A2M	2	398	4	-	2/5/27/28	0/3/3/3
4	OMG	2	373	4	-	1/5/27/28	0/3/3/3
4	2MG	2	978	4	-	0/5/27/28	0/3/3/3
4	B8T	2	4671	4	-	0/7/27/28	0/2/2/2
4	B8W	2	4529	4	-	0/5/27/28	0/3/3/3
4	OMC	2	3887	4	-	1/9/27/28	0/2/2/2
4	A2M	2	3867	4	-	3/5/27/28	0/3/3/3
4	B8T	2	4483	4	-	0/7/27/28	0/2/2/2
4	5MU	2	4083	4	-	0/7/25/26	0/2/2/2
4	B8H	2	4296	4	-	2/7/25/26	0/2/2/2
4	A2M	2	3723	4	-	0/5/27/28	0/3/3/3
4	A2M	2	1524	4	-	1/5/27/28	0/3/3/3
4	OMG	2	2364	4	-	3/5/27/28	0/3/3/3
4	OMC	2	2861	4	-	0/9/27/28	0/2/2/2
4	5MC	2	4335	4	-	0/7/25/26	0/2/2/2
4	7MG	2	4550	4	-	1/7/37/38	0/3/3/3
4	A2M	2	1534	4	-	2/5/27/28	0/3/3/3
4	OMG	2	4196	4	-	2/5/27/28	0/3/3/3
4	OMG	2	4494	4	-	1/5/27/28	0/3/3/3
4	OMG	2	2424	4	-	2/5/27/28	0/3/3/3
4	OMC	2	2365	4	-	0/9/27/28	0/2/2/2
4	E7G	2	2297	4	-	1/9/39/40	0/3/3/3
4	A2M	2	1871	4	-	0/5/27/28	0/3/3/3
4	OMU	2	4306	4	-	0/9/27/28	0/2/2/2
4	OMC	2	4536	4	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OMG	2	4870	4	-	3/5/27/28	0/3/3/3
4	BGH	2	3899	4	-	1/13/43/44	0/3/3/3
4	OMC	2	3701	4	-	7/9/27/28	0/2/2/2
4	A2M	2	1326	4	-	1/5/27/28	0/3/3/3
4	1MA	2	1322	4	-	0/3/25/26	0/3/3/3
4	B8H	2	1860	4	-	2/7/25/26	0/2/2/2
4	B9B	2	1574	4	-	3/7/29/30	0/3/3/3
4	UR3	2	1866	4	-	2/7/25/26	0/2/2/2
4	I4U	2	1659	4	-	1/9/29/30	0/2/2/2
4	OMG	2	4637	4	-	3/5/27/28	0/3/3/3
4	A2M	2	3718	4	-	0/5/27/28	0/3/3/3
4	B8K	2	4690	4	-	0/11/41/42	0/3/3/3
4	B8Q	2	1456	4	-	0/7/42/43	0/2/2/2
4	OMG	2	4623	4	-	0/5/27/28	0/3/3/3
4	7MG	2	1605	4	-	0/7/37/38	0/3/3/3
53	OMU	8	14	53,4	-	1/9/27/28	0/2/2/2
4	A2M	2	2401	4	-	1/5/27/28	0/3/3/3
4	P4U	2	1348	4	-	1/10/29/30	0/2/2/2
4	B8W	2	2380	4	-	2/5/27/28	0/3/3/3
4	B8W	2	4472	4	-	2/5/27/28	0/3/3/3
4	2MG	2	729	4	-	2/5/27/28	0/3/3/3
4	OMG	2	2050	4	-	0/5/27/28	0/3/3/3
4	E7G	2	1797	4	-	2/9/39/40	0/3/3/3
4	P7G	2	1909	4	-	3/10/40/41	0/3/3/3
4	6MZ	2	4220	4	-	2/5/27/28	0/3/3/3
4	UR3	2	4530	4	-	0/7/25/26	0/2/2/2
4	OMG	2	4370	4	-	0/5/27/28	0/3/3/3
4	B9B	2	2754	4	-	4/7/29/30	0/3/3/3
4	P7G	2	3880	4	-	3/10/40/41	0/3/3/3
4	E6G	2	4355	4	-	3/6/28/29	0/3/3/3
4	B9H	2	2786	4	-	0/12/47/48	0/2/2/2
4	OMC	2	2422	4,29	-	1/9/27/28	0/2/2/2
4	MHG	2	4371	4	-	4/16/46/47	0/3/3/3
4	OMU	2	4620	4	-	0/9/27/28	0/2/2/2
4	M7A	2	4564	4	-	0/7/37/38	0/3/3/3
4	OMG	2	1625	4	-	3/5/27/28	0/3/3/3
4	B8K	2	3897	4	-	3/11/41/42	0/3/3/3
4	OMC	2	2804	4	-	0/9/27/28	0/2/2/2

All (572) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	2	4083	5MU	C4-C5	20.58	1.79	1.44
4	2	4083	5MU	C6-N1	16.43	1.66	1.38
4	2	4296	B8H	C6-C5	-16.39	1.11	1.34
4	2	1860	B8H	C6-C5	-16.35	1.12	1.34
4	2	1322	1MA	C2-N3	16.25	1.48	1.29
4	2	4296	B8H	C4-N3	-15.66	1.09	1.38
4	2	1860	B8H	C4-N3	-15.55	1.10	1.38
4	2	1860	B8H	C4-C5	13.36	1.82	1.44
4	2	4296	B8H	C4-C5	13.32	1.82	1.44
4	2	4296	B8H	C6-N1	12.38	1.67	1.36
4	2	1860	B8H	C6-N1	12.28	1.66	1.36
4	2	4083	5MU	C6-C5	-11.74	1.15	1.34
4	2	4083	5MU	C4-N3	-11.07	1.18	1.38
4	2	1659	I4U	C4-N3	10.69	1.45	1.31
4	2	1348	P4U	C4-N3	10.41	1.44	1.31
4	2	4355	E6G	O6-C6	10.16	1.43	1.35
4	2	2786	B9H	C2-N3	9.76	1.49	1.37
4	2	4371	MHG	C8-N9	9.47	1.51	1.46
4	2	2297	E7G	C5-N7	9.45	1.46	1.35
4	2	1797	E7G	C8-N9	9.37	1.51	1.46
4	2	3880	P7G	C8-N9	9.33	1.51	1.46
4	2	4550	7MG	C8-N9	9.31	1.51	1.46
4	2	1797	E7G	C5-N7	9.29	1.46	1.35
4	2	3880	P7G	C5-N7	9.24	1.45	1.35
4	2	1909	P7G	C5-N7	9.23	1.45	1.35
4	2	1909	P7G	C8-N9	9.15	1.51	1.46
4	2	1605	7MG	C8-N9	9.14	1.51	1.46
4	2	4690	B8K	C8-N9	9.14	1.51	1.46
4	2	4335	5MC	C6-C5	9.09	1.49	1.34
4	2	3899	BGH	C8-N9	9.03	1.51	1.46
4	2	1524	A2M	C3'-C4'	-8.94	1.30	1.53
4	2	3867	A2M	C3'-C4'	-8.91	1.30	1.53
4	2	398	A2M	C3'-C4'	-8.90	1.30	1.53
4	2	4371	MHG	C5-N7	8.90	1.45	1.35
4	2	2363	A2M	C3'-C4'	-8.85	1.30	1.53
4	2	3899	BGH	O4'-C1'	8.83	1.62	1.42
4	2	3723	A2M	C3'-C4'	-8.82	1.30	1.53
4	2	3899	BGH	C2'-C1'	-8.82	1.30	1.53
4	2	1871	A2M	C3'-C4'	-8.80	1.30	1.53
4	2	4550	7MG	C5-N7	8.78	1.45	1.35
4	2	3897	B8K	C8-N9	8.77	1.50	1.46
4	2	3718	A2M	C3'-C4'	-8.72	1.30	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	2	1534	A2M	C3'-C4'	-8.72	1.30	1.53
4	2	2401	A2M	C3'-C4'	-8.67	1.30	1.53
4	2	2297	E7G	C8-N9	8.65	1.50	1.46
4	2	4571	A2M	C3'-C4'	-8.64	1.30	1.53
4	2	2522	7MG	C5-N7	8.63	1.45	1.35
4	2	4523	A2M	C3'-C4'	-8.62	1.31	1.53
4	2	1605	7MG	C5-N7	8.60	1.45	1.35
4	2	2522	7MG	C8-N9	8.58	1.50	1.46
4	2	1456	B8Q	C6-C5	8.30	1.52	1.33
4	2	1326	A2M	C3'-C4'	-8.28	1.31	1.53
4	2	4371	MHG	C2-N3	8.07	1.47	1.31
4	2	4529	B8W	C2-N2	7.95	1.49	1.33
4	2	2380	B8W	C2-N2	7.89	1.49	1.33
4	2	4185	B8W	C2-N2	7.87	1.49	1.33
4	2	4472	B8W	C2-N2	7.85	1.49	1.33
4	2	3718	A2M	O4'-C4'	7.83	1.62	1.45
4	2	1326	A2M	O4'-C4'	7.82	1.62	1.45
4	2	1871	A2M	O4'-C4'	7.73	1.62	1.45
4	2	398	A2M	O4'-C4'	7.70	1.62	1.45
4	2	2401	A2M	O4'-C4'	7.69	1.62	1.45
4	2	1534	A2M	O4'-C4'	7.67	1.62	1.45
4	2	4523	A2M	O4'-C4'	7.67	1.62	1.45
4	2	3899	BGH	O4'-C4'	-7.61	1.28	1.45
4	2	3723	A2M	O4'-C4'	7.55	1.61	1.45
4	2	2363	A2M	O4'-C4'	7.52	1.61	1.45
4	2	4483	B8T	C2-N3	7.45	1.51	1.36
4	2	1524	A2M	O4'-C4'	7.38	1.61	1.45
4	2	1524	A2M	O4'-C1'	-7.31	1.30	1.41
4	2	4671	B8T	C2-N3	7.31	1.51	1.36
4	2	3867	A2M	O4'-C4'	7.30	1.61	1.45
4	2	3867	A2M	O4'-C1'	-7.26	1.30	1.41
4	2	4571	A2M	O4'-C4'	7.25	1.61	1.45
4	2	2401	A2M	O4'-C1'	-7.22	1.31	1.41
4	2	4571	A2M	O4'-C1'	-7.19	1.31	1.41
4	2	1534	A2M	O4'-C1'	-7.16	1.31	1.41
4	2	2363	A2M	O4'-C1'	-7.13	1.31	1.41
4	2	4671	B8T	C4-N3	7.13	1.45	1.32
4	2	1866	UR3	C2-N1	7.05	1.48	1.38
4	2	4483	B8T	C4-N3	7.04	1.45	1.32
4	2	398	A2M	O4'-C1'	-7.04	1.31	1.41
4	2	4530	UR3	C2-N1	7.01	1.48	1.38
4	2	3723	A2M	O4'-C1'	-6.98	1.31	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	2	4523	A2M	O4'-C1'	-6.96	1.31	1.41
4	2	4306	OMU	C2-N1	6.95	1.49	1.38
4	2	1326	A2M	O4'-C1'	-6.94	1.31	1.41
4	2	1866	UR3	C6-C5	6.93	1.51	1.35
4	2	3718	A2M	O4'-C1'	-6.92	1.31	1.41
4	2	2786	B9H	C6-C5	6.92	1.48	1.33
4	2	2786	B9H	C2-N1	6.88	1.48	1.38
4	2	1871	A2M	O4'-C1'	-6.86	1.31	1.41
4	2	4620	OMU	C2-N1	6.83	1.49	1.38
4	2	4671	B8T	C6-C5	6.83	1.50	1.35
4	2	978	2MG	C2-N2	6.83	1.48	1.33
4	2	4530	UR3	C6-C5	6.75	1.50	1.35
53	8	14	OMU	C2-N1	6.72	1.49	1.38
4	2	4597	UR3	C6-C5	6.71	1.50	1.35
4	2	4220	6MZ	C6-N6	6.68	1.46	1.35
4	2	1517	2MG	C2-N2	6.67	1.48	1.33
4	2	4483	B8T	C6-C5	6.66	1.50	1.35
4	2	1456	B8Q	C2-N3	6.65	1.46	1.35
4	2	1797	E7G	C4-N9	6.64	1.45	1.37
4	2	3897	B8K	C2-N3	6.61	1.49	1.33
4	2	4371	MHG	C8-N7	6.58	1.52	1.45
4	2	4306	OMU	C2-N3	6.57	1.49	1.38
4	2	4690	B8K	C2-N3	6.51	1.48	1.33
53	8	14	OMU	C2-N3	6.51	1.49	1.38
4	2	729	2MG	C2-N2	6.47	1.47	1.33
4	2	4483	B8T	C4-N4	6.47	1.49	1.35
4	2	4620	OMU	C2-N3	6.47	1.49	1.38
4	2	3880	P7G	C4-N9	6.47	1.44	1.35
4	2	4196	OMG	C2-N3	6.46	1.48	1.33
4	2	3887	OMC	C2-N3	6.44	1.49	1.36
4	2	4335	5MC	C4-N3	6.44	1.45	1.34
4	2	3880	P7G	C8-N7	6.43	1.51	1.45
4	2	4536	OMC	C2-N3	6.41	1.49	1.36
4	2	2861	OMC	C2-N3	6.34	1.49	1.36
4	2	2297	E7G	C8-N7	6.31	1.51	1.45
4	2	3701	OMC	C2-N3	6.31	1.49	1.36
4	2	1625	OMG	C2-N3	6.31	1.48	1.33
4	2	2422	OMC	C2-N3	6.31	1.49	1.36
4	2	4671	B8T	C4-N4	6.29	1.48	1.35
4	2	4371	MHG	C2-N1	6.29	1.46	1.36
4	2	3869	OMC	C2-N3	6.27	1.49	1.36
4	2	3880	P7G	C4-N3	6.27	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	2	1909	P7G	C4-N3	6.23	1.48	1.37
4	2	1659	I4U	C2-N3	6.22	1.49	1.36
4	2	4335	5MC	C2-N3	6.21	1.48	1.36
4	2	2424	OMG	C2-N3	6.19	1.48	1.33
4	2	1909	P7G	C4-N9	6.17	1.44	1.35
4	2	4872	2MG	C2-N2	6.17	1.47	1.33
4	2	2773	OMG	C2-N3	6.17	1.48	1.33
4	2	4870	OMG	C2-N3	6.16	1.48	1.33
4	2	237	B9B	O6-C6	6.15	1.40	1.35
4	2	2804	OMC	C2-N3	6.15	1.48	1.36
4	2	4494	OMG	C2-N3	6.14	1.48	1.33
4	2	2365	OMC	C2-N3	6.12	1.48	1.36
4	2	1883	OMG	C2-N3	6.11	1.48	1.33
4	2	1659	I4U	C6-C5	6.11	1.49	1.35
4	2	1348	P4U	C2-N3	6.10	1.48	1.36
4	2	3701	OMC	C6-C5	6.09	1.49	1.35
4	2	4597	UR3	C2-N3	6.07	1.50	1.39
4	2	4196	OMG	C2-N2	6.06	1.48	1.34
4	2	4870	OMG	C2-N2	6.05	1.48	1.34
4	2	2773	OMG	C2-N2	6.05	1.48	1.34
4	2	1574	B9B	O6-C6	6.05	1.40	1.35
4	2	1625	OMG	C2-N2	6.04	1.48	1.34
4	2	4637	OMG	C2-N3	6.03	1.47	1.33
4	2	4370	OMG	C2-N3	6.03	1.47	1.33
4	2	4370	OMG	C2-N2	6.02	1.48	1.34
4	2	4494	OMG	C2-N2	6.01	1.48	1.34
4	2	1348	P4U	C6-C5	6.01	1.49	1.35
4	2	1316	OMG	C2-N2	5.98	1.48	1.34
4	2	2422	OMC	C6-C5	5.98	1.48	1.35
4	2	1883	OMG	C2-N2	5.97	1.48	1.34
4	2	2424	OMG	C2-N2	5.96	1.48	1.34
4	2	1316	OMG	C2-N3	5.96	1.47	1.33
4	2	3869	OMC	C6-C5	5.95	1.48	1.35
4	2	2861	OMC	C6-C5	5.95	1.48	1.35
4	2	3887	OMC	C6-C5	5.95	1.48	1.35
4	2	373	OMG	C2-N2	5.94	1.48	1.34
4	2	4536	OMC	C6-C5	5.93	1.48	1.35
4	2	4637	OMG	C2-N2	5.93	1.48	1.34
4	2	373	OMG	C2-N3	5.93	1.47	1.33
4	2	3899	BGH	C4-N9	5.92	1.44	1.37
4	2	2364	OMG	C2-N3	5.92	1.47	1.33
4	2	4355	E6G	C2-N2	5.91	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	2	1797	E7G	C4-N3	5.91	1.48	1.34
4	2	1522	OMG	C2-N2	5.91	1.48	1.34
4	2	4597	UR3	C2-N1	5.89	1.47	1.38
4	2	2365	OMC	C6-C5	5.89	1.48	1.35
4	2	1522	OMG	C2-N3	5.89	1.47	1.33
4	2	2364	OMG	C2-N2	5.87	1.48	1.34
4	2	1866	UR3	C2-N3	5.86	1.50	1.39
4	2	1909	P7G	C2-N2	5.85	1.48	1.34
4	2	4623	OMG	C2-N3	5.85	1.47	1.33
4	2	4623	OMG	C2-N2	5.85	1.48	1.34
4	2	3880	P7G	C2-N2	5.84	1.48	1.34
4	2	2804	OMC	C6-C5	5.80	1.48	1.35
4	2	2754	B9B	O6-C6	5.79	1.40	1.35
4	2	1797	E7G	C8-N7	5.78	1.51	1.45
4	2	1797	E7G	C2-N3	5.77	1.47	1.33
4	2	4530	UR3	C2-N3	5.76	1.50	1.39
4	2	237	B9B	C2-N2	5.75	1.45	1.33
4	2	2050	OMG	C2-N2	5.74	1.47	1.34
4	2	4550	7MG	C2-N3	5.72	1.47	1.33
4	2	1605	7MG	C2-N3	5.70	1.46	1.33
4	2	2754	B9B	C2-N2	5.69	1.45	1.33
4	2	2297	E7G	C4-N9	5.69	1.44	1.37
4	2	4371	MHG	C2-N2	5.67	1.46	1.33
4	2	2297	E7G	C2-N3	5.65	1.46	1.33
4	2	4564	M7A	C4-N9	5.64	1.48	1.38
4	2	2297	E7G	C4-N3	5.64	1.47	1.34
4	2	4306	OMU	C6-C5	5.63	1.48	1.35
4	2	3899	BGH	C4-N3	5.62	1.47	1.34
4	2	2050	OMG	C2-N3	5.61	1.46	1.33
4	2	3897	B8K	C4-N9	5.61	1.44	1.37
4	2	4620	OMU	C6-C5	5.59	1.48	1.35
4	2	4550	7MG	C4-N3	5.59	1.47	1.34
4	2	1574	B9B	C2-N2	5.58	1.45	1.33
4	2	1605	7MG	C4-N3	5.56	1.47	1.34
4	2	3899	BGH	C2-N3	5.55	1.46	1.33
4	2	2522	7MG	C2-N3	5.53	1.46	1.33
4	2	4371	MHG	C4-N3	5.48	1.47	1.34
4	2	4690	B8K	C4-N9	5.45	1.44	1.37
4	2	2522	7MG	C4-N3	5.45	1.47	1.34
4	2	4371	MHG	C4-N9	5.42	1.44	1.37
4	2	1605	7MG	C4-N9	5.34	1.43	1.37
4	2	1909	P7G	C8-N7	5.31	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	2	729	2MG	C4-N3	5.27	1.50	1.37
4	2	978	2MG	C4-N3	5.23	1.50	1.37
4	2	4483	B8T	C2-N1	5.21	1.51	1.40
4	2	4550	7MG	C4-N9	5.20	1.43	1.37
53	8	14	OMU	C6-C5	5.20	1.47	1.35
4	2	1797	E7G	C2-N2	5.18	1.46	1.34
4	2	2297	E7G	C2-N2	5.18	1.46	1.34
4	2	1909	P7G	C2-N1	5.18	1.45	1.33
4	2	3701	OMC	C4-N3	5.17	1.44	1.34
4	2	1517	2MG	C4-N3	5.13	1.49	1.37
4	2	2861	OMC	C2-N1	5.10	1.51	1.40
4	2	3880	P7G	C2-N1	5.09	1.45	1.33
4	2	4196	OMG	C4-N3	5.06	1.49	1.37
4	2	2804	OMC	C2-N1	5.05	1.50	1.40
4	2	3887	OMC	C4-N3	5.04	1.44	1.34
4	2	3869	OMC	C4-N3	5.03	1.44	1.34
4	2	2522	7MG	C4-N9	5.00	1.43	1.37
4	2	2365	OMC	C4-N3	4.98	1.44	1.34
4	2	2861	OMC	C4-N3	4.98	1.44	1.34
4	2	2422	OMC	C2-N1	4.96	1.50	1.40
4	2	3887	OMC	C2-N1	4.94	1.50	1.40
4	2	4536	OMC	C4-N3	4.94	1.44	1.34
4	2	2422	OMC	C4-N3	4.94	1.44	1.34
4	2	4536	OMC	C2-N1	4.92	1.50	1.40
4	2	4870	OMG	C4-N3	4.92	1.49	1.37
4	2	3887	OMC	C4-N4	4.88	1.45	1.33
4	2	4536	OMC	C4-N4	4.88	1.45	1.33
4	2	1456	B8Q	C2-N1	4.85	1.45	1.38
4	2	1625	OMG	C4-N3	4.84	1.49	1.37
4	2	3701	OMC	C4-N4	4.83	1.45	1.33
4	2	3869	OMC	C2-N1	4.83	1.50	1.40
4	2	4550	7MG	C2-N2	4.83	1.45	1.34
4	2	2861	OMC	C4-N4	4.83	1.45	1.33
4	2	2422	OMC	C4-N4	4.81	1.45	1.33
4	2	1659	I4U	C5-C4	4.81	1.49	1.43
4	2	3869	OMC	C4-N4	4.80	1.45	1.33
4	2	2804	OMC	C4-N3	4.80	1.44	1.34
4	2	2804	OMC	C4-N4	4.78	1.45	1.33
4	2	3899	BGH	C2-N2	4.78	1.45	1.34
4	2	1348	P4U	O4-C4	4.77	1.40	1.35
4	2	2365	OMC	C4-N4	4.76	1.45	1.33
4	2	2773	OMG	C4-N3	4.75	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	2	1605	7MG	C2-N2	4.75	1.45	1.34
4	2	2424	OMG	C4-N3	4.75	1.48	1.37
4	2	1883	OMG	C4-N3	4.74	1.48	1.37
4	2	4494	OMG	C4-N3	4.73	1.48	1.37
4	2	2522	7MG	C2-N2	4.73	1.45	1.34
4	2	4370	OMG	C4-N3	4.69	1.48	1.37
4	2	4637	OMG	C4-N3	4.68	1.48	1.37
4	2	373	OMG	C4-N3	4.62	1.48	1.37
4	2	1316	OMG	C4-N3	4.61	1.48	1.37
4	2	4872	2MG	C4-N3	4.61	1.48	1.37
4	2	4637	OMG	C6-N1	4.59	1.44	1.37
4	2	1883	OMG	C6-N1	4.58	1.44	1.37
4	2	3899	BGH	C5-N7	4.57	1.47	1.39
4	2	1860	B8H	C2-N3	4.56	1.46	1.38
4	2	4335	5MC	C6-N1	4.55	1.45	1.38
4	2	2364	OMG	C6-N1	4.55	1.44	1.37
4	2	4083	5MU	C2-N3	4.55	1.46	1.38
4	2	4196	OMG	C6-N1	4.55	1.44	1.37
4	2	4870	OMG	C6-N1	4.55	1.44	1.37
4	2	1522	OMG	C4-N3	4.53	1.48	1.37
4	2	2050	OMG	C4-N3	4.53	1.48	1.37
4	2	4494	OMG	C6-N1	4.53	1.44	1.37
4	2	4671	B8T	C2-N1	4.52	1.49	1.40
4	2	4623	OMG	C4-N3	4.52	1.48	1.37
4	2	2364	OMG	C4-N3	4.50	1.48	1.37
4	2	373	OMG	C6-N1	4.50	1.44	1.37
4	2	4370	OMG	C6-N1	4.48	1.44	1.37
4	2	2424	OMG	C6-N1	4.46	1.44	1.37
4	2	1316	OMG	C6-N1	4.45	1.44	1.37
4	2	3897	B8K	C4-N3	4.44	1.44	1.34
4	2	3701	OMC	C2-N1	4.43	1.49	1.40
4	2	1625	OMG	C6-N1	4.42	1.44	1.37
4	2	4296	B8H	C2-N3	4.41	1.45	1.38
4	2	1522	OMG	C6-N1	4.40	1.44	1.37
4	2	4623	OMG	C6-N1	4.40	1.44	1.37
4	2	4690	B8K	C4-N3	4.37	1.44	1.34
4	2	4335	5MC	C4-N4	4.35	1.45	1.34
4	2	2773	OMG	C6-N1	4.34	1.44	1.37
4	2	4564	M7A	C6-N6	4.31	1.45	1.34
4	2	1348	P4U	C5-C4	4.30	1.48	1.43
4	2	2365	OMC	C2-N1	4.29	1.49	1.40
4	2	3897	B8K	C5-C6	4.27	1.54	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	2	4335	5MC	C2-N1	4.23	1.49	1.40
4	2	1517	2MG	C2-N1	4.22	1.43	1.36
4	2	3899	BGH	C5-C6	4.21	1.54	1.43
4	2	978	2MG	C2-N1	4.19	1.43	1.36
4	2	4306	OMU	C4-N3	4.17	1.46	1.38
4	2	1348	P4U	C2-N1	4.17	1.49	1.40
4	2	3897	B8K	C5-N7	4.16	1.46	1.39
4	2	2050	OMG	C6-N1	4.15	1.44	1.37
4	2	1659	I4U	C2-N1	4.15	1.49	1.40
4	2	4690	B8K	C5-C6	4.13	1.54	1.43
4	2	4690	B8K	C5-N7	4.12	1.46	1.39
4	2	1322	1MA	C2-N1	4.10	1.43	1.35
4	2	1322	1MA	C4-N3	4.08	1.50	1.37
4	2	4564	M7A	C5-N7	4.05	1.49	1.39
53	8	14	OMU	C4-N3	4.02	1.45	1.38
4	2	4872	2MG	C2-N1	3.95	1.43	1.36
4	2	729	2MG	C2-N1	3.93	1.43	1.36
4	2	4550	7MG	C5-C6	3.85	1.53	1.43
4	2	4620	OMU	C4-N3	3.85	1.45	1.38
4	2	4671	B8T	C5-C4	3.84	1.49	1.40
4	2	1797	E7G	C5-C6	3.84	1.53	1.43
4	2	2297	E7G	C5-C6	3.83	1.53	1.43
4	2	978	2MG	C6-N1	3.81	1.43	1.37
4	2	1605	7MG	C5-C6	3.72	1.53	1.43
4	2	1517	2MG	C6-N1	3.71	1.43	1.37
4	2	4371	MHG	C5-C6	3.70	1.53	1.43
4	2	1909	P7G	C2-N3	3.69	1.46	1.37
4	2	2522	7MG	C5-C6	3.64	1.52	1.43
4	2	3880	P7G	C2-N3	3.63	1.46	1.37
4	2	1605	7MG	C2-N1	3.63	1.46	1.37
4	2	3897	B8K	C6-N1	3.62	1.45	1.38
4	2	3899	BGH	O2'-C2'	3.60	1.51	1.42
4	2	3899	BGH	C71-N7	3.58	1.47	1.39
4	2	4083	5MU	C2-N1	3.57	1.44	1.38
4	2	4483	B8T	C5-C4	3.56	1.48	1.40
4	2	4550	7MG	C2-N1	3.54	1.46	1.37
4	2	1797	E7G	C2-N1	3.53	1.46	1.37
4	2	4690	B8K	C2-N2	3.52	1.42	1.34
4	2	4872	2MG	C6-N1	3.51	1.43	1.37
4	2	3897	B8K	C2-N2	3.51	1.42	1.34
4	2	4690	B8K	C71-N7	3.50	1.47	1.39
4	2	1909	P7G	C6-N1	3.50	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	2	729	2MG	C6-N1	3.48	1.43	1.37
4	2	4690	B8K	C6-N1	3.48	1.45	1.38
4	2	978	2MG	C5-C6	3.47	1.54	1.47
4	2	4872	2MG	C5-C6	3.46	1.54	1.47
4	2	2522	7MG	C2-N1	3.46	1.46	1.37
4	2	4530	UR3	C6-N1	3.45	1.46	1.38
4	2	4483	B8T	C6-N1	3.45	1.46	1.38
4	2	3887	OMC	C6-N1	3.45	1.46	1.38
4	2	1866	UR3	C6-N1	3.44	1.46	1.38
4	2	3880	P7G	C6-N1	3.44	1.44	1.38
4	2	3899	BGH	C2-N1	3.43	1.46	1.37
4	2	2297	E7G	C2-N1	3.41	1.46	1.37
4	2	3897	B8K	C71-N7	3.39	1.47	1.39
4	2	4550	7MG	C6-N1	3.37	1.45	1.38
4	2	1909	P7G	O6-C6	-3.36	1.18	1.23
4	2	3899	BGH	C6-N1	3.36	1.45	1.38
4	2	4371	MHG	C6-N1	3.35	1.45	1.38
4	2	1348	P4U	C6-N1	3.33	1.46	1.38
4	2	1605	7MG	C6-N1	3.31	1.45	1.38
4	2	4196	OMG	C5-C6	3.31	1.54	1.47
4	2	3869	OMC	C6-N1	3.31	1.46	1.38
4	2	1797	E7G	C6-N1	3.30	1.45	1.38
4	2	1517	2MG	C5-C6	3.30	1.54	1.47
4	2	2364	OMG	C5-C6	3.28	1.54	1.47
4	2	729	2MG	C5-C6	3.28	1.54	1.47
4	2	2522	7MG	C6-N1	3.26	1.44	1.38
4	2	4690	B8K	C2-N1	3.24	1.45	1.37
4	2	3897	B8K	C2-N1	3.24	1.45	1.37
4	2	1659	I4U	C6-N1	3.22	1.45	1.38
4	2	2365	OMC	C6-N1	3.22	1.45	1.38
4	2	2422	OMC	C6-N1	3.22	1.45	1.38
4	2	3880	P7G	C5-C4	3.21	1.43	1.37
4	2	1316	OMG	C5-C6	3.21	1.53	1.47
4	2	2861	OMC	C6-N1	3.21	1.45	1.38
4	2	4623	OMG	C5-C6	3.21	1.53	1.47
4	2	1909	P7G	C5-C4	3.20	1.43	1.37
4	2	4536	OMC	C6-N1	3.18	1.45	1.38
4	2	3723	A2M	C6-N6	3.18	1.45	1.34
4	2	4671	B8T	C6-N1	3.17	1.45	1.38
4	2	3718	A2M	C6-N6	3.16	1.45	1.34
4	2	3701	OMC	C6-N1	3.15	1.45	1.38
4	2	4523	A2M	C6-N6	3.14	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	2	398	A2M	C6-N6	3.14	1.45	1.34
4	2	2297	E7G	C6-N1	3.14	1.44	1.38
4	2	1871	A2M	C6-N6	3.14	1.45	1.34
4	2	1524	A2M	C6-N6	3.14	1.45	1.34
4	2	2050	OMG	C5-C6	3.13	1.53	1.47
4	2	4370	OMG	C5-C6	3.13	1.53	1.47
4	2	373	OMG	C5-C6	3.12	1.53	1.47
4	2	3867	A2M	C6-N6	3.11	1.45	1.34
4	2	2401	A2M	C6-N6	3.11	1.45	1.34
4	2	4637	OMG	C5-C6	3.10	1.53	1.47
4	2	4571	A2M	C6-N6	3.10	1.45	1.34
4	2	1625	OMG	C5-C6	3.10	1.53	1.47
4	2	1326	A2M	C6-N6	3.10	1.45	1.34
4	2	2363	A2M	C6-N6	3.09	1.45	1.34
4	2	2773	OMG	C5-C6	3.09	1.53	1.47
4	2	4494	OMG	C5-C6	3.08	1.53	1.47
4	2	2401	A2M	O3'-C3'	3.08	1.50	1.43
4	2	3880	P7G	O6-C6	-3.08	1.18	1.23
4	2	4870	OMG	C5-C6	3.08	1.53	1.47
4	2	4597	UR3	C6-N1	3.07	1.45	1.38
4	2	2804	OMC	C6-N1	3.07	1.45	1.38
4	2	1534	A2M	C6-N6	3.06	1.45	1.34
4	2	1522	OMG	C5-C6	3.04	1.53	1.47
4	2	1326	A2M	O3'-C3'	3.04	1.50	1.43
53	8	14	OMU	O4-C4	-3.02	1.18	1.24
4	2	4355	E6G	C5-C4	-3.02	1.32	1.40
4	2	4083	5MU	O4-C4	-3.01	1.17	1.23
4	2	4620	OMU	O4-C4	-3.00	1.18	1.24
4	2	1883	OMG	O6-C6	-3.00	1.17	1.23
4	2	1659	I4U	O4-C4	3.00	1.41	1.35
4	2	1517	2MG	C5-C4	-2.97	1.35	1.43
4	2	4872	2MG	C5-C4	-2.96	1.35	1.43
4	2	4306	OMU	O4-C4	-2.93	1.18	1.24
4	2	4306	OMU	C6-N1	2.93	1.45	1.38
4	2	3899	BGH	O3'-C3'	-2.92	1.36	1.43
4	2	3723	A2M	O3'-C3'	2.91	1.49	1.43
4	2	1348	P4U	O2-C2	-2.91	1.18	1.23
4	2	1883	OMG	C5-C6	2.89	1.53	1.47
4	2	1534	A2M	O3'-C3'	2.89	1.49	1.43
4	2	3897	B8K	C5-C4	2.88	1.47	1.38
4	2	3718	A2M	O3'-C3'	2.87	1.49	1.43
4	2	4523	A2M	O3'-C3'	2.86	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	2	1522	OMG	O6-C6	-2.86	1.17	1.23
4	2	4870	OMG	O6-C6	-2.85	1.17	1.23
4	2	4671	B8T	O2-C2	-2.84	1.18	1.23
4	2	4690	B8K	C5-C4	2.84	1.47	1.38
4	2	978	2MG	C5-C4	-2.84	1.35	1.43
4	2	1316	OMG	O6-C6	-2.83	1.17	1.23
4	2	3867	A2M	O3'-C3'	2.83	1.49	1.43
4	2	2363	A2M	O3'-C3'	2.82	1.49	1.43
4	2	2380	B8W	C5-C4	-2.82	1.33	1.40
4	2	2424	OMG	O6-C6	-2.81	1.17	1.23
4	2	2773	OMG	O6-C6	-2.81	1.17	1.23
4	2	2424	OMG	C5-C6	2.80	1.53	1.47
4	2	729	2MG	C5-C4	-2.80	1.35	1.43
4	2	1534	A2M	O2'-C2'	-2.80	1.35	1.42
4	2	4623	OMG	O6-C6	-2.79	1.17	1.23
4	2	4472	B8W	C5-C4	-2.79	1.33	1.40
4	2	2364	OMG	O6-C6	-2.78	1.17	1.23
4	2	1524	A2M	O3'-C3'	2.77	1.49	1.43
4	2	1534	A2M	C5-C4	-2.77	1.33	1.40
4	2	373	OMG	O6-C6	-2.77	1.17	1.23
4	2	237	B9B	C5-C4	-2.77	1.33	1.40
4	2	2365	OMC	O2-C2	-2.77	1.18	1.23
4	2	4370	OMG	O6-C6	-2.77	1.17	1.23
4	2	4637	OMG	O6-C6	-2.76	1.17	1.23
4	2	2754	B9B	C5-C4	-2.76	1.33	1.40
4	2	1574	B9B	C5-C4	-2.76	1.33	1.40
4	2	398	A2M	O3'-C3'	2.76	1.49	1.43
4	2	4494	OMG	O6-C6	-2.76	1.17	1.23
4	2	1871	A2M	O3'-C3'	2.75	1.49	1.43
4	2	4571	A2M	O3'-C3'	2.73	1.49	1.43
4	2	2050	OMG	O6-C6	-2.73	1.17	1.23
4	2	1659	I4U	O2-C2	-2.73	1.18	1.23
4	2	1625	OMG	O6-C6	-2.72	1.17	1.23
4	2	2401	A2M	C5-C4	-2.71	1.33	1.40
4	2	4483	B8T	O2-C2	-2.71	1.18	1.23
4	2	3869	OMC	O2-C2	-2.70	1.18	1.23
4	2	4083	5MU	O2-C2	-2.70	1.18	1.23
4	2	2804	OMC	O2-C2	-2.70	1.18	1.23
4	2	2401	A2M	O2'-C2'	-2.69	1.35	1.42
4	2	3701	OMC	O2-C2	-2.68	1.18	1.23
4	2	4529	B8W	C5-C4	-2.68	1.33	1.40
4	2	2363	A2M	O2'-C2'	-2.68	1.35	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	2	1524	A2M	O2'-C2'	-2.67	1.35	1.42
4	2	4196	OMG	O6-C6	-2.67	1.17	1.23
4	2	2422	OMC	O2-C2	-2.67	1.18	1.23
4	2	4571	A2M	C5-C4	-2.66	1.33	1.40
4	2	1659	I4U	O4-C41	-2.66	1.41	1.47
4	2	3899	BGH	O6-C6	-2.65	1.18	1.23
4	2	398	A2M	O2'-C2'	-2.64	1.35	1.42
4	2	4185	B8W	C5-C4	-2.64	1.33	1.40
4	2	1871	A2M	O2'-C2'	-2.62	1.35	1.42
4	2	2363	A2M	C5-C4	-2.62	1.34	1.40
4	2	4620	OMU	C6-N1	2.62	1.44	1.38
4	2	3867	A2M	O2'-C2'	-2.62	1.35	1.42
4	2	3723	A2M	C5-C4	-2.61	1.34	1.40
4	2	4335	5MC	O2-C2	-2.61	1.18	1.23
4	2	3867	A2M	C5-C4	-2.60	1.34	1.40
4	2	3701	OMC	C5-C4	2.59	1.48	1.42
4	2	4523	A2M	O2'-C2'	-2.59	1.36	1.42
4	2	1524	A2M	C5-C4	-2.58	1.34	1.40
4	2	3723	A2M	O2'-C2'	-2.58	1.36	1.42
4	2	398	A2M	C5-C4	-2.58	1.34	1.40
4	2	2861	OMC	O2-C2	-2.57	1.18	1.23
4	2	3887	OMC	O2-C2	-2.57	1.18	1.23
4	2	2522	7MG	O6-C6	-2.57	1.18	1.23
4	2	1871	A2M	C5-C4	-2.57	1.34	1.40
53	8	14	OMU	C6-N1	2.56	1.44	1.38
4	2	4523	A2M	C5-C4	-2.56	1.34	1.40
4	2	1605	7MG	O6-C6	-2.56	1.18	1.23
4	2	4550	7MG	O6-C6	-2.55	1.18	1.23
4	2	4571	A2M	O2'-C2'	-2.55	1.36	1.42
4	2	4536	OMC	O2-C2	-2.54	1.19	1.23
4	2	373	OMG	C5-C4	-2.54	1.36	1.43
4	2	3718	A2M	O2'-C2'	-2.53	1.36	1.42
4	2	1326	A2M	O2'-C2'	-2.52	1.36	1.42
4	2	4370	OMG	C2-N1	2.52	1.43	1.37
4	2	1883	OMG	C5-C4	-2.51	1.36	1.43
53	8	14	OMU	O2-C2	-2.51	1.18	1.23
4	2	1797	E7G	O6-C6	-2.50	1.18	1.23
4	2	4196	OMG	C2-N1	2.50	1.43	1.37
4	2	1326	A2M	C5-C4	-2.47	1.34	1.40
4	2	4220	6MZ	C5-C4	-2.47	1.34	1.40
4	2	3718	A2M	C5-C4	-2.47	1.34	1.40
4	2	4870	OMG	C2-N1	2.45	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	2	2773	OMG	C2-N1	2.45	1.43	1.37
4	2	1883	OMG	C2-N1	2.44	1.43	1.37
4	2	373	OMG	C2-N1	2.44	1.43	1.37
4	2	4637	OMG	C2-N1	2.43	1.43	1.37
4	2	2050	OMG	C5-C4	-2.43	1.36	1.43
4	2	4494	OMG	C2-N1	2.43	1.43	1.37
4	2	4620	OMU	O2-C2	-2.43	1.18	1.23
4	2	2424	OMG	C2-N1	2.43	1.43	1.37
4	2	1625	OMG	C2-N1	2.42	1.43	1.37
4	2	4523	A2M	C2-N3	2.42	1.36	1.32
4	2	2297	E7G	O6-C6	-2.42	1.19	1.23
4	2	1316	OMG	C5-C4	-2.42	1.36	1.43
4	2	1316	OMG	C2-N1	2.42	1.43	1.37
4	2	1522	OMG	C5-C4	-2.41	1.36	1.43
4	2	4220	6MZ	C2-N3	2.41	1.36	1.32
4	2	1522	OMG	C2-N1	2.40	1.43	1.37
4	2	3887	OMC	C5-C4	2.40	1.48	1.42
4	2	4623	OMG	C2-N1	2.40	1.43	1.37
4	2	2050	OMG	C2-N1	2.39	1.43	1.37
4	2	2364	OMG	C2-N1	2.39	1.43	1.37
4	2	1866	UR3	C4-N3	2.39	1.46	1.40
4	2	4530	UR3	C4-N3	2.38	1.46	1.40
4	2	4306	OMU	C5-C4	2.38	1.48	1.43
4	2	2364	OMG	C5-C4	-2.38	1.37	1.43
4	2	2365	OMC	C5-C4	2.37	1.48	1.42
4	2	3869	OMC	C5-C4	2.36	1.48	1.42
4	2	1326	A2M	C2-N3	2.35	1.35	1.32
4	2	1866	UR3	C5-C4	2.35	1.49	1.43
4	2	1524	A2M	C2-N3	2.34	1.35	1.32
4	2	2861	OMC	C5-C4	2.34	1.48	1.42
4	2	1871	A2M	C2-N3	2.34	1.35	1.32
4	2	1456	B8Q	C6-N1	2.33	1.43	1.38
4	2	4571	A2M	C2-N3	2.33	1.35	1.32
4	2	3723	A2M	C2-N3	2.33	1.35	1.32
4	2	2363	A2M	C2-N3	2.32	1.35	1.32
4	2	2422	OMC	C5-C4	2.32	1.48	1.42
4	2	4371	MHG	O6-C6	-2.30	1.19	1.23
4	2	4637	OMG	C5-C4	-2.30	1.37	1.43
4	2	4623	OMG	C5-C4	-2.30	1.37	1.43
4	2	4870	OMG	C5-C4	-2.30	1.37	1.43
4	2	4597	UR3	C5-C4	2.29	1.49	1.43
4	2	4306	OMU	O2-C2	-2.29	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	2	1534	A2M	C2-N3	2.26	1.35	1.32
4	2	2424	OMG	C5-C4	-2.26	1.37	1.43
53	8	14	OMU	C5-C4	2.25	1.48	1.43
4	2	398	A2M	C2-N3	2.24	1.35	1.32
4	2	4536	OMC	C5-C4	2.24	1.48	1.42
4	2	1322	1MA	C5-C4	-2.23	1.37	1.43
4	2	4620	OMU	C5-C4	2.22	1.48	1.43
4	2	3867	A2M	C2-N3	2.22	1.35	1.32
4	2	2401	A2M	C2-N3	2.22	1.35	1.32
4	2	4597	UR3	C4-N3	2.21	1.45	1.40
4	2	4530	UR3	C5-C4	2.19	1.49	1.43
4	2	4370	OMG	C5-C4	-2.17	1.37	1.43
4	2	3718	A2M	C2-N3	2.17	1.35	1.32
4	2	2786	B9H	C31-N3	-2.16	1.43	1.46
4	2	2786	B9H	C6-N1	2.16	1.43	1.38
4	2	2804	OMC	C5-C4	2.14	1.47	1.42
4	2	4296	B8H	O4-C4	-2.14	1.19	1.23
4	2	4597	UR3	O2-C2	-2.13	1.18	1.22
4	2	3899	BGH	C5-C4	2.12	1.45	1.38
4	2	2773	OMG	C5-C4	-2.11	1.37	1.43
4	2	1322	1MA	CM1-N1	2.11	1.51	1.46
4	2	4494	OMG	C5-C4	-2.10	1.37	1.43
4	2	1456	B8Q	O2-C2	-2.04	1.18	1.22
4	2	1625	OMG	C5-C4	-2.04	1.37	1.43
4	2	3723	A2M	O5'-C5'	-2.03	1.39	1.44
4	2	1860	B8H	O4-C4	-2.01	1.19	1.23

All (356) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	2	1574	B9B	O6-C6-N1	-30.49	93.80	120.12
4	2	2754	B9B	O6-C6-N1	-29.73	94.46	120.12
4	2	237	B9B	O6-C6-N1	-29.09	95.01	120.12
4	2	4564	M7A	C5-C6-N6	13.86	147.41	123.74
4	2	4220	6MZ	C1'-N9-C4	-12.61	104.48	126.64
4	2	4564	M7A	N6-C6-N1	-11.85	92.40	118.35
4	2	1534	A2M	C5-C6-N6	10.80	136.77	120.35
4	2	1871	A2M	C5-C6-N6	10.47	136.26	120.35
4	2	1326	A2M	C5-C6-N6	10.46	136.24	120.35
4	2	3718	A2M	C5-C6-N6	10.45	136.24	120.35
4	2	398	A2M	C5-C6-N6	10.43	136.20	120.35
4	2	1524	A2M	C5-C6-N6	10.42	136.18	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	2	3867	A2M	C5-C6-N6	10.41	136.18	120.35
4	2	2363	A2M	C5-C6-N6	10.38	136.13	120.35
4	2	2401	A2M	C5-C6-N6	10.35	136.07	120.35
4	2	4571	A2M	C5-C6-N6	10.25	135.94	120.35
4	2	4523	A2M	C5-C6-N6	10.08	135.68	120.35
4	2	3723	A2M	C5-C6-N6	9.96	135.49	120.35
4	2	4083	5MU	C5-C4-N3	9.90	123.76	115.31
4	2	4355	E6G	O6-C6-N1	9.88	128.66	120.12
4	2	4597	UR3	C4-N3-C2	-8.37	116.68	124.56
4	2	1534	A2M	N6-C6-N1	-7.84	102.31	118.57
4	2	3867	A2M	N6-C6-N1	-7.34	103.34	118.57
4	2	1871	A2M	N6-C6-N1	-7.32	103.38	118.57
4	2	2401	A2M	N6-C6-N1	-7.32	103.39	118.57
4	2	2363	A2M	N6-C6-N1	-7.30	103.43	118.57
4	2	1524	A2M	N6-C6-N1	-7.28	103.46	118.57
4	2	1326	A2M	N6-C6-N1	-7.21	103.62	118.57
4	2	398	A2M	N6-C6-N1	-7.20	103.62	118.57
4	2	4571	A2M	N6-C6-N1	-7.20	103.63	118.57
4	2	3718	A2M	N6-C6-N1	-7.14	103.76	118.57
4	2	4523	A2M	N6-C6-N1	-7.01	104.02	118.57
4	2	3723	A2M	N6-C6-N1	-6.89	104.28	118.57
4	2	4083	5MU	C5-C6-N1	-6.68	116.46	123.34
4	2	4083	5MU	C4-N3-C2	-6.65	118.74	127.35
4	2	4371	MHG	C2-N3-C4	6.63	120.26	112.04
4	2	4296	B8H	C4-N3-C2	-6.59	118.82	127.35
4	2	4690	B8K	C72-C71-N7	6.44	128.55	118.86
4	2	1871	A2M	N3-C2-N1	-6.42	118.64	128.68
4	2	1860	B8H	C4-N3-C2	-6.40	119.06	127.35
4	2	2401	A2M	N3-C2-N1	-6.40	118.67	128.68
4	2	4220	6MZ	N3-C2-N1	-6.30	118.83	128.68
4	2	1534	A2M	N3-C2-N1	-6.30	118.83	128.68
4	2	398	A2M	N3-C2-N1	-6.29	118.85	128.68
4	2	3723	A2M	N3-C2-N1	-6.27	118.87	128.68
4	2	4523	A2M	N3-C2-N1	-6.27	118.88	128.68
4	2	1524	A2M	N3-C2-N1	-6.27	118.88	128.68
4	2	3867	A2M	N3-C2-N1	-6.26	118.90	128.68
4	2	1326	A2M	N3-C2-N1	-6.24	118.93	128.68
4	2	2363	A2M	N3-C2-N1	-6.23	118.94	128.68
4	2	4571	A2M	N3-C2-N1	-6.21	118.97	128.68
4	2	4355	E6G	N2-C2-N3	6.21	127.91	117.79
4	2	3899	BGH	C72-C71-N7	6.19	128.17	118.86
4	2	2786	B9H	C6-N1-C2	-6.09	116.34	121.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	2	4564	M7A	N3-C2-N1	-6.02	119.18	128.60
4	2	3718	A2M	N3-C2-N1	-5.89	119.48	128.68
4	2	3897	B8K	C72-C71-N7	5.88	127.70	118.86
4	2	4690	B8K	C5-C6-N1	5.78	121.18	110.99
4	2	3899	BGH	C5-C6-N1	5.72	121.07	110.99
4	2	2380	B8W	N2-C2-N3	5.71	127.09	117.79
4	2	3897	B8K	C5-C6-N1	5.69	121.02	110.99
4	2	1860	B8H	N3-C2-N1	5.68	121.27	115.14
4	2	4529	B8W	N2-C2-N3	5.64	126.99	117.79
53	8	14	OMU	C4-N3-C2	-5.63	119.15	126.58
4	2	4296	B8H	N3-C2-N1	5.59	121.18	115.14
4	2	2754	B9B	N3-C2-N1	-5.55	119.82	127.22
4	2	237	B9B	N3-C2-N1	-5.50	119.89	127.22
4	2	1909	P7G	C4-C5-N7	5.49	109.57	106.67
4	2	1456	B8Q	N3-C2-N1	5.46	123.55	117.13
4	2	4355	E6G	N3-C2-N1	-5.43	119.98	127.22
4	2	4185	B8W	N2-C2-N3	5.33	126.47	117.79
4	2	1574	B9B	N3-C2-N1	-5.31	120.14	127.22
4	2	4529	B8W	N3-C2-N1	-5.30	120.15	127.22
4	2	2380	B8W	N3-C2-N1	-5.25	120.22	127.22
4	2	4472	B8W	N2-C2-N3	5.23	126.31	117.79
4	2	1797	E7G	C5-C6-N1	5.22	120.19	110.99
4	2	4185	B8W	N3-C2-N1	-5.21	120.27	127.22
4	2	4472	B8W	N3-C2-N1	-5.21	120.27	127.22
4	2	4306	OMU	C4-N3-C2	-5.21	119.70	126.58
4	2	2786	B9H	C31-N3-C2	5.20	123.71	117.21
4	2	4564	M7A	N3-C4-N9	5.17	133.40	126.87
4	2	4371	MHG	C5-C6-N1	5.16	120.08	110.99
4	2	2297	E7G	C5-C6-N1	5.12	120.01	110.99
4	2	4083	5MU	N3-C2-N1	5.11	121.68	114.89
4	2	1456	B8Q	O2-C2-N3	-5.09	115.47	122.95
4	2	3899	BGH	C2-N3-C4	5.04	121.28	112.30
4	2	1797	E7G	C4-C5-N7	5.03	109.39	104.91
4	2	4472	B8W	O6-C6-N1	5.02	125.98	119.03
4	2	4620	OMU	C4-N3-C2	-5.00	119.99	126.58
4	2	2522	7MG	C5-C6-N1	4.98	119.77	110.99
4	2	1605	7MG	C5-C6-N1	4.96	119.72	110.99
4	2	1456	B8Q	C31-N3-C4	4.95	121.71	114.25
4	2	1797	E7G	C2-N3-C4	4.94	121.10	112.30
4	2	4550	7MG	C5-C6-N1	4.92	119.65	110.99
4	2	4529	B8W	O6-C6-N1	4.89	125.81	119.03
4	2	1322	1MA	N1-C2-N3	-4.88	120.33	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	2	4690	B8K	C2-N3-C4	4.88	121.00	112.30
4	2	3880	P7G	C4-C5-N7	4.88	109.24	106.67
4	2	2297	E7G	C4-C5-N7	4.84	109.22	104.91
4	2	3897	B8K	C2-N3-C4	4.79	120.83	112.30
4	2	4083	5MU	C5M-C5-C6	-4.77	116.48	122.85
4	2	4371	MHG	C4-C5-N7	4.73	109.12	104.91
4	2	4185	B8W	C2-N3-C4	4.71	120.74	115.36
4	2	1866	UR3	C4-N3-C2	-4.71	120.13	124.56
4	2	237	B9B	C2-N3-C4	4.67	120.69	115.36
4	2	4185	B8W	O6-C6-N1	4.59	125.39	119.03
4	2	237	B9B	N2-C2-N3	4.54	125.19	117.79
4	2	2297	E7G	C2-N3-C4	4.53	120.38	112.30
4	2	2754	B9B	C2-N3-C4	4.51	120.51	115.36
4	2	4530	UR3	C4-N3-C2	-4.50	120.33	124.56
4	2	4872	2MG	CM2-N2-C2	-4.49	113.94	123.86
4	2	1574	B9B	C2-N3-C4	4.49	120.48	115.36
4	2	4472	B8W	C2-N3-C4	4.47	120.46	115.36
4	2	4550	7MG	C2-N3-C4	4.46	120.24	112.30
4	2	2522	7MG	C2-N3-C4	4.39	120.12	112.30
4	2	1797	E7G	C5-C4-N3	-4.36	119.82	128.13
4	2	4355	E6G	C2-N3-C4	4.34	120.32	115.36
4	2	1605	7MG	C2-N3-C4	4.34	120.02	112.30
4	2	1659	I4U	C5-C4-N3	-4.34	118.31	124.91
4	2	4690	B8K	C5-C4-N9	4.24	111.85	106.35
4	2	2754	B9B	N2-C2-N3	4.21	124.66	117.79
4	2	3899	BGH	C5-C4-N9	4.21	111.81	106.35
4	2	2380	B8W	C2-N3-C4	4.18	120.13	115.36
4	2	3899	BGH	C4-C5-N7	4.17	108.62	104.91
4	2	4083	5MU	C5M-C5-C4	4.17	123.36	118.77
4	2	1456	B8Q	C6-N1-C2	-4.16	118.06	121.79
4	2	4083	5MU	O4-C4-C5	-4.11	120.14	124.90
4	2	4690	B8K	C4-C5-N7	4.08	108.54	104.91
4	2	3899	BGH	N9-C8-N7	4.08	108.81	103.33
4	2	1322	1MA	C5-C6-N1	4.06	119.95	113.90
4	2	4529	B8W	C1'-N9-C4	-4.05	119.53	126.64
4	2	4355	E6G	C61-O6-C6	-4.04	113.56	117.56
4	2	2804	OMC	O2-C2-N3	-4.02	115.79	122.33
4	2	4529	B8W	C2-N3-C4	4.02	119.95	115.36
4	2	3897	B8K	C5-C4-N9	3.98	111.52	106.35
4	2	4220	6MZ	C2-N1-C6	3.98	120.00	116.59
4	2	1574	B9B	N2-C2-N3	3.92	124.17	117.79
4	2	2297	E7G	C5-C4-N3	-3.91	120.67	128.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	2	2380	B8W	C1'-N9-C4	-3.89	119.81	126.64
4	2	3897	B8K	C4-C5-N7	3.88	108.36	104.91
4	2	2786	B9H	O3'-C3'-C2'	3.80	121.97	111.17
4	2	2380	B8W	O6-C6-N1	3.79	124.28	119.03
4	2	4550	7MG	C5-C4-N9	3.77	111.24	106.35
4	2	4690	B8K	N9-C8-N7	3.77	108.38	103.33
4	2	4620	OMU	N3-C2-N1	3.76	119.88	114.89
4	2	4870	OMG	C5-C6-N1	3.71	120.51	113.95
4	2	1605	7MG	C5-C4-N9	3.70	111.15	106.35
4	2	4371	MHG	C5-C4-N3	-3.69	121.10	128.13
4	2	2522	7MG	C5-C4-N9	3.69	111.14	106.35
4	2	4306	OMU	N3-C2-N1	3.65	119.74	114.89
4	2	1605	7MG	C5-C4-N3	-3.64	121.19	128.13
4	2	2424	OMG	C5-C6-N1	3.63	120.36	113.95
4	2	1883	OMG	C5-C6-N1	3.61	120.32	113.95
4	2	978	2MG	C5-C6-N1	3.60	120.31	113.95
53	8	14	OMU	N3-C2-N1	3.59	119.66	114.89
4	2	4872	2MG	C5-C6-N1	3.59	120.29	113.95
4	2	1316	OMG	C5-C6-N1	3.58	120.28	113.95
4	2	1348	P4U	C5-C4-N3	-3.58	119.46	124.91
4	2	2522	7MG	C5-C4-N3	-3.58	121.31	128.13
4	2	373	OMG	C5-C6-N1	3.57	120.26	113.95
4	2	3897	B8K	N9-C8-N7	3.57	108.12	103.33
4	2	4371	MHG	C2-N1-C6	-3.57	120.38	124.48
4	2	729	2MG	C5-C6-N1	3.56	120.24	113.95
4	2	4296	B8H	C5-C4-N3	3.55	124.62	116.58
4	2	4637	OMG	C5-C6-N1	3.55	120.22	113.95
4	2	4550	7MG	C5-C4-N3	-3.52	121.43	128.13
53	8	14	OMU	C5-C4-N3	3.50	120.08	114.84
4	2	4564	M7A	C2-N3-C4	3.50	120.02	111.75
4	2	1522	OMG	C5-C6-N1	3.49	120.12	113.95
4	2	4371	MHG	C5-C4-N9	3.49	110.88	106.35
4	2	2050	OMG	C5-C6-N1	3.49	120.12	113.95
4	2	4196	OMG	C5-C6-N1	3.49	120.11	113.95
4	2	2297	E7G	C5-C4-N9	3.49	110.87	106.35
4	2	2364	OMG	C5-C6-N1	3.48	120.09	113.95
4	2	1517	2MG	C5-C6-N1	3.48	120.09	113.95
4	2	2773	OMG	C5-C6-N1	3.47	120.08	113.95
4	2	1909	P7G	N9-C8-N7	3.46	108.32	103.38
4	2	4370	OMG	C5-C6-N1	3.45	120.05	113.95
4	2	4306	OMU	C5-C4-N3	3.44	119.98	114.84
4	2	3899	BGH	C5-C4-N3	-3.43	121.59	128.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	2	4494	OMG	C5-C6-N1	3.41	119.98	113.95
4	2	1625	OMG	C5-C6-N1	3.40	119.96	113.95
4	2	2861	OMC	O2-C2-N3	-3.40	116.81	122.33
4	2	4623	OMG	C5-C6-N1	3.38	119.91	113.95
4	2	1860	B8H	C5-C4-N3	3.36	124.18	116.58
4	2	4371	MHG	C72-C71-N7	-3.36	109.10	112.41
4	2	1797	E7G	C5-C4-N9	3.35	110.70	106.35
4	2	4355	E6G	N2-C2-N1	-3.31	112.11	117.25
4	2	4690	B8K	C5-C4-N3	-3.25	121.94	128.13
4	2	2364	OMG	C2-N1-C6	-3.24	119.14	125.10
4	2	4620	OMU	C5-C4-N3	3.20	119.63	114.84
4	2	3897	B8K	C6-C5-C4	-3.20	116.02	122.62
4	2	4335	5MC	C5-C6-N1	-3.20	120.05	123.34
4	2	4637	OMG	C2-N1-C6	-3.18	119.25	125.10
4	2	1625	OMG	C2-N1-C6	-3.17	119.26	125.10
4	2	2424	OMG	C2-N1-C6	-3.17	119.27	125.10
4	2	4472	B8W	C1'-N9-C4	-3.15	121.11	126.64
4	2	4690	B8K	C6-C5-C4	-3.14	116.14	122.62
4	2	2050	OMG	C2-N1-C6	-3.13	119.33	125.10
4	2	1316	OMG	C2-N1-C6	-3.13	119.34	125.10
4	2	3897	B8K	C5-C4-N3	-3.12	122.18	128.13
4	2	1522	OMG	C2-N1-C6	-3.12	119.36	125.10
4	2	4196	OMG	C2-N1-C6	-3.11	119.38	125.10
4	2	4536	OMC	O2-C2-N3	-3.08	117.33	122.33
4	2	4494	OMG	C2-N1-C6	-3.07	119.45	125.10
4	2	4530	UR3	C6-N1-C2	-3.06	119.05	121.79
4	2	1456	B8Q	C1'-N1-C2	3.05	122.14	116.99
4	2	2773	OMG	C2-N1-C6	-3.05	119.48	125.10
53	8	14	OMU	CM2-O2'-C2'	3.05	122.52	114.52
4	2	4483	B8T	O2-C2-N3	-3.04	117.38	122.33
4	2	2422	OMC	O2-C2-N3	-3.04	117.39	122.33
53	8	14	OMU	O4-C4-C5	-3.04	119.82	125.16
4	2	1797	E7G	N9-C8-N7	3.04	107.72	103.38
4	2	4623	OMG	C2-N1-C6	-3.03	119.51	125.10
4	2	1883	OMG	C2-N1-C6	-3.03	119.52	125.10
4	2	3899	BGH	C6-C5-C4	-3.02	116.39	122.62
4	2	373	OMG	C2-N1-C6	-3.01	119.56	125.10
4	2	4370	OMG	C2-N1-C6	-2.99	119.59	125.10
4	2	1860	B8H	O2-C2-N1	-2.96	119.54	122.87
4	2	4196	OMG	CM2-O2'-C2'	2.95	122.26	114.52
4	2	4306	OMU	O4-C4-C5	-2.94	119.99	125.16
4	2	2380	B8W	N2-C2-N1	-2.93	112.69	117.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	2	3867	A2M	C1'-N9-C4	2.91	131.75	126.64
4	2	4870	OMG	C2-N1-C6	-2.90	119.76	125.10
4	2	1909	P7G	C71-N7-C5	2.89	131.35	124.52
4	2	2804	OMC	C1'-N1-C2	2.86	124.80	118.42
4	2	4529	B8W	N2-C2-N1	-2.83	112.86	117.25
4	2	1605	7MG	N9-C8-N7	2.82	107.40	103.38
4	2	3899	BGH	O6-C6-N1	-2.79	114.76	120.12
4	2	2861	OMC	C1'-N1-C2	2.78	124.64	118.42
4	2	2363	A2M	C1'-N9-C4	2.77	131.51	126.64
4	2	4296	B8H	O2-C2-N1	-2.75	119.78	122.87
4	2	4296	B8H	O4-C4-N3	-2.74	114.86	120.12
4	2	1883	OMG	O6-C6-C5	-2.74	119.01	124.37
4	2	2522	7MG	N9-C8-N7	2.74	107.29	103.38
4	2	4690	B8K	O6-C6-N1	-2.73	114.89	120.12
4	2	4597	UR3	C3U-N3-C2	2.72	122.08	117.31
4	2	1456	B8Q	C31-N3-C2	2.70	121.72	117.79
4	2	4371	MHG	N1-C2-N3	-2.70	119.78	123.95
4	2	2804	OMC	O2-C2-N1	2.70	124.46	118.89
4	2	3897	B8K	O6-C6-N1	-2.69	114.96	120.12
4	2	4483	B8T	O3'-C3'-C2'	2.68	120.50	111.82
4	2	1797	E7G	N9-C4-N3	2.68	129.47	125.47
4	2	1322	1MA	C8-N7-C5	2.68	108.09	102.99
4	2	2522	7MG	C4-C5-N7	2.65	109.21	105.53
4	2	2786	B9H	O3'-C3'-C4'	2.64	118.67	111.05
4	2	4620	OMU	O4-C4-C5	-2.63	120.54	125.16
4	2	4671	B8T	C6-C5-C4	2.63	120.18	116.96
4	2	4550	7MG	C4-C5-N7	2.63	109.18	105.53
4	2	2297	E7G	N9-C8-N7	2.62	107.12	103.38
4	2	1797	E7G	C2-N1-C6	-2.62	120.32	125.10
4	2	1605	7MG	C4-C5-N7	2.62	109.16	105.53
4	2	978	2MG	C8-N7-C5	2.61	107.97	102.99
4	2	3880	P7G	N9-C8-N7	2.60	107.10	103.38
4	2	4872	2MG	C8-N7-C5	2.60	107.94	102.99
4	2	2297	E7G	C2-N1-C6	-2.60	120.36	125.10
4	2	1860	B8H	O4-C4-N3	-2.59	115.16	120.12
4	2	237	B9B	C61-O6-C6	-2.57	112.70	117.51
4	2	3887	OMC	O2-C2-N3	-2.57	118.16	122.33
4	2	4185	B8W	N2-C2-N1	-2.57	113.26	117.25
4	2	2424	OMG	O6-C6-C5	-2.56	119.36	124.37
4	2	729	2MG	C8-N7-C5	2.56	107.87	102.99
4	2	4083	5MU	C6-C5-C4	2.55	120.16	118.03
4	2	4483	B8T	O3'-C3'-C4'	2.55	118.42	111.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	2	1517	2MG	C8-N7-C5	2.55	107.84	102.99
4	2	4083	5MU	O2-C2-N1	-2.55	119.40	122.79
4	2	2786	B9H	C1'-N1-C6	2.54	126.38	120.84
4	2	1316	OMG	C8-N7-C5	2.52	107.78	102.99
4	2	4550	7MG	N9-C8-N7	2.50	106.95	103.38
4	2	4690	B8K	C2-N1-C6	-2.50	120.55	125.10
4	2	3718	A2M	C1'-N9-C4	2.47	130.98	126.64
4	2	4472	B8W	N2-C2-N1	-2.46	113.42	117.25
4	2	1605	7MG	C2-N1-C6	-2.45	120.62	125.10
4	2	4571	A2M	C1'-N9-C4	2.44	130.92	126.64
4	2	2754	B9B	C61-O6-C6	-2.43	112.97	117.51
4	2	2522	7MG	C2-N1-C6	-2.41	120.70	125.10
4	2	4523	A2M	C1'-N9-C4	2.41	130.87	126.64
4	2	3723	A2M	C1'-N9-C4	2.39	130.84	126.64
4	2	1625	OMG	O6-C6-C5	-2.39	119.71	124.37
4	2	4564	M7A	C5-C4-N3	-2.39	121.02	126.62
4	2	373	OMG	C8-N7-C5	2.39	107.54	102.99
4	2	3899	BGH	N1-C2-N3	-2.38	118.88	123.32
4	2	3897	B8K	C2-N1-C6	-2.38	120.76	125.10
4	2	1524	A2M	C1'-N9-C4	2.37	130.81	126.64
4	2	4335	5MC	CM5-C5-C6	-2.37	119.68	122.85
4	2	4370	OMG	O6-C6-C5	-2.36	119.76	124.37
4	2	3899	BGH	C2-N1-C6	-2.36	120.79	125.10
4	2	1517	2MG	O6-C6-C5	-2.36	119.76	124.37
4	2	4529	B8W	C2-N1-C6	2.36	119.86	116.08
4	2	4355	E6G	C2-N1-C6	2.35	119.86	116.08
4	2	4536	OMC	C1'-N1-C2	2.35	123.67	118.42
4	2	1522	OMG	C8-N7-C5	2.35	107.47	102.99
4	2	4597	UR3	C3U-N3-C4	2.35	121.24	117.89
4	2	4870	OMG	O6-C6-C5	-2.34	119.79	124.37
4	2	4597	UR3	C6-N1-C2	-2.34	119.69	121.79
4	2	4196	OMG	O6-C6-C5	-2.34	119.81	124.37
4	2	4870	OMG	C8-N7-C5	2.34	107.44	102.99
4	2	1866	UR3	C6-N1-C2	-2.33	119.70	121.79
4	2	4371	MHG	N9-C8-N7	2.33	106.70	103.38
4	2	3869	OMC	O2-C2-N3	-2.32	118.56	122.33
4	2	4637	OMG	C8-N7-C5	2.32	107.41	102.99
4	2	1522	OMG	O6-C6-C5	-2.32	119.84	124.37
4	2	1871	A2M	C1'-N9-C4	2.32	130.71	126.64
4	2	2861	OMC	O2-C2-N1	2.31	123.67	118.89
4	2	4637	OMG	O6-C6-C5	-2.31	119.87	124.37
4	2	4623	OMG	C8-N7-C5	2.30	107.38	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	2	1883	OMG	C8-N7-C5	2.29	107.36	102.99
4	2	4371	MHG	O6-C6-C5	-2.29	121.94	127.54
4	2	4872	2MG	O6-C6-C5	-2.26	119.96	124.37
4	2	2364	OMG	C8-N7-C5	2.26	107.29	102.99
4	2	4494	OMG	O6-C6-C5	-2.25	119.97	124.37
4	2	729	2MG	O6-C6-C5	-2.25	119.98	124.37
4	2	4870	OMG	N1-C2-N3	-2.25	119.12	123.32
4	2	2422	OMC	C1'-N1-C2	2.23	123.40	118.42
4	2	4550	7MG	C2-N1-C6	-2.23	121.04	125.10
4	2	2786	B9H	O2-C2-N1	-2.22	117.52	122.72
4	2	3897	B8K	N1-C2-N3	-2.22	119.19	123.32
4	2	2050	OMG	N2-C2-N1	2.21	121.42	116.71
4	2	1316	OMG	O6-C6-C5	-2.21	120.06	124.37
4	2	978	2MG	O6-C6-C5	-2.21	120.06	124.37
4	2	4690	B8K	N1-C2-N3	-2.21	119.20	123.32
4	2	2050	OMG	C8-N7-C5	2.21	107.19	102.99
4	2	2364	OMG	O6-C6-C5	-2.21	120.06	124.37
4	2	4306	OMU	O2-C2-N1	-2.20	119.86	122.79
4	2	1534	A2M	C1'-N9-C4	2.20	130.51	126.64
4	2	2773	OMG	O6-C6-C5	-2.19	120.09	124.37
4	2	373	OMG	O6-C6-C5	-2.19	120.09	124.37
4	2	1522	OMG	N2-C2-N1	2.18	121.36	116.71
4	2	4550	7MG	C6-C5-C4	-2.16	118.18	122.62
4	2	2364	OMG	N2-C2-N1	2.15	121.30	116.71
4	2	4185	B8W	C1'-N9-C4	-2.14	122.88	126.64
4	2	2380	B8W	C2-N1-C6	2.14	119.52	116.08
4	2	4623	OMG	N2-C2-N1	2.13	121.26	116.71
4	2	4370	OMG	C8-N7-C5	2.12	107.03	102.99
4	2	4196	OMG	C8-N7-C5	2.11	107.02	102.99
4	2	4483	B8T	C6-C5-C4	2.10	119.53	116.96
4	2	2522	7MG	C6-C5-C4	-2.10	118.29	122.62
4	2	4623	OMG	O6-C6-C5	-2.10	120.27	124.37
4	2	4083	5MU	O4-C4-N3	-2.10	116.10	120.12
4	2	2050	OMG	O6-C6-C5	-2.09	120.29	124.37
4	2	4536	OMC	O2-C2-N1	2.09	123.20	118.89
4	2	4371	MHG	C71-N7-C5	2.08	129.45	124.52
4	2	4597	UR3	O2-C2-N3	-2.08	118.40	121.34
4	2	1797	E7G	O6-C6-C5	-2.08	122.44	127.54
4	2	4083	5MU	C6-N1-C2	-2.08	119.19	121.30
4	2	3869	OMC	C6-C5-C4	2.07	120.85	117.50
4	2	4550	7MG	N1-C2-N3	-2.07	119.45	123.32
4	2	1517	2MG	CM2-N2-C2	-2.07	119.29	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	2	4196	OMG	O2'-C2'-C1'	2.07	113.19	109.09
4	2	373	OMG	CM2-O2'-C2'	-2.06	109.13	114.52
4	2	4371	MHG	C6-C5-C4	-2.05	118.40	122.62
4	2	2522	7MG	O6-C6-C5	-2.04	122.53	127.54
4	2	4371	MHG	C21-N2-C2	-2.04	119.36	123.86
4	2	3880	P7G	N3-C2-N1	-2.03	119.54	123.32
4	2	2786	B9H	O2-C2-N3	-2.02	119.51	122.07
4	2	1316	OMG	N2-C2-N1	2.00	120.97	116.71

There are no chirality outliers.

All (113) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
53	8	14	OMU	C1'-C2'-O2'-CM2
4	2	237	B9B	C5-C6-O6-C61
4	2	237	B9B	N1-C6-O6-C61
4	2	237	B9B	C3'-C4'-C5'-O5'
4	2	237	B9B	O4'-C4'-C5'-O5'
4	2	237	B9B	C62-C61-O6-C6
4	2	1348	P4U	N3-C4-O4-C41
4	2	1574	B9B	C5-C6-O6-C61
4	2	1574	B9B	N1-C6-O6-C61
4	2	1574	B9B	C62-C61-O6-C6
4	2	1625	OMG	C3'-C4'-C5'-O5'
4	2	1797	E7G	C3'-C4'-C5'-O5'
4	2	1860	B8H	C3'-C4'-C5'-O5'
4	2	1860	B8H	O4'-C4'-C5'-O5'
4	2	1866	UR3	O4'-C4'-C5'-O5'
4	2	1866	UR3	C3'-C4'-C5'-O5'
4	2	1883	OMG	O4'-C4'-C5'-O5'
4	2	1883	OMG	C3'-C4'-C5'-O5'
4	2	2364	OMG	C1'-C2'-O2'-CM2
4	2	2380	B8W	C5-C6-O6-C61
4	2	2424	OMG	O4'-C4'-C5'-O5'
4	2	2424	OMG	C3'-C4'-C5'-O5'
4	2	2754	B9B	C5-C6-O6-C61
4	2	2754	B9B	N1-C6-O6-C61
4	2	3867	A2M	C3'-C4'-C5'-O5'
4	2	3869	OMC	C2'-C1'-N1-C2
4	2	3869	OMC	C2'-C1'-N1-C6
4	2	3880	P7G	C3'-C4'-C5'-O5'
4	2	3880	P7G	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
4	2	3897	B8K	O4'-C4'-C5'-O5'
4	2	4185	B8W	C5-C6-O6-C61
4	2	4196	OMG	C1'-C2'-O2'-CM2
4	2	4220	6MZ	N1-C6-N6-C9
4	2	4355	E6G	C5-C6-O6-C61
4	2	4355	E6G	N1-C6-O6-C61
4	2	4472	B8W	C5-C6-O6-C61
4	2	4637	OMG	C1'-C2'-O2'-CM2
4	2	398	A2M	O4'-C4'-C5'-O5'
4	2	1517	2MG	C3'-C4'-C5'-O5'
4	2	1797	E7G	O4'-C4'-C5'-O5'
4	2	2364	OMG	O4'-C4'-C5'-O5'
4	2	2773	OMG	C3'-C4'-C5'-O5'
4	2	3867	A2M	O4'-C4'-C5'-O5'
4	2	3897	B8K	C3'-C4'-C5'-O5'
4	2	4371	MHG	O4'-C4'-C5'-O5'
4	2	4870	OMG	C3'-C4'-C5'-O5'
4	2	4872	2MG	O4'-C4'-C5'-O5'
4	2	4472	B8W	N1-C6-O6-C61
4	2	237	B9B	O6-C61-C62-C63
4	2	1517	2MG	O4'-C4'-C5'-O5'
4	2	1625	OMG	O4'-C4'-C5'-O5'
4	2	1909	P7G	O4'-C4'-C5'-O5'
4	2	2364	OMG	C3'-C4'-C5'-O5'
4	2	4637	OMG	O4'-C4'-C5'-O5'
4	2	4870	OMG	O4'-C4'-C5'-O5'
4	2	4872	2MG	C3'-C4'-C5'-O5'
4	2	2380	B8W	N1-C6-O6-C61
4	2	4185	B8W	N1-C6-O6-C61
4	2	4371	MHG	C2'-C1'-N9-C8
4	2	729	2MG	O4'-C4'-C5'-O5'
4	2	398	A2M	C3'-C4'-C5'-O5'
4	2	4296	B8H	C3'-C4'-C5'-O5'
4	2	1909	P7G	C3'-C4'-C5'-O5'
4	2	2773	OMG	O4'-C4'-C5'-O5'
4	2	3869	OMC	O4'-C4'-C5'-O5'
4	2	4296	B8H	O4'-C4'-C5'-O5'
4	2	4523	A2M	O4'-C4'-C5'-O5'
4	2	4637	OMG	C3'-C4'-C5'-O5'
4	2	4523	A2M	C3'-C4'-C5'-O5'
4	2	3880	P7G	N7-C71-C72-C73
4	2	729	2MG	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
4	2	4597	UR3	O4'-C4'-C5'-O5'
4	2	4870	OMG	C4'-C5'-O5'-P
4	2	4494	OMG	C3'-C2'-O2'-CM2
4	2	4523	A2M	C3'-C2'-O2'-CM'
4	2	4371	MHG	C3'-C4'-C5'-O5'
4	2	3701	OMC	C2'-C1'-N1-C6
4	2	4550	7MG	O4'-C4'-C5'-O5'
4	2	373	OMG	C4'-C5'-O5'-P
4	2	1534	A2M	C4'-C5'-O5'-P
4	2	3867	A2M	C4'-C5'-O5'-P
4	2	3869	OMC	C4'-C5'-O5'-P
4	2	3887	OMC	C4'-C5'-O5'-P
4	2	4196	OMG	O4'-C4'-C5'-O5'
4	2	4355	E6G	O4'-C4'-C5'-O5'
4	2	1524	A2M	C3'-C2'-O2'-CM'
4	2	3869	OMC	O4'-C1'-N1-C6
4	2	3897	B8K	C4'-C5'-O5'-P
4	2	2297	E7G	C72-C71-N7-C8
4	2	1326	A2M	C4'-C5'-O5'-P
4	2	4523	A2M	C4'-C5'-O5'-P
4	2	1909	P7G	C72-C71-N7-C8
4	2	2754	B9B	O6-C61-C62-C63
4	2	2401	A2M	C3'-C2'-O2'-CM'
4	2	3701	OMC	O4'-C1'-N1-C6
4	2	1625	OMG	C4'-C5'-O5'-P
4	2	4220	6MZ	C5-C6-N6-C9
4	2	3701	OMC	O4'-C4'-C5'-O5'
4	2	3869	OMC	C3'-C4'-C5'-O5'
4	2	4523	A2M	C1'-C2'-O2'-CM'
4	2	3869	OMC	O4'-C1'-N1-C2
4	2	3899	BGH	O4'-C4'-C5'-O5'
4	2	1517	2MG	C4'-C5'-O5'-P
4	2	3701	OMC	O4'-C1'-N1-C2
4	2	1659	I4U	C43-C41-O4-C4
4	2	2754	B9B	C62-C61-O6-C6
4	2	3701	OMC	C3'-C2'-O2'-CM2
4	2	1534	A2M	O4'-C4'-C5'-O5'
4	2	2422	OMC	O4'-C4'-C5'-O5'
4	2	3701	OMC	C3'-C4'-C5'-O5'
4	2	4597	UR3	C3'-C4'-C5'-O5'
4	2	4371	MHG	O4'-C1'-N9-C8
4	2	3701	OMC	C2'-C1'-N1-C2

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 3 ligands modelled in this entry, 2 are 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	$\#\|Z\| > 2$
59	GDP	A	801	60,61	24,30,30	1.20	2 (8%)	30,47,47	1.41	5 (16%)

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
59	GDP	A	801	60,61	-	2/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	A	801	GDP	C6-N1	-3.47	1.32	1.37
59	A	801	GDP	C2'-C1'	-2.22	1.50	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
59	A	801	GDP	PA-O3A-PB	-3.52	120.74	132.83
59	A	801	GDP	C3'-C2'-C1'	3.26	105.89	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
59	A	801	GDP	C8-N7-C5	2.47	107.69	102.99
59	A	801	GDP	O3B-PB-O2B	2.35	116.63	107.64
59	A	801	GDP	C5-C6-N1	2.32	118.05	113.95

There are no chirality outliers.

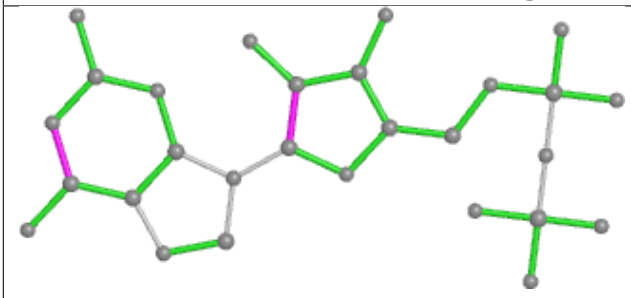
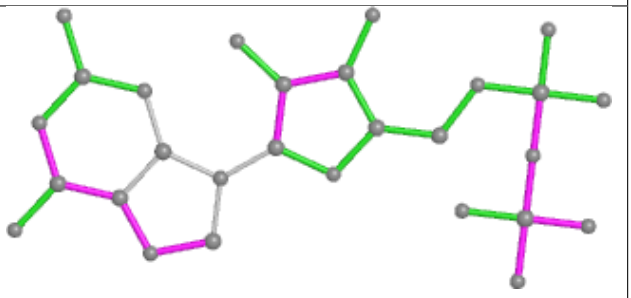
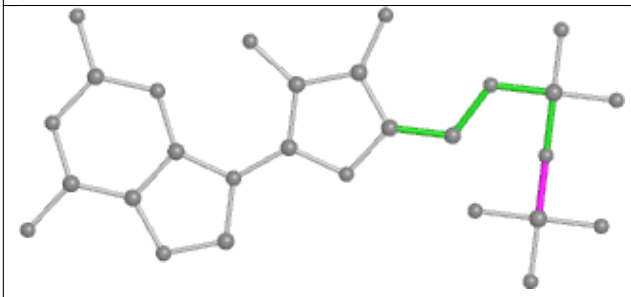
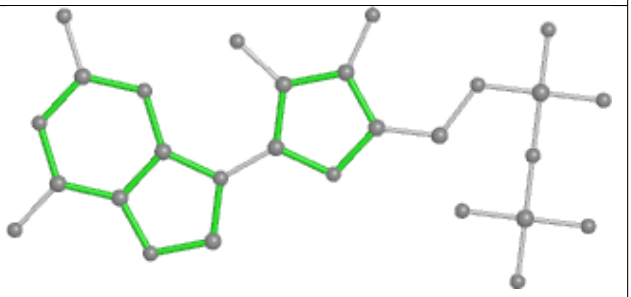
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	A	801	GDP	PA-O3A-PB-O2B
59	A	801	GDP	PA-O3A-PB-O1B

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 GDP A 801	
 Bond lengths	 Bond angles
 Torsions	 Rings

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.

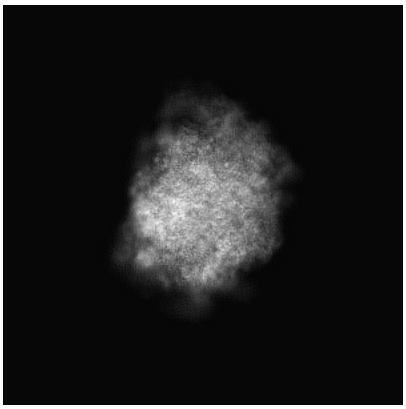
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-35596. These allow visual inspection of the internal detail of the map and identification of artifacts.

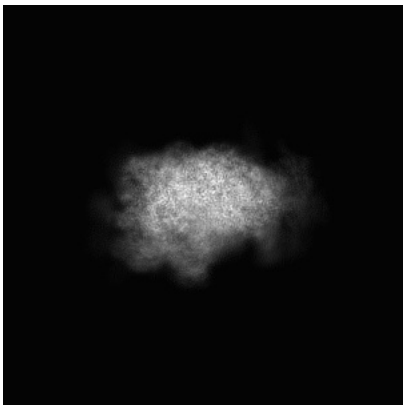
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

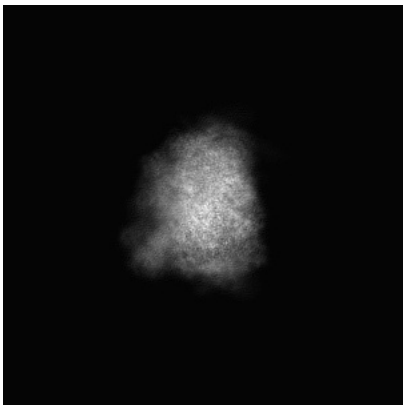
6.1.1 Primary map



X

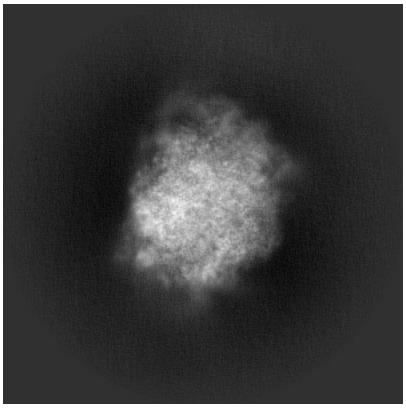


Y

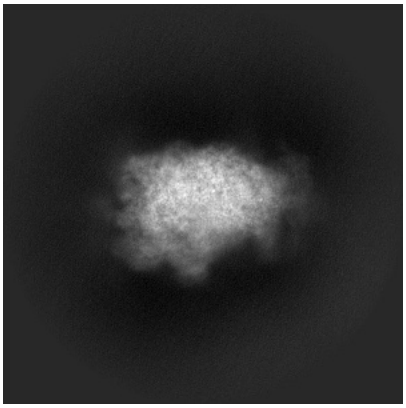


Z

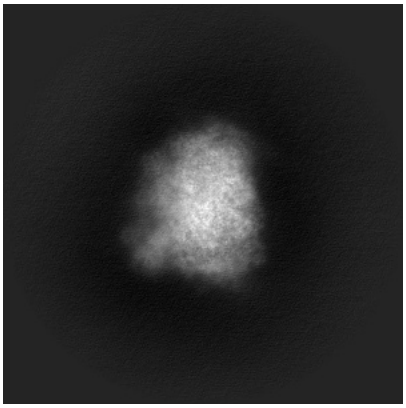
6.1.2 Raw map



X



Y

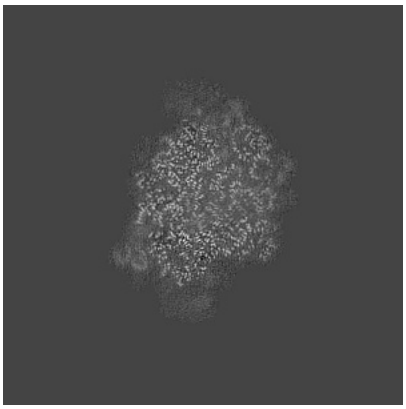


Z

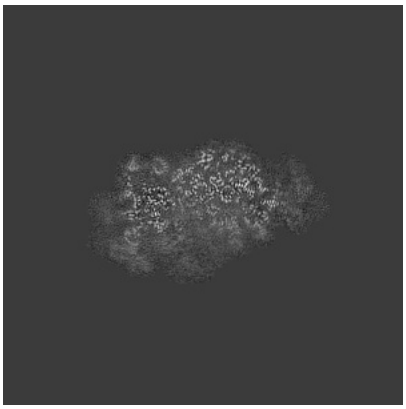
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

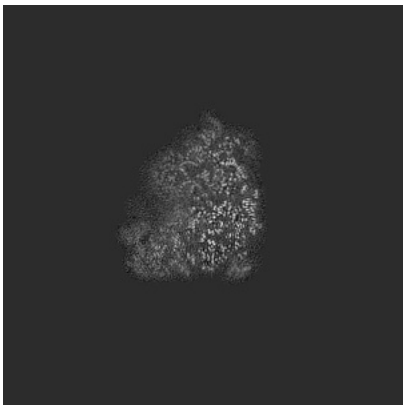
6.2.1 Primary map



X Index: 200

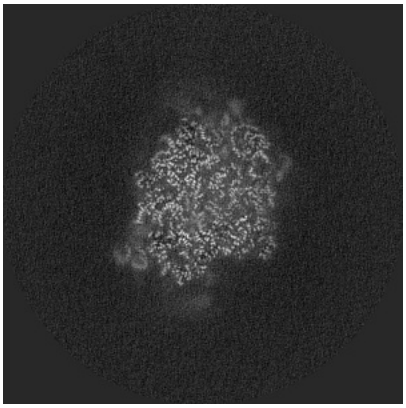


Y Index: 200

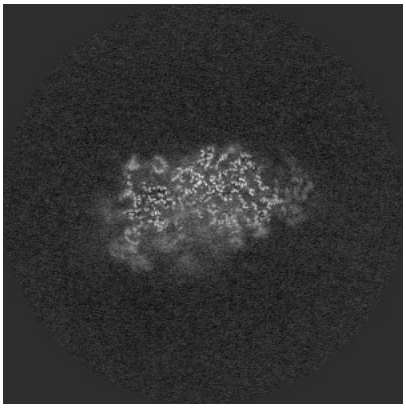


Z Index: 200

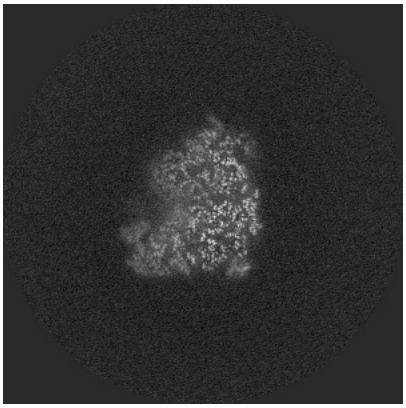
6.2.2 Raw map



X Index: 200



Y Index: 200

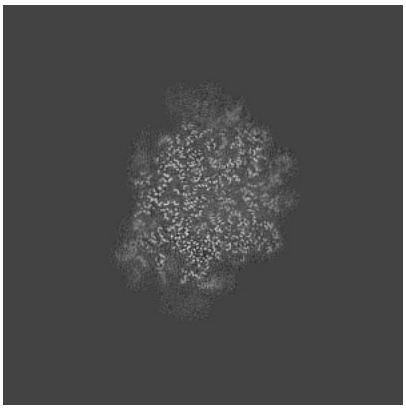


Z Index: 200

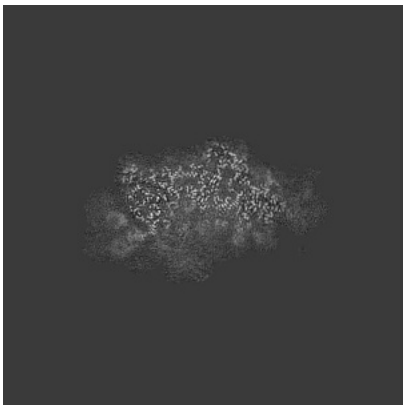
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

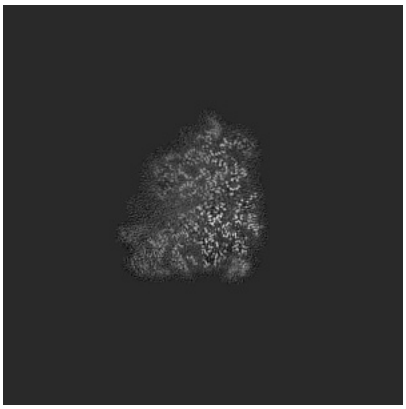
6.3.1 Primary map



X Index: 206

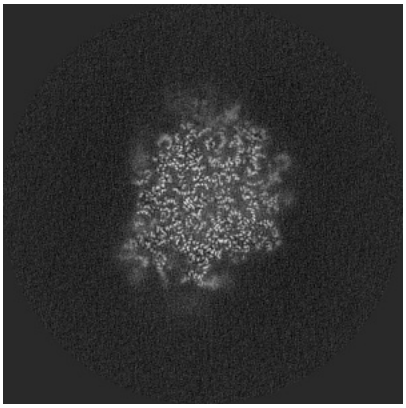


Y Index: 191

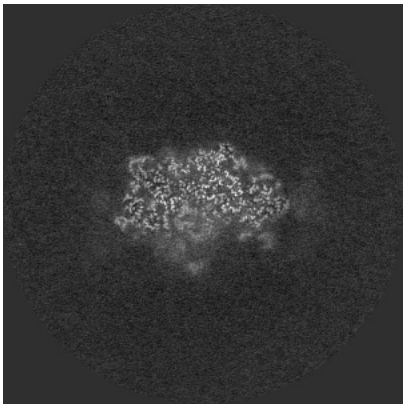


Z Index: 202

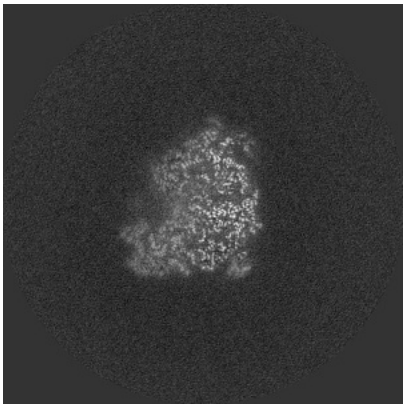
6.3.2 Raw map



X Index: 207



Y Index: 182

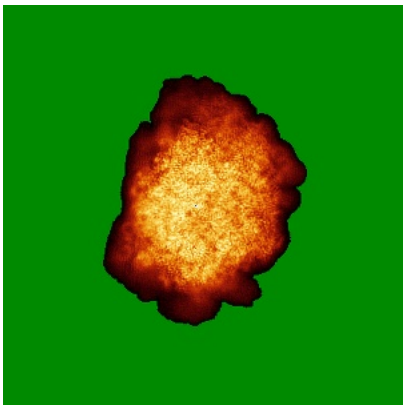


Z Index: 199

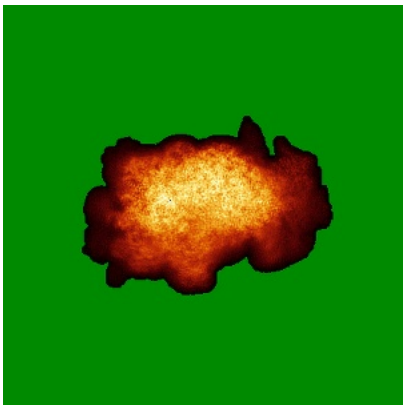
The images above show the largest variance slices of the map in three orthogonal directions.

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

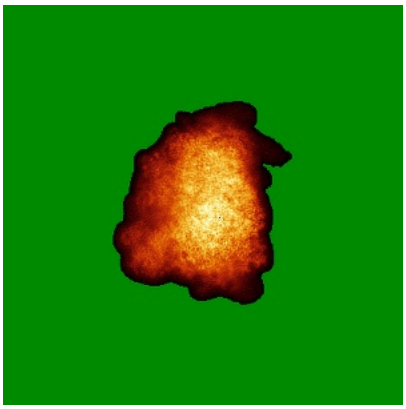
6.4.1 Primary map



X

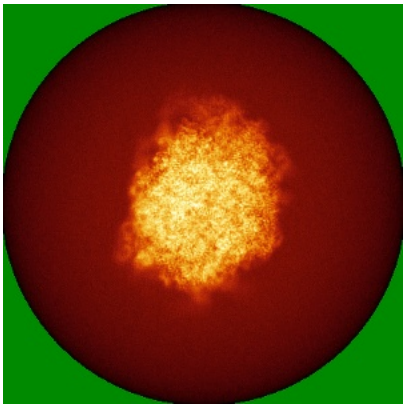


Y

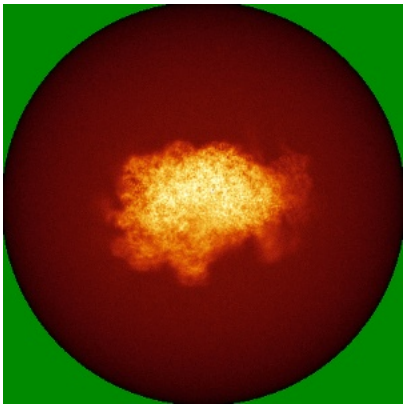


Z

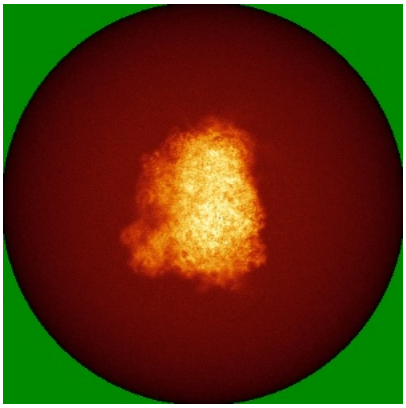
6.4.2 Raw map



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 0.032. 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.

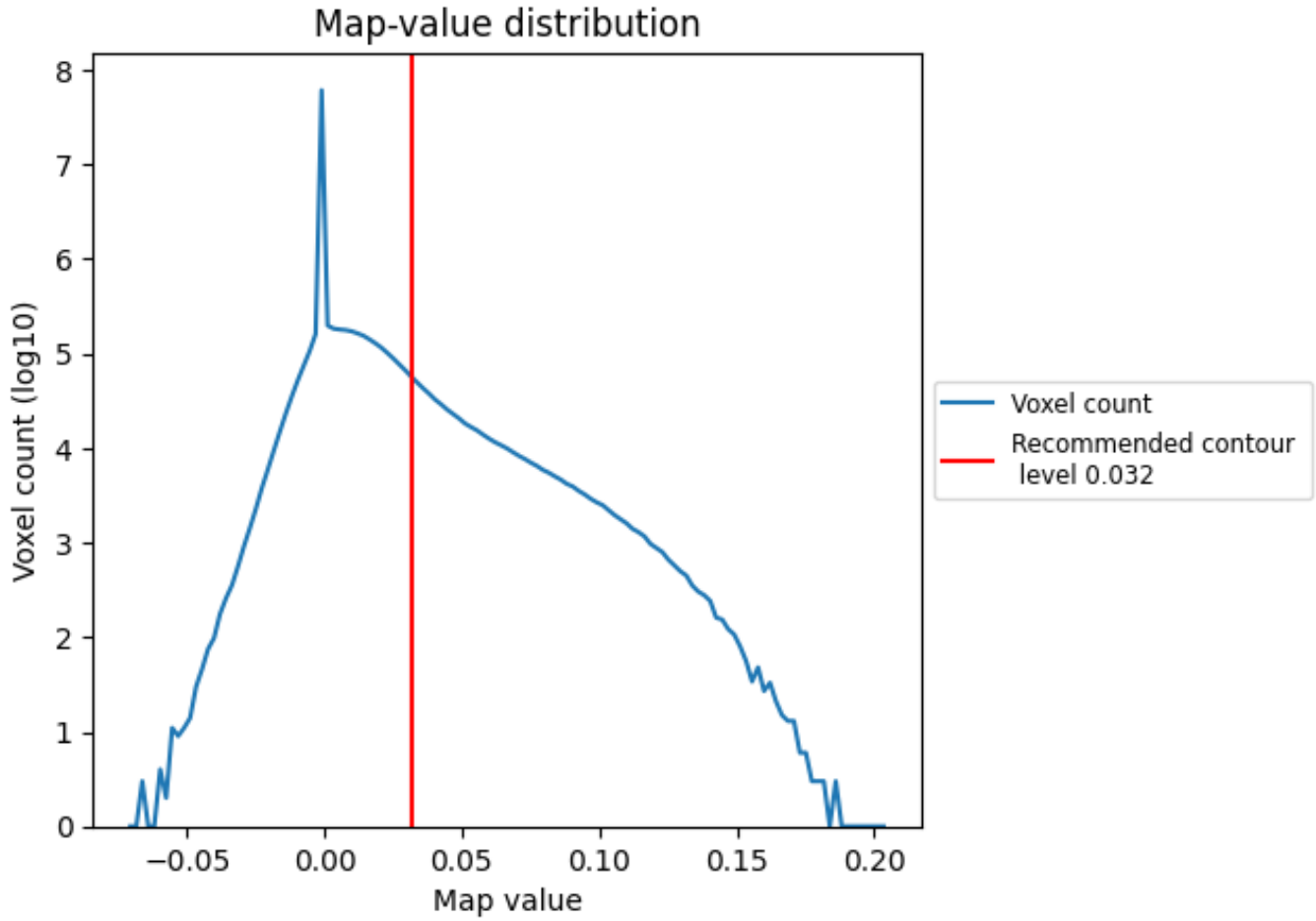
6.6 Mask visualisation (i)

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

7 Map analysis

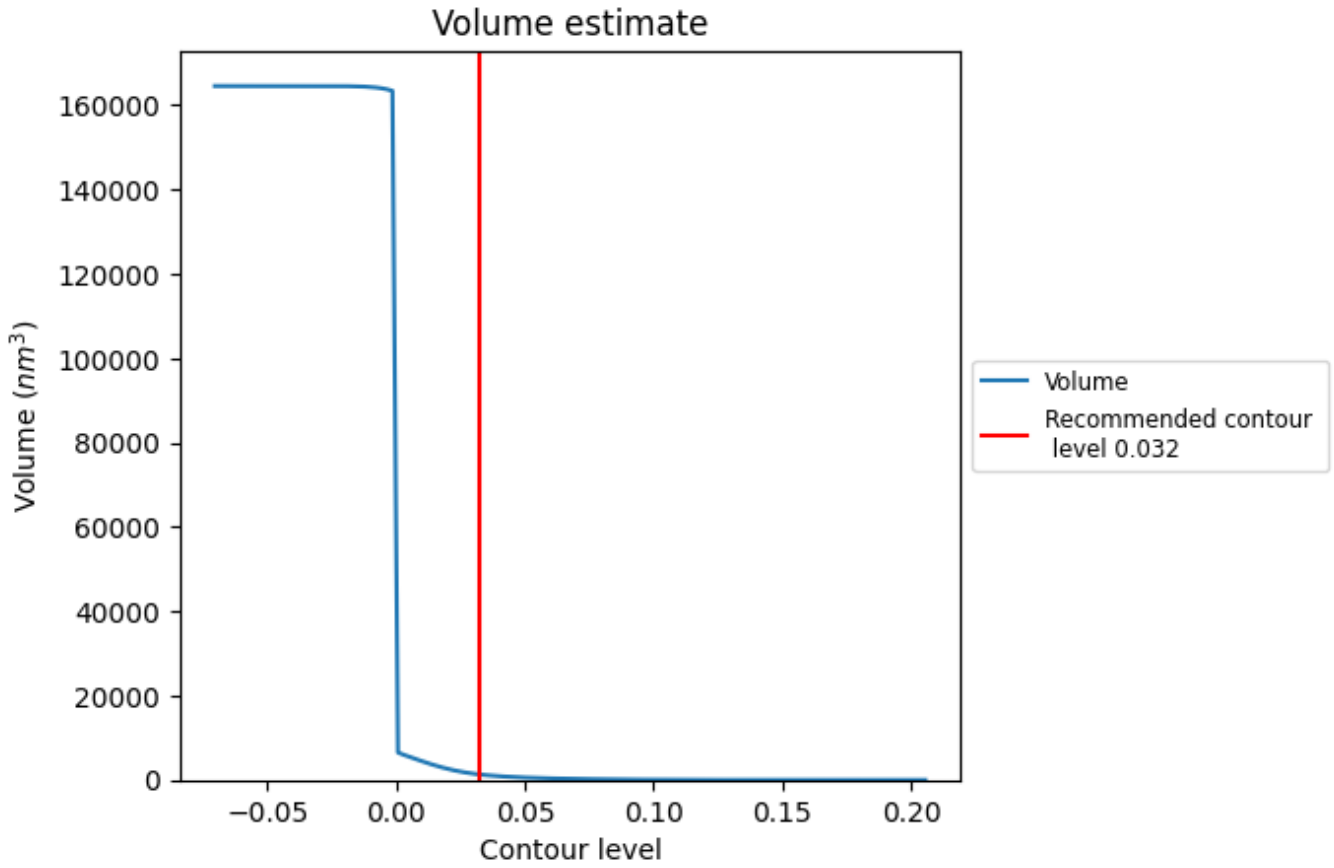
This section contains the results of statistical analysis of the map.

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.

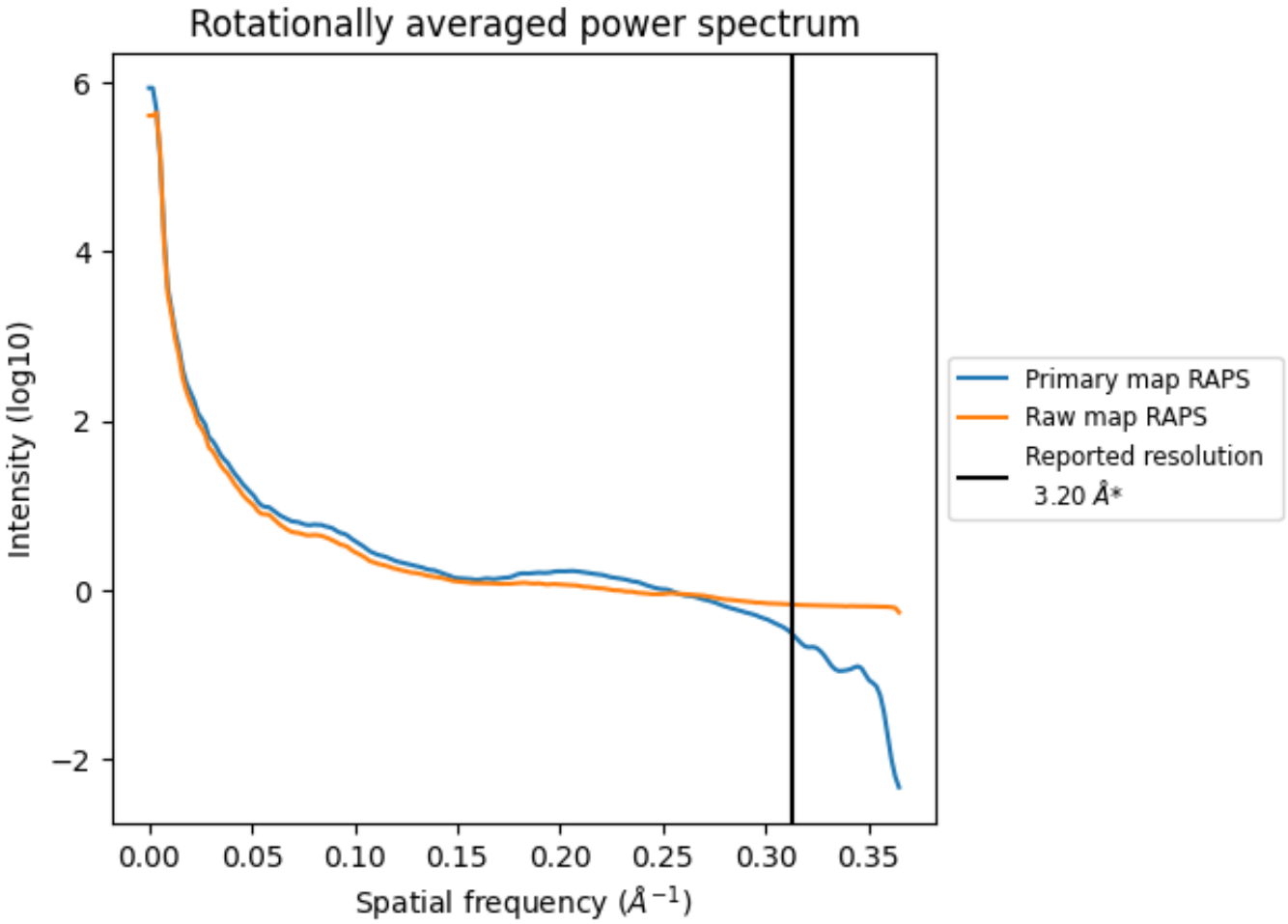
7.2 Volume estimate



The volume at the recommended contour level is 1336 nm^3; this corresponds to an approximate mass of 1207 kDa.

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

7.3 Rotationally averaged power spectrum (i)

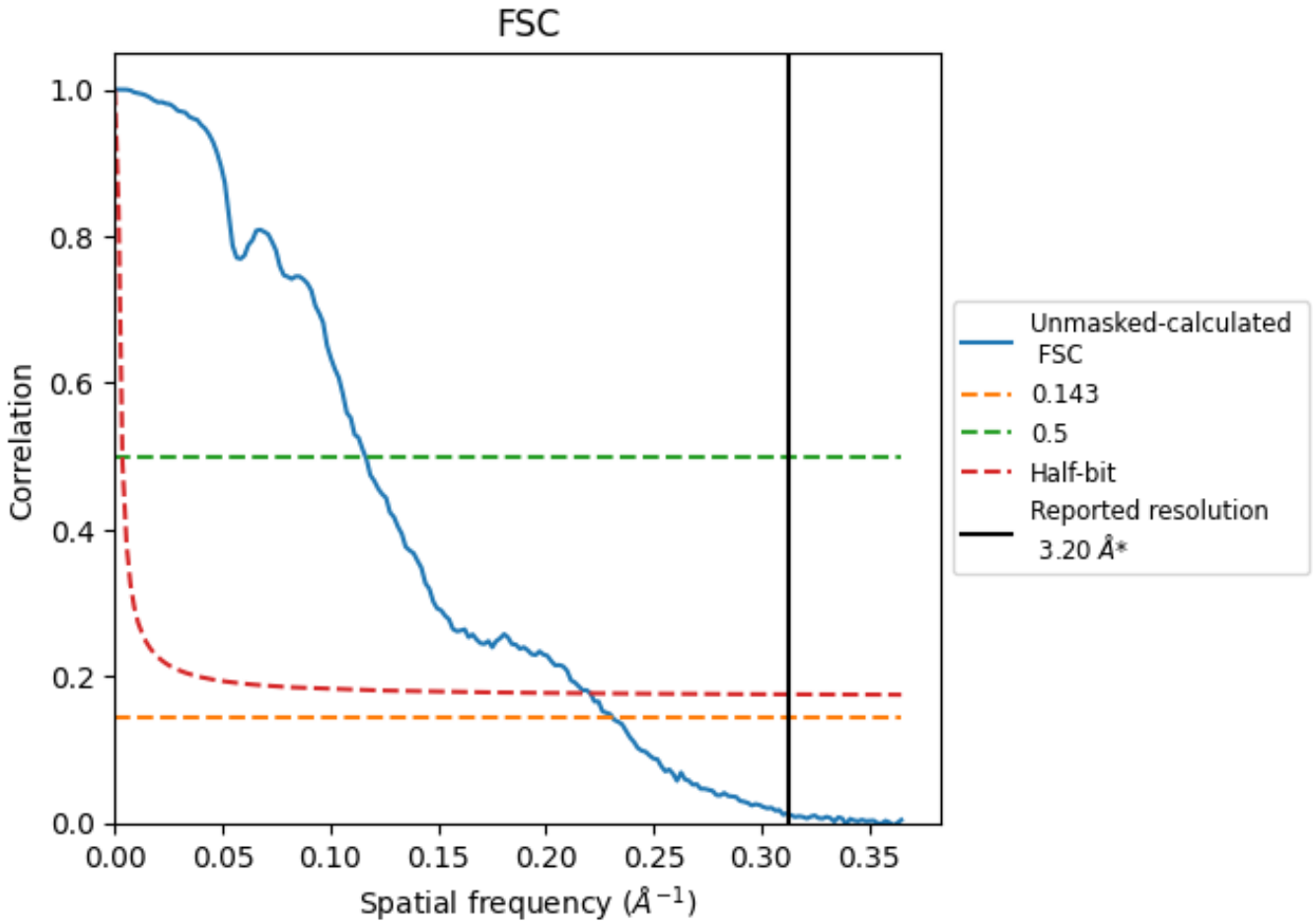


*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



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

8.2 Resolution estimates (i)

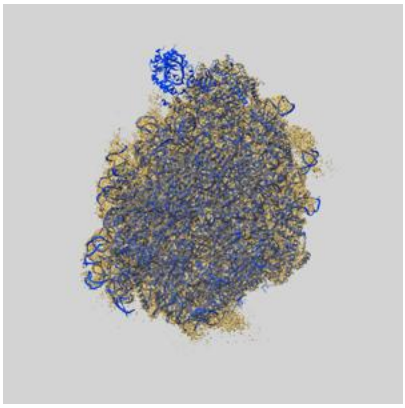
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.33	8.61	4.53

*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 4.33 differs from the reported value 3.2 by more than 10 %

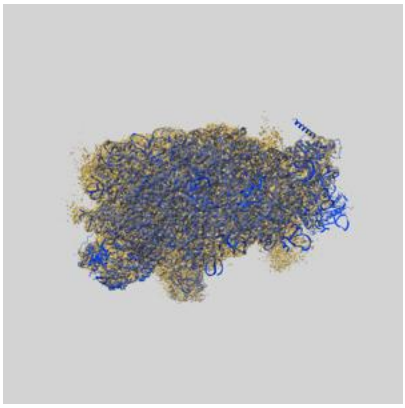
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-35596 and PDB model 8INE. Per-residue inclusion information can be found in section 3 on page 15.

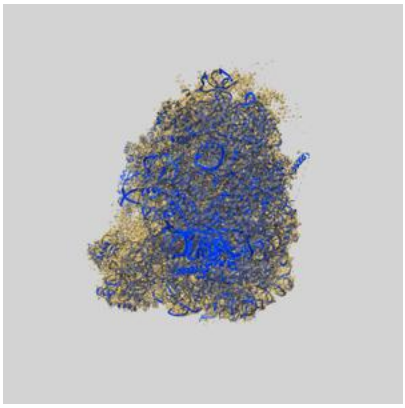
9.1 Map-model overlay



X



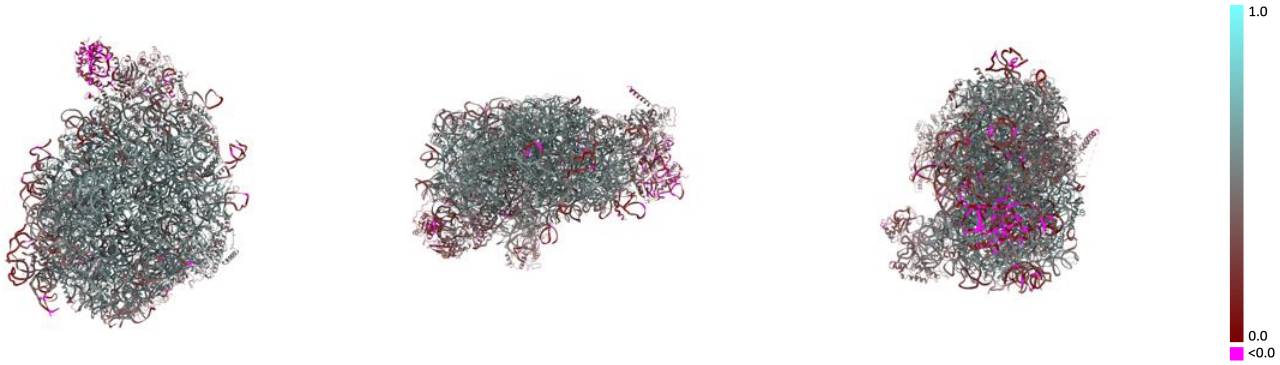
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.032 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.

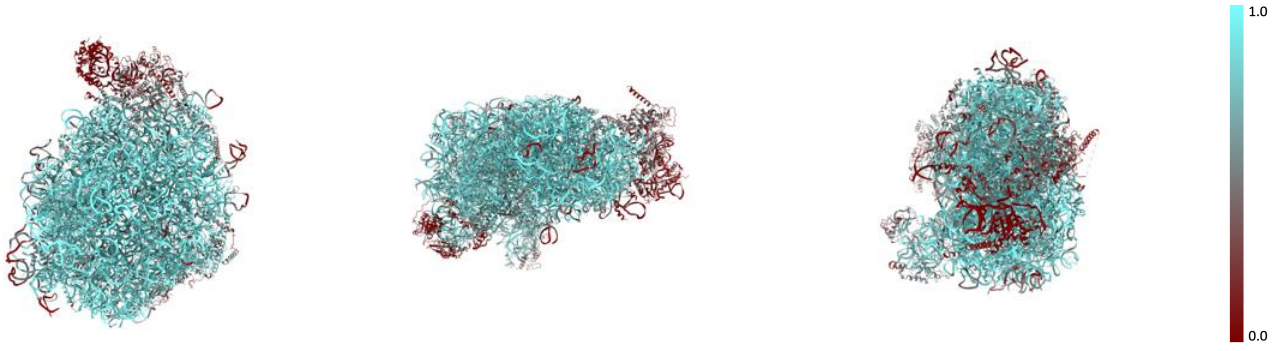
9.2 Q-score mapped to coordinate model



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.

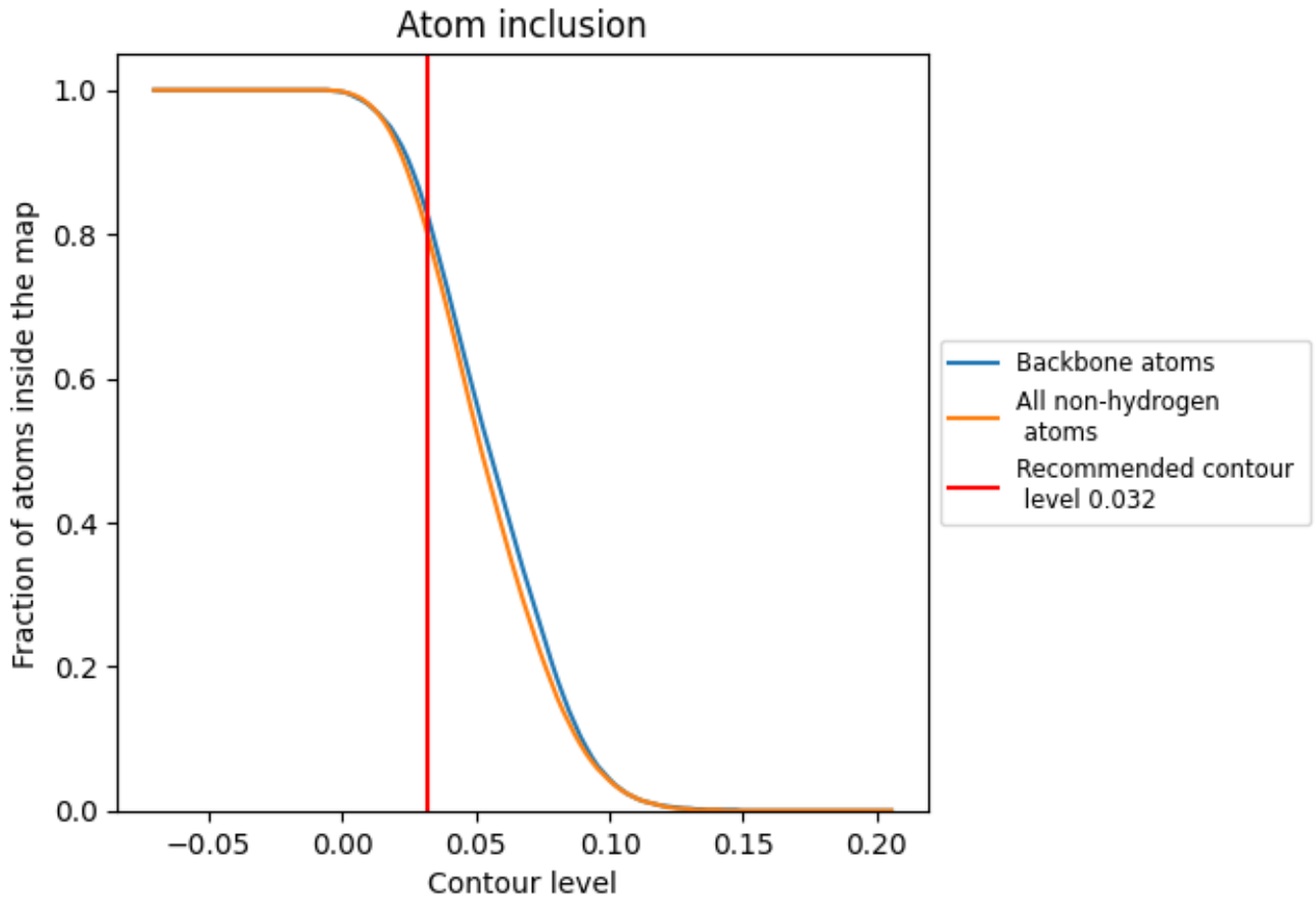
9.3 Atom inclusion mapped to coordinate model



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 (0.032).

9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.032) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7990	0.4650
2	0.8880	0.4730
3	0.2700	0.3550
4	0.6610	0.4320
5	0.8920	0.4310
6	0.7360	0.4760
7	0.7960	0.5070
8	0.9500	0.5390
9	0.5240	0.4330
A	0.5900	0.4300
B	0.8980	0.5460
C	0.7540	0.4210
D	0.9320	0.5500
E	0.7200	0.4710
F	0.8720	0.5320
G	0.7270	0.4600
H	0.8750	0.5320
I	0.8280	0.5090
J	0.1720	0.1510
K	0.8570	0.5060
L	0.9360	0.5530
M	0.9610	0.5670
N	0.4950	0.2850
O	0.7720	0.4920
P	0.9720	0.5740
Q	0.8450	0.5170
R	0.3670	0.3580
S	0.9080	0.5380
T	0.6580	0.3820
U	0.9590	0.5650
V	0.9320	0.5610
W	0.6090	0.4630
X	0.7760	0.4970
Y	0.8680	0.5330
Z	0.9410	0.5630

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Chain	Atom inclusion	Q-score
a	0.8820	0.5190
b	0.9480	0.5700
c	0.8590	0.4840
d	0.7850	0.4840
e	0.8820	0.5270
g	0.8310	0.5110
h	0.8870	0.5420
i	0.8320	0.5070
j	0.8370	0.5130
k	0.9530	0.5640
l	0.9210	0.5480
m	0.8580	0.5210
n	0.9600	0.5760
o	0.7880	0.4690
p	0.9150	0.5380
r	0.6050	0.3620
s	0.2630	0.2070
t	0.1190	0.2320
u	0.0000	0.0970
v	0.4290	0.4110
w	0.4130	0.4110
x	0.0040	0.0100
y	0.1650	0.2130
z	0.6370	0.4350