



## Full wwPDB EM Validation Report ⓘ

Mar 31, 2025 – 08:08 PM JST

PDB ID : 6LSR / pdb\_00006lsr  
EMDB ID : EMD-0963  
Title : Cryo-EM structure of a pre-60S ribosomal subunit - state B  
Authors : Liang, X.; Zuo, M.; Zhang, Y.; Li, N.; Ma, C.; Dong, M.; Gao, N.  
Deposited on : 2020-01-20  
Resolution : 3.13 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](mailto: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>.

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

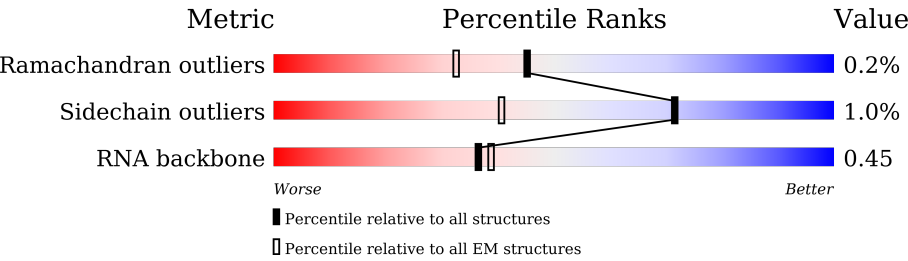
EMDB validation analysis : 0.0.1.dev117  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.42

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.13 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.



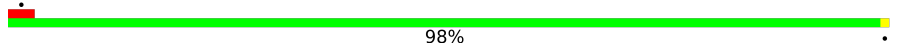



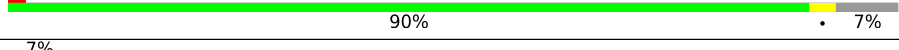

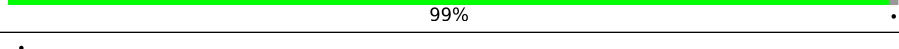
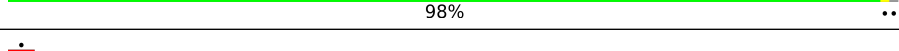
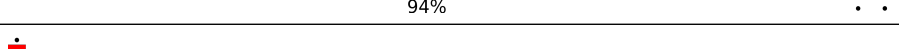
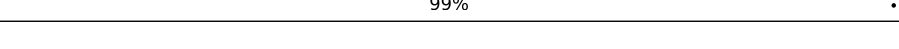
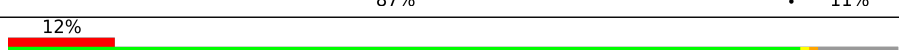

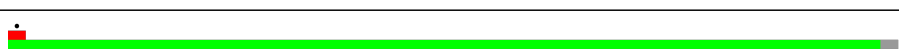
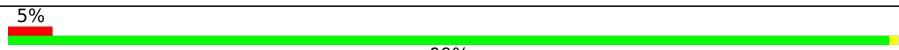
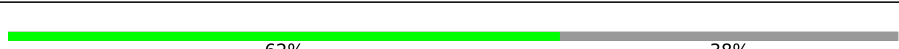

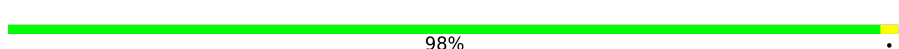
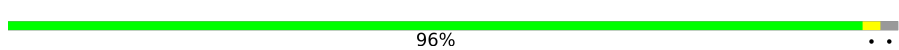
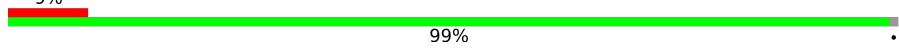
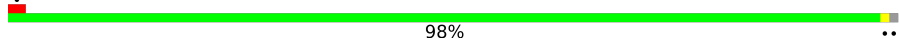
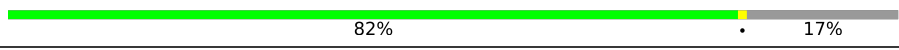
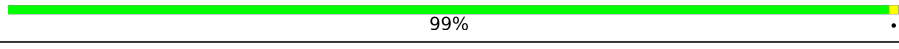

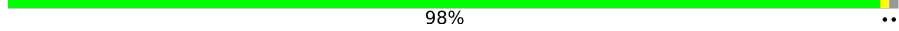

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	477	
2	1	658	
3	2	5070	
4	3	534	
5	5	120	
6	6	245	
7	8	156	
8	A	217	

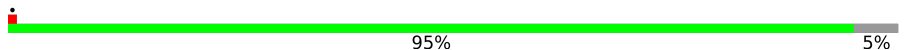
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Mol	Chain	Length	Quality of chain
9	B	403	
10	C	159	
11	D	427	
12	E	115	
13	F	117	
14	G	266	
15	H	123	
16	I	192	
17	K	105	
18	L	148	
19	M	97	
20	N	178	
21	O	70	
22	P	51	
23	Q	211	
24	S	215	
25	T	125	
26	U	204	
27	V	203	
28	W	106	
29	X	92	
30	Y	184	
31	Z	188	
32	a	196	
33	b	176	

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Mol	Chain	Length	Quality of chain
34	c	160	
35	d	128	
36	e	140	
37	f	157	
38	g	156	
39	h	145	
40	i	136	
41	l	137	
42	m	257	
43	r	297	
44	t	135	
45	u	110	
46	v	288	
47	w	248	
48	z	394	

## 2 Entry composition

There are 50 unique types of molecules in this entry. The entry contains 141172 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Zinc finger protein 622.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	190	Total	C	N	O	S	0	0
			1537	968	266	287	16		

- Molecule 2 is a protein called Large subunit GTPase 1 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	1	247	Total	C	N	O	0	0
			988	494	247	247		

- Molecule 3 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	3482	Total	C	N	O	P	0	0
			74786	33362	13689	24254	3481		

- Molecule 4 is a protein called 60S ribosomal export protein NMD3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	255	Total	C	N	O	S	0	0
			2053	1305	358	373	17		

There are 31 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	504	GLY	-	expression tag	UNP Q96D46
3	505	SER	-	expression tag	UNP Q96D46
3	506	GLU	-	expression tag	UNP Q96D46
3	507	ASN	-	expression tag	UNP Q96D46
3	508	LEU	-	expression tag	UNP Q96D46
3	509	TYR	-	expression tag	UNP Q96D46
3	510	PHE	-	expression tag	UNP Q96D46
3	511	GLN	-	expression tag	UNP Q96D46
3	512	GLY	-	expression tag	UNP Q96D46

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Chain	Residue	Modelled	Actual	Comment	Reference
3	513	ASP	-	expression tag	UNP Q96D46
3	514	TYR	-	expression tag	UNP Q96D46
3	515	LYS	-	expression tag	UNP Q96D46
3	516	ASP	-	expression tag	UNP Q96D46
3	517	HIS	-	expression tag	UNP Q96D46
3	518	ASP	-	expression tag	UNP Q96D46
3	519	GLY	-	expression tag	UNP Q96D46
3	520	ASP	-	expression tag	UNP Q96D46
3	521	TYR	-	expression tag	UNP Q96D46
3	522	LYS	-	expression tag	UNP Q96D46
3	523	ASP	-	expression tag	UNP Q96D46
3	524	HIS	-	expression tag	UNP Q96D46
3	525	ASP	-	expression tag	UNP Q96D46
3	526	ILE	-	expression tag	UNP Q96D46
3	527	ASP	-	expression tag	UNP Q96D46
3	528	TYR	-	expression tag	UNP Q96D46
3	529	LYS	-	expression tag	UNP Q96D46
3	530	ASP	-	expression tag	UNP Q96D46
3	531	ASP	-	expression tag	UNP Q96D46
3	532	ASP	-	expression tag	UNP Q96D46
3	533	ASP	-	expression tag	UNP Q96D46
3	534	LYS	-	expression tag	UNP Q96D46

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	224	Total	C	N	O	S	0	0
			1704	1060	294	339	11		

- Molecule 7 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	8	155	Total	C	N	O	P	0	0
			3294	1471	583	1086	154		

- Molecule 8 is a protein called 60S ribosomal protein L10a.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	212	Total	C	N	O	S	0	0
			1708	1092	308	300	8		

- Molecule 9 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	402	Total	C	N	O	S	0	0
			3238	2060	608	556	14		

- Molecule 10 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	C	92	Total	C	N	O	S	0	0
			757	471	166	117	3		

- Molecule 11 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	D	357	Total	C	N	O	S	0	0
			2846	1791	569	472	14		

- Molecule 12 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	E	94	Total	C	N	O	S	0	0
			732	465	130	131	6		

- Molecule 13 is a protein called 60S ribosomal protein L34.

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

- Molecule 14 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	231	Total	C	N	O	S	0	0
			1853	1180	359	310	4		

- Molecule 15 is a protein called 60S ribosomal protein L35.

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

- Molecule 16 is a protein called 60S ribosomal protein L9.

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

- Molecule 17 is a protein called 60S ribosomal protein L36.

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

- Molecule 18 is a protein called 60S ribosomal protein L27a.

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

- Molecule 19 is a protein called 60S ribosomal protein L37.

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

- Molecule 20 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N	162	Total	C	N	O	S	0	0
			1302	823	244	230	5		

- Molecule 21 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	O	68	Total	C	N	O	S	0	0
			559	360	101	97	1		

- Molecule 22 is a protein called 60S ribosomal protein L39.



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

- Molecule 23 is a protein called 60S ribosomal protein L13.

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

- Molecule 24 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	S	134	Total	C	N	O	S	0	0
			1103	707	212	177	7		

- Molecule 25 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	T	107	Total	C	N	O	S	0	0
			888	560	171	155	2		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	V	199	Total	C	N	O	S	0	0
			1634	1053	319	257	5		

- Molecule 28 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	W	105	Total	C	N	O	S	0	0
			862	542	175	139	6		

- Molecule 29 is a protein called 60S ribosomal protein L37a.

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

- Molecule 30 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Y	153	Total	C	N	O	S	0	0
			1242	776	241	216	9		

- Molecule 31 is a protein called 60S ribosomal protein L18.

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

- Molecule 32 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	a	145	Total	C	N	O	S	0	0
			1217	759	262	187	9		

- Molecule 33 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	b	175	Total	C	N	O	S	0	0
			1453	925	283	235	10		

- Molecule 34 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	c	157	Total	C	N	O	S	0	0
			1284	815	250	214	5		

- Molecule 35 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	d	99	Total	C	N	O	S	0	0
			808	518	141	147	2		

- Molecule 36 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	e	129	Total	C	N	O	S	0	0
			969	613	182	169	5		

- Molecule 37 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	f	62	Total	C	N	O	S	0	0
			519	332	101	83	3		

- Molecule 38 is a protein called 60S ribosomal protein L23a.

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

- Molecule 39 is a protein called 60S ribosomal protein L26.

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

- Molecule 40 is a protein called 60S ribosomal protein L27.

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
43	r	275	Total	C	N	O	S	0	0
			2237	1414	405	404	14		

- Molecule 44 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	t	128	Total	C	N	O	S	0	0
			1053	667	216	165	5		

- Molecule 45 is a protein called 60S ribosomal protein L35a.

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

- Molecule 46 is a protein called 60S ribosomal protein L6.

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

- Molecule 47 is a protein called 60S ribosomal protein L7.

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

- Molecule 48 is a protein called Proliferation-associated protein 2G4.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	z	354	Total	C	N	O	S	13	0
			2837	1792	483	543	19		

- Molecule 49 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
49	2	236	Total	Mg	0
			236	236	
49	5	3	Total	Mg	0
			3	3	
49	8	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
49	F	1	Total 1	Mg 1	0
49	a	1	Total 1	Mg 1	0
49	c	1	Total 1	Mg 1	0
49	m	2	Total 2	Mg 2	0
49	w	1	Total 1	Mg 1	0

- Molecule 50 is water.

Mol	Chain	Residues	Atoms		AltConf
50	2	7	Total 7	O 7	0



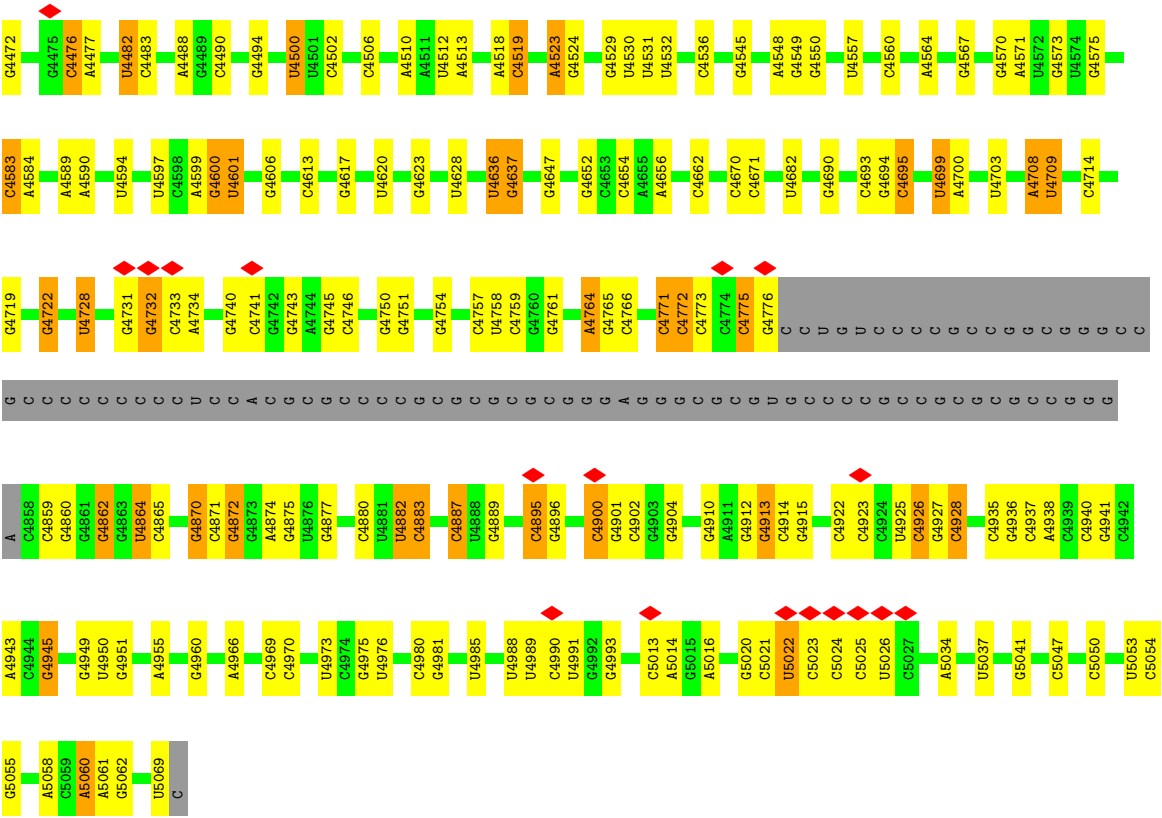




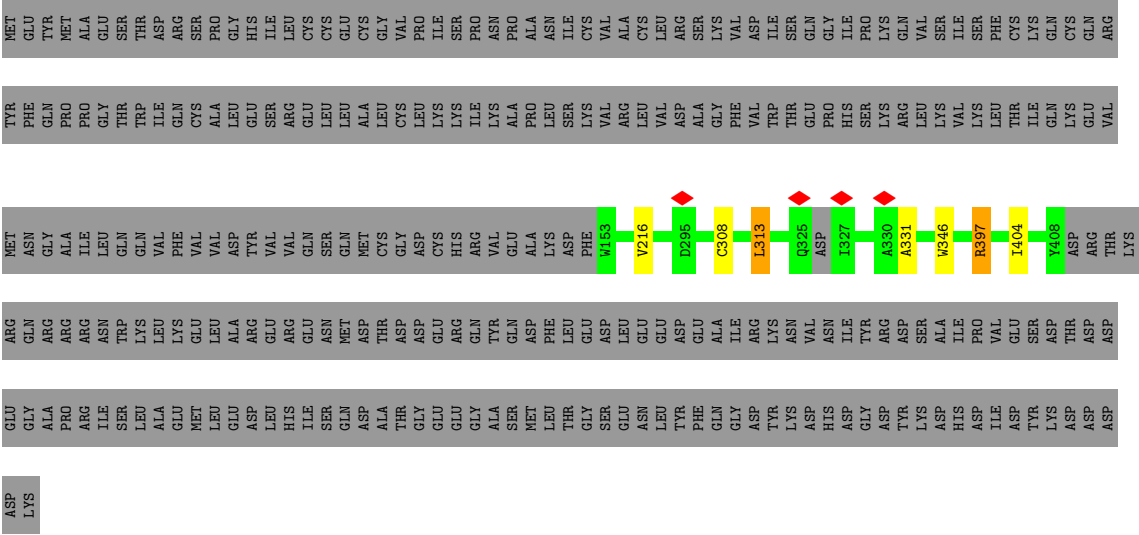




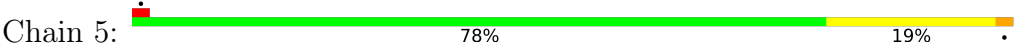




● Molecule 4: 60S ribosomal export protein NMD3

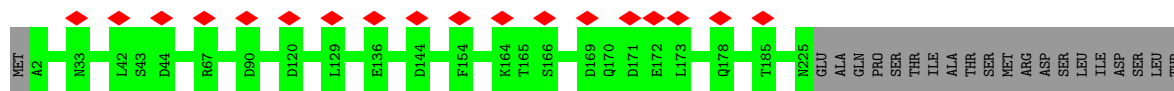


● Molecule 5: 5S rRNA

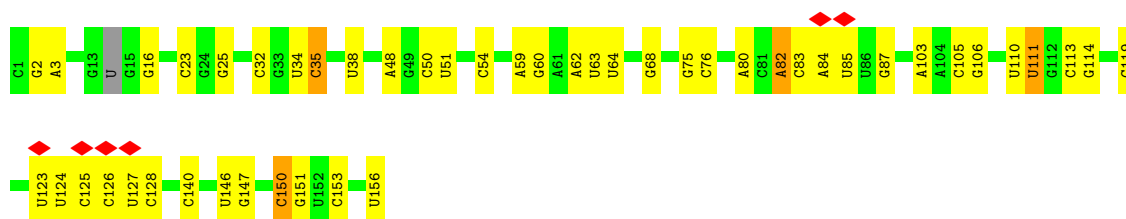




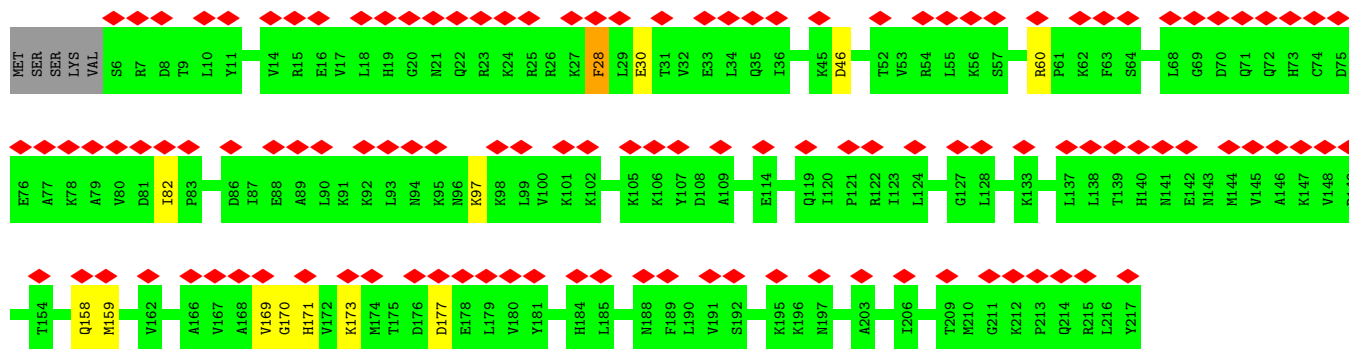
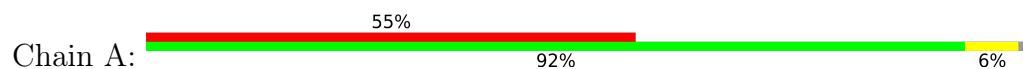
- Molecule 6: Eukaryotic translation initiation factor 6



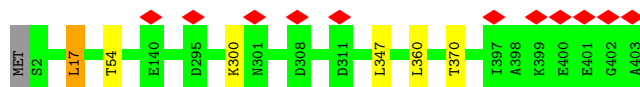
- Molecule 7: 5.8S rRNA



- Molecule 8: 60S ribosomal protein L10a



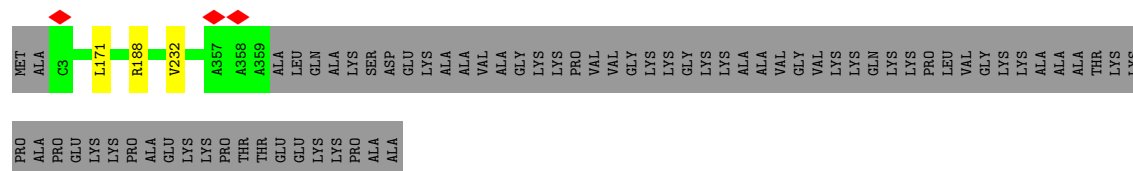
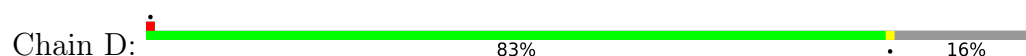
- Molecule 9: 60S ribosomal protein L3



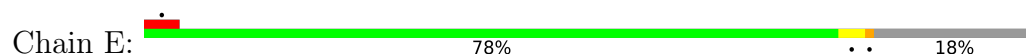
- Molecule 10: 60S ribosomal protein L29



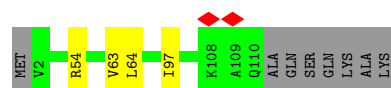
- Molecule 11: 60S ribosomal protein L4



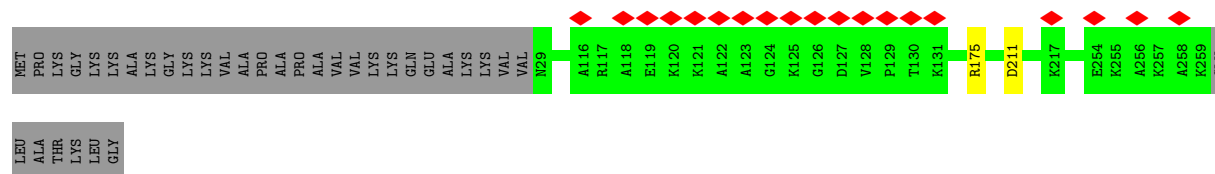
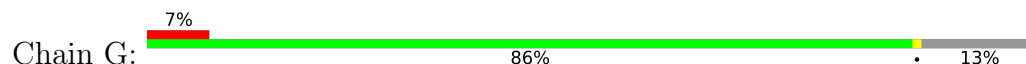
- Molecule 12: 60S ribosomal protein L30



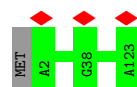
- Molecule 13: 60S ribosomal protein L34



- Molecule 14: 60S ribosomal protein L7a

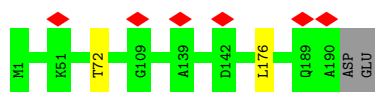


- Molecule 15: 60S ribosomal protein L35



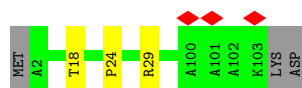
- Molecule 16: 60S ribosomal protein L9

Chain I:  98%



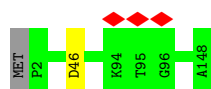
- Molecule 17: 60S ribosomal protein L36

Chain K:  94%



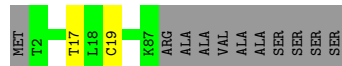
- Molecule 18: 60S ribosomal protein L27a

Chain L:  99%

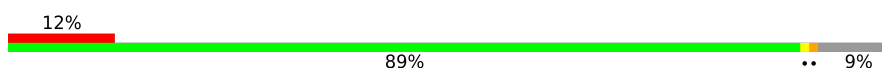


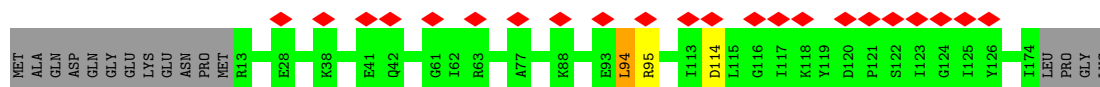
- Molecule 19: 60S ribosomal protein L37

Chain M:  87%



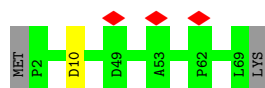
- Molecule 20: 60S ribosomal protein L11

Chain N:  12%



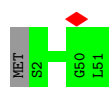
- Molecule 21: 60S ribosomal protein L38

Chain O:  96%

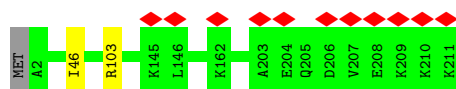


- Molecule 22: 60S ribosomal protein L39

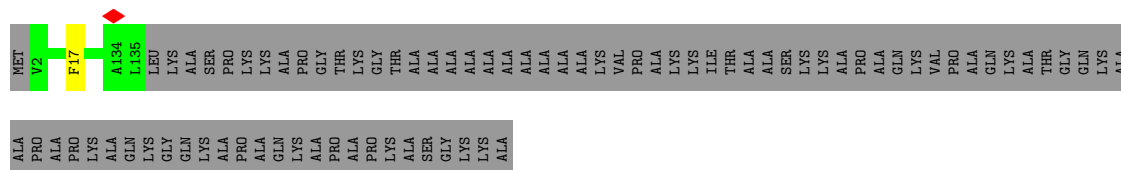
Chain P:  98%



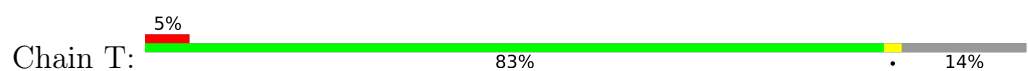
- Molecule 23: 60S ribosomal protein L13



- Molecule 24: 60S ribosomal protein L14



- Molecule 25: 60S ribosomal protein L31



- Molecule 26: 60S ribosomal protein L15



- Molecule 27: 60S ribosomal protein L13a

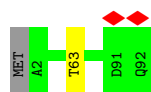


- Molecule 28: 60S ribosomal protein L36a



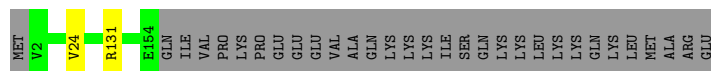
- Molecule 29: 60S ribosomal protein L37a





- Molecule 30: 60S ribosomal protein L17

Chain Y: 82% 17%



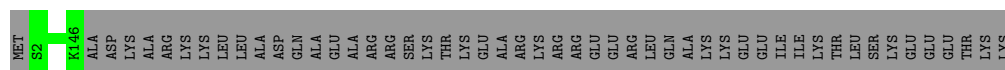
- Molecule 31: 60S ribosomal protein L18

Chain Z: 99% ..



- Molecule 32: 60S ribosomal protein L19

Chain a: 74% 26%



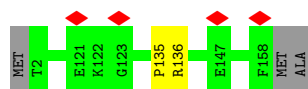
- Molecule 33: 60S ribosomal protein L18a

Chain b: 98% ..



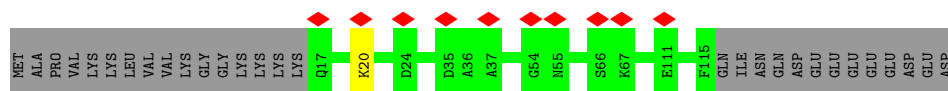
- Molecule 34: 60S ribosomal protein L21

Chain c: 97% ..




- Molecule 35: 60S ribosomal protein L22

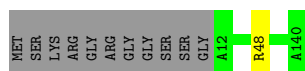
Chain d: 8% 77% 23%



- Molecule 36: 60S ribosomal protein L23

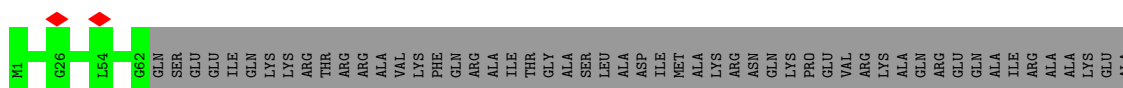


Chain e:  91% 8%




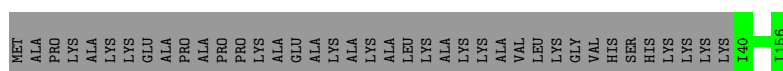
- Molecule 37: 60S ribosomal protein L24

Chain f:  39% 61%




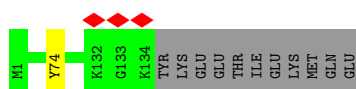
- Molecule 38: 60S ribosomal protein L23a

Chain g:  75% 25%



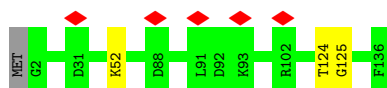
- Molecule 39: 60S ribosomal protein L26

Chain h:  92% 8%




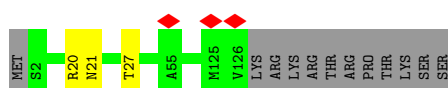
- Molecule 40: 60S ribosomal protein L27

Chain i:  97%



- Molecule 41: 60S ribosomal protein L28

Chain l:  89% 9%

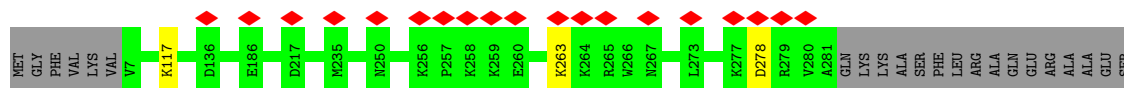
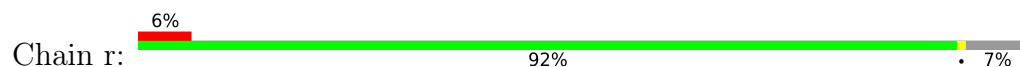


- Molecule 42: 60S ribosomal protein L8

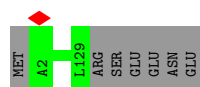
Chain m:  94%



- Molecule 43: 60S ribosomal protein L5



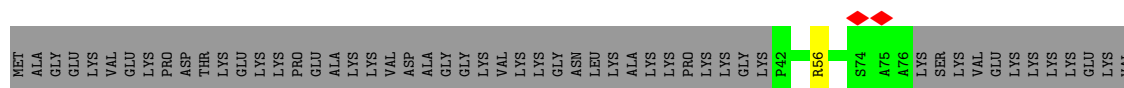
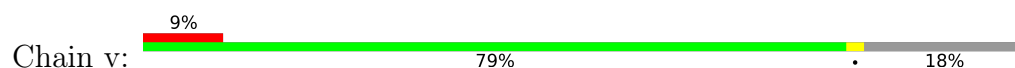
- Molecule 44: 60S ribosomal protein L32



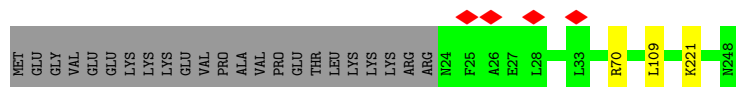
- Molecule 45: 60S ribosomal protein L35a



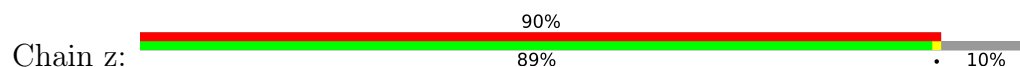
- Molecule 46: 60S ribosomal protein L6



- Molecule 47: 60S ribosomal protein L7



- Molecule 48: Proliferation-associated protein 2G4





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	18819	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	64	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.551	Depositor
Minimum map value	-0.234	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	507.84, 507.84, 507.84	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.058, 1.058, 1.058	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	0	0.40	0/1569	0.65	1/2098 (0.0%)
2	1	0.36	0/976	0.66	0/1199
3	2	1.16	10/81127 (0.0%)	1.28	853/126475 (0.7%)
4	3	0.47	1/2096 (0.0%)	0.64	1/2832 (0.0%)
5	5	0.91	0/2858	1.19	15/4455 (0.3%)
6	6	0.42	0/1728	0.66	0/2352
7	8	4.05	9/3678 (0.2%)	1.69	47/5728 (0.8%)
8	A	0.37	0/1736	0.70	1/2328 (0.0%)
9	B	0.56	0/3306	0.68	2/4424 (0.0%)
10	C	0.39	0/769	0.55	0/1014
11	D	0.56	0/2900	0.64	0/3895
12	E	0.60	2/742 (0.3%)	0.67	0/996
13	F	0.54	0/878	0.69	2/1170 (0.2%)
14	G	0.48	0/1886	0.62	0/2539
15	H	0.47	0/1023	0.60	0/1351
16	I	0.43	0/1537	0.62	1/2066 (0.0%)
17	K	0.45	0/843	0.59	0/1115
18	L	0.56	0/1191	0.61	1/1591 (0.1%)
19	M	0.64	0/720	0.70	1/952 (0.1%)
20	N	0.40	0/1323	0.67	1/1768 (0.1%)
21	O	0.44	0/565	0.57	0/750
22	P	0.56	0/454	0.61	0/599
23	Q	0.51	0/1732	0.60	0/2315
24	S	0.50	0/1125	0.58	0/1505
25	T	0.52	0/903	0.62	1/1216 (0.1%)
26	U	0.60	0/1746	0.65	1/2338 (0.0%)
27	V	0.57	0/1666	0.59	1/2228 (0.0%)
28	W	0.51	0/876	0.62	0/1156
29	X	0.59	0/718	0.62	0/953
30	Y	0.56	0/1268	0.62	0/1701
31	Z	0.58	0/1537	0.69	1/2052 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	a	0.47	0/1233	0.58	0/1633
33	b	0.55	0/1493	0.58	0/2003
34	c	0.55	0/1312	0.61	0/1753
35	d	0.45	0/822	0.68	0/1103
36	e	0.49	0/983	0.68	2/1319 (0.2%)
37	f	0.47	0/532	0.60	0/708
38	g	0.50	0/975	0.63	0/1312
39	h	0.55	0/1132	0.63	0/1504
40	i	0.54	0/1130	0.63	0/1507
41	l	0.54	0/1017	0.59	0/1364
42	m	0.60	0/1936	0.71	1/2596 (0.0%)
43	r	0.48	0/2281	0.60	1/3058 (0.0%)
44	t	0.57	0/1071	0.64	0/1429
45	u	0.62	0/895	0.69	0/1198
46	v	0.45	0/1935	0.67	1/2596 (0.0%)
47	w	0.55	0/1916	0.65	1/2553 (0.0%)
48	z	0.56	0/2911	0.64	2/3913 (0.1%)
All	All	1.12	22/149050 (0.0%)	1.10	938/218710 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	1	0	2
8	A	0	3
9	B	0	1
12	E	0	1
20	N	0	1
21	O	0	1
23	Q	0	1
26	U	0	1
30	Y	0	1
34	c	0	1
35	d	0	1
40	i	0	1
41	l	0	1
42	m	0	1
45	u	0	2
46	v	0	2
47	w	0	1
All	All	0	22

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2	417	G	C2-N2	132.94	2.67	1.34
7	8	16	G	N3-C4	123.93	2.22	1.35
7	8	16	G	C2-N3	106.90	2.18	1.32
7	8	16	G	C6-N1	101.25	2.10	1.39
7	8	16	G	N1-C2	86.95	2.07	1.37
7	8	16	G	C5-C4	81.29	1.95	1.38
7	8	16	G	C5-C6	65.82	2.08	1.42
3	2	417	G	N3-C4	-13.36	1.26	1.35
3	2	417	G	C5-C4	-11.39	1.30	1.38
7	8	16	G	N9-C4	-9.75	1.30	1.38
7	8	16	G	C8-N7	7.73	1.35	1.30
4	3	397	ARG	CA-CB	6.59	1.68	1.53
3	2	2465	C	N1-C6	-6.46	1.33	1.37
3	2	417	G	N9-C4	-5.97	1.33	1.38
12	E	92	CYS	CB-SG	-5.92	1.72	1.81
12	E	52	CYS	CB-SG	-5.92	1.72	1.81
3	2	417	G	N1-C2	5.42	1.42	1.37
3	2	1663	C	C4-C5	-5.36	1.38	1.43
3	2	416	U	C4-C5	-5.35	1.38	1.43
3	2	1577	G	C2-N3	-5.20	1.28	1.32
3	2	2579	G	N9-C4	-5.06	1.33	1.38
7	8	82	A	N9-C4	5.04	1.40	1.37

All (938) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	417	G	C2-N3-C4	38.59	131.19	111.90
7	8	16	G	C2-N3-C4	37.70	130.75	111.90
7	8	16	G	C4-C5-N7	-37.43	95.83	110.80
3	2	417	G	N1-C2-N3	-36.89	101.76	123.90
7	8	16	G	N3-C4-C5	-31.04	113.08	128.60
7	8	16	G	N1-C2-N3	-30.23	105.76	123.90
7	8	16	G	N3-C4-N9	24.79	140.87	126.00
3	2	417	G	N9-C4-C5	23.24	114.70	105.40
7	8	16	G	N7-C8-N9	22.41	124.30	113.10
3	2	417	G	C6-C5-N7	19.43	142.06	130.40
7	8	16	G	C6-C5-N7	19.41	142.05	130.40
7	8	16	G	C5-C6-N1	19.41	121.20	111.50
3	2	417	G	N1-C2-N2	19.02	133.32	116.20
3	2	417	G	C4-C5-N7	-15.06	104.78	110.80
7	8	16	G	N3-C2-N2	15.03	130.42	119.90
3	2	485	C	C2-N1-C1'	14.56	134.82	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	417	G	N3-C4-N9	-14.16	117.50	126.00
3	2	2257	C	C2-N1-C1'	12.21	132.22	118.80
3	2	753	C	N3-C2-O2	-12.16	113.38	121.90
3	2	417	G	C6-N1-C2	11.88	132.23	125.10
3	2	1768	C	N1-C2-O2	11.45	125.77	118.90
3	2	485	C	C6-N1-C1'	-11.21	107.34	120.80
3	2	1768	C	C2-N1-C1'	11.18	131.10	118.80
3	2	2257	C	N1-C2-O2	11.10	125.56	118.90
3	2	180	C	C6-N1-C2	-10.90	115.94	120.30
3	2	485	C	N1-C2-O2	10.81	125.39	118.90
3	2	753	C	N1-C2-O2	10.72	125.33	118.90
3	2	449	C	N1-C2-O2	10.56	125.23	118.90
7	8	16	G	C5-N7-C8	10.46	109.53	104.30
3	2	417	G	C8-N9-C4	-10.45	102.22	106.40
3	2	1715	C	N1-C2-O2	10.36	125.11	118.90
3	2	4557	U	N3-C2-O2	-10.12	115.12	122.20
3	2	925	C	C6-N1-C2	-10.04	116.28	120.30
3	2	1704	C	C6-N1-C2	-10.02	116.29	120.30
3	2	180	C	C5-C6-N1	9.99	125.99	121.00
3	2	4990	C	C2-N1-C1'	9.83	129.61	118.80
3	2	417	G	C8-N9-C1'	9.76	139.69	127.00
3	2	704	C	N1-C2-O2	9.60	124.66	118.90
7	8	16	G	N1-C6-O6	-9.58	114.15	119.90
7	8	147	G	N9-C4-C5	-9.58	101.57	105.40
3	2	449	C	C6-N1-C2	-9.58	116.47	120.30
3	2	655	C	N3-C2-O2	-9.53	115.23	121.90
3	2	1762	C	N1-C2-O2	9.49	124.59	118.90
3	2	1704	C	C2-N1-C1'	9.47	129.21	118.80
3	2	416	U	C2-N1-C1'	9.43	129.01	117.70
3	2	417	G	C4-C5-C6	-9.41	113.15	118.80
7	8	64	U	N3-C2-O2	-9.41	115.61	122.20
3	2	2410	C	C2-N1-C1'	9.37	129.11	118.80
3	2	2410	C	C6-N1-C2	-9.36	116.56	120.30
3	2	1192	C	N3-C2-O2	-9.34	115.36	121.90
3	2	1168	G	N3-C4-N9	-9.31	120.42	126.00
3	2	2257	C	C6-N1-C1'	-9.27	109.67	120.80
3	2	1241	C	C2-N1-C1'	9.26	128.99	118.80
3	2	449	C	N3-C2-O2	-9.24	115.43	121.90
3	2	181	C	N1-C2-O2	9.23	124.44	118.90
3	2	4398	C	N1-C2-O2	9.22	124.44	118.90
3	2	1715	C	C2-N1-C1'	9.18	128.90	118.80
3	2	209	U	C2-N1-C1'	9.17	128.71	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	8	16	G	C8-N9-C1'	9.16	138.91	127.00
3	2	4990	C	C6-N1-C2	-9.12	116.65	120.30
3	2	1768	C	N3-C2-O2	-9.01	115.59	121.90
3	2	1447	C	N3-C2-O2	-8.94	115.64	121.90
3	2	4902	C	C2-N1-C1'	8.90	128.59	118.80
3	2	449	C	C2-N1-C1'	8.88	128.57	118.80
7	8	51	U	N3-C2-O2	-8.83	116.02	122.20
3	2	100	C	C2-N1-C1'	8.82	128.51	118.80
3	2	3598	C	N1-C2-O2	8.82	124.19	118.90
3	2	4601	U	C5-C6-N1	8.82	127.11	122.70
3	2	655	C	N1-C2-O2	8.73	124.14	118.90
7	8	147	G	C4-C5-N7	8.69	114.28	110.80
3	2	181	C	N3-C2-O2	-8.65	115.85	121.90
3	2	1241	C	N1-C2-O2	8.59	124.05	118.90
3	2	4945	G	C5-C6-N1	8.57	115.79	111.50
3	2	654	C	N1-C2-O2	8.52	124.01	118.90
3	2	1762	C	C2-N1-C1'	8.47	128.12	118.80
3	2	1081	C	N1-C2-O2	8.46	123.98	118.90
3	2	1762	C	N3-C2-O2	-8.46	115.98	121.90
7	8	16	G	N1-C2-N2	8.41	123.77	116.20
3	2	489	C	N1-C2-O2	8.39	123.93	118.90
3	2	4476	C	N1-C2-O2	8.38	123.93	118.90
3	2	1704	C	N1-C2-O2	8.35	123.91	118.90
3	2	264	C	C6-N1-C2	-8.35	116.96	120.30
3	2	4682	U	N1-C2-O2	8.34	128.63	122.80
3	2	1447	C	C6-N1-C2	-8.32	116.97	120.30
7	8	51	U	N1-C2-O2	8.32	128.62	122.80
3	2	4303	C	N3-C2-O2	-8.25	116.13	121.90
3	2	1731	C	C5-C6-N1	8.24	125.12	121.00
3	2	4990	C	N1-C2-O2	8.24	123.85	118.90
3	2	704	C	C2-N1-C1'	8.23	127.86	118.80
3	2	753	C	C6-N1-C2	-8.23	117.01	120.30
3	2	2410	C	C5-C6-N1	8.22	125.11	121.00
3	2	115	C	N1-C2-O2	8.22	123.83	118.90
3	2	1663	C	C5-C6-N1	8.21	125.10	121.00
3	2	4895	C	N3-C2-O2	-8.20	116.16	121.90
3	2	4557	U	C2-N1-C1'	8.20	127.53	117.70
3	2	1620	U	N3-C2-O2	-8.19	116.47	122.20
3	2	1768	C	C6-N1-C1'	-8.19	110.98	120.80
3	2	416	U	N3-C2-O2	-8.12	116.52	122.20
3	2	4926	C	N1-C2-O2	8.11	123.77	118.90
3	2	1704	C	C5-C6-N1	8.11	125.05	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	485	C	C5-C6-N1	8.10	125.05	121.00
3	2	472	C	C2-N1-C1'	8.09	127.70	118.80
3	2	4895	C	N1-C2-O2	8.08	123.75	118.90
7	8	16	G	C4-N9-C1'	-8.07	116.01	126.50
3	2	4682	U	N3-C2-O2	-8.03	116.58	122.20
3	2	1243	C	N1-C2-O2	7.99	123.69	118.90
3	2	4601	U	C2-N1-C1'	7.95	127.24	117.70
3	2	3636	C	C6-N1-C2	-7.92	117.13	120.30
26	U	134	LEU	CA-CB-CG	7.91	133.49	115.30
3	2	654	C	N3-C2-O2	-7.91	116.37	121.90
7	8	147	G	C8-N9-C1'	-7.88	116.75	127.00
3	2	1715	C	N3-C2-O2	-7.87	116.39	121.90
3	2	1050	C	C6-N1-C2	-7.86	117.16	120.30
3	2	673	C	C2-N1-C1'	7.84	127.42	118.80
3	2	1241	C	C6-N1-C2	-7.84	117.17	120.30
3	2	2561	C	C6-N1-C2	-7.83	117.17	120.30
3	2	2465	C	C5-C6-N1	7.82	124.91	121.00
3	2	4945	G	N3-C4-N9	7.75	130.65	126.00
3	2	115	C	N3-C2-O2	-7.74	116.48	121.90
3	2	4557	U	N1-C2-O2	7.73	128.21	122.80
3	2	1628	C	C6-N1-C2	-7.73	117.21	120.30
3	2	704	C	N3-C2-O2	-7.71	116.51	121.90
3	2	115	C	C2-N1-C1'	7.69	127.26	118.80
3	2	4775	C	N1-C2-O2	7.67	123.50	118.90
3	2	1241	C	N3-C2-O2	-7.65	116.54	121.90
3	2	2096	G	C4-N9-C1'	7.65	136.45	126.50
3	2	77	U	N3-C2-O2	-7.62	116.86	122.20
3	2	2900	U	N1-C2-O2	7.62	128.14	122.80
3	2	1378	C	N1-C2-O2	7.62	123.47	118.90
3	2	1662	C	C6-N1-C2	-7.62	117.25	120.30
3	2	4709	U	C5-C6-N1	7.61	126.51	122.70
3	2	985	C	C2-N1-C1'	7.59	127.15	118.80
3	2	1704	C	N3-C2-O2	-7.59	116.59	121.90
3	2	987	C	C6-N1-C2	-7.57	117.27	120.30
3	2	4926	C	C2-N1-C1'	7.56	127.11	118.80
3	2	41	C	C6-N1-C2	-7.55	117.28	120.30
3	2	672	C	C2-N1-C1'	7.54	127.10	118.80
3	2	672	C	N1-C2-O2	7.54	123.42	118.90
3	2	100	C	N1-C2-O2	7.54	123.42	118.90
3	2	220	C	C5-C6-N1	7.53	124.77	121.00
3	2	220	C	N1-C2-O2	7.53	123.42	118.90
3	2	1821	G	N3-C4-C5	-7.51	124.84	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	1417	C	C2-N1-C1'	7.51	127.06	118.80
3	2	1216	C	C2-N1-C1'	7.50	127.05	118.80
3	2	1245	C	C5-C6-N1	7.50	124.75	121.00
3	2	4775	C	C2-N1-C1'	7.49	127.04	118.80
3	2	4766	C	C6-N1-C2	-7.48	117.31	120.30
3	2	1731	C	C6-N1-C2	-7.46	117.31	120.30
3	2	10	A	N1-C2-N3	-7.46	125.57	129.30
3	2	512	U	N3-C2-O2	-7.43	117.00	122.20
3	2	2627	C	C2-N1-C1'	7.43	126.98	118.80
3	2	1821	G	N3-C4-N9	7.41	130.44	126.00
3	2	2583	C	C6-N1-C2	-7.39	117.34	120.30
3	2	2528	G	C4-N9-C1'	7.38	136.10	126.50
3	2	2900	U	N3-C2-O2	-7.37	117.04	122.20
3	2	9	C	C6-N1-C2	-7.36	117.36	120.30
3	2	1168	G	C4-N9-C1'	-7.35	116.94	126.50
3	2	1168	G	C8-N9-C1'	7.35	136.56	127.00
3	2	1446	C	N1-C2-O2	7.35	123.31	118.90
3	2	3598	C	N3-C2-O2	-7.34	116.76	121.90
3	2	449	C	C5-C6-N1	7.33	124.66	121.00
3	2	4928	C	C2-N1-C1'	7.33	126.86	118.80
3	2	512	U	N1-C2-O2	7.32	127.92	122.80
3	2	1446	C	C2-N1-C1'	7.31	126.84	118.80
3	2	1168	G	C6-C5-N7	7.31	134.78	130.40
3	2	4476	C	N3-C2-O2	-7.29	116.80	121.90
3	2	673	C	C5-C6-N1	7.28	124.64	121.00
3	2	2583	C	N3-C2-O2	-7.28	116.81	121.90
3	2	416	U	N1-C2-O2	7.27	127.89	122.80
7	8	64	U	N1-C2-O2	7.27	127.89	122.80
36	e	48	ARG	NE-CZ-NH1	7.25	123.92	120.30
3	2	4990	C	N3-C2-O2	-7.25	116.83	121.90
3	2	1216	C	N1-C2-O2	7.23	123.24	118.90
3	2	3696	C	C6-N1-C2	-7.22	117.41	120.30
3	2	1821	G	C4-N9-C1'	7.22	135.88	126.50
3	2	100	C	N3-C2-O2	-7.21	116.85	121.90
3	2	3788	C	C6-N1-C2	-7.21	117.42	120.30
3	2	41	C	C5-C6-N1	7.21	124.60	121.00
3	2	1763	C	P-O3'-C3'	7.21	128.35	119.70
3	2	654	C	C2-N1-C1'	7.18	126.70	118.80
7	8	147	G	C6-C5-N7	-7.18	126.09	130.40
3	2	4078	C	C5-C6-N1	7.18	124.59	121.00
3	2	217	C	N1-C2-O2	7.17	123.20	118.90
3	2	2257	C	N3-C2-O2	-7.16	116.89	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	2257	C	C5-C6-N1	7.14	124.57	121.00
3	2	2528	G	N3-C4-N9	7.13	130.28	126.00
3	2	4928	C	N3-C2-O2	-7.13	116.91	121.90
3	2	4601	U	N1-C2-O2	7.09	127.76	122.80
3	2	3866	C	C5-C6-N1	7.09	124.54	121.00
3	2	3637	U	N3-C2-O2	-7.07	117.25	122.20
7	8	111	U	C2-N1-C1'	7.06	126.17	117.70
3	2	914	U	P-O3'-C3'	7.05	128.16	119.70
3	2	2505	C	C2-N1-C1'	7.05	126.56	118.80
3	2	1193	C	C6-N1-C2	-7.05	117.48	120.30
3	2	4078	C	C6-N1-C2	-7.04	117.48	120.30
3	2	2579	G	N3-C4-N9	-7.04	121.78	126.00
3	2	2653	C	C6-N1-C2	-7.03	117.49	120.30
3	2	148	C	C6-N1-C2	-7.01	117.49	120.30
3	2	1439	C	C2-N1-C1'	7.01	126.52	118.80
3	2	2103	G	C4-N9-C1'	7.01	135.62	126.50
3	2	4145	C	N1-C2-O2	7.01	123.10	118.90
3	2	1050	C	C5-C6-N1	7.00	124.50	121.00
3	2	1192	C	N1-C2-O2	6.99	123.09	118.90
3	2	4990	C	C5-C6-N1	6.99	124.50	121.00
3	2	4303	C	C2-N1-C1'	6.99	126.48	118.80
3	2	4882	U	C2-N1-C1'	6.96	126.05	117.70
3	2	498	C	N1-C2-O2	6.95	123.07	118.90
3	2	1340	C	C5-C6-N1	6.94	124.47	121.00
3	2	417	G	C4-N9-C1'	-6.94	117.48	126.50
3	2	418	A	N7-C8-N9	6.93	117.27	113.80
3	2	969	C	C2-N1-C1'	6.92	126.41	118.80
3	2	1620	U	N1-C2-O2	6.92	127.64	122.80
3	2	1740	C	C6-N1-C2	-6.92	117.53	120.30
3	2	1566	C	C5-C6-N1	6.92	124.46	121.00
3	2	992	C	N1-C2-O2	6.91	123.04	118.90
3	2	1633	G	P-O3'-C3'	6.89	127.97	119.70
3	2	4728	U	N1-C2-O2	6.89	127.62	122.80
7	8	82	A	C2-N3-C4	6.89	114.04	110.60
3	2	322	C	N1-C2-O2	6.88	123.03	118.90
3	2	322	C	C6-N1-C2	-6.88	117.55	120.30
3	2	1378	C	N3-C2-O2	-6.87	117.09	121.90
3	2	4732	G	C8-N9-C4	-6.87	103.65	106.40
3	2	2675	G	P-O3'-C3'	6.87	127.95	119.70
3	2	1789	C	N1-C2-O2	6.87	123.02	118.90
3	2	1666	C	C6-N1-C2	-6.86	117.56	120.30
7	8	147	G	C4-N9-C1'	6.86	135.42	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	655	C	C6-N1-C2	-6.85	117.56	120.30
7	8	16	G	C5-C6-O6	-6.84	124.50	128.60
3	2	4940	C	N1-C2-O2	6.83	123.00	118.90
3	2	4926	C	N3-C2-O2	-6.83	117.12	121.90
3	2	3680	U	N1-C2-O2	6.82	127.58	122.80
3	2	987	C	C5-C6-N1	6.82	124.41	121.00
3	2	969	C	N1-C2-O2	6.82	122.99	118.90
3	2	96	U	N3-C2-O2	-6.81	117.43	122.20
3	2	2454	U	N3-C2-O2	-6.79	117.44	122.20
3	2	4772	C	C5-C6-N1	6.79	124.40	121.00
3	2	489	C	N3-C2-O2	-6.79	117.15	121.90
3	2	282	C	N3-C2-O2	-6.79	117.15	121.90
3	2	2561	C	C5-C6-N1	6.78	124.39	121.00
3	2	4258	C	C5-C6-N1	6.78	124.39	121.00
3	2	1081	C	N3-C2-O2	-6.76	117.17	121.90
3	2	4709	U	C2-N1-C1'	6.75	125.80	117.70
3	2	4303	C	N1-C2-O2	6.74	122.94	118.90
7	8	51	U	C2-N1-C1'	6.74	125.79	117.70
3	2	1447	C	N1-C2-O2	6.74	122.94	118.90
3	2	1893	C	C5-C6-N1	6.72	124.36	121.00
3	2	1188	C	C6-N1-C2	-6.71	117.62	120.30
3	2	2084	C	P-O3'-C3'	6.71	127.75	119.70
3	2	1726	U	N3-C2-O2	-6.70	117.51	122.20
3	2	3882	C	N1-C2-O2	6.69	122.91	118.90
3	2	1367	C	C2-N1-C1'	6.68	126.14	118.80
3	2	4993	G	N3-C4-N9	-6.67	122.00	126.00
3	2	2255	C	C2-N1-C1'	6.67	126.14	118.80
3	2	4882	U	N1-C2-O2	6.67	127.47	122.80
9	B	360	LEU	CA-CB-CG	6.66	130.62	115.30
3	2	1662	C	C5-C6-N1	6.66	124.33	121.00
3	2	4766	C	C2-N1-C1'	6.65	126.12	118.80
3	2	2760	G	P-O3'-C3'	6.64	127.67	119.70
3	2	925	C	N3-C2-O2	-6.64	117.25	121.90
3	2	2563	C	N1-C2-O2	6.62	122.87	118.90
3	2	963	G	C4-N9-C1'	6.62	135.10	126.50
3	2	1726	U	N1-C2-O2	6.61	127.43	122.80
3	2	4662	C	C6-N1-C2	-6.61	117.66	120.30
3	2	2615	C	N1-C2-O2	6.61	122.86	118.90
3	2	3598	C	C6-N1-C2	-6.60	117.66	120.30
3	2	4766	C	C5-C6-N1	6.60	124.30	121.00
3	2	704	C	C6-N1-C2	-6.59	117.66	120.30
3	2	4229	U	N3-C2-O2	-6.59	117.59	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	1763	C	OP1-P-O3'	6.58	119.69	105.20
3	2	2560	C	C5-C6-N1	6.58	124.29	121.00
47	w	109	LEU	CA-CB-CG	6.58	130.42	115.30
3	2	2103	G	C8-N9-C1'	-6.56	118.47	127.00
3	2	4926	C	C6-N1-C2	-6.56	117.67	120.30
3	2	4945	G	C5-C6-O6	-6.56	124.66	128.60
3	2	2465	C	C6-N1-C2	-6.55	117.68	120.30
3	2	2409	U	N1-C2-N3	6.55	118.83	114.90
3	2	1853	G	C4-N9-C1'	6.54	135.00	126.50
3	2	4969	C	C6-N1-C2	-6.54	117.68	120.30
3	2	2409	U	N3-C2-O2	-6.54	117.62	122.20
3	2	274	C	C6-N1-C2	-6.53	117.69	120.30
3	2	4923	C	C2-N1-C1'	6.53	125.98	118.80
3	2	5016	A	O4'-C1'-N9	6.53	113.42	108.20
5	5	67	C	C6-N1-C2	-6.53	117.69	120.30
3	2	1293	G	N3-C4-C5	-6.53	125.34	128.60
3	2	2499	C	C6-N1-C2	-6.52	117.69	120.30
3	2	2528	G	N3-C4-C5	-6.52	125.34	128.60
3	2	220	C	C2-N1-C1'	6.50	125.95	118.80
3	2	2084	C	OP2-P-O3'	6.49	119.47	105.20
3	2	220	C	C6-N1-C2	-6.48	117.71	120.30
3	2	2033	A	P-O3'-C3'	6.48	127.47	119.70
48	z	281	ARG	NE-CZ-NH1	6.47	123.53	120.30
3	2	1243	C	C2-N1-C1'	6.46	125.91	118.80
3	2	2416	G	P-O3'-C3'	6.46	127.45	119.70
3	2	209	U	C6-N1-C1'	-6.45	112.17	121.20
3	2	1715	C	C6-N1-C2	-6.45	117.72	120.30
3	2	217	C	C2-N1-C1'	6.45	125.89	118.80
3	2	925	C	C5-C6-N1	6.43	124.22	121.00
3	2	3863	C	C5-C6-N1	6.43	124.22	121.00
3	2	14	C	C6-N1-C2	-6.42	117.73	120.30
3	2	4206	C	C6-N1-C2	-6.42	117.73	120.30
3	2	4490	C	C6-N1-C2	-6.41	117.73	120.30
3	2	264	C	C5-C6-N1	6.41	124.20	121.00
3	2	1099	C	N3-C2-O2	-6.41	117.41	121.90
7	8	140	C	C6-N1-C2	-6.41	117.74	120.30
3	2	1207	C	C6-N1-C2	-6.40	117.74	120.30
3	2	2392	C	C6-N1-C2	-6.40	117.74	120.30
3	2	1085	C	C6-N1-C2	-6.37	117.75	120.30
3	2	3840	U	N3-C2-O2	-6.37	117.75	122.20
3	2	4120	U	C2-N1-C1'	6.36	125.33	117.70
3	2	4902	C	N1-C2-O2	6.36	122.72	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	416	U	C6-N1-C2	-6.36	117.19	121.00
3	2	4601	U	N3-C2-O2	-6.35	117.75	122.20
3	2	1245	C	N1-C2-O2	6.34	122.71	118.90
3	2	2096	G	C8-N9-C1'	-6.33	118.77	127.00
3	2	488	G	C6-C5-N7	-6.32	126.61	130.40
3	2	1340	C	C6-N1-C2	-6.32	117.77	120.30
3	2	1168	G	N9-C4-C5	6.32	107.93	105.40
3	2	1438	U	O4'-C1'-N1	6.31	113.25	108.20
3	2	1086	C	C6-N1-C2	-6.30	117.78	120.30
3	2	673	C	C6-N1-C2	-6.29	117.79	120.30
3	2	2791	C	C6-N1-C2	-6.28	117.79	120.30
3	2	489	C	C2-N1-C1'	6.28	125.70	118.80
3	2	2627	C	C6-N1-C2	-6.28	117.79	120.30
3	2	1187	G	N3-C4-N9	6.27	129.76	126.00
3	2	3802	U	C2-N1-C1'	6.27	125.22	117.70
3	2	1715	C	C6-N1-C1'	-6.27	113.28	120.80
3	2	1273	G	C6-C5-N7	-6.26	126.65	130.40
3	2	2729	C	C5-C6-N1	6.25	124.12	121.00
3	2	322	C	N3-C2-O2	-6.25	117.53	121.90
3	2	2814	C	N1-C2-O2	6.24	122.64	118.90
3	2	2528	G	C8-N9-C1'	-6.24	118.89	127.00
3	2	4923	C	C6-N1-C2	-6.23	117.81	120.30
3	2	195	C	C6-N1-C2	-6.21	117.81	120.30
3	2	141	C	C5-C6-N1	6.21	124.11	121.00
3	2	1276	C	C6-N1-C2	-6.21	117.82	120.30
3	2	4902	C	C6-N1-C2	-6.21	117.82	120.30
3	2	4923	C	C5-C6-N1	6.20	124.10	121.00
3	2	3696	C	C2-N1-C1'	6.20	125.62	118.80
3	2	498	C	C6-N1-C2	-6.19	117.82	120.30
3	2	1249	C	C5-C6-N1	6.19	124.10	121.00
27	V	141	LEU	CA-CB-CG	6.19	129.53	115.30
3	2	2262	G	C4-N9-C1'	6.18	134.54	126.50
3	2	3925	U	N3-C2-O2	-6.18	117.87	122.20
3	2	4303	C	C6-N1-C2	-6.18	117.83	120.30
3	2	4398	C	N3-C2-O2	-6.18	117.58	121.90
3	2	485	C	C6-N1-C2	-6.17	117.83	120.30
3	2	2096	G	N3-C4-N9	6.17	129.70	126.00
3	2	100	C	C6-N1-C1'	-6.17	113.40	120.80
3	2	282	C	N1-C2-O2	6.16	122.60	118.90
3	2	343	C	C6-N1-C2	-6.16	117.83	120.30
3	2	1418	C	C6-N1-C2	-6.16	117.83	120.30
3	2	4773	C	N1-C2-O2	6.16	122.60	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	3905	A	O4'-C1'-N9	6.16	113.13	108.20
3	2	3788	C	P-O3'-C3'	6.16	127.09	119.70
3	2	9	C	C5-C6-N1	6.15	124.07	121.00
3	2	4583	C	O4'-C1'-N1	6.14	113.12	108.20
3	2	1441	C	C6-N1-C2	-6.14	117.85	120.30
3	2	2579	G	N9-C4-C5	6.13	107.85	105.40
3	2	4775	C	N3-C2-O2	-6.13	117.61	121.90
3	2	3781	C	C6-N1-C2	-6.12	117.85	120.30
3	2	4229	U	N1-C2-O2	6.12	127.08	122.80
3	2	100	C	O4'-C1'-N1	6.12	113.09	108.20
3	2	3636	C	C5-C6-N1	6.11	124.06	121.00
3	2	1168	G	N3-C4-C5	6.11	131.65	128.60
3	2	1674	C	C6-N1-C2	-6.11	117.86	120.30
3	2	3802	U	N3-C2-O2	-6.11	117.93	122.20
3	2	4145	C	C6-N1-C2	-6.11	117.86	120.30
3	2	2262	G	N3-C4-N9	6.10	129.66	126.00
3	2	2410	C	N1-C2-O2	6.09	122.56	118.90
3	2	4902	C	C6-N1-C1'	-6.09	113.49	120.80
3	2	2675	G	N3-C4-N9	6.09	129.65	126.00
3	2	4728	U	N3-C2-O2	-6.08	117.94	122.20
3	2	447	C	C6-N1-C2	-6.08	117.87	120.30
3	2	2579	G	N3-C2-N2	-6.08	115.64	119.90
3	2	2454	U	N1-C2-O2	6.08	127.05	122.80
3	2	1607	C	N3-C2-O2	-6.07	117.65	121.90
3	2	4476	C	C2-N1-C1'	6.07	125.47	118.80
13	F	64	LEU	CA-CB-CG	6.07	129.26	115.30
3	2	1439	C	C6-N1-C2	-6.07	117.87	120.30
4	3	313	LEU	CB-CG-CD2	-6.06	100.70	111.00
3	2	1494	U	N3-C2-O2	-6.05	117.96	122.20
3	2	3788	C	C5-C6-N1	6.05	124.03	121.00
3	2	4118	U	N3-C2-O2	-6.05	117.97	122.20
3	2	4714	C	C6-N1-C2	-6.05	117.88	120.30
3	2	1080	C	C6-N1-C2	-6.05	117.88	120.30
3	2	516	C	N1-C2-O2	6.04	122.52	118.90
3	2	488	G	N3-C4-N9	6.03	129.62	126.00
3	2	972	C	C6-N1-C2	-6.03	117.89	120.30
3	2	1762	C	C6-N1-C1'	-6.03	113.57	120.80
3	2	3866	C	C6-N1-C2	-6.03	117.89	120.30
3	2	4945	G	C2-N3-C4	6.03	114.91	111.90
3	2	3926	C	N1-C2-O2	6.02	122.51	118.90
48	z	281	ARG	NE-CZ-NH2	-6.02	117.29	120.30
3	2	3680	U	N3-C2-O2	-6.02	117.99	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	M	19	CYS	CA-CB-SG	6.02	124.83	114.00
3	2	4601	U	C6-N1-C2	-6.01	117.39	121.00
3	2	3778	U	C2-N1-C1'	6.01	124.91	117.70
3	2	4887	C	C2-N1-C1'	6.01	125.41	118.80
3	2	3920	U	C2-N1-C1'	6.01	124.91	117.70
3	2	3870	C	C5-C6-N1	6.00	124.00	121.00
3	2	1254	A	C2-N3-C4	6.00	113.60	110.60
3	2	2362	U	C2-N1-C1'	6.00	124.90	117.70
3	2	4990	C	C6-N1-C1'	-5.99	113.61	120.80
3	2	1182	C	C6-N1-C2	-5.99	117.90	120.30
3	2	343	C	C5-C6-N1	5.99	123.99	121.00
3	2	1821	G	C8-N9-C1'	-5.99	119.21	127.00
3	2	205	C	C6-N1-C2	-5.99	117.91	120.30
5	5	34	C	N1-C2-O2	5.98	122.49	118.90
3	2	1768	C	C6-N1-C2	-5.98	117.91	120.30
3	2	4099	G	O4'-C1'-N9	5.97	112.98	108.20
3	2	26	C	C6-N1-C2	-5.97	117.91	120.30
8	A	170	GLY	N-CA-C	5.97	128.02	113.10
3	2	657	C	C2-N1-C1'	5.96	125.36	118.80
3	2	1080	C	N1-C2-O2	5.96	122.48	118.90
7	8	150	C	N1-C2-O2	5.96	122.48	118.90
36	e	48	ARG	NE-CZ-NH2	-5.96	117.32	120.30
3	2	1081	C	C2-N1-C1'	5.96	125.35	118.80
3	2	4764	A	C6-N1-C2	5.96	122.17	118.60
3	2	657	C	N1-C2-O2	5.95	122.47	118.90
3	2	3870	C	C6-N1-C2	-5.95	117.92	120.30
3	2	4945	G	N3-C4-C5	-5.95	125.63	128.60
3	2	485	C	N3-C2-O2	-5.95	117.74	121.90
3	2	1467	C	C6-N1-C2	-5.94	117.92	120.30
3	2	4229	U	C2-N1-C1'	5.94	124.83	117.70
3	2	4600	G	P-O3'-C3'	5.94	126.83	119.70
3	2	1598	C	C6-N1-C2	-5.94	117.92	120.30
3	2	3826	C	C6-N1-C2	-5.94	117.92	120.30
7	8	35	C	C6-N1-C2	-5.94	117.92	120.30
3	2	2726	G	N3-C4-C5	-5.93	125.63	128.60
3	2	1275	G	N3-C4-N9	-5.93	122.44	126.00
7	8	146	U	C6-N1-C2	-5.93	117.44	121.00
3	2	1607	C	C6-N1-C2	-5.92	117.93	120.30
3	2	1245	C	C2-N1-C1'	5.92	125.32	118.80
3	2	2255	C	N1-C2-O2	5.91	122.45	118.90
3	2	4764	A	N1-C2-N3	-5.91	126.34	129.30
3	2	1293	G	N3-C4-N9	5.91	129.55	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	1245	C	C6-N1-C2	-5.91	117.94	120.30
3	2	3598	C	C2-N1-C1'	5.90	125.29	118.80
3	2	4900	C	C6-N1-C2	-5.90	117.94	120.30
3	2	719	C	C6-N1-C2	-5.89	117.94	120.30
3	2	258	G	N9-C4-C5	-5.89	103.05	105.40
3	2	1882	U	C5-C4-O4	-5.88	122.37	125.90
3	2	4862	G	N3-C4-N9	5.88	129.53	126.00
3	2	2560	C	C6-N1-C2	-5.88	117.95	120.30
3	2	1273	G	N9-C4-C5	-5.88	103.05	105.40
3	2	1708	G	N3-C4-N9	5.88	129.53	126.00
3	2	2653	C	C5-C6-N1	5.88	123.94	121.00
3	2	4708	A	C4-N9-C1'	5.88	136.88	126.30
3	2	1439	C	C5-C6-N1	5.87	123.93	121.00
3	2	4360	U	N3-C2-O2	-5.87	118.09	122.20
3	2	274	C	C5-C6-N1	5.86	123.93	121.00
3	2	1367	C	N1-C2-O2	5.86	122.42	118.90
3	2	390	C	C5-C6-N1	5.85	123.93	121.00
3	2	1792	U	N3-C2-O2	-5.85	118.11	122.20
3	2	1663	C	C6-N1-C2	-5.85	117.96	120.30
3	2	2281	U	C2-N1-C1'	5.85	124.72	117.70
3	2	345	C	C6-N1-C2	-5.84	117.96	120.30
5	5	29	C	N1-C2-O2	5.84	122.40	118.90
7	8	147	G	N3-C4-N9	5.84	129.50	126.00
3	2	2729	C	C2-N1-C1'	5.83	125.22	118.80
3	2	4772	C	N1-C2-O2	5.83	122.40	118.90
3	2	4372	U	N3-C2-O2	-5.83	118.12	122.20
3	2	260	C	C6-N1-C2	-5.83	117.97	120.30
3	2	472	C	C5-C6-N1	5.83	123.91	121.00
3	2	274	C	C2-N1-C1'	5.82	125.21	118.80
3	2	1068	G	N3-C4-N9	5.82	129.49	126.00
3	2	4281	A	N7-C8-N9	5.82	116.71	113.80
3	2	1957	U	N3-C2-O2	-5.82	118.13	122.20
3	2	2505	C	C6-N1-C1'	-5.82	113.82	120.80
3	2	1632	A	C2-N3-C4	5.81	113.51	110.60
3	2	2416	G	OP2-P-O3'	5.81	117.99	105.20
3	2	1853	G	C8-N9-C1'	-5.81	119.45	127.00
3	2	1929	A	C4-N9-C1'	5.81	136.75	126.30
3	2	74	G	C8-N9-C1'	-5.81	119.45	127.00
3	2	1413	C	C5-C6-N1	5.81	123.90	121.00
3	2	4145	C	C5-C6-N1	5.81	123.90	121.00
3	2	992	C	C2-N1-C1'	5.80	125.18	118.80
3	2	417	G	N1-C6-O6	-5.80	116.42	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	5	76	U	N1-C2-O2	5.80	126.86	122.80
3	2	4895	C	C6-N1-C2	-5.80	117.98	120.30
3	2	1241	C	C6-N1-C1'	-5.79	113.85	120.80
3	2	1327	C	C6-N1-C2	-5.79	117.98	120.30
3	2	2817	C	C6-N1-C2	-5.79	117.98	120.30
3	2	3636	C	N3-C2-O2	-5.79	117.84	121.90
3	2	4482	U	C2-N1-C1'	5.79	124.65	117.70
31	Z	28	LEU	CA-CB-CG	5.79	128.62	115.30
3	2	1241	C	C5-C6-N1	5.79	123.89	121.00
3	2	141	C	C6-N1-C2	-5.79	117.98	120.30
3	2	269	G	C6-C5-N7	-5.78	126.93	130.40
3	2	2096	G	N3-C4-C5	-5.78	125.71	128.60
3	2	516	C	C6-N1-C2	-5.78	117.99	120.30
3	2	1633	G	OP1-P-O3'	5.78	117.91	105.20
3	2	216	C	C5-C6-N1	5.77	123.89	121.00
3	2	4773	C	N3-C2-O2	-5.77	117.86	121.90
3	2	1216	C	C6-N1-C1'	-5.77	113.88	120.80
7	8	76	C	C5-C6-N1	5.77	123.88	121.00
3	2	1893	C	C2-N1-C1'	5.77	125.14	118.80
3	2	360	A	N9-C1'-C2'	5.76	121.49	114.00
3	2	1590	C	P-O3'-C3'	5.76	126.61	119.70
3	2	1597	G	O4'-C1'-N9	5.76	112.81	108.20
3	2	27	C	C6-N1-C2	-5.76	118.00	120.30
3	2	68	U	N3-C2-O2	-5.76	118.17	122.20
3	2	360	A	C5-N7-C8	-5.76	101.02	103.90
3	2	4883	C	C5-C6-N1	5.75	123.87	121.00
3	2	4466	C	C6-N1-C2	-5.74	118.00	120.30
3	2	2593	C	C6-N1-C2	-5.74	118.00	120.30
3	2	2899	C	N1-C2-O2	5.74	122.34	118.90
5	5	24	C	C6-N1-C2	-5.74	118.00	120.30
3	2	2607	C	N1-C2-O2	5.73	122.34	118.90
3	2	2900	U	C2-N1-C1'	5.73	124.58	117.70
3	2	4913	G	P-O3'-C3'	5.73	126.58	119.70
3	2	2094	G	C4-N9-C1'	5.73	133.95	126.50
3	2	4096	C	N3-C4-N4	5.73	122.01	118.00
3	2	2072	C	C6-N1-C2	-5.72	118.01	120.30
3	2	4709	U	N1-C2-O2	5.72	126.81	122.80
3	2	181	C	O4'-C1'-N1	5.72	112.78	108.20
3	2	2409	U	C4-C5-C6	5.72	123.13	119.70
3	2	4887	C	N1-C2-O2	5.71	122.33	118.90
3	2	472	C	C6-N1-C1'	-5.71	113.95	120.80
3	2	4281	A	O4'-C1'-N9	5.71	112.77	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	8	111	U	N3-C2-O2	-5.71	118.20	122.20
3	2	387	G	O4'-C1'-N9	5.70	112.76	108.20
3	2	1273	G	N3-C4-N9	5.70	129.42	126.00
3	2	2478	C	N1-C2-O2	5.70	122.32	118.90
3	2	77	U	N1-C2-O2	5.70	126.79	122.80
3	2	753	C	N3-C4-N4	-5.70	114.01	118.00
3	2	2362	U	C5-C6-N1	5.70	125.55	122.70
3	2	1580	C	C6-N1-C2	-5.70	118.02	120.30
3	2	365	U	N3-C2-O2	-5.70	118.21	122.20
5	5	76	U	N3-C2-O2	-5.69	118.22	122.20
3	2	3696	C	C5-C6-N1	5.69	123.84	121.00
3	2	4902	C	C5-C6-N1	5.69	123.84	121.00
18	L	46	ASP	CB-CG-OD1	5.69	123.42	118.30
3	2	406	C	P-O3'-C3'	5.68	126.52	119.70
3	2	2667	C	N1-C2-O2	5.68	122.31	118.90
3	2	4145	C	N3-C2-O2	-5.68	117.92	121.90
3	2	4398	C	C2-N1-C1'	5.68	125.05	118.80
3	2	50	C	C6-N1-C2	-5.68	118.03	120.30
3	2	1853	G	N3-C4-C5	-5.68	125.76	128.60
3	2	1417	C	C6-N1-C2	-5.67	118.03	120.30
3	2	3863	C	C6-N1-C2	-5.67	118.03	120.30
3	2	1273	G	C8-N9-C1'	-5.67	119.63	127.00
3	2	2593	C	C5-C6-N1	5.66	123.83	121.00
3	2	4502	C	N1-C2-O2	5.65	122.29	118.90
3	2	4973	U	N3-C2-O2	-5.65	118.25	122.20
20	N	94	LEU	CA-CB-CG	5.64	128.28	115.30
3	2	209	U	N3-C2-O2	-5.64	118.25	122.20
3	2	282	C	C6-N1-C2	-5.64	118.04	120.30
3	2	2683	C	C6-N1-C2	-5.64	118.05	120.30
5	5	29	C	C6-N1-C2	-5.63	118.05	120.30
3	2	4215	C	C6-N1-C2	-5.63	118.05	120.30
3	2	217	C	C6-N1-C2	-5.63	118.05	120.30
3	2	1192	C	C6-N1-C2	-5.63	118.05	120.30
3	2	3667	C	C6-N1-C2	-5.63	118.05	120.30
3	2	3882	C	C2-N1-C1'	5.63	124.99	118.80
3	2	1651	G	C4-N9-C1'	5.62	133.81	126.50
3	2	3670	C	N1-C2-O2	5.62	122.27	118.90
5	5	34	C	N3-C2-O2	-5.62	117.97	121.90
3	2	742	G	N3-C4-N9	5.62	129.37	126.00
3	2	2615	C	N3-C2-O2	-5.62	117.97	121.90
3	2	3637	U	N1-C2-O2	5.62	126.73	122.80
3	2	2534	C	C6-N1-C2	-5.62	118.05	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	2814	C	N3-C2-O2	-5.62	117.97	121.90
3	2	3673	C	P-O3'-C3'	5.62	126.44	119.70
3	2	446	C	C5-C6-N1	5.61	123.81	121.00
3	2	1884	C	C6-N1-C2	-5.61	118.06	120.30
3	2	3853	U	C2-N1-C1'	5.61	124.43	117.70
3	2	1494	U	N1-C2-O2	5.60	126.72	122.80
3	2	2563	C	N3-C2-O2	-5.60	117.98	121.90
3	2	100	C	C6-N1-C2	-5.60	118.06	120.30
3	2	257	C	C5-C6-N1	5.60	123.80	121.00
3	2	2892	C	N1-C2-O2	5.60	122.26	118.90
3	2	2257	C	C6-N1-C2	-5.59	118.06	120.30
3	2	4171	C	C6-N1-C2	-5.59	118.06	120.30
3	2	1708	G	N3-C4-C5	-5.58	125.81	128.60
3	2	258	G	N3-C4-N9	5.58	129.35	126.00
3	2	4695	C	N1-C2-O2	5.58	122.25	118.90
46	v	254	ASP	CB-CG-OD1	5.58	123.32	118.30
3	2	3926	C	C6-N1-C2	-5.58	118.07	120.30
3	2	2627	C	N1-C2-O2	5.58	122.25	118.90
3	2	4613	C	N1-C2-O2	5.57	122.24	118.90
3	2	3775	A	O4'-C1'-N9	5.57	112.66	108.20
3	2	4928	C	N1-C2-O2	5.57	122.24	118.90
7	8	147	G	C5-N7-C8	-5.57	101.52	104.30
3	2	74	G	C4-N9-C1'	5.57	133.74	126.50
3	2	498	C	N3-C2-O2	-5.57	118.00	121.90
3	2	3778	U	N1-C2-O2	5.57	126.70	122.80
3	2	365	U	N1-C2-O2	5.56	126.69	122.80
3	2	200	U	O4'-C1'-N1	5.56	112.65	108.20
3	2	4880	C	N1-C2-O2	5.56	122.23	118.90
3	2	1429	C	C2-N1-C1'	5.56	124.91	118.80
3	2	436	C	N1-C2-O2	5.55	122.23	118.90
3	2	2579	G	N1-C6-O6	-5.55	116.57	119.90
3	2	513	U	N1-C2-O2	5.55	126.69	122.80
3	2	4923	C	N1-C2-O2	5.55	122.23	118.90
3	2	4882	U	C5-C6-N1	5.55	125.47	122.70
3	2	195	C	C2-N1-C1'	5.54	124.90	118.80
3	2	2561	C	N1-C2-O2	5.54	122.23	118.90
3	2	4146	G	N3-C4-N9	5.54	129.33	126.00
3	2	5022	U	N1-C2-O2	5.54	126.68	122.80
3	2	85	G	O4'-C1'-N9	5.54	112.63	108.20
3	2	4145	C	C2-N1-C1'	5.54	124.89	118.80
3	2	360	A	OP2-P-O3'	5.53	117.38	105.20
7	8	146	U	C6-N1-C1'	5.53	128.94	121.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	472	C	N1-C2-O2	5.53	122.22	118.90
3	2	1847	C	C5-C6-N1	5.53	123.77	121.00
3	2	2627	C	C5-C6-N1	5.53	123.76	121.00
7	8	16	G	C4-C5-C6	5.52	122.11	118.80
3	2	4926	C	C5-C6-N1	5.51	123.76	121.00
3	2	654	C	C6-N1-C2	-5.51	118.10	120.30
3	2	2410	C	C6-N1-C1'	-5.50	114.20	120.80
3	2	2589	C	C6-N1-C2	-5.50	118.10	120.30
3	2	716	C	C6-N1-C2	-5.50	118.10	120.30
3	2	3598	C	C5-C6-N1	5.50	123.75	121.00
3	2	137	G	C8-N9-C4	-5.49	104.20	106.40
3	2	1077	C	C6-N1-C2	-5.49	118.10	120.30
3	2	1715	C	C5-C6-N1	5.49	123.75	121.00
3	2	488	G	C4-N9-C1'	5.49	133.64	126.50
3	2	3781	C	C5-C6-N1	5.49	123.75	121.00
3	2	1395	U	N3-C2-O2	-5.49	118.36	122.20
3	2	1607	C	N1-C2-O2	5.49	122.19	118.90
5	5	34	C	C6-N1-C2	-5.49	118.11	120.30
3	2	2783	A	N1-C2-N3	-5.48	126.56	129.30
3	2	2532	C	N1-C2-O2	5.48	122.19	118.90
3	2	2303	C	C6-N1-C2	-5.48	118.11	120.30
3	2	4862	G	C6-C5-N7	-5.47	127.12	130.40
3	2	337	U	C5-C6-N1	5.47	125.44	122.70
3	2	112	C	C2-N1-C1'	5.47	124.82	118.80
3	2	4158	C	C2-N1-C1'	5.47	124.82	118.80
3	2	5020	G	C4-N9-C1'	5.47	133.61	126.50
7	8	111	U	N1-C2-O2	5.47	126.63	122.80
7	8	128	C	O4'-C1'-N1	5.47	112.58	108.20
3	2	4162	C	N1-C2-O2	5.47	122.18	118.90
3	2	79	C	C6-N1-C2	-5.46	118.11	120.30
3	2	390	C	C6-N1-C2	-5.46	118.11	120.30
3	2	925	C	C6-N1-C1'	5.46	127.36	120.80
3	2	969	C	N3-C2-O2	-5.46	118.08	121.90
3	2	1578	U	C5-C6-N1	5.46	125.43	122.70
3	2	971	U	N1-C2-O2	5.46	126.62	122.80
3	2	963	G	C8-N9-C1'	-5.46	119.91	127.00
3	2	4068	U	C2-N1-C1'	5.46	124.25	117.70
3	2	2853	C	N1-C2-O2	5.46	122.17	118.90
5	5	29	C	C2-N1-C1'	5.45	124.80	118.80
7	8	146	U	C5-C6-N1	5.45	125.43	122.70
3	2	3693	U	N1-C2-O2	5.45	126.62	122.80
9	B	17	LEU	CA-CB-CG	5.45	127.83	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	1187	G	N3-C4-C5	-5.45	125.88	128.60
3	2	4162	C	C2-N1-C1'	5.45	124.79	118.80
3	2	4940	C	N3-C2-O2	-5.45	118.09	121.90
3	2	515	C	N1-C2-O2	5.44	122.17	118.90
3	2	4259	C	C6-N1-C2	-5.44	118.12	120.30
3	2	133	C	N1-C2-O2	5.44	122.16	118.90
3	2	2046	G	O4'-C1'-N9	5.44	112.55	108.20
3	2	4728	U	C2-N1-C1'	5.44	124.23	117.70
3	2	2281	U	C5-C6-N1	5.44	125.42	122.70
3	2	4940	C	C2-N1-C1'	5.44	124.78	118.80
3	2	1807	C	C6-N1-C2	-5.44	118.13	120.30
3	2	3920	U	N3-C2-O2	-5.43	118.40	122.20
3	2	86	U	N3-C2-O2	-5.43	118.40	122.20
3	2	209	U	N1-C2-O2	5.43	126.60	122.80
3	2	1632	A	C4-N9-C1'	5.43	136.07	126.30
3	2	3685	C	C5-C6-N1	5.43	123.72	121.00
3	2	2850	A	C4-N9-C1'	5.43	136.07	126.30
3	2	4882	U	N3-C2-O2	-5.43	118.40	122.20
3	2	228	C	C6-N1-C2	-5.43	118.13	120.30
3	2	1187	G	C8-N9-C1'	-5.43	119.94	127.00
3	2	122	U	N3-C2-O2	-5.42	118.40	122.20
3	2	673	C	N1-C2-O2	5.42	122.15	118.90
3	2	148	C	C5-C6-N1	5.42	123.71	121.00
3	2	1187	G	C4-N9-C1'	5.42	133.54	126.50
3	2	2038	U	N3-C2-O2	-5.42	118.41	122.20
3	2	4772	C	C2-N1-C1'	5.42	124.76	118.80
5	5	63	C	O4'-C1'-N1	5.41	112.53	108.20
3	2	217	C	N3-C2-O2	-5.41	118.11	121.90
3	2	269	G	C4-N9-C1'	5.41	133.53	126.50
3	2	4171	C	N1-C2-O2	5.41	122.15	118.90
3	2	3844	U	C5-C6-N1	5.41	125.40	122.70
3	2	4714	C	C5-C6-N1	5.40	123.70	121.00
3	2	258	G	N3-C2-N2	5.40	123.68	119.90
3	2	4928	C	C6-N1-C1'	-5.40	114.32	120.80
3	2	4864	U	N1-C2-O2	5.40	126.58	122.80
3	2	2802	C	C6-N1-C2	-5.40	118.14	120.30
3	2	345	C	C5-C6-N1	5.39	123.70	121.00
3	2	672	C	C6-N1-C1'	-5.39	114.33	120.80
3	2	2892	C	C2-N1-C1'	5.39	124.73	118.80
3	2	3778	U	N3-C2-O2	-5.39	118.42	122.20
3	2	4775	C	C6-N1-C2	-5.39	118.14	120.30
3	2	1293	G	C4-N9-C1'	5.39	133.50	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	F	97	ILE	CG1-CB-CG2	-5.39	99.55	111.40
3	2	4068	U	N1-C2-O2	5.39	126.57	122.80
3	2	4865	C	C5-C6-N1	5.39	123.69	121.00
3	2	1439	C	N1-C2-O2	5.38	122.13	118.90
3	2	2561	C	C2-N3-C4	5.38	122.59	119.90
3	2	115	C	C6-N1-C2	-5.38	118.15	120.30
3	2	217	C	C5-C6-N1	5.38	123.69	121.00
3	2	2819	U	N3-C2-O2	-5.38	118.43	122.20
3	2	4519	C	N1-C2-O2	5.38	122.13	118.90
3	2	1188	C	C5-C6-N1	5.38	123.69	121.00
3	2	753	C	C5-C4-N4	5.38	123.96	120.20
3	2	985	C	C6-N1-C2	-5.37	118.15	120.30
3	2	652	G	C8-N9-C1'	-5.37	120.02	127.00
3	2	1446	C	N3-C2-O2	-5.37	118.14	121.90
3	2	1566	C	C2-N1-C1'	5.37	124.71	118.80
3	2	1703	C	N1-C2-O2	5.37	122.12	118.90
3	2	1081	C	C6-N1-C2	-5.37	118.15	120.30
3	2	3892	U	N3-C2-O2	-5.37	118.44	122.20
25	T	46	LEU	CA-CB-CG	-5.37	102.95	115.30
3	2	5037	U	N3-C2-O2	-5.37	118.44	122.20
3	2	4557	U	C6-N1-C1'	-5.36	113.69	121.20
3	2	4945	G	C4-C5-N7	5.36	112.94	110.80
3	2	416	U	C6-N1-C1'	-5.36	113.69	121.20
3	2	1704	C	O4'-C1'-N1	5.36	112.49	108.20
3	2	704	C	C5-C6-N1	5.36	123.68	121.00
3	2	2724	G	N3-C4-C5	-5.36	125.92	128.60
3	2	4969	C	C5-C6-N1	5.36	123.68	121.00
3	2	4199	C	N1-C2-O2	5.36	122.11	118.90
3	2	4243	C	C6-N1-C2	-5.36	118.16	120.30
3	2	4887	C	C6-N1-C2	-5.35	118.16	120.30
3	2	3826	C	C5-C6-N1	5.35	123.67	121.00
3	2	1929	A	N7-C8-N9	5.35	116.47	113.80
3	2	4887	C	N3-C2-O2	-5.35	118.16	121.90
3	2	1447	C	C2-N1-C1'	5.35	124.68	118.80
3	2	3838	U	N3-C2-O2	-5.34	118.46	122.20
3	2	416	U	C5-C6-N1	5.34	125.37	122.70
3	2	4594	U	N3-C2-O2	-5.34	118.46	122.20
3	2	4973	U	N1-C2-O2	5.34	126.54	122.80
3	2	4302	U	N3-C2-O2	-5.34	118.46	122.20
3	2	1579	C	C6-N1-C2	-5.33	118.17	120.30
3	2	4613	C	C6-N1-C2	-5.33	118.17	120.30
3	2	1197	C	C6-N1-C2	-5.32	118.17	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	2727	C	C6-N1-C2	-5.32	118.17	120.30
3	2	4463	U	O4'-C1'-N1	5.32	112.46	108.20
3	2	467	U	C2-N1-C1'	5.32	124.08	117.70
3	2	1906	U	N1-C2-O2	5.31	126.52	122.80
3	2	2304	U	N3-C2-O2	-5.31	118.48	122.20
3	2	2850	A	C8-N9-C4	-5.31	103.68	105.80
1	0	439	LEU	CA-CB-CG	5.30	127.50	115.30
3	2	675	C	C6-N1-C2	-5.30	118.18	120.30
42	m	102	LEU	CA-CB-CG	5.30	127.50	115.30
3	2	4198	G	N3-C4-N9	5.30	129.18	126.00
3	2	413	G	C4-N9-C1'	5.30	133.39	126.50
3	2	7	C	C6-N1-C2	-5.29	118.18	120.30
7	8	50	C	N1-C2-O2	5.29	122.08	118.90
3	2	446	C	C6-N1-C2	-5.29	118.18	120.30
3	2	1848	C	C6-N1-C2	-5.29	118.18	120.30
3	2	53	C	C6-N1-C2	-5.29	118.18	120.30
3	2	71	C	C6-N1-C1'	5.29	127.15	120.80
3	2	220	C	N3-C2-O2	-5.29	118.20	121.90
3	2	4241	C	N1-C2-O2	5.28	122.07	118.90
3	2	1552	G	O4'-C1'-N9	5.28	112.43	108.20
3	2	1538	U	N3-C2-O2	-5.28	118.50	122.20
5	5	28	C	N1-C2-O2	5.28	122.07	118.90
3	2	4506	C	C6-N1-C2	-5.28	118.19	120.30
3	2	86	U	N1-C2-O2	5.28	126.49	122.80
3	2	1168	G	N3-C2-N2	-5.27	116.21	119.90
3	2	1294	A	O4'-C1'-N9	5.27	112.42	108.20
3	2	1704	C	C6-N1-C1'	-5.27	114.47	120.80
3	2	4399	U	N3-C2-O2	-5.27	118.51	122.20
3	2	1384	C	C6-N1-C2	-5.27	118.19	120.30
3	2	1666	C	C5-C6-N1	5.27	123.64	121.00
3	2	2520	C	C6-N1-C2	-5.27	118.19	120.30
3	2	704	C	C6-N1-C1'	-5.26	114.48	120.80
3	2	1762	C	C6-N1-C2	-5.26	118.19	120.30
3	2	3924	C	C6-N1-C2	-5.26	118.19	120.30
3	2	4068	U	N3-C2-O2	-5.26	118.52	122.20
3	2	941	C	C6-N1-C2	-5.26	118.20	120.30
3	2	1273	G	C4-N9-C1'	5.26	133.34	126.50
3	2	4722	G	C2-N3-C4	5.26	114.53	111.90
3	2	4980	C	C5-C6-N1	5.26	123.63	121.00
3	2	1853	G	N3-C4-N9	5.26	129.16	126.00
3	2	4654	C	C6-N1-C2	-5.26	118.20	120.30
3	2	1203	G	N3-C4-N9	5.25	129.15	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	504	G	C2-N3-C4	5.25	114.52	111.90
3	2	1446	C	C6-N1-C1'	-5.25	114.50	120.80
3	2	4703	U	N3-C2-O2	-5.25	118.53	122.20
3	2	969	C	C6-N1-C1'	-5.24	114.51	120.80
3	2	1663	C	N1-C2-O2	5.24	122.05	118.90
3	2	657	C	C5-C6-N1	5.24	123.62	121.00
3	2	1080	C	N3-C2-O2	-5.24	118.23	121.90
3	2	4981	G	C4-N9-C1'	5.24	133.31	126.50
3	2	691	C	C6-N1-C2	-5.24	118.21	120.30
3	2	2338	C	C6-N1-C2	-5.24	118.21	120.30
3	2	4771	C	C5-C6-N1	5.24	123.62	121.00
3	2	1203	G	C4-N9-C1'	5.23	133.30	126.50
3	2	4880	C	N3-C2-O2	-5.23	118.24	121.90
3	2	4926	C	O4'-C1'-N1	5.22	112.38	108.20
3	2	1068	G	N3-C4-C5	-5.22	125.99	128.60
3	2	1708	G	C4-N9-C1'	5.22	133.28	126.50
3	2	2094	G	C8-N9-C1'	-5.22	120.22	127.00
3	2	4340	U	C5-C6-N1	5.22	125.31	122.70
3	2	1386	C	N1-C2-O2	5.21	122.03	118.90
3	2	2362	U	N1-C2-O2	5.21	126.45	122.80
3	2	2561	C	C2-N1-C1'	5.21	124.53	118.80
3	2	155	C	N3-C2-O2	-5.21	118.25	121.90
7	8	119	C	C6-N1-C2	-5.21	118.22	120.30
3	2	985	C	C6-N1-C1'	-5.21	114.55	120.80
3	2	1915	C	C2-N1-C1'	5.21	124.53	118.80
3	2	1344	C	C6-N1-C2	-5.20	118.22	120.30
3	2	2499	C	C5-C6-N1	5.20	123.60	121.00
3	2	963	G	N7-C8-N9	5.20	115.70	113.10
3	2	986	C	C6-N1-C2	-5.20	118.22	120.30
3	2	3685	C	C6-N1-C2	-5.20	118.22	120.30
3	2	4342	C	N1-C2-O2	5.20	122.02	118.90
3	2	4361	U	N3-C2-O2	-5.19	118.56	122.20
3	2	1789	C	N3-C2-O2	-5.19	118.27	121.90
3	2	250	C	C6-N1-C2	-5.18	118.23	120.30
3	2	3622	C	C5-C6-N1	5.18	123.59	121.00
3	2	2817	C	C5-C6-N1	5.18	123.59	121.00
3	2	115	C	C6-N1-C1'	-5.17	114.59	120.80
3	2	3926	C	C2-N1-C1'	5.17	124.49	118.80
3	2	322	C	C5-C6-N1	5.17	123.59	121.00
3	2	1514	U	N1-C2-O2	5.17	126.42	122.80
3	2	4682	U	C2-N1-C1'	5.17	123.91	117.70
3	2	4199	C	N3-C2-O2	-5.17	118.28	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	4900	C	C2-N1-C1'	5.17	124.49	118.80
3	2	417	G	C5-N7-C8	5.17	106.88	104.30
3	2	4183	G	N3-C4-C5	-5.17	126.02	128.60
3	2	4399	U	N1-C2-O2	5.17	126.42	122.80
3	2	4289	U	C2-N1-C1'	5.17	123.90	117.70
3	2	2094	G	N3-C4-N9	5.17	129.10	126.00
3	2	1821	G	C2-N3-C4	5.16	114.48	111.90
3	2	2262	G	C8-N9-C1'	-5.16	120.29	127.00
3	2	4880	C	C6-N1-C2	-5.16	118.23	120.30
3	2	4341	C	N3-C2-O2	-5.16	118.29	121.90
3	2	258	G	C4-C5-N7	5.16	112.86	110.80
5	5	4	U	N1-C2-O2	5.16	126.41	122.80
3	2	691	C	C5-C6-N1	5.16	123.58	121.00
3	2	3641	U	C5-C6-N1	-5.15	120.12	122.70
3	2	4372	U	N1-C2-O2	5.15	126.41	122.80
3	2	4973	U	C2-N1-C1'	5.15	123.88	117.70
16	I	176	LEU	CA-CB-CG	5.15	127.14	115.30
3	2	2262	G	N3-C4-C5	-5.15	126.03	128.60
7	8	54	C	N1-C2-O2	5.15	121.99	118.90
7	8	50	C	N3-C2-O2	-5.14	118.30	121.90
3	2	4342	C	C5-C6-N1	5.14	123.57	121.00
3	2	1731	C	N1-C2-O2	5.14	121.98	118.90
3	2	49	U	N3-C2-O2	-5.14	118.60	122.20
3	2	2667	C	N3-C2-O2	-5.14	118.30	121.90
3	2	2860	C	C6-N1-C2	-5.14	118.25	120.30
3	2	4258	C	C6-N1-C2	-5.14	118.25	120.30
3	2	110	C	C6-N1-C2	-5.13	118.25	120.30
3	2	4138	C	N1-C2-O2	5.13	121.98	118.90
3	2	2534	C	C5-C6-N1	5.13	123.57	121.00
3	2	974	C	C6-N1-C2	-5.13	118.25	120.30
3	2	2447	U	N3-C2-O2	-5.13	118.61	122.20
3	2	5022	U	N3-C2-O2	-5.13	118.61	122.20
3	2	1929	A	C2-N3-C4	5.12	113.16	110.60
3	2	2249	C	C6-N1-C2	-5.12	118.25	120.30
7	8	32	C	C6-N1-C2	-5.12	118.25	120.30
3	2	3939	G	N3-C4-C5	-5.12	126.04	128.60
3	2	4162	C	N3-C2-O2	-5.12	118.32	121.90
3	2	4694	G	C4-N9-C1'	5.12	133.16	126.50
3	2	1216	C	N3-C2-O2	-5.12	118.32	121.90
3	2	137	G	N7-C8-N9	5.12	115.66	113.10
3	2	2819	U	N1-C2-O2	5.12	126.38	122.80
3	2	4364	G	N1-C6-O6	-5.12	116.83	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	1074	G	N3-C4-N9	5.11	129.07	126.00
3	2	4714	C	N1-C2-O2	5.11	121.97	118.90
3	2	250	C	C2-N1-C1'	5.11	124.42	118.80
3	2	1243	C	C5-C6-N1	5.11	123.55	121.00
3	2	1068	G	C4-N9-C1'	5.11	133.14	126.50
3	2	1187	G	C5-C6-O6	-5.10	125.54	128.60
3	2	1686	C	N1-C2-O2	5.10	121.96	118.90
3	2	436	C	N3-C2-O2	-5.10	118.33	121.90
3	2	2362	U	N3-C2-O2	-5.10	118.63	122.20
3	2	742	G	N3-C4-C5	-5.09	126.05	128.60
3	2	2639	U	O4'-C1'-N1	5.09	112.28	108.20
7	8	147	G	N1-C6-O6	5.09	122.96	119.90
3	2	2351	C	C6-N1-C2	-5.09	118.26	120.30
3	2	4261	C	C6-N1-C2	-5.09	118.26	120.30
3	2	3926	C	C5-C6-N1	5.09	123.55	121.00
3	2	2689	C	C5-C6-N1	5.09	123.54	121.00
3	2	5020	G	C8-N9-C1'	-5.09	120.39	127.00
3	2	3832	U	N3-C2-O2	-5.08	118.64	122.20
3	2	4360	U	N1-C2-O2	5.08	126.36	122.80
3	2	1767	A	C2-N3-C4	5.08	113.14	110.60
3	2	5060	A	C3'-C2'-C1'	5.08	105.56	101.50
3	2	672	C	C5-C6-N1	5.07	123.54	121.00
3	2	971	U	C2-N1-C1'	5.07	123.79	117.70
3	2	4928	C	O4'-C1'-N1	5.07	112.26	108.20
3	2	4970	C	C2-N1-C1'	5.07	124.38	118.80
3	2	1879	C	C6-N1-C2	-5.07	118.27	120.30
3	2	14	C	C5-C6-N1	5.07	123.53	121.00
3	2	1720	C	C6-N1-C2	-5.07	118.27	120.30
3	2	294	G	C2-N3-C4	5.06	114.43	111.90
3	2	992	C	N3-C2-O2	-5.06	118.36	121.90
3	2	1430	C	C6-N1-C2	-5.06	118.28	120.30
3	2	1602	U	N3-C2-O2	-5.06	118.66	122.20
3	2	499	G	C8-N9-C4	-5.06	104.38	106.40
5	5	24	C	C5-C6-N1	5.06	123.53	121.00
3	2	4883	C	C6-N1-C2	-5.06	118.28	120.30
3	2	673	C	C6-N1-C1'	-5.06	114.73	120.80
3	2	1167	C	C6-N1-C2	-5.06	118.28	120.30
3	2	4758	U	C5-C6-N1	5.06	125.23	122.70
3	2	1249	C	C6-N1-C2	-5.06	118.28	120.30
3	2	216	C	C6-N1-C2	-5.05	118.28	120.30
3	2	1298	C	C6-N1-C2	-5.05	118.28	120.30
3	2	1644	C	C5-C6-N1	5.05	123.53	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	10	A	C2-N3-C4	5.05	113.12	110.60
3	2	3693	U	N3-C2-O2	-5.05	118.67	122.20
3	2	4341	C	N1-C2-O2	5.05	121.93	118.90
3	2	504	G	C4-N9-C1'	5.05	133.06	126.50
3	2	934	C	N1-C2-O2	5.05	121.93	118.90
3	2	2593	C	C2-N1-C1'	5.05	124.35	118.80
3	2	1286	C	C6-N1-C2	-5.04	118.28	120.30
3	2	1417	C	C6-N1-C1'	-5.04	114.75	120.80
3	2	4502	C	C6-N1-C2	-5.04	118.28	120.30
3	2	656	C	C5-C6-N1	5.04	123.52	121.00
3	2	1598	C	N1-C2-O2	5.03	121.92	118.90
3	2	1243	C	N3-C2-O2	-5.03	118.38	121.90
3	2	1915	C	N3-C2-O2	-5.03	118.38	121.90
3	2	276	C	C6-N1-C2	-5.03	118.29	120.30
3	2	1441	C	C6-N1-C1'	5.03	126.83	120.80
3	2	1906	U	N3-C2-O2	-5.03	118.68	122.20
3	2	4900	C	N1-C2-O2	5.03	121.92	118.90
3	2	2524	U	N3-C2-O2	-5.03	118.68	122.20
3	2	4699	U	OP1-P-O3'	5.03	116.26	105.20
3	2	233	U	C2-N1-C1'	5.02	123.73	117.70
3	2	4775	C	C6-N1-C1'	-5.02	114.77	120.80
7	8	113	C	C6-N1-C2	-5.02	118.29	120.30
3	2	504	G	N3-C4-C5	-5.02	126.09	128.60
3	2	4862	G	C4-C5-N7	5.02	112.81	110.80
3	2	4922	C	C6-N1-C2	-5.02	118.29	120.30
3	2	218	A	C4-N9-C1'	5.02	135.33	126.30
3	2	1468	C	C6-N1-C2	-5.02	118.29	120.30
3	2	1602	U	C5-C6-N1	5.02	125.21	122.70
3	2	2499	C	C2-N1-C1'	5.01	124.31	118.80
3	2	245	C	C5-C6-N1	5.01	123.51	121.00
3	2	472	C	C6-N1-C2	-5.01	118.30	120.30
3	2	1863	U	N3-C2-O2	-5.01	118.69	122.20
3	2	2072	C	C5-C6-N1	5.01	123.50	121.00
3	2	946	C	C6-N1-C2	-5.01	118.30	120.30
3	2	4862	G	C4-N9-C1'	5.01	133.01	126.50
5	5	43	U	N1-C2-O2	5.01	126.30	122.80
43	r	278	ASP	CB-CG-OD1	5.01	122.81	118.30
3	2	18	C	N1-C2-O2	5.00	121.90	118.90
3	2	2729	C	C6-N1-C2	-5.00	118.30	120.30
3	2	406	C	C2'-C3'-O3'	5.00	121.71	113.70

There are no chirality outliers.

All (22) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1	502	ARG	Peptide
2	1	503	PRO	Peptide
8	A	158	GLN	Peptide
8	A	46	ASP	Peptide
8	A	82	ILE	Peptide
9	B	17	LEU	Peptide
12	E	52	CYS	Peptide
20	N	94	LEU	Peptide
21	O	10	ASP	Peptide
23	Q	46	ILE	Peptide
26	U	147	ASP	Peptide
30	Y	131	ARG	Peptide
34	c	135	PRO	Peptide
35	d	20	LYS	Peptide
40	i	124	THR	Peptide
41	l	20	ARG	Peptide
42	m	54	ARG	Peptide
45	u	103	VAL	Peptide
45	u	106	TYR	Peptide
46	v	129	GLY	Peptide
46	v	203	ILE	Peptide
47	w	221	LYS	Peptide

## 5.2 Too-close contacts [i](#)

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	0	184/477 (39%)	158 (86%)	25 (14%)	1 (0%)	25 55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	1	223/658 (34%)	183 (82%)	40 (18%)	0	100	100
4	3	251/534 (47%)	227 (90%)	23 (9%)	1 (0%)	30	60
6	6	222/245 (91%)	208 (94%)	14 (6%)	0	100	100
8	A	210/217 (97%)	184 (88%)	22 (10%)	4 (2%)	6	25
9	B	400/403 (99%)	372 (93%)	28 (7%)	0	100	100
10	C	88/159 (55%)	84 (96%)	4 (4%)	0	100	100
11	D	355/427 (83%)	326 (92%)	28 (8%)	1 (0%)	37	65
12	E	92/115 (80%)	82 (89%)	10 (11%)	0	100	100
13	F	107/117 (92%)	104 (97%)	3 (3%)	0	100	100
14	G	229/266 (86%)	212 (93%)	17 (7%)	0	100	100
15	H	120/123 (98%)	114 (95%)	6 (5%)	0	100	100
16	I	188/192 (98%)	169 (90%)	19 (10%)	0	100	100
17	K	100/105 (95%)	92 (92%)	7 (7%)	1 (1%)	13	40
18	L	145/148 (98%)	131 (90%)	14 (10%)	0	100	100
19	M	84/97 (87%)	79 (94%)	5 (6%)	0	100	100
20	N	160/178 (90%)	146 (91%)	14 (9%)	0	100	100
21	O	66/70 (94%)	64 (97%)	2 (3%)	0	100	100
22	P	48/51 (94%)	45 (94%)	3 (6%)	0	100	100
23	Q	208/211 (99%)	188 (90%)	20 (10%)	0	100	100
24	S	132/215 (61%)	125 (95%)	7 (5%)	0	100	100
25	T	105/125 (84%)	96 (91%)	9 (9%)	0	100	100
26	U	201/204 (98%)	190 (94%)	9 (4%)	2 (1%)	13	40
27	V	197/203 (97%)	189 (96%)	8 (4%)	0	100	100
28	W	103/106 (97%)	95 (92%)	8 (8%)	0	100	100
29	X	89/92 (97%)	85 (96%)	4 (4%)	0	100	100
30	Y	151/184 (82%)	140 (93%)	11 (7%)	0	100	100
31	Z	185/188 (98%)	174 (94%)	11 (6%)	0	100	100
32	a	143/196 (73%)	136 (95%)	7 (5%)	0	100	100
33	b	173/176 (98%)	163 (94%)	10 (6%)	0	100	100
34	c	155/160 (97%)	145 (94%)	9 (6%)	1 (1%)	22	51
35	d	97/128 (76%)	87 (90%)	10 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	e	127/140 (91%)	119 (94%)	8 (6%)	0	100	100
37	f	60/157 (38%)	57 (95%)	3 (5%)	0	100	100
38	g	115/156 (74%)	104 (90%)	11 (10%)	0	100	100
39	h	132/145 (91%)	123 (93%)	9 (7%)	0	100	100
40	i	133/136 (98%)	125 (94%)	7 (5%)	1 (1%)	16	45
41	l	123/137 (90%)	116 (94%)	6 (5%)	1 (1%)	16	45
42	m	246/257 (96%)	221 (90%)	24 (10%)	1 (0%)	30	60
43	r	273/297 (92%)	252 (92%)	21 (8%)	0	100	100
44	t	126/135 (93%)	115 (91%)	11 (9%)	0	100	100
45	u	107/110 (97%)	97 (91%)	8 (8%)	2 (2%)	6	25
46	v	231/288 (80%)	206 (89%)	24 (10%)	1 (0%)	30	60
47	w	224/248 (90%)	211 (94%)	13 (6%)	0	100	100
48	z	363/394 (92%)	354 (98%)	9 (2%)	0	100	100
All	All	7471/9370 (80%)	6893 (92%)	561 (8%)	17 (0%)	45	72

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
46	v	226	ARG
4	3	331	ALA
8	A	28	PHE
8	A	159	MET
8	A	169	VAL
8	A	173	LYS
17	K	24	PRO
41	l	21	ASN
34	c	136	ARG
40	i	125	GLY
45	u	80	ASN
11	D	232	VAL
45	u	107	PRO
26	U	84	PRO
26	U	83	LYS
42	m	55	GLY
1	0	245	PRO



### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	165/404 (41%)	162 (98%)	3 (2%)	54	74
4	3	235/485 (48%)	229 (97%)	6 (3%)	41	65
6	6	194/213 (91%)	194 (100%)	0	100	100
8	A	191/196 (97%)	185 (97%)	6 (3%)	35	60
9	B	348/349 (100%)	344 (99%)	4 (1%)	70	83
10	C	77/126 (61%)	77 (100%)	0	100	100
11	D	298/348 (86%)	296 (99%)	2 (1%)	81	89
12	E	79/97 (81%)	77 (98%)	2 (2%)	42	66
13	F	94/100 (94%)	92 (98%)	2 (2%)	48	70
14	G	195/223 (87%)	193 (99%)	2 (1%)	73	85
15	H	109/110 (99%)	109 (100%)	0	100	100
16	I	169/171 (99%)	168 (99%)	1 (1%)	84	91
17	K	86/89 (97%)	84 (98%)	2 (2%)	45	67
18	L	120/121 (99%)	120 (100%)	0	100	100
19	M	73/80 (91%)	72 (99%)	1 (1%)	62	79
20	N	136/149 (91%)	134 (98%)	2 (2%)	60	78
21	O	63/65 (97%)	63 (100%)	0	100	100
22	P	47/48 (98%)	47 (100%)	0	100	100
23	Q	176/177 (99%)	175 (99%)	1 (1%)	84	91
24	S	114/161 (71%)	113 (99%)	1 (1%)	75	86
25	T	98/110 (89%)	96 (98%)	2 (2%)	50	71
26	U	171/172 (99%)	171 (100%)	0	100	100
27	V	171/174 (98%)	168 (98%)	3 (2%)	54	74
28	W	93/94 (99%)	93 (100%)	0	100	100
29	X	74/75 (99%)	73 (99%)	1 (1%)	62	79
30	Y	134/163 (82%)	133 (99%)	1 (1%)	81	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	Z	164/165 (99%)	164 (100%)	0	100	100
32	a	131/175 (75%)	131 (100%)	0	100	100
33	b	156/157 (99%)	154 (99%)	2 (1%)	65	80
34	c	138/140 (99%)	138 (100%)	0	100	100
35	d	89/115 (77%)	89 (100%)	0	100	100
36	e	100/107 (94%)	100 (100%)	0	100	100
37	f	54/126 (43%)	54 (100%)	0	100	100
38	g	105/133 (79%)	105 (100%)	0	100	100
39	h	124/135 (92%)	123 (99%)	1 (1%)	79	88
40	i	117/118 (99%)	116 (99%)	1 (1%)	75	86
41	l	109/121 (90%)	108 (99%)	1 (1%)	75	86
42	m	190/199 (96%)	186 (98%)	4 (2%)	48	70
43	r	232/250 (93%)	230 (99%)	2 (1%)	75	86
44	t	114/121 (94%)	114 (100%)	0	100	100
45	u	88/89 (99%)	86 (98%)	2 (2%)	45	67
46	v	208/252 (82%)	205 (99%)	3 (1%)	62	79
47	w	195/215 (91%)	193 (99%)	2 (1%)	73	85
48	z	316/336 (94%)	314 (99%)	2 (1%)	84	91
All	All	6340/7454 (85%)	6278 (99%)	62 (1%)	71	85

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	334	PHE
1	0	350	ARG
1	0	476	ARG
4	3	216	VAL
4	3	308	CYS
4	3	313	LEU
4	3	346	TRP
4	3	397	ARG
4	3	404	ILE
8	A	28	PHE
8	A	30	GLU
8	A	60	ARG
8	A	97	LYS

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Mol	Chain	Res	Type
8	A	171	HIS
8	A	177	ASP
9	B	54	THR
9	B	300	LYS
9	B	347	LEU
9	B	370	THR
11	D	171	LEU
11	D	188	ARG
12	E	23	LYS
12	E	91	VAL
13	F	54	ARG
13	F	63	VAL
14	G	175	ARG
14	G	211	ASP
16	I	72	THR
17	K	18	THR
17	K	29	ARG
19	M	17	THR
20	N	95	ARG
20	N	114	ASP
23	Q	103	ARG
24	S	17	PHE
25	T	100	ASN
25	T	114	PHE
27	V	34	VAL
27	V	49	ARG
27	V	92	THR
29	X	63	THR
30	Y	24	VAL
33	b	38	VAL
33	b	87	ARG
39	h	74	TYR
40	i	52	LYS
41	l	27	THR
42	m	45	VAL
42	m	143	THR
42	m	157	VAL
42	m	169	VAL
43	r	117	LYS
43	r	263	LYS
45	u	25	THR
45	u	109	ARG

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Mol	Chain	Res	Type
46	v	56	ARG
46	v	99	ASP
46	v	223	ARG
47	w	70[A]	ARG
47	w	70[B]	ARG
48	z	274	ASP
48	z	288	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	233	GLN
1	0	393	HIS
4	3	270	GLN
4	3	358	GLN
4	3	364	HIS
4	3	382	ASN
4	3	391	ASN
6	6	68	HIS
6	6	106	ASN
6	6	145	GLN
6	6	157	GLN
6	6	162	HIS
8	A	171	HIS
8	A	200	ASN
9	B	167	GLN
9	B	204	GLN
9	B	281	ASN
10	C	49	HIS
10	C	60	ASN
11	D	38	ASN
11	D	61	GLN
11	D	119	GLN
13	F	3	GLN
14	G	195	HIS
14	G	208	ASN
14	G	227	ASN
15	H	101	ASN
15	H	108	GLN
16	I	39	ASN
16	I	42	ASN
20	N	46	GLN

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Mol	Chain	Res	Type
20	N	104	ASN
21	O	58	GLN
24	S	66	HIS
24	S	125	ASN
25	T	100	ASN
27	V	167	HIS
28	W	18	HIS
28	W	45	GLN
28	W	51	GLN
29	X	56	HIS
30	Y	21	ASN
30	Y	34	GLN
30	Y	80	GLN
30	Y	116	HIS
30	Y	118	GLN
31	Z	44	ASN
31	Z	188	ASN
33	b	23	HIS
33	b	173	ASN
35	d	41	GLN
35	d	55	ASN
36	e	77	HIS
37	f	59	HIS
38	g	73	HIS
38	g	151	ASN
39	h	20	ASN
40	i	78	ASN
41	l	6	GLN
42	m	132	ASN
42	m	194	ASN
43	r	81	HIS
43	r	195	HIS
43	r	225	GLN
44	t	107	ASN
45	u	20	ASN
46	v	190	HIS
46	v	211	HIS
46	v	268	GLN
47	w	63	GLN
48	z	242	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	2	3436/5070 (67%)	902 (26%)	23 (0%)
5	5	119/120 (99%)	20 (16%)	0
7	8	153/156 (98%)	35 (22%)	0
All	All	3708/5346 (69%)	957 (25%)	23 (0%)

All (957) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	2	2	G
3	2	10	A
3	2	18	C
3	2	25	A
3	2	39	A
3	2	42	A
3	2	48	G
3	2	56	A
3	2	59	A
3	2	64	A
3	2	65	A
3	2	67	C
3	2	69	A
3	2	73	A
3	2	74	G
3	2	75	G
3	2	91	G
3	2	98	A
3	2	108	A
3	2	109	G
3	2	110	C
3	2	119	G
3	2	120	A
3	2	127	G
3	2	128	C
3	2	131	C
3	2	132	G
3	2	133	C
3	2	134	G
3	2	135	G
3	2	136	C
3	2	141	C
3	2	143	C
3	2	146	G
3	2	151	G

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Mol	Chain	Res	Type
3	2	157	U
3	2	159	C
3	2	165	A
3	2	172	C
3	2	177	G
3	2	180	C
3	2	181	C
3	2	183	C
3	2	184	U
3	2	185	C
3	2	188	G
3	2	189	G
3	2	200	U
3	2	207	G
3	2	209	U
3	2	216	C
3	2	218	A
3	2	219	G
3	2	220	C
3	2	225	G
3	2	233	U
3	2	234	G
3	2	236	G
3	2	250	C
3	2	254	G
3	2	256	G
3	2	257	C
3	2	260	C
3	2	261	G
3	2	262	G
3	2	263	G
3	2	265	C
3	2	278	G
3	2	279	A
3	2	280	G
3	2	297	U
3	2	306	A
3	2	315	G
3	2	316	U
3	2	340	C
3	2	341	G
3	2	347	A

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Mol	Chain	Res	Type
3	2	348	G
3	2	349	A
3	2	350	C
3	2	361	C
3	2	362	A
3	2	363	A
3	2	380	U
3	2	387	G
3	2	388	A
3	2	406	C
3	2	407	A
3	2	408	A
3	2	412	G
3	2	413	G
3	2	433	A
3	2	449	C
3	2	450	G
3	2	452	A
3	2	453	G
3	2	454	U
3	2	457	G
3	2	458	C
3	2	467	U
3	2	484	U
3	2	485	C
3	2	486	C
3	2	489	C
3	2	493	G
3	2	494	U
3	2	497	G
3	2	498	C
3	2	499	G
3	2	500	G
3	2	501	C
3	2	502	C
3	2	503	C
3	2	504	G
3	2	505	G
3	2	507	G
3	2	508	G
3	2	509	A
3	2	510	U

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Mol	Chain	Res	Type
3	2	511	C
3	2	512	U
3	2	513	U
3	2	514	U
3	2	515	C
3	2	517	C
3	2	518	G
3	2	519	C
3	2	643	C
3	2	644	G
3	2	645	G
3	2	646	G
3	2	653	U
3	2	656	C
3	2	657	C
3	2	659	G
3	2	660	A
3	2	665	C
3	2	667	A
3	2	668	C
3	2	670	G
3	2	673	C
3	2	685	C
3	2	686	A
3	2	687	U
3	2	696	C
3	2	697	G
3	2	703	G
3	2	704	C
3	2	705	G
3	2	708	G
3	2	731	G
3	2	738	C
3	2	739	G
3	2	746	A
3	2	749	G
3	2	753	C
3	2	756	G
3	2	757	G
3	2	760	G
3	2	904	C
3	2	905	C

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Mol	Chain	Res	Type
3	2	906	C
3	2	907	C
3	2	912	G
3	2	913	U
3	2	914	U
3	2	915	A
3	2	916	C
3	2	917	A
3	2	918	G
3	2	923	C
3	2	924	C
3	2	925	C
3	2	932	A
3	2	933	G
3	2	934	C
3	2	935	A
3	2	936	C
3	2	937	U
3	2	941	C
3	2	943	A
3	2	944	A
3	2	945	U
3	2	956	A
3	2	959	G
3	2	960	A
3	2	961	G
3	2	962	C
3	2	965	G
3	2	966	A
3	2	967	C
3	2	971	U
3	2	977	C
3	2	978	2MG
3	2	982	U
3	2	985	C
3	2	989	U
3	2	990	C
3	2	991	C
3	2	992	C
3	2	993	G
3	2	995	C
3	2	1048	G

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Mol	Chain	Res	Type
3	2	1049	C
3	2	1051	G
3	2	1065	G
3	2	1068	G
3	2	1070	G
3	2	1071	C
3	2	1072	C
3	2	1075	G
3	2	1078	A
3	2	1080	C
3	2	1083	U
3	2	1084	C
3	2	1095	A
3	2	1098	G
3	2	1171	G
3	2	1172	C
3	2	1173	G
3	2	1174	G
3	2	1176	C
3	2	1178	G
3	2	1179	U
3	2	1180	C
3	2	1181	C
3	2	1182	C
3	2	1183	C
3	2	1185	G
3	2	1187	G
3	2	1189	G
3	2	1191	C
3	2	1199	G
3	2	1202	C
3	2	1203	G
3	2	1204	C
3	2	1210	C
3	2	1211	G
3	2	1214	C
3	2	1215	C
3	2	1217	G
3	2	1218	G
3	2	1222	A
3	2	1241	C
3	2	1242	G

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Mol	Chain	Res	Type
3	2	1253	G
3	2	1254	A
3	2	1255	A
3	2	1259	G
3	2	1260	G
3	2	1261	G
3	2	1262	G
3	2	1263	A
3	2	1264	C
3	2	1265	G
3	2	1266	G
3	2	1267	C
3	2	1269	G
3	2	1270	A
3	2	1271	G
3	2	1272	C
3	2	1273	G
3	2	1274	A
3	2	1275	G
3	2	1280	C
3	2	1281	G
3	2	1284	G
3	2	1287	G
3	2	1289	C
3	2	1293	G
3	2	1294	A
3	2	1295	C
3	2	1296	G
3	2	1301	C
3	2	1302	U
3	2	1303	A
3	2	1314	C
3	2	1324	A
3	2	1326	A2M
3	2	1337	A
3	2	1354	A
3	2	1358	G
3	2	1359	G
3	2	1365	C
3	2	1366	G
3	2	1367	C
3	2	1370	G

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Mol	Chain	Res	Type
3	2	1377	G
3	2	1378	C
3	2	1379	C
3	2	1387	A
3	2	1394	G
3	2	1397	A
3	2	1399	G
3	2	1403	G
3	2	1404	G
3	2	1405	C
3	2	1407	C
3	2	1408	G
3	2	1409	C
3	2	1410	U
3	2	1411	C
3	2	1412	G
3	2	1420	A
3	2	1425	G
3	2	1435	G
3	2	1437	C
3	2	1438	U
3	2	1439	C
3	2	1441	C
3	2	1443	A
3	2	1446	C
3	2	1447	C
3	2	1458	C
3	2	1459	A
3	2	1482	G
3	2	1483	C
3	2	1493	G
3	2	1497	A
3	2	1498	G
3	2	1502	G
3	2	1514	U
3	2	1515	A
3	2	1517	2MG
3	2	1518	A
3	2	1522	OMG
3	2	1525	A
3	2	1534	A2M
3	2	1547	A

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Mol	Chain	Res	Type
3	2	1566	C
3	2	1578	U
3	2	1586	G
3	2	1591	U
3	2	1596	U
3	2	1597	G
3	2	1621	A
3	2	1624	G
3	2	1625	OMG
3	2	1626	G
3	2	1627	G
3	2	1631	A
3	2	1632	A
3	2	1633	G
3	2	1634	A
3	2	1638	A
3	2	1640	C
3	2	1641	G
3	2	1642	A
3	2	1651	G
3	2	1654	G
3	2	1655	C
3	2	1661	C
3	2	1676	C
3	2	1677	PSU
3	2	1678	C
3	2	1679	A
3	2	1681	G
3	2	1686	C
3	2	1694	C
3	2	1697	G
3	2	1699	A
3	2	1700	G
3	2	1701	A
3	2	1703	C
3	2	1704	C
3	2	1705	G
3	2	1706	A
3	2	1707	C
3	2	1708	G
3	2	1709	C
3	2	1715	C

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Mol	Chain	Res	Type
3	2	1716	G
3	2	1719	A
3	2	1734	G
3	2	1763	C
3	2	1764	G
3	2	1765	A
3	2	1766	A
3	2	1768	C
3	2	1769	G
3	2	1772	C
3	2	1773	U
3	2	1774	C
3	2	1790	U
3	2	1804	A
3	2	1806	G
3	2	1809	C
3	2	1810	G
3	2	1815	G
3	2	1820	C
3	2	1821	G
3	2	1822	U
3	2	1829	G
3	2	1836	G
3	2	1837	A
3	2	1842	G
3	2	1855	G
3	2	1862	U
3	2	1863	U
3	2	1866	UR3
3	2	1867	A
3	2	1869	G
3	2	1872	G
3	2	1873	A
3	2	1881	C
3	2	1883	OMG
3	2	1891	A
3	2	1892	A
3	2	1893	C
3	2	1897	A
3	2	1918	U
3	2	1919	G
3	2	1920	C

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Mol	Chain	Res	Type
3	2	1922	G
3	2	1925	G
3	2	1931	C
3	2	1932	A
3	2	1935	C
3	2	1940	G
3	2	1943	A
3	2	1948	G
3	2	1951	G
3	2	1952	G
3	2	1959	U
3	2	1960	A
3	2	1961	G
3	2	1962	A
3	2	1963	C
3	2	2024	G
3	2	2025	A
3	2	2026	A
3	2	2033	A
3	2	2034	G
3	2	2046	G
3	2	2048	U
3	2	2055	G
3	2	2056	G
3	2	2069	A
3	2	2070	U
3	2	2071	A
3	2	2084	C
3	2	2085	G
3	2	2089	G
3	2	2090	U
3	2	2091	C
3	2	2092	G
3	2	2093	A
3	2	2094	G
3	2	2095	A
3	2	2096	G
3	2	2097	U
3	2	2098	G
3	2	2100	A
3	2	2101	C
3	2	2103	G

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Mol	Chain	Res	Type
3	2	2104	G
3	2	2106	G
3	2	2108	G
3	2	2111	G
3	2	2112	G
3	2	2251	G
3	2	2252	G
3	2	2253	A
3	2	2256	C
3	2	2259	G
3	2	2262	G
3	2	2263	A
3	2	2280	G
3	2	2289	C
3	2	2300	A
3	2	2301	G
3	2	2305	U
3	2	2313	A
3	2	2316	G
3	2	2331	G
3	2	2332	A
3	2	2333	G
3	2	2345	G
3	2	2348	G
3	2	2351	C
3	2	2357	G
3	2	2360	A
3	2	2364	OMG
3	2	2382	A
3	2	2395	A
3	2	2396	A
3	2	2397	G
3	2	2398	U
3	2	2402	G
3	2	2408	U
3	2	2417	A
3	2	2422	OMC
3	2	2424	OMG
3	2	2425	U
3	2	2437	C
3	2	2441	C
3	2	2447	U

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Mol	Chain	Res	Type
3	2	2450	G
3	2	2453	A
3	2	2460	A
3	2	2465	C
3	2	2467	U
3	2	2471	G
3	2	2474	G
3	2	2475	G
3	2	2478	C
3	2	2480	G
3	2	2481	G
3	2	2483	G
3	2	2484	A
3	2	2485	U
3	2	2486	G
3	2	2487	G
3	2	2488	C
3	2	2489	C
3	2	2490	U
3	2	2491	C
3	2	2492	C
3	2	2494	U
3	2	2503	G
3	2	2504	C
3	2	2505	C
3	2	2506	G
3	2	2511	A
3	2	2512	A
3	2	2513	A
3	2	2514	G
3	2	2519	U
3	2	2520	C
3	2	2532	C
3	2	2537	A
3	2	2544	G
3	2	2546	G
3	2	2547	G
3	2	2553	A
3	2	2554	U
3	2	2555	G
3	2	2562	G
3	2	2566	G

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Mol	Chain	Res	Type
3	2	2569	G
3	2	2573	A
3	2	2583	C
3	2	2587	A
3	2	2589	C
3	2	2596	G
3	2	2618	G
3	2	2627	C
3	2	2638	G
3	2	2652	G
3	2	2653	C
3	2	2659	A
3	2	2661	U
3	2	2662	G
3	2	2663	G
3	2	2664	G
3	2	2669	C
3	2	2670	C
3	2	2673	G
3	2	2675	G
3	2	2676	A
3	2	2687	U
3	2	2694	G
3	2	2695	A
3	2	2696	A
3	2	2697	A
3	2	2705	G
3	2	2724	G
3	2	2726	G
3	2	2732	G
3	2	2739	C
3	2	2742	G
3	2	2743	A
3	2	2746	A
3	2	2756	G
3	2	2761	U
3	2	2763	U
3	2	2764	A
3	2	2769	U
3	2	2770	C
3	2	2773	OMG
3	2	2788	U

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Mol	Chain	Res	Type
3	2	2790	U
3	2	2793	G
3	2	2794	C
3	2	2800	G
3	2	2814	C
3	2	2815	A
3	2	2822	G
3	2	2825	A
3	2	2826	U
3	2	2827	G
3	2	2829	U
3	2	2835	A
3	2	2838	G
3	2	2848	G
3	2	2850	A
3	2	2855	G
3	2	2870	A
3	2	2876	G
3	2	2877	G
3	2	2879	A
3	2	2886	U
3	2	2900	U
3	2	3604	A
3	2	3605	C
3	2	3615	G
3	2	3619	G
3	2	3626	G
3	2	3630	A
3	2	3635	A
3	2	3644	U
3	2	3662	A
3	2	3664	G
3	2	3670	C
3	2	3673	C
3	2	3674	G
3	2	3680	U
3	2	3691	G
3	2	3692	A
3	2	3706	C
3	2	3711	A
3	2	3713	U
3	2	3714	G

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Mol	Chain	Res	Type
3	2	3728	A
3	2	3729	PSU
3	2	3735	G
3	2	3736	A
3	2	3748	A
3	2	3750	G
3	2	3776	G
3	2	3777	G
3	2	3784	A
3	2	3785	A2M
3	2	3789	C
3	2	3799	A
3	2	3802	U
3	2	3811	G
3	2	3812	C
3	2	3813	A
3	2	3814	U
3	2	3817	A
3	2	3818	U
3	2	3819	G
3	2	3823	G
3	2	3838	U
3	2	3839	G
3	2	3840	U
3	2	3851	U
3	2	3867	A2M
3	2	3876	A
3	2	3877	A
3	2	3878	C
3	2	3879	G
3	2	3881	G
3	2	3892	U
3	2	3898	G
3	2	3901	A
3	2	3902	A
3	2	3906	A
3	2	3907	G
3	2	3908	A
3	2	3910	C
3	2	3915	U
3	2	3922	G
3	2	3923	A

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Mol	Chain	Res	Type
3	2	3925	U
3	2	3926	C
3	2	3938	G
3	2	3939	G
3	2	3941	G
3	2	3944	G
3	2	3946	G
3	2	4076	G
3	2	4084	G
3	2	4086	G
3	2	4088	C
3	2	4097	G
3	2	4098	A
3	2	4099	G
3	2	4101	C
3	2	4102	C
3	2	4103	C
3	2	4104	G
3	2	4105	A
3	2	4106	G
3	2	4107	G
3	2	4108	G
3	2	4111	U
3	2	4112	C
3	2	4113	U
3	2	4114	C
3	2	4115	G
3	2	4116	C
3	2	4117	U
3	2	4118	U
3	2	4119	C
3	2	4127	A
3	2	4133	C
3	2	4138	C
3	2	4139	G
3	2	4140	C
3	2	4141	G
3	2	4142	C
3	2	4143	G
3	2	4145	C
3	2	4146	G
3	2	4148	C

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Mol	Chain	Res	Type
3	2	4157	A
3	2	4162	C
3	2	4163	U
3	2	4170	A
3	2	4177	C
3	2	4183	G
3	2	4184	G
3	2	4191	G
3	2	4195	G
3	2	4196	OMG
3	2	4206	C
3	2	4212	A
3	2	4224	A
3	2	4228	G
3	2	4229	U
3	2	4233	A
3	2	4234	A
3	2	4251	A
3	2	4254	G
3	2	4256	A
3	2	4257	A
3	2	4265	U
3	2	4268	A
3	2	4271	A
3	2	4272	G
3	2	4273	A
3	2	4281	A
3	2	4282	A
3	2	4291	G
3	2	4304	A
3	2	4305	G
3	2	4312	U
3	2	4313	A
3	2	4314	C
3	2	4319	C
3	2	4326	G
3	2	4329	G
3	2	4330	G
3	2	4332	C
3	2	4349	C
3	2	4354	U
3	2	4364	G

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Mol	Chain	Res	Type
3	2	4372	U
3	2	4373	G
3	2	4374	U
3	2	4376	A
3	2	4377	G
3	2	4378	A
3	2	4379	A
3	2	4380	A
3	2	4387	C
3	2	4394	A
3	2	4398	C
3	2	4400	G
3	2	4403	PSU
3	2	4443	C
3	2	4444	C
3	2	4448	G
3	2	4450	PSU
3	2	4451	G
3	2	4453	C
3	2	4464	A
3	2	4466	C
3	2	4471	U
3	2	4476	C
3	2	4477	A
3	2	4482	U
3	2	4488	A
3	2	4500	PSU
3	2	4510	A
3	2	4512	U
3	2	4513	A
3	2	4518	A
3	2	4519	C
3	2	4523	A2M
3	2	4524	G
3	2	4532	U
3	2	4545	G
3	2	4548	A
3	2	4549	G
3	2	4560	C
3	2	4567	G
3	2	4570	G
3	2	4573	G

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Mol	Chain	Res	Type
3	2	4575	G
3	2	4583	C
3	2	4584	A
3	2	4589	A
3	2	4590	A
3	2	4599	A
3	2	4600	G
3	2	4601	U
3	2	4606	G
3	2	4617	G
3	2	4636	PSU
3	2	4637	OMG
3	2	4647	G
3	2	4652	G
3	2	4656	A
3	2	4670	C
3	2	4693	C
3	2	4695	C
3	2	4700	A
3	2	4708	A
3	2	4709	U
3	2	4719	G
3	2	4722	G
3	2	4728	U
3	2	4731	G
3	2	4732	G
3	2	4733	C
3	2	4734	A
3	2	4740	G
3	2	4741	C
3	2	4743	G
3	2	4745	G
3	2	4746	C
3	2	4750	G
3	2	4751	G
3	2	4754	G
3	2	4757	C
3	2	4759	C
3	2	4761	G
3	2	4764	A
3	2	4765	G
3	2	4771	C

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Mol	Chain	Res	Type
3	2	4772	C
3	2	4775	C
3	2	4776	G
3	2	4859	C
3	2	4860	G
3	2	4862	G
3	2	4864	U
3	2	4870	OMG
3	2	4871	C
3	2	4872	2MG
3	2	4874	A
3	2	4875	G
3	2	4877	G
3	2	4882	U
3	2	4883	C
3	2	4887	C
3	2	4889	G
3	2	4895	C
3	2	4896	G
3	2	4900	C
3	2	4901	G
3	2	4904	G
3	2	4910	G
3	2	4912	G
3	2	4914	C
3	2	4915	G
3	2	4925	U
3	2	4926	C
3	2	4927	G
3	2	4928	C
3	2	4935	C
3	2	4936	G
3	2	4937	C
3	2	4938	A
3	2	4941	G
3	2	4943	A
3	2	4945	G
3	2	4949	G
3	2	4950	U
3	2	4951	G
3	2	4955	A
3	2	4960	G

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Mol	Chain	Res	Type
3	2	4966	A
3	2	4975	G
3	2	4976	U
3	2	4985	U
3	2	4988	U
3	2	4989	U
3	2	4991	U
3	2	5013	C
3	2	5014	A
3	2	5021	C
3	2	5022	U
3	2	5023	C
3	2	5024	C
3	2	5025	C
3	2	5026	U
3	2	5034	A
3	2	5041	G
3	2	5047	C
3	2	5050	C
3	2	5053	U
3	2	5054	C
3	2	5055	G
3	2	5058	A
3	2	5060	A
3	2	5061	A
3	2	5062	G
3	2	5069	U
5	5	4	U
5	5	5	A
5	5	11	A
5	5	13	A
5	5	22	A
5	5	24	C
5	5	38	U
5	5	42	A
5	5	53	U
5	5	54	A
5	5	61	G
5	5	62	U
5	5	63	C
5	5	64	G
5	5	70	G

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Mol	Chain	Res	Type
5	5	71	G
5	5	74	A
5	5	100	A
5	5	106	G
5	5	110	G
7	8	2	G
7	8	3	A
7	8	23	C
7	8	25	G
7	8	34	U
7	8	35	C
7	8	38	U
7	8	48	A
7	8	59	A
7	8	60	G
7	8	62	A
7	8	63	U
7	8	68	G
7	8	75	G
7	8	80	A
7	8	82	A
7	8	83	C
7	8	84	A
7	8	85	U
7	8	87	G
7	8	103	A
7	8	105	C
7	8	106	G
7	8	110	U
7	8	111	U
7	8	114	G
7	8	123	U
7	8	124	U
7	8	125	C
7	8	126	C
7	8	127	U
7	8	150	C
7	8	151	G
7	8	153	C
7	8	156	U

All (23) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	2	406	C
3	2	504	G
3	2	914	U
3	2	955	G
3	2	1082	C
3	2	1517	2MG
3	2	1633	G
3	2	1763	C
3	2	1773	U
3	2	2033	A
3	2	2084	C
3	2	2416	G
3	2	2675	G
3	2	2760	G
3	2	3614	G
3	2	3673	C
3	2	3788	C
3	2	4378	A
3	2	4600	G
3	2	4699	U
3	2	4913	G
3	2	5022	U
3	2	5060	A

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

98 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	$\# Z  > 2$
3	PSU	2	4403	3	18,21,22	1.07	1 (5%)	22,30,33	1.57	5 (22%)
3	PSU	2	4450	3	18,21,22	1.07	2 (11%)	22,30,33	2.02	5 (22%)
3	OMC	2	2804	3	19,22,23	2.64	7 (36%)	26,31,34	0.81	0
3	E6G	2	4355	3	20,27,28	5.90	9 (45%)	22,39,42	2.70	9 (40%)
3	B8Q	2	1456	3	17,22,23	2.85	4 (23%)	22,32,35	2.24	6 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	OMC	2	2365	49,3	19,22,23	2.69	7 (36%)	26,31,34	0.72	0
3	A2M	2	3785	3	18,25,26	4.00	7 (38%)	18,36,39	3.09	3 (16%)
3	B8H	2	4296	3	19,22,23	6.83	7 (36%)	22,32,35	2.40	5 (22%)
3	OMG	2	3792	3	18,26,27	2.32	7 (38%)	19,38,41	1.38	4 (21%)
3	OMG	2	2364	3	18,26,27	2.20	7 (38%)	19,38,41	1.61	3 (15%)
3	UR3	2	4530	3	19,22,23	2.75	7 (36%)	26,32,35	1.45	5 (19%)
3	A2M	2	2401	3	18,25,26	4.11	8 (44%)	18,36,39	3.06	3 (16%)
3	2MG	2	729	3	18,26,27	2.26	7 (38%)	16,38,41	1.44	3 (18%)
3	OMG	2	2424	49,3	18,26,27	2.39	7 (38%)	19,38,41	1.64	4 (21%)
3	B8K	2	3897	3	24,28,29	4.32	16 (66%)	30,42,45	2.51	12 (40%)
3	2MG	2	1517	3	18,26,27	2.36	7 (38%)	16,38,41	1.77	5 (31%)
3	P7G	2	1909	3	24,28,29	4.26	11 (45%)	27,41,44	1.76	3 (11%)
3	A2M	2	1534	49,3	18,25,26	4.18	7 (38%)	18,36,39	2.86	4 (22%)
3	OMC	2	4536	3	19,22,23	2.73	7 (36%)	26,31,34	0.75	0
3	A2M	2	1326	49,3	18,25,26	4.11	6 (33%)	18,36,39	3.00	3 (16%)
3	A2M	2	3825	3	18,25,26	4.21	7 (38%)	18,36,39	3.15	3 (16%)
3	P7G	2	3880	3	24,28,29	4.22	11 (45%)	27,41,44	1.71	5 (18%)
3	OMC	2	2861	3	19,22,23	2.76	7 (36%)	26,31,34	0.66	0
3	5MC	2	4335	3	18,22,23	3.29	7 (38%)	26,32,35	1.16	2 (7%)
3	PSU	2	1582	3	18,21,22	1.07	1 (5%)	22,30,33	1.76	4 (18%)
3	B8W	2	4529	4,3	18,26,27	6.22	9 (50%)	21,38,41	3.04	9 (42%)
3	OMG	2	1625	49,3	18,26,27	2.27	7 (38%)	19,38,41	1.53	4 (21%)
3	A2M	2	1524	3	18,25,26	4.14	7 (38%)	18,36,39	3.15	4 (22%)
3	OMG	2	4196	3	18,26,27	2.48	8 (44%)	19,38,41	1.51	4 (21%)
3	B9H	2	2786	3	20,25,26	2.69	5 (25%)	22,35,38	2.62	7 (31%)
3	B8T	2	4483	3	19,22,23	3.47	8 (42%)	26,31,34	0.84	1 (3%)
3	B8W	2	4472	3	18,26,27	6.10	7 (38%)	21,38,41	2.18	5 (23%)
3	7MG	2	2522	3	22,26,27	3.14	10 (45%)	29,39,42	2.01	7 (24%)
3	5MC	2	3782	49,3	18,22,23	3.31	7 (38%)	26,32,35	1.15	3 (11%)
3	B8W	2	4185	3	18,26,27	6.19	7 (38%)	21,38,41	2.45	7 (33%)
3	OMC	2	2422	30,49,3	19,22,23	2.76	7 (36%)	26,31,34	1.43	3 (11%)
3	OMG	2	1522	3	18,26,27	2.31	7 (38%)	19,38,41	1.61	4 (21%)
3	B8H	2	1860	3	19,22,23	6.84	7 (36%)	22,32,35	2.50	5 (22%)
3	B8W	2	2380	3	18,26,27	6.11	7 (38%)	21,38,41	2.28	6 (28%)
3	A2M	2	4571	3	18,25,26	4.20	7 (38%)	18,36,39	3.02	4 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PSU	2	3729	3	18,21,22	1.03	2 (11%)	22,30,33	1.74	4 (18%)
3	OMG	2	373	3	18,26,27	2.25	7 (38%)	19,38,41	1.53	4 (21%)
3	PSU	2	3715	3	18,21,22	1.04	1 (5%)	22,30,33	1.49	3 (13%)
3	OMC	2	3887	3	19,22,23	2.84	7 (36%)	26,31,34	1.00	1 (3%)
3	BGH	2	3899	3	25,29,30	4.17	16 (64%)	31,43,46	2.53	12 (38%)
3	1MA	2	1322	49,3	16,25,26	3.69	4 (25%)	18,37,40	1.77	3 (16%)
3	OMC	2	3909	3	19,22,23	2.96	8 (42%)	26,31,34	1.44	4 (15%)
3	E7G	2	1797	3	24,27,28	3.54	11 (45%)	30,40,43	2.21	9 (30%)
3	B9B	2	2754	3	21,28,29	5.58	8 (38%)	23,40,43	2.13	5 (21%)
3	OMG	2	2773	3	18,26,27	2.44	8 (44%)	19,38,41	1.65	5 (26%)
3	5MU	2	4083	3	19,22,23	4.68	7 (36%)	28,32,35	3.85	10 (35%)
3	A2M	2	3718	3	18,25,26	4.22	6 (33%)	18,36,39	3.18	3 (16%)
3	B8W	2	4129	3	18,26,27	6.18	7 (38%)	21,38,41	2.70	9 (42%)
3	2MG	2	4872	27,24,3	18,26,27	2.24	7 (38%)	16,38,41	1.45	3 (18%)
3	OMG	2	4637	3	18,26,27	2.33	7 (38%)	19,38,41	1.70	4 (21%)
3	OMC	2	3701	49,3	19,22,23	2.61	8 (42%)	26,31,34	0.95	1 (3%)
3	E7G	2	2297	3	24,27,28	3.43	11 (45%)	30,40,43	2.17	9 (30%)
3	A2M	2	398	3	18,25,26	4.17	6 (33%)	18,36,39	3.19	3 (16%)
3	A2M	2	3723	3	18,25,26	4.25	7 (38%)	18,36,39	3.00	4 (22%)
3	A2M	2	1871	3	18,25,26	4.31	6 (33%)	18,36,39	2.91	3 (16%)
3	B8K	2	4690	3	24,28,29	4.33	16 (66%)	30,42,45	2.55	12 (40%)
3	PSU	2	1677	3	18,21,22	1.31	3 (16%)	22,30,33	2.08	5 (22%)
3	MHG	2	4371	4,3	29,32,33	3.68	12 (41%)	34,46,49	2.20	10 (29%)
3	PSU	2	4636	3	18,21,22	1.17	3 (16%)	22,30,33	1.95	4 (18%)
3	OMU	2	4306	3	19,22,23	2.75	7 (36%)	26,31,34	1.74	5 (19%)
3	OMC	2	3869	3	19,22,23	2.74	7 (36%)	26,31,34	0.75	0
3	UR3	2	4597	3	19,22,23	2.78	6 (31%)	26,32,35	1.24	2 (7%)
3	7MG	2	4550	3	22,26,27	3.11	10 (45%)	29,39,42	2.05	10 (34%)
3	OMG	2	4623	3	18,26,27	2.31	8 (44%)	19,38,41	1.61	3 (15%)
3	I4U	2	4194	3	21,24,25	4.84	16 (76%)	27,34,37	1.60	6 (22%)
3	B9B	2	1574	3,32	21,28,29	5.73	8 (38%)	23,40,43	2.17	5 (21%)
3	I4U	2	1659	49,3	21,24,25	4.57	15 (71%)	27,34,37	1.31	3 (11%)
3	B9B	2	237	3	21,28,29	5.59	9 (42%)	23,40,43	2.51	6 (26%)
3	PSU	2	4293	3	18,21,22	1.12	2 (11%)	22,30,33	1.76	4 (18%)
3	OMG	2	4870	33,24,3	18,26,27	2.50	8 (44%)	19,38,41	1.47	6 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PSU	2	4442	3	18,21,22	1.20	1 (5%)	22,30,33	1.65	4 (18%)
3	OMG	2	4370	3	18,26,27	2.27	8 (44%)	19,38,41	1.46	4 (21%)
3	PSU	2	4500	3	18,21,22	1.09	3 (16%)	22,30,33	1.99	5 (22%)
3	OMG	2	1883	3	18,26,27	2.24	6 (33%)	19,38,41	1.53	5 (26%)
3	PSU	2	1683	3	18,21,22	1.13	1 (5%)	22,30,33	1.84	3 (13%)
3	PSU	2	2508	3	18,21,22	1.03	1 (5%)	22,30,33	1.58	3 (13%)
3	B8T	2	4671	3	19,22,23	3.27	8 (42%)	26,31,34	1.12	1 (3%)
3	M7A	2	4564	3	20,25,26	1.90	4 (20%)	28,37,40	3.91	7 (25%)
3	7MG	2	1605	3	22,26,27	2.99	10 (45%)	29,39,42	2.04	9 (31%)
3	A2M	2	3867	3	18,25,26	4.11	6 (33%)	18,36,39	2.81	3 (16%)
3	2MG	2	978	3	18,26,27	2.33	7 (38%)	16,38,41	1.61	4 (25%)
3	OMU	2	4620	36,3	19,22,23	2.82	8 (42%)	26,31,34	2.02	8 (30%)
3	A2M	2	2363	49,3	18,25,26	4.13	7 (38%)	18,36,39	3.41	3 (16%)
3	PSU	2	4628	3	18,21,22	0.99	1 (5%)	22,30,33	1.87	4 (18%)
3	6MZ	2	4220	3	18,25,26	1.84	3 (16%)	16,36,39	3.88	3 (18%)
3	PSU	2	4531	3	18,21,22	1.04	1 (5%)	22,30,33	1.83	4 (18%)
3	P4U	2	1348	31,3	21,24,25	3.50	8 (38%)	27,33,36	1.14	2 (7%)
3	UR3	2	1866	3	19,22,23	3.01	6 (31%)	26,32,35	1.65	4 (15%)
3	A2M	2	4523	3	18,25,26	4.17	7 (38%)	18,36,39	3.19	5 (27%)
3	OMG	2	2050	3	18,26,27	2.26	7 (38%)	19,38,41	1.57	3 (15%)
3	OMG	2	1316	49,3	18,26,27	2.35	8 (44%)	19,38,41	1.78	5 (26%)
3	OMG	2	4494	3	18,26,27	2.31	7 (38%)	19,38,41	1.57	4 (21%)
3	5MC	2	4447	49,3	18,22,23	3.17	7 (38%)	26,32,35	1.67	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
3	PSU	2	4403	3	-	5/7/25/26	0/2/2/2
3	PSU	2	4450	3	-	5/7/25/26	0/2/2/2
3	OMC	2	2804	3	-	0/9/27/28	0/2/2/2
3	E6G	2	4355	3	-	5/6/28/29	0/3/3/3
3	B8Q	2	1456	3	-	0/7/42/43	0/2/2/2
3	OMC	2	2365	49,3	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A2M	2	3785	3	-	3/5/27/28	0/3/3/3
3	B8H	2	4296	3	-	2/7/25/26	0/2/2/2
3	OMG	2	3792	3	-	0/5/27/28	0/3/3/3
3	OMG	2	2364	3	-	2/5/27/28	0/3/3/3
3	UR3	2	4530	3	-	1/7/25/26	0/2/2/2
3	A2M	2	2401	3	-	2/5/27/28	0/3/3/3
3	2MG	2	729	3	-	2/5/27/28	0/3/3/3
3	OMG	2	2424	49,3	-	2/5/27/28	0/3/3/3
3	B8K	2	3897	3	-	3/11/41/42	0/3/3/3
3	2MG	2	1517	3	-	1/5/27/28	0/3/3/3
3	P7G	2	1909	3	-	3/10/40/41	0/3/3/3
3	A2M	2	1534	49,3	-	2/5/27/28	0/3/3/3
3	OMC	2	4536	3	-	0/9/27/28	0/2/2/2
3	A2M	2	1326	49,3	-	1/5/27/28	0/3/3/3
3	A2M	2	3825	3	-	1/5/27/28	0/3/3/3
3	P7G	2	3880	3	-	4/10/40/41	0/3/3/3
3	OMC	2	2861	3	-	0/9/27/28	0/2/2/2
3	5MC	2	4335	3	-	0/7/25/26	0/2/2/2
3	PSU	2	1582	3	-	0/7/25/26	0/2/2/2
3	B8W	2	4529	4,3	-	2/5/27/28	0/3/3/3
3	OMG	2	1625	49,3	-	2/5/27/28	0/3/3/3
3	A2M	2	1524	3	-	2/5/27/28	0/3/3/3
3	OMG	2	4196	3	-	2/5/27/28	0/3/3/3
3	B9H	2	2786	3	-	2/12/47/48	0/2/2/2
3	B8T	2	4483	3	-	0/7/27/28	0/2/2/2
3	B8W	2	4472	3	-	4/5/27/28	0/3/3/3
3	7MG	2	2522	3	-	0/7/37/38	0/3/3/3
3	5MC	2	3782	49,3	-	0/7/25/26	0/2/2/2
3	B8W	2	4185	3	-	2/5/27/28	0/3/3/3
3	OMC	2	2422	30,49,3	-	2/9/27/28	0/2/2/2
3	OMG	2	1522	3	-	0/5/27/28	0/3/3/3
3	B8H	2	1860	3	-	2/7/25/26	0/2/2/2
3	B8W	2	2380	3	-	4/5/27/28	0/3/3/3
3	A2M	2	4571	3	-	0/5/27/28	0/3/3/3
3	PSU	2	3729	3	-	2/7/25/26	0/2/2/2
3	OMG	2	373	3	-	1/5/27/28	0/3/3/3
3	PSU	2	3715	3	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMC	2	3887	3	-	1/9/27/28	0/2/2/2
3	BGH	2	3899	3	-	0/13/43/44	0/3/3/3
3	1MA	2	1322	49,3	-	1/3/25/26	0/3/3/3
3	OMC	2	3909	3	-	2/9/27/28	0/2/2/2
3	E7G	2	1797	3	-	2/9/39/40	0/3/3/3
3	B9B	2	2754	3	-	5/7/29/30	0/3/3/3
3	OMG	2	2773	3	-	2/5/27/28	0/3/3/3
3	5MU	2	4083	3	-	0/7/25/26	0/2/2/2
3	A2M	2	3718	3	-	0/5/27/28	0/3/3/3
3	B8W	2	4129	3	-	2/5/27/28	0/3/3/3
3	2MG	2	4872	27,24,3	-	2/5/27/28	0/3/3/3
3	OMG	2	4637	3	-	2/5/27/28	0/3/3/3
3	OMC	2	3701	49,3	-	4/9/27/28	0/2/2/2
3	E7G	2	2297	3	-	3/9/39/40	0/3/3/3
3	A2M	2	398	3	-	2/5/27/28	0/3/3/3
3	A2M	2	3723	3	-	0/5/27/28	0/3/3/3
3	A2M	2	1871	3	-	2/5/27/28	0/3/3/3
3	B8K	2	4690	3	-	0/11/41/42	0/3/3/3
3	PSU	2	1677	3	-	4/7/25/26	0/2/2/2
3	MHG	2	4371	4,3	-	8/16/46/47	0/3/3/3
3	PSU	2	4636	3	-	4/7/25/26	0/2/2/2
3	OMU	2	4306	3	-	1/9/27/28	0/2/2/2
3	OMC	2	3869	3	-	0/9/27/28	0/2/2/2
3	UR3	2	4597	3	-	0/7/25/26	0/2/2/2
3	7MG	2	4550	3	-	2/7/37/38	0/3/3/3
3	OMG	2	4623	3	-	0/5/27/28	0/3/3/3
3	I4U	2	4194	3	-	0/9/29/30	0/2/2/2
3	B9B	2	1574	3,32	-	3/7/29/30	0/3/3/3
3	I4U	2	1659	49,3	-	3/9/29/30	0/2/2/2
3	B9B	2	237	3	-	5/7/29/30	0/3/3/3
3	PSU	2	4293	3	-	0/7/25/26	0/2/2/2
3	OMG	2	4870	33,24,3	-	3/5/27/28	0/3/3/3
3	PSU	2	4442	3	-	0/7/25/26	0/2/2/2
3	OMG	2	4370	3	-	1/5/27/28	0/3/3/3
3	PSU	2	4500	3	-	3/7/25/26	0/2/2/2
3	OMG	2	1883	3	-	2/5/27/28	0/3/3/3
3	PSU	2	1683	3	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	2	2508	3	-	0/7/25/26	0/2/2/2
3	B8T	2	4671	3	-	0/7/27/28	0/2/2/2
3	M7A	2	4564	3	-	0/7/37/38	0/3/3/3
3	7MG	2	1605	3	-	0/7/37/38	0/3/3/3
3	A2M	2	3867	3	-	2/5/27/28	0/3/3/3
3	2MG	2	978	3	-	2/5/27/28	0/3/3/3
3	OMU	2	4620	36,3	-	1/9/27/28	0/2/2/2
3	A2M	2	2363	49,3	-	0/5/27/28	0/3/3/3
3	PSU	2	4628	3	-	0/7/25/26	0/2/2/2
3	6MZ	2	4220	3	-	2/5/27/28	0/3/3/3
3	PSU	2	4531	3	-	1/7/25/26	0/2/2/2
3	P4U	2	1348	31,3	-	1/10/29/30	0/2/2/2
3	UR3	2	1866	3	-	2/7/25/26	0/2/2/2
3	A2M	2	4523	3	-	2/5/27/28	0/3/3/3
3	OMG	2	2050	3	-	0/5/27/28	0/3/3/3
3	OMG	2	1316	49,3	-	0/5/27/28	0/3/3/3
3	OMG	2	4494	3	-	1/5/27/28	0/3/3/3
3	5MC	2	4447	49,3	-	4/7/25/26	0/2/2/2

All (683) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2	4472	B8W	O4'-C1'	17.68	1.65	1.41
3	2	4129	B8W	O4'-C1'	17.62	1.65	1.41
3	2	2380	B8W	O4'-C1'	17.50	1.65	1.41
3	2	4529	B8W	O4'-C1'	17.37	1.65	1.41
3	2	4185	B8W	O4'-C1'	17.34	1.65	1.41
3	2	1860	B8H	C6-C5	-16.87	1.11	1.34
3	2	4296	B8H	C6-C5	-16.85	1.11	1.34
3	2	237	B9B	C2'-C1'	-16.77	1.28	1.53
3	2	1574	B9B	C2'-C1'	-16.70	1.28	1.53
3	2	4296	B8H	C4-N3	-16.48	1.08	1.38
3	2	4355	E6G	C2'-C1'	-16.37	1.28	1.53
3	2	1860	B8H	C4-N3	-16.25	1.08	1.38
3	2	4185	B8W	C2'-C1'	-15.89	1.29	1.53
3	2	2754	B9B	C2'-C1'	-15.72	1.29	1.53
3	2	4129	B8W	C2'-C1'	-15.43	1.30	1.53
3	2	4355	E6G	O4'-C1'	15.43	1.62	1.41
3	2	2380	B8W	C2'-C1'	-15.39	1.30	1.53
3	2	1871	A2M	O4'-C1'	15.34	1.62	1.41
3	2	1574	B9B	O4'-C1'	15.18	1.62	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2	2754	B9B	O4'-C1'	15.16	1.62	1.41
3	2	4529	B8W	C2'-C1'	-15.02	1.31	1.53
3	2	3723	A2M	O4'-C1'	14.97	1.62	1.41
3	2	3718	A2M	O4'-C1'	14.97	1.62	1.41
3	2	398	A2M	O4'-C1'	14.78	1.61	1.41
3	2	4472	B8W	C2'-C1'	-14.76	1.31	1.53
3	2	3825	A2M	O4'-C1'	14.74	1.61	1.41
3	2	4523	A2M	O4'-C1'	14.62	1.61	1.41
3	2	1534	A2M	O4'-C1'	14.48	1.61	1.41
3	2	1524	A2M	O4'-C1'	14.48	1.61	1.41
3	2	1326	A2M	O4'-C1'	14.47	1.61	1.41
3	2	3867	A2M	O4'-C1'	14.43	1.61	1.41
3	2	4571	A2M	O4'-C1'	14.42	1.61	1.41
3	2	2401	A2M	O4'-C1'	14.40	1.61	1.41
3	2	237	B9B	O4'-C1'	14.24	1.60	1.41
3	2	2363	A2M	O4'-C1'	14.09	1.60	1.41
3	2	3785	A2M	O4'-C1'	13.64	1.60	1.41
3	2	1322	1MA	C2-N3	13.31	1.45	1.29
3	2	1860	B8H	C4-C5	12.98	1.81	1.44
3	2	4296	B8H	C4-C5	12.75	1.80	1.44
3	2	3880	P7G	C8-N9	12.14	1.52	1.46
3	2	1860	B8H	C6-N1	11.84	1.65	1.36
3	2	4296	B8H	C6-N1	11.72	1.65	1.36
3	2	1909	P7G	C8-N9	11.71	1.52	1.46
3	2	1659	I4U	C3'-C2'	-10.57	1.24	1.53
3	2	4194	I4U	C3'-C2'	-10.57	1.24	1.53
3	2	4083	5MU	C6-N1	10.49	1.55	1.38
3	2	4690	B8K	C3'-C4'	-10.47	1.26	1.53
3	2	3897	B8K	C3'-C4'	-10.10	1.27	1.53
3	2	1909	P7G	C5-N7	10.07	1.46	1.35
3	2	4083	5MU	C2-N1	10.05	1.54	1.38
3	2	4194	I4U	C4-N3	9.96	1.44	1.31
3	2	3899	BGH	C3'-C4'	-9.92	1.27	1.53
3	2	3897	B8K	O4'-C4'	9.87	1.67	1.45
3	2	1348	P4U	C4-N3	9.66	1.43	1.31
3	2	4690	B8K	O4'-C4'	9.48	1.66	1.45
3	2	4529	B8W	C2-N2	9.20	1.52	1.33
3	2	3899	BGH	O4'-C4'	9.11	1.65	1.45
3	2	3880	P7G	C5-N7	9.01	1.45	1.35
3	2	1659	I4U	C4-N3	8.92	1.42	1.31
3	2	4335	5MC	C6-C5	8.75	1.49	1.34
3	2	2297	E7G	C5-N7	8.70	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2	4083	5MU	C4-C5	8.70	1.59	1.44
3	2	3782	5MC	C6-C5	8.63	1.48	1.34
3	2	4083	5MU	C4-N3	-8.46	1.23	1.38
3	2	1797	E7G	C8-N9	8.44	1.50	1.46
3	2	4371	MHG	C5-N7	8.36	1.45	1.35
3	2	4355	E6G	O4'-C4'	-8.36	1.26	1.45
3	2	1797	E7G	C5-N7	8.35	1.45	1.35
3	2	1456	B8Q	C6-C5	8.30	1.52	1.33
3	2	237	B9B	O4'-C4'	-8.29	1.26	1.45
3	2	2786	B9H	C2-N3	8.28	1.47	1.37
3	2	4447	5MC	C6-C5	8.23	1.48	1.34
3	2	1574	B9B	O4'-C4'	-8.21	1.26	1.45
3	2	4371	MHG	C8-N9	8.07	1.50	1.46
3	2	4129	B8W	C2-N2	8.07	1.50	1.33
3	2	2297	E7G	C8-N9	8.05	1.50	1.46
3	2	4472	B8W	C2-N2	8.03	1.50	1.33
3	2	2754	B9B	O4'-C4'	-7.72	1.27	1.45
3	2	1866	UR3	C2-N1	7.70	1.49	1.38
3	2	1659	I4U	O4'-C4'	-7.69	1.27	1.45
3	2	4185	B8W	C2-N2	7.60	1.49	1.33
3	2	2522	7MG	C5-N7	7.42	1.44	1.35
3	2	4571	A2M	O4'-C4'	-7.27	1.28	1.45
3	2	4194	I4U	O4'-C4'	-7.27	1.28	1.45
3	2	4550	7MG	C5-N7	7.25	1.44	1.35
3	2	2363	A2M	O4'-C4'	-7.23	1.28	1.45
3	2	2380	B8W	C2-N2	7.23	1.48	1.33
3	2	1605	7MG	C5-N7	7.14	1.43	1.35
3	2	4483	B8T	C2-N3	7.10	1.50	1.36
3	2	1524	A2M	O4'-C4'	-7.00	1.29	1.45
3	2	4371	MHG	C2-N3	7.00	1.45	1.31
3	2	4483	B8T	C4-N3	6.92	1.44	1.32
3	2	4530	UR3	C2-N1	6.82	1.48	1.38
3	2	1534	A2M	O4'-C4'	-6.80	1.29	1.45
3	2	1866	UR3	C6-C5	6.80	1.50	1.35
3	2	4523	A2M	O4'-C4'	-6.79	1.29	1.45
3	2	3723	A2M	O4'-C4'	-6.78	1.29	1.45
3	2	3825	A2M	O4'-C4'	-6.74	1.29	1.45
3	2	4483	B8T	C6-C5	6.73	1.50	1.35
3	2	4550	7MG	C8-N9	6.72	1.49	1.46
3	2	3718	A2M	O4'-C4'	-6.70	1.30	1.45
3	2	3880	P7G	C4-N3	6.69	1.49	1.37
3	2	4355	E6G	O6-C6	6.68	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2	1456	B8Q	C2-N3	6.66	1.46	1.35
3	2	1348	P4U	C2-N3	6.63	1.49	1.36
3	2	4371	MHG	C8-N7	6.62	1.52	1.45
3	2	3785	A2M	O4'-C4'	-6.60	1.30	1.45
3	2	4671	B8T	C6-C5	6.59	1.50	1.35
3	2	2754	B9B	O6-C6	6.57	1.40	1.35
3	2	4597	UR3	C2-N1	6.57	1.48	1.38
3	2	398	A2M	O4'-C4'	-6.55	1.30	1.45
3	2	1326	A2M	O4'-C4'	-6.51	1.30	1.45
3	2	4597	UR3	C6-C5	6.48	1.50	1.35
3	2	4671	B8T	C2-N3	6.44	1.49	1.36
3	2	2401	A2M	O4'-C4'	-6.44	1.30	1.45
3	2	4194	I4U	C6-C5	6.40	1.49	1.35
3	2	3867	A2M	O4'-C4'	-6.40	1.30	1.45
3	2	1871	A2M	O4'-C4'	-6.37	1.30	1.45
3	2	4530	UR3	C6-C5	6.34	1.49	1.35
3	2	4620	OMU	C2-N3	6.30	1.49	1.38
3	2	2522	7MG	C8-N9	6.28	1.49	1.46
3	2	1909	P7G	C4-N3	6.16	1.48	1.37
3	2	4306	OMU	C2-N3	6.16	1.48	1.38
3	2	4220	6MZ	C6-N6	6.15	1.45	1.35
3	2	4620	OMU	C2-N1	6.13	1.48	1.38
3	2	3909	OMC	C2-N3	6.11	1.48	1.36
3	2	1866	UR3	C2-N3	6.08	1.50	1.39
3	2	4194	I4U	C2-N3	6.07	1.48	1.36
3	2	4483	B8T	C4-N4	6.06	1.48	1.35
3	2	3887	OMC	C2-N3	6.04	1.48	1.36
3	2	3897	B8K	O4'-C1'	-6.01	1.27	1.42
3	2	4671	B8T	C4-N3	6.00	1.43	1.32
3	2	2861	OMC	C2-N3	5.99	1.48	1.36
3	2	1348	P4U	C6-C5	5.94	1.48	1.35
3	2	1574	B9B	O6-C6	5.94	1.40	1.35
3	2	4371	MHG	C2-N1	5.88	1.46	1.36
3	2	3887	OMC	C6-C5	5.85	1.48	1.35
3	2	2786	B9H	C6-C5	5.82	1.46	1.33
3	2	4536	OMC	C2-N3	5.79	1.48	1.36
3	2	4371	MHG	C2-N2	5.79	1.46	1.33
3	2	4671	B8T	C4-N4	5.77	1.47	1.35
3	2	2422	OMC	C6-C5	5.76	1.48	1.35
3	2	2365	OMC	C2-N3	5.76	1.48	1.36
3	2	3782	5MC	C4-N3	5.75	1.43	1.34
3	2	1659	I4U	C6-C5	5.74	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2	4690	B8K	O4'-C1'	-5.73	1.28	1.42
3	2	2804	OMC	C2-N3	5.69	1.47	1.36
3	2	3701	OMC	C6-C5	5.69	1.48	1.35
3	2	3782	5MC	C2-N3	5.68	1.47	1.36
3	2	3869	OMC	C2-N3	5.67	1.47	1.36
3	2	2861	OMC	C6-C5	5.66	1.48	1.35
3	2	4690	B8K	C2-N3	5.65	1.46	1.33
3	2	3909	OMC	C6-C5	5.65	1.48	1.35
3	2	4529	B8W	O4'-C4'	-5.65	1.32	1.45
3	2	4536	OMC	C6-C5	5.64	1.48	1.35
3	2	3869	OMC	C6-C5	5.61	1.48	1.35
3	2	4690	B8K	C8-N9	5.60	1.49	1.46
3	2	4196	OMG	C2-N3	5.59	1.46	1.33
3	2	1909	P7G	C2-N2	5.58	1.47	1.34
3	2	4335	5MC	C4-N3	5.55	1.43	1.34
3	2	2365	OMC	C6-C5	5.54	1.47	1.35
3	2	4185	B8W	O4'-C4'	-5.54	1.32	1.45
3	2	4306	OMU	C2-N1	5.52	1.47	1.38
3	2	4083	5MU	C6-C5	5.51	1.43	1.34
3	2	4129	B8W	O4'-C4'	-5.48	1.32	1.45
3	2	1659	I4U	C2-N3	5.48	1.47	1.36
3	2	4870	OMG	C2-N3	5.48	1.46	1.33
3	2	1797	E7G	C2-N3	5.47	1.46	1.33
3	2	3897	B8K	C2-N3	5.47	1.46	1.33
3	2	2380	B8W	O4'-C4'	-5.46	1.32	1.45
3	2	2754	B9B	C2-N2	5.41	1.44	1.33
3	2	4597	UR3	C2-N3	5.40	1.49	1.39
3	2	4371	MHG	C4-N3	5.40	1.47	1.34
3	2	237	B9B	O6-C6	5.40	1.39	1.35
3	2	2804	OMC	C6-C5	5.39	1.47	1.35
3	2	1797	E7G	C4-N3	5.38	1.47	1.34
3	2	2422	OMC	C2-N3	5.38	1.47	1.36
3	2	1909	P7G	C2-N1	5.34	1.46	1.33
3	2	3701	OMC	C2-N3	5.34	1.47	1.36
3	2	237	B9B	C2-N2	5.33	1.44	1.33
3	2	4306	OMU	C6-C5	5.32	1.47	1.35
3	2	4447	5MC	C2-N3	5.32	1.47	1.36
3	2	4335	5MC	C2-N3	5.28	1.47	1.36
3	2	3880	P7G	C2-N2	5.28	1.46	1.34
3	2	3899	BGH	C4-N3	5.27	1.46	1.34
3	2	4472	B8W	O4'-C4'	-5.26	1.33	1.45
3	2	2522	7MG	C2-N3	5.25	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2	4355	E6G	C2-N2	5.25	1.44	1.33
3	2	1605	7MG	C2-N3	5.24	1.45	1.33
3	2	4447	5MC	C4-N3	5.24	1.43	1.34
3	2	2424	OMG	C2-N3	5.23	1.45	1.33
3	2	2773	OMG	C2-N3	5.21	1.45	1.33
3	2	1574	B9B	C2-N2	5.20	1.44	1.33
3	2	4194	I4U	C3'-C4'	5.13	1.66	1.53
3	2	4620	OMU	C6-C5	5.12	1.47	1.35
3	2	4185	B8W	O3'-C3'	-5.11	1.30	1.43
3	2	1517	2MG	C2-N2	5.11	1.44	1.33
3	2	3909	OMC	C2-N1	5.08	1.51	1.40
3	2	2297	E7G	C2-N3	5.06	1.45	1.33
3	2	4530	UR3	C2-N3	5.05	1.48	1.39
3	2	3792	OMG	C2-N3	5.05	1.45	1.33
3	2	3899	BGH	O4'-C1'	-5.03	1.30	1.42
3	2	4637	OMG	C2-N3	5.01	1.45	1.33
3	2	1348	P4U	O4-C4	5.01	1.40	1.35
3	2	4494	OMG	C2-N3	5.00	1.45	1.33
3	2	3899	BGH	C8-N9	4.99	1.48	1.46
3	2	3899	BGH	C2-N3	4.98	1.45	1.33
3	2	1605	7MG	C4-N3	4.98	1.46	1.34
3	2	4370	OMG	C2-N3	4.96	1.45	1.33
3	2	2050	OMG	C2-N3	4.96	1.45	1.33
3	2	729	2MG	C2-N2	4.96	1.44	1.33
3	2	2297	E7G	C4-N3	4.95	1.46	1.34
3	2	4472	B8W	O3'-C3'	-4.94	1.31	1.43
3	2	3897	B8K	C8-N9	4.93	1.48	1.46
3	2	1625	OMG	C2-N3	4.93	1.45	1.33
3	2	4550	7MG	C4-N3	4.87	1.45	1.34
3	2	4690	B8K	C4-N3	4.85	1.45	1.34
3	2	4550	7MG	C2-N3	4.85	1.44	1.33
3	2	3880	P7G	C2-N1	4.84	1.44	1.33
3	2	2522	7MG	C4-N3	4.84	1.45	1.34
3	2	3909	OMC	C4-N4	4.82	1.45	1.33
3	2	4623	OMG	C2-N3	4.82	1.44	1.33
3	2	1348	P4U	C5-C4	4.80	1.49	1.43
3	2	978	2MG	C2-N2	4.79	1.44	1.33
3	2	1316	OMG	C2-N3	4.79	1.44	1.33
3	2	4564	M7A	C6-N6	4.76	1.46	1.34
3	2	4196	OMG	C4-N3	4.76	1.48	1.37
3	2	729	2MG	C4-N3	4.75	1.48	1.37
3	2	3897	B8K	C4-N3	4.74	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2	1797	E7G	C2-N2	4.74	1.45	1.34
3	2	4194	I4U	C1'-N1	-4.73	1.33	1.47
3	2	4371	MHG	C4-N9	4.72	1.43	1.37
3	2	2364	OMG	C2-N3	4.72	1.44	1.33
3	2	3909	OMC	C4-N3	4.71	1.44	1.34
3	2	4529	B8W	O3'-C3'	-4.70	1.31	1.43
3	2	1522	OMG	C2-N3	4.70	1.44	1.33
3	2	4872	2MG	C2-N2	4.69	1.43	1.33
3	2	2422	OMC	C4-N4	4.65	1.44	1.33
3	2	4129	B8W	O3'-C3'	-4.64	1.32	1.43
3	2	2422	OMC	C2-N1	4.64	1.50	1.40
3	2	3897	B8K	O2'-C2'	-4.63	1.32	1.43
3	2	3792	OMG	C4-N3	4.63	1.48	1.37
3	2	4870	OMG	C4-N3	4.63	1.48	1.37
3	2	3880	P7G	C4-N9	4.60	1.42	1.35
3	2	3887	OMC	C4-N4	4.60	1.44	1.33
3	2	1517	2MG	C4-N3	4.59	1.48	1.37
3	2	1659	I4U	C1'-N1	-4.59	1.34	1.47
3	2	2297	E7G	C2-N2	4.58	1.45	1.34
3	2	978	2MG	C4-N3	4.56	1.48	1.37
3	2	2773	OMG	C4-N3	4.55	1.48	1.37
3	2	3887	OMC	C4-N3	4.55	1.43	1.34
3	2	1909	P7G	C6-N1	4.54	1.46	1.38
3	2	2861	OMC	C4-N4	4.54	1.44	1.33
3	2	1883	OMG	C2-N3	4.54	1.44	1.33
3	2	4690	B8K	O2'-C2'	-4.53	1.32	1.43
3	2	3869	OMC	C4-N4	4.53	1.44	1.33
3	2	3899	BGH	C2-N2	4.52	1.44	1.34
3	2	1605	7MG	C8-N9	4.50	1.48	1.46
3	2	373	OMG	C2-N3	4.50	1.44	1.33
3	2	1605	7MG	C2-N2	4.48	1.44	1.34
3	2	2050	OMG	C4-N3	4.46	1.48	1.37
3	2	2365	OMC	C4-N4	4.45	1.44	1.33
3	2	4370	OMG	C4-N3	4.43	1.48	1.37
3	2	2861	OMC	C4-N3	4.42	1.43	1.34
3	2	2380	B8W	O3'-C3'	-4.41	1.32	1.43
3	2	4494	OMG	C4-N3	4.40	1.48	1.37
3	2	2786	B9H	C2-N1	4.40	1.44	1.38
3	2	1797	E7G	C4-N9	4.39	1.42	1.37
3	2	2522	7MG	C2-N2	4.38	1.44	1.34
3	2	3869	OMC	C4-N3	4.38	1.43	1.34
3	2	4442	PSU	C6-C5	4.38	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2	4550	7MG	C2-N2	4.37	1.44	1.34
3	2	4536	OMC	C4-N4	4.37	1.44	1.33
3	2	3899	BGH	C71-N7	4.34	1.49	1.39
3	2	4623	OMG	C4-N3	4.34	1.47	1.37
3	2	4637	OMG	C4-N3	4.33	1.47	1.37
3	2	2804	OMC	C4-N4	4.33	1.44	1.33
3	2	3897	B8K	C4-N9	4.32	1.42	1.37
3	2	978	2MG	C2-N1	4.32	1.43	1.36
3	2	1625	OMG	C4-N3	4.30	1.47	1.37
3	2	3899	BGH	O2'-C2'	-4.29	1.31	1.42
3	2	2804	OMC	C4-N3	4.29	1.43	1.34
3	2	1522	OMG	C4-N3	4.27	1.47	1.37
3	2	2365	OMC	C4-N3	4.26	1.43	1.34
3	2	4872	2MG	C4-N3	4.25	1.47	1.37
3	2	4536	OMC	C4-N3	4.25	1.43	1.34
3	2	1909	P7G	C4-N9	4.23	1.41	1.35
3	2	4483	B8T	C2-N1	4.21	1.49	1.40
3	2	1659	I4U	C3'-C4'	4.21	1.63	1.53
3	2	1797	E7G	C8-N7	4.19	1.49	1.45
3	2	1316	OMG	C4-N3	4.19	1.47	1.37
3	2	1883	OMG	C4-N3	4.19	1.47	1.37
3	2	2424	OMG	C4-N3	4.19	1.47	1.37
3	2	373	OMG	C4-N3	4.19	1.47	1.37
3	2	3701	OMC	C4-N4	4.18	1.43	1.33
3	2	4564	M7A	C4-N9	4.17	1.46	1.38
3	2	4194	I4U	O4'-C1'	4.17	1.51	1.42
3	2	4690	B8K	C5-N7	4.13	1.46	1.39
3	2	4690	B8K	C4-N9	4.13	1.42	1.37
3	2	3880	P7G	O6-C6	-4.11	1.17	1.23
3	2	3880	P7G	C8-N7	4.11	1.49	1.45
3	2	4335	5MC	C6-N1	4.10	1.45	1.38
3	2	3897	B8K	C5-N7	4.08	1.46	1.39
3	2	3782	5MC	C4-N4	4.07	1.44	1.34
3	2	4447	5MC	C4-N4	4.06	1.44	1.34
3	2	3887	OMC	C2-N1	4.06	1.48	1.40
3	2	1605	7MG	C4-N9	4.06	1.42	1.37
3	2	2364	OMG	C4-N3	4.05	1.47	1.37
3	2	1659	I4U	O4'-C1'	4.03	1.51	1.42
3	2	3701	OMC	C4-N3	4.01	1.42	1.34
3	2	3880	P7G	C6-N1	3.97	1.45	1.38
3	2	4870	OMG	C6-N1	3.95	1.43	1.37
3	2	4564	M7A	C5-N7	3.94	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2	2297	E7G	C8-N7	3.94	1.49	1.45
3	2	4196	OMG	C2-N2	3.93	1.43	1.34
3	2	1517	2MG	C2-N1	3.93	1.43	1.36
3	2	3899	BGH	C5-N7	3.92	1.46	1.39
3	2	4335	5MC	C4-N4	3.92	1.44	1.34
3	2	4671	B8T	C2-N1	3.91	1.48	1.40
3	2	2861	OMC	C2-N1	3.91	1.48	1.40
3	2	2422	OMC	C4-N3	3.89	1.42	1.34
3	2	2773	OMG	C6-N1	3.89	1.43	1.37
3	2	1659	I4U	C2-N1	3.89	1.48	1.40
3	2	1909	P7G	C5-C4	3.88	1.45	1.37
3	2	1909	P7G	O6-C6	-3.87	1.17	1.23
3	2	4194	I4U	C2-N1	3.86	1.48	1.40
3	2	729	2MG	C2-N1	3.84	1.42	1.36
3	2	4194	I4U	C5-C4	3.84	1.48	1.43
3	2	1348	P4U	C2-N1	3.84	1.48	1.40
3	2	2773	OMG	C2-N2	3.83	1.43	1.34
3	2	3782	5MC	C6-N1	3.82	1.44	1.38
3	2	3897	B8K	C2-N2	3.80	1.43	1.34
3	2	2424	OMG	C2-N2	3.79	1.43	1.34
3	2	4296	B8H	C2-N3	3.79	1.44	1.38
3	2	4447	5MC	C6-N1	3.77	1.44	1.38
3	2	1322	1MA	C2-N1	3.76	1.42	1.35
3	2	4196	OMG	C6-N1	3.76	1.43	1.37
3	2	4870	OMG	C2-N2	3.75	1.43	1.34
3	2	4637	OMG	C2-N2	3.74	1.43	1.34
3	2	4872	2MG	C2-N1	3.74	1.42	1.36
3	2	1860	B8H	C2-N3	3.73	1.44	1.38
3	2	1522	OMG	C2-N2	3.73	1.43	1.34
3	2	373	OMG	C2-N2	3.73	1.43	1.34
3	2	3782	5MC	C2-N1	3.72	1.48	1.40
3	2	2804	OMC	C2-N1	3.72	1.48	1.40
3	2	3899	BGH	C2-N1	3.70	1.46	1.37
3	2	1883	OMG	C2-N2	3.69	1.43	1.34
3	2	4403	PSU	C6-C5	3.69	1.39	1.35
3	2	4550	7MG	C4-N9	3.67	1.42	1.37
3	2	1348	P4U	C6-N1	3.67	1.46	1.38
3	2	4690	B8K	C2-N2	3.66	1.42	1.34
3	2	4494	OMG	C2-N2	3.66	1.42	1.34
3	2	4083	5MU	O4-C4	-3.64	1.16	1.23
3	2	4335	5MC	C2-N1	3.63	1.47	1.40
3	2	1625	OMG	C2-N2	3.63	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2	2522	7MG	C4-N9	3.62	1.41	1.37
3	2	4690	B8K	C5-C6	3.62	1.52	1.43
3	2	3880	P7G	C2-N3	3.61	1.46	1.37
3	2	1522	OMG	C5-C4	-3.61	1.33	1.43
3	2	1797	E7G	C2-N1	3.61	1.46	1.37
3	2	2297	E7G	C4-N9	3.60	1.41	1.37
3	2	3792	OMG	C2-N2	3.60	1.42	1.34
3	2	4447	5MC	O2-C2	-3.59	1.17	1.23
3	2	4623	OMG	C2-N2	3.59	1.42	1.34
3	2	3701	OMC	C2-N1	3.59	1.47	1.40
3	2	1659	I4U	O2-C2	-3.59	1.17	1.23
3	2	4671	B8T	C5-C4	3.58	1.48	1.40
3	2	2365	OMC	C2-N1	3.58	1.47	1.40
3	2	3869	OMC	C2-N1	3.57	1.47	1.40
3	2	3880	P7G	C5-C4	3.56	1.44	1.37
3	2	4355	E6G	O3'-C3'	-3.55	1.34	1.43
3	2	3899	BGH	C6-N1	3.55	1.45	1.38
3	2	4620	OMU	C4-N3	3.54	1.44	1.38
3	2	4306	OMU	C4-N3	3.53	1.44	1.38
3	2	4371	MHG	C5-C6	3.52	1.52	1.43
3	2	4690	B8K	O6-C6	-3.51	1.16	1.23
3	2	3899	BGH	O6-C6	-3.50	1.16	1.23
3	2	4306	OMU	O4-C4	-3.50	1.17	1.24
3	2	1316	OMG	C2-N2	3.49	1.42	1.34
3	2	1909	P7G	C2-N3	3.49	1.46	1.37
3	2	4483	B8T	C5-C4	3.48	1.48	1.40
3	2	4536	OMC	O2-C2	-3.47	1.17	1.23
3	2	2364	OMG	C2-N2	3.46	1.42	1.34
3	2	1316	OMG	C5-C4	-3.46	1.34	1.43
3	2	1574	B9B	O2'-C2'	3.45	1.51	1.43
3	2	2297	E7G	C2-N1	3.45	1.46	1.37
3	2	4083	5MU	O2-C2	-3.44	1.16	1.23
3	2	3785	A2M	C5-C4	-3.44	1.31	1.40
3	2	4370	OMG	C2-N2	3.43	1.42	1.34
3	2	4447	5MC	C2-N1	3.43	1.47	1.40
3	2	4571	A2M	O3'-C3'	-3.43	1.34	1.43
3	2	2424	OMG	C6-N1	3.43	1.43	1.37
3	2	1322	1MA	C4-N3	3.43	1.48	1.37
3	2	1909	P7G	C8-N7	3.43	1.49	1.45
3	2	2364	OMG	C5-C4	-3.43	1.34	1.43
3	2	4597	UR3	C6-N1	3.41	1.46	1.38
3	2	3825	A2M	O3'-C3'	-3.40	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2	3897	B8K	C2-N1	3.40	1.46	1.37
3	2	4194	I4U	O2-C2	-3.38	1.17	1.23
3	2	2754	B9B	O2'-C2'	3.38	1.50	1.43
3	2	373	OMG	C5-C4	-3.38	1.34	1.43
3	2	3897	B8K	C5-C6	3.38	1.52	1.43
3	2	1866	UR3	C6-N1	3.36	1.46	1.38
3	2	1574	B9B	C5-C4	-3.36	1.32	1.40
3	2	4536	OMC	C2-N1	3.35	1.47	1.40
3	2	1677	PSU	C6-C5	3.34	1.39	1.35
3	2	1574	B9B	O3'-C3'	-3.34	1.35	1.43
3	2	1517	2MG	C6-N1	3.33	1.42	1.37
3	2	2401	A2M	O3'-C3'	-3.33	1.35	1.43
3	2	4371	MHG	C6-N1	3.32	1.45	1.38
3	2	1883	OMG	C5-C4	-3.32	1.34	1.43
3	2	2050	OMG	C2-N2	3.32	1.42	1.34
3	2	237	B9B	O3'-C3'	-3.30	1.35	1.43
3	2	4620	OMU	O4-C4	-3.29	1.18	1.24
3	2	1871	A2M	O3'-C3'	-3.29	1.35	1.43
3	2	1625	OMG	C5-C4	-3.29	1.34	1.43
3	2	1534	A2M	C5-C4	-3.28	1.32	1.40
3	2	2363	A2M	C5-C4	-3.28	1.32	1.40
3	2	4637	OMG	C5-C4	-3.27	1.34	1.43
3	2	4636	PSU	C6-C5	3.27	1.39	1.35
3	2	4531	PSU	C6-C5	3.27	1.39	1.35
3	2	4623	OMG	C5-C4	-3.26	1.34	1.43
3	2	3869	OMC	O2-C2	-3.24	1.17	1.23
3	2	1524	A2M	O3'-C3'	-3.24	1.35	1.43
3	2	2050	OMG	C5-C4	-3.23	1.34	1.43
3	2	398	A2M	O3'-C3'	-3.22	1.35	1.43
3	2	3897	B8K	O6-C6	-3.22	1.17	1.23
3	2	4671	B8T	O2-C2	-3.21	1.17	1.23
3	2	2422	OMC	O2-C2	-3.21	1.17	1.23
3	2	4530	UR3	C6-N1	3.21	1.45	1.38
3	2	1326	A2M	O3'-C3'	-3.20	1.35	1.43
3	2	1871	A2M	C6-N6	3.20	1.45	1.34
3	2	2363	A2M	O3'-C3'	-3.19	1.35	1.43
3	2	3867	A2M	O3'-C3'	-3.19	1.35	1.43
3	2	4306	OMU	O2-C2	-3.18	1.17	1.23
3	2	3899	BGH	C4-N9	3.18	1.41	1.37
3	2	978	2MG	C6-N1	3.18	1.42	1.37
3	2	3909	OMC	O2-C2	-3.18	1.17	1.23
3	2	4494	OMG	C6-N1	3.18	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2	3715	PSU	C6-C5	3.17	1.39	1.35
3	2	1316	OMG	C6-N1	3.17	1.42	1.37
3	2	2424	OMG	C5-C4	-3.17	1.35	1.43
3	2	1517	2MG	C5-C4	-3.16	1.35	1.43
3	2	2522	7MG	C5-C6	3.16	1.51	1.43
3	2	4194	I4U	O4-C4	3.16	1.41	1.35
3	2	4550	7MG	O6-C6	-3.15	1.17	1.23
3	2	3718	A2M	C5-C4	-3.14	1.32	1.40
3	2	4450	PSU	C6-C5	3.14	1.39	1.35
3	2	2522	7MG	C2-N1	3.14	1.45	1.37
3	2	237	B9B	C5-C4	-3.14	1.32	1.40
3	2	4355	E6G	O2'-C2'	3.14	1.50	1.43
3	2	4335	5MC	O2-C2	-3.14	1.17	1.23
3	2	4872	2MG	C5-C6	3.12	1.53	1.47
3	2	3909	OMC	C6-N1	3.11	1.45	1.38
3	2	3792	OMG	C6-N1	3.11	1.42	1.37
3	2	4523	A2M	O3'-C3'	-3.11	1.35	1.43
3	2	2401	A2M	C5-C4	-3.10	1.32	1.40
3	2	1316	OMG	O6-C6	-3.09	1.17	1.23
3	2	1522	OMG	O6-C6	-3.09	1.17	1.23
3	2	2754	B9B	C5-C4	-3.09	1.32	1.40
3	2	3782	5MC	O2-C2	-3.08	1.18	1.23
3	2	3867	A2M	C5-C4	-3.08	1.32	1.40
3	2	3897	B8K	O3'-C3'	3.07	1.50	1.43
3	2	4571	A2M	C5-C4	-3.07	1.32	1.40
3	2	1871	A2M	C5-C4	-3.07	1.32	1.40
3	2	1605	7MG	C2-N1	3.07	1.45	1.37
3	2	1326	A2M	C5-C4	-3.07	1.32	1.40
3	2	3723	A2M	C6-N6	3.06	1.45	1.34
3	2	4194	I4U	O2'-C2'	3.06	1.50	1.43
3	2	237	B9B	O2'-C2'	3.06	1.50	1.43
3	2	2773	OMG	C5-C4	-3.06	1.35	1.43
3	2	3869	OMC	C6-N1	3.05	1.45	1.38
3	2	4494	OMG	C5-C4	-3.05	1.35	1.43
3	2	2365	OMC	O2-C2	-3.04	1.18	1.23
3	2	3723	A2M	O3'-C3'	-3.04	1.35	1.43
3	2	1605	7MG	C5-C6	3.04	1.51	1.43
3	2	4637	OMG	C6-N1	3.04	1.42	1.37
3	2	1524	A2M	C5-C4	-3.03	1.32	1.40
3	2	4220	6MZ	C5-C4	-3.03	1.32	1.40
3	2	398	A2M	C5-C4	-3.02	1.32	1.40
3	2	1582	PSU	C6-C5	3.02	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2	4536	OMC	C6-N1	3.02	1.45	1.38
3	2	1524	A2M	C6-N6	3.01	1.45	1.34
3	2	3899	BGH	C5-C6	3.01	1.51	1.43
3	2	4523	A2M	C5-C4	-3.00	1.33	1.40
3	2	4483	B8T	C6-N1	2.99	1.45	1.38
3	2	3825	A2M	C5-C4	-2.99	1.33	1.40
3	2	4371	MHG	C72-C71	2.99	1.58	1.52
3	2	4872	2MG	C6-N1	2.99	1.42	1.37
3	2	1456	B8Q	C2-N1	2.99	1.42	1.38
3	2	3718	A2M	O3'-C3'	-2.98	1.35	1.43
3	2	4620	OMU	O2-C2	-2.98	1.17	1.23
3	2	1625	OMG	C6-N1	2.98	1.42	1.37
3	2	2424	OMG	O6-C6	-2.98	1.17	1.23
3	2	4637	OMG	O6-C6	-2.98	1.17	1.23
3	2	4870	OMG	C5-C4	-2.98	1.35	1.43
3	2	4523	A2M	C6-N6	2.97	1.44	1.34
3	2	4370	OMG	C6-N1	2.97	1.42	1.37
3	2	373	OMG	C6-N1	2.97	1.42	1.37
3	2	3887	OMC	C6-N1	2.96	1.45	1.38
3	2	3825	A2M	C6-N6	2.96	1.44	1.34
3	2	1659	I4U	O4-C4	2.96	1.41	1.35
3	2	1534	A2M	O3'-C3'	-2.96	1.36	1.43
3	2	3723	A2M	C5-C4	-2.96	1.33	1.40
3	2	2804	OMC	O2-C2	-2.94	1.18	1.23
3	2	4355	E6G	C5-C4	-2.94	1.33	1.40
3	2	1871	A2M	O2'-C2'	2.94	1.50	1.42
3	2	4370	OMG	C5-C4	-2.94	1.35	1.43
3	2	978	2MG	C5-C6	2.93	1.53	1.47
3	2	2050	OMG	O6-C6	-2.93	1.17	1.23
3	2	3785	A2M	O3'-C3'	-2.93	1.36	1.43
3	2	1797	E7G	C5-C6	2.92	1.51	1.43
3	2	4623	OMG	O6-C6	-2.92	1.17	1.23
3	2	1883	OMG	O6-C6	-2.91	1.17	1.23
3	2	2754	B9B	O3'-C3'	-2.91	1.36	1.43
3	2	3785	A2M	O2'-C2'	2.90	1.50	1.42
3	2	2861	OMC	C6-N1	2.90	1.45	1.38
3	2	4690	B8K	C2-N1	2.89	1.44	1.37
3	2	3887	OMC	O2-C2	-2.89	1.18	1.23
3	2	2297	E7G	O6-C6	-2.89	1.18	1.23
3	2	4872	2MG	C5-C4	-2.89	1.35	1.43
3	2	3718	A2M	C6-N6	2.88	1.44	1.34
3	2	3897	B8K	C6-N1	2.88	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2	1322	1MA	C5-C4	-2.88	1.35	1.43
3	2	2522	7MG	O6-C6	-2.86	1.18	1.23
3	2	2297	E7G	C5-C6	2.86	1.50	1.43
3	2	978	2MG	C5-C4	-2.86	1.35	1.43
3	2	2365	OMC	C6-N1	2.85	1.44	1.38
3	2	2422	OMC	C6-N1	2.85	1.44	1.38
3	2	3867	A2M	C6-N6	2.84	1.44	1.34
3	2	1883	OMG	C6-N1	2.84	1.42	1.37
3	2	1605	7MG	O6-C6	-2.84	1.18	1.23
3	2	1797	E7G	O6-C6	-2.83	1.18	1.23
3	2	4571	A2M	C6-N6	2.82	1.44	1.34
3	2	1522	OMG	C6-N1	2.82	1.42	1.37
3	2	1534	A2M	C6-N6	2.81	1.44	1.34
3	2	2401	A2M	C6-N6	2.81	1.44	1.34
3	2	4483	B8T	O2-C2	-2.81	1.18	1.23
3	2	4293	PSU	C6-C5	2.81	1.38	1.35
3	2	2363	A2M	C6-N6	2.81	1.44	1.34
3	2	3723	A2M	O2'-C2'	2.80	1.49	1.42
3	2	3792	OMG	C5-C4	-2.80	1.35	1.43
3	2	3701	OMC	O2-C2	-2.79	1.18	1.23
3	2	2364	OMG	O6-C6	-2.78	1.17	1.23
3	2	4623	OMG	C6-N1	2.77	1.42	1.37
3	2	398	A2M	C6-N6	2.77	1.44	1.34
3	2	3701	OMC	C6-N1	2.76	1.44	1.38
3	2	3785	A2M	C6-N6	2.76	1.44	1.34
3	2	2861	OMC	O2-C2	-2.76	1.18	1.23
3	2	4185	B8W	C5-C4	-2.75	1.33	1.40
3	2	2786	B9H	C6-N1	2.73	1.44	1.38
3	2	729	2MG	C5-C4	-2.73	1.36	1.43
3	2	2522	7MG	C6-N1	2.72	1.43	1.38
3	2	4870	OMG	C2-N1	2.71	1.44	1.37
3	2	373	OMG	O6-C6	-2.70	1.17	1.23
3	2	4196	OMG	O6-C6	-2.69	1.17	1.23
3	2	1659	I4U	C5-C4	2.69	1.46	1.43
3	2	4550	7MG	C5-C6	2.68	1.50	1.43
3	2	4529	B8W	O2'-C2'	2.67	1.49	1.43
3	2	4370	OMG	O6-C6	-2.67	1.17	1.23
3	2	1517	2MG	O6-C6	-2.67	1.17	1.23
3	2	4550	7MG	C2-N1	2.67	1.44	1.37
3	2	3825	A2M	O2'-C2'	2.67	1.49	1.42
3	2	4623	OMG	C5-C6	2.65	1.52	1.47
3	2	4129	B8W	O2'-C2'	2.65	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2	1659	I4U	O2'-C2'	2.65	1.49	1.43
3	2	2380	B8W	C5-C4	-2.65	1.33	1.40
3	2	2297	E7G	C6-N1	2.64	1.43	1.38
3	2	1797	E7G	C6-N1	2.64	1.43	1.38
3	2	2380	B8W	O2'-C2'	2.64	1.49	1.43
3	2	4690	B8K	C71-N7	2.62	1.45	1.39
3	2	4671	B8T	C6-N1	2.62	1.44	1.38
3	2	2786	B9H	O2-C2	-2.62	1.17	1.22
3	2	1326	A2M	C6-N6	2.60	1.43	1.34
3	2	4494	OMG	C5-C6	2.60	1.52	1.47
3	2	729	2MG	C5-C6	2.60	1.52	1.47
3	2	3718	A2M	O2'-C2'	2.59	1.49	1.42
3	2	2363	A2M	O2'-C2'	2.59	1.49	1.42
3	2	3792	OMG	O6-C6	-2.59	1.18	1.23
3	2	1659	I4U	C6-N1	2.58	1.44	1.38
3	2	3897	B8K	C71-N7	2.57	1.45	1.39
3	2	1326	A2M	O2'-C2'	2.56	1.49	1.42
3	2	2804	OMC	C6-N1	2.56	1.44	1.38
3	2	4870	OMG	O6-C6	-2.55	1.18	1.23
3	2	4196	OMG	C2-N1	2.55	1.44	1.37
3	2	4494	OMG	O6-C6	-2.54	1.18	1.23
3	2	1456	B8Q	C6-N1	2.54	1.44	1.38
3	2	4196	OMG	C5-C4	-2.53	1.36	1.43
3	2	4529	B8W	C5-C4	-2.53	1.34	1.40
3	2	4194	I4U	C6-N1	2.53	1.44	1.38
3	2	1625	OMG	O6-C6	-2.52	1.18	1.23
3	2	4296	B8H	O4-C4	-2.52	1.18	1.23
3	2	398	A2M	O2'-C2'	2.52	1.49	1.42
3	2	4690	B8K	C6-N1	2.52	1.43	1.38
3	2	4550	7MG	C6-N1	2.52	1.43	1.38
3	2	2773	OMG	O6-C6	-2.51	1.18	1.23
3	2	4371	MHG	O6-C6	-2.50	1.18	1.23
3	2	4472	B8W	O2'-C2'	2.48	1.48	1.43
3	2	4690	B8K	O3'-C3'	2.48	1.48	1.43
3	2	2050	OMG	C6-N1	2.47	1.41	1.37
3	2	2364	OMG	C6-N1	2.47	1.41	1.37
3	2	3867	A2M	O2'-C2'	2.47	1.48	1.42
3	2	3825	A2M	O5'-C5'	-2.46	1.38	1.44
3	2	729	2MG	O6-C6	-2.46	1.18	1.23
3	2	2508	PSU	C6-C5	2.45	1.38	1.35
3	2	1860	B8H	O4-C4	-2.44	1.18	1.23
3	2	1534	A2M	O2'-C2'	2.43	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2	4571	A2M	O2'-C2'	2.43	1.48	1.42
3	2	3792	OMG	C5-C6	2.42	1.52	1.47
3	2	1605	7MG	C6-N1	2.42	1.43	1.38
3	2	4370	OMG	C5-C6	2.41	1.52	1.47
3	2	978	2MG	O6-C6	-2.41	1.18	1.23
3	2	237	B9B	O5'-C5'	-2.40	1.38	1.44
3	2	1534	A2M	O5'-C5'	-2.40	1.38	1.44
3	2	4529	B8W	C6-N1	2.40	1.35	1.31
3	2	3785	A2M	O5'-C5'	-2.40	1.38	1.44
3	2	4306	OMU	C6-N1	2.40	1.43	1.38
3	2	4355	E6G	O5'-C5'	-2.40	1.38	1.44
3	2	2050	OMG	C5-C6	2.40	1.52	1.47
3	2	4196	OMG	C5-C6	2.40	1.52	1.47
3	2	3899	BGH	O5'-C5'	-2.39	1.38	1.44
3	2	4870	OMG	C5-C6	2.38	1.52	1.47
3	2	2773	OMG	C2-N1	2.38	1.43	1.37
3	2	4872	2MG	O6-C6	-2.38	1.18	1.23
3	2	4185	B8W	O2'-C2'	2.36	1.48	1.43
3	2	2364	OMG	C5-C6	2.36	1.52	1.47
3	2	2401	A2M	O2'-C2'	2.36	1.48	1.42
3	2	373	OMG	C5-C6	2.35	1.52	1.47
3	2	3723	A2M	O5'-C5'	-2.34	1.39	1.44
3	2	2424	OMG	C2-N1	2.32	1.43	1.37
3	2	4194	I4U	O5'-C5'	-2.31	1.39	1.44
3	2	1316	OMG	C5-C6	2.31	1.52	1.47
3	2	729	2MG	C6-N1	2.30	1.41	1.37
3	2	1866	UR3	C4-N3	2.30	1.45	1.40
3	2	4620	OMU	C6-N1	2.28	1.43	1.38
3	2	4472	B8W	C5-C4	-2.27	1.34	1.40
3	2	1625	OMG	C5-C6	2.26	1.52	1.47
3	2	4500	PSU	C6-C5	2.26	1.38	1.35
3	2	2363	A2M	O5'-C5'	-2.25	1.39	1.44
3	2	2773	OMG	C5-C6	2.23	1.51	1.47
3	2	4529	B8W	C8-N7	-2.23	1.30	1.34
3	2	1683	PSU	C4-C5	-2.22	1.37	1.44
3	2	4523	A2M	O2'-C2'	2.22	1.48	1.42
3	2	4523	A2M	O5'-C5'	-2.21	1.39	1.44
3	2	3729	PSU	C6-C5	2.21	1.37	1.35
3	2	4571	A2M	O5'-C5'	-2.21	1.39	1.44
3	2	1677	PSU	C4-C5	-2.20	1.37	1.44
3	2	3729	PSU	C4-C5	-2.20	1.37	1.44
3	2	1860	B8H	C2-N1	-2.19	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2	1348	P4U	O2-C2	-2.19	1.19	1.23
3	2	2401	A2M	O5'-C5'	-2.19	1.39	1.44
3	2	4194	I4U	O3'-C3'	2.19	1.48	1.43
3	2	1677	PSU	O4'-C1'	-2.18	1.40	1.43
3	2	4597	UR3	C5-C4	2.17	1.49	1.43
3	2	4500	PSU	C4-C5	-2.17	1.38	1.44
3	2	1522	OMG	C5-C6	2.16	1.51	1.47
3	2	1517	2MG	C5-C6	2.15	1.51	1.47
3	2	4500	PSU	O4'-C1'	-2.15	1.40	1.43
3	2	1524	A2M	O5'-C5'	-2.15	1.39	1.44
3	2	4636	PSU	C4-C5	-2.14	1.38	1.44
3	2	4530	UR3	O2-C2	-2.14	1.18	1.22
3	2	4129	B8W	C5-C4	-2.13	1.35	1.40
3	2	1659	I4U	O5'-C5'	-2.12	1.39	1.44
3	2	4530	UR3	C4-N3	2.12	1.45	1.40
3	2	4564	M7A	C5-C6	-2.12	1.35	1.40
3	2	4450	PSU	C4-C5	-2.11	1.38	1.44
3	2	4220	6MZ	C2-N3	2.09	1.35	1.32
3	2	3701	OMC	C5-C4	2.08	1.47	1.42
3	2	4637	OMG	C5-C6	2.08	1.51	1.47
3	2	4628	PSU	O4'-C1'	-2.07	1.41	1.43
3	2	4636	PSU	O4'-C1'	-2.07	1.41	1.43
3	2	1316	OMG	C2-N1	2.07	1.42	1.37
3	2	1866	UR3	C5-C4	2.06	1.49	1.43
3	2	3909	OMC	C5-C4	2.06	1.47	1.42
3	2	4530	UR3	C5-C4	2.05	1.49	1.43
3	2	4597	UR3	O2-C2	-2.05	1.18	1.22
3	2	4370	OMG	C2-N1	2.04	1.42	1.37
3	2	4620	OMU	O3'-C3'	2.03	1.47	1.43
3	2	2401	A2M	C6-C5	-2.02	1.35	1.43
3	2	4296	B8H	C2-N1	-2.01	1.34	1.38
3	2	4293	PSU	C4-C5	-2.01	1.38	1.44
3	2	1524	A2M	O2'-C2'	2.01	1.47	1.42
3	2	4623	OMG	C2-N1	2.00	1.42	1.37

All (444) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	4564	M7A	C5-C6-N6	13.91	147.49	123.74
3	2	4220	6MZ	C1'-N9-C4	-13.75	102.49	126.64
3	2	4083	5MU	C5-C4-N3	12.98	126.39	115.31
3	2	4564	M7A	N6-C6-N1	-11.44	93.29	118.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	2363	A2M	C5-C6-N6	10.30	136.01	120.35
3	2	3718	A2M	C5-C6-N6	9.86	135.34	120.35
3	2	4523	A2M	C5-C6-N6	9.60	134.94	120.35
3	2	398	A2M	C5-C6-N6	9.59	134.92	120.35
3	2	4083	5MU	C5-C6-N1	-9.58	113.48	123.34
3	2	1524	A2M	C5-C6-N6	9.54	134.85	120.35
3	2	3825	A2M	C5-C6-N6	9.33	134.53	120.35
3	2	2401	A2M	C5-C6-N6	9.26	134.42	120.35
3	2	3785	A2M	C5-C6-N6	9.10	134.18	120.35
3	2	1326	A2M	C5-C6-N6	8.87	133.84	120.35
3	2	4571	A2M	C5-C6-N6	8.86	133.82	120.35
3	2	3723	A2M	C5-C6-N6	8.84	133.79	120.35
3	2	1871	A2M	C5-C6-N6	8.42	133.15	120.35
3	2	1534	A2M	C5-C6-N6	8.36	133.06	120.35
3	2	3867	A2M	C5-C6-N6	8.25	132.89	120.35
3	2	2786	B9H	C31-N3-C2	7.69	126.82	117.21
3	2	4529	B8W	N3-C2-N1	-7.41	117.33	127.22
3	2	2363	A2M	N6-C6-N1	-7.36	103.29	118.57
3	2	4529	B8W	C2-N3-C4	7.23	123.62	115.36
3	2	237	B9B	O6-C6-N1	-7.15	113.95	120.12
3	2	1860	B8H	C4-N3-C2	-6.99	118.30	127.35
3	2	3718	A2M	N6-C6-N1	-6.89	104.26	118.57
3	2	4296	B8H	C4-N3-C2	-6.89	118.43	127.35
3	2	398	A2M	N6-C6-N1	-6.73	104.60	118.57
3	2	3880	P7G	C4-C5-N7	6.72	110.22	106.67
3	2	3825	A2M	N6-C6-N1	-6.68	104.72	118.57
3	2	3785	A2M	N6-C6-N1	-6.64	104.79	118.57
3	2	1524	A2M	N6-C6-N1	-6.63	104.82	118.57
3	2	4523	A2M	N6-C6-N1	-6.55	104.98	118.57
3	2	1871	A2M	N3-C2-N1	-6.52	118.49	128.68
3	2	1860	B8H	N3-C2-N1	6.44	122.10	115.14
3	2	1326	A2M	N6-C6-N1	-6.38	105.34	118.57
3	2	4564	M7A	N3-C2-N1	-6.37	118.63	128.60
3	2	2401	A2M	N6-C6-N1	-6.26	105.57	118.57
3	2	4447	5MC	C5-C6-N1	-6.25	116.91	123.34
3	2	4355	E6G	N2-C2-N3	6.16	127.82	117.79
3	2	3867	A2M	N6-C6-N1	-6.14	105.83	118.57
3	2	2401	A2M	N3-C2-N1	-6.12	119.12	128.68
3	2	4220	6MZ	N3-C2-N1	-6.11	119.13	128.68
3	2	398	A2M	N3-C2-N1	-6.08	119.17	128.68
3	2	3723	A2M	N3-C2-N1	-6.08	119.18	128.68
3	2	2363	A2M	N3-C2-N1	-6.04	119.23	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	4690	B8K	C5-C6-N1	6.03	121.62	110.99
3	2	4371	MHG	C2-N3-C4	6.03	119.51	112.04
3	2	1456	B8Q	C31-N3-C4	6.01	123.31	114.25
3	2	4571	A2M	N6-C6-N1	-5.99	106.13	118.57
3	2	1326	A2M	N3-C2-N1	-5.99	119.31	128.68
3	2	3897	B8K	C72-C71-N7	5.99	127.87	118.86
3	2	4571	A2M	N3-C2-N1	-5.92	119.42	128.68
3	2	3723	A2M	N6-C6-N1	-5.87	106.39	118.57
3	2	1534	A2M	N6-C6-N1	-5.85	106.42	118.57
3	2	3825	A2M	N3-C2-N1	-5.80	119.61	128.68
3	2	3785	A2M	N3-C2-N1	-5.77	119.66	128.68
3	2	4564	M7A	N3-C4-N9	5.74	134.12	126.87
3	2	4690	B8K	C72-C71-N7	5.71	127.44	118.86
3	2	1322	1MA	N1-C2-N3	-5.69	119.38	126.02
3	2	4083	5MU	O4-C4-C5	-5.68	118.31	124.90
3	2	4296	B8H	N3-C2-N1	5.68	121.28	115.14
3	2	237	B9B	N3-C2-N1	-5.65	119.68	127.22
3	2	1871	A2M	N6-C6-N1	-5.63	106.89	118.57
3	2	4129	B8W	N2-C2-N3	5.62	126.96	117.79
3	2	1524	A2M	N3-C2-N1	-5.62	119.90	128.68
3	2	2786	B9H	C6-N1-C2	-5.55	116.82	121.79
3	2	1534	A2M	N3-C2-N1	-5.54	120.02	128.68
3	2	4129	B8W	N3-C2-N1	-5.54	119.83	127.22
3	2	3899	BGH	C5-C6-N1	5.50	120.69	110.99
3	2	1797	E7G	C4-C5-N7	5.49	109.80	104.91
3	2	4083	5MU	C4-N3-C2	-5.48	120.25	127.35
3	2	1574	B9B	O6-C6-N1	-5.48	115.40	120.12
3	2	4083	5MU	N3-C2-N1	5.43	122.10	114.89
3	2	2297	E7G	C5-C6-N1	5.41	120.53	110.99
3	2	4620	OMU	C4-N3-C2	-5.41	119.44	126.58
3	2	4523	A2M	N3-C2-N1	-5.40	120.23	128.68
3	2	2297	E7G	C4-C5-N7	5.39	109.70	104.91
3	2	1456	B8Q	N3-C2-N1	5.38	123.46	117.13
3	2	2754	B9B	N3-C2-N1	-5.35	120.09	127.22
3	2	3718	A2M	N3-C2-N1	-5.33	120.35	128.68
3	2	1677	PSU	N1-C2-N3	5.33	121.17	115.13
3	2	3899	BGH	C4-C5-N7	5.30	109.63	104.91
3	2	4306	OMU	C4-N3-C2	-5.29	119.60	126.58
3	2	4450	PSU	N1-C2-N3	5.27	121.10	115.13
3	2	1574	B9B	N3-C2-N1	-5.26	120.21	127.22
3	2	4185	B8W	N3-C2-N1	-5.25	120.21	127.22
3	2	4355	E6G	N3-C2-N1	-5.25	120.22	127.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	2522	7MG	C5-C6-N1	5.25	120.24	110.99
3	2	4636	PSU	C4-N3-C2	-5.21	118.84	126.34
3	2	3867	A2M	N3-C2-N1	-5.20	120.55	128.68
3	2	4355	E6G	O6-C6-N1	5.18	124.60	120.12
3	2	1909	P7G	C4-C5-N7	5.16	109.39	106.67
3	2	4690	B8K	C4-C5-N7	5.16	109.50	104.91
3	2	4550	7MG	C5-C6-N1	5.16	120.09	110.99
3	2	3897	B8K	C5-C6-N1	5.13	120.03	110.99
3	2	1677	PSU	C4-N3-C2	-5.11	118.97	126.34
3	2	4185	B8W	C2-N3-C4	5.11	121.19	115.36
3	2	4529	B8W	C4-C5-N7	-5.11	104.08	109.40
3	2	1797	E7G	C5-C6-N1	5.10	119.97	110.99
3	2	2754	B9B	O6-C6-N1	-5.09	115.73	120.12
3	2	4472	B8W	N3-C2-N1	-5.09	120.43	127.22
3	2	4531	PSU	N1-C2-N3	5.04	120.84	115.13
3	2	4500	PSU	N1-C2-N3	5.03	120.83	115.13
3	2	4628	PSU	N1-C2-N3	4.98	120.78	115.13
3	2	4500	PSU	C4-N3-C2	-4.96	119.20	126.34
3	2	4450	PSU	C4-N3-C2	-4.93	119.24	126.34
3	2	1605	7MG	C5-C6-N1	4.93	119.67	110.99
3	2	4371	MHG	C5-C6-N1	4.91	119.65	110.99
3	2	4371	MHG	C4-C5-N7	4.90	109.27	104.91
3	2	1582	PSU	N1-C2-N3	4.88	120.66	115.13
3	2	3899	BGH	C72-C71-N7	4.88	126.19	118.86
3	2	4129	B8W	O6-C6-C5	4.84	122.92	116.01
3	2	4636	PSU	N1-C2-N3	4.83	120.61	115.13
3	2	237	B9B	C2-N3-C4	4.83	120.87	115.36
3	2	3897	B8K	C4-C5-N7	4.82	109.20	104.91
3	2	1683	PSU	C4-N3-C2	-4.77	119.47	126.34
3	2	1866	UR3	C1'-N1-C2	4.67	124.88	116.99
3	2	4550	7MG	C2-N3-C4	4.66	120.60	112.30
3	2	4628	PSU	C4-N3-C2	-4.62	119.69	126.34
3	2	1683	PSU	N1-C2-N3	4.59	120.33	115.13
3	2	4293	PSU	N1-C2-N3	4.59	120.33	115.13
3	2	2754	B9B	C2-N3-C4	4.58	120.58	115.36
3	2	4442	PSU	N1-C2-N3	4.58	120.31	115.13
3	2	2422	OMC	O2-C2-N3	-4.53	114.97	122.33
3	2	4530	UR3	C4-N3-C2	-4.50	120.32	124.56
3	2	1909	P7G	N9-C8-N7	4.49	109.79	103.38
3	2	4597	UR3	C4-N3-C2	-4.48	120.34	124.56
3	2	4690	B8K	C2-N3-C4	4.46	120.25	112.30
3	2	4531	PSU	C4-N3-C2	-4.46	119.91	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	4355	E6G	C2-N3-C4	4.46	120.45	115.36
3	2	2380	B8W	C3'-C2'-C1'	4.45	107.69	100.98
3	2	3729	PSU	N1-C2-N3	4.45	120.17	115.13
3	2	4529	B8W	O6-C6-C5	4.44	122.36	116.01
3	2	2522	7MG	C2-N3-C4	4.44	120.21	112.30
3	2	2297	E7G	C2-N3-C4	4.43	120.20	112.30
3	2	3899	BGH	C2-N3-C4	4.41	120.15	112.30
3	2	4185	B8W	N2-C2-N3	4.41	124.97	117.79
3	2	1582	PSU	C4-N3-C2	-4.40	119.99	126.34
3	2	4620	OMU	N3-C2-N1	4.40	120.73	114.89
3	2	1797	E7G	C2-N3-C4	4.39	120.13	112.30
3	2	3897	B8K	C2-N3-C4	4.37	120.08	112.30
3	2	4472	B8W	C2-N3-C4	4.34	120.32	115.36
3	2	1517	2MG	C5-C6-N1	4.32	121.59	113.95
3	2	1456	B8Q	O2-C2-N3	-4.30	116.64	122.95
3	2	3899	BGH	N9-C8-N7	4.28	109.08	103.33
3	2	4293	PSU	C4-N3-C2	-4.27	120.19	126.34
3	2	1909	P7G	C71-N7-C5	4.26	134.62	124.52
3	2	4194	I4U	C5-C4-N3	-4.24	118.45	124.91
3	2	2380	B8W	N3-C2-N1	-4.17	121.66	127.22
3	2	1574	B9B	C2-N3-C4	4.12	120.07	115.36
3	2	4306	OMU	N3-C2-N1	4.11	120.34	114.89
3	2	4335	5MC	C5-C6-N1	-4.10	119.12	123.34
3	2	2380	B8W	O6-C6-N1	4.09	124.71	119.03
3	2	1605	7MG	C2-N3-C4	4.09	119.58	112.30
3	2	3729	PSU	C4-N3-C2	-4.08	120.46	126.34
3	2	4637	OMG	C5-C6-N1	4.07	121.13	113.95
3	2	4083	5MU	C5M-C5-C4	4.03	123.21	118.77
3	2	4442	PSU	C4-N3-C2	-4.03	120.54	126.34
3	2	1797	E7G	C5-C4-N3	-4.03	120.46	128.13
3	2	1866	UR3	C6-N1-C2	-4.03	118.18	121.79
3	2	2508	PSU	C4-N3-C2	-4.02	120.55	126.34
3	2	4129	B8W	C2-N3-C4	3.99	119.92	115.36
3	2	3909	OMC	O2-C2-N3	-3.99	115.83	122.33
3	2	2508	PSU	N1-C2-N3	3.93	119.59	115.13
3	2	4472	B8W	N2-C2-N3	3.93	124.19	117.79
3	2	4472	B8W	O6-C6-N1	3.90	124.44	119.03
3	2	4083	5MU	C5M-C5-C6	-3.90	117.64	122.85
3	2	4403	PSU	N1-C2-N3	3.88	119.53	115.13
3	2	1522	OMG	C5-C6-N1	3.87	120.79	113.95
3	2	3715	PSU	N1-C2-N3	3.83	119.46	115.13
3	2	2380	B8W	N2-C2-N3	3.82	124.02	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	1866	UR3	C4-N3-C2	-3.79	121.00	124.56
3	2	1316	OMG	C5-C6-N1	3.78	120.63	113.95
3	2	2050	OMG	C5-C6-N1	3.78	120.63	113.95
3	2	2364	OMG	C5-C6-N1	3.76	120.60	113.95
3	2	4129	B8W	C2-N1-C6	3.75	122.11	116.08
3	2	3897	B8K	N9-C8-N7	3.75	108.36	103.33
3	2	1605	7MG	C5-C4-N3	-3.73	121.02	128.13
3	2	1860	B8H	C5-C4-N3	3.68	124.91	116.58
3	2	4494	OMG	C5-C6-N1	3.68	120.45	113.95
3	2	2424	OMG	C5-C6-N1	3.68	120.44	113.95
3	2	2522	7MG	C5-C4-N9	3.66	111.10	106.35
3	2	1348	P4U	C5-C4-N3	-3.66	119.34	124.91
3	2	1659	I4U	C5-C4-N3	-3.66	119.35	124.91
3	2	1322	1MA	C5-C6-N1	3.65	119.34	113.90
3	2	4296	B8H	C5-C4-N3	3.65	124.84	116.58
3	2	2522	7MG	C5-C4-N3	-3.64	121.19	128.13
3	2	4185	B8W	O6-C6-N1	3.63	124.07	119.03
3	2	2773	OMG	C5-C6-N1	3.63	120.36	113.95
3	2	4690	B8K	C5-C4-N9	3.63	111.05	106.35
3	2	4371	MHG	C2-N1-C6	-3.62	120.32	124.48
3	2	1625	OMG	C5-C6-N1	3.62	120.34	113.95
3	2	1605	7MG	N9-C8-N7	3.61	108.55	103.38
3	2	2786	B9H	O3'-C3'-C2'	3.60	121.38	111.17
3	2	4371	MHG	C5-C4-N9	3.59	111.01	106.35
3	2	2786	B9H	C32-C31-N3	3.57	119.93	112.47
3	2	2786	B9H	O2-C2-N1	-3.57	114.37	122.72
3	2	978	2MG	C5-C6-N1	3.57	120.25	113.95
3	2	4623	OMG	C5-C6-N1	3.57	120.25	113.95
3	2	3715	PSU	C4-N3-C2	-3.56	121.20	126.34
3	2	4403	PSU	C4-N3-C2	-3.56	121.21	126.34
3	2	978	2MG	CM2-N2-C2	-3.56	116.00	123.86
3	2	4220	6MZ	C2-N1-C6	3.55	119.63	116.59
3	2	4872	2MG	C5-C6-N1	3.52	120.17	113.95
3	2	2297	E7G	C5-C4-N3	-3.52	121.42	128.13
3	2	3909	OMC	C1'-N1-C2	3.51	126.25	118.42
3	2	4447	5MC	CM5-C5-C6	-3.50	118.17	122.85
3	2	4550	7MG	C5-C4-N3	-3.50	121.46	128.13
3	2	1517	2MG	O6-C6-C5	-3.49	117.55	124.37
3	2	729	2MG	C5-C6-N1	3.48	120.09	113.95
3	2	2380	B8W	C2-N3-C4	3.47	119.32	115.36
3	2	3897	B8K	C5-C4-N9	3.46	110.83	106.35
3	2	4690	B8K	N9-C8-N7	3.43	107.93	103.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	1883	OMG	C5-C6-N1	3.42	119.99	113.95
3	2	1860	B8H	O2-C2-N1	-3.41	119.03	122.87
3	2	4355	E6G	N2-C2-N1	-3.41	111.95	117.25
3	2	373	OMG	C5-C6-N1	3.39	119.95	113.95
3	2	4296	B8H	O2-C2-N1	-3.36	119.08	122.87
3	2	4370	OMG	C5-C6-N1	3.36	119.88	113.95
3	2	4637	OMG	C2-N1-C6	-3.34	118.94	125.10
3	2	1316	OMG	C2-N1-C6	-3.33	118.96	125.10
3	2	4196	OMG	C5-C6-N1	3.33	119.83	113.95
3	2	4306	OMU	C5-C4-N3	3.32	119.81	114.84
3	2	237	B9B	C3'-C2'-C1'	3.32	105.98	100.98
3	2	2364	OMG	C2-N1-C6	-3.28	119.05	125.10
3	2	4690	B8K	C6-C5-C4	-3.28	115.85	122.62
3	2	2424	OMG	C2-N1-C6	-3.28	119.05	125.10
3	2	3899	BGH	C6-C5-C4	-3.27	115.88	122.62
3	2	4620	OMU	C5-C4-N3	3.26	119.72	114.84
3	2	2754	B9B	C3'-C2'-C1'	3.26	105.88	100.98
3	2	4371	MHG	C72-C71-N7	3.26	115.61	112.41
3	2	4529	B8W	C2-N1-C6	3.25	121.30	116.08
3	2	4450	PSU	C6-C5-C4	3.22	120.45	118.20
3	2	1625	OMG	C2-N1-C6	-3.21	119.19	125.10
3	2	2050	OMG	C2-N1-C6	-3.21	119.19	125.10
3	2	4371	MHG	C5-C4-N3	-3.17	122.09	128.13
3	2	1605	7MG	C4-C5-N7	3.17	109.93	105.53
3	2	3792	OMG	C5-C6-N1	3.17	119.54	113.95
3	2	3729	PSU	C6-N1-C2	-3.13	119.48	122.68
3	2	4531	PSU	C6-N1-C2	-3.13	119.48	122.68
3	2	1605	7MG	C5-C4-N9	3.13	110.41	106.35
3	2	4620	OMU	O4-C4-C5	-3.11	119.69	125.16
3	2	4196	OMG	C2-N1-C6	-3.11	119.37	125.10
3	2	1574	B9B	C1'-N9-C4	-3.09	121.21	126.64
3	2	4620	OMU	O3'-C3'-C4'	3.09	119.99	111.05
3	2	4564	M7A	C2-N3-C4	3.08	119.04	111.75
3	2	3899	BGH	C5-C4-N9	3.07	110.33	106.35
3	2	4494	OMG	C2-N1-C6	-3.07	119.44	125.10
3	2	4550	7MG	C4-C5-N7	3.07	109.79	105.53
3	2	2773	OMG	C2-N1-C6	-3.07	119.45	125.10
3	2	4083	5MU	O2-C2-N1	-3.06	118.71	122.79
3	2	1883	OMG	C2-N1-C6	-3.06	119.47	125.10
3	2	4623	OMG	C2-N1-C6	-3.06	119.47	125.10
3	2	4550	7MG	C5-C4-N9	3.05	110.31	106.35
3	2	4500	PSU	C6-C5-C4	3.04	120.32	118.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	3729	PSU	O2-C2-N1	-3.04	119.45	122.79
3	2	4370	OMG	C2-N1-C6	-3.01	119.55	125.10
3	2	4628	PSU	O2-C2-N1	-3.01	119.48	122.79
3	2	4531	PSU	O2-C2-N1	-2.99	119.50	122.79
3	2	2773	OMG	O6-C6-C5	-2.97	118.58	124.37
3	2	1316	OMG	C8-N7-C5	2.97	108.64	102.99
3	2	1797	E7G	C5-C4-N9	2.96	110.19	106.35
3	2	2424	OMG	O6-C6-C5	-2.96	118.59	124.37
3	2	4671	B8T	C6-C5-C4	2.95	120.57	116.96
3	2	2297	E7G	C5-C4-N9	2.95	110.18	106.35
3	2	4293	PSU	O2-C2-N1	-2.94	119.55	122.79
3	2	4355	E6G	O4'-C4'-C3'	-2.92	99.34	105.11
3	2	4623	OMG	C8-N7-C5	2.91	108.53	102.99
3	2	2522	7MG	C2-N1-C6	-2.90	119.80	125.10
3	2	1683	PSU	O2-C2-N1	-2.89	119.61	122.79
3	2	1677	PSU	O2-C2-N1	-2.89	119.61	122.79
3	2	4194	I4U	C3'-C2'-C1'	2.88	106.91	101.43
3	2	4129	B8W	C4-C5-N7	-2.88	106.40	109.40
3	2	373	OMG	C2-N1-C6	-2.87	119.82	125.10
3	2	4870	OMG	N1-C2-N3	-2.86	117.97	123.32
3	2	4530	UR3	C1'-N1-C2	2.85	121.81	116.99
3	2	1860	B8H	O4-C4-N3	-2.85	114.65	120.12
3	2	2297	E7G	C2-N1-C6	-2.85	119.91	125.10
3	2	4690	B8K	C5-C4-N3	-2.84	122.72	128.13
3	2	3897	B8K	C6-C5-C4	-2.84	116.77	122.62
3	2	4870	OMG	C5-C6-N1	2.82	118.94	113.95
3	2	2364	OMG	C8-N7-C5	2.82	108.36	102.99
3	2	1522	OMG	C2-N1-C6	-2.80	119.94	125.10
3	2	2297	E7G	O6-C6-C5	-2.77	120.73	127.54
3	2	1582	PSU	C6-N1-C2	-2.77	119.85	122.68
3	2	4293	PSU	C6-N1-C2	-2.77	119.85	122.68
3	2	4628	PSU	C6-N1-C2	-2.77	119.85	122.68
3	2	373	OMG	C8-N7-C5	2.76	108.25	102.99
3	2	4637	OMG	O6-C6-C5	-2.74	119.02	124.37
3	2	1677	PSU	C6-N1-C2	-2.74	119.88	122.68
3	2	2786	B9H	O3'-C3'-C4'	2.74	118.96	111.05
3	2	1316	OMG	O6-C6-C5	-2.74	119.03	124.37
3	2	4355	E6G	C2-N1-C6	2.73	120.46	116.08
3	2	3897	B8K	C5-C4-N3	-2.71	122.96	128.13
3	2	1797	E7G	N9-C8-N7	2.69	107.23	103.38
3	2	2050	OMG	C8-N7-C5	2.68	108.10	102.99
3	2	3899	BGH	N1-C2-N3	-2.68	118.32	123.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	1456	B8Q	C31-N3-C2	2.68	121.68	117.79
3	2	1456	B8Q	C1'-N1-C2	2.67	121.50	116.99
3	2	1677	PSU	C6-C5-C4	2.67	120.06	118.20
3	2	1456	B8Q	C6-N1-C2	-2.67	119.40	121.79
3	2	4306	OMU	O2-C2-N1	-2.66	119.26	122.79
3	2	3792	OMG	C2-N1-C6	-2.65	120.21	125.10
3	2	2773	OMG	C8-N7-C5	2.65	108.04	102.99
3	2	1522	OMG	C8-N7-C5	2.65	108.03	102.99
3	2	1883	OMG	O6-C6-C5	-2.64	119.21	124.37
3	2	4083	5MU	C6-N1-C2	-2.64	118.62	121.30
3	2	4129	B8W	C5-C6-N1	-2.64	118.23	123.26
3	2	4530	UR3	O2-C2-N3	-2.63	117.63	121.34
3	2	4196	OMG	O6-C6-C5	-2.63	119.23	124.37
3	2	3899	BGH	O6-C6-C5	-2.62	121.11	127.54
3	2	4370	OMG	C8-N7-C5	2.62	107.98	102.99
3	2	1797	E7G	C2-N1-C6	-2.61	120.33	125.10
3	2	4872	2MG	C8-N7-C5	2.61	107.97	102.99
3	2	1605	7MG	C2-N1-C6	-2.61	120.33	125.10
3	2	4129	B8W	N2-C2-N1	-2.60	113.21	117.25
3	2	1866	UR3	O2-C2-N3	-2.60	117.68	121.34
3	2	1797	E7G	N9-C4-N3	2.60	129.35	125.47
3	2	2522	7MG	C4-C5-N7	2.59	109.13	105.53
3	2	4450	PSU	C6-N1-C2	-2.58	120.05	122.68
3	2	2422	OMC	O2-C2-N1	2.58	124.21	118.89
3	2	3899	BGH	N2-C2-N1	2.57	122.19	116.71
3	2	4442	PSU	C6-N1-C2	-2.57	120.05	122.68
3	2	4403	PSU	C6-N1-C2	-2.57	120.06	122.68
3	2	4494	OMG	C8-N7-C5	2.57	107.88	102.99
3	2	3897	B8K	N1-C2-N3	-2.56	118.54	123.32
3	2	4296	B8H	O4-C4-N3	-2.54	115.24	120.12
3	2	978	2MG	C8-N7-C5	2.54	107.83	102.99
3	2	4690	B8K	C2-N1-C6	-2.53	120.49	125.10
3	2	3792	OMG	C8-N7-C5	2.53	107.80	102.99
3	2	1797	E7G	O6-C6-C5	-2.53	121.35	127.54
3	2	1524	A2M	O4'-C4'-C3'	-2.52	100.12	105.11
3	2	4450	PSU	O2-C2-N1	-2.52	120.02	122.79
3	2	3887	OMC	O2-C2-N3	-2.52	118.23	122.33
3	2	4083	5MU	O4-C4-N3	-2.52	115.29	120.12
3	2	4637	OMG	C8-N7-C5	2.51	107.77	102.99
3	2	4550	7MG	O6-C6-C5	-2.49	121.44	127.54
3	2	3897	B8K	O6-C6-C5	-2.49	121.44	127.54
3	2	2422	OMC	C1'-N1-C2	2.48	123.95	118.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	4306	OMU	O4-C4-C5	-2.47	120.81	125.16
3	2	1574	B9B	C3'-C2'-C1'	2.47	104.69	100.98
3	2	2786	B9H	C1'-N1-C6	2.46	126.20	120.84
3	2	4529	B8W	C3'-C2'-C1'	2.45	104.67	100.98
3	2	4529	B8W	N2-C2-N1	2.45	121.07	117.25
3	2	3897	B8K	N2-C2-N1	2.45	121.93	116.71
3	2	4620	OMU	O2-C2-N1	-2.45	119.53	122.79
3	2	3899	BGH	C5-C4-N3	-2.44	123.49	128.13
3	2	4196	OMG	C8-N7-C5	2.42	107.60	102.99
3	2	4870	OMG	C8-N7-C5	2.41	107.59	102.99
3	2	4185	B8W	C1'-N9-C4	-2.41	122.40	126.64
3	2	4371	MHG	O6-C6-C5	-2.41	121.63	127.54
3	2	2424	OMG	C8-N7-C5	2.41	107.58	102.99
3	2	1625	OMG	O6-C6-C5	-2.41	119.67	124.37
3	2	1625	OMG	C8-N7-C5	2.40	107.57	102.99
3	2	4550	7MG	N1-C2-N3	-2.40	118.84	123.32
3	2	2380	B8W	C1'-N9-C4	-2.40	122.42	126.64
3	2	1517	2MG	CM2-N2-C2	-2.40	118.57	123.86
3	2	4472	B8W	C2-N1-C6	2.40	119.93	116.08
3	2	2522	7MG	O6-C6-C5	-2.39	121.67	127.54
3	2	4194	I4U	C5'-C4'-C3'	-2.39	106.22	115.18
3	2	1883	OMG	C8-N7-C5	2.39	107.54	102.99
3	2	4403	PSU	O2-C2-N1	-2.39	120.16	122.79
3	2	3880	P7G	N2-C2-N3	2.38	121.78	116.71
3	2	3715	PSU	C6-N1-C2	-2.38	120.25	122.68
3	2	3880	P7G	N9-C8-N7	2.38	106.78	103.38
3	2	4636	PSU	C6-C5-C4	2.37	119.86	118.20
3	2	729	2MG	C8-N7-C5	2.37	107.50	102.99
3	2	4371	MHG	N1-C2-N3	-2.36	120.30	123.95
3	2	4530	UR3	C6-N1-C2	-2.36	119.67	121.79
3	2	3897	B8K	O4'-C1'-C2'	-2.36	101.50	106.64
3	2	4597	UR3	C6-N1-C2	-2.35	119.69	121.79
3	2	3909	OMC	O2-C2-N1	2.33	123.71	118.89
3	2	1605	7MG	O6-C6-C5	-2.33	121.82	127.54
3	2	4529	B8W	N2-C2-N3	2.33	121.59	117.79
3	2	3880	P7G	C71-N7-C5	2.32	130.01	124.52
3	2	1522	OMG	N1-C2-N3	-2.31	119.00	123.32
3	2	4530	UR3	C3U-N3-C4	2.31	121.18	117.89
3	2	4550	7MG	C6-C5-C4	-2.30	117.88	122.62
3	2	1316	OMG	N2-C2-N1	2.30	121.61	116.71
3	2	4690	B8K	N1-C2-N3	-2.28	119.06	123.32
3	2	4500	PSU	O2-C2-N1	-2.28	120.28	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	3782	5MC	C5-C4-N3	-2.27	119.22	121.67
3	2	4870	OMG	C2-N1-C6	-2.26	120.93	125.10
3	2	4500	PSU	C6-N1-C2	-2.26	120.38	122.68
3	2	1348	P4U	O2-C2-N3	-2.25	118.67	122.33
3	2	4194	I4U	C2'-C3'-C4'	2.25	107.01	102.64
3	2	3899	BGH	O4'-C4'-C3'	-2.25	100.67	105.11
3	2	4194	I4U	O4-C41-C43	2.23	113.08	107.14
3	2	3782	5MC	O2-C2-N3	-2.23	118.71	122.33
3	2	1322	1MA	C8-N7-C5	2.23	107.23	102.99
3	2	3782	5MC	C5-C6-N1	-2.21	121.06	123.34
3	2	4872	2MG	CM2-N2-C2	-2.20	119.00	123.86
3	2	1582	PSU	O2-C2-N1	-2.20	120.37	122.79
3	2	4494	OMG	O6-C6-C5	-2.20	120.08	124.37
3	2	1517	2MG	C3'-C2'-C1'	2.19	104.27	100.98
3	2	1517	2MG	C8-N7-C5	2.19	107.16	102.99
3	2	4185	B8W	C2-N1-C6	2.19	119.59	116.08
3	2	3909	OMC	C1'-N1-C6	-2.18	116.08	120.84
3	2	4550	7MG	C2-N1-C6	-2.18	121.13	125.10
3	2	1534	A2M	O3'-C3'-C4'	-2.18	104.76	111.05
3	2	4371	MHG	C6-C5-C4	-2.18	118.14	122.62
3	2	237	B9B	C1'-N9-C4	-2.17	122.82	126.64
3	2	978	2MG	O6-C6-C5	-2.17	120.13	124.37
3	2	237	B9B	C2-N1-C6	2.16	119.55	116.08
3	2	4355	E6G	C2'-C3'-C4'	-2.15	98.46	102.64
3	2	4523	A2M	O4'-C4'-C3'	-2.15	100.85	105.11
3	2	4690	B8K	O6-C6-C5	-2.15	122.27	127.54
3	2	4403	PSU	O4-C4-N3	-2.15	116.00	120.12
3	2	4335	5MC	O2-C2-N3	-2.14	118.85	122.33
3	2	1659	I4U	O2-C2-N3	-2.14	118.86	122.33
3	2	4194	I4U	O4'-C4'-C3'	2.14	109.34	105.11
3	2	373	OMG	O6-C6-C5	-2.13	120.22	124.37
3	2	2297	E7G	C6-C5-C4	-2.13	118.24	122.62
3	2	4355	E6G	C5-C6-N1	-2.13	119.21	123.26
3	2	3792	OMG	O6-C6-C5	-2.13	120.22	124.37
3	2	4129	B8W	C3'-C2'-C1'	2.12	104.17	100.98
3	2	4529	B8W	C5-C6-N1	-2.11	119.24	123.26
3	2	2297	E7G	N9-C8-N7	2.11	106.40	103.38
3	2	4564	M7A	C2-N1-C6	2.11	122.39	118.77
3	2	4620	OMU	O3'-C3'-C2'	2.11	117.16	111.17
3	2	4690	B8K	O6-C6-N1	-2.09	116.11	120.12
3	2	4620	OMU	C6-N1-C2	-2.09	118.32	120.99
3	2	1883	OMG	N2-C2-N1	2.08	121.14	116.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	4564	M7A	C5-C4-N3	-2.08	121.74	126.62
3	2	4442	PSU	O2-C2-N1	-2.08	120.50	122.79
3	2	1605	7MG	N9-C4-N3	2.08	128.57	125.47
3	2	4370	OMG	O6-C6-C5	-2.07	120.32	124.37
3	2	4550	7MG	N9-C8-N7	2.07	106.34	103.38
3	2	2754	B9B	N2-C2-N3	2.05	121.13	117.79
3	2	4870	OMG	N2-C2-N1	2.05	121.08	116.71
3	2	4185	B8W	C3'-C2'-C1'	2.04	104.06	100.98
3	2	4571	A2M	C5'-C4'-C3'	-2.04	107.53	115.18
3	2	3701	OMC	C5-C6-N1	-2.04	118.39	121.81
3	2	1659	I4U	O4'-C4'-C3'	-2.04	101.08	105.11
3	2	4870	OMG	O6-C6-C5	-2.03	120.40	124.37
3	2	4483	B8T	C6-C5-C4	2.03	119.45	116.96
3	2	2773	OMG	N2-C2-N1	2.03	121.04	116.71
3	2	2508	PSU	O2-C2-N1	-2.02	120.56	122.79
3	2	3723	A2M	O4'-C4'-C3'	-2.02	101.12	105.11
3	2	4523	A2M	C1'-N9-C4	-2.02	123.09	126.64
3	2	3880	P7G	N3-C2-N1	-2.02	119.56	123.32
3	2	4636	PSU	O4'-C1'-C2'	2.02	107.99	105.14
3	2	729	2MG	CM2-N2-C2	-2.01	119.43	123.86

There are no chirality outliers.

All (158) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	2	237	B9B	C5-C6-O6-C61
3	2	237	B9B	N1-C6-O6-C61
3	2	237	B9B	O4'-C4'-C5'-O5'
3	2	1348	P4U	N3-C4-O4-C41
3	2	1574	B9B	C5-C6-O6-C61
3	2	1574	B9B	N1-C6-O6-C61
3	2	1625	OMG	C3'-C4'-C5'-O5'
3	2	1677	PSU	C3'-C4'-C5'-O5'
3	2	1797	E7G	O4'-C4'-C5'-O5'
3	2	1883	OMG	O4'-C4'-C5'-O5'
3	2	1883	OMG	C3'-C4'-C5'-O5'
3	2	1909	P7G	C72-C71-N7-C5
3	2	2297	E7G	C3'-C4'-C5'-O5'
3	2	2297	E7G	O4'-C4'-C5'-O5'
3	2	2364	OMG	O4'-C4'-C5'-O5'
3	2	2380	B8W	C5-C6-O6-C61
3	2	2424	OMG	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
3	2	2754	B9B	C5-C6-O6-C61
3	2	2754	B9B	N1-C6-O6-C61
3	2	2786	B9H	C32-C31-N3-C2
3	2	2786	B9H	C32-C31-N3-C4
3	2	3701	OMC	C2'-C1'-N1-C2
3	2	3701	OMC	C2'-C1'-N1-C6
3	2	3867	A2M	O4'-C4'-C5'-O5'
3	2	3867	A2M	C3'-C4'-C5'-O5'
3	2	3880	P7G	O4'-C4'-C5'-O5'
3	2	3897	B8K	O4'-C4'-C5'-O5'
3	2	4129	B8W	C5-C6-O6-C61
3	2	4129	B8W	N1-C6-O6-C61
3	2	4185	B8W	C5-C6-O6-C61
3	2	4185	B8W	N1-C6-O6-C61
3	2	4196	OMG	O4'-C4'-C5'-O5'
3	2	4196	OMG	C3'-C4'-C5'-O5'
3	2	4306	OMU	C1'-C2'-O2'-CM2
3	2	4355	E6G	C3'-C4'-C5'-O5'
3	2	4355	E6G	O4'-C4'-C5'-O5'
3	2	4355	E6G	C5-C6-O6-C61
3	2	4355	E6G	N1-C6-O6-C61
3	2	4371	MHG	O4'-C4'-C5'-O5'
3	2	4371	MHG	C71-C72-C73-C75
3	2	4403	PSU	C2'-C1'-C5-C4
3	2	4403	PSU	O4'-C1'-C5-C4
3	2	4403	PSU	O4'-C1'-C5-C6
3	2	4403	PSU	C3'-C4'-C5'-O5'
3	2	4403	PSU	O4'-C4'-C5'-O5'
3	2	4450	PSU	C2'-C1'-C5-C4
3	2	4472	B8W	C5-C6-O6-C61
3	2	4472	B8W	N1-C6-O6-C61
3	2	4472	B8W	C3'-C4'-C5'-O5'
3	2	4472	B8W	O4'-C4'-C5'-O5'
3	2	4500	PSU	C3'-C4'-C5'-O5'
3	2	4523	A2M	O4'-C4'-C5'-O5'
3	2	4529	B8W	C5-C6-O6-C61
3	2	4529	B8W	N1-C6-O6-C61
3	2	4620	OMU	C1'-C2'-O2'-CM2
3	2	4636	PSU	C2'-C1'-C5-C6
3	2	4636	PSU	O4'-C1'-C5-C6
3	2	4636	PSU	C3'-C4'-C5'-O5'
3	2	4636	PSU	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
3	2	4637	OMG	O4'-C4'-C5'-O5'
3	2	4870	OMG	C3'-C4'-C5'-O5'
3	2	237	B9B	C3'-C4'-C5'-O5'
3	2	398	A2M	O4'-C4'-C5'-O5'
3	2	1677	PSU	O4'-C4'-C5'-O5'
3	2	1797	E7G	C3'-C4'-C5'-O5'
3	2	1866	UR3	O4'-C4'-C5'-O5'
3	2	2364	OMG	C3'-C4'-C5'-O5'
3	2	2424	OMG	O4'-C4'-C5'-O5'
3	2	2773	OMG	O4'-C4'-C5'-O5'
3	2	3729	PSU	O4'-C4'-C5'-O5'
3	2	3785	A2M	O4'-C4'-C5'-O5'
3	2	3785	A2M	C3'-C4'-C5'-O5'
3	2	3897	B8K	C3'-C4'-C5'-O5'
3	2	4450	PSU	O4'-C4'-C5'-O5'
3	2	4500	PSU	O4'-C4'-C5'-O5'
3	2	4523	A2M	C3'-C4'-C5'-O5'
3	2	4637	OMG	C3'-C4'-C5'-O5'
3	2	4870	OMG	O4'-C4'-C5'-O5'
3	2	4872	2MG	O4'-C4'-C5'-O5'
3	2	978	2MG	C3'-C4'-C5'-O5'
3	2	1860	B8H	O4'-C4'-C5'-O5'
3	2	1866	UR3	C3'-C4'-C5'-O5'
3	2	2773	OMG	C3'-C4'-C5'-O5'
3	2	3880	P7G	C3'-C4'-C5'-O5'
3	2	4450	PSU	C3'-C4'-C5'-O5'
3	2	4872	2MG	C3'-C4'-C5'-O5'
3	2	3880	P7G	N7-C71-C72-C73
3	2	1909	P7G	C72-C71-N7-C8
3	2	4355	E6G	C62-C61-O6-C6
3	2	3729	PSU	C3'-C4'-C5'-O5'
3	2	4371	MHG	C71-C72-C73-C74
3	2	237	B9B	O6-C61-C62-C63
3	2	729	2MG	O4'-C4'-C5'-O5'
3	2	4220	6MZ	C3'-C4'-C5'-O5'
3	2	398	A2M	C3'-C4'-C5'-O5'
3	2	978	2MG	O4'-C4'-C5'-O5'
3	2	1625	OMG	O4'-C4'-C5'-O5'
3	2	1659	I4U	O4'-C4'-C5'-O5'
3	2	1871	A2M	O4'-C4'-C5'-O5'
3	2	4220	6MZ	O4'-C4'-C5'-O5'
3	2	4296	B8H	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
3	2	1909	P7G	N7-C71-C72-C73
3	2	4371	MHG	C75-C73-C74-C76
3	2	729	2MG	C3'-C4'-C5'-O5'
3	2	4296	B8H	C3'-C4'-C5'-O5'
3	2	4371	MHG	C2'-C1'-N9-C8
3	2	1574	B9B	O6-C61-C62-C63
3	2	1860	B8H	C3'-C4'-C5'-O5'
3	2	4447	5MC	C2'-C1'-N1-C6
3	2	2754	B9B	O4'-C4'-C5'-O5'
3	2	2297	E7G	C72-C71-N7-C8
3	2	2401	A2M	C3'-C2'-O2'-CM'
3	2	3897	B8K	C4'-C5'-O5'-P
3	2	2754	B9B	C3'-C4'-C5'-O5'
3	2	2754	B9B	O6-C61-C62-C63
3	2	4447	5MC	O4'-C1'-N1-C6
3	2	4371	MHG	C72-C71-N7-C5
3	2	2380	B8W	N1-C6-O6-C61
3	2	373	OMG	C4'-C5'-O5'-P
3	2	2380	B8W	O4'-C4'-C5'-O5'
3	2	4530	UR3	O4'-C4'-C5'-O5'
3	2	4550	7MG	O4'-C4'-C5'-O5'
3	2	4447	5MC	C2'-C1'-N1-C2
3	2	1517	2MG	C4'-C5'-O5'-P
3	2	4500	PSU	C4'-C5'-O5'-P
3	2	4870	OMG	C4'-C5'-O5'-P
3	2	3701	OMC	O4'-C1'-N1-C6
3	2	1524	A2M	C3'-C2'-O2'-CM'
3	2	3825	A2M	C3'-C2'-O2'-CM'
3	2	3701	OMC	O4'-C1'-N1-C2
3	2	4447	5MC	O4'-C1'-N1-C2
3	2	1534	A2M	C4'-C5'-O5'-P
3	2	2422	OMC	O4'-C4'-C5'-O5'
3	2	3880	P7G	C72-C71-N7-C8
3	2	4371	MHG	C72-C71-N7-C8
3	2	1677	PSU	O4'-C1'-C5-C4
3	2	4450	PSU	O4'-C1'-C5-C4
3	2	4531	PSU	O4'-C1'-C5-C4
3	2	4370	OMG	C3'-C2'-O2'-CM2
3	2	4494	OMG	C3'-C2'-O2'-CM2
3	2	1326	A2M	C4'-C5'-O5'-P
3	2	3887	OMC	C4'-C5'-O5'-P
3	2	1534	A2M	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
3	2	4371	MHG	O4'-C1'-N9-C8
3	2	3909	OMC	C2'-C1'-N1-C6
3	2	1871	A2M	C3'-C4'-C5'-O5'
3	2	1524	A2M	C1'-C2'-O2'-CM'
3	2	2401	A2M	C1'-C2'-O2'-CM'
3	2	1322	1MA	O4'-C4'-C5'-O5'
3	2	1677	PSU	O4'-C1'-C5-C6
3	2	4450	PSU	O4'-C1'-C5-C6
3	2	3909	OMC	C2'-C1'-N1-C2
3	2	1659	I4U	C42-C41-O4-C4
3	2	1659	I4U	C43-C41-O4-C4
3	2	3785	A2M	C3'-C2'-O2'-CM'
3	2	2380	B8W	C3'-C4'-C5'-O5'
3	2	4550	7MG	C3'-C4'-C5'-O5'
3	2	2422	OMC	C2'-C1'-N1-C2

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 246 ligands modelled in this entry, 246 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

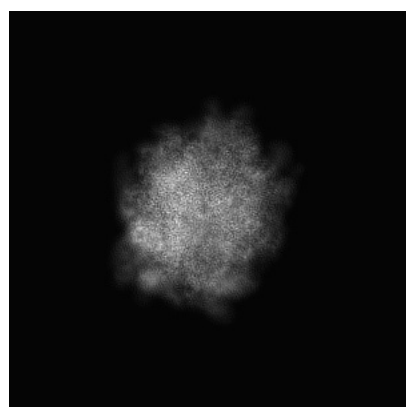
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0963. These allow visual inspection of the internal detail of the map and identification of artifacts.

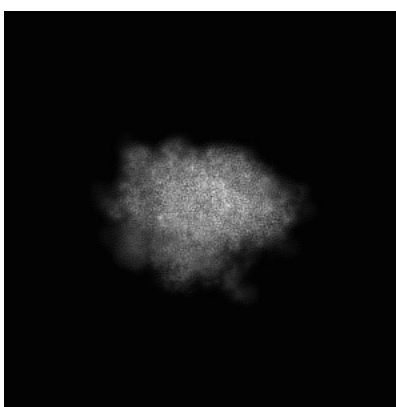
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

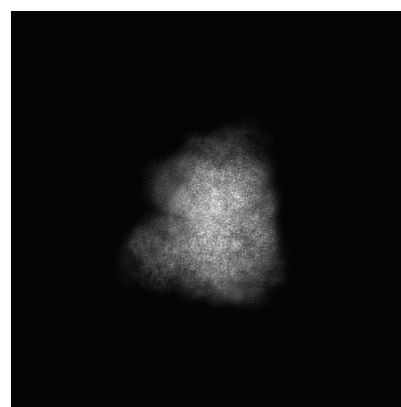
#### 6.1.1 Primary map



X



Y

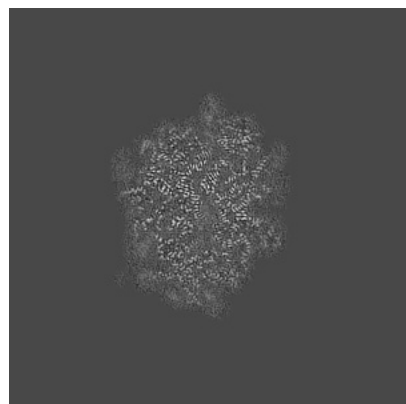


Z

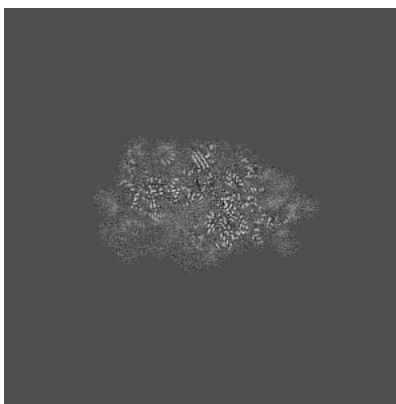
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

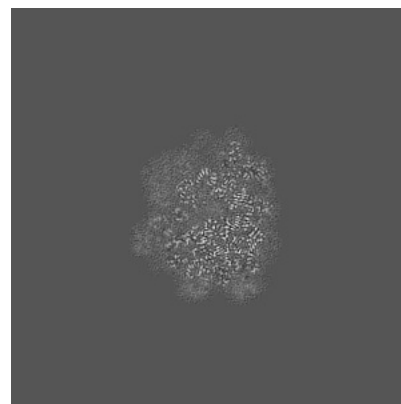
#### 6.2.1 Primary map



X Index: 240



Y Index: 240

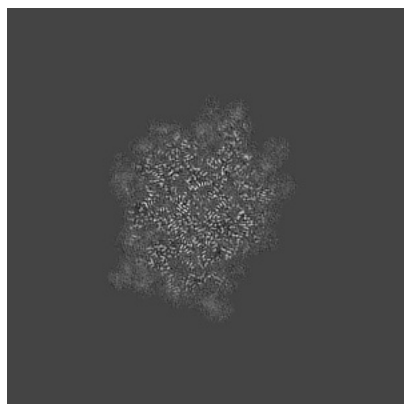


Z Index: 240

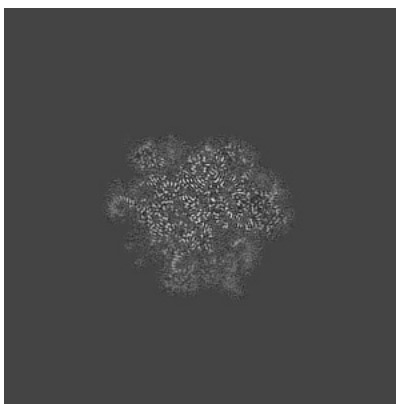
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

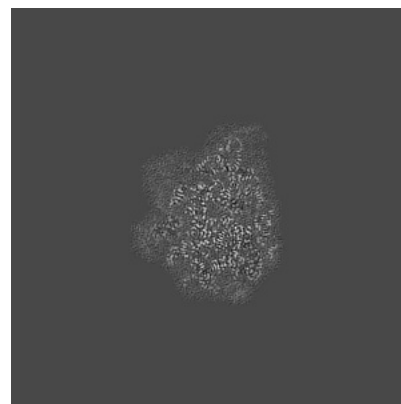
### 6.3.1 Primary map



X Index: 253



Y Index: 201

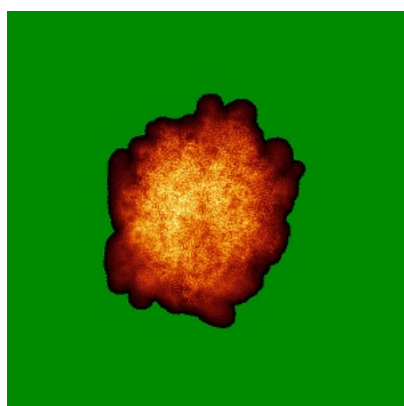


Z Index: 251

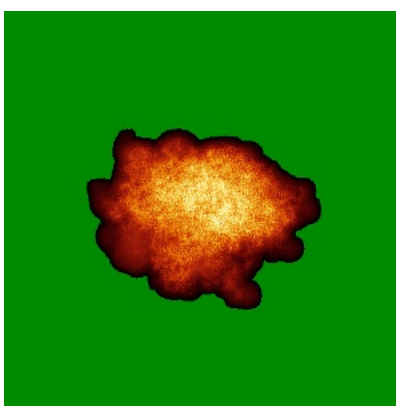
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

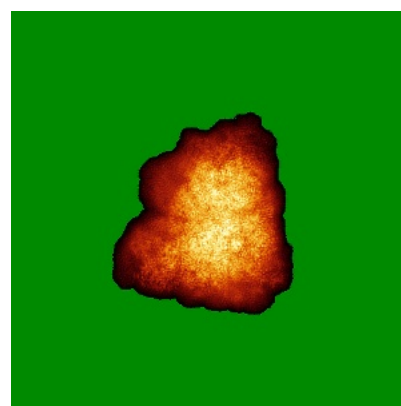
### 6.4.1 Primary map



X



Y

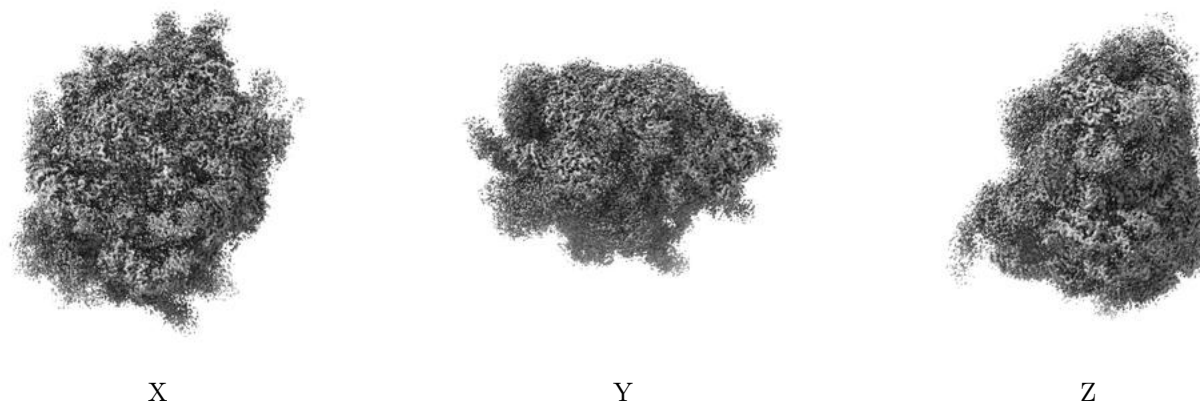


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

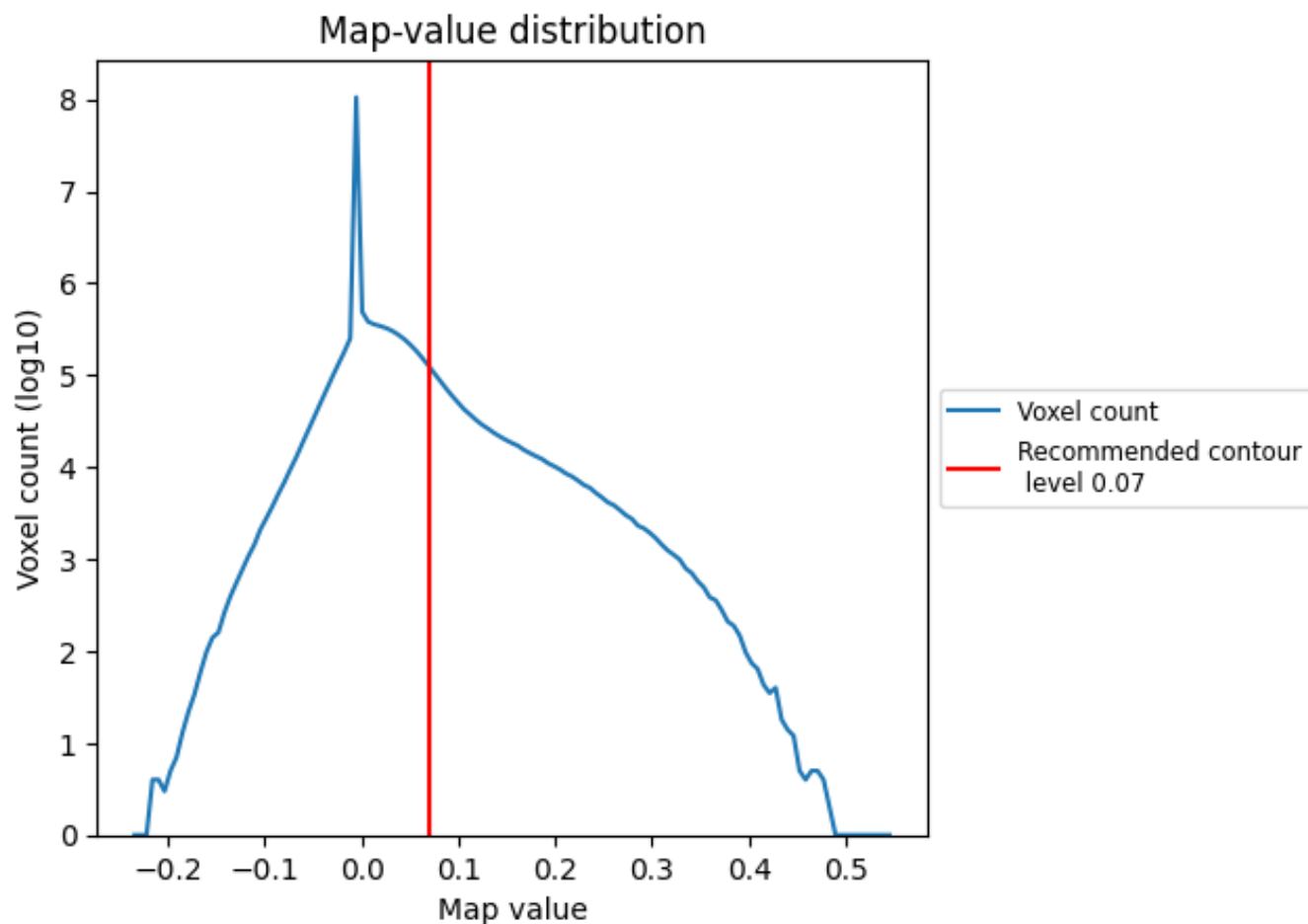
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

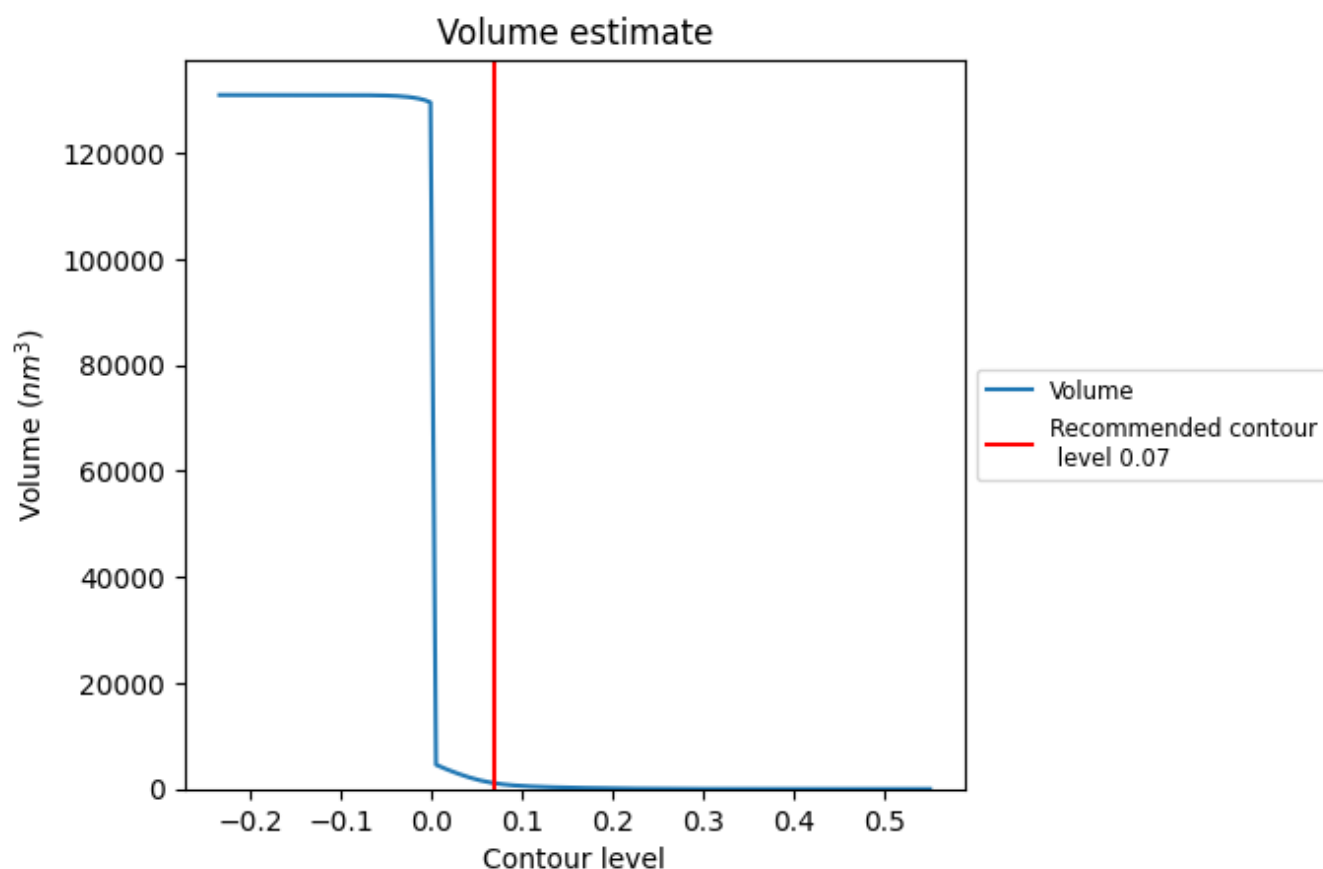
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

## 7.2 Volume estimate [i](#)

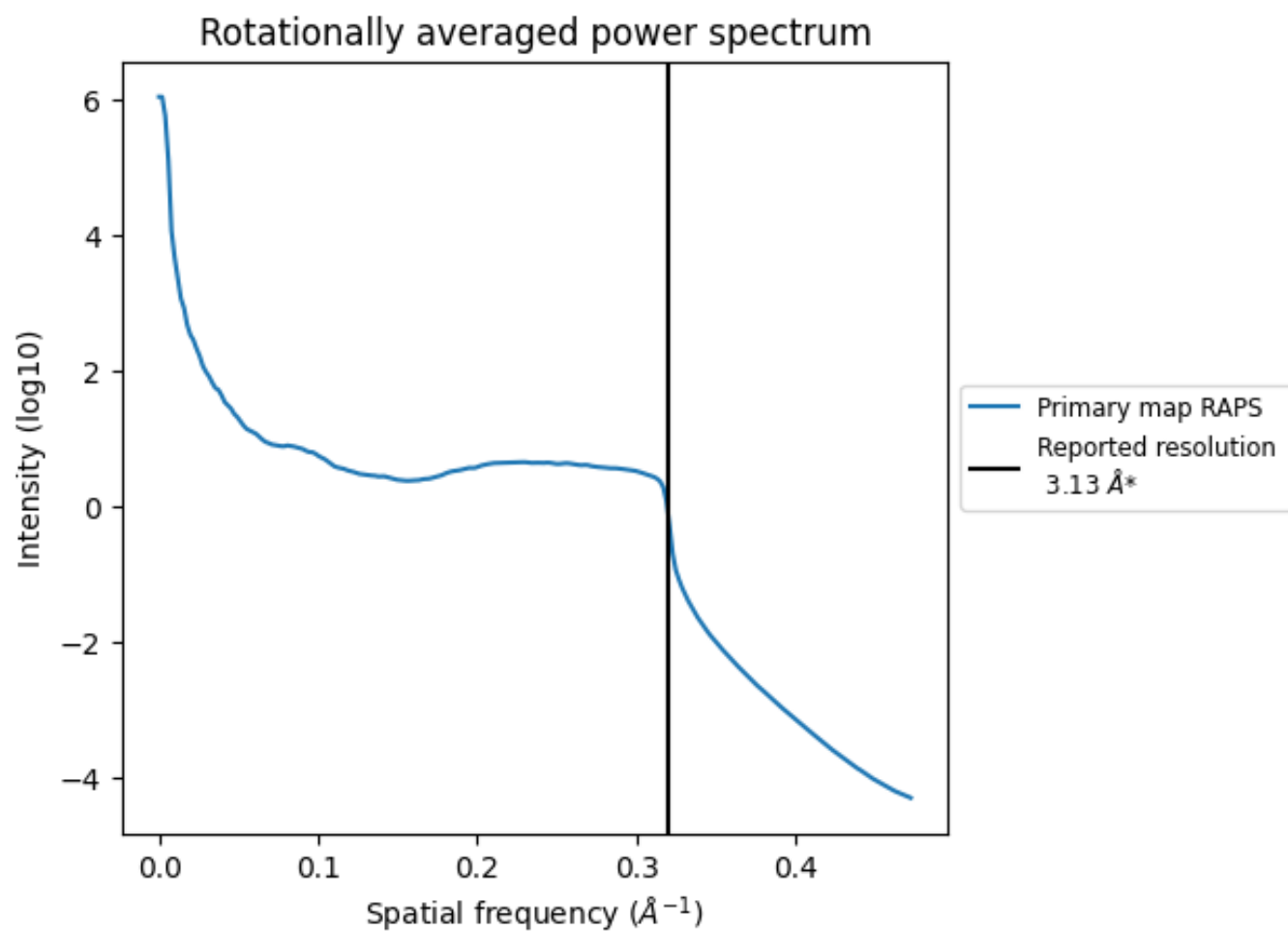


The volume at the recommended contour level is 1084  $\text{nm}^3$ ; this corresponds to an approximate mass of 979 kDa.

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 ⓘ



\*Reported resolution corresponds to spatial frequency of 0.319  $\text{\AA}^{-1}$

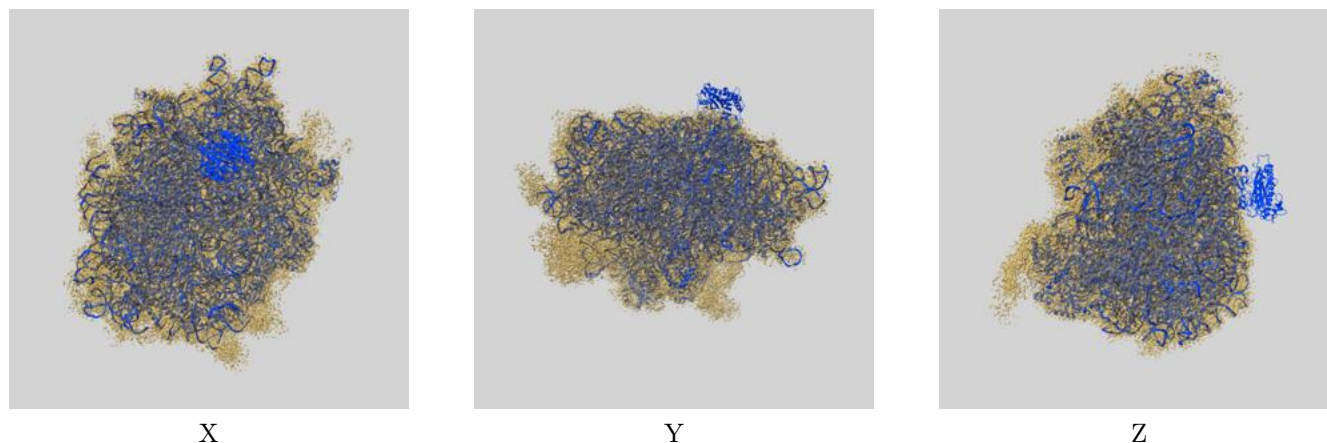
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [i](#)

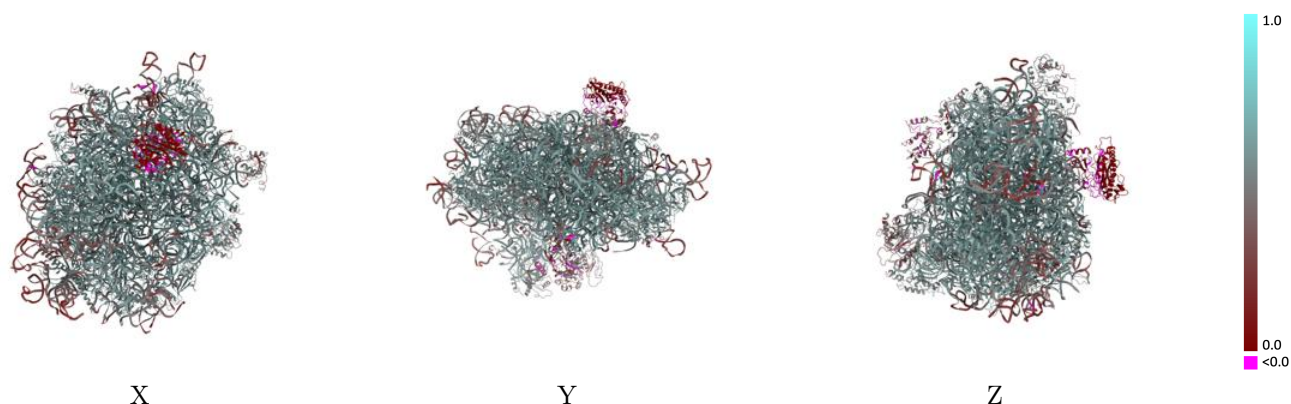
This section contains information regarding the fit between EMDB map EMD-0963 and PDB model 6LSR. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

### 9.1 Map-model overlay [i](#)



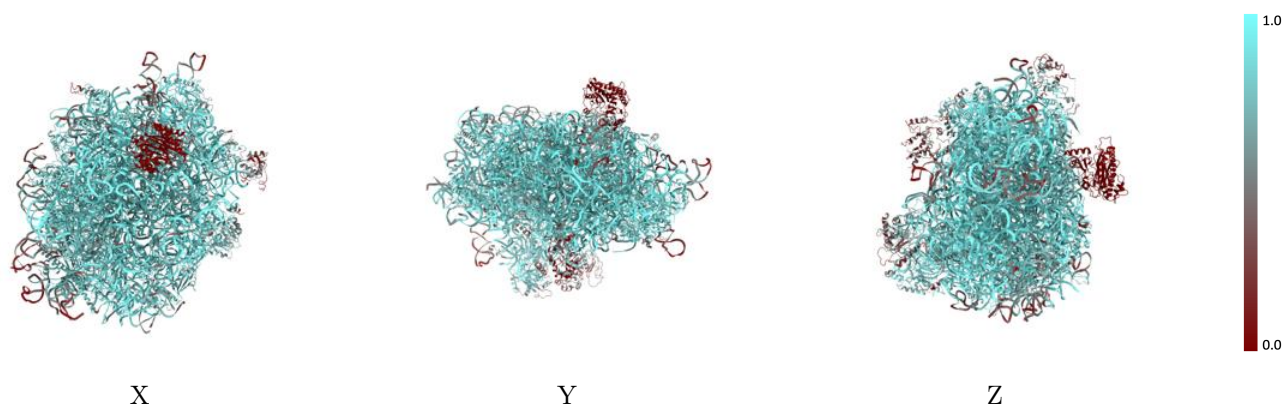
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



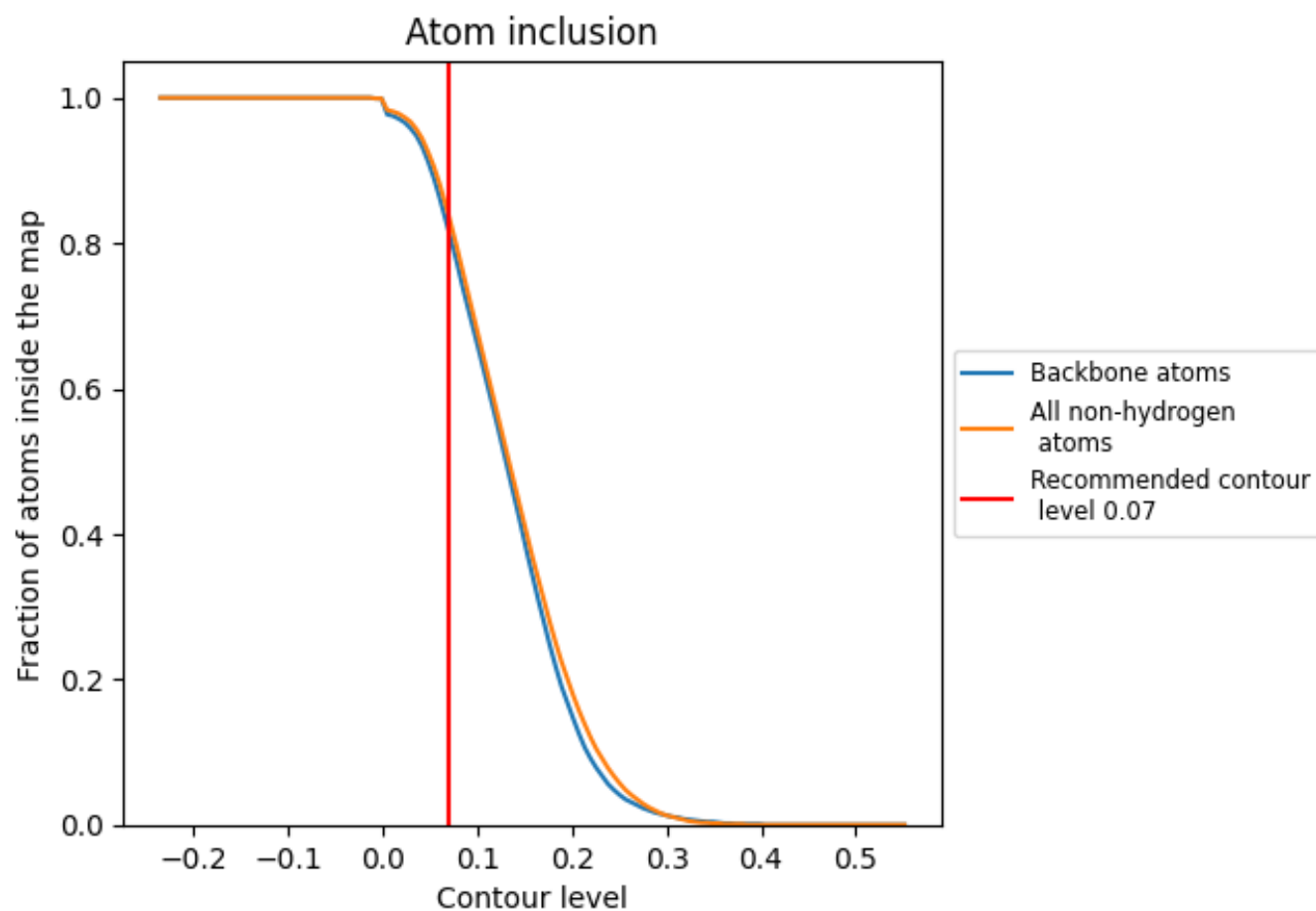
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.07).







































































## 9.4 Atom inclusion ⓘ



At the recommended contour level, 82% of all backbone atoms, 84% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8380	 0.5320
0	 0.5020	 0.4460
1	 0.3130	 0.2480
2	 0.8730	 0.5340
3	 0.8300	 0.5350
5	 0.9430	 0.5660
6	 0.6740	 0.4860
8	 0.9210	 0.5590
A	 0.3870	 0.3470
B	 0.8710	 0.5770
C	 0.8140	 0.5190
D	 0.9140	 0.5890
E	 0.8010	 0.5350
F	 0.8950	 0.5820
G	 0.8060	 0.5430
H	 0.8470	 0.5710
I	 0.8080	 0.5500
K	 0.8300	 0.5470
L	 0.9340	 0.6080
M	 0.9520	 0.6010
N	 0.6780	 0.4610
O	 0.7510	 0.5350
P	 0.9290	 0.5950
Q	 0.8430	 0.5670
S	 0.8770	 0.5680
T	 0.8440	 0.5730
U	 0.9590	 0.6120
V	 0.9130	 0.5880
W	 0.8450	 0.5550
X	 0.8470	 0.5610
Y	 0.9100	 0.5940
Z	 0.9320	 0.5970
a	 0.8980	 0.5770
b	 0.9210	 0.5870
c	 0.8710	 0.5710



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Chain	Atom inclusion	Q-score
d	 0.7220	 0.4980
e	 0.8810	 0.5780
f	 0.8120	 0.5590
g	 0.8690	 0.5640
h	 0.8770	 0.5760
i	 0.8160	 0.5560
l	 0.8990	 0.5810
m	 0.9320	 0.5970
r	 0.7870	 0.5330
t	 0.9350	 0.5980
u	 0.9530	 0.6020
v	 0.7760	 0.5240
w	 0.9040	 0.5830
z	 0.0120	 0.0200