Full wwPDB EM Validation Report ⓘ

Nov 6, 2023 – 11:08 AM JST

PDB ID	:	8IDT
EMDB ID	:	EMD-35370
Title	:	human nuclear pre-60S ribosomal particle - State G
Authors	:	Zhang, Y.; Gao, N.
Deposited on	:	2023-02-14
Resolution	:	2.80 Å(reported)

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

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

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

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

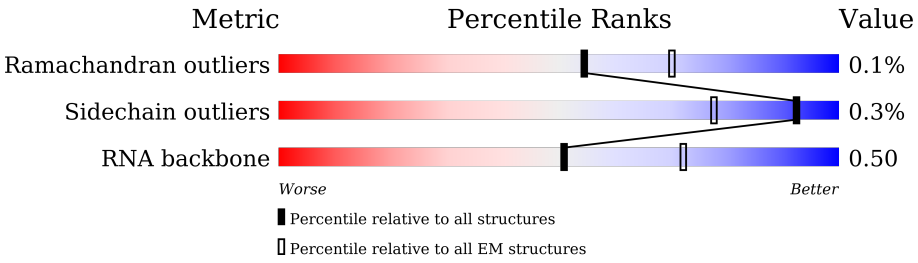
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	5	120	71% 27%
2	6	245	9% 99%
3	7	163	82% 17%
4	8	156	6% 58% 38%
5	9	134	43% 69% 28%
6	B	403	99%
7	C	159	11% 58% 42%
8	D	427	83% 16%

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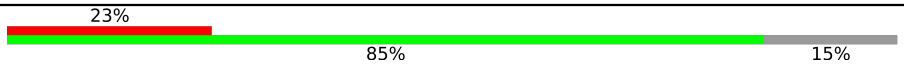
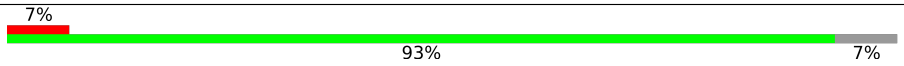
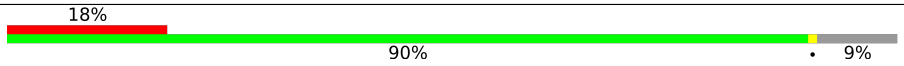
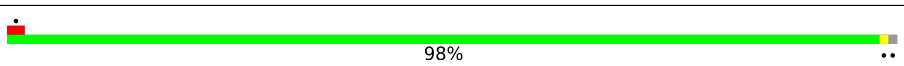
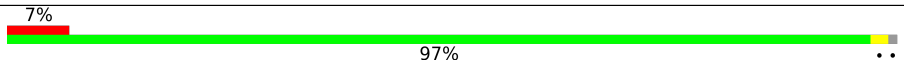
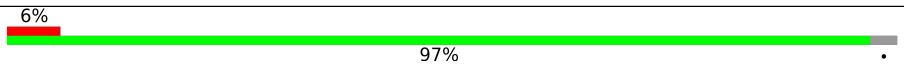
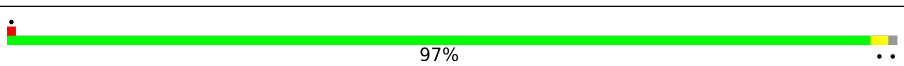
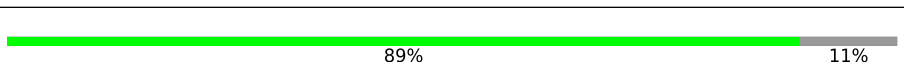
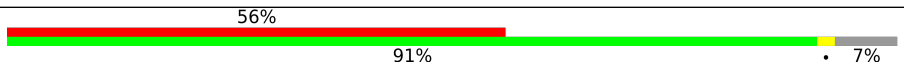
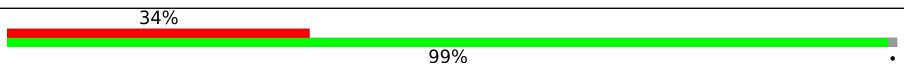
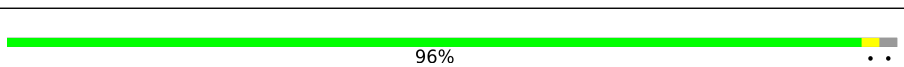
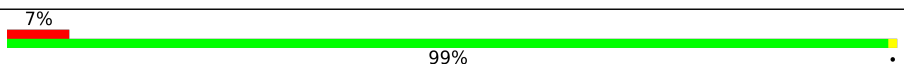
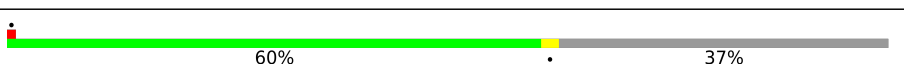
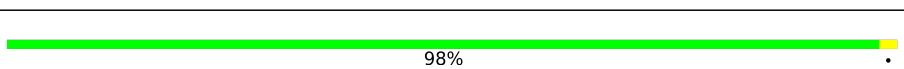
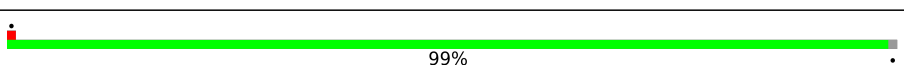
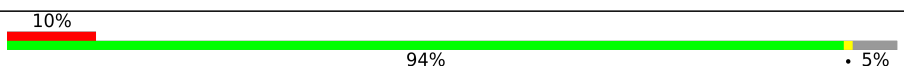
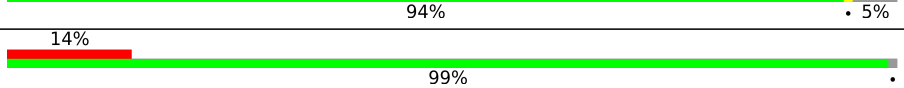
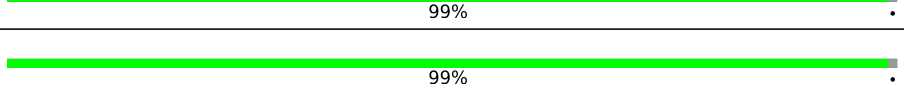
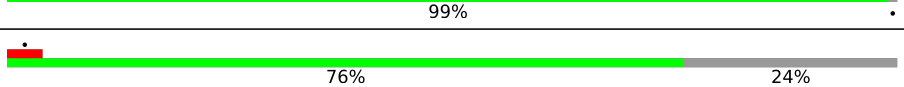
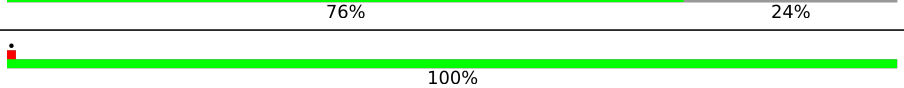
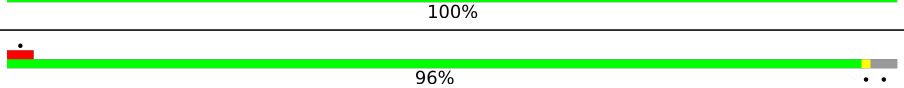
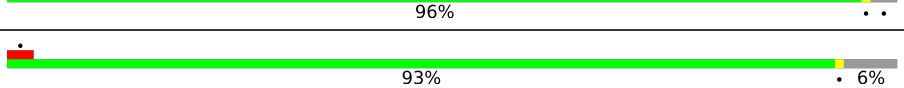
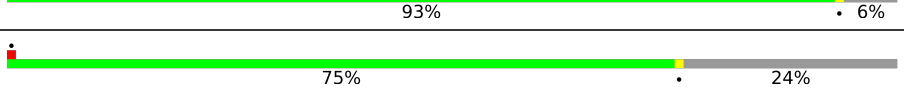
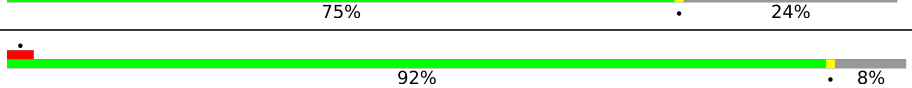
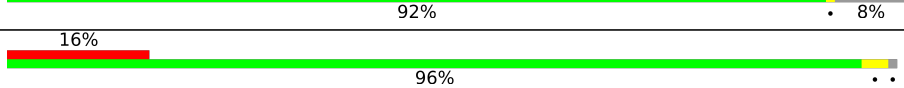
Mol	Chain	Length	Quality of chain
9	E	115	
10	F	117	
11	G	266	
12	H	123	
13	I	192	
14	K	105	
15	L	148	
16	M	97	
17	N	178	
18	O	70	
19	P	51	
20	Q	211	
21	S	215	
22	U	204	
23	V	203	
24	W	106	
25	X	92	
26	Z	188	
27	a	196	
28	b	176	
29	c	160	
30	e	140	
31	g	156	
32	h	145	
33	i	136	

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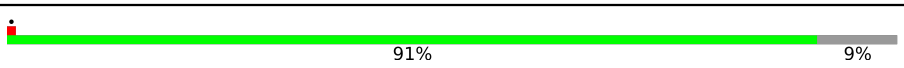
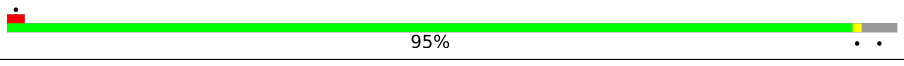
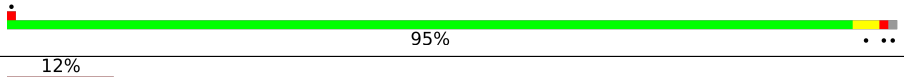
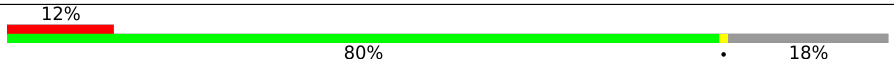
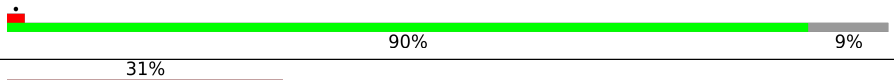
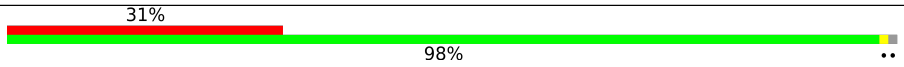
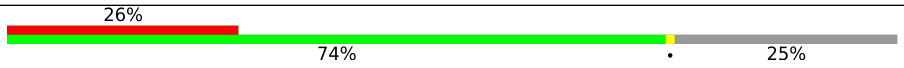
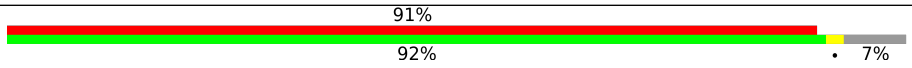
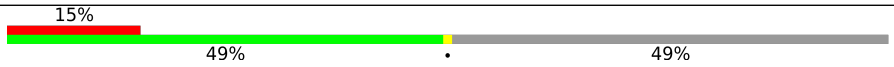
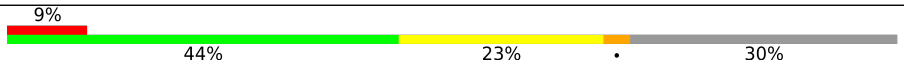
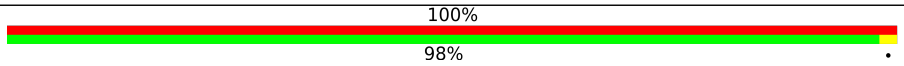
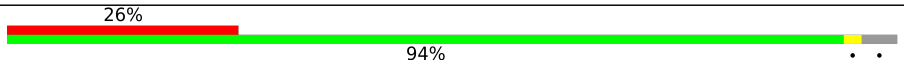
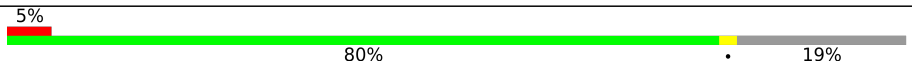
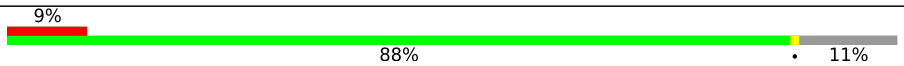
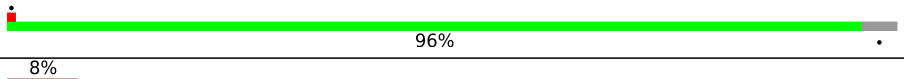
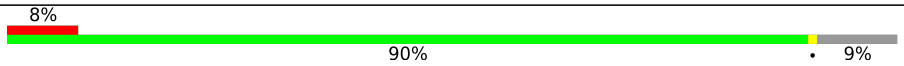
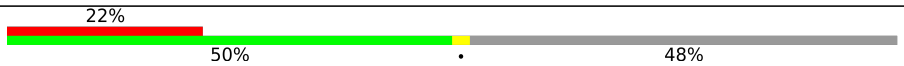
Mol	Chain	Length	Quality of chain
34	l	137	
35	m	257	
36	n	110	
37	o	288	
38	p	248	
39	r	297	
40	A	731	
41	R	203	
42	J	239	
43	T	99	
44	2	5054	
45	y	165	
46	4	634	
47	d	128	
48	j	125	
49	k	135	
50	Y	184	
51	z	129	

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 147681 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	5	120	2558	1141	456	842	119	0	0

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	9	97	793	484	171	134	4	0	0

- Molecule 6 is a protein called 60S ribosomal protein L3.

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

- Molecule 7 is a protein called 60S ribosomal protein L29.

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 14 is a protein called 60S ribosomal protein L36.

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

- Molecule 15 is a protein called 60S ribosomal protein L27a.

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

- Molecule 16 is a protein called 60S ribosomal protein L37.

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

- Molecule 17 is a protein called 60S ribosomal protein L11.

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 24 is a protein called 60S ribosomal protein L36a.

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

- Molecule 25 is a protein called 60S ribosomal protein L37a.

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

- Molecule 26 is a protein called 60S ribosomal protein L18.

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

- Molecule 27 is a protein called 60S ribosomal protein L19.

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

- Molecule 28 is a protein called 60S ribosomal protein L18a.

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

- Molecule 29 is a protein called 60S ribosomal protein L21.

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

- Molecule 30 is a protein called 60S ribosomal protein L23.

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

- Molecule 31 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	g	118	Total	C	N	O	S	0	0
			967	618	181	167	1		

- Molecule 32 is a protein called 60S ribosomal protein L26.

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

- Molecule 33 is a protein called 60S ribosomal protein L27.

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

- Molecule 34 is a protein called 60S ribosomal protein L28.

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

- Molecule 35 is a protein called 60S ribosomal protein L8.

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

- Molecule 36 is a protein called 60S ribosomal protein L35a.

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

- Molecule 37 is a protein called 60S ribosomal protein L6.

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

- Molecule 38 is a protein called 60S ribosomal protein L7.

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

- Molecule 39 is a protein called 60S ribosomal protein L5.

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

- Molecule 40 is a protein called G Protein Nucleolar 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	A	307	Total	C	N	O	S	0	0
			2460	1576	419	457	8		

- Molecule 41 is a protein called Translation machinery-associated protein 16.

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

- Molecule 42 is a protein called mRNA turnover protein 4 homolog.

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

- Molecule 43 is a protein called Leydig cell tumor 10 kDa protein homolog.

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

- Molecule 44 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	2	3524	Total	C	N	O	P	0	0
			75681	33754	13848	24556	3523		

- Molecule 45 is a protein called 60S ribosomal protein L12.

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

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

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

- Molecule 47 is a protein called 60S ribosomal protein L22.

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

- Molecule 48 is a protein called 60S ribosomal protein L31.

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

- Molecule 49 is a protein called 60S ribosomal protein L32.

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

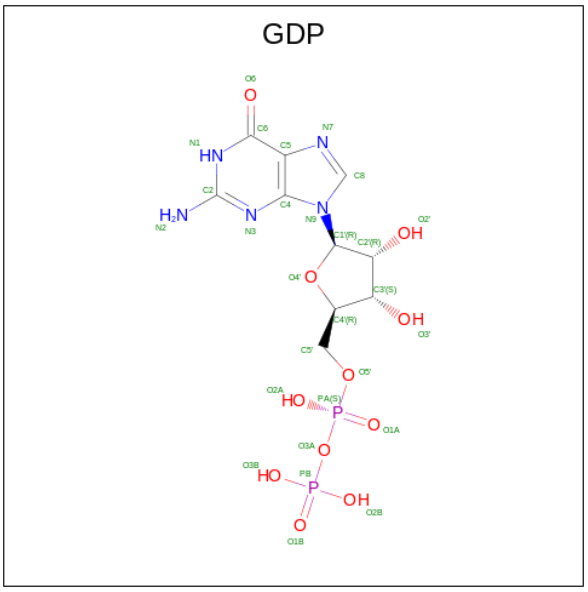
- Molecule 50 is a protein called 60S ribosomal protein L17.

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

- Molecule 51 is a protein called Protein LLP homolog.

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

- Molecule 52 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

- Molecule 53 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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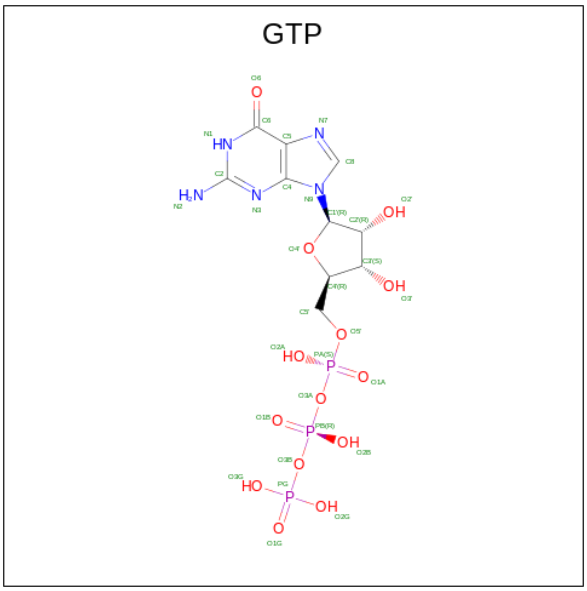
Mol	Chain	Residues	Atoms	AltConf
53	4	1	Total Mg 1 1	0

- Molecule 54 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 55 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



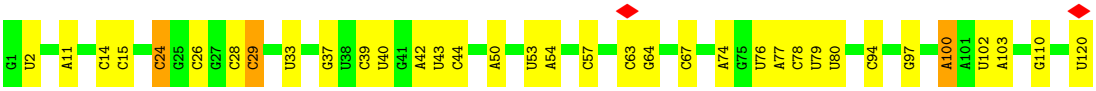
Mol	Chain	Residues	Atoms	AltConf
55	4	1	Total C N O P 32 10 5 14 3	0

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.

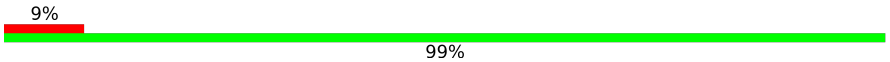
- Molecule 1: 5S rRNA

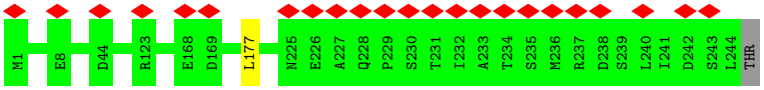
Chain 5:



- Molecule 2: Eukaryotic translation initiation factor 6

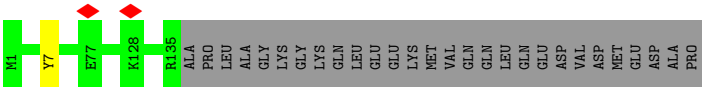
Chain 6:





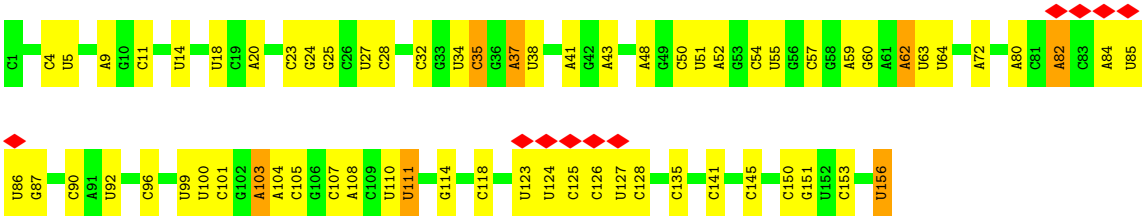
- Molecule 3: Probable ribosome biogenesis protein RLP24

Chain 7:



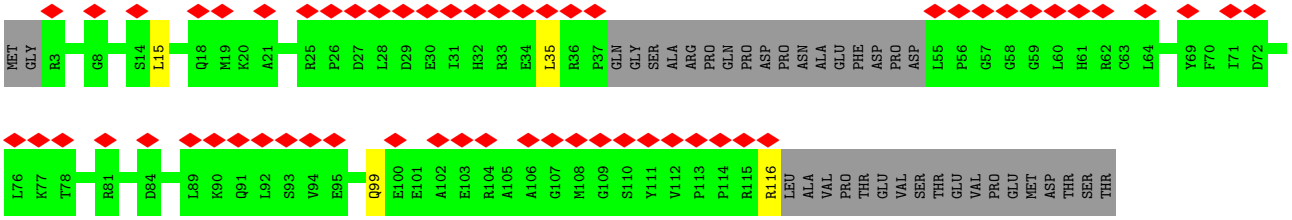
- Molecule 4: 5.8S rRNA

Chain 8:

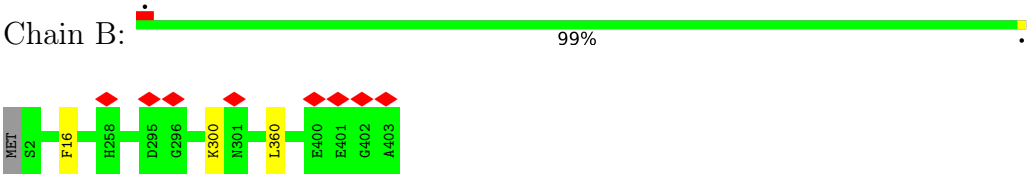


- Molecule 5: Zinc finger protein 593

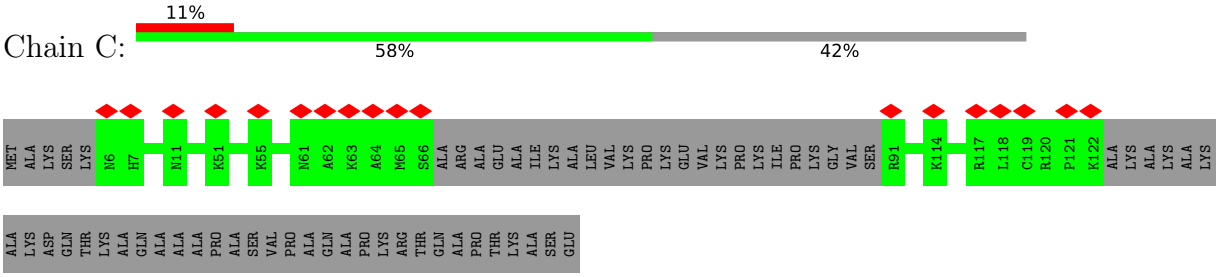
Chain 9:



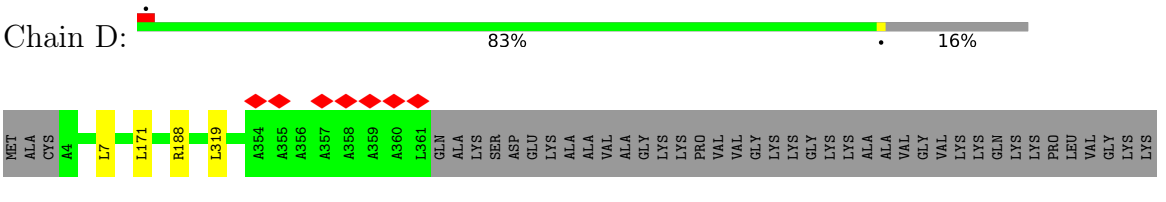
• Molecule 6: 60S ribosomal protein L3



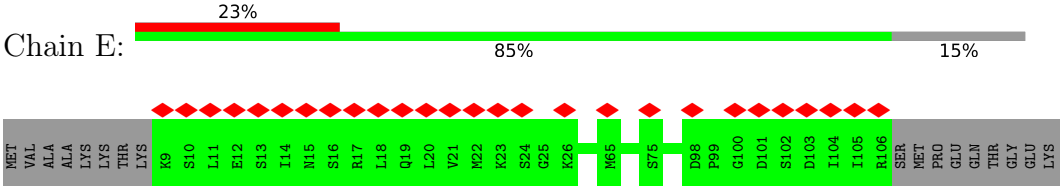
• Molecule 7: 60S ribosomal protein L29



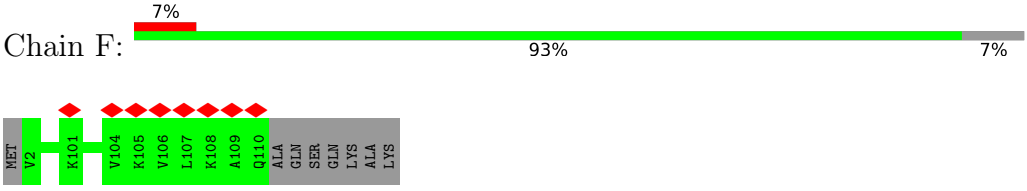
• Molecule 8: 60S ribosomal protein L4



• Molecule 9: 60S ribosomal protein L30

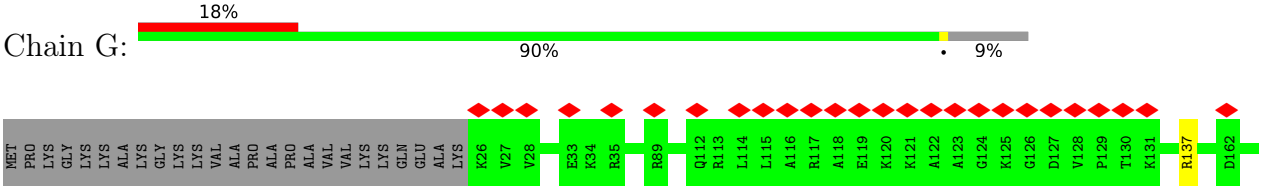


• Molecule 10: 60S ribosomal protein L34



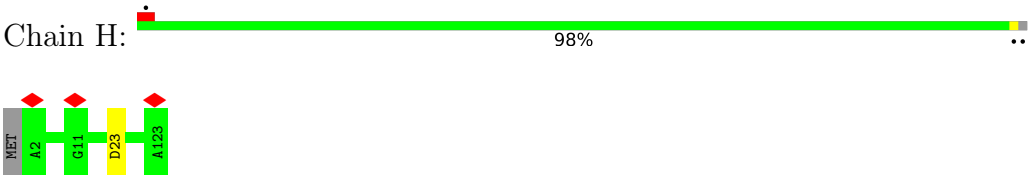
• Molecule 11: 60S ribosomal protein L7a

Chain G:



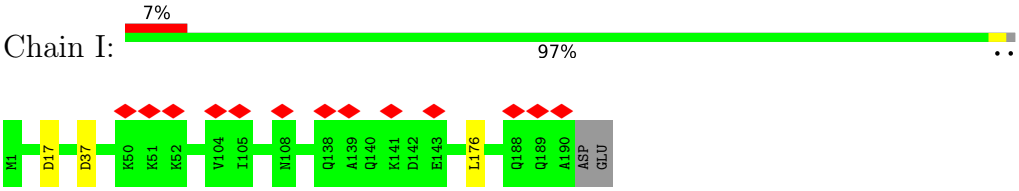
• Molecule 12: 60S ribosomal protein L35

Chain H:



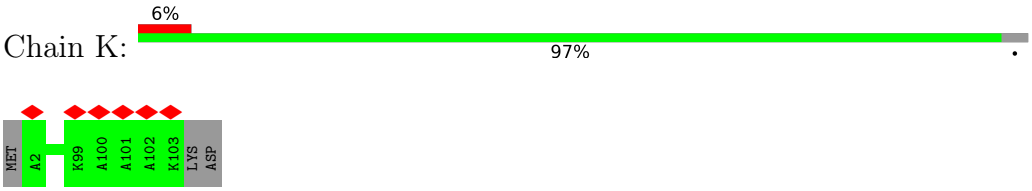
• Molecule 13: 60S ribosomal protein L9

Chain I:



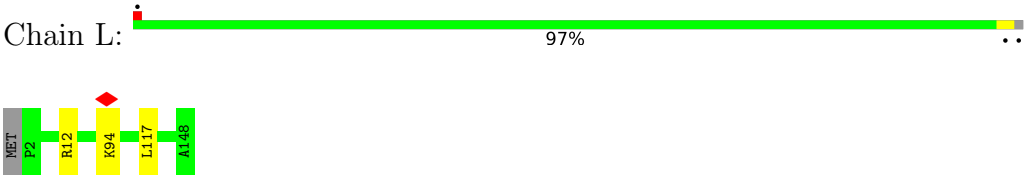
• Molecule 14: 60S ribosomal protein L36

Chain K:



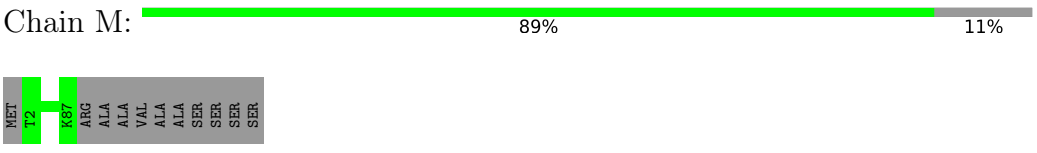
• Molecule 15: 60S ribosomal protein L27a

Chain L:



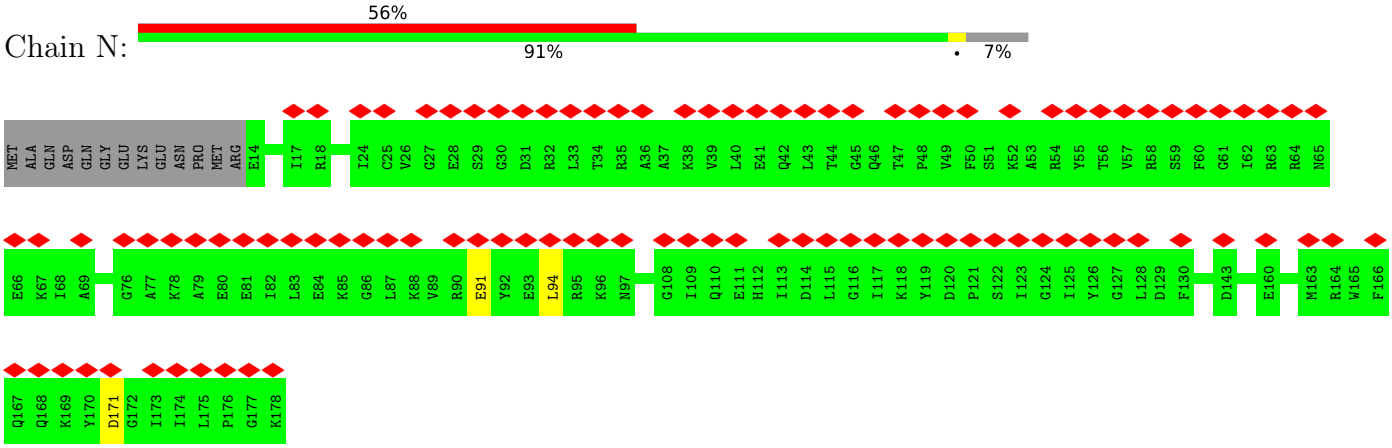
• Molecule 16: 60S ribosomal protein L37

Chain M:



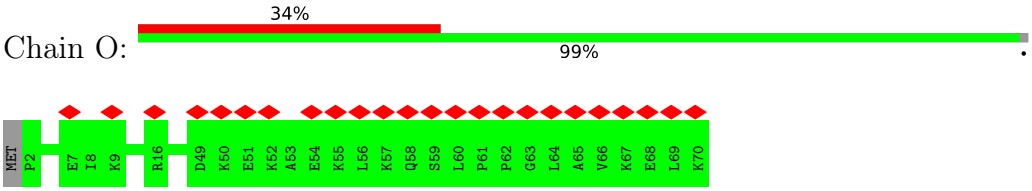
• Molecule 17: 60S ribosomal protein L11

Chain N:



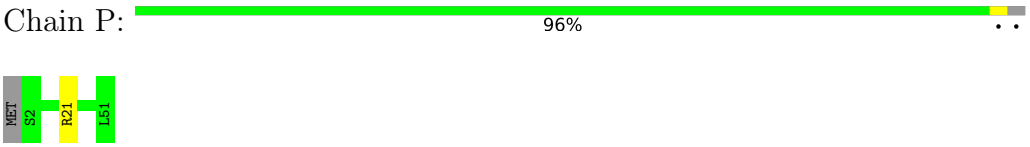
• Molecule 18: 60S ribosomal protein L38

Chain O:



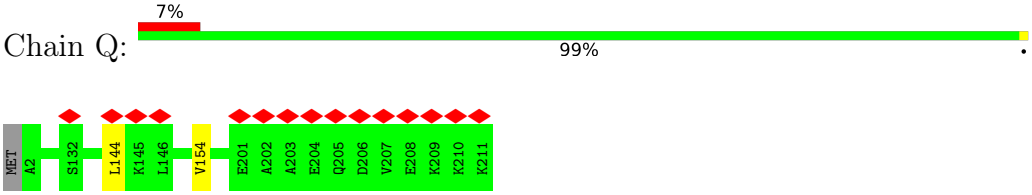
• Molecule 19: 60S ribosomal protein L39

Chain P:



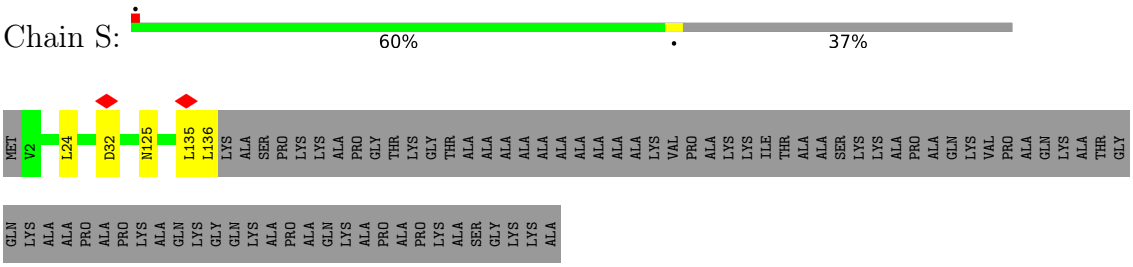
• Molecule 20: 60S ribosomal protein L13

Chain Q:



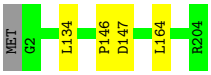
• Molecule 21: 60S ribosomal protein L14

Chain S:



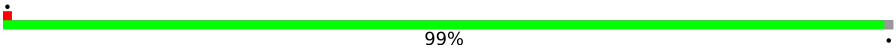
• Molecule 22: 60S ribosomal protein L15

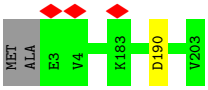
Chain U:



• Molecule 23: 60S ribosomal protein L13a

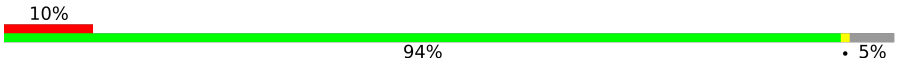
Chain V:

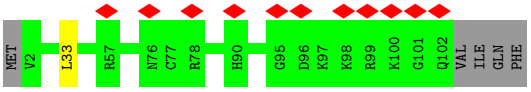




• Molecule 24: 60S ribosomal protein L36a

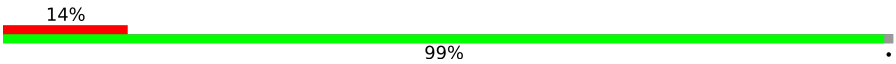
Chain W:

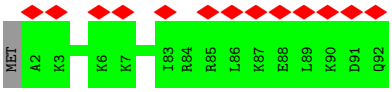




• Molecule 25: 60S ribosomal protein L37a

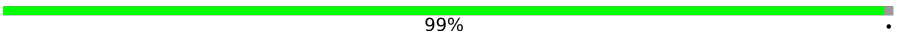
Chain X:





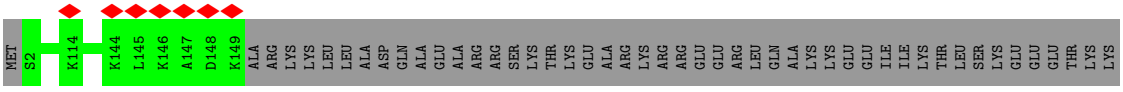
• Molecule 26: 60S ribosomal protein L18

Chain Z:



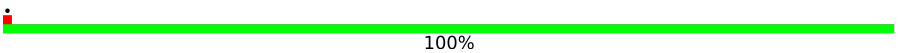
• Molecule 27: 60S ribosomal protein L19

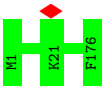
Chain a:



• Molecule 28: 60S ribosomal protein L18a

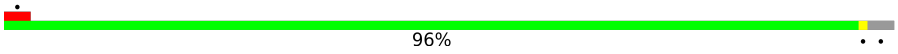
Chain b:

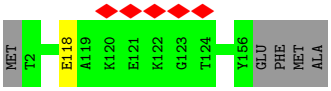




• Molecule 29: 60S ribosomal protein L21

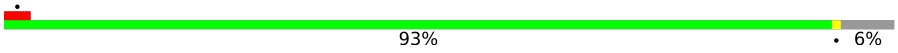
Chain c:

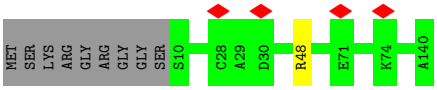




• Molecule 30: 60S ribosomal protein L23

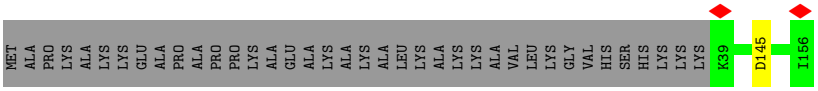
Chain e:





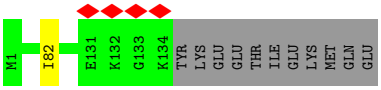
• Molecule 31: 60S ribosomal protein L23a

Chain g:



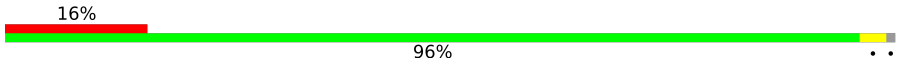
• Molecule 32: 60S ribosomal protein L26

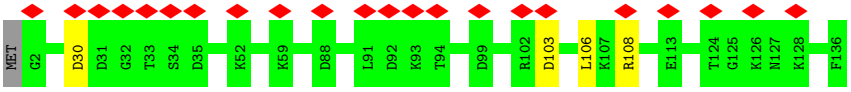
Chain h:



• Molecule 33: 60S ribosomal protein L27

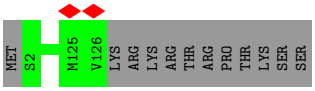
Chain i:





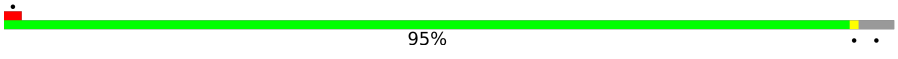
• Molecule 34: 60S ribosomal protein L28

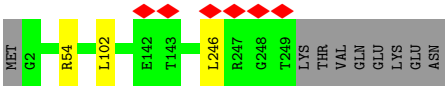
Chain l:



• Molecule 35: 60S ribosomal protein L8

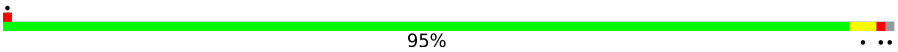
Chain m:

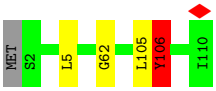




• Molecule 36: 60S ribosomal protein L35a

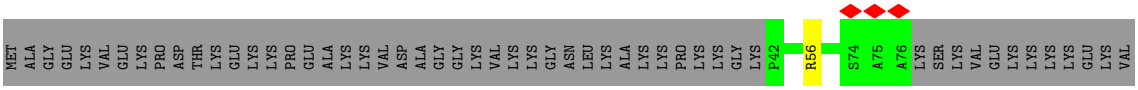
Chain n:

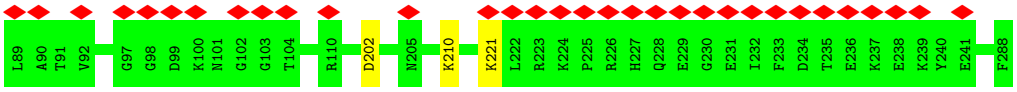




• Molecule 37: 60S ribosomal protein L6

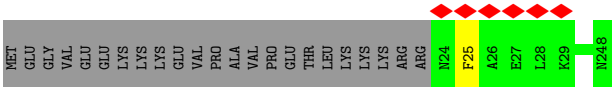
Chain o:





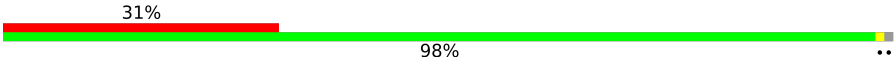
• Molecule 38: 60S ribosomal protein L7

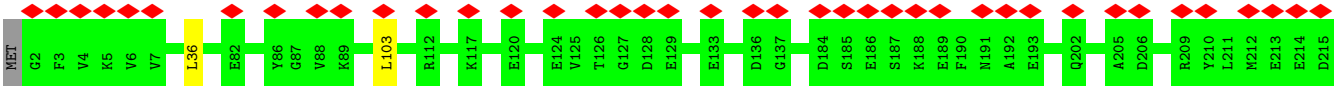
Chain p:

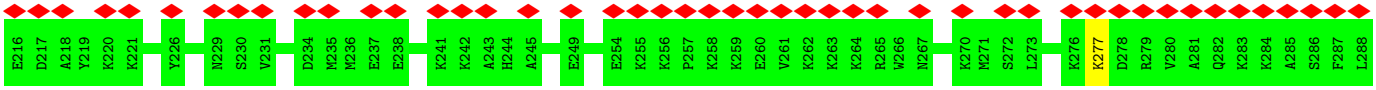


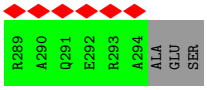
• Molecule 39: 60S ribosomal protein L5

Chain r:



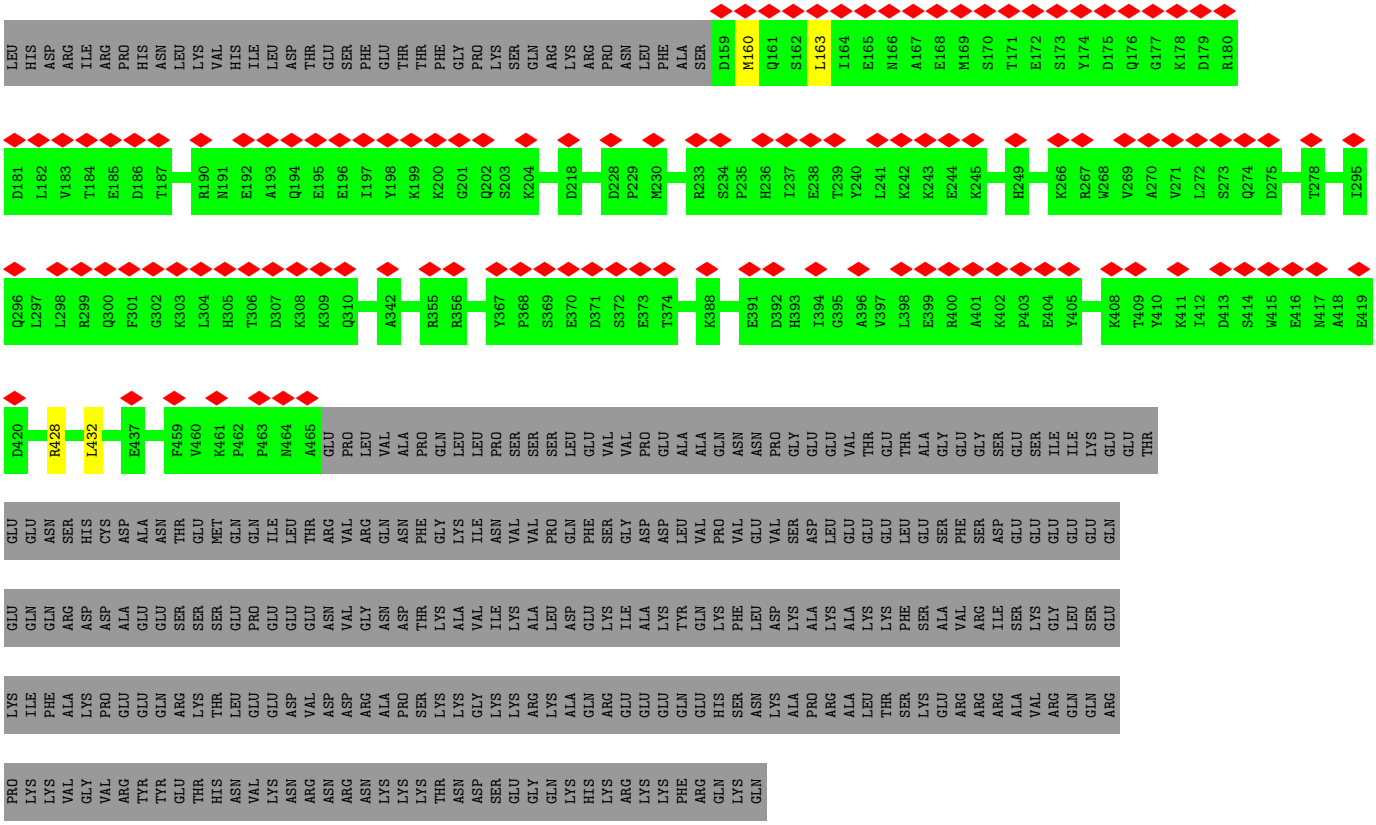






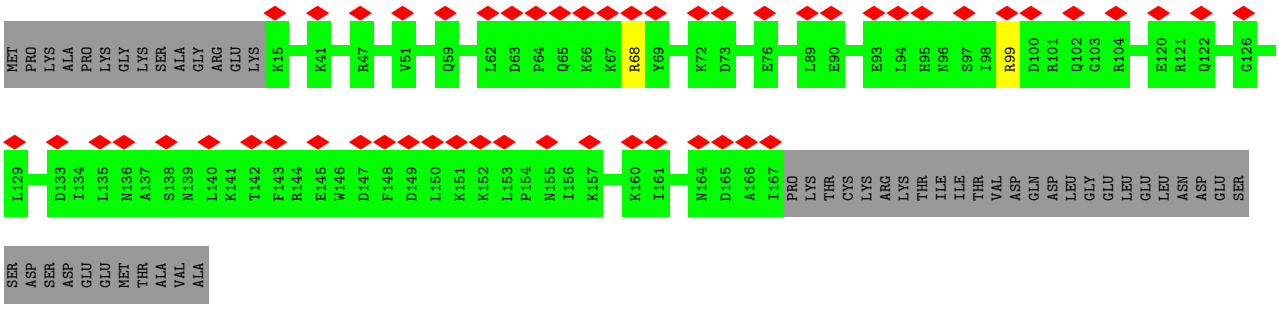
• Molecule 40: G Protein Nucleolar 2

Chain A:



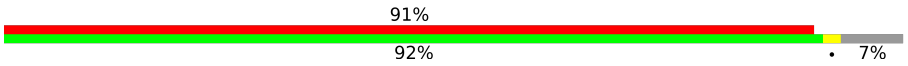
• Molecule 41: Translation machinery-associated protein 16

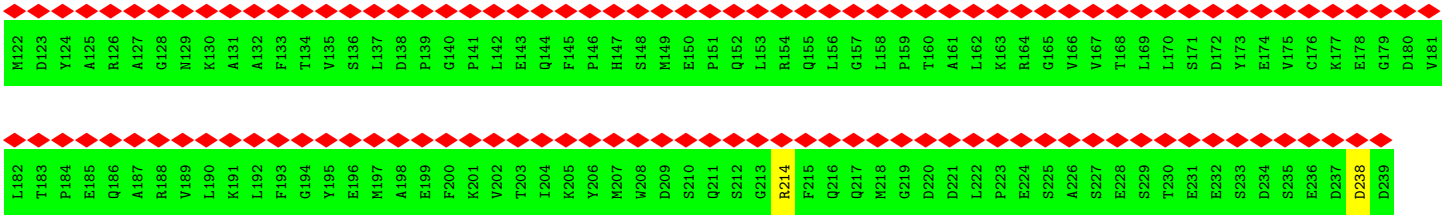
Chain R:



• Molecule 42: mRNA turnover protein 4 homolog

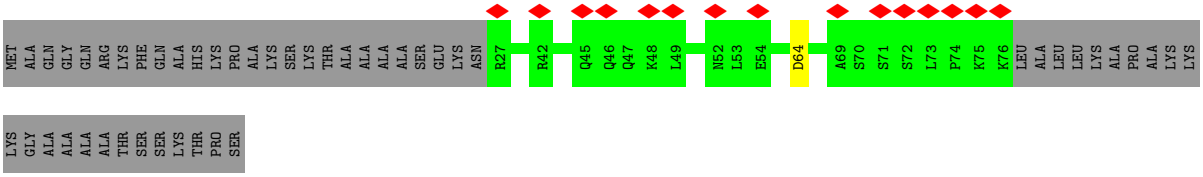
Chain J:





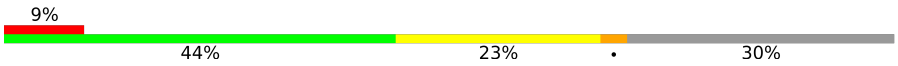
• Molecule 43: Leydig cell tumor 10 kDa protein homolog

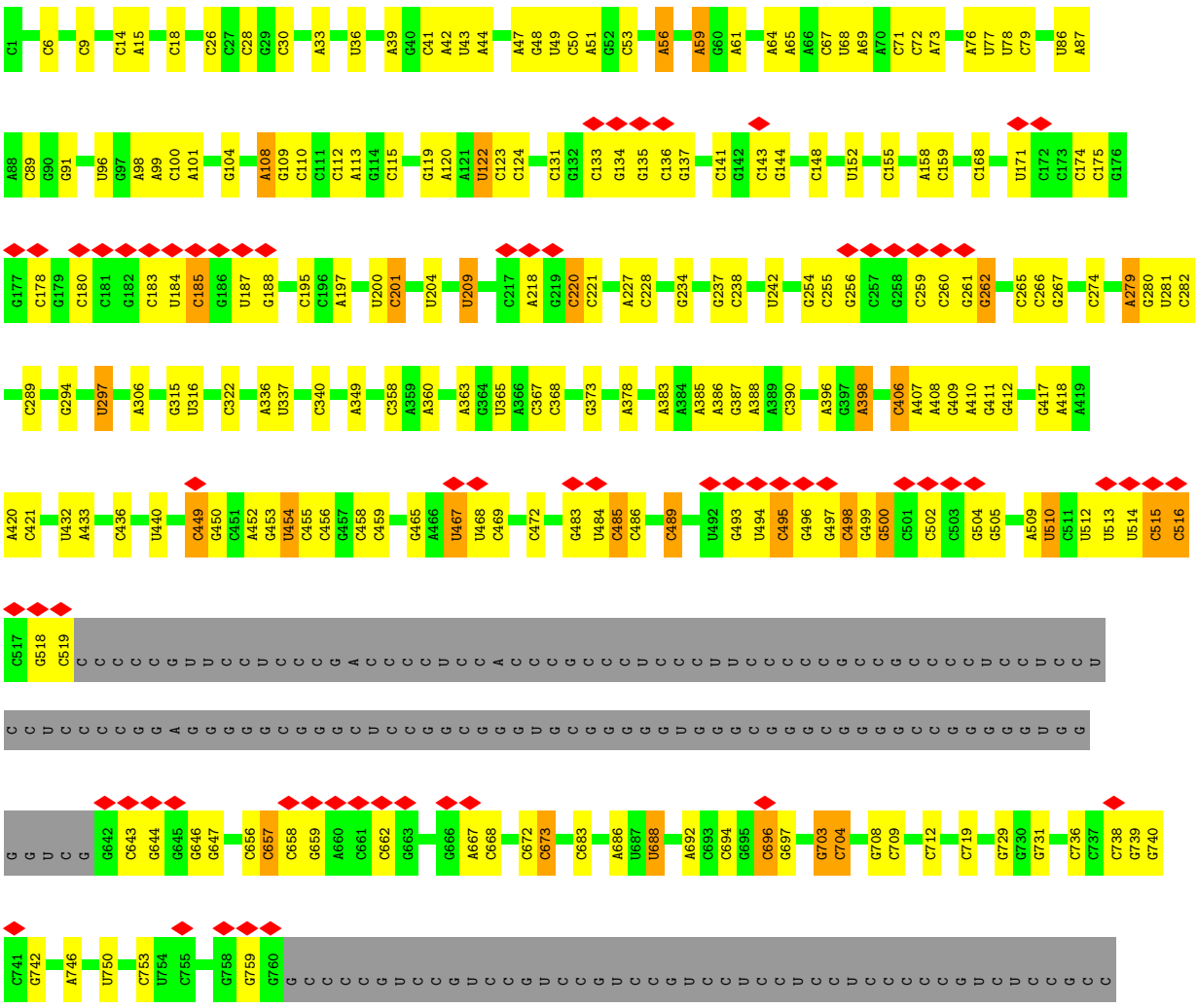
Chain T:

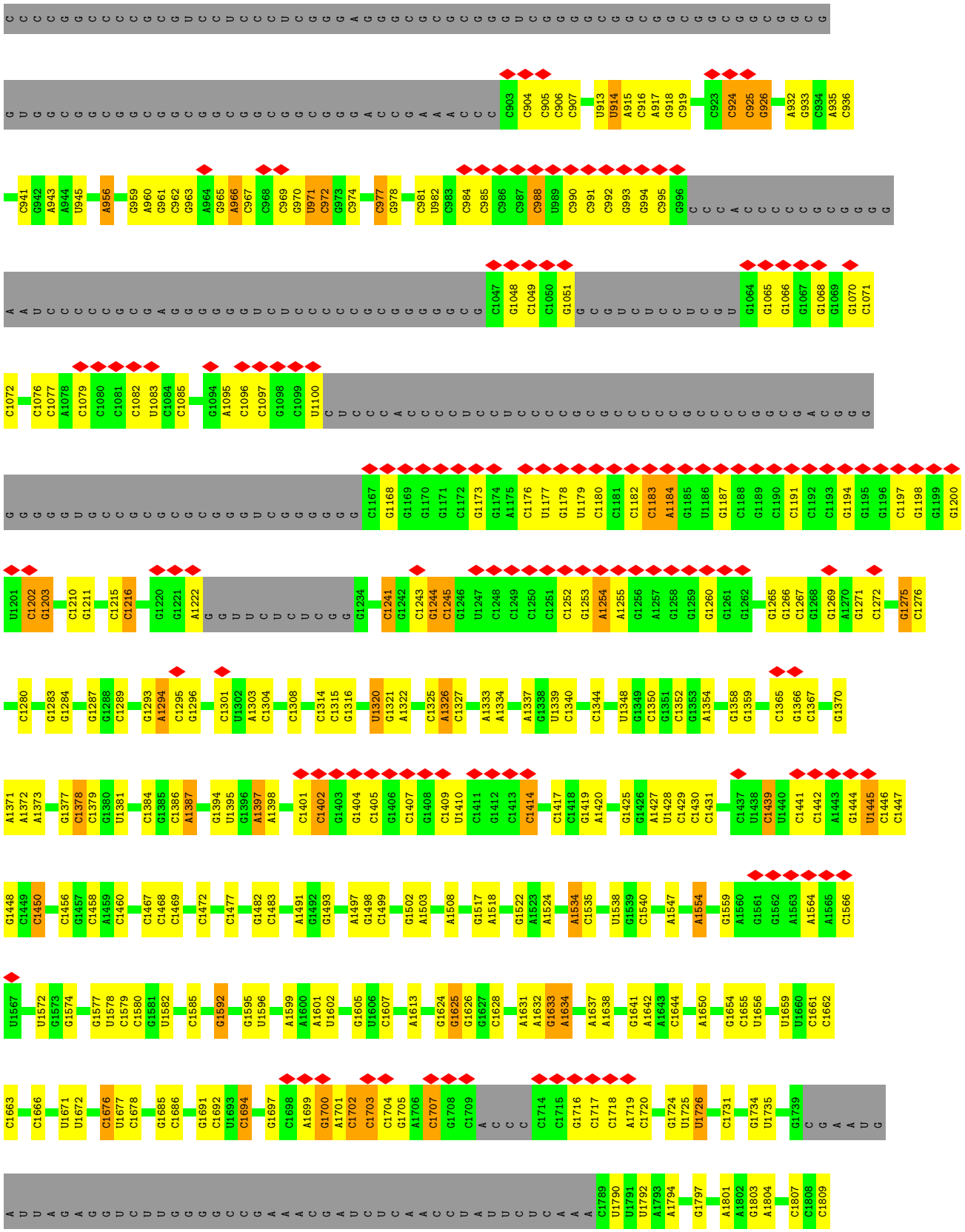


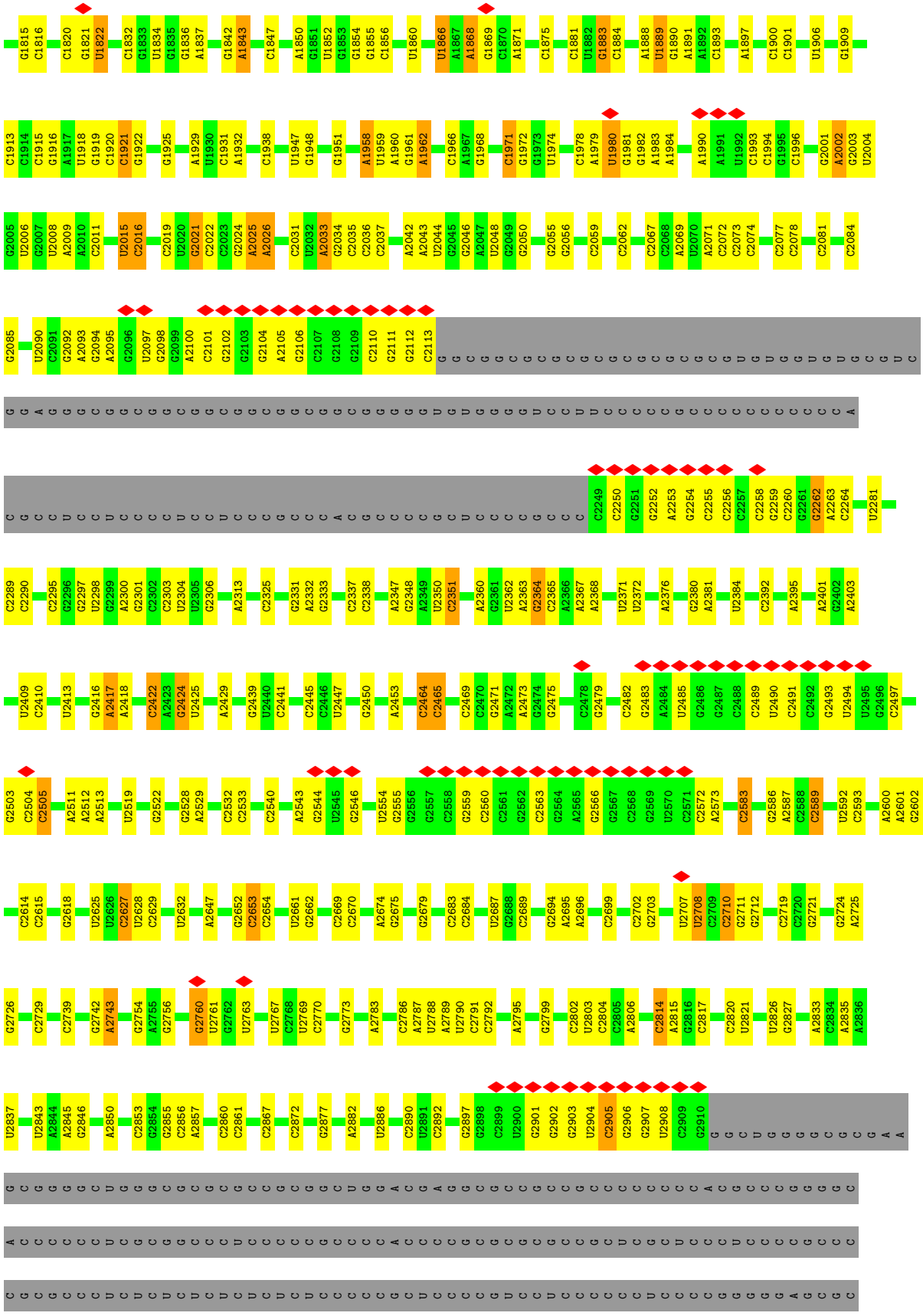
• Molecule 44: 28S rRNA

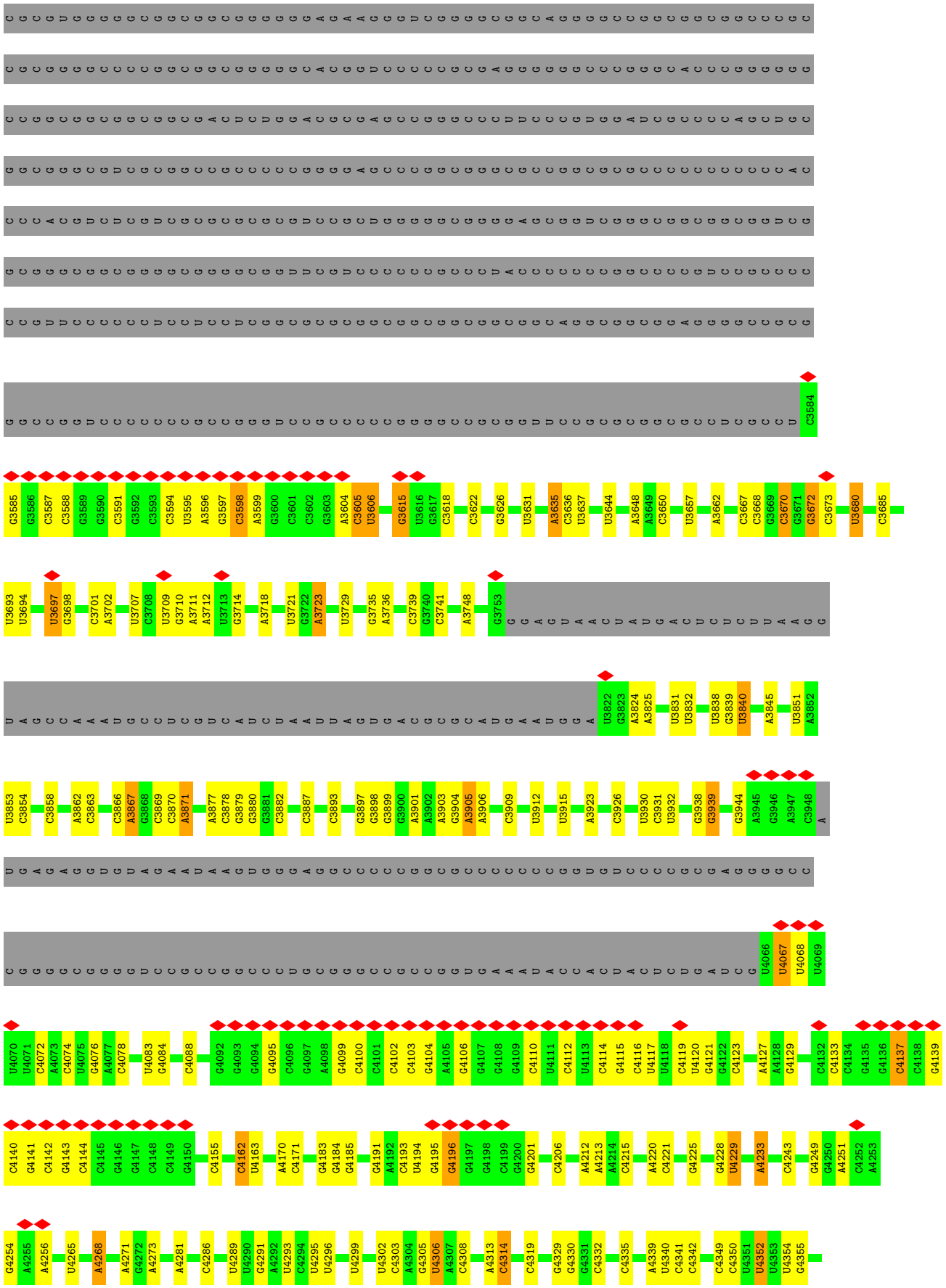
Chain 2:

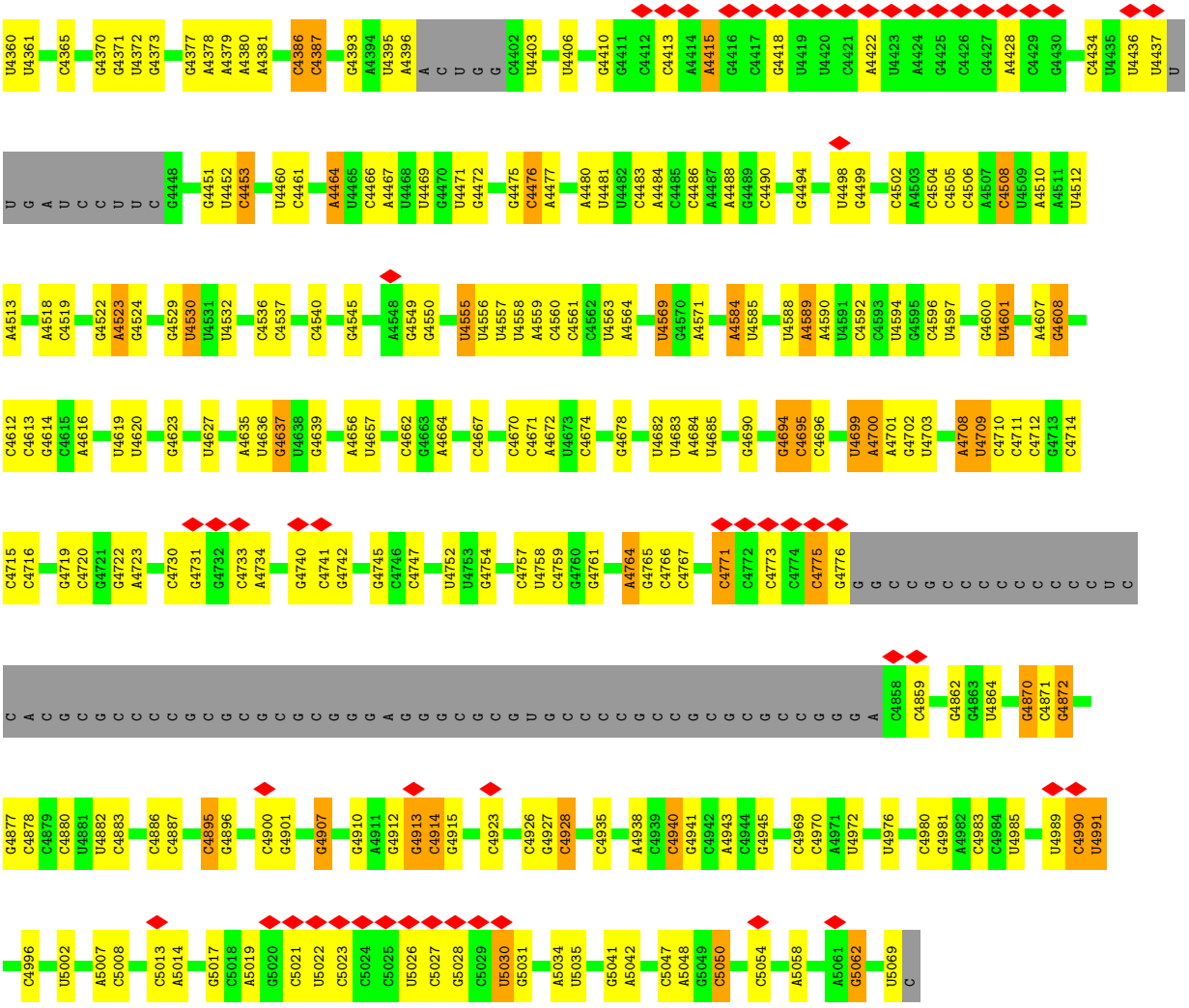






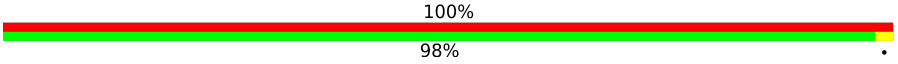


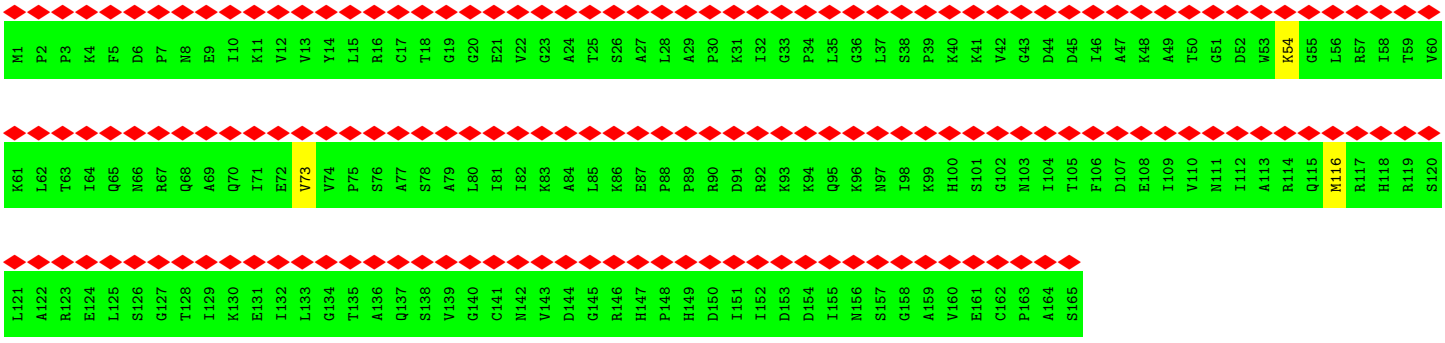




• Molecule 45: 60S ribosomal protein L12

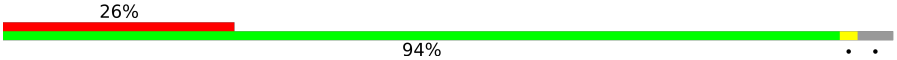
Chain y:

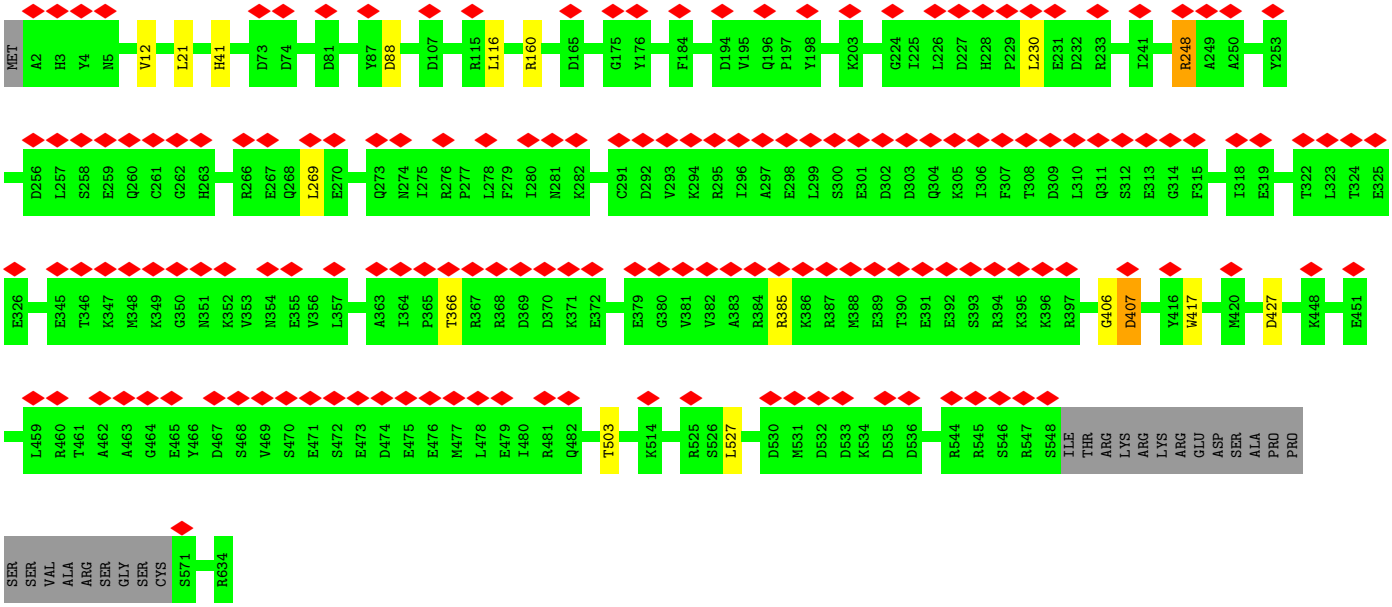




• Molecule 46: GTP-binding protein 4

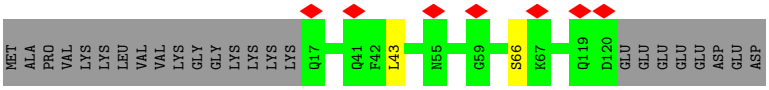
Chain 4:





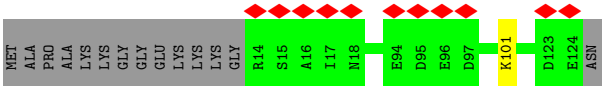
• Molecule 47: 60S ribosomal protein L22

Chain d:



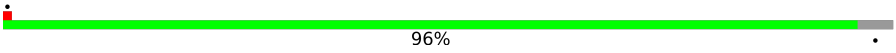
• Molecule 48: 60S ribosomal protein L31

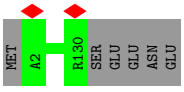
Chain j:



• Molecule 49: 60S ribosomal protein L32

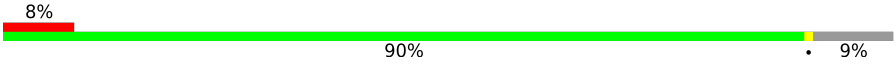
Chain k:

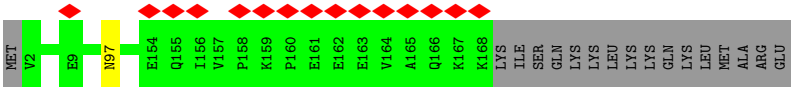




• Molecule 50: 60S ribosomal protein L17

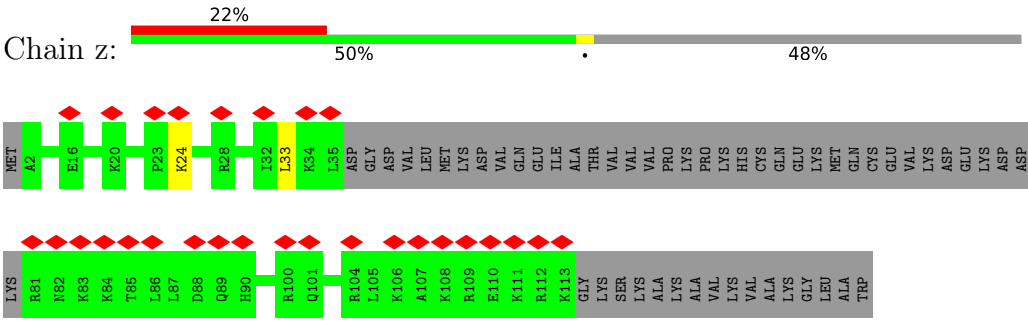
Chain Y:





• Molecule 51: Protein LLP homolog

Chain z:


22%
50%
48%
MET A2 E16 K20 P23 K24 R28 I32 L33 K34 L35 ASP GLY ASP VAL LEU MET LYS ASP VAL GLN GLU ILE ALA THR VAL VAL VAL PRO LYS PRO LYS HIS CYS GLN GLU LYS MET GLN CYS GLU VAL LYS ASP GLU LYS ASP ASP MET LYS MET GLU THR ASP ILE
LYS R81 N82 K83 K84 T85 L86 L87 D88 Q89 H90 R100 Q101 R104 L105 K106 A107 K108 R109 E110 K111 R112 K113 GLY LYS SER LYS ALA LYS ALA VAL LYS VAL ALA LYS GLY LEU ALA TRP

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	175116	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	0.312	Depositor
Minimum map value	-0.098	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.045	Depositor
Map size (Å)	548.0, 548.0, 548.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.37, 1.37, 1.37	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	5	0.45	0/2858	1.37	46/4455 (1.0%)
2	6	0.35	0/1877	0.74	1/2554 (0.0%)
3	7	0.39	0/1181	0.75	1/1563 (0.1%)
4	8	0.52	0/3679	1.44	74/5732 (1.3%)
5	9	0.32	0/808	0.83	2/1076 (0.2%)
6	B	0.33	0/3315	0.71	1/4435 (0.0%)
7	C	0.29	0/777	0.67	0/1026
8	D	0.33	0/2907	0.78	4/3905 (0.1%)
9	E	0.30	0/774	0.65	0/1038
10	F	0.30	0/878	0.73	0/1170
11	G	0.34	0/1971	0.71	1/2651 (0.0%)
12	H	0.32	0/1023	0.68	1/1351 (0.1%)
13	I	0.34	0/1537	0.79	3/2066 (0.1%)
14	K	0.31	0/843	0.67	0/1115
15	L	0.31	0/1191	0.69	2/1591 (0.1%)
16	M	0.35	0/720	0.74	0/952
17	N	0.37	0/1341	0.81	2/1793 (0.1%)
18	O	0.32	0/575	0.69	0/761
19	P	0.32	0/454	0.72	0/599
20	Q	0.35	0/1732	0.75	1/2315 (0.0%)
21	S	0.36	0/1133	0.76	4/1516 (0.3%)
22	U	0.31	0/1746	0.73	4/2338 (0.2%)
23	V	0.34	0/1682	0.66	1/2250 (0.0%)
24	W	0.31	0/840	0.73	1/1107 (0.1%)
25	X	0.30	0/718	0.63	0/953
26	Z	0.31	0/1537	0.72	0/2052
27	a	0.31	0/1255	0.70	0/1662
28	b	0.34	0/1501	0.66	0/2013
29	c	0.36	0/1291	0.72	1/1725 (0.1%)
30	e	0.38	0/993	0.71	0/1332
31	g	0.30	0/984	0.66	1/1323 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	h	0.35	0/1132	0.72	1/1504 (0.1%)
33	i	0.40	0/1130	0.82	3/1507 (0.2%)
34	l	0.31	0/1017	0.70	0/1364
35	m	0.34	0/1936	0.76	2/2596 (0.1%)
36	n	0.31	0/895	0.79	4/1198 (0.3%)
37	o	0.34	0/1935	0.78	1/2596 (0.0%)
38	p	0.37	0/1916	0.74	1/2553 (0.0%)
39	r	0.33	0/2428	0.71	2/3252 (0.1%)
40	A	0.31	0/2515	0.58	2/3403 (0.1%)
41	R	0.35	0/1317	0.63	0/1757
42	J	0.36	0/1844	0.71	2/2476 (0.1%)
43	T	0.31	0/396	0.77	1/522 (0.2%)
44	2	0.48	3/82562 (0.0%)	1.39	1341/128718 (1.0%)
45	y	0.31	0/1269	0.74	2/1712 (0.1%)
46	4	0.36	0/5099	0.79	13/6840 (0.2%)
47	d	0.38	0/864	0.81	2/1160 (0.2%)
48	j	0.32	0/933	0.70	0/1256
49	k	0.31	0/1082	0.70	0/1443
50	Y	0.31	0/1383	0.62	0/1856
51	z	0.33	0/587	0.75	1/767 (0.1%)
All	All	0.43	3/156361 (0.0%)	1.18	1529/228899 (0.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	B	0	1
17	N	0	1
20	Q	0	1
35	m	0	1
36	n	0	1
42	J	0	1
46	4	0	1
All	All	0	7

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	2	1929	A	N9-C4	5.71	1.41	1.37
44	2	1632	A	N9-C4	5.13	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	2	485	C	N1-C2	5.03	1.45	1.40

All (1529) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	2	485	C	C2-N1-C1'	14.98	135.28	118.80
44	2	495	C	N1-C2-O2	13.24	126.85	118.90
44	2	495	C	C2-N1-C1'	12.95	133.05	118.80
44	2	4502	C	N1-C2-O2	12.46	126.38	118.90
44	2	753	C	N1-C2-O2	12.38	126.33	118.90
44	2	485	C	N1-C2-O2	12.32	126.30	118.90
44	2	4502	C	N3-C2-O2	-11.68	113.72	121.90
44	2	467	U	N1-C2-O2	11.63	130.94	122.80
44	2	1216	C	N1-C2-O2	11.38	125.73	118.90
44	2	4926	C	N1-C2-O2	11.37	125.72	118.90
44	2	467	U	N3-C2-O2	-11.31	114.28	122.20
44	2	1994	C	C2-N1-C1'	11.23	131.16	118.80
44	2	495	C	N3-C2-O2	-11.17	114.08	121.90
44	2	100	C	N1-C2-O2	11.10	125.56	118.90
44	2	753	C	N3-C2-O2	-11.07	114.15	121.90
44	2	1703	C	N1-C2-O2	11.06	125.53	118.90
4	8	128	C	N1-C2-O2	11.04	125.52	118.90
44	2	467	U	C2-N1-C1'	10.98	130.88	117.70
4	8	128	C	C6-N1-C2	-10.82	115.97	120.30
44	2	3587	C	N1-C2-O2	10.81	125.39	118.90
44	2	753	C	C6-N1-C2	-10.76	116.00	120.30
8	D	171	LEU	CA-CB-CG	10.76	140.04	115.30
44	2	1921	C	N1-C2-O2	10.71	125.33	118.90
44	2	100	C	C2-N1-C1'	10.64	130.50	118.80
44	2	1216	C	C2-N1-C1'	10.61	130.47	118.80
44	2	77	U	N3-C2-O2	-10.59	114.78	122.20
44	2	1325	C	N1-C2-O2	10.57	125.25	118.90
44	2	485	C	C6-N1-C2	-10.51	116.09	120.30
44	2	516	C	N1-C2-O2	10.48	125.19	118.90
44	2	2025	A	C2-N3-C4	10.48	115.84	110.60
46	4	230	LEU	CA-CB-CG	10.45	139.34	115.30
44	2	1325	C	C2-N1-C1'	10.43	130.28	118.80
4	8	128	C	C5-C6-N1	10.39	126.20	121.00
44	2	4502	C	C6-N1-C2	-10.36	116.16	120.30
44	2	2820	C	N1-C2-O2	10.35	125.11	118.90
44	2	495	C	C6-N1-C2	-10.29	116.18	120.30
44	2	1994	C	N1-C2-O2	10.25	125.05	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	2	4926	C	C2-N1-C1'	10.25	130.08	118.80
44	2	485	C	C6-N1-C1'	-10.23	108.52	120.80
44	2	1856	C	N1-C2-O2	10.23	125.04	118.90
44	2	4613	C	N1-C2-O2	10.22	125.03	118.90
44	2	100	C	N3-C2-O2	-10.17	114.78	121.90
44	2	2860	C	N1-C2-O2	10.11	124.97	118.90
44	2	753	C	C2-N1-C1'	9.96	129.76	118.80
44	2	4453	C	N1-C2-O2	9.91	124.84	118.90
8	D	319	LEU	CA-CB-CG	9.90	138.08	115.30
44	2	516	C	N3-C2-O2	-9.90	114.97	121.90
44	2	485	C	C5-C6-N1	9.84	125.92	121.00
44	2	1325	C	N3-C2-O2	-9.83	115.02	121.90
44	2	4758	U	N3-C2-O2	-9.83	115.32	122.20
44	2	4887	C	N1-C2-O2	9.80	124.78	118.90
44	2	4229	U	N3-C2-O2	-9.77	115.36	122.20
44	2	4758	U	N1-C2-O2	9.76	129.63	122.80
44	2	4476	C	C2-N1-C1'	9.74	129.51	118.80
44	2	4476	C	N1-C2-O2	9.68	124.71	118.90
44	2	4682	U	N3-C2-O2	-9.57	115.50	122.20
4	8	128	C	C2-N1-C1'	9.56	129.31	118.80
44	2	1971	C	C6-N1-C2	-9.51	116.50	120.30
44	2	4709	U	N3-C2-O2	-9.49	115.56	122.20
44	2	1325	C	C6-N1-C2	-9.45	116.52	120.30
44	2	1971	C	C2-N1-C1'	9.45	129.19	118.80
44	2	4608	G	C8-N9-C4	-9.45	102.62	106.40
44	2	2627	C	C6-N1-C2	-9.43	116.53	120.30
12	H	23	ASP	CB-CG-OD2	9.41	126.77	118.30
44	2	4608	G	N7-C8-N9	9.40	117.80	113.10
44	2	2860	C	C6-N1-C2	-9.39	116.54	120.30
44	2	4758	U	C2-N1-C1'	9.39	128.97	117.70
44	2	1703	C	C2-N1-C1'	9.33	129.06	118.80
44	2	4682	U	N1-C2-O2	9.31	129.32	122.80
44	2	3636	C	C6-N1-C2	-9.28	116.59	120.30
6	B	360	LEU	CA-CB-CG	9.25	136.58	115.30
44	2	96	U	N3-C2-O2	-9.22	115.74	122.20
44	2	4926	C	N3-C2-O2	-9.21	115.45	121.90
44	2	4709	U	N1-C2-O2	9.19	129.23	122.80
43	T	64	ASP	CB-CG-OD2	9.18	126.56	118.30
44	2	1458	C	N1-C2-O2	9.18	124.41	118.90
44	2	4505	C	C6-N1-C2	-9.18	116.63	120.30
44	2	1921	C	C6-N1-C2	-9.18	116.63	120.30
44	2	2262	G	C4-N9-C1'	9.15	138.39	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	2	1216	C	N3-C2-O2	-9.13	115.51	121.90
44	2	2016	C	C6-N1-C2	-9.11	116.65	120.30
37	o	202	ASP	CB-CG-OD1	9.09	126.48	118.30
44	2	4471	U	N3-C2-O2	-9.08	115.84	122.20
44	2	220	C	N1-C2-O2	9.05	124.33	118.90
44	2	77	U	N1-C2-O2	8.97	129.08	122.80
44	2	1183	C	N1-C2-O2	8.96	124.28	118.90
44	2	1921	C	N3-C2-O2	-8.95	115.64	121.90
44	2	1241	C	N1-C2-O2	8.94	124.27	118.90
44	2	4453	C	C2-N1-C1'	8.93	128.62	118.80
44	2	495	C	C6-N1-C1'	-8.90	110.12	120.80
44	2	2026	A	O4'-C1'-N9	8.89	115.32	108.20
44	2	2410	C	C6-N1-C2	-8.88	116.75	120.30
44	2	4613	C	N3-C2-O2	-8.80	115.74	121.90
4	8	128	C	N3-C2-O2	-8.79	115.75	121.90
44	2	4502	C	C2-N1-C1'	8.79	128.47	118.80
44	2	2262	G	N3-C4-N9	8.78	131.27	126.00
44	2	4612	C	N1-C2-O2	8.77	124.16	118.90
44	2	1414	C	C6-N1-C2	-8.77	116.79	120.30
44	2	2016	C	C5-C6-N1	8.76	125.38	121.00
44	2	3587	C	N3-C2-O2	-8.76	115.77	121.90
44	2	1191	C	N3-C2-O2	-8.74	115.78	121.90
44	2	1994	C	N3-C2-O2	-8.72	115.79	121.90
44	2	1703	C	N3-C2-O2	-8.71	115.80	121.90
33	i	103	ASP	CB-CG-OD2	8.70	126.13	118.30
44	2	3587	C	C6-N1-C2	-8.70	116.82	120.30
44	2	657	C	N1-C2-O2	8.68	124.11	118.90
44	2	2262	G	N3-C4-C5	-8.68	124.26	128.60
44	2	4504	C	N1-C2-O2	8.67	124.10	118.90
44	2	1889	U	N1-C2-O2	8.66	128.86	122.80
44	2	485	C	N3-C2-O2	-8.63	115.86	121.90
4	8	64	U	N3-C2-O2	-8.62	116.17	122.20
44	2	4360	U	N3-C2-O2	-8.59	116.19	122.20
44	2	1889	U	N3-C2-O2	-8.59	116.19	122.20
44	2	1929	A	C2-N3-C4	8.55	114.88	110.60
44	2	1340	C	C5-C6-N1	8.55	125.27	121.00
44	2	115	C	C2-N1-C1'	8.53	128.19	118.80
44	2	498	C	N1-C2-O2	8.53	124.02	118.90
44	2	115	C	N1-C2-O2	8.51	124.01	118.90
44	2	4505	C	C2-N1-C1'	8.51	128.16	118.80
44	2	1726	U	N3-C2-O2	-8.50	116.25	122.20
44	2	4314	C	N1-C2-O2	8.50	124.00	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	2	2860	C	N3-C2-O2	-8.49	115.96	121.90
46	4	407	ASP	CB-CG-OD1	8.47	125.93	118.30
44	2	1320	U	N3-C2-O2	-8.47	116.27	122.20
44	2	112	C	C6-N1-C2	-8.45	116.92	120.30
44	2	4293	U	N3-C2-O2	-8.44	116.29	122.20
44	2	1856	C	N3-C2-O2	-8.44	115.99	121.90
44	2	1607	C	N1-C2-O2	8.43	123.96	118.90
44	2	4215	C	N1-C2-O2	8.41	123.95	118.90
44	2	112	C	C2-N1-C1'	8.40	128.04	118.80
44	2	2820	C	N3-C2-O2	-8.39	116.02	121.90
44	2	1320	U	N1-C2-O2	8.39	128.67	122.80
44	2	1216	C	C6-N1-C2	-8.39	116.95	120.30
44	2	1702	C	N1-C2-O2	8.36	123.92	118.90
44	2	4171	C	N1-C2-O2	8.36	123.92	118.90
44	2	1340	C	C6-N1-C2	-8.35	116.96	120.30
44	2	1191	C	N1-C2-O2	8.33	123.90	118.90
44	2	2710	C	N1-C2-O2	8.32	123.89	118.90
44	2	4505	C	N1-C2-O2	8.31	123.88	118.90
44	2	1079	C	N1-C2-O2	8.28	123.87	118.90
44	2	4880	C	N1-C2-O2	8.27	123.86	118.90
44	2	2410	C	C5-C6-N1	8.27	125.13	121.00
44	2	656	C	N1-C2-O2	8.26	123.85	118.90
44	2	2627	C	C5-C6-N1	8.26	125.13	121.00
44	2	1176	C	N1-C2-O2	8.25	123.85	118.90
2	6	177	LEU	CA-CB-CG	8.22	134.21	115.30
44	2	516	C	C6-N1-C2	-8.21	117.02	120.30
44	2	1632	A	C2-N3-C4	8.20	114.70	110.60
44	2	4887	C	N3-C2-O2	-8.20	116.16	121.90
44	2	1856	C	C6-N1-C2	-8.19	117.02	120.30
44	2	4229	U	N1-C2-O2	8.19	128.53	122.80
44	2	1731	C	C6-N1-C2	-8.18	117.03	120.30
44	2	4243	C	C6-N1-C2	-8.18	117.03	120.30
44	2	498	C	C6-N1-C2	-8.18	117.03	120.30
44	2	2710	C	C2-N1-C1'	8.18	127.80	118.80
44	2	2351	C	C6-N1-C2	-8.18	117.03	120.30
44	2	1607	C	N3-C2-O2	-8.17	116.18	121.90
44	2	1241	C	C2-N1-C1'	8.16	127.78	118.80
44	2	100	C	C6-N1-C2	-8.16	117.04	120.30
44	2	1655	C	N1-C2-O2	8.13	123.78	118.90
44	2	972	C	N1-C2-O2	8.13	123.78	118.90
44	2	1445	U	N1-C2-O2	8.11	128.48	122.80
44	2	2362	U	N3-C2-O2	-8.11	116.52	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	2	489	C	C6-N1-C2	-8.10	117.06	120.30
44	2	494	U	N3-C2-O2	-8.10	116.53	122.20
44	2	2009	A	N1-C6-N6	-8.10	113.74	118.60
44	2	1971	C	C5-C6-N1	8.09	125.05	121.00
44	2	2563	C	N1-C2-O2	8.08	123.75	118.90
44	2	1445	U	N3-C2-O2	-8.07	116.55	122.20
44	2	4972	U	N3-C2-O2	-8.06	116.56	122.20
44	2	175	C	C6-N1-C2	-8.03	117.09	120.30
44	2	4747	C	C2-N1-C1'	8.03	127.63	118.80
44	2	2528	G	C4-N9-C1'	8.03	136.94	126.50
44	2	4505	C	C5-C6-N1	8.02	125.01	121.00
44	2	175	C	N3-C2-O2	-7.99	116.31	121.90
44	2	3587	C	C2-N1-C1'	7.99	127.59	118.80
44	2	2410	C	C2-N1-C1'	7.99	127.59	118.80
1	5	28	C	C6-N1-C2	-7.97	117.11	120.30
44	2	1702	C	C2-N1-C1'	7.96	127.56	118.80
44	2	4476	C	N3-C2-O2	-7.96	116.33	121.90
44	2	4766	C	C6-N1-C2	-7.95	117.12	120.30
44	2	242	U	N3-C2-O2	-7.93	116.65	122.20
44	2	2627	C	C2-N1-C1'	7.93	127.52	118.80
44	2	4747	C	C6-N1-C2	-7.93	117.13	120.30
44	2	1254	A	C2-N3-C4	7.89	114.54	110.60
44	2	4293	U	N1-C2-O2	7.87	128.31	122.80
44	2	1405	C	N1-C2-O2	7.86	123.62	118.90
44	2	2589	C	C6-N1-C2	-7.86	117.16	120.30
44	2	322	C	N1-C2-O2	7.86	123.61	118.90
44	2	489	C	C2-N1-C1'	7.85	127.44	118.80
44	2	50	C	N1-C2-O2	7.85	123.61	118.90
44	2	4471	U	N1-C2-O2	7.84	128.29	122.80
44	2	3926	C	N1-C2-O2	7.84	123.60	118.90
44	2	4453	C	N3-C2-O2	-7.82	116.42	121.90
44	2	4674	C	C6-N1-C2	-7.82	117.17	120.30
44	2	1402	C	N1-C2-O2	7.81	123.58	118.90
13	I	176	LEU	CA-CB-CG	7.79	133.23	115.30
44	2	1414	C	C5-C6-N1	7.79	124.89	121.00
44	2	2760	G	P-O3'-C3'	7.79	129.05	119.70
44	2	494	U	N1-C2-O2	7.79	128.25	122.80
44	2	656	C	C6-N1-C2	-7.77	117.19	120.30
44	2	2410	C	N1-C2-O2	7.77	123.56	118.90
44	2	914	U	P-O3'-C3'	7.75	129.00	119.70
44	2	515	C	C6-N1-C2	-7.74	117.20	120.30
1	5	76	U	N3-C2-O2	-7.72	116.80	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	2	4864	U	N3-C2-O2	-7.71	116.80	122.20
44	2	1971	C	N1-C2-O2	7.71	123.53	118.90
44	2	1320	U	C2-N1-C1'	7.71	126.95	117.70
44	2	50	C	C6-N1-C2	-7.70	117.22	120.30
44	2	1726	U	N1-C2-O2	7.70	128.19	122.80
44	2	972	C	C6-N1-C2	-7.68	117.23	120.30
44	2	1994	C	C6-N1-C1'	-7.68	111.59	120.80
44	2	2262	G	C8-N9-C1'	-7.67	117.03	127.00
44	2	195	C	C6-N1-C2	-7.66	117.23	120.30
44	2	4360	U	N1-C2-O2	7.66	128.16	122.80
44	2	1079	C	C6-N1-C2	-7.63	117.25	120.30
44	2	2072	C	C6-N1-C2	-7.63	117.25	120.30
44	2	1994	C	C6-N1-C2	-7.61	117.26	120.30
44	2	4864	U	N1-C2-O2	7.61	128.13	122.80
44	2	4613	C	C6-N1-C2	-7.61	117.26	120.30
44	2	1472	C	C6-N1-C2	-7.61	117.26	120.30
44	2	1458	C	N3-C2-O2	-7.59	116.58	121.90
44	2	1921	C	C2-N1-C1'	7.58	127.14	118.80
44	2	4662	C	C6-N1-C2	-7.58	117.27	120.30
44	2	3657	U	N3-C2-O2	-7.57	116.90	122.20
4	8	51	U	N1-C2-O2	7.56	128.09	122.80
44	2	1822	U	N3-C2-O2	-7.54	116.92	122.20
4	8	28	C	C6-N1-C2	-7.54	117.28	120.30
44	2	1655	C	C6-N1-C2	-7.52	117.29	120.30
44	2	4969	C	C6-N1-C2	-7.51	117.29	120.30
44	2	1655	C	N3-C2-O2	-7.51	116.64	121.90
44	2	1816	C	C6-N1-C2	-7.51	117.30	120.30
44	2	3637	U	N3-C2-O2	-7.51	116.94	122.20
36	n	105	LEU	C-N-CA	7.51	140.47	121.70
44	2	2033	A	P-O3'-C3'	7.51	128.71	119.70
44	2	3636	C	N3-C2-O2	-7.51	116.64	121.90
22	U	147	ASP	CB-CG-OD2	7.50	125.05	118.30
1	5	28	C	N1-C2-O2	7.50	123.40	118.90
44	2	1980	U	P-O3'-C3'	7.49	128.69	119.70
44	2	2026	A	C2-N3-C4	7.48	114.34	110.60
44	2	2026	A	N1-C6-N6	-7.48	114.11	118.60
44	2	2022	C	N1-C2-O2	7.46	123.37	118.90
44	2	4747	C	N1-C2-O2	7.45	123.37	118.90
1	5	76	U	N1-C2-O2	7.44	128.01	122.80
44	2	96	U	N1-C2-O2	7.44	128.01	122.80
4	8	51	U	N3-C2-O2	-7.43	117.00	122.20
44	2	3615	G	N3-C4-N9	7.43	130.46	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	2	5035	U	N3-C2-O2	-7.42	117.01	122.20
44	2	3636	C	N1-C2-O2	7.41	123.34	118.90
44	2	4775	C	C2-N1-C1'	7.40	126.94	118.80
44	2	1731	C	C5-C6-N1	7.40	124.70	121.00
44	2	2281	U	N1-C2-O2	7.40	127.98	122.80
22	U	146	PRO	C-N-CA	7.39	140.17	121.70
44	2	112	C	N1-C2-O2	7.38	123.33	118.90
44	2	4171	C	C6-N1-C2	-7.38	117.35	120.30
44	2	907	C	C6-N1-C2	-7.37	117.35	120.30
44	2	3631	U	N3-C2-O2	-7.37	117.04	122.20
44	2	1395	U	N3-C2-O2	-7.37	117.04	122.20
44	2	4773	C	C6-N1-C2	-7.37	117.35	120.30
44	2	1183	C	C6-N1-C2	-7.36	117.36	120.30
44	2	2814	C	N1-C2-O2	7.36	123.32	118.90
44	2	1915	C	N3-C2-O2	-7.36	116.75	121.90
44	2	4395	U	N1-C2-O2	7.35	127.95	122.80
44	2	1183	C	N3-C2-O2	-7.35	116.75	121.90
44	2	1790	U	N1-C2-O2	7.35	127.94	122.80
44	2	220	C	C6-N1-C2	-7.34	117.36	120.30
44	2	2008	U	C2-N1-C1'	7.33	126.50	117.70
44	2	174	C	N1-C2-O2	7.33	123.30	118.90
44	2	1429	C	C6-N1-C2	-7.33	117.37	120.30
44	2	2860	C	C5-C6-N1	7.33	124.66	121.00
44	2	4887	C	C6-N1-C2	-7.33	117.37	120.30
44	2	4395	U	C2-N1-C1'	7.32	126.49	117.70
44	2	4928	C	C2-N1-C1'	7.32	126.85	118.80
44	2	2820	C	C6-N1-C2	-7.32	117.37	120.30
44	2	4340	U	N3-C2-O2	-7.32	117.08	122.20
44	2	115	C	N3-C2-O2	-7.31	116.78	121.90
4	8	101	C	C6-N1-C2	-7.31	117.38	120.30
44	2	1915	C	N1-C2-O2	7.30	123.28	118.90
44	2	1822	U	N1-C2-O2	7.30	127.91	122.80
44	2	1241	C	N3-C2-O2	-7.28	116.80	121.90
44	2	2802	C	C6-N1-C2	-7.27	117.39	120.30
44	2	498	C	N3-C2-O2	-7.26	116.82	121.90
44	2	1079	C	C5-C6-N1	7.25	124.63	121.00
44	2	2837	U	N3-C2-O2	-7.25	117.12	122.20
44	2	1676	C	OP2-P-O3'	7.24	121.14	105.20
44	2	4395	U	N3-C2-O2	-7.23	117.14	122.20
1	5	24	C	N1-C2-O2	7.23	123.24	118.90
44	2	1216	C	C5-C6-N1	7.23	124.62	121.00
44	2	2783	A	N1-C2-N3	-7.23	125.69	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	2	4314	C	N3-C2-O2	-7.22	116.85	121.90
44	2	4926	C	C6-N1-C2	-7.21	117.42	120.30
44	2	2528	G	N3-C4-C5	-7.20	125.00	128.60
1	5	24	C	C6-N1-C2	-7.20	117.42	120.30
44	2	2729	C	C6-N1-C2	-7.20	117.42	120.30
44	2	3622	C	N1-C2-O2	7.20	123.22	118.90
44	2	4303	C	C2-N1-C1'	7.20	126.72	118.80
44	2	2362	U	N1-C2-O2	7.19	127.84	122.80
44	2	495	C	C5-C6-N1	7.19	124.60	121.00
44	2	1921	C	C5-C6-N1	7.19	124.59	121.00
44	2	4341	C	N1-C2-O2	7.18	123.21	118.90
44	2	4162	C	N1-C2-O2	7.17	123.20	118.90
44	2	1079	C	C2-N1-C1'	7.17	126.69	118.80
44	2	4747	C	C5-C6-N1	7.16	124.58	121.00
4	8	118	C	C6-N1-C2	-7.16	117.44	120.30
44	2	4612	C	C6-N1-C2	-7.16	117.44	120.30
1	5	39	C	N1-C2-O2	7.16	123.19	118.90
44	2	2026	A	N9-C4-C5	7.15	108.66	105.80
44	2	4612	C	N3-C2-O2	-7.15	116.89	121.90
44	2	281	U	N3-C2-O2	-7.15	117.20	122.20
44	2	2856	C	N1-C2-O2	7.15	123.19	118.90
44	2	1176	C	C6-N1-C2	-7.14	117.44	120.30
44	2	1402	C	N3-C2-O2	-7.14	116.90	121.90
44	2	294	G	N3-C4-N9	7.13	130.28	126.00
44	2	4133	C	C6-N1-C2	-7.13	117.45	120.30
44	2	4537	C	N1-C2-O2	7.13	123.18	118.90
4	8	32	C	N1-C2-O2	7.13	123.18	118.90
44	2	4206	C	C6-N1-C2	-7.12	117.45	120.30
44	2	68	U	N3-C2-O2	-7.12	117.22	122.20
44	2	4352	U	N3-C2-O2	-7.12	117.22	122.20
44	2	4887	C	C2-N1-C1'	7.11	126.62	118.80
44	2	1405	C	C6-N1-C2	-7.09	117.46	120.30
44	2	1097	C	C5-C6-N1	7.09	124.54	121.00
44	2	4709	U	C2-N1-C1'	7.09	126.20	117.70
44	2	753	C	C5-C6-N1	7.08	124.54	121.00
44	2	4504	C	N3-C2-O2	-7.08	116.95	121.90
44	2	472	C	C6-N1-C2	-7.07	117.47	120.30
44	2	322	C	C6-N1-C2	-7.06	117.48	120.30
44	2	455	C	C6-N1-C2	-7.05	117.48	120.30
44	2	4627	U	N3-C2-O2	-7.05	117.26	122.20
44	2	2417	A	O4'-C1'-N9	7.05	113.84	108.20
44	2	4340	U	N1-C2-O2	7.04	127.73	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	2	1243	C	C6-N1-C2	-7.04	117.48	120.30
44	2	1671	U	N3-C2-O2	-7.04	117.27	122.20
44	2	4481	U	N3-C2-O2	-7.04	117.27	122.20
4	8	150	C	N1-C2-O2	7.04	123.12	118.90
44	2	3739	C	C6-N1-C2	-7.04	117.48	120.30
44	2	1367	C	C2-N1-C1'	7.04	126.54	118.80
44	2	2528	G	N3-C4-N9	7.03	130.22	126.00
44	2	220	C	N3-C2-O2	-7.03	116.98	121.90
44	2	925	C	C6-N1-C2	-7.03	117.49	120.30
44	2	1607	C	C6-N1-C2	-7.03	117.49	120.30
44	2	3702	A	C2-N3-C4	7.03	114.11	110.60
44	2	4972	U	N1-C2-O2	7.03	127.72	122.80
44	2	1097	C	C6-N1-C2	-7.02	117.49	120.30
44	2	274	C	C6-N1-C2	-7.02	117.49	120.30
44	2	4880	C	N3-C2-O2	-7.02	116.99	121.90
44	2	67	C	C6-N1-C2	-7.02	117.49	120.30
36	n	5	LEU	CA-CB-CG	7.02	131.44	115.30
44	2	4215	C	N3-C2-O2	-7.02	116.99	121.90
44	2	489	C	N1-C2-O2	7.01	123.11	118.90
44	2	282	C	N1-C2-O2	7.01	123.11	118.90
44	2	467	U	C6-N1-C1'	-7.00	111.40	121.20
44	2	489	C	C5-C6-N1	7.00	124.50	121.00
44	2	972	C	N3-C2-O2	-7.00	117.00	121.90
4	8	54	C	C6-N1-C2	-6.99	117.50	120.30
44	2	2532	C	C6-N1-C2	-6.99	117.50	120.30
44	2	100	C	C6-N1-C1'	-6.99	112.42	120.80
44	2	2281	U	N3-C2-O2	-6.97	117.32	122.20
44	2	4926	C	C6-N1-C1'	-6.97	112.44	120.80
44	2	1906	U	N3-C2-O2	-6.96	117.33	122.20
44	2	3615	G	C4-N9-C1'	6.96	135.54	126.50
44	2	4171	C	N3-C2-O2	-6.96	117.03	121.90
44	2	719	C	C6-N1-C2	-6.95	117.52	120.30
44	2	1790	U	N3-C2-O2	-6.95	117.33	122.20
44	2	656	C	N3-C2-O2	-6.94	117.04	121.90
44	2	1702	C	N3-C2-O2	-6.94	117.05	121.90
44	2	2710	C	N3-C2-O2	-6.94	117.05	121.90
44	2	3905	A	P-O3'-C3'	6.93	128.02	119.70
44	2	2351	C	C2-N1-C1'	6.93	126.42	118.80
44	2	4342	C	C6-N1-C2	-6.93	117.53	120.30
44	2	2464	C	O4'-C1'-N1	6.92	113.74	108.20
44	2	2627	C	N1-C2-O2	6.92	123.05	118.90
44	2	1628	C	C6-N1-C2	-6.92	117.53	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	2	1414	C	C2-N1-C1'	6.91	126.40	118.80
44	2	2615	C	N1-C2-O2	6.91	123.04	118.90
4	8	64	U	N1-C2-O2	6.90	127.63	122.80
1	5	14	C	C6-N1-C2	-6.90	117.54	120.30
44	2	3650	C	C6-N1-C2	-6.89	117.54	120.30
44	2	449	C	N1-C2-O2	6.89	123.03	118.90
44	2	4913	G	P-O3'-C3'	6.88	127.96	119.70
44	2	907	C	C2-N1-C1'	6.88	126.37	118.80
44	2	1731	C	N1-C2-O2	6.88	123.03	118.90
4	8	35	C	C6-N1-C2	-6.88	117.55	120.30
44	2	2892	C	C2-N1-C1'	6.88	126.36	118.80
44	2	985	C	C6-N1-C2	-6.87	117.55	120.30
44	2	1216	C	C6-N1-C1'	-6.87	112.55	120.80
44	2	4601	U	N1-C2-O2	6.87	127.61	122.80
44	2	1703	C	C6-N1-C2	-6.87	117.55	120.30
44	2	1401	C	C6-N1-C2	-6.86	117.56	120.30
17	N	171	ASP	CB-CG-OD1	6.86	124.47	118.30
44	2	406	C	P-O3'-C3'	6.85	127.92	119.70
44	2	1958	A	C2-N3-C4	6.85	114.03	110.60
44	2	4895	C	N1-C2-O2	6.85	123.01	118.90
44	2	1386	C	C6-N1-C2	-6.85	117.56	120.30
44	2	2015	U	P-O3'-C3'	6.84	127.91	119.70
44	2	2351	C	C5-C6-N1	6.84	124.42	121.00
44	2	472	C	N1-C2-O2	6.83	123.00	118.90
44	2	2337	C	C6-N1-C2	-6.83	117.57	120.30
44	2	3587	C	C5-C6-N1	6.83	124.41	121.00
44	2	4627	U	N1-C2-O2	6.82	127.57	122.80
44	2	4342	C	N1-C2-O2	6.82	122.99	118.90
44	2	4775	C	N1-C2-O2	6.82	122.99	118.90
44	2	1720	C	C6-N1-C2	-6.81	117.58	120.30
44	2	2791	C	C6-N1-C2	-6.80	117.58	120.30
44	2	1889	U	C2-N1-C1'	6.80	125.86	117.70
44	2	1378	C	C2-N1-C1'	6.79	126.27	118.80
44	2	2025	A	N1-C2-N3	-6.79	125.91	129.30
44	2	2592	U	N3-C2-O2	-6.79	117.45	122.20
44	2	2837	U	N1-C2-O2	6.79	127.55	122.80
44	2	4614	G	C5-C6-O6	6.78	132.67	128.60
44	2	242	U	N1-C2-O2	6.78	127.54	122.80
44	2	971	U	C2-N1-C1'	6.78	125.83	117.70
4	8	43	A	C2-N3-C4	6.77	113.99	110.60
44	2	657	C	N3-C2-O2	-6.77	117.16	121.90
44	2	4314	C	C6-N1-C2	-6.77	117.59	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	2	367	C	C6-N1-C2	-6.76	117.59	120.30
44	2	3840	U	N3-C2-O2	-6.76	117.47	122.20
44	2	4078	C	C6-N1-C2	-6.76	117.60	120.30
44	2	4601	U	N3-C2-O2	-6.76	117.47	122.20
44	2	963	G	C4-N9-C1'	6.75	135.28	126.50
44	2	4481	U	N1-C2-O2	6.75	127.53	122.80
44	2	50	C	N3-C2-O2	-6.74	117.18	121.90
44	2	3615	G	N3-C4-C5	-6.74	125.23	128.60
33	i	30	ASP	CB-CG-OD1	6.74	124.36	118.30
44	2	1663	C	C6-N1-C2	-6.74	117.61	120.30
44	2	4773	C	C2-N1-C1'	6.73	126.20	118.80
44	2	4766	C	C2-N1-C1'	6.73	126.20	118.80
44	2	2563	C	N3-C2-O2	-6.72	117.20	121.90
4	8	32	C	C6-N1-C2	-6.72	117.61	120.30
44	2	112	C	C5-C6-N1	6.71	124.36	121.00
44	2	281	U	N1-C2-O2	6.71	127.49	122.80
44	2	2031	C	N1-C2-O2	6.71	122.92	118.90
24	W	33	LEU	CA-CB-CG	6.70	130.71	115.30
44	2	4766	C	C5-C6-N1	6.70	124.35	121.00
44	2	2845	A	C2-N3-C4	6.70	113.95	110.60
44	2	4764	A	N1-C2-N3	-6.69	125.95	129.30
44	2	1656	U	N3-C2-O2	-6.69	117.52	122.20
44	2	1906	U	N1-C2-O2	6.68	127.48	122.80
44	2	2008	U	N1-C2-O2	6.68	127.48	122.80
44	2	4476	C	C6-N1-C1'	-6.68	112.78	120.80
44	2	4712	C	C6-N1-C2	-6.68	117.63	120.30
44	2	365	U	N3-C2-O2	-6.67	117.53	122.20
44	2	4361	U	N3-C2-O2	-6.66	117.54	122.20
44	2	4522	G	C4-N9-C1'	6.66	135.16	126.50
44	2	2860	C	C2-N1-C1'	6.65	126.12	118.80
44	2	4308	C	N1-C2-O2	6.65	122.89	118.90
44	2	3866	C	C6-N1-C2	-6.64	117.64	120.30
44	2	4123	C	N1-C2-O2	6.64	122.89	118.90
44	2	4453	C	C6-N1-C1'	-6.64	112.83	120.80
44	2	1663	C	C5-C6-N1	6.63	124.32	121.00
44	2	1929	A	C4-N9-C1'	6.63	138.24	126.30
44	2	704	C	N1-C2-O2	6.63	122.88	118.90
44	2	3637	U	N1-C2-O2	6.63	127.44	122.80
44	2	1633	G	P-O3'-C3'	6.62	127.64	119.70
44	2	2533	C	C6-N1-C2	-6.62	117.65	120.30
44	2	3631	U	N1-C2-O2	6.62	127.43	122.80
44	2	1809	C	C6-N1-C2	-6.61	117.66	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	2	1676	C	P-O3'-C3'	6.61	127.63	119.70
44	2	4996	C	C6-N1-C2	-6.61	117.66	120.30
44	2	1469	C	C6-N1-C2	-6.61	117.66	120.30
44	2	4365	C	C6-N1-C2	-6.61	117.66	120.30
44	2	1197	C	C6-N1-C2	-6.60	117.66	120.30
1	5	78	C	C6-N1-C2	-6.59	117.66	120.30
44	2	1582	U	N3-C2-O2	-6.59	117.59	122.20
44	2	1472	C	C2-N1-C1'	6.58	126.04	118.80
44	2	4880	C	C6-N1-C2	-6.58	117.67	120.30
20	Q	144	LEU	CA-CB-CG	6.58	130.44	115.30
44	2	515	C	C5-C6-N1	6.58	124.29	121.00
44	2	2482	C	C6-N1-C2	-6.58	117.67	120.30
44	2	4708	A	C2-N3-C4	6.57	113.89	110.60
44	2	1197	C	N1-C2-O2	6.57	122.84	118.90
44	2	2528	G	C8-N9-C1'	-6.56	118.47	127.00
44	2	1096	C	C6-N1-C2	-6.56	117.68	120.30
44	2	4714	C	N1-C2-O2	6.56	122.83	118.90
44	2	673	C	C6-N1-C2	-6.55	117.68	120.30
44	2	4773	C	N1-C2-O2	6.54	122.82	118.90
44	2	1816	C	C2-N1-C1'	6.53	125.98	118.80
4	8	150	C	C6-N1-C2	-6.51	117.69	120.30
44	2	365	U	N1-C2-O2	6.51	127.36	122.80
44	2	1445	U	C2-N1-C1'	6.50	125.50	117.70
4	8	54	C	N1-C2-O2	6.50	122.80	118.90
47	d	43	LEU	CA-CB-CG	6.50	130.24	115.30
44	2	4476	C	C6-N1-C2	-6.49	117.70	120.30
44	2	1662	C	C6-N1-C2	-6.49	117.70	120.30
44	2	322	C	N3-C2-O2	-6.49	117.36	121.90
44	2	1735	U	N3-C2-O2	-6.48	117.66	122.20
44	2	2892	C	C6-N1-C2	-6.48	117.71	120.30
44	2	282	C	N3-C2-O2	-6.47	117.37	121.90
44	2	1477	C	C6-N1-C2	-6.47	117.71	120.30
44	2	1325	C	O4'-C1'-N1	6.47	113.38	108.20
44	2	228	C	C6-N1-C2	-6.46	117.71	120.30
44	2	1405	C	N3-C2-O2	-6.46	117.38	121.90
44	2	220	C	C5-C6-N1	6.45	124.23	121.00
44	2	1176	C	C5-C6-N1	6.45	124.22	121.00
44	2	1401	C	N1-C2-O2	6.45	122.77	118.90
44	2	1472	C	C5-C6-N1	6.45	124.23	121.00
44	2	1592	G	C4-N9-C1'	6.45	134.88	126.50
44	2	1176	C	N3-C2-O2	-6.43	117.40	121.90
44	2	1428	U	N3-C2-O2	-6.43	117.70	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	2	2856	C	C6-N1-C2	-6.43	117.73	120.30
44	2	4773	C	C5-C6-N1	6.43	124.21	121.00
44	2	9	C	C6-N1-C2	-6.42	117.73	120.30
44	2	472	C	C2-N1-C1'	6.42	125.86	118.80
1	5	29	C	N1-C2-O2	6.42	122.75	118.90
44	2	28	C	C6-N1-C2	-6.41	117.73	120.30
44	2	4387	C	N1-C2-O2	6.41	122.75	118.90
44	2	2589	C	C5-C6-N1	6.41	124.21	121.00
44	2	3893	C	C6-N1-C2	-6.41	117.74	120.30
44	2	4308	C	C6-N1-C2	-6.41	117.74	120.30
44	2	155	C	N1-C2-O2	6.40	122.74	118.90
1	5	102	U	N3-C2-O2	-6.40	117.72	122.20
44	2	2814	C	C2-N1-C1'	6.40	125.84	118.80
44	2	1816	C	C5-C6-N1	6.40	124.20	121.00
44	2	1325	C	C5-C6-N1	6.40	124.20	121.00
44	2	4928	C	N1-C2-O2	6.40	122.74	118.90
44	2	2260	C	C2-N1-C1'	6.40	125.84	118.80
44	2	4133	C	C2-N1-C1'	6.39	125.83	118.80
44	2	209	U	N1-C2-O2	6.39	127.27	122.80
35	m	246	LEU	CA-CB-CG	6.38	129.99	115.30
44	2	1325	C	C6-N1-C1'	-6.38	113.14	120.80
44	2	220	C	C2-N1-C1'	6.38	125.82	118.80
44	2	1666	C	C6-N1-C2	-6.38	117.75	120.30
44	2	4945	G	N3-C4-N9	6.38	129.83	126.00
4	8	111	U	C2-N1-C1'	6.37	125.35	117.70
44	2	4700	A	C2-N3-C4	6.37	113.78	110.60
44	2	1809	C	C2-N1-C1'	6.36	125.80	118.80
44	2	5008	C	C6-N1-C2	-6.36	117.75	120.30
31	g	145	ASP	CB-CG-OD2	6.36	124.03	118.30
44	2	3693	U	N3-C2-O2	-6.36	117.75	122.20
44	2	86	U	N3-C2-O2	-6.36	117.75	122.20
44	2	515	C	N1-C2-O2	6.36	122.71	118.90
44	2	1856	C	C2-N1-C1'	6.36	125.79	118.80
4	8	103	A	N1-C2-N3	-6.35	126.12	129.30
44	2	1856	C	C5-C6-N1	6.35	124.17	121.00
44	2	4133	C	C5-C6-N1	6.35	124.17	121.00
1	5	28	C	N3-C2-O2	-6.34	117.46	121.90
44	2	985	C	C2-N1-C1'	6.34	125.78	118.80
44	2	1672	U	N3-C2-O2	-6.34	117.76	122.20
44	2	2031	C	C6-N1-C2	-6.34	117.76	120.30
44	2	4352	U	N1-C2-O2	6.34	127.24	122.80
44	2	3622	C	C6-N1-C2	-6.34	117.76	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	2	2371	U	N3-C2-O2	-6.33	117.77	122.20
44	2	2563	C	C6-N1-C2	-6.33	117.77	120.30
44	2	36	U	N3-C2-O2	-6.33	117.77	122.20
44	2	3882	C	C6-N1-C2	-6.33	117.77	120.30
44	2	294	G	N3-C4-C5	-6.33	125.44	128.60
44	2	2892	C	N1-C2-O2	6.33	122.69	118.90
44	2	1671	U	N1-C2-O2	6.32	127.22	122.80
44	2	1367	C	N1-C2-O2	6.32	122.69	118.90
1	5	44	C	N1-C2-O2	6.31	122.68	118.90
44	2	2867	C	C6-N1-C2	-6.30	117.78	120.30
44	2	4342	C	N3-C2-O2	-6.30	117.49	121.90
1	5	28	C	C5-C6-N1	6.30	124.15	121.00
44	2	4537	C	N3-C2-O2	-6.30	117.49	121.90
44	2	972	C	C5-C6-N1	6.30	124.15	121.00
44	2	3926	C	C6-N1-C2	-6.30	117.78	120.30
4	8	118	C	C5-C6-N1	6.29	124.15	121.00
44	2	4563	U	N3-C2-O2	-6.29	117.80	122.20
44	2	2362	U	C2-N1-C1'	6.28	125.24	117.70
44	2	2033	A	N1-C2-N3	-6.28	126.16	129.30
44	2	294	G	C4-N9-C1'	6.28	134.66	126.50
44	2	2022	C	N3-C2-O2	-6.27	117.51	121.90
44	2	4991	U	N3-C2-O2	-6.27	117.81	122.20
44	2	1822	U	C2-N1-C1'	6.27	125.22	117.70
44	2	4243	C	C5-C6-N1	6.27	124.13	121.00
44	2	694	C	N1-C2-O2	6.27	122.66	118.90
44	2	2019	C	C6-N1-C2	-6.26	117.80	120.30
44	2	4694	G	N3-C4-C5	-6.26	125.47	128.60
44	2	2281	U	C5-C6-N1	6.25	125.83	122.70
44	2	4674	C	C5-C6-N1	6.25	124.12	121.00
40	A	163	LEU	CA-CB-CG	6.25	129.67	115.30
44	2	2351	C	N1-C2-O2	6.25	122.65	118.90
44	2	2059	C	C6-N1-C2	-6.24	117.80	120.30
44	2	3926	C	N3-C2-O2	-6.24	117.53	121.90
44	2	1577	G	C2-N3-C4	6.24	115.02	111.90
44	2	44	A	C2-N3-C4	6.23	113.72	110.60
44	2	657	C	C6-N1-C2	-6.23	117.81	120.30
44	2	4215	C	C6-N1-C2	-6.23	117.81	120.30
44	2	2850	A	C2-N3-C4	6.23	113.72	110.60
44	2	4766	C	N1-C2-O2	6.23	122.64	118.90
44	2	498	C	C5-C6-N1	6.22	124.11	121.00
44	2	4341	C	C6-N1-C2	-6.22	117.81	120.30
44	2	4522	G	N3-C4-C5	-6.21	125.49	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	2	657	C	C2-N1-C1'	6.20	125.62	118.80
44	2	1197	C	C5-C6-N1	6.20	124.10	121.00
44	2	4504	C	C6-N1-C2	-6.20	117.82	120.30
44	2	2026	A	C5-C6-N1	6.19	120.80	117.70
44	2	3912	U	N3-C2-O2	-6.19	117.87	122.20
22	U	164	LEU	CA-CB-CG	6.18	129.52	115.30
44	2	1582	U	N1-C2-O2	6.18	127.13	122.80
44	2	1703	C	C6-N1-C1'	-6.18	113.39	120.80
44	2	4710	C	C6-N1-C2	-6.18	117.83	120.30
44	2	4714	C	C6-N1-C2	-6.18	117.83	120.30
44	2	4561	C	C6-N1-C2	-6.18	117.83	120.30
44	2	1538	U	N3-C2-O2	-6.17	117.88	122.20
44	2	2372	U	N3-C2-O2	-6.17	117.88	122.20
44	2	696	C	C6-N1-C2	-6.17	117.83	120.30
44	2	1315	C	C6-N1-C2	-6.17	117.83	120.30
44	2	4537	C	C6-N1-C2	-6.17	117.83	120.30
44	2	2094	G	C4-N9-C1'	6.16	134.51	126.50
1	5	57	C	C6-N1-C2	-6.16	117.84	120.30
44	2	4133	C	N1-C2-O2	6.16	122.59	118.90
1	5	67	C	C6-N1-C2	-6.16	117.84	120.30
4	8	101	C	C2-N1-C1'	6.16	125.57	118.80
44	2	906	C	C2-N1-C1'	6.16	125.57	118.80
44	2	1901	C	C6-N1-C2	-6.15	117.84	120.30
44	2	2802	C	C5-C6-N1	6.15	124.08	121.00
44	2	2019	C	N1-C2-O2	6.15	122.59	118.90
44	2	2337	C	N1-C2-O2	6.15	122.59	118.90
44	2	2482	C	C5-C6-N1	6.15	124.07	121.00
44	2	1176	C	C2-N1-C1'	6.15	125.56	118.80
44	2	2439	G	C4-N9-C1'	6.15	134.49	126.50
44	2	2615	C	N3-C2-O2	-6.15	117.60	121.90
44	2	2062	C	C6-N1-C2	-6.14	117.84	120.30
44	2	2872	C	C6-N1-C2	-6.14	117.84	120.30
4	8	28	C	C5-C6-N1	6.13	124.07	121.00
44	2	1809	C	N1-C2-O2	6.13	122.58	118.90
44	2	4303	C	N3-C2-O2	-6.13	117.61	121.90
44	2	262	G	N1-C6-O6	-6.13	116.22	119.90
44	2	2072	C	C5-C6-N1	6.13	124.06	121.00
44	2	1579	C	C6-N1-C2	-6.13	117.85	120.30
44	2	14	C	C6-N1-C2	-6.12	117.85	120.30
44	2	3606	U	N3-C2-O2	-6.12	117.92	122.20
44	2	4695	C	N1-C2-O2	6.12	122.57	118.90
44	2	1884	C	C6-N1-C2	-6.12	117.85	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	2	3615	G	C8-N9-C1'	-6.12	119.04	127.00
44	2	1832	C	N1-C2-O2	6.12	122.57	118.90
44	2	4403	U	N1-C2-O2	6.12	127.08	122.80
4	8	55	U	N3-C2-O2	-6.12	117.92	122.20
44	2	3693	U	N1-C2-O2	6.11	127.08	122.80
44	2	30	C	C6-N1-C2	-6.11	117.86	120.30
44	2	4393	G	C5-C6-O6	6.11	132.26	128.60
44	2	71	C	C6-N1-C2	-6.11	117.86	120.30
44	2	390	C	C6-N1-C2	-6.11	117.86	120.30
44	2	472	C	C5-C6-N1	6.11	124.05	121.00
44	2	1731	C	C2-N1-C1'	6.10	125.51	118.80
4	8	135	C	C6-N1-C2	-6.10	117.86	120.30
44	2	26	C	C6-N1-C2	-6.09	117.86	120.30
44	2	1656	U	N1-C2-O2	6.09	127.07	122.80
44	2	2281	U	C2-N1-C1'	6.09	125.01	117.70
44	2	2532	C	N1-C2-O2	6.09	122.56	118.90
44	2	1726	U	C2-N1-C1'	6.09	125.01	117.70
44	2	1958	A	N1-C2-N3	-6.08	126.26	129.30
44	2	2532	C	C5-C6-N1	6.08	124.04	121.00
44	2	4970	C	C6-N1-C2	-6.08	117.87	120.30
46	4	406	GLY	C-N-CA	6.08	136.91	121.70
44	2	924	C	C6-N1-C2	-6.08	117.87	120.30
44	2	385	A	N1-C2-N3	-6.08	126.26	129.30
44	2	4299	U	N3-C2-O2	-6.08	117.94	122.20
4	8	90	C	C6-N1-C2	-6.08	117.87	120.30
44	2	907	C	N1-C2-O2	6.07	122.54	118.90
44	2	4710	C	C5-C6-N1	6.06	124.03	121.00
1	5	43	U	N3-C2-O2	-6.06	117.96	122.20
44	2	907	C	C5-C6-N1	6.06	124.03	121.00
44	2	2260	C	N1-C2-O2	6.06	122.53	118.90
44	2	4709	U	C6-N1-C2	-6.06	117.36	121.00
44	2	672	C	N1-C2-O2	6.05	122.53	118.90
44	2	115	C	C6-N1-C2	-6.05	117.88	120.30
44	2	1450	C	C6-N1-C2	-6.05	117.88	120.30
44	2	289	C	C6-N1-C2	-6.04	117.88	120.30
44	2	2820	C	C2-N1-C1'	6.04	125.45	118.80
44	2	2856	C	N3-C2-O2	-6.04	117.67	121.90
44	2	1414	C	N1-C2-O2	6.04	122.52	118.90
44	2	4403	U	N3-C2-O2	-6.04	117.97	122.20
44	2	78	U	N3-C2-O2	-6.03	117.98	122.20
44	2	4293	U	C2-N1-C1'	6.03	124.94	117.70
44	2	4555	U	P-O3'-C3'	6.03	126.94	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	2	204	U	N3-C2-O2	-6.03	117.98	122.20
44	2	4639	G	N3-C4-C5	-6.03	125.58	128.60
44	2	5008	C	N1-C2-O2	6.03	122.52	118.90
1	5	24	C	N3-C2-O2	-6.03	117.68	121.90
44	2	2337	C	C5-C6-N1	6.03	124.01	121.00
44	2	3939	G	N3-C4-C5	-6.03	125.59	128.60
44	2	4341	C	N3-C2-O2	-6.02	117.68	121.90
44	2	1893	C	C6-N1-C2	-6.02	117.89	120.30
44	2	3739	C	C2-N1-C1'	6.02	125.42	118.80
44	2	155	C	N3-C2-O2	-6.02	117.69	121.90
44	2	494	U	C2-N1-C1'	6.02	124.92	117.70
44	2	1672	U	N1-C2-O2	6.02	127.01	122.80
44	2	1096	C	C5-C6-N1	6.02	124.01	121.00
44	2	1577	G	N3-C2-N2	-6.02	115.69	119.90
44	2	1735	U	N1-C2-O2	6.02	127.01	122.80
44	2	3670	C	N1-C2-O2	6.02	122.51	118.90
44	2	4088	C	C6-N1-C2	-6.02	117.89	120.30
44	2	2008	U	N3-C2-O2	-6.01	117.99	122.20
46	4	503	THR	C-N-CA	6.01	136.74	121.70
44	2	4758	U	C6-N1-C1'	-6.01	112.78	121.20
44	2	36	U	N1-C2-O2	6.01	127.01	122.80
4	8	32	C	N3-C2-O2	-6.00	117.70	121.90
44	2	4303	C	N1-C2-O2	6.00	122.50	118.90
44	2	209	U	N3-C2-O2	-6.00	118.00	122.20
44	2	656	C	C5-C6-N1	6.00	124.00	121.00
44	2	1293	G	N3-C4-C5	-6.00	125.60	128.60
44	2	4928	C	N3-C2-O2	-6.00	117.70	121.90
44	2	14	C	N3-C2-O2	-6.00	117.70	121.90
44	2	2853	C	N1-C2-O2	6.00	122.50	118.90
44	2	4171	C	C5-C6-N1	6.00	124.00	121.00
44	2	1915	C	C6-N1-C2	-5.99	117.90	120.30
44	2	4206	C	N1-C2-O2	5.99	122.50	118.90
46	4	230	LEU	CB-CG-CD1	5.99	121.18	111.00
44	2	688	U	N3-C2-O2	-5.99	118.01	122.20
1	5	24	C	C5-C6-N1	5.99	123.99	121.00
44	2	1978	C	C6-N1-C2	-5.99	117.91	120.30
44	2	4752	U	N3-C2-O2	-5.98	118.01	122.20
44	2	294	G	C2-N3-C4	5.98	114.89	111.90
44	2	4471	U	C2-N1-C1'	5.98	124.88	117.70
44	2	148	C	C6-N1-C2	-5.98	117.91	120.30
44	2	406	C	C6-N1-C2	-5.98	117.91	120.30
44	2	4505	C	N3-C2-O2	-5.98	117.72	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	2	1381	U	N3-C2-O2	-5.98	118.02	122.20
44	2	4683	U	N3-C2-O2	-5.98	118.02	122.20
44	2	1378	C	C6-N1-C1'	-5.97	113.64	120.80
44	2	4308	C	N3-C2-O2	-5.97	117.72	121.90
44	2	1294	A	O4'-C1'-N9	5.97	112.97	108.20
44	2	14	C	N1-C2-O2	5.97	122.48	118.90
44	2	2403	A	C2-N3-C4	5.97	113.58	110.60
44	2	467	U	C6-N1-C2	-5.96	117.42	121.00
44	2	1405	C	C5-C6-N1	5.96	123.98	121.00
44	2	2002	A	C2-N3-C4	5.96	113.58	110.60
44	2	1428	U	N1-C2-O2	5.96	126.97	122.80
44	2	1429	C	C5-C6-N1	5.96	123.98	121.00
44	2	2019	C	C2-N1-C1'	5.96	125.35	118.80
44	2	2886	U	N3-C2-O2	-5.96	118.03	122.20
4	8	150	C	N3-C2-O2	-5.96	117.73	121.90
44	2	4864	U	C2-N1-C1'	5.96	124.85	117.70
44	2	122	U	N3-C2-O2	-5.95	118.03	122.20
44	2	4508	C	N1-C2-O2	5.95	122.47	118.90
44	2	4752	U	N1-C2-O2	5.95	126.97	122.80
46	4	269	LEU	CA-CB-CG	5.95	128.98	115.30
44	2	2465	C	C6-N1-C2	-5.95	117.92	120.30
44	2	4120	U	C2-N1-C1'	5.95	124.83	117.70
1	5	43	U	N1-C2-O2	5.94	126.96	122.80
44	2	712	C	C6-N1-C2	-5.94	117.92	120.30
44	2	926	G	N3-C4-C5	-5.94	125.63	128.60
44	2	2445	C	C6-N1-C2	-5.94	117.92	120.30
1	5	2	U	N3-C2-O2	-5.94	118.04	122.20
44	2	4434	C	N1-C2-O2	5.93	122.46	118.90
44	2	4508	C	C6-N1-C2	-5.93	117.93	120.30
44	2	4502	C	C5-C6-N1	5.93	123.97	121.00
44	2	2505	C	C6-N1-C2	-5.93	117.93	120.30
44	2	4162	C	C2-N1-C1'	5.92	125.32	118.80
21	S	32	ASP	CB-CG-OD1	5.92	123.63	118.30
44	2	294	G	C8-N9-C1'	-5.92	119.30	127.00
44	2	1308	C	C6-N1-C2	-5.92	117.93	120.30
44	2	1402	C	C6-N1-C2	-5.92	117.93	120.30
44	2	4709	U	C5-C6-N1	5.92	125.66	122.70
44	2	195	C	C5-C6-N1	5.91	123.96	121.00
44	2	3680	U	N3-C2-O2	-5.91	118.06	122.20
44	2	4612	C	C5-C6-N1	5.91	123.95	121.00
44	2	3831	U	N1-C2-O2	5.91	126.94	122.80
44	2	4469	U	N3-C2-O2	-5.90	118.07	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	2	2016	C	N1-C2-O2	5.90	122.44	118.90
44	2	2439	G	N3-C4-N9	5.90	129.54	126.00
1	5	14	C	C5-C6-N1	5.90	123.95	121.00
44	2	274	C	C5-C6-N1	5.89	123.95	121.00
44	2	2625	U	N3-C2-O2	-5.89	118.08	122.20
44	2	274	C	C2-N1-C1'	5.89	125.27	118.80
39	r	103	LEU	CA-CB-CG	5.88	128.83	115.30
44	2	41	C	C6-N1-C2	-5.88	117.95	120.30
44	2	1632	A	N1-C2-N3	-5.88	126.36	129.30
44	2	3831	U	N3-C2-O2	-5.88	118.08	122.20
44	2	4303	C	C6-N1-C2	-5.88	117.95	120.30
1	5	78	C	C5-C6-N1	5.88	123.94	121.00
44	2	4361	U	N1-C2-O2	5.88	126.92	122.80
44	2	3882	C	C2-N1-C1'	5.88	125.27	118.80
4	8	51	U	C2-N1-C1'	5.88	124.75	117.70
44	2	2071	A	C2-N3-C4	5.88	113.54	110.60
44	2	2792	C	C6-N1-C2	-5.88	117.95	120.30
44	2	1472	C	N1-C2-O2	5.87	122.42	118.90
44	2	3680	U	N1-C2-O2	5.87	126.91	122.80
44	2	2710	C	C6-N1-C1'	-5.87	113.75	120.80
44	2	3851	U	N3-C2-O2	-5.87	118.09	122.20
44	2	2325	C	C6-N1-C2	-5.87	117.95	120.30
44	2	1703	C	C5-C6-N1	5.87	123.93	121.00
44	2	963	G	N3-C4-C5	-5.87	125.67	128.60
44	2	1790	U	C2-N1-C1'	5.86	124.73	117.70
44	2	5035	U	N1-C2-O2	5.86	126.90	122.80
22	U	134	LEU	CA-CB-CG	5.85	128.76	115.30
44	2	2803	U	N3-C2-O2	-5.85	118.10	122.20
44	2	124	C	C6-N1-C2	-5.85	117.96	120.30
4	8	5	U	N3-C2-O2	-5.85	118.11	122.20
44	2	1592	G	N3-C4-C5	-5.85	125.68	128.60
4	8	118	C	C2-N1-C1'	5.84	125.23	118.80
44	2	516	C	C5-C6-N1	5.84	123.92	121.00
1	5	102	U	N1-C2-O2	5.84	126.89	122.80
44	2	4350	C	C6-N1-C2	-5.84	117.96	120.30
44	2	963	G	N3-C4-N9	5.84	129.50	126.00
44	2	1913	C	C6-N1-C2	-5.83	117.97	120.30
44	2	4940	C	N1-C2-O2	5.83	122.40	118.90
4	8	11	C	C6-N1-C2	-5.83	117.97	120.30
44	2	141	C	N1-C2-O2	5.83	122.40	118.90
44	2	3618	C	C6-N1-C2	-5.83	117.97	120.30
1	5	80	U	N3-C2-O2	-5.83	118.12	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	8	101	C	N1-C2-O2	5.83	122.39	118.90
44	2	4561	C	C2-N1-C1'	5.83	125.21	118.80
44	2	2290	C	N1-C2-O2	5.82	122.39	118.90
44	2	4926	C	C5-C6-N1	5.82	123.91	121.00
44	2	1243	C	N1-C2-O2	5.82	122.39	118.90
44	2	704	C	C2-N1-C1'	5.82	125.20	118.80
44	2	2026	A	C6-C5-N7	5.81	136.37	132.30
44	2	4710	C	C2-N1-C1'	5.81	125.19	118.80
44	2	3622	C	N3-C2-O2	-5.80	117.84	121.90
44	2	688	U	N1-C2-O2	5.80	126.86	122.80
44	2	4685	U	N3-C2-O2	-5.80	118.14	122.20
44	2	1401	C	C5-C6-N1	5.79	123.90	121.00
44	2	985	C	N1-C2-O2	5.79	122.38	118.90
44	2	1183	C	C5-C6-N1	5.79	123.90	121.00
44	2	673	C	C5-C6-N1	5.79	123.89	121.00
44	2	2767	U	N3-C2-O2	-5.79	118.15	122.20
44	2	2905	C	C6-N1-C2	-5.79	117.98	120.30
44	2	500	G	O4'-C1'-N9	5.79	112.83	108.20
44	2	2371	U	N1-C2-O2	5.79	126.85	122.80
44	2	4923	C	C6-N1-C2	-5.79	117.99	120.30
44	2	449	C	C2-N1-C1'	5.78	125.16	118.80
4	8	54	C	C5-C6-N1	5.78	123.89	121.00
44	2	112	C	N3-C2-O2	-5.77	117.86	121.90
44	2	712	C	C5-C6-N1	5.77	123.89	121.00
44	2	100	C	O4'-C1'-N1	5.77	112.82	108.20
44	2	906	C	C6-N1-C2	-5.77	117.99	120.30
44	2	1832	C	C6-N1-C2	-5.76	118.00	120.30
44	2	2791	C	C2-N1-C1'	5.76	125.14	118.80
44	2	4469	U	N1-C2-O2	5.76	126.83	122.80
44	2	1458	C	C6-N1-C2	-5.76	118.00	120.30
44	2	4923	C	N1-C2-O2	5.76	122.35	118.90
46	4	12	VAL	CA-CB-CG1	5.76	119.54	110.90
44	2	1644	C	C6-N1-C2	-5.75	118.00	120.30
44	2	2384	U	N3-C2-O2	-5.75	118.17	122.20
44	2	115	C	C6-N1-C1'	-5.75	113.90	120.80
44	2	3932	U	N3-C2-O2	-5.75	118.18	122.20
44	2	386	A	C2-N3-C4	5.75	113.47	110.60
44	2	1183	C	C2-N1-C1'	5.75	125.12	118.80
44	2	4683	U	N1-C2-O2	5.75	126.82	122.80
44	2	201	C	C6-N1-C2	-5.74	118.00	120.30
44	2	1726	U	C6-N1-C2	-5.74	117.56	121.00
44	2	2892	C	C5-C6-N1	5.74	123.87	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	2	4712	C	N1-C2-O2	5.74	122.34	118.90
44	2	4716	C	C6-N1-C2	-5.74	118.00	120.30
44	2	467	U	C5-C6-N1	5.74	125.57	122.70
44	2	498	C	C2-N1-C1'	5.74	125.11	118.80
44	2	322	C	C5-C6-N1	5.74	123.87	121.00
44	2	1241	C	C6-N1-C1'	-5.74	113.92	120.80
44	2	1381	U	N1-C2-O2	5.74	126.81	122.80
44	2	1429	C	C2-N1-C1'	5.74	125.11	118.80
8	D	7	LEU	CA-CB-CG	5.73	128.48	115.30
44	2	1401	C	C2-N1-C1'	5.73	125.11	118.80
44	2	4682	U	C2-N1-C1'	5.73	124.58	117.70
44	2	4711	C	C6-N1-C2	-5.73	118.01	120.30
44	2	297	U	N3-C2-O2	-5.73	118.19	122.20
44	2	365	U	C2-N1-C1'	5.73	124.57	117.70
4	8	32	C	C2-N1-C1'	5.72	125.10	118.80
44	2	2025	A	C8-N9-C4	-5.72	103.51	105.80
44	2	1460	C	C6-N1-C2	-5.72	118.01	120.30
44	2	1592	G	N3-C4-N9	5.72	129.43	126.00
44	2	2843	U	N3-C2-O2	-5.72	118.20	122.20
44	2	4243	C	C2-N1-C1'	5.72	125.09	118.80
44	2	4522	G	N3-C4-N9	5.72	129.43	126.00
44	2	4895	C	C2-N1-C1'	5.71	125.09	118.80
13	I	17	ASP	CB-CG-OD2	5.71	123.44	118.30
44	2	977	C	N1-C2-O2	5.71	122.33	118.90
44	2	2392	C	C6-N1-C2	-5.71	118.02	120.30
44	2	3882	C	C5-C6-N1	5.71	123.85	121.00
44	2	5050	C	N1-C2-O2	5.71	122.32	118.90
44	2	1720	C	C5-C6-N1	5.71	123.85	121.00
44	2	2729	C	C2-N1-C1'	5.70	125.07	118.80
44	2	50	C	C5-C6-N1	5.70	123.85	121.00
44	2	1809	C	C5-C6-N1	5.70	123.85	121.00
44	2	4711	C	C5-C6-N1	5.70	123.85	121.00
44	2	4886	C	N1-C2-O2	5.70	122.32	118.90
11	G	253	LEU	CA-CB-CG	5.70	128.40	115.30
44	2	1243	C	C2-N1-C1'	5.70	125.06	118.80
44	2	4406	U	C2-N1-C1'	5.70	124.54	117.70
44	2	3636	C	C5-C6-N1	5.69	123.85	121.00
44	2	204	U	N1-C2-O2	5.69	126.78	122.80
4	8	101	C	C5-C6-N1	5.69	123.84	121.00
4	8	80	A	C2-N3-C4	5.68	113.44	110.60
44	2	3657	U	N1-C2-O2	5.68	126.78	122.80
44	2	4764	A	C6-N1-C2	5.68	122.01	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	103	A	C2-N3-C4	5.68	113.44	110.60
44	2	336	A	C2-N3-C4	5.67	113.44	110.60
4	8	90	C	C5-C6-N1	5.67	123.84	121.00
32	h	82	ILE	CG1-CB-CG2	-5.67	98.92	111.40
8	D	171	LEU	CB-CG-CD1	-5.67	101.36	111.00
44	2	1720	C	N1-C2-O2	5.67	122.30	118.90
44	2	4387	C	N3-C2-O2	-5.67	117.93	121.90
44	2	3832	U	N3-C2-O2	-5.67	118.23	122.20
44	2	4490	C	C6-N1-C2	-5.67	118.03	120.30
44	2	68	U	N1-C2-O2	5.67	126.77	122.80
44	2	238	C	C6-N1-C2	-5.67	118.03	120.30
44	2	971	U	N1-C2-O2	5.67	126.77	122.80
44	2	4563	U	N1-C2-O2	5.67	126.77	122.80
44	2	3853	U	N3-C2-O2	-5.66	118.24	122.20
44	2	4639	G	C2-N3-C4	5.66	114.73	111.90
45	y	73	VAL	CG1-CB-CG2	-5.66	101.84	110.90
44	2	1994	C	O4'-C1'-N1	5.66	112.73	108.20
44	2	282	C	C6-N1-C2	-5.66	118.04	120.30
44	2	2031	C	N3-C2-O2	-5.66	117.94	121.90
44	2	30	C	C2-N1-C1'	5.66	125.02	118.80
44	2	3851	U	N1-C2-O2	5.66	126.76	122.80
44	2	3870	C	C5-C6-N1	5.66	123.83	121.00
44	2	4985	U	N3-C2-O2	-5.65	118.24	122.20
4	8	100	U	N3-C2-O2	-5.65	118.25	122.20
44	2	981	C	C6-N1-C2	-5.65	118.04	120.30
44	2	2783	A	C6-N1-C2	5.65	121.99	118.60
44	2	2729	C	C5-C6-N1	5.64	123.82	121.00
44	2	4701	A	N1-C2-N3	-5.64	126.48	129.30
44	2	2022	C	C6-N1-C2	-5.64	118.04	120.30
44	2	4464	A	C2-N3-C4	5.64	113.42	110.60
44	2	703	G	C4-N9-C1'	5.63	133.82	126.50
44	2	2465	C	N1-C2-O2	5.63	122.28	118.90
47	d	66	SER	C-N-CA	5.63	135.78	121.70
29	c	118	GLU	N-CA-CB	5.63	120.73	110.60
44	2	4386	C	C6-N1-C2	-5.63	118.05	120.30
44	2	56	A	N1-C2-N3	-5.62	126.49	129.30
15	L	12	ARG	CA-CB-CG	5.62	125.77	113.40
23	V	190	ASP	CB-CG-OD1	5.62	123.36	118.30
44	2	516	C	C2-N1-C1'	5.62	124.98	118.80
44	2	4213	A	N1-C2-N3	-5.62	126.49	129.30
44	2	750	U	N3-C2-O2	-5.62	118.27	122.20
44	2	4613	C	C2-N1-C1'	5.62	124.98	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	8	99	U	N3-C2-O2	-5.62	118.27	122.20
44	2	1929	A	C8-N9-C1'	-5.62	117.59	127.70
4	8	4	C	C6-N1-C2	-5.61	118.05	120.30
42	J	30	LEU	CB-CG-CD1	5.61	120.54	111.00
44	2	926	G	N3-C4-N9	5.61	129.37	126.00
44	2	2410	C	N3-C2-O2	-5.61	117.97	121.90
44	2	4969	C	C5-C6-N1	5.61	123.81	121.00
44	2	365	U	C5-C6-N1	5.61	125.50	122.70
44	2	3831	U	C2-N1-C1'	5.61	124.43	117.70
44	2	2298	U	N3-C2-O2	-5.61	118.28	122.20
44	2	1707	C	C6-N1-C2	-5.61	118.06	120.30
44	2	1929	A	N3-C4-N9	5.60	131.88	127.40
44	2	2403	A	N1-C2-N3	-5.60	126.50	129.30
1	5	2	U	N1-C2-O2	5.60	126.72	122.80
44	2	1915	C	C2-N1-C1'	5.60	124.96	118.80
44	2	1245	C	C6-N1-C2	-5.60	118.06	120.30
44	2	1671	U	C2-N1-C1'	5.60	124.42	117.70
44	2	4878	C	C6-N1-C2	-5.59	118.06	120.30
44	2	5042	A	N1-C2-N3	-5.59	126.50	129.30
44	2	2528	G	C2-N3-C4	5.59	114.69	111.90
44	2	67	C	C5-C6-N1	5.59	123.79	121.00
46	4	41	HIS	C-N-CA	5.59	135.67	121.70
44	2	1439	C	C6-N1-C2	-5.58	118.07	120.30
44	2	1468	C	C6-N1-C2	-5.58	118.07	120.30
44	2	2074	C	C6-N1-C2	-5.58	118.07	120.30
38	p	25	PHE	CB-CG-CD1	5.58	124.71	120.80
44	2	3858	C	C6-N1-C2	-5.58	118.07	120.30
44	2	4476	C	O4'-C1'-N1	5.58	112.66	108.20
44	2	274	C	N1-C2-O2	5.58	122.25	118.90
44	2	1350	C	C6-N1-C2	-5.58	118.07	120.30
44	2	4700	A	N1-C2-N3	-5.58	126.51	129.30
44	2	4703	U	N3-C2-O2	-5.58	118.30	122.20
44	2	1450	C	C2-N1-C1'	5.57	124.93	118.80
44	2	1535	C	C6-N1-C2	-5.57	118.07	120.30
44	2	3870	C	C6-N1-C2	-5.57	118.07	120.30
44	2	925	C	C5-C6-N1	5.57	123.79	121.00
44	2	358	C	C6-N1-C2	-5.57	118.07	120.30
44	2	1577	G	C8-N9-C4	-5.56	104.17	106.40
44	2	86	U	N1-C2-O2	5.56	126.69	122.80
44	2	1245	C	C5-C6-N1	5.56	123.78	121.00
44	2	2303	C	C6-N1-C2	-5.56	118.08	120.30
44	2	1077	C	C6-N1-C2	-5.56	118.08	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	2	1726	U	C5-C6-N1	5.56	125.48	122.70
44	2	4532	U	N3-C2-O2	-5.56	118.31	122.20
44	2	3685	C	C6-N1-C2	-5.55	118.08	120.30
44	2	174	C	N3-C2-O2	-5.55	118.01	121.90
44	2	1293	G	N3-C4-N9	5.55	129.33	126.00
15	L	117	LEU	CA-CB-CG	5.55	128.06	115.30
44	2	3668	C	C6-N1-C2	-5.55	118.08	120.30
44	2	4880	C	C2-N1-C1'	5.55	124.90	118.80
4	8	50	C	C6-N1-C2	-5.54	118.08	120.30
44	2	100	C	C5-C6-N1	5.54	123.77	121.00
44	2	1671	U	C6-N1-C2	-5.54	117.67	121.00
44	2	4588	U	N3-C2-O2	-5.54	118.32	122.20
4	8	54	C	N3-C2-O2	-5.54	118.02	121.90
17	N	91	GLU	CA-CB-CG	5.54	125.59	113.40
44	2	510	U	N3-C2-O2	-5.54	118.32	122.20
44	2	1417	C	N1-C2-O2	5.54	122.22	118.90
44	2	1820	C	C6-N1-C2	-5.54	118.08	120.30
44	2	3605	C	C2-N1-C1'	5.54	124.89	118.80
44	2	2572	C	C6-N1-C2	-5.54	118.08	120.30
44	2	4229	U	C2-N1-C1'	5.54	124.34	117.70
44	2	2806	A	N1-C2-N3	-5.54	126.53	129.30
44	2	2019	C	C5-C6-N1	5.53	123.77	121.00
44	2	977	C	C6-N1-C2	-5.53	118.09	120.30
44	2	3697	U	C6-N1-C2	-5.53	117.68	121.00
44	2	3739	C	N1-C2-O2	5.53	122.22	118.90
44	2	1203	G	N3-C4-N9	5.52	129.31	126.00
51	z	33	LEU	CA-CB-CG	5.52	128.00	115.30
44	2	1632	A	C4-N9-C1'	5.52	136.24	126.30
44	2	2009	A	C2-N3-C4	5.52	113.36	110.60
44	2	963	G	C8-N9-C1'	-5.51	119.83	127.00
44	2	1276	C	C6-N1-C2	-5.51	118.09	120.30
44	2	4120	U	N1-C2-O2	5.51	126.66	122.80
4	8	107	C	C6-N1-C2	-5.51	118.10	120.30
44	2	3606	U	N1-C2-O2	5.51	126.66	122.80
44	2	4694	G	N3-C4-N9	5.51	129.30	126.00
36	n	106	TYR	N-CA-C	5.50	125.86	111.00
44	2	1577	G	N1-C6-O6	-5.50	116.60	119.90
44	2	2081	C	C6-N1-C2	-5.50	118.10	120.30
44	2	1971	C	C6-N1-C1'	-5.50	114.20	120.80
44	2	2439	G	C8-N9-C1'	-5.50	119.85	127.00
44	2	2592	U	N1-C2-O2	5.50	126.65	122.80
35	m	102	LEU	CA-CB-CG	5.50	127.95	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	2	454	U	N3-C2-O2	-5.50	118.35	122.20
44	2	753	C	C6-N1-C1'	-5.50	114.20	120.80
44	2	2304	U	N3-C2-O2	-5.50	118.35	122.20
44	2	2886	U	N1-C2-O2	5.50	126.65	122.80
44	2	4155	C	C6-N1-C2	-5.50	118.10	120.30
44	2	2699	C	C6-N1-C2	-5.50	118.10	120.30
44	2	2325	C	N3-C2-O2	-5.49	118.05	121.90
44	2	4476	C	C5-C6-N1	5.49	123.75	121.00
44	2	1275	G	O4'-C1'-N9	5.49	112.59	108.20
21	S	135	LEU	CA-CB-CG	5.49	127.93	115.30
44	2	2073	C	C6-N1-C2	-5.49	118.10	120.30
44	2	2304	U	N1-C2-O2	5.49	126.64	122.80
44	2	2684	C	C6-N1-C2	-5.49	118.10	120.30
44	2	1508	A	N1-C2-N3	-5.49	126.56	129.30
44	2	242	U	C6-N1-C2	-5.49	117.71	121.00
44	2	2006	U	N3-C2-O2	-5.49	118.36	122.20
44	2	1585	C	C6-N1-C2	-5.48	118.11	120.30
44	2	4413	C	C6-N1-C2	-5.48	118.11	120.30
44	2	469	C	C6-N1-C2	-5.48	118.11	120.30
44	2	2684	C	C5-C6-N1	5.48	123.74	121.00
44	2	3863	C	C6-N1-C2	-5.48	118.11	120.30
44	2	18	C	C6-N1-C2	-5.48	118.11	120.30
44	2	4608	G	C6-C5-N7	-5.48	127.11	130.40
44	2	966	A	N7-C8-N9	5.48	116.54	113.80
44	2	1994	C	C5-C6-N1	5.48	123.74	121.00
44	2	3866	C	C5-C6-N1	5.48	123.74	121.00
5	9	35	LEU	CA-CB-CG	5.48	127.90	115.30
44	2	417	G	O4'-C1'-N9	5.48	112.58	108.20
44	2	2409	U	N1-C2-N3	5.48	118.19	114.90
44	2	242	U	C2-N1-C1'	5.47	124.27	117.70
44	2	1634	A	N1-C2-N3	-5.47	126.56	129.30
44	2	2820	C	C5-C6-N1	5.47	123.74	121.00
44	2	43	U	N3-C2-O2	-5.47	118.37	122.20
44	2	3912	U	N1-C2-O2	5.46	126.62	122.80
44	2	3939	G	N3-C4-N9	5.46	129.28	126.00
44	2	3741	C	C6-N1-C2	-5.46	118.11	120.30
44	2	1427	A	N1-C2-N3	-5.45	126.57	129.30
44	2	4694	G	C2-N3-C4	5.45	114.63	111.90
44	2	1971	C	N3-C2-O2	-5.45	118.08	121.90
44	2	4072	C	C6-N1-C2	-5.45	118.12	120.30
4	8	82	A	C2-N3-C4	5.45	113.33	110.60
44	2	1702	C	C6-N1-C1'	-5.45	114.26	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	2	3622	C	C5-C6-N1	5.45	123.72	121.00
44	2	719	C	C5-C6-N1	5.45	123.72	121.00
44	2	3882	C	N1-C2-O2	5.45	122.17	118.90
1	5	76	U	C2-N1-C1'	5.45	124.23	117.70
44	2	2036	C	C6-N1-C2	-5.45	118.12	120.30
44	2	673	C	N1-C2-O2	5.44	122.17	118.90
44	2	2629	C	N1-C2-O2	5.44	122.17	118.90
1	5	39	C	C6-N1-C2	-5.44	118.12	120.30
44	2	1671	U	C5-C6-N1	5.44	125.42	122.70
44	2	2603	C	C6-N1-C2	-5.44	118.12	120.30
44	2	2362	U	C6-N1-C2	-5.43	117.74	121.00
44	2	2439	G	N3-C4-C5	-5.43	125.88	128.60
44	2	5008	C	N3-C2-O2	-5.43	118.10	121.90
44	2	1801	A	N1-C2-N3	-5.43	126.58	129.30
44	2	2264	C	N1-C2-O2	5.43	122.16	118.90
44	2	4722	G	C4-N9-C1'	5.43	133.56	126.50
44	2	1243	C	C5-C6-N1	5.43	123.72	121.00
44	2	3840	U	N1-C2-O2	5.43	126.60	122.80
44	2	4137	C	C6-N1-C2	-5.43	118.13	120.30
44	2	49	U	N3-C2-O2	-5.43	118.40	122.20
44	2	3901	A	C2-N3-C4	5.43	113.31	110.60
44	2	1216	C	O4'-C1'-N1	5.42	112.54	108.20
44	2	1344	C	C6-N1-C2	-5.42	118.13	120.30
44	2	2853	C	C6-N1-C2	-5.42	118.13	120.30
44	2	4162	C	N3-C2-O2	-5.42	118.10	121.90
44	2	981	C	C5-C6-N1	5.42	123.71	121.00
44	2	1794	A	C2-N3-C4	5.42	113.31	110.60
44	2	1352	C	C6-N1-C2	-5.42	118.13	120.30
44	2	1580	C	C6-N1-C2	-5.42	118.13	120.30
44	2	4714	C	N3-C2-O2	-5.42	118.11	121.90
44	2	2497	C	N1-C2-O2	5.42	122.15	118.90
44	2	3870	C	N1-C2-O2	5.42	122.15	118.90
44	2	3905	A	OP2-P-O3'	5.42	117.11	105.20
13	I	37	ASP	CB-CG-OD2	5.41	123.17	118.30
4	8	4	C	C5-C6-N1	5.41	123.70	121.00
44	2	185	C	C6-N1-C2	-5.41	118.14	120.30
44	2	4589	A	N1-C2-N3	-5.41	126.59	129.30
44	2	1540	C	C6-N1-C2	-5.41	118.14	120.30
44	2	4664	A	N1-C2-N3	-5.41	126.60	129.30
44	2	5030	U	C5-C6-N1	5.41	125.40	122.70
44	2	4506	C	N1-C2-O2	5.41	122.14	118.90
44	2	2803	U	N1-C2-O2	5.41	126.58	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	2	2729	C	N1-C2-O2	5.40	122.14	118.90
44	2	180	C	C5-C6-N1	5.40	123.70	121.00
44	2	1893	C	N1-C2-O2	5.40	122.14	118.90
44	2	1993	C	C6-N1-C2	-5.40	118.14	120.30
44	2	18	C	N1-C2-O2	5.40	122.14	118.90
44	2	227	A	N1-C2-N3	-5.40	126.60	129.30
44	2	408	A	N1-C2-N3	-5.40	126.60	129.30
44	2	30	C	N1-C2-O2	5.40	122.14	118.90
44	2	1315	C	C5-C6-N1	5.40	123.70	121.00
44	2	1320	U	C5-C6-N1	5.39	125.39	122.70
1	5	29	C	N3-C2-O2	-5.39	118.13	121.90
44	2	5042	A	C2-N3-C4	5.39	113.30	110.60
44	2	2791	C	C5-C6-N1	5.39	123.69	121.00
44	2	1535	C	N1-C2-O2	5.39	122.13	118.90
44	2	1304	C	C6-N1-C2	-5.38	118.15	120.30
44	2	1592	G	C8-N9-C1'	-5.38	120.00	127.00
44	2	4775	C	N3-C2-O2	-5.38	118.13	121.90
44	2	458	C	C6-N1-C2	-5.38	118.15	120.30
44	2	2814	C	N3-C2-O2	-5.38	118.13	121.90
44	2	3650	C	C5-C6-N1	5.38	123.69	121.00
44	2	4403	U	C2-N1-C1'	5.38	124.16	117.70
44	2	4206	C	C5-C6-N1	5.38	123.69	121.00
44	2	4887	C	C5-C6-N1	5.38	123.69	121.00
44	2	510	U	N1-C2-O2	5.38	126.56	122.80
44	2	4067	U	N3-C2-O2	-5.38	118.44	122.20
46	4	21	LEU	CA-CB-CG	5.38	127.67	115.30
44	2	406	C	C2'-C3'-O3'	5.37	122.30	113.70
44	2	1079	C	N3-C2-O2	-5.37	118.14	121.90
44	2	2683	C	C6-N1-C2	-5.37	118.15	120.30
44	2	4981	G	N3-C4-C5	-5.37	125.92	128.60
44	2	4508	C	C5-C6-N1	5.37	123.68	121.00
44	2	4926	C	O4'-C1'-N1	5.37	112.49	108.20
44	2	101	A	N1-C2-N3	-5.36	126.62	129.30
44	2	1469	C	C5-C6-N1	5.36	123.68	121.00
44	2	1395	U	N1-C2-O2	5.36	126.55	122.80
44	2	2332	A	N1-C2-N3	-5.36	126.62	129.30
1	5	39	C	N3-C2-O2	-5.36	118.15	121.90
44	2	4710	C	N1-C2-O2	5.36	122.12	118.90
44	2	4715	C	N3-C2-O2	-5.36	118.15	121.90
44	2	1397	A	N1-C2-N3	-5.36	126.62	129.30
44	2	2338	C	C6-N1-C2	-5.36	118.16	120.30
44	2	4561	C	N1-C2-O2	5.36	122.11	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	57	C	C5-C6-N1	5.35	123.68	121.00
44	2	26	C	C2-N1-C1'	5.35	124.69	118.80
44	2	1966	C	C6-N1-C2	-5.35	118.16	120.30
44	2	4289	U	N3-C2-O2	-5.35	118.45	122.20
44	2	1203	G	C4-N9-C1'	5.35	133.46	126.50
44	2	2262	G	C2-N3-C4	5.35	114.57	111.90
44	2	2821	U	N3-C2-O2	-5.35	118.45	122.20
44	2	3893	C	C5-C6-N1	5.35	123.67	121.00
44	2	390	C	C5-C6-N1	5.35	123.67	121.00
44	2	1599	A	C2-N3-C4	5.35	113.27	110.60
44	2	1694	C	C6-N1-C2	-5.35	118.16	120.30
1	5	39	C	C5-C6-N1	5.35	123.67	121.00
44	2	1320	U	C6-N1-C2	-5.35	117.79	121.00
44	2	2625	U	N1-C2-O2	5.35	126.54	122.80
44	2	2078	C	C6-N1-C2	-5.34	118.16	120.30
44	2	1373	A	N1-C2-N3	-5.34	126.63	129.30
44	2	1702	C	C6-N1-C2	-5.34	118.16	120.30
44	2	4990	C	C6-N1-C2	-5.34	118.16	120.30
44	2	1499	C	C6-N1-C2	-5.34	118.17	120.30
44	2	1339	U	N3-C2-O2	-5.33	118.47	122.20
44	2	4299	U	N1-C2-O2	5.33	126.53	122.80
44	2	436	C	C6-N1-C2	-5.33	118.17	120.30
44	2	2035	C	C6-N1-C2	-5.33	118.17	120.30
44	2	4594	U	N3-C2-O2	-5.33	118.47	122.20
4	8	62	A	N1-C2-N3	-5.33	126.64	129.30
44	2	4639	G	N3-C4-N9	5.33	129.20	126.00
44	2	3926	C	C5-C6-N1	5.33	123.66	121.00
44	2	4120	U	N3-C2-O2	-5.33	118.47	122.20
44	2	4596	C	N1-C2-O2	5.33	122.09	118.90
44	2	185	C	N1-C2-O2	5.32	122.09	118.90
44	2	4467	A	N1-C2-N3	-5.32	126.64	129.30
44	2	2497	C	C6-N1-C2	-5.31	118.17	120.30
44	2	657	C	C5-C6-N1	5.31	123.66	121.00
44	2	1993	C	C2-N1-C1'	5.31	124.64	118.80
44	2	2067	C	N1-C2-O2	5.31	122.09	118.90
44	2	4532	U	N1-C2-O2	5.31	126.52	122.80
44	2	89	C	C6-N1-C2	-5.31	118.18	120.30
44	2	4907	G	N3-C4-C5	-5.31	125.95	128.60
44	2	5050	C	N3-C2-O2	-5.31	118.19	121.90
4	8	96	C	C6-N1-C2	-5.30	118.18	120.30
44	2	365	U	C6-N1-C2	-5.30	117.82	121.00
44	2	1978	C	N1-C2-O2	5.30	122.08	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	2	337	U	N3-C2-O2	-5.30	118.49	122.20
4	8	37	A	N1-C2-N3	-5.29	126.65	129.30
4	8	108	A	N1-C2-N3	-5.29	126.65	129.30
33	i	106	LEU	CA-CB-CG	5.29	127.47	115.30
44	2	201	C	N1-C2-O2	5.29	122.07	118.90
44	2	1717	C	C6-N1-C2	-5.29	118.18	120.30
44	2	4715	C	N1-C2-O2	5.29	122.07	118.90
44	2	4723	A	C2-N3-C4	5.29	113.24	110.60
44	2	1884	C	N1-C2-O2	5.29	122.07	118.90
4	8	35	C	C5-C6-N1	5.28	123.64	121.00
4	8	9	A	N1-C2-N3	-5.28	126.66	129.30
44	2	914	U	C5-C4-O4	-5.28	122.73	125.90
44	2	3930	U	N3-C2-O2	-5.28	118.50	122.20
44	2	2094	G	N3-C4-N9	5.28	129.17	126.00
44	2	1662	C	C5-C6-N1	5.28	123.64	121.00
44	2	4286	C	C6-N1-C2	-5.28	118.19	120.30
44	2	4289	U	N1-C2-O2	5.28	126.49	122.80
44	2	4302	U	N1-C2-O2	5.28	126.49	122.80
44	2	4714	C	C5-C6-N1	5.28	123.64	121.00
44	2	4302	U	N3-C2-O2	-5.28	118.51	122.20
44	2	4667	C	C6-N1-C2	-5.28	118.19	120.30
44	2	3739	C	C5-C6-N1	5.27	123.64	121.00
1	5	14	C	C2-N1-C1'	5.27	124.60	118.80
44	2	643	C	C6-N1-C2	-5.27	118.19	120.30
44	2	454	U	N1-C2-O2	5.27	126.49	122.80
44	2	4747	C	N3-C2-O2	-5.27	118.21	121.90
4	8	118	C	N1-C2-O2	5.27	122.06	118.90
39	r	36	LEU	CA-CB-CG	5.27	127.42	115.30
44	2	1184	A	C2-N3-C4	5.27	113.23	110.60
44	2	1792	U	N3-C2-O2	-5.27	118.51	122.20
44	2	2689	C	C6-N1-C2	-5.27	118.19	120.30
44	2	3939	G	C4-N9-C1'	5.27	133.35	126.50
44	2	4137	C	C5-C6-N1	5.27	123.63	121.00
44	2	515	C	C2-N1-C1'	5.27	124.59	118.80
44	2	2264	C	C6-N1-C2	-5.27	118.19	120.30
44	2	1572	U	N3-C2-O2	-5.26	118.52	122.20
44	2	3702	A	N1-C2-N3	-5.26	126.67	129.30
44	2	4767	C	C6-N1-C2	-5.26	118.19	120.30
44	2	5007	A	N1-C2-N3	-5.26	126.67	129.30
44	2	2094	G	N3-C4-C5	-5.26	125.97	128.60
44	2	1384	C	C6-N1-C2	-5.26	118.19	120.30
44	2	449	C	N3-C2-O2	-5.26	118.22	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	39	C	C2-N1-C1'	5.26	124.58	118.80
44	2	124	C	C5-C6-N1	5.26	123.63	121.00
44	2	1725	U	N3-C2-O2	-5.25	118.52	122.20
21	S	24	LEU	CA-CB-CG	5.25	127.38	115.30
44	2	1333	A	N1-C2-N3	-5.25	126.67	129.30
44	2	1293	G	C4-N9-C1'	5.25	133.33	126.50
44	2	2295	C	C6-N1-C2	-5.25	118.20	120.30
21	S	136	LEU	CA-CB-CG	5.25	127.37	115.30
44	2	2077	C	C6-N1-C2	-5.25	118.20	120.30
44	2	2882	A	C2-N3-C4	5.25	113.22	110.60
44	2	386	A	N1-C2-N3	-5.25	126.68	129.30
46	4	116	LEU	CB-CG-CD2	5.25	119.92	111.00
44	2	1832	C	C5-C6-N1	5.24	123.62	121.00
44	2	4981	G	C4-N9-C1'	5.24	133.32	126.50
44	2	977	C	C2-N1-C1'	5.24	124.57	118.80
44	2	1686	C	C6-N1-C2	-5.24	118.20	120.30
44	2	1700	G	N3-C4-C5	-5.24	125.98	128.60
44	2	2465	C	C2-N1-C1'	5.24	124.57	118.80
44	2	4927	G	C4-N9-C1'	5.24	133.31	126.50
44	2	2533	C	N1-C2-O2	5.23	122.04	118.90
44	2	180	C	C6-N1-C2	-5.23	118.21	120.30
44	2	4460	U	N3-C2-O2	-5.23	118.54	122.20
44	2	472	C	N3-C2-O2	-5.23	118.24	121.90
44	2	935	A	N1-C2-N3	-5.23	126.69	129.30
44	2	2026	A	C6-N1-C2	-5.23	115.46	118.60
44	2	3667	C	C6-N1-C2	-5.23	118.21	120.30
44	2	4313	A	N1-C2-N3	-5.23	126.69	129.30
44	2	2653	C	C6-N1-C2	-5.22	118.21	120.30
44	2	421	C	C6-N1-C2	-5.22	118.21	120.30
44	2	972	C	C2-N1-C1'	5.22	124.55	118.80
44	2	4880	C	C5-C6-N1	5.22	123.61	121.00
44	2	3714	G	C4-N9-C1'	5.22	133.28	126.50
44	2	418	A	N1-C2-N3	-5.22	126.69	129.30
44	2	2593	C	C6-N1-C2	-5.22	118.21	120.30
44	2	1202	C	C6-N1-C2	-5.21	118.21	120.30
45	y	116	MET	CA-CB-CG	5.21	122.16	113.30
44	2	694	C	N3-C2-O2	-5.21	118.25	121.90
44	2	1327	C	C6-N1-C2	-5.21	118.22	120.30
44	2	2026	A	C4-C5-N7	-5.21	108.09	110.70
44	2	1417	C	C6-N1-C2	-5.21	118.22	120.30
44	2	2890	C	C6-N1-C2	-5.21	118.22	120.30
44	2	4981	G	N3-C4-N9	5.21	129.13	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	8	18	U	N3-C2-O2	-5.21	118.55	122.20
44	2	76	A	N1-C2-N3	-5.21	126.69	129.30
44	2	683	C	N1-C2-O2	5.21	122.03	118.90
1	5	79	U	N3-C2-O2	-5.21	118.56	122.20
44	2	696	C	C5-C6-N1	5.21	123.60	121.00
4	8	18	U	N1-C2-O2	5.20	126.44	122.80
44	2	1386	C	C5-C6-N1	5.20	123.60	121.00
4	8	27	U	N3-C2-O2	-5.20	118.56	122.20
44	2	61	A	N1-C2-N3	-5.20	126.70	129.30
44	2	985	C	C5-C6-N1	5.20	123.60	121.00
44	2	2413	U	N3-C2-O2	-5.20	118.56	122.20
44	2	2532	C	C2-N1-C1'	5.20	124.52	118.80
44	2	4471	U	C6-N1-C2	-5.20	117.88	121.00
44	2	656	C	C2-N1-C1'	5.19	124.51	118.80
44	2	2362	U	C5-C6-N1	5.19	125.30	122.70
44	2	4233	A	C2-N3-C4	5.19	113.20	110.60
44	2	4293	U	C6-N1-C2	-5.19	117.88	121.00
44	2	4715	C	C6-N1-C2	-5.19	118.22	120.30
4	8	156	U	N3-C2-O2	-5.19	118.57	122.20
44	2	87	A	N1-C2-N3	-5.19	126.70	129.30
44	2	1430	C	C6-N1-C2	-5.19	118.22	120.30
44	2	1085	C	C6-N1-C2	-5.19	118.22	120.30
44	2	485	C	OP1-P-O3'	5.18	116.61	105.20
44	2	1254	A	N1-C2-N3	-5.18	126.71	129.30
44	2	5002	U	N3-C2-O2	-5.18	118.57	122.20
44	2	385	A	OP1-P-O3'	5.18	116.60	105.20
44	2	4694	G	C4-N9-C1'	5.18	133.24	126.50
44	2	4764	A	C4-C5-C6	-5.18	114.41	117.00
44	2	4983	C	C6-N1-C2	-5.18	118.23	120.30
44	2	1822	U	C6-N1-C2	-5.18	117.89	121.00
44	2	2817	C	C6-N1-C2	-5.18	118.23	120.30
44	2	4206	C	C2-N1-C1'	5.18	124.50	118.80
44	2	4907	G	N3-C4-N9	5.18	129.11	126.00
44	2	378	A	N1-C2-N3	-5.18	126.71	129.30
44	2	4914	C	C6-N1-C2	-5.18	118.23	120.30
44	2	1847	C	C6-N1-C2	-5.17	118.23	120.30
44	2	1794	A	N1-C2-N3	-5.17	126.71	129.30
44	2	974	C	C6-N1-C2	-5.17	118.23	120.30
44	2	2347	A	N1-C2-N3	-5.17	126.71	129.30
44	2	1822	U	C5-C6-N1	5.17	125.28	122.70
1	5	94	C	C6-N1-C2	-5.17	118.23	120.30
4	8	153	C	C6-N1-C2	-5.17	118.23	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	2	2614	C	C6-N1-C2	-5.17	118.23	120.30
44	2	1893	C	C5-C6-N1	5.17	123.58	121.00
44	2	123	C	C6-N1-C2	-5.17	118.23	120.30
44	2	436	C	N1-C2-O2	5.17	122.00	118.90
44	2	2845	A	N1-C2-N3	-5.17	126.72	129.30
1	5	44	C	N3-C2-O2	-5.16	118.29	121.90
44	2	1996	C	C6-N1-C2	-5.16	118.23	120.30
44	2	4613	C	C5-C6-N1	5.16	123.58	121.00
4	8	111	U	N3-C2-O2	-5.16	118.59	122.20
44	2	1429	C	N1-C2-O2	5.16	122.00	118.90
44	2	1692	C	C6-N1-C2	-5.16	118.24	120.30
44	2	2867	C	C2-N1-C1'	5.16	124.48	118.80
44	2	4672	A	N1-C2-N3	-5.16	126.72	129.30
4	8	111	U	N1-C2-O2	5.16	126.41	122.80
5	9	15	LEU	CA-CB-CG	5.16	127.16	115.30
44	2	1477	C	C5-C6-N1	5.16	123.58	121.00
44	2	1962	A	C2-N3-C4	5.16	113.18	110.60
44	2	4913	G	OP2-P-O3'	5.16	116.55	105.20
44	2	1097	C	C2-N1-C1'	5.16	124.47	118.80
44	2	1655	C	C5-C6-N1	5.16	123.58	121.00
44	2	4585	U	N3-C2-O2	-5.16	118.59	122.20
4	8	72	A	N1-C2-N3	-5.16	126.72	129.30
44	2	459	C	N1-C2-O2	5.16	121.99	118.90
44	2	1244	G	C4-N9-C1'	5.16	133.20	126.50
44	2	1572	U	N1-C2-O2	5.16	126.41	122.80
44	2	1847	C	C5-C6-N1	5.16	123.58	121.00
44	2	2540	C	C6-N1-C2	-5.16	118.24	120.30
4	8	145	C	C6-N1-C2	-5.15	118.24	120.30
44	2	4461	C	C6-N1-C2	-5.15	118.24	120.30
44	2	4619	U	N3-C2-O2	-5.15	118.59	122.20
44	2	5050	C	C6-N1-C2	-5.15	118.24	120.30
4	8	55	U	N1-C2-O2	5.15	126.41	122.80
44	2	1431	C	C6-N1-C2	-5.15	118.24	120.30
44	2	2473	A	N1-C2-N3	-5.15	126.72	129.30
44	2	3598	C	N1-C2-O2	5.15	121.99	118.90
44	2	3871	A	N1-C2-N3	-5.15	126.72	129.30
44	2	2628	U	N3-C2-O2	-5.15	118.60	122.20
44	2	485	C	C2-N3-C4	5.15	122.47	119.90
44	2	2381	A	N1-C2-N3	-5.15	126.73	129.30
44	2	3605	C	C6-N1-C2	-5.15	118.24	120.30
44	2	2026	A	C5'-C4'-C3'	5.15	124.23	116.00
44	2	1468	C	C5-C6-N1	5.14	123.57	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	2	2417	A	N1-C2-N3	-5.14	126.73	129.30
44	2	2600	A	N1-C2-N3	-5.14	126.73	129.30
44	2	4601	U	C2-N1-C1'	5.14	123.87	117.70
44	2	26	C	N1-C2-O2	5.14	121.99	118.90
44	2	1852	U	N1-C2-O2	5.14	126.40	122.80
44	2	4123	C	N3-C2-O2	-5.14	118.30	121.90
44	2	1467	C	C6-N1-C2	-5.14	118.24	120.30
44	2	2429	A	C2-N3-C4	5.14	113.17	110.60
44	2	3707	U	N3-C2-O2	-5.14	118.60	122.20
44	2	5048	A	N1-C2-N3	-5.14	126.73	129.30
44	2	5062	G	N3-C4-N9	5.14	129.08	126.00
44	2	1852	U	N3-C2-O2	-5.14	118.60	122.20
46	4	527	LEU	CA-CB-CG	5.14	127.11	115.30
44	2	3635	A	N1-C2-N3	-5.13	126.73	129.30
44	2	4639	G	C4-N9-C1'	5.13	133.18	126.50
44	2	1790	U	C5-C6-N1	5.13	125.27	122.70
44	2	2409	U	C6-N1-C2	-5.13	117.92	121.00
44	2	4206	C	N3-C2-O2	-5.13	118.31	121.90
44	2	4608	G	C5-N7-C8	-5.13	101.73	104.30
4	8	128	C	C6-N1-C1'	-5.13	114.64	120.80
44	2	1801	A	C2-N3-C4	5.13	113.17	110.60
44	2	4592	C	C6-N1-C2	-5.13	118.25	120.30
44	2	966	A	C2-N3-C4	5.13	113.17	110.60
44	2	1387	A	N1-C2-N3	-5.13	126.73	129.30
44	2	4696	C	N1-C2-O2	5.13	121.98	118.90
44	2	974	C	N1-C2-O2	5.13	121.98	118.90
44	2	1076	C	C6-N1-C2	-5.13	118.25	120.30
44	2	1850	A	N1-C2-N3	-5.13	126.74	129.30
44	2	2022	C	C2-N1-C1'	5.13	124.44	118.80
44	2	2376	A	N1-C2-N3	-5.13	126.74	129.30
44	2	3854	C	C6-N1-C2	-5.13	118.25	120.30
44	2	4588	U	N1-C2-O2	5.13	126.39	122.80
46	4	248	ARG	CA-CB-CG	5.13	124.68	113.40
44	2	228	C	C5-C6-N1	5.13	123.56	121.00
44	2	694	C	C6-N1-C2	-5.13	118.25	120.30
44	2	2632	U	N3-C2-O2	-5.13	118.61	122.20
4	8	72	A	C2-N3-C4	5.12	113.16	110.60
44	2	4775	C	C6-N1-C1'	-5.12	114.65	120.80
44	2	455	C	C5-C6-N1	5.12	123.56	121.00
44	2	1868	A	N1-C2-N3	-5.12	126.74	129.30
44	2	2025	A	P-O3'-C3'	5.12	125.85	119.70
1	5	15	C	C6-N1-C2	-5.12	118.25	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	2	2603	C	C5-C6-N1	5.12	123.56	121.00
44	2	4699	U	OP1-P-O3'	5.12	116.47	105.20
44	2	1334	A	N1-C2-N3	-5.12	126.74	129.30
44	2	3604	A	C2-N3-C4	5.12	113.16	110.60
44	2	2702	C	C6-N1-C2	-5.12	118.25	120.30
44	2	4233	A	N1-C2-N3	-5.12	126.74	129.30
44	2	956	A	N1-C2-N3	-5.11	126.74	129.30
44	2	1602	U	N3-C2-O2	-5.11	118.62	122.20
1	5	77	A	N1-C2-N3	-5.11	126.74	129.30
44	2	47	A	N1-C2-N3	-5.11	126.74	129.30
44	2	279	A	N1-C2-N3	-5.11	126.75	129.30
44	2	4927	G	N3-C4-C5	-5.11	126.05	128.60
44	2	59	A	N1-C2-N3	-5.11	126.75	129.30
1	5	26	C	N1-C2-O2	5.11	121.97	118.90
44	2	297	U	N1-C2-O2	5.11	126.37	122.80
44	2	924	C	C5-C6-N1	5.11	123.55	121.00
44	2	1554	A	N1-C2-N3	-5.11	126.75	129.30
44	2	2708	U	N1-C2-O2	5.11	126.37	122.80
44	2	3931	C	C6-N1-C2	-5.11	118.26	120.30
44	2	2337	C	N3-C2-O2	-5.10	118.33	121.90
4	8	141	C	C5-C6-N1	5.10	123.55	121.00
44	2	363	A	N1-C2-N3	-5.10	126.75	129.30
44	2	1289	C	N3-C2-O2	-5.10	118.33	121.90
44	2	1491	A	N1-C2-N3	-5.10	126.75	129.30
44	2	2035	C	C5-C6-N1	5.10	123.55	121.00
44	2	383	A	N1-C2-N3	-5.10	126.75	129.30
44	2	3845	A	N1-C2-N3	-5.10	126.75	129.30
44	2	51	A	N1-C2-N3	-5.10	126.75	129.30
44	2	2094	G	C8-N9-C1'	-5.10	120.38	127.00
44	2	3741	C	N3-C2-O2	-5.10	118.33	121.90
44	2	360	A	N1-C2-N3	-5.09	126.75	129.30
44	2	3721	U	N3-C2-O2	-5.09	118.63	122.20
44	2	4319	C	C6-N1-C2	-5.09	118.26	120.30
1	5	26	C	C6-N1-C2	-5.09	118.26	120.30
1	5	42	A	C2-N3-C4	5.09	113.15	110.60
4	8	150	C	C5-C6-N1	5.09	123.55	121.00
44	2	53	C	C6-N1-C2	-5.09	118.26	120.30
44	2	1401	C	N3-C2-O2	-5.09	118.34	121.90
44	2	5021	C	C6-N1-C2	-5.09	118.26	120.30
44	2	919	C	N1-C2-O2	5.09	121.95	118.90
44	2	1293	G	C2-N3-C4	5.09	114.44	111.90
44	2	2290	C	C6-N1-C2	-5.09	118.27	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	2	2787	A	N1-C2-N3	-5.09	126.76	129.30
44	2	388	A	N1-C2-N3	-5.09	126.76	129.30
44	2	41	C	C5-C6-N1	5.09	123.54	121.00
44	2	1947	U	N1-C2-O2	5.09	126.36	122.80
44	2	2583	C	C6-N1-C2	-5.09	118.27	120.30
44	2	4127	A	N1-C2-N3	-5.09	126.76	129.30
44	2	1644	C	C5-C6-N1	5.08	123.54	121.00
44	2	49	U	N1-C2-O2	5.08	126.36	122.80
44	2	2360	A	N1-C2-N3	-5.08	126.76	129.30
42	J	30	LEU	CA-CB-CG	5.08	126.99	115.30
44	2	168	C	C6-N1-C2	-5.08	118.27	120.30
44	2	3862	A	N1-C2-N3	-5.08	126.76	129.30
44	2	4619	U	N1-C2-O2	5.08	126.36	122.80
44	2	1807	C	N1-C2-O2	5.08	121.95	118.90
44	2	2563	C	C2-N1-C1'	5.08	124.39	118.80
44	2	2743	A	N1-C2-N3	-5.08	126.76	129.30
44	2	33	A	N1-C2-N3	-5.08	126.76	129.30
44	2	4559	A	N1-C2-N3	-5.08	126.76	129.30
46	4	417	TRP	CA-CB-CG	5.08	123.35	113.70
44	2	1203	G	N3-C4-C5	-5.08	126.06	128.60
44	2	1875	C	N1-C2-O2	5.08	121.95	118.90
44	2	1978	C	C5-C6-N1	5.08	123.54	121.00
44	2	2367	A	N1-C2-N3	-5.08	126.76	129.30
44	2	4708	A	N1-C2-N3	-5.08	126.76	129.30
44	2	4758	U	O4'-C1'-N1	5.08	112.26	108.20
44	2	4480	A	N1-C2-N3	-5.07	126.76	129.30
44	2	4522	G	C8-N9-C1'	-5.07	120.41	127.00
44	2	2016	C	C2-N1-C1'	5.07	124.38	118.80
44	2	15	A	N1-C2-N3	-5.07	126.77	129.30
44	2	2654	C	C6-N1-C2	-5.07	118.27	120.30
44	2	4074	C	C2-N1-C1'	5.07	124.37	118.80
44	2	99	A	N1-C2-N3	-5.07	126.77	129.30
44	2	1477	C	C2-N1-C1'	5.07	124.37	118.80
44	2	2872	C	C5-C6-N1	5.07	123.53	121.00
1	5	29	C	C6-N1-C2	-5.06	118.28	120.30
44	2	1731	C	N3-C2-O2	-5.06	118.36	121.90
44	2	4616	A	N1-C2-N3	-5.06	126.77	129.30
40	A	432	LEU	CA-CB-CG	5.06	126.94	115.30
44	2	988	C	C6-N1-C2	-5.06	118.28	120.30
44	2	4569	U	N3-C2-O2	-5.06	118.66	122.20
4	8	20	A	N1-C2-N3	-5.06	126.77	129.30
44	2	2298	U	N1-C2-O2	5.06	126.34	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	2	2627	C	N3-C2-O2	-5.05	118.36	121.90
44	2	4286	C	C5-C6-N1	5.05	123.53	121.00
44	2	4980	C	C6-N1-C2	-5.05	118.28	120.30
44	2	1601	A	N1-C2-N3	-5.05	126.77	129.30
44	2	1843	A	N1-C2-N3	-5.05	126.77	129.30
4	8	92	U	N3-C2-O2	-5.05	118.66	122.20
44	2	221	C	C6-N1-C2	-5.05	118.28	120.30
44	2	2262	G	C6-C5-N7	-5.05	127.37	130.40
44	2	4486	C	N1-C2-O2	5.05	121.93	118.90
1	5	76	U	C6-N1-C2	-5.05	117.97	121.00
44	2	4540	C	C6-N1-C2	-5.05	118.28	120.30
4	8	57	C	N1-C2-O2	5.04	121.93	118.90
44	2	367	C	C5-C6-N1	5.04	123.52	121.00
44	2	2304	U	C2-N1-C1'	5.04	123.75	117.70
44	2	2368	A	N1-C2-N3	-5.04	126.78	129.30
44	2	4584	A	N1-C2-N3	-5.04	126.78	129.30
44	2	2037	C	C6-N1-C2	-5.04	118.28	120.30
44	2	3668	C	C2-N1-C1'	5.04	124.34	118.80
44	2	3853	U	N1-C2-O2	5.04	126.33	122.80
44	2	709	C	C6-N1-C2	-5.04	118.29	120.30
44	2	1267	C	N3-C2-O2	-5.04	118.38	121.90
1	5	100	A	N1-C2-N3	-5.03	126.78	129.30
44	2	1929	A	N1-C2-N3	-5.03	126.78	129.30
3	7	7	TYR	C-N-CA	5.03	134.28	121.70
44	2	368	C	C6-N1-C2	-5.03	118.29	120.30
44	2	971	U	N3-C2-O2	-5.03	118.68	122.20
44	2	3615	G	C2-N3-C4	5.03	114.42	111.90
44	2	4722	G	N3-C4-N9	5.03	129.02	126.00
44	2	1372	A	N1-C2-N3	-5.03	126.79	129.30
44	2	4477	A	N1-C2-N3	-5.03	126.79	129.30
44	2	2008	U	C6-N1-C1'	-5.03	114.16	121.20
44	2	2856	C	C5-C6-N1	5.03	123.51	121.00
44	2	2833	A	C2-N3-C4	5.02	113.11	110.60
44	2	4193	C	C2-N1-C1'	5.02	124.33	118.80
44	2	2647	A	C2-N3-C4	5.02	113.11	110.60
44	2	4078	C	C5-C6-N1	5.02	123.51	121.00
44	2	4350	C	N1-C2-O2	5.02	121.91	118.90
44	2	420	A	N1-C2-N3	-5.02	126.79	129.30
44	2	3622	C	C2-N1-C1'	5.02	124.32	118.80
44	2	3672	G	N3-C4-N9	5.02	129.01	126.00
44	2	4477	A	C2-N3-C4	5.02	113.11	110.60
44	2	4928	C	C6-N1-C1'	-5.02	114.78	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	2	4771	C	C5-C6-N1	5.02	123.51	121.00
44	2	1395	U	C6-N1-C2	-5.02	117.99	121.00
44	2	1993	C	N1-C2-O2	5.02	121.91	118.90
44	2	1197	C	N3-C2-O2	-5.01	118.39	121.90
44	2	113	A	N1-C2-N3	-5.01	126.79	129.30
44	2	2021	G	N3-C4-C5	-5.01	126.09	128.60
44	2	79	C	C6-N1-C2	-5.01	118.30	120.30
44	2	1367	C	N3-C2-O2	-5.01	118.39	121.90
44	2	1607	C	C2-N1-C1'	5.01	124.31	118.80
44	2	5062	G	N3-C4-C5	-5.01	126.09	128.60
44	2	4268	A	N1-C2-N3	-5.01	126.80	129.30
4	8	32	C	C5-C6-N1	5.01	123.50	121.00
36	n	62	GLY	C-N-CA	5.01	134.22	121.70
44	2	736	C	C6-N1-C2	-5.01	118.30	120.30
44	2	1599	A	N1-C2-N3	-5.01	126.80	129.30
44	2	3694	U	N3-C2-O2	-5.01	118.70	122.20
44	2	108	A	N1-C2-N3	-5.00	126.80	129.30
44	2	4945	G	C4-N9-C1'	5.00	133.01	126.50
4	8	41	A	N1-C2-N3	-5.00	126.80	129.30
44	2	5019	A	N1-C2-N3	-5.00	126.80	129.30
44	2	2031	C	C2-N1-C1'	5.00	124.30	118.80
44	2	2073	C	C5-C6-N1	5.00	123.50	121.00

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
46	4	248	ARG	Peptide
6	B	16	PHE	Peptide
42	J	238	ASP	Peptide
17	N	94	LEU	Peptide
20	Q	154	VAL	Peptide
35	m	54	ARG	Peptide
36	n	106	TYR	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	6	242/245 (99%)	227 (94%)	15 (6%)	0	100	100
3	7	133/163 (82%)	129 (97%)	4 (3%)	0	100	100
5	9	93/134 (69%)	81 (87%)	11 (12%)	1 (1%)	14	41
6	B	401/403 (100%)	382 (95%)	19 (5%)	0	100	100
7	C	89/159 (56%)	86 (97%)	3 (3%)	0	100	100
8	D	356/427 (83%)	335 (94%)	21 (6%)	0	100	100
9	E	96/115 (84%)	94 (98%)	2 (2%)	0	100	100
10	F	107/117 (92%)	104 (97%)	3 (3%)	0	100	100
11	G	240/266 (90%)	231 (96%)	9 (4%)	0	100	100
12	H	120/123 (98%)	116 (97%)	4 (3%)	0	100	100
13	I	188/192 (98%)	179 (95%)	9 (5%)	0	100	100
14	K	100/105 (95%)	93 (93%)	7 (7%)	0	100	100
15	L	145/148 (98%)	137 (94%)	8 (6%)	0	100	100
16	M	84/97 (87%)	79 (94%)	5 (6%)	0	100	100
17	N	163/178 (92%)	147 (90%)	16 (10%)	0	100	100
18	O	67/70 (96%)	62 (92%)	5 (8%)	0	100	100
19	P	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
20	Q	208/211 (99%)	193 (93%)	15 (7%)	0	100	100
21	S	133/215 (62%)	125 (94%)	8 (6%)	0	100	100
22	U	201/204 (98%)	192 (96%)	9 (4%)	0	100	100
23	V	199/203 (98%)	192 (96%)	7 (4%)	0	100	100
24	W	99/106 (93%)	95 (96%)	4 (4%)	0	100	100
25	X	89/92 (97%)	86 (97%)	3 (3%)	0	100	100
26	Z	185/188 (98%)	179 (97%)	6 (3%)	0	100	100
27	a	146/196 (74%)	142 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	b	174/176 (99%)	169 (97%)	5 (3%)	0	100	100
29	c	153/160 (96%)	148 (97%)	5 (3%)	0	100	100
30	e	129/140 (92%)	117 (91%)	12 (9%)	0	100	100
31	g	116/156 (74%)	114 (98%)	2 (2%)	0	100	100
32	h	132/145 (91%)	130 (98%)	2 (2%)	0	100	100
33	i	133/136 (98%)	124 (93%)	9 (7%)	0	100	100
34	l	123/137 (90%)	115 (94%)	8 (6%)	0	100	100
35	m	246/257 (96%)	221 (90%)	25 (10%)	0	100	100
36	n	107/110 (97%)	103 (96%)	3 (3%)	1 (1%)	17	46
37	o	231/288 (80%)	214 (93%)	17 (7%)	0	100	100
38	p	224/248 (90%)	216 (96%)	8 (4%)	0	100	100
39	r	291/297 (98%)	279 (96%)	12 (4%)	0	100	100
40	A	305/731 (42%)	300 (98%)	4 (1%)	1 (0%)	41	72
41	R	151/203 (74%)	148 (98%)	2 (1%)	1 (1%)	22	53
42	J	221/239 (92%)	206 (93%)	15 (7%)	0	100	100
43	T	48/99 (48%)	48 (100%)	0	0	100	100
45	y	163/165 (99%)	158 (97%)	5 (3%)	0	100	100
46	4	607/634 (96%)	559 (92%)	44 (7%)	4 (1%)	22	53
47	d	102/128 (80%)	95 (93%)	7 (7%)	0	100	100
48	j	109/125 (87%)	104 (95%)	5 (5%)	0	100	100
49	k	127/135 (94%)	121 (95%)	6 (5%)	0	100	100
50	Y	165/184 (90%)	158 (96%)	7 (4%)	0	100	100
51	z	63/129 (49%)	59 (94%)	3 (5%)	1 (2%)	9	31
All	All	8052/9430 (85%)	7638 (95%)	405 (5%)	9 (0%)	54	81

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
36	n	106	TYR
5	9	99	GLN
51	z	24	LYS
40	A	160	MET
46	4	88	ASP
46	4	427	ASP

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Mol	Chain	Res	Type
41	R	99	ARG
46	4	407	ASP
46	4	366	THR

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	6	212/213 (100%)	212 (100%)	0	100	100
3	7	126/149 (85%)	126 (100%)	0	100	100
5	9	82/114 (72%)	81 (99%)	1 (1%)	71	92
6	B	349/349 (100%)	348 (100%)	1 (0%)	92	98
7	C	78/126 (62%)	78 (100%)	0	100	100
8	D	298/348 (86%)	297 (100%)	1 (0%)	92	98
9	E	83/97 (86%)	83 (100%)	0	100	100
10	F	94/100 (94%)	94 (100%)	0	100	100
11	G	204/223 (92%)	202 (99%)	2 (1%)	76	93
12	H	109/110 (99%)	109 (100%)	0	100	100
13	I	169/171 (99%)	169 (100%)	0	100	100
14	K	86/89 (97%)	86 (100%)	0	100	100
15	L	120/121 (99%)	119 (99%)	1 (1%)	81	94
16	M	73/80 (91%)	73 (100%)	0	100	100
17	N	138/149 (93%)	138 (100%)	0	100	100
18	O	64/65 (98%)	64 (100%)	0	100	100
19	P	47/48 (98%)	46 (98%)	1 (2%)	53	84
20	Q	176/177 (99%)	176 (100%)	0	100	100
21	S	115/161 (71%)	114 (99%)	1 (1%)	78	94
22	U	171/172 (99%)	171 (100%)	0	100	100
23	V	173/174 (99%)	173 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
24	W	89/94 (95%)	89 (100%)	0	100 100
25	X	74/75 (99%)	74 (100%)	0	100 100
26	Z	164/165 (99%)	164 (100%)	0	100 100
27	a	133/175 (76%)	133 (100%)	0	100 100
28	b	157/157 (100%)	157 (100%)	0	100 100
29	c	136/140 (97%)	136 (100%)	0	100 100
30	e	101/107 (94%)	100 (99%)	1 (1%)	76 93
31	g	106/133 (80%)	106 (100%)	0	100 100
32	h	124/135 (92%)	124 (100%)	0	100 100
33	i	117/118 (99%)	116 (99%)	1 (1%)	78 94
34	l	109/121 (90%)	109 (100%)	0	100 100
35	m	190/199 (96%)	190 (100%)	0	100 100
36	n	88/89 (99%)	88 (100%)	0	100 100
37	o	208/252 (82%)	205 (99%)	3 (1%)	67 90
38	p	195/215 (91%)	195 (100%)	0	100 100
39	r	246/250 (98%)	245 (100%)	1 (0%)	91 97
40	A	272/654 (42%)	271 (100%)	1 (0%)	91 97
41	R	141/184 (77%)	140 (99%)	1 (1%)	84 95
42	J	199/214 (93%)	197 (99%)	2 (1%)	76 93
43	T	43/76 (57%)	43 (100%)	0	100 100
45	y	137/137 (100%)	136 (99%)	1 (1%)	84 95
46	4	554/574 (96%)	552 (100%)	2 (0%)	91 97
47	d	94/115 (82%)	94 (100%)	0	100 100
48	j	101/110 (92%)	100 (99%)	1 (1%)	76 93
49	k	115/121 (95%)	115 (100%)	0	100 100
50	Y	147/163 (90%)	146 (99%)	1 (1%)	84 95
51	z	61/115 (53%)	61 (100%)	0	100 100
All	All	7068/8124 (87%)	7045 (100%)	23 (0%)	92 98

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	9	116	ARG

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Mol	Chain	Res	Type
6	B	300	LYS
8	D	188	ARG
11	G	137[A]	ARG
11	G	137[B]	ARG
15	L	94	LYS
19	P	21	ARG
21	S	125	ASN
30	e	48	ARG
33	i	108	ARG
37	o	56	ARG
37	o	210	LYS
37	o	221	LYS
39	r	277	LYS
40	A	428	ARG
41	R	68	ARG
42	J	118	LYS
42	J	214	ARG
45	y	54	LYS
46	4	160	ARG
46	4	385	ARG
48	j	101	LYS
50	Y	97	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
15	L	66	ASN
28	b	77	ASN
35	m	215	ASN
42	J	50	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	5	119/120 (99%)	16 (13%)	0
4	8	155/156 (99%)	31 (20%)	0
44	2	3481/5054 (68%)	776 (22%)	15 (0%)
All	All	3755/5330 (70%)	823 (21%)	15 (0%)

All (823) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	5	11	A
1	5	24	C
1	5	29	C
1	5	33	U
1	5	37	G
1	5	40	U
1	5	50	A
1	5	53	U
1	5	54	A
1	5	63	C
1	5	64	G
1	5	74	A
1	5	97	G
1	5	100	A
1	5	110	G
1	5	120	U
4	8	23	C
4	8	24	G
4	8	25	G
4	8	34	U
4	8	35	C
4	8	37	A
4	8	38	U
4	8	48	A
4	8	52	A
4	8	59	A
4	8	60	G
4	8	62	A
4	8	63	U
4	8	82	A
4	8	84	A
4	8	85	U
4	8	86	U
4	8	87	G
4	8	103	A
4	8	104	A
4	8	105	C
4	8	110	U
4	8	111	U
4	8	114	G
4	8	123	U
4	8	124	U
4	8	125	C

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Mol	Chain	Res	Type
4	8	126	C
4	8	127	U
4	8	151	G
4	8	156	U
44	2	6	C
44	2	39	A
44	2	42	A
44	2	48	G
44	2	56	A
44	2	59	A
44	2	64	A
44	2	65	A
44	2	69	A
44	2	72	C
44	2	73	A
44	2	91	G
44	2	98	A
44	2	104	G
44	2	108	A
44	2	109	G
44	2	110	C
44	2	119	G
44	2	120	A
44	2	122	U
44	2	131	C
44	2	133	C
44	2	134	G
44	2	135	G
44	2	136	C
44	2	137	G
44	2	143	C
44	2	144	G
44	2	152	U
44	2	158	A
44	2	159	C
44	2	171	U
44	2	178	C
44	2	183	C
44	2	184	U
44	2	185	C
44	2	187	U
44	2	188	G

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Mol	Chain	Res	Type
44	2	197	A
44	2	200	U
44	2	201	C
44	2	209	U
44	2	218	A
44	2	220	C
44	2	234	G
44	2	254	G
44	2	255	C
44	2	256	G
44	2	259	C
44	2	260	C
44	2	261	G
44	2	262	G
44	2	265	C
44	2	266	C
44	2	267	G
44	2	279	A
44	2	280	G
44	2	297	U
44	2	306	A
44	2	315	G
44	2	316	U
44	2	340	C
44	2	349	A
44	2	387	G
44	2	396	A
44	2	398	A2M
44	2	407	A
44	2	409	G
44	2	410	A
44	2	411	G
44	2	412	G
44	2	432	U
44	2	433	A
44	2	440	U
44	2	449	C
44	2	450	G
44	2	452	A
44	2	453	G
44	2	454	U
44	2	456	C

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Mol	Chain	Res	Type
44	2	465	G
44	2	467	U
44	2	468	U
44	2	483	G
44	2	484	U
44	2	485	C
44	2	486	C
44	2	489	C
44	2	493	G
44	2	495	C
44	2	496	G
44	2	497	G
44	2	498	C
44	2	499	G
44	2	500	G
44	2	502	C
44	2	504	G
44	2	505	G
44	2	509	A
44	2	510	U
44	2	512	U
44	2	513	U
44	2	514	U
44	2	515	C
44	2	516	C
44	2	518	G
44	2	519	C
44	2	644	G
44	2	646	G
44	2	647	G
44	2	657	C
44	2	658	C
44	2	659	G
44	2	662	C
44	2	667	A
44	2	668	C
44	2	673	C
44	2	686	A
44	2	688	U
44	2	692	A
44	2	696	C
44	2	697	G

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Mol	Chain	Res	Type
44	2	703	G
44	2	704	C
44	2	708	G
44	2	731	G
44	2	738	C
44	2	739	G
44	2	740	G
44	2	742	G
44	2	746	A
44	2	759	G
44	2	904	C
44	2	905	C
44	2	913	U
44	2	914	U
44	2	915	A
44	2	916	C
44	2	917	A
44	2	918	G
44	2	924	C
44	2	925	C
44	2	926	G
44	2	932	A
44	2	933	G
44	2	936	C
44	2	941	C
44	2	943	A
44	2	945	U
44	2	956	A
44	2	959	G
44	2	960	A
44	2	961	G
44	2	962	C
44	2	965	G
44	2	966	A
44	2	967	C
44	2	969	C
44	2	970	G
44	2	971	U
44	2	972	C
44	2	977	C
44	2	982	U
44	2	984	C

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Mol	Chain	Res	Type
44	2	988	C
44	2	990	C
44	2	991	C
44	2	992	C
44	2	993	G
44	2	994	G
44	2	995	C
44	2	1048	G
44	2	1049	C
44	2	1051	G
44	2	1065	G
44	2	1066	G
44	2	1068	G
44	2	1070	G
44	2	1071	C
44	2	1072	C
44	2	1082	C
44	2	1083	U
44	2	1095	A
44	2	1100	U
44	2	1168	G
44	2	1173	G
44	2	1177	U
44	2	1178	G
44	2	1179	U
44	2	1180	C
44	2	1182	C
44	2	1183	C
44	2	1184	A
44	2	1187	G
44	2	1194	G
44	2	1198	G
44	2	1200	G
44	2	1202	C
44	2	1203	G
44	2	1210	C
44	2	1211	G
44	2	1215	C
44	2	1216	C
44	2	1222	A
44	2	1241	C
44	2	1244	G

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Mol	Chain	Res	Type
44	2	1245	C
44	2	1252	C
44	2	1253	G
44	2	1254	A
44	2	1255	A
44	2	1260	G
44	2	1265	G
44	2	1266	G
44	2	1269	G
44	2	1271	G
44	2	1272	C
44	2	1275	G
44	2	1280	C
44	2	1283	G
44	2	1284	G
44	2	1287	G
44	2	1294	A
44	2	1295	C
44	2	1296	G
44	2	1301	C
44	2	1303	A
44	2	1314	C
44	2	1320	U
44	2	1321	G
44	2	1322	A
44	2	1326	A2M
44	2	1337	A
44	2	1354	A
44	2	1358	G
44	2	1359	G
44	2	1365	C
44	2	1366	G
44	2	1370	G
44	2	1371	A
44	2	1377	G
44	2	1378	C
44	2	1379	C
44	2	1387	A
44	2	1394	G
44	2	1397	A
44	2	1398	A
44	2	1402	C

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Mol	Chain	Res	Type
44	2	1404	G
44	2	1407	C
44	2	1409	C
44	2	1410	U
44	2	1414	C
44	2	1419	G
44	2	1420	A
44	2	1425	G
44	2	1439	C
44	2	1441	C
44	2	1442	C
44	2	1444	G
44	2	1445	U
44	2	1446	C
44	2	1447	C
44	2	1448	G
44	2	1450	C
44	2	1482	G
44	2	1483	C
44	2	1493	G
44	2	1497	A
44	2	1498	G
44	2	1502	G
44	2	1503	A
44	2	1518	A
44	2	1534	A2M
44	2	1547	A
44	2	1554	A
44	2	1559	G
44	2	1564	A
44	2	1566	C
44	2	1578	U
44	2	1592	G
44	2	1595	G
44	2	1596	U
44	2	1613	A
44	2	1624	G
44	2	1625	OMG
44	2	1626	G
44	2	1631	A
44	2	1633	G
44	2	1634	A

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Mol	Chain	Res	Type
44	2	1637	A
44	2	1638	A
44	2	1641	G
44	2	1642	A
44	2	1650	A
44	2	1654	G
44	2	1661	C
44	2	1676	C
44	2	1677	U
44	2	1678	C
44	2	1685	G
44	2	1691	G
44	2	1694	C
44	2	1697	G
44	2	1699	A
44	2	1700	G
44	2	1701	A
44	2	1702	C
44	2	1703	C
44	2	1704	C
44	2	1705	G
44	2	1707	C
44	2	1716	G
44	2	1718	C
44	2	1719	A
44	2	1724	G
44	2	1726	U
44	2	1734	G
44	2	1803	G
44	2	1804	A
44	2	1815	G
44	2	1821	G
44	2	1822	U
44	2	1834	U
44	2	1836	G
44	2	1837	A
44	2	1842	G
44	2	1843	A
44	2	1854	G
44	2	1855	G
44	2	1866	UR3
44	2	1868	A

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Mol	Chain	Res	Type
44	2	1869	G
44	2	1881	C
44	2	1883	OMG
44	2	1888	A
44	2	1889	U
44	2	1890	G
44	2	1891	A
44	2	1897	A
44	2	1900	C
44	2	1916	G
44	2	1918	U
44	2	1919	G
44	2	1920	C
44	2	1921	C
44	2	1922	G
44	2	1925	G
44	2	1931	C
44	2	1932	A
44	2	1938	C
44	2	1948	G
44	2	1951	G
44	2	1958	A
44	2	1959	U
44	2	1960	A
44	2	1961	G
44	2	1962	A
44	2	1968	G
44	2	1971	C
44	2	1972	G
44	2	1974	U
44	2	1979	A
44	2	1980	U
44	2	1981	G
44	2	1982	G
44	2	1983	A
44	2	1984	A
44	2	1990	A
44	2	2001	G
44	2	2002	A
44	2	2003	G
44	2	2004	U
44	2	2011	C

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Mol	Chain	Res	Type
44	2	2016	C
44	2	2021	G
44	2	2024	G
44	2	2025	A
44	2	2026	A
44	2	2033	A
44	2	2034	G
44	2	2042	A
44	2	2043	A
44	2	2044	U
44	2	2046	G
44	2	2048	U
44	2	2055	G
44	2	2056	G
44	2	2069	A
44	2	2084	C
44	2	2085	G
44	2	2090	U
44	2	2092	G
44	2	2093	A
44	2	2095	A
44	2	2097	U
44	2	2098	G
44	2	2100	A
44	2	2101	C
44	2	2102	G
44	2	2104	G
44	2	2105	A
44	2	2106	G
44	2	2110	C
44	2	2111	G
44	2	2112	G
44	2	2113	C
44	2	2250	C
44	2	2252	G
44	2	2253	A
44	2	2254	G
44	2	2255	C
44	2	2256	C
44	2	2258	C
44	2	2259	G
44	2	2262	G

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Mol	Chain	Res	Type
44	2	2263	A
44	2	2289	C
44	2	2300	A
44	2	2301	G
44	2	2306	G
44	2	2313	A
44	2	2331	G
44	2	2333	G
44	2	2348	G
44	2	2350	U
44	2	2351	C
44	2	2364	OMG
44	2	2395	A
44	2	2416	G
44	2	2417	A
44	2	2418	A
44	2	2422	OMC
44	2	2424	OMG
44	2	2425	U
44	2	2441	C
44	2	2447	U
44	2	2450	G
44	2	2453	A
44	2	2464	C
44	2	2465	C
44	2	2469	C
44	2	2471	G
44	2	2475	G
44	2	2479	G
44	2	2483	G
44	2	2485	U
44	2	2489	C
44	2	2490	U
44	2	2491	C
44	2	2493	G
44	2	2494	U
44	2	2503	G
44	2	2504	C
44	2	2505	C
44	2	2511	A
44	2	2512	A
44	2	2513	A

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Mol	Chain	Res	Type
44	2	2519	U
44	2	2529	A
44	2	2543	A
44	2	2544	G
44	2	2546	G
44	2	2554	U
44	2	2555	G
44	2	2559	G
44	2	2560	C
44	2	2566	G
44	2	2573	A
44	2	2583	C
44	2	2586	G
44	2	2587	A
44	2	2589	C
44	2	2601	A
44	2	2602	G
44	2	2618	G
44	2	2627	C
44	2	2652	G
44	2	2653	C
44	2	2661	U
44	2	2662	G
44	2	2669	C
44	2	2670	C
44	2	2674	A
44	2	2675	G
44	2	2679	G
44	2	2687	U
44	2	2694	G
44	2	2695	A
44	2	2696	A
44	2	2703	G
44	2	2707	U
44	2	2708	U
44	2	2710	C
44	2	2711	G
44	2	2712	G
44	2	2719	C
44	2	2721	G
44	2	2724	G
44	2	2725	A

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Mol	Chain	Res	Type
44	2	2726	G
44	2	2739	C
44	2	2742	G
44	2	2743	A
44	2	2756	G
44	2	2761	U
44	2	2763	U
44	2	2769	U
44	2	2770	C
44	2	2788	U
44	2	2789	A
44	2	2790	U
44	2	2795	A
44	2	2799	G
44	2	2814	C
44	2	2815	A
44	2	2826	U
44	2	2827	G
44	2	2835	A
44	2	2846	G
44	2	2855	G
44	2	2857	A
44	2	2877	G
44	2	2897	G
44	2	2901	G
44	2	2902	G
44	2	2903	G
44	2	2904	U
44	2	2905	C
44	2	2906	G
44	2	2907	G
44	2	2908	U
44	2	3585	G
44	2	3588	C
44	2	3591	C
44	2	3594	C
44	2	3595	U
44	2	3596	A
44	2	3597	G
44	2	3598	C
44	2	3599	A
44	2	3605	C

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Mol	Chain	Res	Type
44	2	3606	U
44	2	3615	G
44	2	3626	G
44	2	3635	A
44	2	3644	U
44	2	3648	A
44	2	3662	A
44	2	3670	C
44	2	3672	G
44	2	3673	C
44	2	3680	U
44	2	3697	U
44	2	3698	G
44	2	3709	U
44	2	3710	G
44	2	3711	A
44	2	3712	A
44	2	3723	A2M
44	2	3729	U
44	2	3735	G
44	2	3736	A
44	2	3748	A
44	2	3824	A
44	2	3838	U
44	2	3839	G
44	2	3840	U
44	2	3867	A2M
44	2	3871	A
44	2	3877	A
44	2	3878	C
44	2	3879	G
44	2	3898	G
44	2	3903	A
44	2	3904	G
44	2	3905	A
44	2	3906	A
44	2	3915	U
44	2	3923	A
44	2	3938	G
44	2	3939	G
44	2	3944	G
44	2	4067	U

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Mol	Chain	Res	Type
44	2	4068	U
44	2	4076	G
44	2	4084	G
44	2	4095	G
44	2	4099	G
44	2	4100	C
44	2	4102	C
44	2	4103	C
44	2	4104	G
44	2	4106	G
44	2	4110	C
44	2	4112	C
44	2	4114	C
44	2	4115	G
44	2	4116	C
44	2	4117	U
44	2	4119	C
44	2	4121	G
44	2	4137	C
44	2	4139	G
44	2	4140	C
44	2	4141	G
44	2	4142	C
44	2	4143	G
44	2	4144	C
44	2	4162	C
44	2	4163	U
44	2	4170	A
44	2	4183	G
44	2	4184	G
44	2	4191	G
44	2	4194	U
44	2	4195	G
44	2	4196	OMG
44	2	4201	G
44	2	4212	A
44	2	4221	C
44	2	4225	G
44	2	4228	G
44	2	4229	U
44	2	4233	A
44	2	4249	G

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Mol	Chain	Res	Type
44	2	4251	A
44	2	4254	G
44	2	4256	A
44	2	4265	U
44	2	4268	A
44	2	4271	A
44	2	4273	A
44	2	4281	A
44	2	4291	G
44	2	4295	U
44	2	4305	G
44	2	4306	OMU
44	2	4314	C
44	2	4329	G
44	2	4330	G
44	2	4332	C
44	2	4339	A
44	2	4349	C
44	2	4352	U
44	2	4354	U
44	2	4372	U
44	2	4373	G
44	2	4377	G
44	2	4378	A
44	2	4379	A
44	2	4380	A
44	2	4381	A
44	2	4386	C
44	2	4387	C
44	2	4396	A
44	2	4410	G
44	2	4415	1MA
44	2	4418	G
44	2	4422	A
44	2	4428	A
44	2	4436	U
44	2	4437	U
44	2	4451	G
44	2	4452	U
44	2	4453	C
44	2	4464	A
44	2	4466	C

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Mol	Chain	Res	Type
44	2	4475	G
44	2	4476	C
44	2	4484	A
44	2	4488	A
44	2	4498	U
44	2	4499	G
44	2	4508	C
44	2	4510	A
44	2	4512	U
44	2	4513	A
44	2	4518	A
44	2	4519	C
44	2	4523	A2M
44	2	4524	G
44	2	4530	UR3
44	2	4545	G
44	2	4549	G
44	2	4555	U
44	2	4556	U
44	2	4557	U
44	2	4558	U
44	2	4560	C
44	2	4569	U
44	2	4584	A
44	2	4589	A
44	2	4590	A
44	2	4600	G
44	2	4601	U
44	2	4607	A
44	2	4608	G
44	2	4635	A
44	2	4636	U
44	2	4637	OMG
44	2	4656	A
44	2	4657	U
44	2	4670	C
44	2	4678	G
44	2	4684	A
44	2	4694	G
44	2	4695	C
44	2	4700	A
44	2	4702	G

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Mol	Chain	Res	Type
44	2	4708	A
44	2	4709	U
44	2	4719	G
44	2	4720	C
44	2	4730	C
44	2	4731	G
44	2	4733	C
44	2	4734	A
44	2	4740	G
44	2	4741	C
44	2	4742	G
44	2	4745	G
44	2	4754	G
44	2	4757	C
44	2	4759	C
44	2	4761	G
44	2	4764	A
44	2	4765	G
44	2	4771	C
44	2	4775	C
44	2	4776	G
44	2	4859	C
44	2	4862	G
44	2	4870	OMG
44	2	4871	C
44	2	4872	2MG
44	2	4877	G
44	2	4882	U
44	2	4883	C
44	2	4895	C
44	2	4896	G
44	2	4900	C
44	2	4901	G
44	2	4907	G
44	2	4910	G
44	2	4912	G
44	2	4914	C
44	2	4915	G
44	2	4928	C
44	2	4935	C
44	2	4938	A
44	2	4940	C

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Mol	Chain	Res	Type
44	2	4941	G
44	2	4943	A
44	2	4976	U
44	2	4989	U
44	2	4990	C
44	2	4991	U
44	2	5013	C
44	2	5014	A
44	2	5017	G
44	2	5022	U
44	2	5023	C
44	2	5026	U
44	2	5027	C
44	2	5028	G
44	2	5030	U
44	2	5031	G
44	2	5034	A
44	2	5041	G
44	2	5047	C
44	2	5050	C
44	2	5054	C
44	2	5058	A
44	2	5062	G
44	2	5069	U

All (15) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
44	2	406	C
44	2	914	U
44	2	1633	G
44	2	1676	C
44	2	1980	U
44	2	2015	U
44	2	2033	A
44	2	2760	G
44	2	3596	A
44	2	3905	A
44	2	4378	A
44	2	4498	U
44	2	4555	U
44	2	4699	U

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Mol	Chain	Res	Type
44	2	4913	G

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

80 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	$\#\|Z\| > 2$
44	OMC	2	4536	44	19,22,23	3.00	8 (42%)	26,31,34	1.15	3 (11%)
44	7MG	2	1605	44	22,26,27	3.79	10 (45%)	29,39,42	1.96	8 (27%)
44	OMG	2	2424	44	18,26,27	2.85	8 (44%)	19,38,41	1.49	3 (15%)
44	OMG	2	4870	44	18,26,27	2.87	8 (44%)	19,38,41	1.58	4 (21%)
44	A2M	2	3825	44	18,25,26	3.61	8 (44%)	18,36,39	3.37	3 (16%)
44	2MG	2	729	44	18,26,27	2.62	6 (33%)	16,38,41	1.38	3 (18%)
44	OMG	2	1625	44	18,26,27	2.87	8 (44%)	19,38,41	1.42	4 (21%)
44	A2M	2	3723	44	18,25,26	3.57	8 (44%)	18,36,39	3.41	4 (22%)
44	M7A	2	4564	44	20,25,26	1.98	3 (15%)	28,37,40	3.90	6 (21%)
44	5MC	2	4335	44	18,22,23	3.56	7 (38%)	26,32,35	1.07	2 (7%)
44	OMU	2	4306	44	19,22,23	3.02	8 (42%)	26,31,34	1.70	4 (15%)
44	B8K	2	4690	44	24,28,29	3.31	12 (50%)	30,42,45	2.64	12 (40%)
44	B9B	2	2754	44	21,28,29	2.02	3 (14%)	23,40,43	6.49	4 (17%)
44	UR3	2	4597	44	19,22,23	2.76	6 (31%)	26,32,35	2.11	6 (23%)
44	E7G	2	1797	44	24,27,28	4.04	11 (45%)	30,40,43	2.29	10 (33%)
44	UR3	2	4530	44	19,22,23	2.87	7 (36%)	26,32,35	1.34	2 (7%)
44	A2M	2	1534	44	18,25,26	3.60	8 (44%)	18,36,39	3.62	4 (22%)
44	OMG	2	2773	44	18,26,27	2.85	8 (44%)	19,38,41	1.47	5 (26%)
44	7MG	2	2522	44	22,26,27	3.67	10 (45%)	29,39,42	2.00	9 (31%)
44	OMC	2	2861	44	19,22,23	3.03	8 (42%)	26,31,34	1.06	2 (7%)
44	A2M	2	3867	44	18,25,26	3.61	8 (44%)	18,36,39	3.42	4 (22%)
44	B8H	2	4296	44	19,22,23	6.77	6 (31%)	22,32,35	2.30	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
44	B8W	2	4472	44	18,26,27	2.12	2 (11%)	21,38,41	2.63	7 (33%)
44	B8T	2	4671	44	19,22,23	3.55	8 (42%)	26,31,34	0.97	1 (3%)
44	OMG	2	4370	44	18,26,27	2.81	8 (44%)	19,38,41	1.50	5 (26%)
44	OMC	2	3909	44	19,22,23	3.04	8 (42%)	26,31,34	1.23	3 (11%)
44	A2M	2	2401	44	18,25,26	3.60	8 (44%)	18,36,39	3.39	3 (16%)
44	OMG	2	1316	44	18,26,27	2.80	8 (44%)	19,38,41	1.62	5 (26%)
44	A2M	2	4571	44	18,25,26	3.59	8 (44%)	18,36,39	3.40	4 (22%)
44	BGH	2	3899	44	25,29,30	4.56	17 (68%)	31,43,46	2.61	12 (38%)
44	UR3	2	1866	44	19,22,23	2.91	6 (31%)	26,32,35	1.31	2 (7%)
44	A2M	2	398	44	18,25,26	3.59	8 (44%)	18,36,39	3.47	4 (22%)
44	6MZ	2	4220	44	18,25,26	1.89	3 (16%)	16,36,39	3.68	3 (18%)
44	2MG	2	4872	44	18,26,27	2.54	6 (33%)	16,38,41	1.80	4 (25%)
44	E7G	2	2297	44	24,27,28	3.93	11 (45%)	30,40,43	2.14	9 (30%)
44	OMG	2	4196	44	18,26,27	2.96	7 (38%)	19,38,41	1.65	6 (31%)
44	OMG	2	1883	44	18,26,27	2.82	8 (44%)	19,38,41	1.56	6 (31%)
4	OMU	8	14	4,44	19,22,23	2.91	8 (42%)	26,31,34	1.80	6 (23%)
44	2MG	2	1517	44	18,26,27	2.68	6 (33%)	16,38,41	1.57	3 (18%)
44	OMC	2	2804	44	19,22,23	2.94	8 (42%)	26,31,34	1.22	3 (11%)
44	OMC	2	2422	44,50	19,22,23	2.98	8 (42%)	26,31,34	1.10	2 (7%)
44	A2M	2	1524	44	18,25,26	3.61	8 (44%)	18,36,39	3.42	4 (22%)
44	5MU	2	4083	44	19,22,23	7.23	8 (42%)	28,32,35	3.38	10 (35%)
44	OMC	2	3887	44	19,22,23	3.03	8 (42%)	26,31,34	0.92	1 (3%)
44	B8H	2	1860	44	19,22,23	6.75	6 (31%)	22,32,35	2.28	5 (22%)
44	B8W	2	4129	44	18,26,27	2.11	2 (11%)	21,38,41	2.49	8 (38%)
44	B8W	2	4185	44	18,26,27	2.11	2 (11%)	21,38,41	2.48	7 (33%)
44	1MA	2	4415	44	16,25,26	4.35	5 (31%)	18,37,40	1.69	3 (16%)
44	OMG	2	2364	44	18,26,27	2.78	8 (44%)	19,38,41	1.56	5 (26%)
44	P7G	2	1909	44	24,28,29	3.96	11 (45%)	27,41,44	1.59	4 (14%)
44	E6G	2	4355	44	20,27,28	2.77	3 (15%)	22,39,42	3.04	7 (31%)
44	B8T	2	4483	44	19,22,23	3.64	8 (42%)	26,31,34	1.31	3 (11%)
44	B8K	2	3897	44	24,28,29	3.41	11 (45%)	30,42,45	2.54	11 (36%)
44	OMC	2	3869	44	19,22,23	3.04	8 (42%)	26,31,34	1.63	5 (19%)
44	B9B	2	1574	44	21,28,29	1.94	3 (14%)	23,40,43	6.41	5 (21%)
44	OMG	2	1522	44	18,26,27	2.76	8 (44%)	19,38,41	1.51	5 (26%)
44	7MG	2	4550	44	22,26,27	3.84	10 (45%)	29,39,42	1.96	9 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
44	B9B	2	237	44	21,28,29	1.97	3 (14%)	23,40,43	6.57	5 (21%)
44	B8W	2	4529	44	18,26,27	2.13	2 (11%)	21,38,41	2.69	7 (33%)
44	OMC	2	3701	44	19,22,23	2.98	8 (42%)	26,31,34	0.82	0
44	A2M	2	3718	44	18,25,26	3.59	8 (44%)	18,36,39	3.42	4 (22%)
44	OMC	2	2365	44	19,22,23	2.91	8 (42%)	26,31,34	0.82	0
44	MHG	2	4371	44	29,32,33	3.94	11 (37%)	34,46,49	2.32	12 (35%)
44	P7G	2	3880	44	24,28,29	4.04	11 (45%)	27,41,44	1.53	4 (14%)
44	OMG	2	4637	44	18,26,27	2.78	8 (44%)	19,38,41	1.56	5 (26%)
44	B9H	2	2786	44	20,25,26	3.35	4 (20%)	22,35,38	2.75	7 (31%)
44	B8W	2	2380	44	18,26,27	2.03	2 (11%)	21,38,41	2.36	6 (28%)
44	OMU	2	4620	44	19,22,23	2.94	8 (42%)	26,31,34	1.67	5 (19%)
44	A2M	2	4523	44	18,25,26	3.57	8 (44%)	18,36,39	3.39	4 (22%)
44	OMG	2	2050	44	18,26,27	2.77	8 (44%)	19,38,41	1.55	5 (26%)
44	OMG	2	4494	44	18,26,27	2.87	8 (44%)	19,38,41	1.46	4 (21%)
44	2MG	2	978	44	18,26,27	2.68	6 (33%)	16,38,41	1.41	4 (25%)
44	OMG	2	4623	44	18,26,27	2.72	8 (44%)	19,38,41	1.58	4 (21%)
44	I4U	2	1659	44	21,24,25	3.50	9 (42%)	27,34,37	1.31	2 (7%)
44	B8Q	2	1456	44	17,22,23	2.97	5 (29%)	22,32,35	2.39	6 (27%)
44	A2M	2	1326	44	18,25,26	3.69	9 (50%)	18,36,39	3.50	4 (22%)
44	OMG	2	373	44	18,26,27	2.85	8 (44%)	19,38,41	1.66	5 (26%)
44	A2M	2	2363	44	18,25,26	3.59	8 (44%)	18,36,39	3.38	4 (22%)
44	A2M	2	1871	44	18,25,26	3.58	8 (44%)	18,36,39	3.40	3 (16%)
44	P4U	2	1348	44	21,24,25	3.52	8 (38%)	27,33,36	1.09	2 (7%)

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
44	OMC	2	4536	44	-	0/9/27/28	0/2/2/2
44	7MG	2	1605	44	-	0/7/37/38	0/3/3/3
44	OMG	2	2424	44	-	2/5/27/28	0/3/3/3
44	OMG	2	4870	44	-	3/5/27/28	0/3/3/3
44	A2M	2	3825	44	-	0/5/27/28	0/3/3/3
44	2MG	2	729	44	-	1/5/27/28	0/3/3/3
44	OMG	2	1625	44	-	2/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	A2M	2	3723	44	-	2/5/27/28	0/3/3/3
44	M7A	2	4564	44	-	0/7/37/38	0/3/3/3
44	5MC	2	4335	44	-	0/7/25/26	0/2/2/2
44	OMU	2	4306	44	-	0/9/27/28	0/2/2/2
44	B8K	2	4690	44	-	1/11/41/42	0/3/3/3
44	B9B	2	2754	44	-	3/7/29/30	0/3/3/3
44	UR3	2	4597	44	-	0/7/25/26	0/2/2/2
44	E7G	2	1797	44	-	2/9/39/40	0/3/3/3
44	UR3	2	4530	44	-	0/7/25/26	0/2/2/2
44	A2M	2	1534	44	-	1/5/27/28	0/3/3/3
44	OMG	2	2773	44	-	1/5/27/28	0/3/3/3
44	7MG	2	2522	44	-	0/7/37/38	0/3/3/3
44	OMC	2	2861	44	-	0/9/27/28	0/2/2/2
44	A2M	2	3867	44	-	2/5/27/28	0/3/3/3
44	B8H	2	4296	44	-	2/7/25/26	0/2/2/2
44	B8W	2	4472	44	-	1/5/27/28	0/3/3/3
44	B8T	2	4671	44	-	0/7/27/28	0/2/2/2
44	OMG	2	4370	44	-	0/5/27/28	0/3/3/3
44	OMC	2	3909	44	-	0/9/27/28	0/2/2/2
44	A2M	2	2401	44	-	1/5/27/28	0/3/3/3
44	OMG	2	1316	44	-	1/5/27/28	0/3/3/3
44	A2M	2	4571	44	-	0/5/27/28	0/3/3/3
44	BGH	2	3899	44	-	0/13/43/44	0/3/3/3
44	UR3	2	1866	44	-	2/7/25/26	0/2/2/2
44	A2M	2	398	44	-	2/5/27/28	0/3/3/3
44	6MZ	2	4220	44	-	0/5/27/28	0/3/3/3
44	2MG	2	4872	44	-	2/5/27/28	0/3/3/3
44	E7G	2	2297	44	-	1/9/39/40	0/3/3/3
44	OMG	2	4196	44	-	2/5/27/28	0/3/3/3
44	OMG	2	1883	44	-	2/5/27/28	0/3/3/3
4	OMU	8	14	4,44	-	1/9/27/28	0/2/2/2
44	2MG	2	1517	44	-	3/5/27/28	0/3/3/3
44	OMC	2	2804	44	-	0/9/27/28	0/2/2/2
44	OMC	2	2422	44,50	-	1/9/27/28	0/2/2/2
44	A2M	2	1524	44	-	2/5/27/28	0/3/3/3
44	5MU	2	4083	44	-	0/7/25/26	0/2/2/2
44	OMC	2	3887	44	-	1/9/27/28	0/2/2/2
44	B8H	2	1860	44	-	0/7/25/26	0/2/2/2
44	B8W	2	4129	44	-	2/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	B8W	2	4185	44	-	2/5/27/28	0/3/3/3
44	1MA	2	4415	44	-	3/3/25/26	0/3/3/3
44	OMG	2	2364	44	-	2/5/27/28	0/3/3/3
44	P7G	2	1909	44	-	2/10/40/41	0/3/3/3
44	E6G	2	4355	44	-	2/6/28/29	0/3/3/3
44	B8T	2	4483	44	-	0/7/27/28	0/2/2/2
44	B8K	2	3897	44	-	3/11/41/42	0/3/3/3
44	OMC	2	3869	44	-	5/9/27/28	0/2/2/2
44	B9B	2	1574	44	-	3/7/29/30	0/3/3/3
44	OMG	2	1522	44	-	0/5/27/28	0/3/3/3
44	7MG	2	4550	44	-	0/7/37/38	0/3/3/3
44	B9B	2	237	44	-	5/7/29/30	0/3/3/3
44	B8W	2	4529	44	-	0/5/27/28	0/3/3/3
44	OMC	2	3701	44	-	4/9/27/28	0/2/2/2
44	A2M	2	3718	44	-	0/5/27/28	0/3/3/3
44	OMC	2	2365	44	-	0/9/27/28	0/2/2/2
44	MHG	2	4371	44	-	3/16/46/47	0/3/3/3
44	P7G	2	3880	44	-	4/10/40/41	0/3/3/3
44	OMG	2	4637	44	-	3/5/27/28	0/3/3/3
44	B9H	2	2786	44	-	1/12/47/48	0/2/2/2
44	B8W	2	2380	44	-	2/5/27/28	0/3/3/3
44	OMU	2	4620	44	-	0/9/27/28	0/2/2/2
44	A2M	2	4523	44	-	3/5/27/28	0/3/3/3
44	OMG	2	2050	44	-	0/5/27/28	0/3/3/3
44	OMG	2	4494	44	-	0/5/27/28	0/3/3/3
44	2MG	2	978	44	-	0/5/27/28	0/3/3/3
44	OMG	2	4623	44	-	0/5/27/28	0/3/3/3
44	I4U	2	1659	44	-	2/9/29/30	0/2/2/2
44	B8Q	2	1456	44	-	0/7/42/43	0/2/2/2
44	A2M	2	1326	44	-	3/5/27/28	0/3/3/3
44	OMG	2	373	44	-	1/5/27/28	0/3/3/3
44	A2M	2	2363	44	-	0/5/27/28	0/3/3/3
44	A2M	2	1871	44	-	0/5/27/28	0/3/3/3
44	P4U	2	1348	44	-	2/10/29/30	0/2/2/2

All (590) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	2	4083	5MU	C4-C5	20.75	1.79	1.44
44	2	4296	B8H	C6-C5	-16.42	1.11	1.34
44	2	1860	B8H	C6-C5	-16.38	1.11	1.34
44	2	4415	1MA	C2-N3	16.04	1.48	1.29
44	2	4083	5MU	C6-N1	15.93	1.65	1.38
44	2	4296	B8H	C4-N3	-15.69	1.09	1.38
44	2	1860	B8H	C4-N3	-15.52	1.10	1.38
44	2	1860	B8H	C4-C5	13.28	1.82	1.44
44	2	4296	B8H	C4-C5	13.24	1.81	1.44
44	2	1860	B8H	C6-N1	12.21	1.66	1.36
44	2	4296	B8H	C6-N1	12.20	1.66	1.36
44	2	4083	5MU	C6-C5	-11.57	1.15	1.34
44	2	4083	5MU	C4-N3	-11.16	1.18	1.38
44	2	2786	B9H	C2-N3	10.52	1.50	1.37
44	2	1659	I4U	C4-N3	10.25	1.44	1.31
44	2	1348	P4U	C4-N3	10.20	1.44	1.31
44	2	4355	E6G	O6-C6	10.19	1.43	1.35
44	2	4371	MHG	C8-N9	9.60	1.51	1.46
44	2	2297	E7G	C5-N7	9.50	1.46	1.35
44	2	3880	P7G	C5-N7	9.38	1.46	1.35
44	2	4550	7MG	C8-N9	9.36	1.51	1.46
44	2	1797	E7G	C5-N7	9.33	1.46	1.35
44	2	1797	E7G	C8-N9	9.28	1.51	1.46
44	2	1605	7MG	C8-N9	9.22	1.51	1.46
44	2	3897	B8K	C8-N9	9.10	1.51	1.46
44	2	1909	P7G	C5-N7	9.10	1.45	1.35
44	2	4335	5MC	C6-C5	9.07	1.49	1.34
44	2	4371	MHG	C5-N7	9.02	1.45	1.35
44	2	1326	A2M	C3'-C4'	-8.98	1.30	1.53
44	2	4550	7MG	C5-N7	8.88	1.45	1.35
44	2	3899	BGH	O4'-C1'	8.87	1.63	1.42
44	2	3867	A2M	C3'-C4'	-8.84	1.30	1.53
44	2	3880	P7G	C8-N9	8.84	1.50	1.46
44	2	3899	BGH	C2'-C1'	-8.81	1.30	1.53
44	2	1524	A2M	C3'-C4'	-8.80	1.30	1.53
44	2	2297	E7G	C8-N9	8.80	1.50	1.46
44	2	1534	A2M	C3'-C4'	-8.79	1.30	1.53
44	2	4690	B8K	C8-N9	8.79	1.50	1.46
44	2	1871	A2M	C3'-C4'	-8.78	1.30	1.53
44	2	398	A2M	C3'-C4'	-8.76	1.30	1.53
44	2	3718	A2M	C3'-C4'	-8.74	1.30	1.53
44	2	4571	A2M	C3'-C4'	-8.73	1.30	1.53
44	2	1909	P7G	C8-N9	8.71	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	2	3825	A2M	C3'-C4'	-8.70	1.30	1.53
44	2	2363	A2M	C3'-C4'	-8.69	1.30	1.53
44	2	3723	A2M	C3'-C4'	-8.65	1.30	1.53
44	2	2522	7MG	C5-N7	8.65	1.45	1.35
44	2	2401	A2M	C3'-C4'	-8.62	1.31	1.53
44	2	1605	7MG	C5-N7	8.60	1.45	1.35
44	2	4523	A2M	C3'-C4'	-8.59	1.31	1.53
44	2	3899	BGH	C8-N9	8.46	1.50	1.46
44	2	2522	7MG	C8-N9	8.37	1.50	1.46
44	2	1456	B8Q	C6-C5	8.23	1.51	1.33
44	2	4371	MHG	C2-N3	8.13	1.47	1.31
44	2	4129	B8W	C2-N2	8.03	1.50	1.33
44	2	4529	B8W	C2-N2	8.00	1.49	1.33
44	2	4185	B8W	C2-N2	7.87	1.49	1.33
44	2	4472	B8W	C2-N2	7.83	1.49	1.33
44	2	1871	A2M	O4'-C4'	7.74	1.62	1.45
44	2	3718	A2M	O4'-C4'	7.69	1.62	1.45
44	2	3825	A2M	O4'-C4'	7.68	1.62	1.45
44	2	398	A2M	O4'-C4'	7.65	1.62	1.45
44	2	4483	B8T	C2-N3	7.62	1.51	1.36
44	2	1534	A2M	O4'-C4'	7.61	1.62	1.45
44	2	2401	A2M	O4'-C4'	7.60	1.62	1.45
44	2	1326	A2M	O4'-C1'	-7.60	1.30	1.41
44	2	3899	BGH	O4'-C4'	-7.60	1.28	1.45
44	2	1326	A2M	O4'-C4'	7.59	1.62	1.45
44	2	4523	A2M	O4'-C4'	7.56	1.61	1.45
44	2	3867	A2M	O4'-C1'	-7.53	1.30	1.41
44	2	2363	A2M	O4'-C4'	7.50	1.61	1.45
44	2	3723	A2M	O4'-C4'	7.49	1.61	1.45
44	2	2380	B8W	C2-N2	7.47	1.48	1.33
44	2	4571	A2M	O4'-C4'	7.43	1.61	1.45
44	2	1524	A2M	O4'-C4'	7.41	1.61	1.45
44	2	1524	A2M	O4'-C1'	-7.31	1.30	1.41
44	2	2786	B9H	C2-N1	7.29	1.49	1.38
44	2	4483	B8T	C4-N3	7.26	1.45	1.32
44	2	4671	B8T	C2-N3	7.26	1.51	1.36
44	2	4571	A2M	O4'-C1'	-7.25	1.31	1.41
44	2	3867	A2M	O4'-C4'	7.23	1.61	1.45
44	2	2401	A2M	O4'-C1'	-7.19	1.31	1.41
44	2	4523	A2M	O4'-C1'	-7.17	1.31	1.41
44	2	2363	A2M	O4'-C1'	-7.17	1.31	1.41
44	2	3825	A2M	O4'-C1'	-7.15	1.31	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	2	398	A2M	O4'-C1'	-7.14	1.31	1.41
44	2	3723	A2M	O4'-C1'	-7.14	1.31	1.41
44	2	1534	A2M	O4'-C1'	-7.11	1.31	1.41
44	2	1866	UR3	C2-N1	7.10	1.48	1.38
44	2	4306	OMU	C2-N1	7.04	1.49	1.38
44	2	3718	A2M	O4'-C1'	-7.02	1.31	1.41
44	2	4671	B8T	C4-N3	6.97	1.44	1.32
44	2	4620	OMU	C2-N1	6.91	1.49	1.38
44	2	4530	UR3	C2-N1	6.91	1.48	1.38
44	2	1871	A2M	O4'-C1'	-6.83	1.31	1.41
44	2	1866	UR3	C6-C5	6.79	1.50	1.35
44	2	4671	B8T	C6-C5	6.78	1.50	1.35
44	2	4220	6MZ	C6-N6	6.76	1.46	1.35
4	8	14	OMU	C2-N1	6.76	1.49	1.38
44	2	978	2MG	C2-N2	6.75	1.48	1.33
44	2	2786	B9H	C6-C5	6.74	1.48	1.33
44	2	4597	UR3	C6-C5	6.70	1.50	1.35
44	2	1517	2MG	C2-N2	6.69	1.48	1.33
44	2	1456	B8Q	C2-N3	6.64	1.46	1.35
44	2	4306	OMU	C2-N3	6.63	1.49	1.38
44	2	3909	OMC	C6-C5	6.62	1.50	1.35
44	2	4530	UR3	C6-C5	6.59	1.50	1.35
44	2	3897	B8K	C2-N3	6.59	1.49	1.33
44	2	4690	B8K	C2-N3	6.57	1.49	1.33
44	2	1797	E7G	C4-N9	6.54	1.45	1.37
44	2	4483	B8T	C6-C5	6.53	1.50	1.35
44	2	729	2MG	C2-N2	6.50	1.47	1.33
44	2	4196	OMG	C2-N3	6.46	1.48	1.33
44	2	4620	OMU	C2-N3	6.43	1.49	1.38
44	2	3880	P7G	C4-N9	6.43	1.44	1.35
44	2	4335	5MC	C4-N3	6.42	1.45	1.34
4	8	14	OMU	C2-N3	6.39	1.49	1.38
44	2	4536	OMC	C2-N3	6.39	1.49	1.36
44	2	3869	OMC	C2-N3	6.38	1.49	1.36
44	2	4371	MHG	C8-N7	6.38	1.51	1.45
44	2	2754	B9B	O6-C6	6.37	1.40	1.35
44	2	3887	OMC	C2-N3	6.36	1.49	1.36
44	2	2861	OMC	C2-N3	6.34	1.49	1.36
44	2	1909	P7G	C4-N3	6.26	1.48	1.37
44	2	2422	OMC	C2-N3	6.24	1.49	1.36
44	2	3880	P7G	C4-N3	6.24	1.48	1.37
44	2	4671	B8T	C4-N4	6.20	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	2	4483	B8T	C4-N4	6.20	1.48	1.35
44	2	4872	2MG	C2-N2	6.19	1.47	1.33
44	2	3701	OMC	C2-N3	6.18	1.48	1.36
44	2	4371	MHG	C2-N1	6.18	1.46	1.36
44	2	1909	P7G	C4-N9	6.13	1.44	1.35
44	2	1625	OMG	C2-N3	6.12	1.48	1.33
44	2	3701	OMC	C6-C5	6.11	1.49	1.35
44	2	2424	OMG	C2-N3	6.11	1.48	1.33
44	2	4335	5MC	C2-N3	6.10	1.48	1.36
44	2	2804	OMC	C2-N3	6.10	1.48	1.36
44	2	1659	I4U	C6-C5	6.10	1.49	1.35
44	2	4494	OMG	C2-N3	6.09	1.48	1.33
44	2	4597	UR3	C2-N3	6.09	1.50	1.39
44	2	4870	OMG	C2-N3	6.08	1.48	1.33
44	2	4196	OMG	C2-N2	6.06	1.48	1.34
44	2	1625	OMG	C2-N2	6.04	1.48	1.34
44	2	1659	I4U	C2-N3	6.04	1.48	1.36
44	2	2297	E7G	C8-N7	6.03	1.51	1.45
44	2	2424	OMG	C2-N2	5.98	1.48	1.34
44	2	2365	OMC	C2-N3	5.98	1.48	1.36
44	2	1348	P4U	C2-N3	5.98	1.48	1.36
44	2	2861	OMC	C6-C5	5.95	1.48	1.35
44	2	2773	OMG	C2-N3	5.94	1.47	1.33
44	2	4494	OMG	C2-N2	5.94	1.48	1.34
44	2	2773	OMG	C2-N2	5.93	1.48	1.34
44	2	3887	OMC	C6-C5	5.93	1.48	1.35
44	2	2365	OMC	C6-C5	5.93	1.48	1.35
44	2	4536	OMC	C6-C5	5.92	1.48	1.35
44	2	373	OMG	C2-N2	5.92	1.48	1.34
44	2	1348	P4U	C6-C5	5.92	1.48	1.35
44	2	4870	OMG	C2-N2	5.91	1.48	1.34
44	2	1883	OMG	C2-N2	5.90	1.48	1.34
44	2	1797	E7G	C8-N7	5.90	1.51	1.45
44	2	1883	OMG	C2-N3	5.90	1.47	1.33
44	2	2422	OMC	C6-C5	5.90	1.48	1.35
44	2	373	OMG	C2-N3	5.87	1.47	1.33
44	2	4370	OMG	C2-N2	5.86	1.48	1.34
44	2	4355	E6G	C2-N2	5.85	1.45	1.33
44	2	1797	E7G	C4-N3	5.84	1.48	1.34
44	2	4637	OMG	C2-N2	5.84	1.48	1.34
44	2	2364	OMG	C2-N2	5.83	1.48	1.34
44	2	4597	UR3	C2-N1	5.83	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	2	1866	UR3	C2-N3	5.82	1.50	1.39
44	2	3880	P7G	C8-N7	5.82	1.51	1.45
44	2	237	B9B	O6-C6	5.81	1.40	1.35
44	2	2804	OMC	C6-C5	5.81	1.48	1.35
44	2	3899	BGH	C4-N9	5.80	1.44	1.37
44	2	3880	P7G	C2-N2	5.79	1.48	1.34
44	2	1522	OMG	C2-N2	5.79	1.48	1.34
44	2	1909	P7G	C2-N2	5.79	1.47	1.34
44	2	4306	OMU	C6-C5	5.78	1.48	1.35
44	2	4370	OMG	C2-N3	5.78	1.47	1.33
44	2	1574	B9B	O6-C6	5.77	1.40	1.35
44	2	3897	B8K	C4-N9	5.75	1.44	1.37
44	2	4530	UR3	C2-N3	5.75	1.50	1.39
44	2	1316	OMG	C2-N3	5.75	1.47	1.33
44	2	3869	OMC	C2-N1	5.73	1.52	1.40
44	2	2050	OMG	C2-N2	5.73	1.47	1.34
44	2	4637	OMG	C2-N3	5.72	1.47	1.33
44	2	1316	OMG	C2-N2	5.70	1.47	1.34
44	2	4371	MHG	C4-N9	5.70	1.44	1.37
44	2	1797	E7G	C2-N3	5.67	1.46	1.33
44	2	2297	E7G	C4-N3	5.67	1.47	1.34
44	2	3899	BGH	C4-N3	5.66	1.47	1.34
44	2	237	B9B	C2-N2	5.66	1.45	1.33
44	2	1522	OMG	C2-N3	5.65	1.46	1.33
44	2	4550	7MG	C2-N3	5.65	1.46	1.33
44	2	4620	OMU	C6-C5	5.65	1.48	1.35
44	2	4564	M7A	C4-N9	5.65	1.48	1.38
44	2	3869	OMC	C6-C5	5.64	1.48	1.35
44	2	1909	P7G	C8-N7	5.64	1.51	1.45
44	2	2050	OMG	C2-N3	5.64	1.46	1.33
44	2	4371	MHG	C2-N2	5.62	1.45	1.33
44	2	2754	B9B	C2-N2	5.62	1.45	1.33
44	2	4623	OMG	C2-N2	5.62	1.47	1.34
44	2	2364	OMG	C2-N3	5.62	1.46	1.33
44	2	2297	E7G	C2-N3	5.57	1.46	1.33
44	2	3909	OMC	C2-N3	5.55	1.47	1.36
44	2	3899	BGH	C2-N3	5.54	1.46	1.33
44	2	3909	OMC	C4-N4	5.53	1.47	1.33
44	2	4371	MHG	C4-N3	5.53	1.47	1.34
44	2	4550	7MG	C4-N3	5.51	1.47	1.34
44	2	1574	B9B	C2-N2	5.51	1.44	1.33
44	2	1605	7MG	C4-N3	5.47	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	2	2522	7MG	C2-N3	5.47	1.46	1.33
44	2	2297	E7G	C4-N9	5.47	1.44	1.37
44	2	1605	7MG	C2-N3	5.43	1.46	1.33
44	2	4623	OMG	C2-N3	5.40	1.46	1.33
44	2	1517	2MG	C4-N3	5.37	1.50	1.37
44	2	2522	7MG	C4-N3	5.35	1.47	1.34
44	2	729	2MG	C4-N3	5.35	1.50	1.37
4	8	14	OMU	C6-C5	5.30	1.47	1.35
44	2	4690	B8K	C4-N9	5.18	1.43	1.37
44	2	978	2MG	C4-N3	5.17	1.49	1.37
44	2	1797	E7G	C2-N2	5.16	1.46	1.34
44	2	3880	P7G	C2-N1	5.15	1.45	1.33
44	2	4483	B8T	C2-N1	5.12	1.51	1.40
44	2	4550	7MG	C4-N9	5.09	1.43	1.37
44	2	3887	OMC	C4-N3	5.09	1.44	1.34
44	2	2297	E7G	C2-N2	5.08	1.46	1.34
44	2	1456	B8Q	C2-N1	5.07	1.45	1.38
44	2	4196	OMG	C4-N3	5.06	1.49	1.37
44	2	2861	OMC	C2-N1	5.05	1.50	1.40
44	2	1605	7MG	C4-N9	5.04	1.43	1.37
44	2	3701	OMC	C4-N3	4.99	1.44	1.34
44	2	2861	OMC	C4-N3	4.95	1.44	1.34
44	2	4536	OMC	C4-N3	4.94	1.44	1.34
44	2	1909	P7G	C2-N1	4.93	1.45	1.33
44	2	2422	OMC	C2-N1	4.90	1.50	1.40
44	2	2861	OMC	C4-N4	4.88	1.45	1.33
44	2	3899	BGH	C2-N2	4.87	1.45	1.34
44	2	4536	OMC	C4-N4	4.87	1.45	1.33
44	2	4536	OMC	C2-N1	4.86	1.50	1.40
44	2	3869	OMC	C4-N4	4.85	1.45	1.33
44	2	3887	OMC	C4-N4	4.83	1.45	1.33
44	2	2522	7MG	C4-N9	4.83	1.43	1.37
44	2	2804	OMC	C4-N4	4.82	1.45	1.33
44	2	4494	OMG	C4-N3	4.82	1.49	1.37
44	2	3701	OMC	C4-N4	4.81	1.45	1.33
44	2	1625	OMG	C4-N3	4.81	1.49	1.37
44	2	2422	OMC	C4-N3	4.81	1.44	1.34
44	2	3869	OMC	C4-N3	4.79	1.44	1.34
44	2	2365	OMC	C4-N3	4.79	1.44	1.34
44	2	1348	P4U	O4-C4	4.78	1.40	1.35
44	2	2804	OMC	C4-N3	4.78	1.44	1.34
44	2	2804	OMC	C2-N1	4.77	1.50	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	2	2422	OMC	C4-N4	4.77	1.45	1.33
44	2	3909	OMC	C4-N3	4.77	1.44	1.34
44	2	4870	OMG	C4-N3	4.74	1.48	1.37
44	2	2365	OMC	C4-N4	4.74	1.45	1.33
44	2	1605	7MG	C2-N2	4.73	1.45	1.34
44	2	3887	OMC	C2-N1	4.71	1.50	1.40
44	2	2522	7MG	C2-N2	4.70	1.45	1.34
44	2	4550	7MG	C2-N2	4.69	1.45	1.34
44	2	2424	OMG	C4-N3	4.69	1.48	1.37
44	2	2364	OMG	C6-N1	4.66	1.44	1.37
44	2	1659	I4U	C5-C4	4.65	1.49	1.43
44	2	2773	OMG	C4-N3	4.63	1.48	1.37
44	2	373	OMG	C4-N3	4.60	1.48	1.37
44	2	4370	OMG	C6-N1	4.57	1.44	1.37
44	2	2424	OMG	C6-N1	4.57	1.44	1.37
44	2	4196	OMG	C6-N1	4.55	1.44	1.37
44	2	3897	B8K	C4-N3	4.54	1.45	1.34
44	2	4494	OMG	C6-N1	4.52	1.44	1.37
44	2	1883	OMG	C4-N3	4.52	1.48	1.37
44	2	373	OMG	C6-N1	4.52	1.44	1.37
44	2	4370	OMG	C4-N3	4.50	1.48	1.37
44	2	4872	2MG	C4-N3	4.50	1.48	1.37
44	2	2050	OMG	C4-N3	4.49	1.48	1.37
44	2	3899	BGH	C5-N7	4.49	1.47	1.39
44	2	2773	OMG	C6-N1	4.49	1.44	1.37
44	2	4671	B8T	C2-N1	4.48	1.49	1.40
44	2	1316	OMG	C6-N1	4.48	1.44	1.37
44	2	4690	B8K	C4-N3	4.48	1.44	1.34
44	2	4335	5MC	C6-N1	4.47	1.45	1.38
44	2	1860	B8H	C2-N3	4.46	1.45	1.38
44	2	4870	OMG	C6-N1	4.46	1.44	1.37
44	2	1883	OMG	C6-N1	4.44	1.44	1.37
44	2	4637	OMG	C4-N3	4.44	1.48	1.37
44	2	4623	OMG	C6-N1	4.44	1.44	1.37
44	2	4083	5MU	C2-N3	4.43	1.45	1.38
44	2	1522	OMG	C6-N1	4.43	1.44	1.37
44	2	4637	OMG	C6-N1	4.42	1.44	1.37
44	2	2050	OMG	C6-N1	4.41	1.44	1.37
44	2	4335	5MC	C4-N4	4.38	1.45	1.34
44	2	1316	OMG	C4-N3	4.38	1.48	1.37
44	2	2364	OMG	C4-N3	4.37	1.48	1.37
44	2	1659	I4U	C2-N1	4.35	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	2	1522	OMG	C4-N3	4.34	1.47	1.37
44	2	1625	OMG	C6-N1	4.34	1.44	1.37
44	2	3701	OMC	C2-N1	4.32	1.49	1.40
44	2	1348	P4U	C2-N1	4.31	1.49	1.40
44	2	3909	OMC	C2-N1	4.26	1.49	1.40
44	2	1348	P4U	C5-C4	4.26	1.48	1.43
44	2	4335	5MC	C2-N1	4.26	1.49	1.40
44	2	4296	B8H	C2-N3	4.26	1.45	1.38
44	2	4690	B8K	C5-N7	4.25	1.46	1.39
44	2	2365	OMC	C2-N1	4.24	1.49	1.40
44	2	3897	B8K	C5-C6	4.23	1.54	1.43
44	2	3899	BGH	C5-C6	4.22	1.54	1.43
44	2	978	2MG	C2-N1	4.20	1.43	1.36
44	2	3897	B8K	C5-N7	4.18	1.46	1.39
44	2	4564	M7A	C6-N6	4.16	1.44	1.34
44	2	4623	OMG	C4-N3	4.11	1.47	1.37
44	2	4415	1MA	C2-N1	4.11	1.43	1.35
44	2	4415	1MA	C4-N3	4.09	1.50	1.37
44	2	1517	2MG	C2-N1	4.01	1.43	1.36
44	2	4306	OMU	C4-N3	4.00	1.45	1.38
4	8	14	OMU	C4-N3	3.99	1.45	1.38
44	2	4564	M7A	C5-N7	3.97	1.49	1.39
44	2	729	2MG	C2-N1	3.96	1.43	1.36
44	2	4872	2MG	C2-N1	3.95	1.43	1.36
44	2	4690	B8K	C5-C6	3.94	1.53	1.43
44	2	4671	B8T	C5-C4	3.84	1.49	1.40
44	2	4371	MHG	C5-C6	3.83	1.53	1.43
44	2	1797	E7G	C5-C6	3.80	1.53	1.43
44	2	4550	7MG	C5-C6	3.74	1.53	1.43
44	2	2297	E7G	C5-C6	3.71	1.53	1.43
44	2	3880	P7G	C2-N3	3.71	1.46	1.37
44	2	4620	OMU	C4-N3	3.70	1.45	1.38
44	2	4872	2MG	C5-C6	3.68	1.54	1.47
44	2	1605	7MG	C5-C6	3.66	1.53	1.43
44	2	4690	B8K	C71-N7	3.65	1.47	1.39
44	2	1909	P7G	C2-N3	3.63	1.46	1.37
44	2	3899	BGH	O2'-C2'	3.63	1.51	1.42
44	2	978	2MG	C6-N1	3.63	1.43	1.37
44	2	1605	7MG	C2-N1	3.61	1.46	1.37
44	2	3897	B8K	C6-N1	3.61	1.45	1.38
44	2	1909	P7G	O6-C6	-3.54	1.18	1.23
44	2	3897	B8K	C71-N7	3.52	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	2	2522	7MG	C5-C6	3.52	1.52	1.43
44	2	3880	P7G	C6-N1	3.51	1.44	1.38
44	2	4872	2MG	C6-N1	3.51	1.43	1.37
44	2	3899	BGH	C71-N7	3.51	1.47	1.39
44	2	3887	OMC	C6-N1	3.50	1.46	1.38
44	2	3909	OMC	C6-N1	3.49	1.46	1.38
44	2	2522	7MG	C2-N1	3.47	1.46	1.37
44	2	3897	B8K	C2-N2	3.47	1.42	1.34
44	2	4530	UR3	C6-N1	3.47	1.46	1.38
44	2	1517	2MG	C6-N1	3.43	1.43	1.37
44	2	4550	7MG	C2-N1	3.42	1.46	1.37
44	2	4690	B8K	C6-N1	3.41	1.45	1.38
44	2	4483	B8T	C5-C4	3.41	1.48	1.40
44	2	4690	B8K	C2-N2	3.40	1.42	1.34
44	2	2297	E7G	C2-N1	3.40	1.46	1.37
44	2	3899	BGH	C6-N1	3.40	1.45	1.38
44	2	729	2MG	C5-C6	3.40	1.54	1.47
44	2	1866	UR3	C6-N1	3.40	1.46	1.38
44	2	1659	I4U	C6-N1	3.39	1.46	1.38
44	2	978	2MG	C5-C6	3.38	1.54	1.47
44	2	1517	2MG	C5-C6	3.38	1.54	1.47
44	2	4483	B8T	C6-N1	3.37	1.46	1.38
44	2	1348	P4U	C6-N1	3.37	1.46	1.38
44	2	3869	OMC	C6-N1	3.37	1.46	1.38
44	2	1316	OMG	C5-C6	3.36	1.54	1.47
44	2	1909	P7G	C6-N1	3.36	1.44	1.38
44	2	4623	OMG	C5-C6	3.35	1.54	1.47
44	2	4083	5MU	C2-N1	3.34	1.43	1.38
44	2	1797	E7G	C2-N1	3.33	1.45	1.37
44	2	2773	OMG	C5-C6	3.33	1.54	1.47
44	2	4870	OMG	C5-C6	3.32	1.54	1.47
44	2	4196	OMG	C5-C6	3.31	1.54	1.47
44	2	2365	OMC	C6-N1	3.30	1.45	1.38
44	2	4550	7MG	C6-N1	3.28	1.44	1.38
44	2	3880	P7G	C5-C4	3.27	1.43	1.37
44	2	1605	7MG	C6-N1	3.26	1.44	1.38
44	2	3899	BGH	C2-N1	3.25	1.45	1.37
44	2	373	OMG	C5-C6	3.25	1.54	1.47
44	2	2861	OMC	C6-N1	3.25	1.45	1.38
44	2	3897	B8K	C2-N1	3.24	1.45	1.37
44	2	4371	MHG	C6-N1	3.22	1.44	1.38
44	2	729	2MG	C6-N1	3.22	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	2	4370	OMG	C5-C6	3.21	1.53	1.47
44	2	1909	P7G	C5-C4	3.19	1.43	1.37
44	2	2297	E7G	C6-N1	3.18	1.44	1.38
44	2	2422	OMC	C6-N1	3.18	1.45	1.38
44	2	1326	A2M	C6-N6	3.17	1.45	1.34
44	2	3723	A2M	C6-N6	3.17	1.45	1.34
44	2	4637	OMG	C5-C6	3.17	1.53	1.47
44	2	4494	OMG	C5-C6	3.15	1.53	1.47
44	2	3825	A2M	C6-N6	3.15	1.45	1.34
44	2	1524	A2M	C6-N6	3.14	1.45	1.34
44	2	4536	OMC	C6-N1	3.14	1.45	1.38
44	2	1871	A2M	C6-N6	3.13	1.45	1.34
44	2	2804	OMC	C6-N1	3.13	1.45	1.38
44	2	1797	E7G	C6-N1	3.13	1.44	1.38
44	2	3701	OMC	C6-N1	3.12	1.45	1.38
44	2	398	A2M	C6-N6	3.12	1.45	1.34
44	2	3880	P7G	O6-C6	-3.12	1.18	1.23
44	2	2401	A2M	C6-N6	3.11	1.45	1.34
44	2	2522	7MG	C6-N1	3.10	1.44	1.38
44	2	1625	OMG	C5-C6	3.10	1.53	1.47
44	2	2050	OMG	C5-C6	3.10	1.53	1.47
44	2	3867	A2M	C6-N6	3.09	1.45	1.34
44	2	1883	OMG	O6-C6	-3.09	1.17	1.23
44	2	3718	A2M	C6-N6	3.08	1.45	1.34
44	2	4597	UR3	C6-N1	3.08	1.45	1.38
44	2	4523	A2M	C6-N6	3.08	1.45	1.34
44	2	2364	OMG	C5-C6	3.07	1.53	1.47
44	2	4690	B8K	C2-N1	3.06	1.45	1.37
44	2	4671	B8T	C6-N1	3.06	1.45	1.38
44	2	2401	A2M	O3'-C3'	3.06	1.50	1.43
44	2	4355	E6G	C5-C4	-3.05	1.32	1.40
44	2	4571	A2M	C6-N6	3.04	1.45	1.34
44	2	1522	OMG	C5-C6	3.04	1.53	1.47
44	2	1534	A2M	C6-N6	3.04	1.45	1.34
44	2	4872	2MG	C5-C4	-3.02	1.35	1.43
44	2	4306	OMU	O4-C4	-3.01	1.18	1.24
44	2	2363	A2M	C6-N6	2.98	1.44	1.34
44	2	1348	P4U	O2-C2	-2.98	1.18	1.23
44	2	4620	OMU	O4-C4	-2.97	1.18	1.24
4	8	14	OMU	O4-C4	-2.96	1.18	1.24
44	2	1534	A2M	O3'-C3'	2.96	1.49	1.43
44	2	1659	I4U	O2-C2	-2.95	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	2	2050	OMG	O6-C6	-2.94	1.17	1.23
44	2	4083	5MU	O2-C2	-2.93	1.17	1.23
44	2	4083	5MU	O4-C4	-2.92	1.18	1.23
44	2	1574	B9B	C5-C4	-2.92	1.33	1.40
44	2	3723	A2M	O3'-C3'	2.92	1.49	1.43
44	2	3825	A2M	O3'-C3'	2.91	1.49	1.43
44	2	1326	A2M	O3'-C3'	2.91	1.49	1.43
44	2	373	OMG	O6-C6	-2.91	1.17	1.23
44	2	2380	B8W	C5-C4	-2.90	1.33	1.40
44	2	2363	A2M	O3'-C3'	2.89	1.49	1.43
44	2	237	B9B	C5-C4	-2.89	1.33	1.40
44	2	4671	B8T	O2-C2	-2.89	1.18	1.23
44	2	3718	A2M	O3'-C3'	2.89	1.49	1.43
44	2	3867	A2M	O3'-C3'	2.89	1.49	1.43
44	2	4472	B8W	C5-C4	-2.89	1.33	1.40
44	2	1316	OMG	O6-C6	-2.88	1.17	1.23
44	2	4623	OMG	O6-C6	-2.88	1.17	1.23
44	2	3899	BGH	O3'-C3'	-2.86	1.36	1.43
44	2	3909	OMC	C5-C4	2.86	1.49	1.42
44	2	3897	B8K	C5-C4	2.85	1.47	1.38
44	2	2365	OMC	O2-C2	-2.84	1.18	1.23
44	2	4637	OMG	O6-C6	-2.84	1.17	1.23
44	2	4306	OMU	C6-N1	2.84	1.44	1.38
44	2	1522	OMG	O6-C6	-2.84	1.17	1.23
44	2	1524	A2M	O3'-C3'	2.83	1.49	1.43
44	2	398	A2M	O3'-C3'	2.82	1.49	1.43
44	2	1517	2MG	C5-C4	-2.82	1.35	1.43
44	2	4571	A2M	O3'-C3'	2.81	1.49	1.43
44	2	1871	A2M	O3'-C3'	2.81	1.49	1.43
44	2	2364	OMG	O6-C6	-2.81	1.17	1.23
44	2	4523	A2M	O3'-C3'	2.80	1.49	1.43
44	2	2424	OMG	C5-C6	2.80	1.53	1.47
44	2	3899	BGH	O6-C6	-2.80	1.18	1.23
44	2	2804	OMC	O2-C2	-2.78	1.18	1.23
44	2	1524	A2M	O2'-C2'	-2.78	1.35	1.42
44	2	1883	OMG	C5-C6	2.77	1.53	1.47
44	2	978	2MG	C5-C4	-2.77	1.36	1.43
44	2	4870	OMG	O6-C6	-2.77	1.17	1.23
44	2	1659	I4U	O4-C4	2.77	1.40	1.35
44	2	2422	OMC	O2-C2	-2.77	1.18	1.23
44	2	3701	OMC	O2-C2	-2.76	1.18	1.23
44	2	4494	OMG	O6-C6	-2.76	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	2	2522	7MG	O6-C6	-2.76	1.18	1.23
44	2	2424	OMG	O6-C6	-2.75	1.17	1.23
44	2	729	2MG	C5-C4	-2.75	1.36	1.43
44	2	2773	OMG	O6-C6	-2.74	1.17	1.23
44	2	2363	A2M	C5-C4	-2.74	1.33	1.40
44	2	1326	A2M	O2'-C2'	-2.74	1.35	1.42
44	2	4529	B8W	C5-C4	-2.74	1.33	1.40
44	2	2401	A2M	C5-C4	-2.73	1.33	1.40
44	2	2754	B9B	C5-C4	-2.73	1.33	1.40
44	2	4185	B8W	C5-C4	-2.73	1.33	1.40
44	2	4483	B8T	O2-C2	-2.73	1.18	1.23
44	2	4620	OMU	C6-N1	2.73	1.44	1.38
44	2	1625	OMG	O6-C6	-2.71	1.17	1.23
44	2	1659	I4U	O4-C41	-2.71	1.40	1.47
44	2	1534	A2M	O2'-C2'	-2.71	1.35	1.42
44	2	2401	A2M	O2'-C2'	-2.70	1.35	1.42
44	2	2363	A2M	O2'-C2'	-2.70	1.35	1.42
44	2	4690	B8K	C5-C4	2.69	1.46	1.38
44	2	4370	OMG	O6-C6	-2.69	1.17	1.23
44	2	4335	5MC	O2-C2	-2.69	1.18	1.23
44	2	3825	A2M	C5-C4	-2.68	1.33	1.40
44	2	1534	A2M	C5-C4	-2.68	1.33	1.40
44	2	3909	OMC	O2-C2	-2.68	1.18	1.23
44	2	3723	A2M	C5-C4	-2.67	1.33	1.40
4	8	14	OMU	C6-N1	2.67	1.44	1.38
44	2	4571	A2M	O2'-C2'	-2.67	1.35	1.42
44	2	4196	OMG	O6-C6	-2.67	1.17	1.23
4	8	14	OMU	O2-C2	-2.66	1.18	1.23
44	2	1871	A2M	C5-C4	-2.66	1.33	1.40
44	2	398	A2M	C5-C4	-2.65	1.33	1.40
44	2	1524	A2M	C5-C4	-2.65	1.33	1.40
44	2	4536	OMC	O2-C2	-2.65	1.18	1.23
44	2	1883	OMG	C5-C4	-2.65	1.36	1.43
44	2	2861	OMC	O2-C2	-2.65	1.18	1.23
44	2	4550	7MG	O6-C6	-2.65	1.18	1.23
44	2	3701	OMC	C5-C4	2.64	1.49	1.42
44	2	4523	A2M	C5-C4	-2.64	1.34	1.40
44	2	3825	A2M	O2'-C2'	-2.61	1.35	1.42
44	2	4571	A2M	C5-C4	-2.61	1.34	1.40
44	2	3887	OMC	O2-C2	-2.61	1.18	1.23
44	2	3718	A2M	O2'-C2'	-2.60	1.35	1.42
44	2	4620	OMU	O2-C2	-2.60	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	2	3867	A2M	O2'-C2'	-2.60	1.36	1.42
44	2	4523	A2M	O2'-C2'	-2.60	1.36	1.42
44	2	3867	A2M	C5-C4	-2.59	1.34	1.40
44	2	1605	7MG	O6-C6	-2.58	1.18	1.23
44	2	398	A2M	O2'-C2'	-2.56	1.36	1.42
44	2	1871	A2M	O2'-C2'	-2.55	1.36	1.42
44	2	2297	E7G	O6-C6	-2.55	1.18	1.23
44	2	373	OMG	C5-C4	-2.54	1.36	1.43
44	2	3718	A2M	C5-C4	-2.54	1.34	1.40
44	2	4220	6MZ	C5-C4	-2.52	1.34	1.40
44	2	4370	OMG	C2-N1	2.52	1.43	1.37
44	2	2773	OMG	C2-N1	2.51	1.43	1.37
44	2	1316	OMG	C5-C4	-2.51	1.36	1.43
44	2	4196	OMG	C2-N1	2.50	1.43	1.37
44	2	3723	A2M	O2'-C2'	-2.49	1.36	1.42
44	2	1797	E7G	O6-C6	-2.49	1.18	1.23
44	2	3869	OMC	O2-C2	-2.47	1.19	1.23
44	2	1326	A2M	C5-C4	-2.47	1.34	1.40
44	2	2364	OMG	C5-C4	-2.47	1.36	1.43
44	2	4494	OMG	C2-N1	2.45	1.43	1.37
44	2	1522	OMG	C2-N1	2.45	1.43	1.37
44	2	1522	OMG	C5-C4	-2.44	1.36	1.43
44	2	1625	OMG	C2-N1	2.43	1.43	1.37
44	2	4637	OMG	C2-N1	2.41	1.43	1.37
44	2	2364	OMG	C2-N1	2.40	1.43	1.37
44	2	4623	OMG	C5-C4	-2.40	1.37	1.43
44	2	2424	OMG	C2-N1	2.40	1.43	1.37
44	2	2050	OMG	C2-N1	2.39	1.43	1.37
44	2	2050	OMG	C5-C4	-2.39	1.37	1.43
44	2	2861	OMC	C5-C4	2.39	1.48	1.42
44	2	3887	OMC	C5-C4	2.38	1.48	1.42
44	2	4623	OMG	C2-N1	2.37	1.43	1.37
44	2	4306	OMU	O2-C2	-2.36	1.18	1.23
44	2	1326	A2M	C2-N3	2.36	1.35	1.32
44	2	1316	OMG	C2-N1	2.36	1.43	1.37
44	2	4870	OMG	C2-N1	2.35	1.43	1.37
44	2	1866	UR3	C4-N3	2.35	1.46	1.40
44	2	4530	UR3	C4-N3	2.35	1.46	1.40
44	2	3867	A2M	C2-N3	2.35	1.35	1.32
44	2	4371	MHG	O6-C6	-2.33	1.19	1.23
44	2	373	OMG	C2-N1	2.33	1.43	1.37
44	2	1524	A2M	C2-N3	2.31	1.35	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	2	1883	OMG	C2-N1	2.31	1.43	1.37
44	2	4306	OMU	C5-C4	2.31	1.48	1.43
44	2	1871	A2M	C2-N3	2.30	1.35	1.32
44	2	2365	OMC	C5-C4	2.30	1.48	1.42
44	2	4870	OMG	C5-C4	-2.30	1.37	1.43
44	2	4637	OMG	C5-C4	-2.29	1.37	1.43
44	2	4220	6MZ	C2-N3	2.29	1.35	1.32
44	2	2786	B9H	C6-N1	2.29	1.43	1.38
44	2	4415	1MA	C5-C4	-2.29	1.37	1.43
44	2	1456	B8Q	C6-N1	2.28	1.43	1.38
44	2	4129	B8W	C5-C4	-2.28	1.34	1.40
44	2	4597	UR3	C5-C4	2.28	1.49	1.43
44	2	1534	A2M	C2-N3	2.28	1.35	1.32
44	2	4370	OMG	C5-C4	-2.27	1.37	1.43
44	2	1866	UR3	C5-C4	2.27	1.49	1.43
44	2	4523	A2M	C2-N3	2.26	1.35	1.32
44	2	4597	UR3	O2-C2	-2.26	1.18	1.22
44	2	2422	OMC	C5-C4	2.26	1.48	1.42
44	2	4571	A2M	C2-N3	2.26	1.35	1.32
4	8	14	OMU	C5-C4	2.25	1.48	1.43
44	2	2424	OMG	C5-C4	-2.24	1.37	1.43
44	2	4620	OMU	C5-C4	2.23	1.48	1.43
44	2	3825	A2M	C2-N3	2.21	1.35	1.32
44	2	2773	OMG	C5-C4	-2.21	1.37	1.43
44	2	4296	B8H	O4-C4	-2.19	1.19	1.23
44	2	4494	OMG	C5-C4	-2.18	1.37	1.43
44	2	1625	OMG	C5-C4	-2.18	1.37	1.43
44	2	3723	A2M	C2-N3	2.16	1.35	1.32
44	2	4536	OMC	C5-C4	2.16	1.47	1.42
44	2	2363	A2M	C2-N3	2.16	1.35	1.32
44	2	2401	A2M	C2-N3	2.16	1.35	1.32
44	2	1326	A2M	O5'-C5'	-2.11	1.39	1.44
44	2	398	A2M	C2-N3	2.11	1.35	1.32
44	2	4530	UR3	C5-C4	2.10	1.49	1.43
44	2	2804	OMC	C5-C4	2.10	1.47	1.42
44	2	4690	B8K	O6-C6	-2.10	1.19	1.23
44	2	4415	1MA	CM1-N1	2.08	1.50	1.46
44	2	1456	B8Q	O2-C2	-2.06	1.18	1.22
44	2	1860	B8H	O4-C4	-2.05	1.19	1.23
44	2	3899	BGH	C5-C4	2.02	1.44	1.38
44	2	3718	A2M	C2-N3	2.02	1.35	1.32
44	2	3869	OMC	C5-C4	2.01	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	2	4530	UR3	O2-C2	-2.01	1.18	1.22

All (389) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	2	237	B9B	O6-C6-N1	-29.95	94.27	120.12
44	2	2754	B9B	O6-C6-N1	-29.72	94.47	120.12
44	2	1574	B9B	O6-C6-N1	-29.42	94.72	120.12
44	2	4564	M7A	C5-C6-N6	13.78	147.27	123.74
44	2	4220	6MZ	C1'-N9-C4	-12.45	104.76	126.64
44	2	4564	M7A	N6-C6-N1	-11.61	92.92	118.35
44	2	1534	A2M	C5-C6-N6	10.93	136.97	120.35
44	2	3718	A2M	C5-C6-N6	10.62	136.49	120.35
44	2	398	A2M	C5-C6-N6	10.58	136.44	120.35
44	2	1326	A2M	C5-C6-N6	10.48	136.28	120.35
44	2	3723	A2M	C5-C6-N6	10.36	136.10	120.35
44	2	3867	A2M	C5-C6-N6	10.29	135.99	120.35
44	2	1871	A2M	C5-C6-N6	10.28	135.98	120.35
44	2	4571	A2M	C5-C6-N6	10.28	135.97	120.35
44	2	2401	A2M	C5-C6-N6	10.26	135.95	120.35
44	2	3825	A2M	C5-C6-N6	10.24	135.91	120.35
44	2	1524	A2M	C5-C6-N6	10.21	135.87	120.35
44	2	4523	A2M	C5-C6-N6	10.16	135.78	120.35
44	2	4083	5MU	C5-C4-N3	10.14	123.97	115.31
44	2	2363	A2M	C5-C6-N6	10.02	135.59	120.35
44	2	4355	E6G	O6-C6-N1	9.07	127.96	120.12
44	2	4597	UR3	C4-N3-C2	-8.62	116.44	124.56
44	2	1534	A2M	N6-C6-N1	-7.87	102.24	118.57
44	2	4083	5MU	C5-C6-N1	-7.82	115.30	123.34
44	2	398	A2M	N6-C6-N1	-7.47	103.06	118.57
44	2	2786	B9H	C31-N3-C2	7.37	126.42	117.21
44	2	3718	A2M	N6-C6-N1	-7.34	103.33	118.57
44	2	1326	A2M	N6-C6-N1	-7.30	103.42	118.57
44	2	1524	A2M	N6-C6-N1	-7.23	103.57	118.57
44	2	3867	A2M	N6-C6-N1	-7.23	103.57	118.57
44	2	2786	B9H	C6-N1-C2	-7.23	115.31	121.79
44	2	1871	A2M	N6-C6-N1	-7.19	103.64	118.57
44	2	2401	A2M	N6-C6-N1	-7.18	103.66	118.57
44	2	4571	A2M	N6-C6-N1	-7.16	103.70	118.57
44	2	4523	A2M	N6-C6-N1	-7.16	103.71	118.57
44	2	3723	A2M	N6-C6-N1	-7.11	103.81	118.57
44	2	2363	A2M	N6-C6-N1	-7.07	103.90	118.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	2	4083	5MU	C4-N3-C2	-7.00	118.29	127.35
44	2	3825	A2M	N6-C6-N1	-6.99	104.07	118.57
44	2	4371	MHG	C2-N3-C4	6.78	120.44	112.04
44	2	3825	A2M	N3-C2-N1	-6.56	118.43	128.68
44	2	4296	B8H	C4-N3-C2	-6.55	118.87	127.35
44	2	3723	A2M	N3-C2-N1	-6.47	118.57	128.68
44	2	4690	B8K	C72-C71-N7	6.46	128.58	118.86
44	2	4523	A2M	N3-C2-N1	-6.45	118.59	128.68
44	2	1871	A2M	N3-C2-N1	-6.43	118.62	128.68
44	2	1860	B8H	C4-N3-C2	-6.43	119.02	127.35
44	2	2401	A2M	N3-C2-N1	-6.42	118.64	128.68
44	2	2363	A2M	N3-C2-N1	-6.42	118.65	128.68
44	2	4472	B8W	O6-C6-N1	6.40	127.91	119.03
44	2	1524	A2M	N3-C2-N1	-6.34	118.77	128.68
44	2	1534	A2M	N3-C2-N1	-6.27	118.87	128.68
44	2	398	A2M	N3-C2-N1	-6.27	118.88	128.68
44	2	4564	M7A	N3-C2-N1	-6.26	118.81	128.60
44	2	4220	6MZ	N3-C2-N1	-6.26	118.90	128.68
44	2	4355	E6G	N2-C2-N3	6.22	127.93	117.79
44	2	4571	A2M	N3-C2-N1	-6.21	118.97	128.68
44	2	3897	B8K	C72-C71-N7	6.17	128.15	118.86
44	2	3867	A2M	N3-C2-N1	-6.17	119.04	128.68
44	2	1326	A2M	N3-C2-N1	-6.15	119.06	128.68
44	2	4690	B8K	C5-C6-N1	6.12	121.77	110.99
44	2	3899	BGH	C72-C71-N7	6.02	127.91	118.86
44	2	3718	A2M	N3-C2-N1	-5.83	119.57	128.68
44	2	1456	B8Q	N3-C2-N1	5.78	123.92	117.13
44	2	3899	BGH	C5-C6-N1	5.76	121.13	110.99
44	2	2380	B8W	N2-C2-N3	5.73	127.14	117.79
44	2	3897	B8K	C5-C6-N1	5.73	121.09	110.99
44	2	237	B9B	N3-C2-N1	-5.72	119.59	127.22
44	2	4129	B8W	N2-C2-N3	5.72	127.11	117.79
44	2	3880	P7G	C4-C5-N7	5.57	109.61	106.67
44	2	4529	B8W	N2-C2-N3	5.55	126.83	117.79
44	2	4355	E6G	N3-C2-N1	-5.54	119.84	127.22
44	2	1860	B8H	N3-C2-N1	5.52	121.11	115.14
44	2	2754	B9B	N3-C2-N1	-5.50	119.88	127.22
44	2	4129	B8W	N3-C2-N1	-5.47	119.92	127.22
44	2	1909	P7G	C4-C5-N7	5.46	109.55	106.67
44	2	4185	B8W	N3-C2-N1	-5.44	119.97	127.22
44	2	4296	B8H	N3-C2-N1	5.44	121.02	115.14
4	8	14	OMU	C4-N3-C2	-5.40	119.45	126.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	2	4185	B8W	N2-C2-N3	5.38	126.55	117.79
44	2	1574	B9B	N3-C2-N1	-5.37	120.06	127.22
44	2	4564	M7A	N3-C4-N9	5.36	133.64	126.87
44	2	1797	E7G	C5-C6-N1	5.32	120.36	110.99
44	2	1456	B8Q	C31-N3-C4	5.32	122.26	114.25
44	2	4472	B8W	N2-C2-N3	5.30	126.42	117.79
44	2	4306	OMU	C4-N3-C2	-5.24	119.67	126.58
44	2	4529	B8W	N3-C2-N1	-5.19	120.31	127.22
44	2	1456	B8Q	O2-C2-N3	-5.17	115.36	122.95
44	2	2297	E7G	C5-C6-N1	5.16	120.08	110.99
44	2	4371	MHG	C5-C6-N1	5.14	120.05	110.99
44	2	3899	BGH	C2-N3-C4	5.12	121.43	112.30
44	2	4472	B8W	N3-C2-N1	-5.11	120.41	127.22
44	2	4529	B8W	O6-C6-N1	5.10	126.10	119.03
44	2	1797	E7G	C2-N3-C4	5.09	121.38	112.30
44	2	1797	E7G	C4-C5-N7	5.09	109.43	104.91
44	2	4415	1MA	N1-C2-N3	-5.04	120.14	126.02
44	2	4185	B8W	C2-N3-C4	4.98	121.05	115.36
44	2	4550	7MG	C5-C6-N1	4.97	119.76	110.99
44	2	2522	7MG	C5-C6-N1	4.96	119.73	110.99
44	2	4083	5MU	N3-C2-N1	4.94	121.45	114.89
44	2	3897	B8K	C2-N3-C4	4.93	121.08	112.30
44	2	3869	OMC	O2-C2-N3	-4.93	114.32	122.33
44	2	4371	MHG	C4-C5-N7	4.89	109.26	104.91
44	2	4620	OMU	C4-N3-C2	-4.88	120.14	126.58
44	2	4083	5MU	C5M-C5-C6	-4.88	116.33	122.85
44	2	2297	E7G	C4-C5-N7	4.86	109.24	104.91
44	2	4690	B8K	C2-N3-C4	4.86	120.95	112.30
44	2	1605	7MG	C5-C6-N1	4.85	119.53	110.99
44	2	2380	B8W	N3-C2-N1	-4.77	120.86	127.22
44	2	237	B9B	C2-N3-C4	4.76	120.80	115.36
44	2	4690	B8K	C4-C5-N7	4.76	109.14	104.91
44	2	4529	B8W	C1'-N9-C4	-4.74	118.31	126.64
44	2	2754	B9B	C2-N3-C4	4.71	120.74	115.36
44	2	1866	UR3	C4-N3-C2	-4.71	120.13	124.56
44	2	4872	2MG	CM2-N2-C2	-4.69	113.49	123.86
44	2	237	B9B	N2-C2-N3	4.69	125.44	117.79
44	2	4530	UR3	C4-N3-C2	-4.62	120.22	124.56
44	2	2297	E7G	C2-N3-C4	4.57	120.44	112.30
44	2	4185	B8W	O6-C6-N1	4.55	125.33	119.03
44	2	3899	BGH	C5-C4-N9	4.46	112.14	106.35
44	2	1797	E7G	C5-C4-N3	-4.45	119.64	128.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	2	4355	E6G	C2-N3-C4	4.43	120.42	115.36
44	2	1659	I4U	C5-C4-N3	-4.42	118.19	124.91
44	2	4550	7MG	C2-N3-C4	4.41	120.16	112.30
44	2	1574	B9B	C2-N3-C4	4.37	120.35	115.36
44	2	4472	B8W	C2-N3-C4	4.37	120.35	115.36
44	2	4129	B8W	C2-N3-C4	4.35	120.32	115.36
44	2	2522	7MG	C2-N3-C4	4.33	120.01	112.30
44	2	2754	B9B	N2-C2-N3	4.32	124.84	117.79
44	2	1605	7MG	C2-N3-C4	4.24	119.85	112.30
44	2	4220	6MZ	C2-N1-C6	4.11	120.11	116.59
44	2	3899	BGH	N9-C8-N7	4.11	108.84	103.33
44	2	1456	B8Q	C6-N1-C2	-4.10	118.12	121.79
44	2	3897	B8K	C5-C4-N9	4.06	111.62	106.35
44	2	3897	B8K	C4-C5-N7	4.01	108.48	104.91
44	2	4529	B8W	C2-N3-C4	4.01	119.93	115.36
44	2	4083	5MU	O4-C4-C5	-3.99	120.28	124.90
44	2	1574	B9B	N2-C2-N3	3.96	124.25	117.79
44	2	4620	OMU	N3-C2-N1	3.95	120.14	114.89
44	2	4371	MHG	C5-C4-N3	-3.92	120.66	128.13
44	2	1605	7MG	C5-C4-N9	3.92	111.43	106.35
44	2	4306	OMU	N3-C2-N1	3.91	120.08	114.89
44	2	4083	5MU	C5M-C5-C4	3.91	123.07	118.77
44	2	2380	B8W	C2-N3-C4	3.90	119.81	115.36
44	2	4415	1MA	C5-C6-N1	3.89	119.69	113.90
44	2	3899	BGH	C4-C5-N7	3.88	108.36	104.91
44	2	4690	B8K	C5-C4-N9	3.86	111.36	106.35
44	2	4690	B8K	N9-C8-N7	3.86	108.51	103.33
44	2	2786	B9H	O3'-C3'-C2'	3.85	122.11	111.17
44	2	2380	B8W	O6-C6-N1	3.84	124.36	119.03
44	2	1517	2MG	C5-C6-N1	3.79	120.64	113.95
4	8	14	OMU	N3-C2-N1	3.77	119.89	114.89
44	2	2297	E7G	C5-C4-N3	-3.75	120.99	128.13
44	2	3897	B8K	N9-C8-N7	3.72	108.32	103.33
44	2	4872	2MG	C5-C6-N1	3.71	120.50	113.95
44	2	1883	OMG	C5-C6-N1	3.66	120.42	113.95
44	2	373	OMG	C5-C6-N1	3.64	120.38	113.95
44	2	4870	OMG	C5-C6-N1	3.63	120.37	113.95
44	2	2522	7MG	C5-C4-N9	3.62	111.05	106.35
44	2	1348	P4U	C5-C4-N3	-3.62	119.41	124.91
44	2	4296	B8H	C5-C4-N3	3.60	124.73	116.58
44	2	4129	B8W	O6-C6-C5	3.60	121.16	116.01
44	2	4371	MHG	C2-N1-C6	-3.57	120.37	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	8	14	OMU	C5-C4-N3	3.54	120.14	114.84
44	2	729	2MG	C5-C6-N1	3.54	120.20	113.95
44	2	1316	OMG	C5-C6-N1	3.54	120.20	113.95
44	2	3899	BGH	C5-C4-N3	-3.52	121.43	128.13
44	2	4550	7MG	C5-C4-N9	3.51	110.91	106.35
44	2	3869	OMC	C1'-N1-C2	3.51	126.25	118.42
44	2	978	2MG	C5-C6-N1	3.51	120.14	113.95
44	2	2297	E7G	C5-C4-N9	3.50	110.89	106.35
44	2	4196	OMG	C5-C6-N1	3.49	120.11	113.95
44	2	2522	7MG	C5-C4-N3	-3.49	121.48	128.13
44	2	2050	OMG	C5-C6-N1	3.48	120.11	113.95
44	2	4550	7MG	C5-C4-N3	-3.48	121.50	128.13
44	2	2424	OMG	C5-C6-N1	3.47	120.09	113.95
44	2	1860	B8H	C5-C4-N3	3.47	124.44	116.58
44	2	2804	OMC	O2-C2-N3	-3.46	116.71	122.33
44	2	4637	OMG	C5-C6-N1	3.45	120.04	113.95
44	2	4494	OMG	C5-C6-N1	3.44	120.03	113.95
44	2	1605	7MG	C5-C4-N3	-3.43	121.60	128.13
44	2	2364	OMG	C5-C6-N1	3.41	119.97	113.95
44	2	4564	M7A	C2-N3-C4	3.39	119.75	111.75
44	2	4371	MHG	C5-C4-N9	3.38	110.74	106.35
44	2	4690	B8K	C6-C5-C4	-3.38	115.65	122.62
44	2	4472	B8W	O6-C6-C5	-3.38	111.18	116.01
44	2	2380	B8W	N2-C2-N1	-3.38	112.00	117.25
44	2	2773	OMG	C5-C6-N1	3.38	119.91	113.95
44	2	1797	E7G	C5-C4-N9	3.37	110.72	106.35
44	2	1625	OMG	C5-C6-N1	3.34	119.84	113.95
44	2	1909	P7G	N9-C8-N7	3.32	108.13	103.38
44	2	4306	OMU	C5-C4-N3	3.32	119.80	114.84
44	2	4370	OMG	C5-C6-N1	3.29	119.76	113.95
44	2	2422	OMC	O2-C2-N3	-3.29	116.98	122.33
44	2	1522	OMG	C5-C6-N1	3.28	119.75	113.95
44	2	4637	OMG	C2-N1-C6	-3.23	119.14	125.10
44	2	4355	E6G	N2-C2-N1	-3.23	112.23	117.25
44	2	3897	B8K	C6-C5-C4	-3.21	116.01	122.62
44	2	3897	B8K	C5-C4-N3	-3.20	122.03	128.13
44	2	4623	OMG	C5-C6-N1	3.18	119.57	113.95
44	2	4129	B8W	C2-N1-C6	3.14	121.13	116.08
44	2	1316	OMG	C2-N1-C6	-3.14	119.32	125.10
44	2	2363	A2M	C1'-N9-C4	3.13	132.15	126.64
44	2	4597	UR3	C3U-N3-C2	3.13	122.80	117.31
44	2	4690	B8K	C5-C4-N3	-3.11	122.20	128.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	2	4196	OMG	C2-N1-C6	-3.11	119.38	125.10
44	2	2380	B8W	C1'-N9-C4	-3.10	121.19	126.64
44	2	4870	OMG	C2-N1-C6	-3.09	119.40	125.10
44	2	4623	OMG	C2-N1-C6	-3.08	119.43	125.10
44	2	4620	OMU	C5-C4-N3	3.08	119.44	114.84
44	2	4536	OMC	O2-C2-N3	-3.08	117.33	122.33
44	2	4083	5MU	C6-C5-C4	3.07	120.60	118.03
44	2	2050	OMG	C2-N1-C6	-3.05	119.48	125.10
44	2	2424	OMG	C2-N1-C6	-3.05	119.49	125.10
44	2	373	OMG	C2-N1-C6	-3.04	119.50	125.10
44	2	4530	UR3	C6-N1-C2	-3.04	119.07	121.79
44	2	2786	B9H	C32-C31-N3	3.02	118.78	112.47
44	2	4370	OMG	C2-N1-C6	-3.02	119.54	125.10
44	2	2522	7MG	N9-C8-N7	3.02	107.69	103.38
44	2	3899	BGH	C6-C5-C4	-3.01	116.41	122.62
44	2	2861	OMC	O2-C2-N3	-3.01	117.44	122.33
4	8	14	OMU	O4-C4-C5	-3.00	119.88	125.16
44	2	3869	OMC	O2-C2-N1	2.99	125.07	118.89
44	2	1797	E7G	N9-C8-N7	2.99	107.65	103.38
44	2	4494	OMG	C2-N1-C6	-2.97	119.63	125.10
44	2	2773	OMG	C2-N1-C6	-2.96	119.65	125.10
44	2	1605	7MG	N9-C8-N7	2.95	107.60	103.38
44	2	2364	OMG	C2-N1-C6	-2.95	119.67	125.10
44	2	4196	OMG	CM2-O2'-C2'	2.95	122.26	114.52
44	2	1456	B8Q	C1'-N1-C2	2.93	121.93	116.99
44	2	1883	OMG	C2-N1-C6	-2.92	119.72	125.10
44	2	1522	OMG	C2-N1-C6	-2.92	119.72	125.10
44	2	4571	A2M	C1'-N9-C4	2.92	131.76	126.64
44	2	1456	B8Q	C31-N3-C2	2.86	121.95	117.79
44	2	4671	B8T	C6-C5-C4	2.86	120.46	116.96
44	2	2786	B9H	O2-C2-N1	-2.86	116.03	122.72
44	2	1625	OMG	C2-N1-C6	-2.85	119.84	125.10
44	2	2786	B9H	C1'-N1-C6	2.84	127.03	120.84
44	2	4335	5MC	C5-C6-N1	-2.84	120.42	123.34
44	2	2522	7MG	C4-C5-N7	2.83	109.46	105.53
44	2	4296	B8H	O2-C2-N1	-2.83	119.69	122.87
44	2	4529	B8W	N2-C2-N1	-2.82	112.87	117.25
44	2	4623	OMG	N2-C2-N1	2.81	122.69	116.71
44	2	1797	E7G	N9-C4-N3	2.79	129.63	125.47
44	2	1860	B8H	O2-C2-N1	-2.78	119.74	122.87
44	2	3899	BGH	O6-C6-N1	-2.77	114.81	120.12
44	2	3867	A2M	C1'-N9-C4	2.76	131.49	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	2	4129	B8W	N2-C2-N1	-2.75	112.97	117.25
44	2	2786	B9H	O3'-C3'-C4'	2.75	119.01	111.05
44	2	4415	1MA	C8-N7-C5	2.74	108.20	102.99
44	2	4483	B8T	O3'-C3'-C2'	2.73	120.66	111.82
44	2	4306	OMU	O4-C4-C5	-2.72	120.37	125.16
44	2	1659	I4U	O2-C2-N3	-2.72	117.90	122.33
44	2	3880	P7G	N9-C8-N7	2.71	107.25	103.38
44	2	4296	B8H	O4-C4-N3	-2.69	114.96	120.12
44	2	4550	7MG	C4-C5-N7	2.69	109.27	105.53
44	2	4083	5MU	O2-C2-N1	-2.68	119.23	122.79
44	2	1909	P7G	C71-N7-C5	2.66	130.81	124.52
44	2	1316	OMG	N2-C2-N1	2.65	122.36	116.71
44	2	4872	2MG	C8-N7-C5	2.65	108.04	102.99
44	2	4597	UR3	C6-N1-C2	-2.64	119.42	121.79
44	2	4371	MHG	N1-C2-N3	-2.64	119.87	123.95
44	2	1605	7MG	C4-C5-N7	2.64	109.19	105.53
44	2	4472	B8W	N2-C2-N1	-2.63	113.17	117.25
44	2	2297	E7G	N9-C8-N7	2.62	107.12	103.38
44	2	1860	B8H	O4-C4-N3	-2.62	115.10	120.12
44	2	1797	E7G	C2-N1-C6	-2.61	120.34	125.10
44	2	4185	B8W	C1'-N9-C4	-2.61	122.06	126.64
44	2	2364	OMG	N2-C2-N1	2.60	122.26	116.71
44	2	3909	OMC	C5-C4-N4	2.60	124.66	120.57
44	2	4129	B8W	C4-C5-N7	-2.60	106.69	109.40
44	2	3909	OMC	O2-C2-N3	-2.59	118.12	122.33
44	2	2804	OMC	C1'-N1-C2	2.58	124.19	118.42
44	2	4483	B8T	O3'-C3'-C4'	2.58	118.52	111.05
44	2	978	2MG	C8-N7-C5	2.58	107.91	102.99
44	2	3899	BGH	O4'-C1'-N9	2.57	112.80	109.30
44	2	373	OMG	C8-N7-C5	2.56	107.87	102.99
44	2	1517	2MG	O6-C6-C5	-2.55	119.39	124.37
44	2	4620	OMU	O4-C4-C5	-2.54	120.69	125.16
44	2	3897	B8K	O6-C6-N1	-2.54	115.25	120.12
44	2	4371	MHG	N9-C8-N7	2.54	107.01	103.38
44	2	4690	B8K	C2-N1-C6	-2.53	120.48	125.10
44	2	729	2MG	C8-N7-C5	2.53	107.80	102.99
44	2	2424	OMG	O6-C6-C5	-2.52	119.45	124.37
44	2	4355	E6G	C2-N1-C6	2.51	120.12	116.08
44	2	2050	OMG	N2-C2-N1	2.51	122.06	116.71
44	2	2804	OMC	O2-C2-N1	2.51	124.07	118.89
44	2	1517	2MG	C8-N7-C5	2.50	107.76	102.99
44	2	1326	A2M	C1'-N9-C4	2.47	130.99	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	2	4483	B8T	O2-C2-N3	-2.47	118.32	122.33
44	2	3869	OMC	C6-N1-C2	-2.46	116.23	120.49
44	2	4335	5MC	CM5-C5-C6	-2.45	119.57	122.85
44	2	2297	E7G	C2-N1-C6	-2.45	120.63	125.10
44	2	237	B9B	C61-O6-C6	-2.45	112.94	117.51
44	2	4355	E6G	C61-O6-C6	-2.43	115.15	117.56
44	2	1883	OMG	O6-C6-C5	-2.43	119.62	124.37
44	2	4536	OMC	C1'-N1-C2	2.43	123.84	118.42
44	2	4185	B8W	N2-C2-N1	-2.43	113.48	117.25
44	2	2861	OMC	C1'-N1-C2	2.42	123.83	118.42
44	2	4870	OMG	C8-N7-C5	2.42	107.60	102.99
44	2	1524	A2M	C1'-N9-C4	2.42	130.90	126.64
44	2	1316	OMG	C8-N7-C5	2.42	107.60	102.99
44	2	4597	UR3	O2-C2-N3	-2.42	117.94	121.34
44	2	3899	BGH	C2-N1-C6	-2.40	120.73	125.10
44	2	3899	BGH	N1-C2-N3	-2.39	118.86	123.32
44	2	3718	A2M	C1'-N9-C4	2.37	130.81	126.64
44	2	3897	B8K	N1-C2-N3	-2.37	118.90	123.32
44	2	4690	B8K	O6-C6-N1	-2.36	115.60	120.12
44	2	1522	OMG	N2-C2-N1	2.35	121.72	116.71
44	2	4690	B8K	N1-C2-N3	-2.34	118.95	123.32
44	2	4472	B8W	C1'-N9-C4	-2.34	122.53	126.64
44	2	2522	7MG	C2-N1-C6	-2.34	120.83	125.10
44	2	1574	B9B	C61-O6-C6	-2.34	113.14	117.51
44	2	4637	OMG	C8-N7-C5	2.34	107.44	102.99
44	2	4196	OMG	O6-C6-C5	-2.34	119.81	124.37
44	2	3887	OMC	O2-C2-N3	-2.34	118.53	122.33
44	2	1605	7MG	C2-N1-C6	-2.33	120.84	125.10
44	2	1883	OMG	C8-N7-C5	2.32	107.42	102.99
44	2	4623	OMG	C8-N7-C5	2.32	107.42	102.99
44	2	4637	OMG	N2-C2-N1	2.32	121.65	116.71
44	2	4370	OMG	N2-C2-N1	2.32	121.64	116.71
44	2	3897	B8K	C2-N1-C6	-2.31	120.89	125.10
44	2	4129	B8W	C5-C6-N1	-2.30	118.89	123.26
44	2	4523	A2M	C1'-N9-C4	2.29	130.66	126.64
44	2	4550	7MG	C2-N1-C6	-2.28	120.95	125.10
44	2	4564	M7A	C5-C4-N3	-2.28	121.28	126.62
44	2	4083	5MU	O4-C4-N3	-2.27	115.76	120.12
44	2	1625	OMG	O6-C6-C5	-2.27	119.94	124.37
44	2	2364	OMG	C8-N7-C5	2.26	107.30	102.99
44	2	4620	OMU	O2-C2-N1	-2.24	119.80	122.79
44	2	1316	OMG	O6-C6-C5	-2.24	120.00	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	2	373	OMG	O6-C6-C5	-2.23	120.01	124.37
44	2	4550	7MG	N9-C8-N7	2.23	106.57	103.38
44	2	978	2MG	O6-C6-C5	-2.22	120.04	124.37
44	2	1522	OMG	C8-N7-C5	2.22	107.21	102.99
44	2	4494	OMG	O6-C6-C5	-2.21	120.06	124.37
4	8	14	OMU	C1'-N1-C2	2.21	121.57	117.57
44	2	3880	P7G	C71-N7-C5	2.20	129.73	124.52
44	2	2050	OMG	O6-C6-C5	-2.20	120.07	124.37
44	2	1348	P4U	O2-C2-N3	-2.20	118.75	122.33
44	2	4370	OMG	C8-N7-C5	2.20	107.18	102.99
44	2	4550	7MG	C6-C5-C4	-2.19	118.11	122.62
44	2	3909	OMC	C5-C4-N3	-2.19	117.61	121.33
44	2	3869	OMC	C6-C5-C4	2.19	121.03	117.50
44	2	4870	OMG	O6-C6-C5	-2.18	120.11	124.37
44	2	729	2MG	O6-C6-C5	-2.18	120.12	124.37
44	2	4370	OMG	O6-C6-C5	-2.17	120.13	124.37
44	2	2773	OMG	C8-N7-C5	2.17	107.12	102.99
44	2	4529	B8W	C2-N1-C6	2.16	119.55	116.08
44	2	2364	OMG	O6-C6-C5	-2.15	120.17	124.37
44	2	1522	OMG	O6-C6-C5	-2.15	120.18	124.37
44	2	2773	OMG	N2-C2-N1	2.14	121.28	116.71
44	2	4371	MHG	O6-C6-C5	-2.14	122.29	127.54
44	2	2522	7MG	C6-C5-C4	-2.14	118.21	122.62
44	2	2297	E7G	C6-C5-C4	-2.13	118.23	122.62
44	2	1866	UR3	C6-N1-C2	-2.13	119.88	121.79
44	2	2522	7MG	O6-C6-C5	-2.12	122.33	127.54
44	2	3723	A2M	C1'-N9-C4	2.12	130.36	126.64
44	2	398	A2M	C1'-N9-C4	2.12	130.36	126.64
44	2	2050	OMG	C8-N7-C5	2.12	107.02	102.99
44	2	4196	OMG	C8-N7-C5	2.11	107.02	102.99
44	2	4637	OMG	O6-C6-C5	-2.10	120.26	124.37
44	2	1605	7MG	C6-C5-C4	-2.10	118.28	122.62
44	2	1883	OMG	N2-C2-N1	2.10	121.19	116.71
44	2	4371	MHG	N9-C4-N3	2.10	128.60	125.47
44	2	4494	OMG	C8-N7-C5	2.09	106.98	102.99
44	2	1534	A2M	C1'-N9-C4	2.09	130.32	126.64
44	2	2297	E7G	O6-C6-C5	-2.09	122.41	127.54
44	2	373	OMG	N2-C2-N1	2.08	121.14	116.71
44	2	2422	OMC	C1'-N1-C2	2.08	123.05	118.42
44	2	4371	MHG	C71-N7-C5	2.07	129.43	124.52
44	2	4196	OMG	O2'-C2'-C1'	2.07	113.19	109.09
44	2	978	2MG	CM2-N2-C2	-2.06	119.32	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	2	1797	E7G	O6-C6-C5	-2.04	122.53	127.54
44	2	4550	7MG	N1-C2-N3	-2.04	119.52	123.32
44	2	1797	E7G	N1-C2-N3	-2.04	119.52	123.32
44	2	1883	OMG	N1-C2-N3	-2.03	119.52	123.32
4	8	14	OMU	CM2-O2'-C2'	2.03	119.86	114.52
44	2	4597	UR3	C5-C6-N1	-2.03	118.40	121.81
44	2	4872	2MG	O6-C6-C5	-2.03	120.40	124.37
44	2	3880	P7G	N3-C2-N1	-2.03	119.53	123.32
44	2	1625	OMG	C8-N7-C5	2.03	106.86	102.99
44	2	2773	OMG	O6-C6-C5	-2.03	120.41	124.37
44	2	4371	MHG	C71-C72-C73	-2.02	108.53	114.20
44	2	4185	B8W	C2-N1-C6	2.02	119.32	116.08
44	2	1909	P7G	N2-C2-N3	2.01	121.00	116.71
44	2	4536	OMC	O2-C2-N1	2.00	123.03	118.89
44	2	4597	UR3	C3U-N3-C4	2.00	120.75	117.89
44	2	4690	B8K	O6-C6-C5	-2.00	122.63	127.54

There are no chirality outliers.

All (101) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	8	14	OMU	C1'-C2'-O2'-CM2
44	2	237	B9B	C5-C6-O6-C61
44	2	237	B9B	N1-C6-O6-C61
44	2	237	B9B	C3'-C4'-C5'-O5'
44	2	237	B9B	O4'-C4'-C5'-O5'
44	2	398	A2M	O4'-C4'-C5'-O5'
44	2	1348	P4U	N3-C4-O4-C41
44	2	1574	B9B	C5-C6-O6-C61
44	2	1574	B9B	N1-C6-O6-C61
44	2	1625	OMG	C3'-C4'-C5'-O5'
44	2	1797	E7G	C3'-C4'-C5'-O5'
44	2	1797	E7G	O4'-C4'-C5'-O5'
44	2	1883	OMG	O4'-C4'-C5'-O5'
44	2	1883	OMG	C3'-C4'-C5'-O5'
44	2	2364	OMG	O4'-C4'-C5'-O5'
44	2	2380	B8W	C5-C6-O6-C61
44	2	2380	B8W	N1-C6-O6-C61
44	2	2424	OMG	O4'-C4'-C5'-O5'
44	2	2424	OMG	C3'-C4'-C5'-O5'
44	2	2754	B9B	C5-C6-O6-C61
44	2	2754	B9B	N1-C6-O6-C61

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Mol	Chain	Res	Type	Atoms
44	2	3867	A2M	O4'-C4'-C5'-O5'
44	2	3867	A2M	C3'-C4'-C5'-O5'
44	2	3869	OMC	O4'-C1'-N1-C2
44	2	3869	OMC	O4'-C1'-N1-C6
44	2	3880	P7G	O4'-C4'-C5'-O5'
44	2	3897	B8K	O4'-C4'-C5'-O5'
44	2	4129	B8W	C5-C6-O6-C61
44	2	4129	B8W	N1-C6-O6-C61
44	2	4185	B8W	C5-C6-O6-C61
44	2	4185	B8W	N1-C6-O6-C61
44	2	4196	OMG	C1'-C2'-O2'-CM2
44	2	4355	E6G	C5-C6-O6-C61
44	2	4355	E6G	N1-C6-O6-C61
44	2	4415	1MA	O4'-C4'-C5'-O5'
44	2	4637	OMG	O4'-C4'-C5'-O5'
44	2	4637	OMG	C3'-C4'-C5'-O5'
44	2	4870	OMG	C3'-C4'-C5'-O5'
44	2	398	A2M	C3'-C4'-C5'-O5'
44	2	1909	P7G	O4'-C4'-C5'-O5'
44	2	2364	OMG	C3'-C4'-C5'-O5'
44	2	3723	A2M	O4'-C4'-C5'-O5'
44	2	3880	P7G	C3'-C4'-C5'-O5'
44	2	3897	B8K	C3'-C4'-C5'-O5'
44	2	4371	MHG	O4'-C4'-C5'-O5'
44	2	4415	1MA	C3'-C4'-C5'-O5'
44	2	4870	OMG	O4'-C4'-C5'-O5'
44	2	4872	2MG	O4'-C4'-C5'-O5'
44	2	3880	P7G	N7-C71-C72-C73
44	2	1866	UR3	O4'-C4'-C5'-O5'
44	2	1909	P7G	C3'-C4'-C5'-O5'
44	2	3723	A2M	C3'-C4'-C5'-O5'
44	2	4872	2MG	C3'-C4'-C5'-O5'
44	2	3701	OMC	C2'-C1'-N1-C6
44	2	1866	UR3	C3'-C4'-C5'-O5'
44	2	3701	OMC	C2'-C1'-N1-C2
44	2	3869	OMC	C2'-C1'-N1-C6
44	2	1625	OMG	O4'-C4'-C5'-O5'
44	2	4523	A2M	O4'-C4'-C5'-O5'
44	2	1574	B9B	C62-C61-O6-C6
44	2	4523	A2M	C3'-C4'-C5'-O5'
44	2	4371	MHG	C2'-C1'-N9-C8
44	2	1517	2MG	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
44	2	4472	B8W	C5-C6-O6-C61
44	2	3701	OMC	O4'-C1'-N1-C2
44	2	3701	OMC	O4'-C1'-N1-C6
44	2	4870	OMG	C4'-C5'-O5'-P
44	2	4296	B8H	O4'-C4'-C5'-O5'
44	2	3869	OMC	C2'-C1'-N1-C2
44	2	3869	OMC	C3'-C2'-O2'-CM2
44	2	1326	A2M	C4'-C5'-O5'-P
44	2	1326	A2M	C3'-C4'-C5'-O5'
44	2	4296	B8H	C3'-C4'-C5'-O5'
44	2	3880	P7G	C72-C71-N7-C8
44	2	373	OMG	C4'-C5'-O5'-P
44	2	4196	OMG	O4'-C4'-C5'-O5'
44	2	1524	A2M	C3'-C2'-O2'-CM'
44	2	2401	A2M	C3'-C2'-O2'-CM'
44	2	2786	B9H	C32-C31-N3-C2
44	2	1348	P4U	O4-C41-C42-C43
44	2	3897	B8K	C4'-C5'-O5'-P
44	2	729	2MG	O4'-C4'-C5'-O5'
44	2	2297	E7G	C72-C71-N7-C8
44	2	3887	OMC	C4'-C5'-O5'-P
44	2	2422	OMC	O4'-C4'-C5'-O5'
44	2	1659	I4U	C42-C41-O4-C4
44	2	2773	OMG	C3'-C2'-O2'-CM2
44	2	4371	MHG	O4'-C1'-N9-C8
44	2	4415	1MA	C4'-C5'-O5'-P
44	2	1326	A2M	O4'-C4'-C5'-O5'
44	2	1534	A2M	O4'-C4'-C5'-O5'
44	2	1524	A2M	C1'-C2'-O2'-CM'
44	2	4637	OMG	C1'-C2'-O2'-CM2
44	2	1316	OMG	O4'-C4'-C5'-O5'
44	2	1517	2MG	C3'-C4'-C5'-O5'
44	2	1659	I4U	C43-C41-O4-C4
44	2	237	B9B	C62-C61-O6-C6
44	2	2754	B9B	C62-C61-O6-C6
44	2	4523	A2M	C4'-C5'-O5'-P
44	2	4690	B8K	O4'-C4'-C5'-O5'
44	2	1517	2MG	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
52	GDP	A	801	53,54	24,30,30	1.20	2 (8%)	30,47,47	1.41	5 (16%)
55	GTP	4	701	46,53	26,34,34	1.12	2 (7%)	32,54,54	1.64	7 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	GDP	A	801	53,54	-	2/12/32/32	0/3/3/3
55	GTP	4	701	46,53	-	2/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	4	701	GTP	C5-C6	-3.90	1.39	1.47
52	A	801	GDP	C6-N1	-3.47	1.32	1.37
52	A	801	GDP	C2'-C1'	-2.22	1.50	1.53
55	4	701	GTP	C2-N3	2.14	1.38	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	A	801	GDP	PA-O3A-PB	-3.52	120.74	132.83
55	4	701	GTP	C5-C6-N1	3.50	120.14	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	4	701	GTP	C3'-C2'-C1'	3.38	106.06	100.98
52	A	801	GDP	C3'-C2'-C1'	3.26	105.89	100.98
55	4	701	GTP	C2-N1-C6	-3.03	119.51	125.10
55	4	701	GTP	PB-O3B-PG	-3.02	122.45	132.83
55	4	701	GTP	PA-O3A-PB	-2.93	122.76	132.83
55	4	701	GTP	C8-N7-C5	2.86	108.43	102.99
52	A	801	GDP	C8-N7-C5	2.47	107.69	102.99
52	A	801	GDP	O3B-PB-O2B	2.35	116.63	107.64
52	A	801	GDP	C5-C6-N1	2.32	118.05	113.95
55	4	701	GTP	O6-C6-C5	-2.16	120.15	124.37

There are no chirality outliers.

All (4) torsion outliers are listed below:

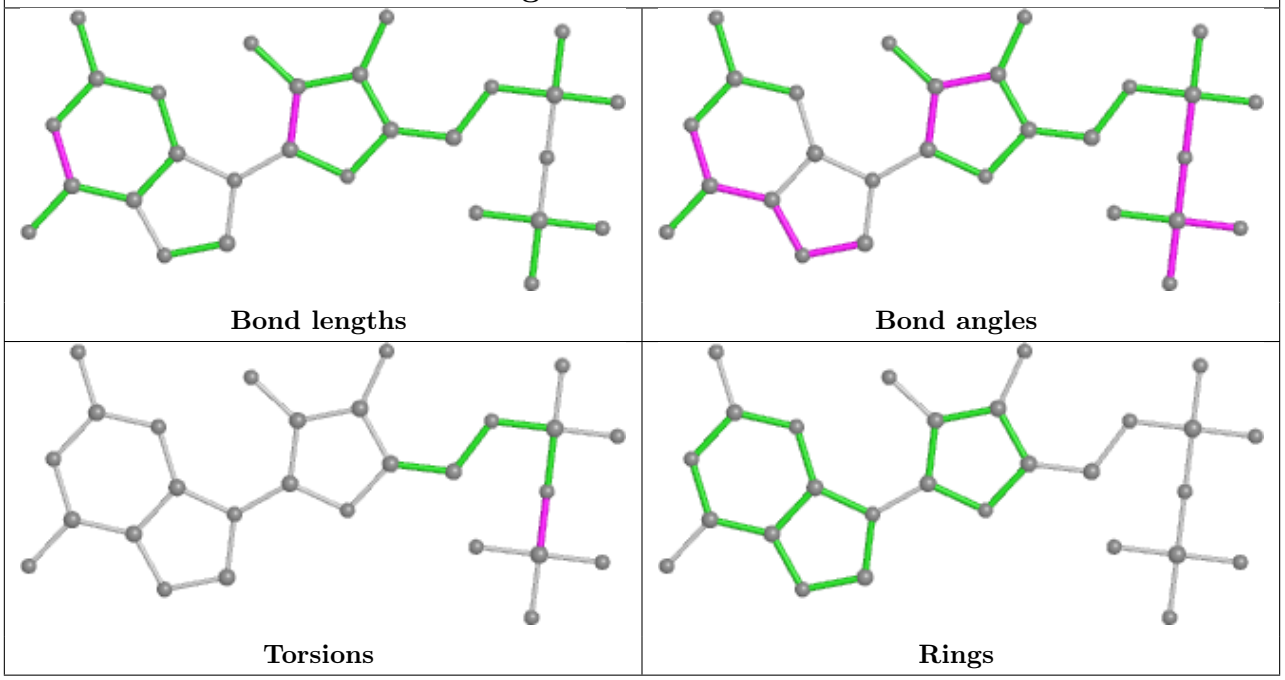
Mol	Chain	Res	Type	Atoms
52	A	801	GDP	PA-O3A-PB-O2B
55	4	701	GTP	C4'-C5'-O5'-PA
52	A	801	GDP	PA-O3A-PB-O1B
55	4	701	GTP	C5'-O5'-PA-O1A

There are no ring outliers.

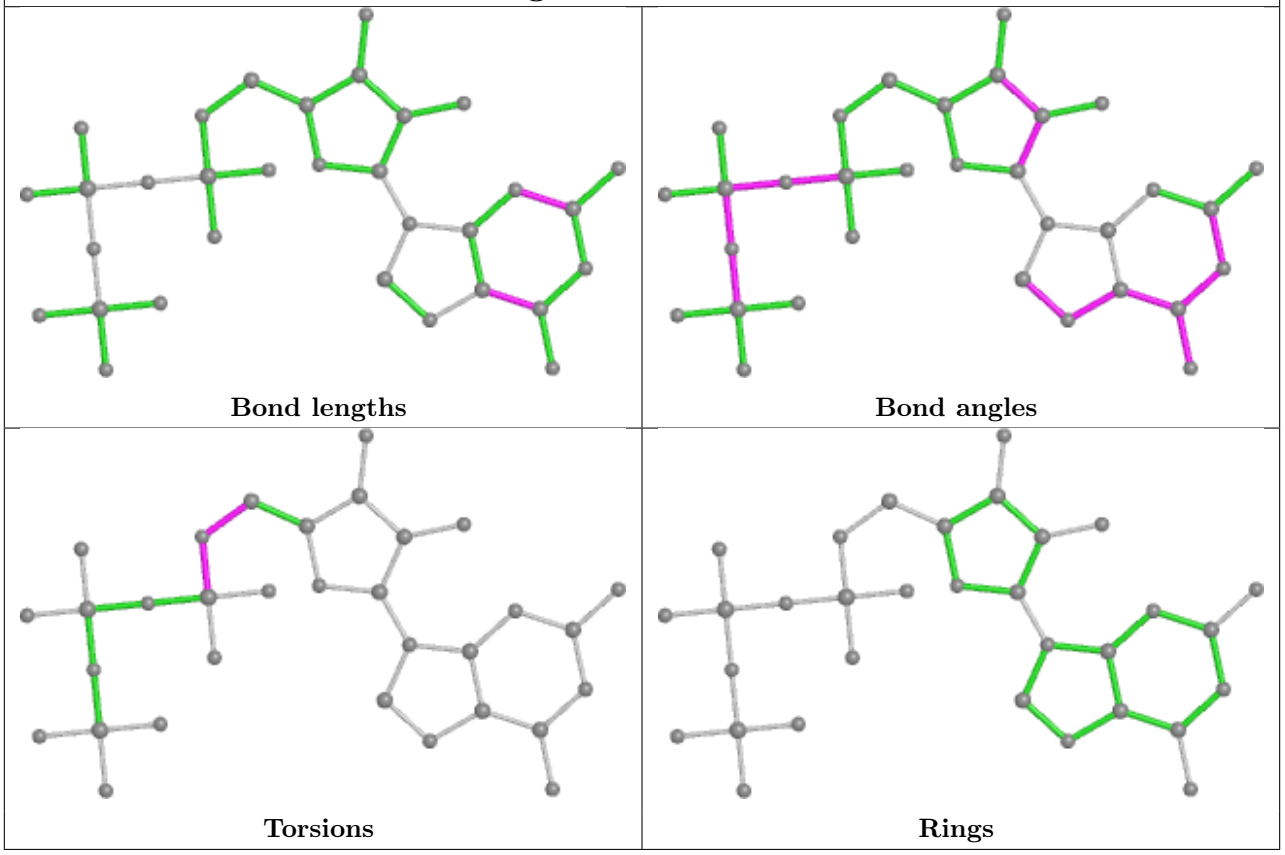
No monomer is involved in short contacts.

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

Ligand GDP A 801



Ligand GTP 4 701



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.

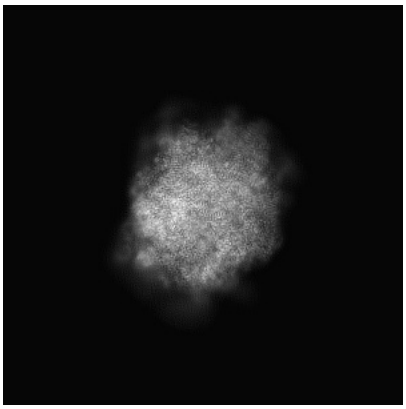
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-35370. These allow visual inspection of the internal detail of the map and identification of artifacts.

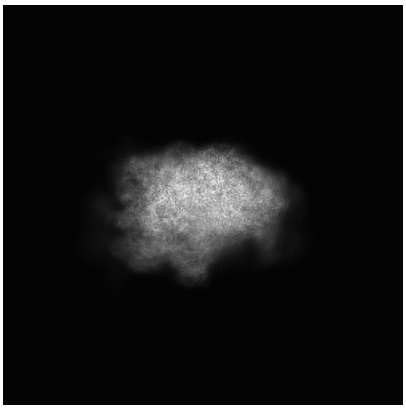
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

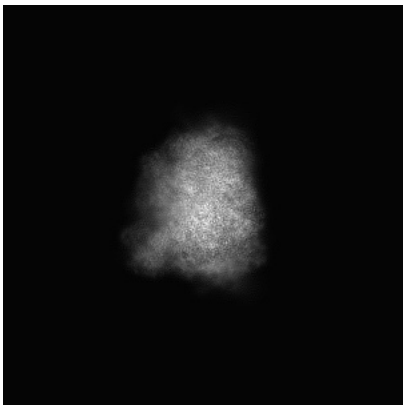
6.1.1 Primary map



X

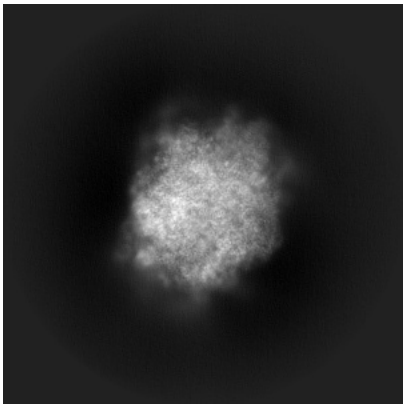


Y

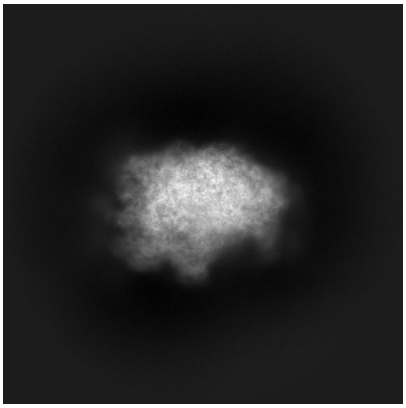


Z

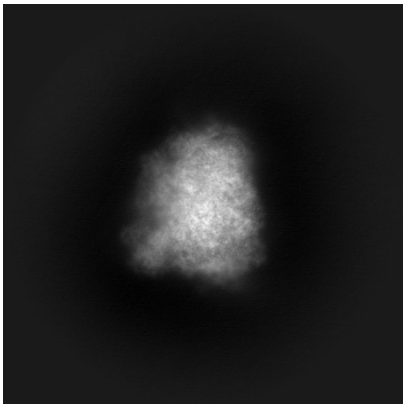
6.1.2 Raw map



X



Y

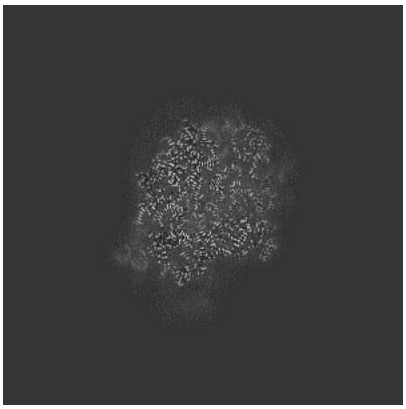


Z

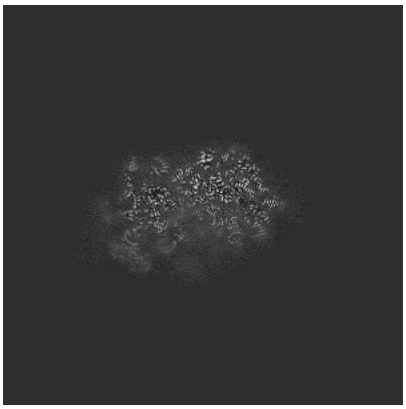
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

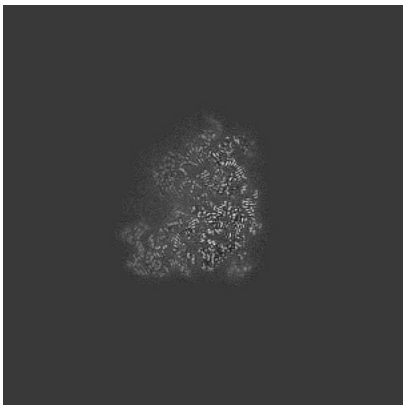
6.2.1 Primary map



X Index: 200

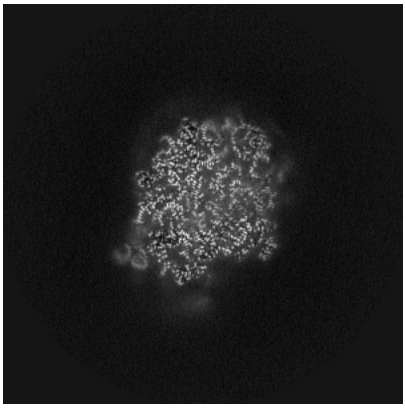


Y Index: 200

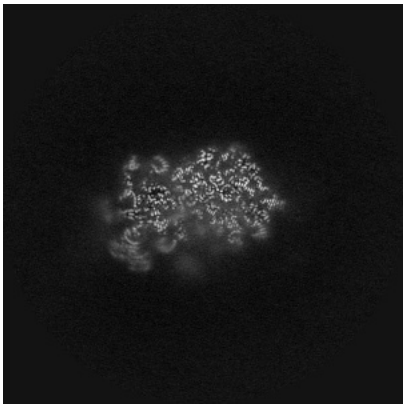


Z Index: 200

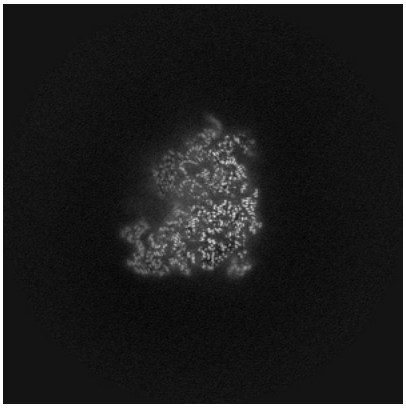
6.2.2 Raw map



X Index: 200



Y Index: 200

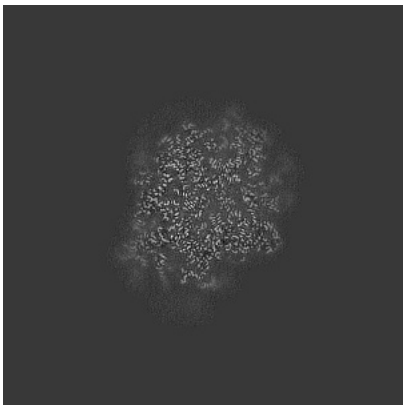


Z Index: 200

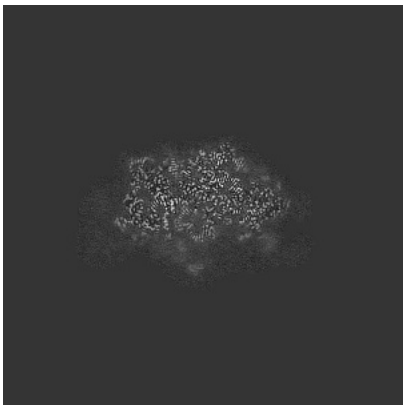
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

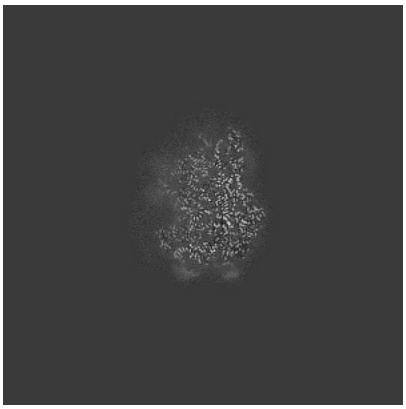
6.3.1 Primary map



X Index: 206

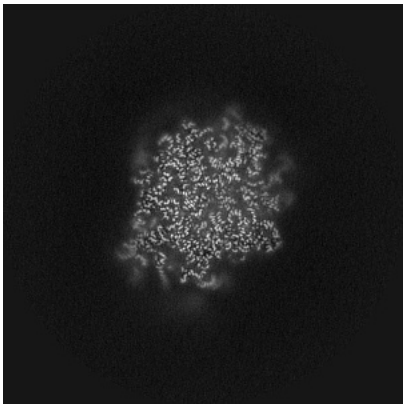


Y Index: 182

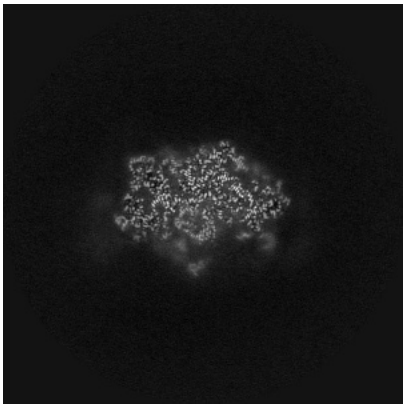


Z Index: 215

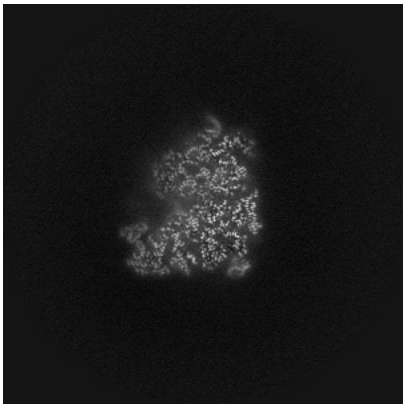
6.3.2 Raw map



X Index: 206



Y Index: 181

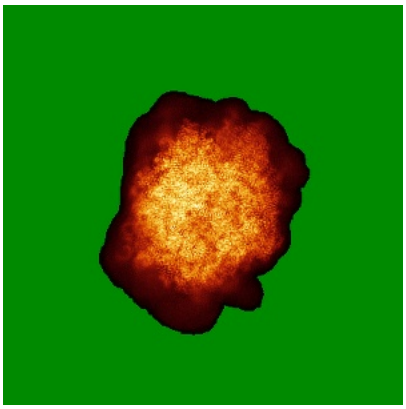


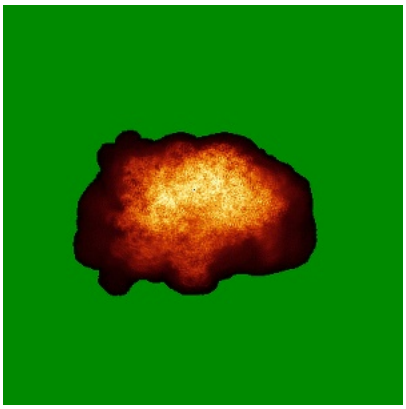
Z Index: 201

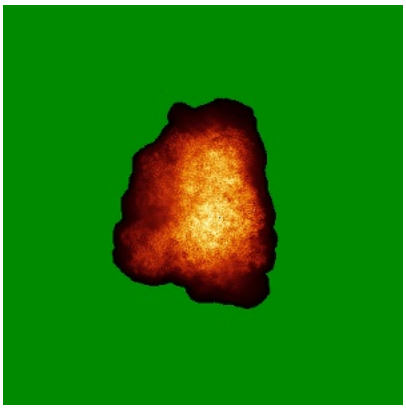
The images above show the largest variance slices of the map in three orthogonal directions.

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

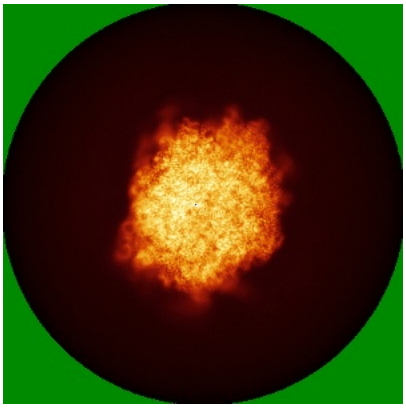
6.4.1 Primary map

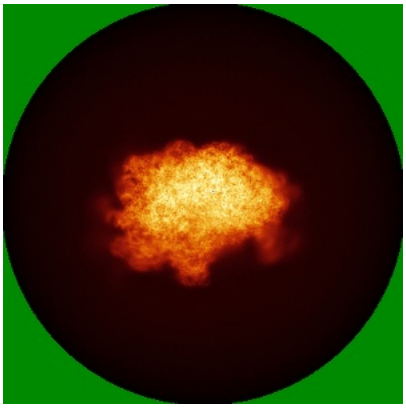

X

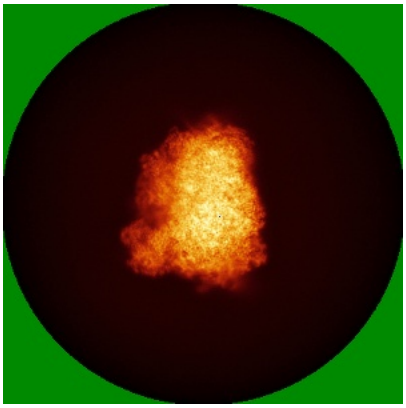

Y


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 0.045. 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.

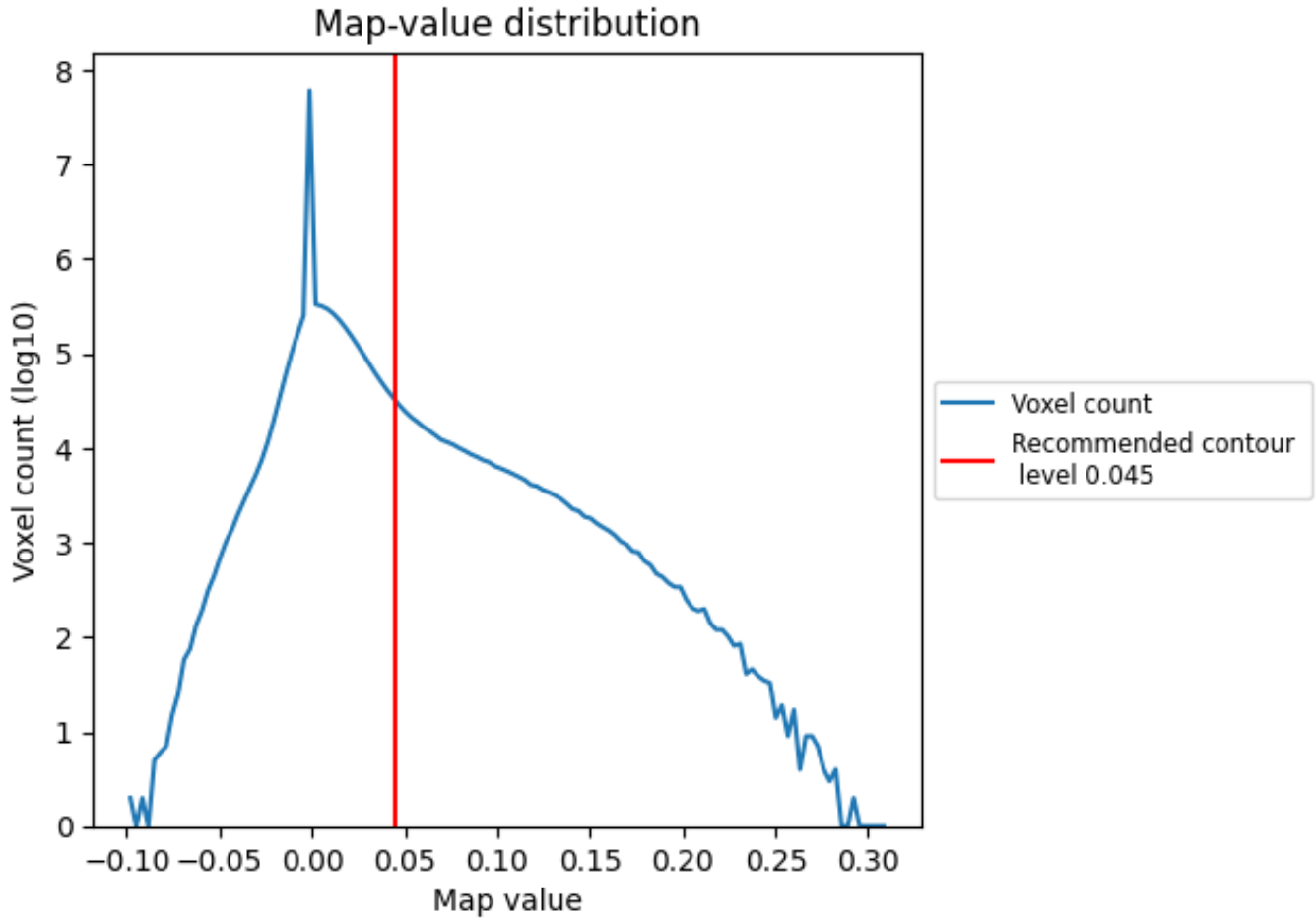
6.6 Mask visualisation (i)

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

7 Map analysis

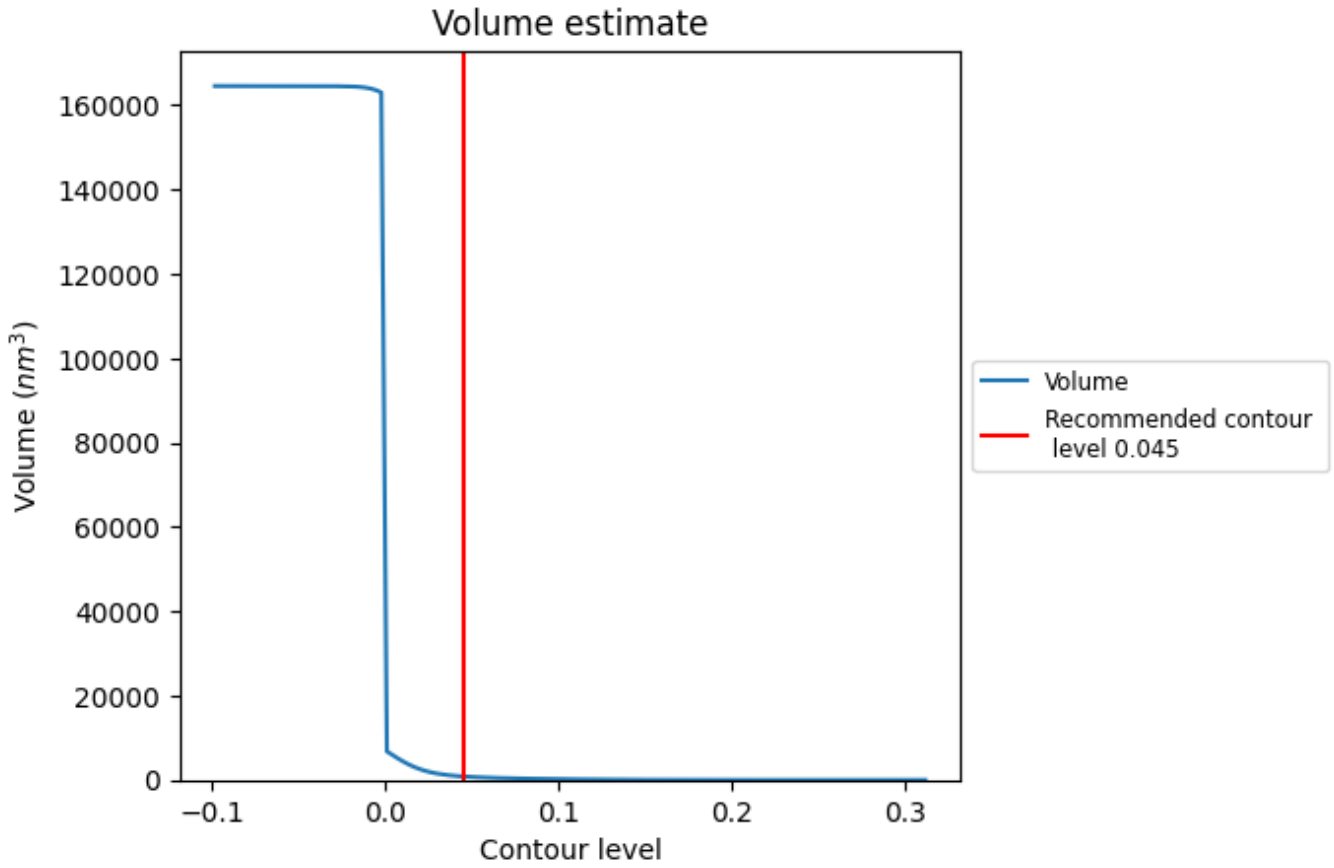
This section contains the results of statistical analysis of the map.

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.

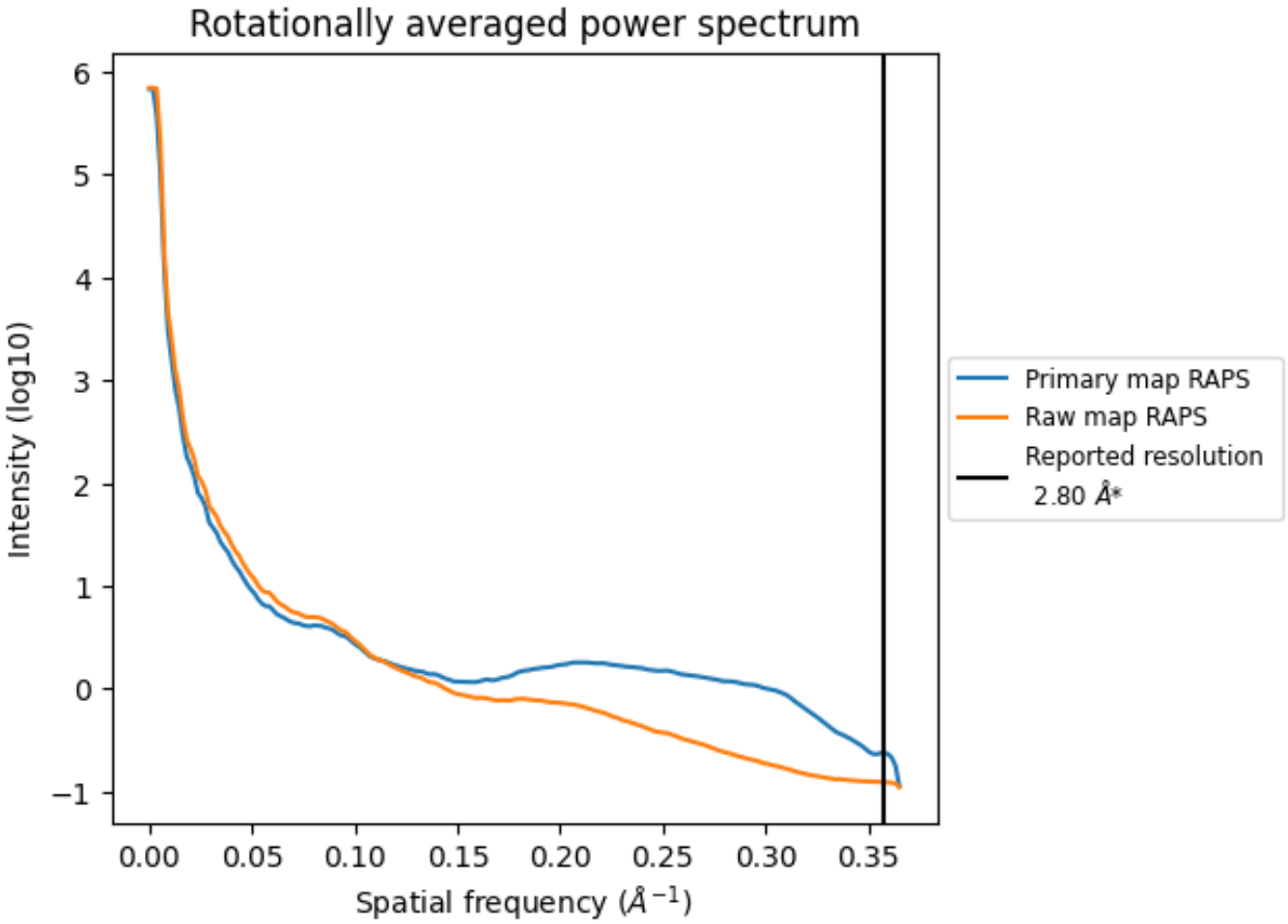
7.2 Volume estimate



The volume at the recommended contour level is 836 nm^3; this corresponds to an approximate mass of 755 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)

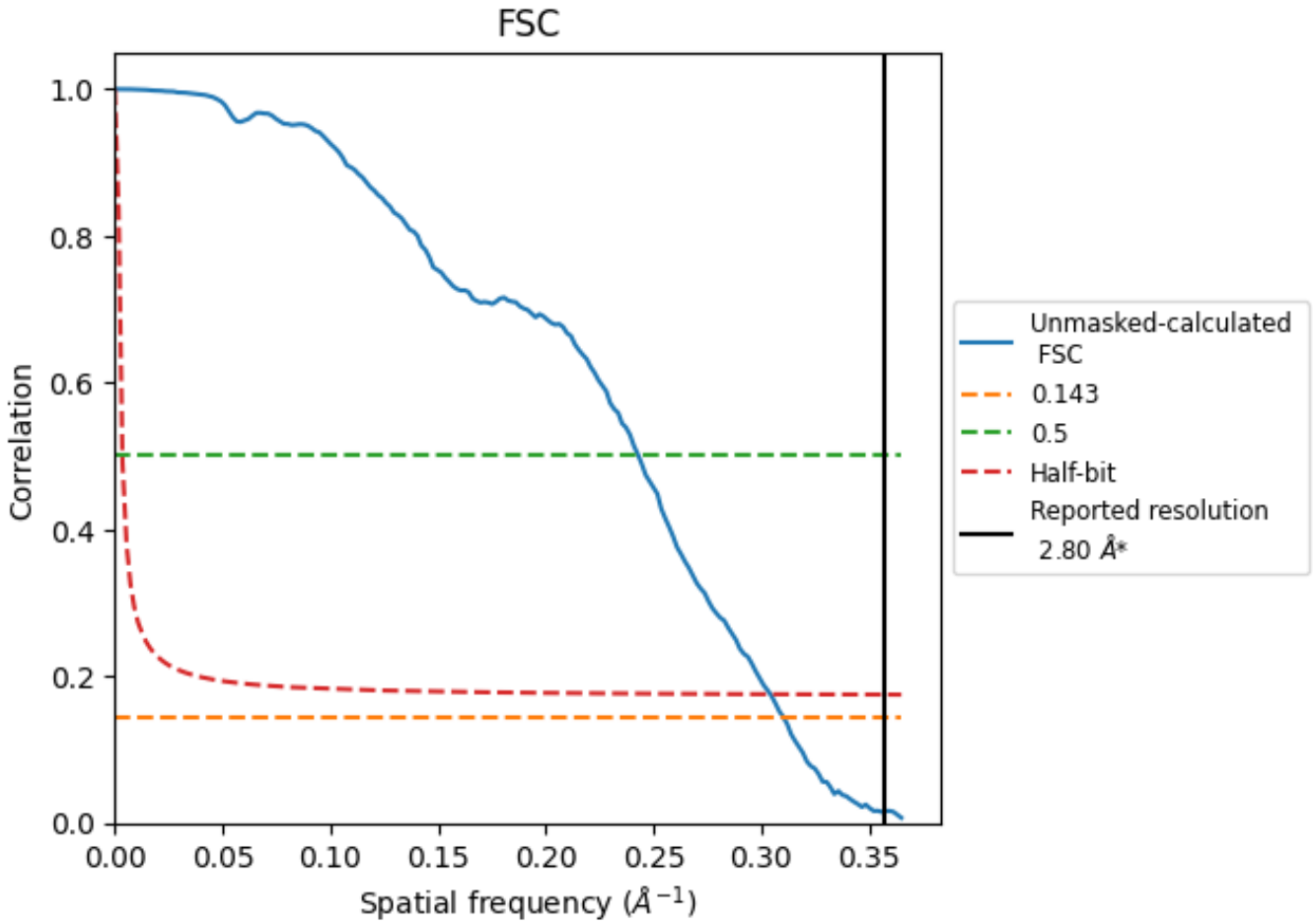


*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

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 0.357 Å^{-1}

8.2 Resolution estimates (i)

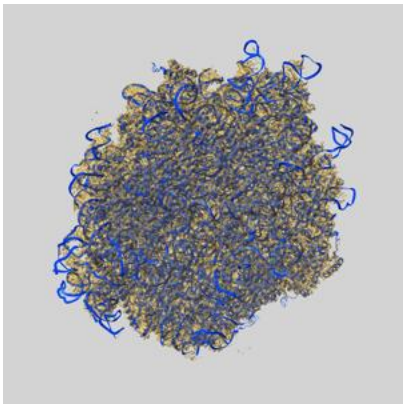
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.22	4.12	3.29

*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 3.22 differs from the reported value 2.8 by more than 10 %

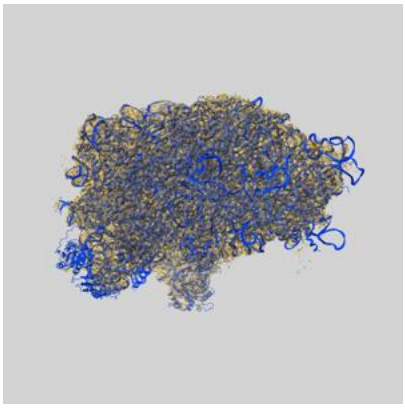
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-35370 and PDB model 8IDT. Per-residue inclusion information can be found in section 3 on page 14.

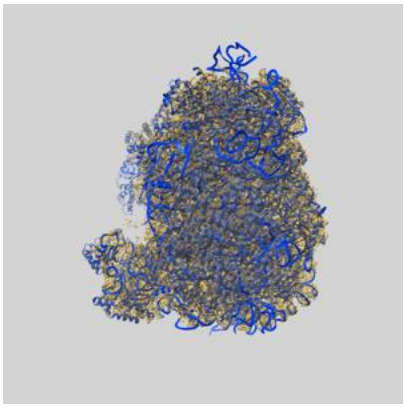
9.1 Map-model overlay



X



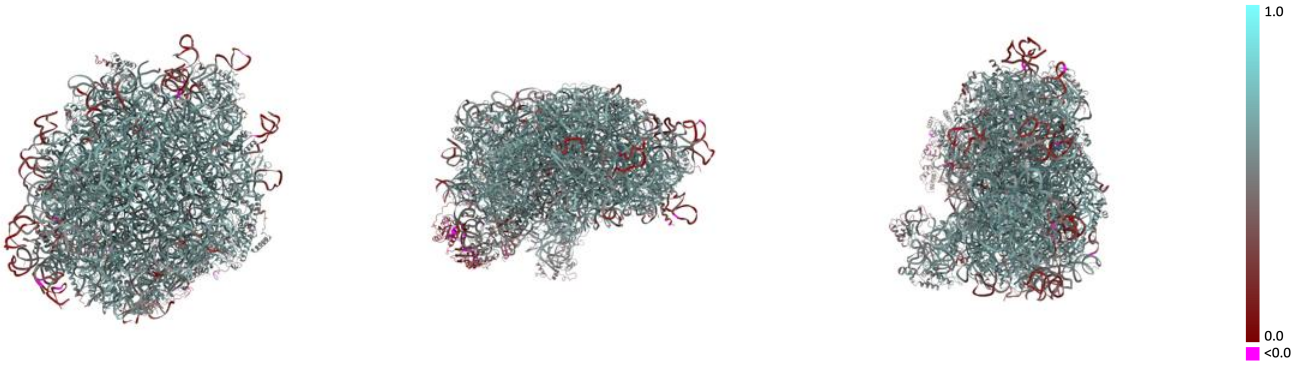
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

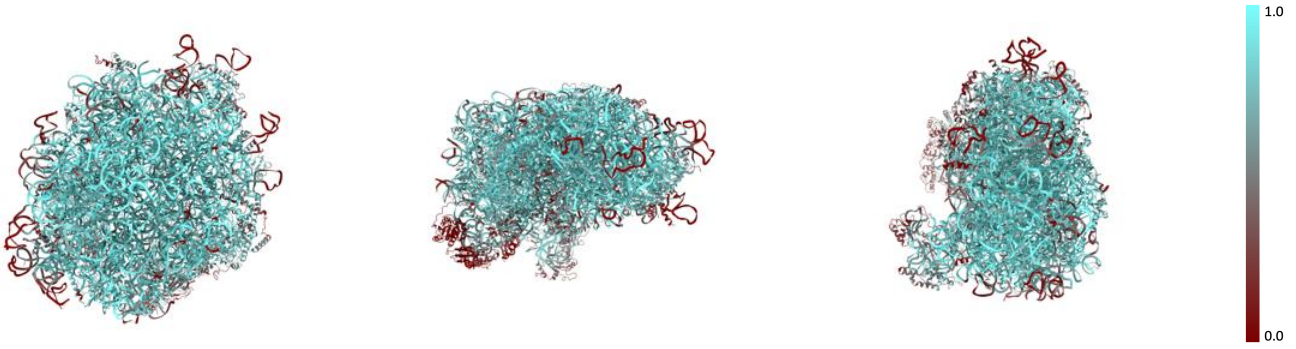
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

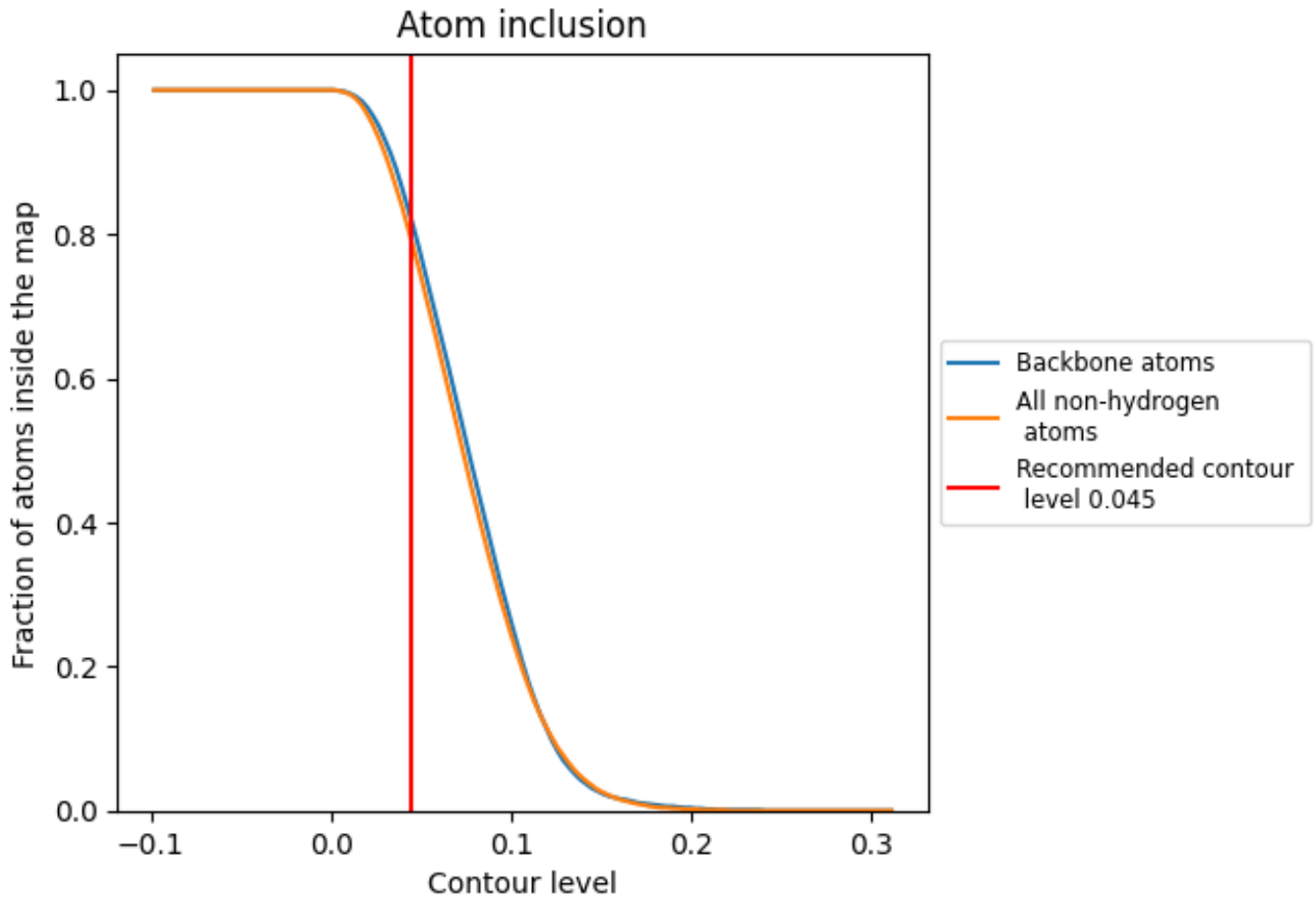
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.045).

9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 79% 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 (0.045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7910	0.5500
2	0.8320	0.5460
4	0.6000	0.4920
5	0.8910	0.5750
6	0.7140	0.5450
7	0.8060	0.5820
8	0.9220	0.5940
9	0.3770	0.4980
A	0.4620	0.5310
B	0.8960	0.6100
C	0.6720	0.5150
D	0.9220	0.6120
E	0.5600	0.5360
F	0.8450	0.5860
G	0.6810	0.5200
H	0.8420	0.5950
I	0.7840	0.5710
J	0.0470	0.1950
K	0.8180	0.5860
L	0.9260	0.6220
M	0.9520	0.6190
N	0.3540	0.4200
O	0.6140	0.5230
P	0.9690	0.6220
Q	0.8290	0.5770
R	0.4980	0.5180
S	0.8750	0.5950
T	0.5200	0.5110
U	0.9620	0.6320
V	0.9120	0.6080
W	0.7270	0.5800
X	0.7280	0.5670
Y	0.8490	0.5990
Z	0.9400	0.6330
a	0.8080	0.5880

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Chain	Atom inclusion	Q-score
b	0.9340	0.6260
c	0.8400	0.5810
d	0.7320	0.5550
e	0.8610	0.5910
g	0.8650	0.6000
h	0.8650	0.5980
i	0.6720	0.5570
j	0.8290	0.5890
k	0.9380	0.6230
l	0.9200	0.6100
m	0.8700	0.5950
n	0.9480	0.6280
o	0.7250	0.5330
p	0.9030	0.6060
r	0.5570	0.5000
y	0.0200	0.2250
z	0.4800	0.4980