



## Full wwPDB EM Validation Report ⓘ

Mar 31, 2025 – 07:59 PM JST

PDB ID : 6LQM / pdb\_00006lqm  
EMDB ID : EMD-0948  
Title : Cryo-EM structure of a pre-60S ribosomal subunit - state C  
Authors : Liang, X.; Zuo, M.; Zhang, Y.; Li, N.; Ma, C.; Dong, M.; Gao, N.  
Deposited on : 2020-01-14  
Resolution : 3.09 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:

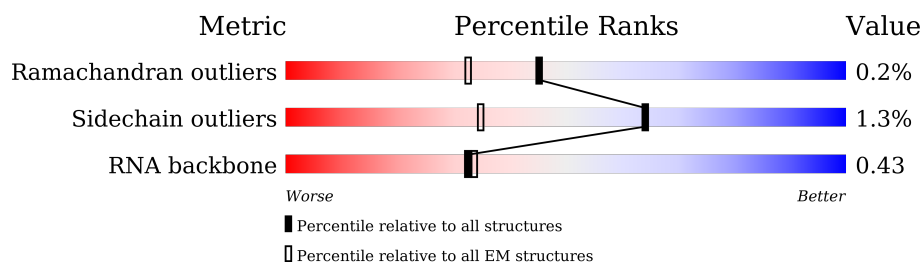
EMDB validation analysis : 0.0.1.dev117  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson 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 3.09 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.






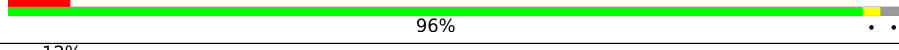

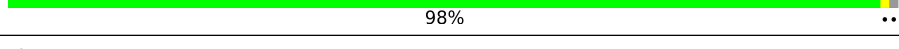
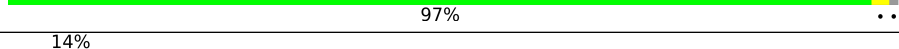
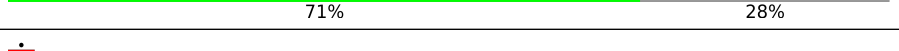
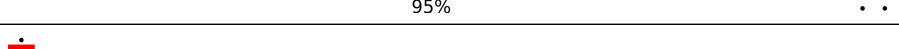
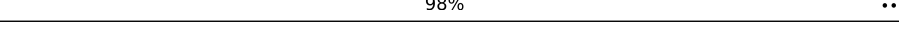
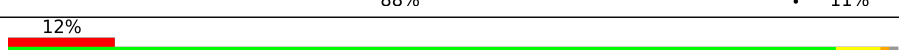
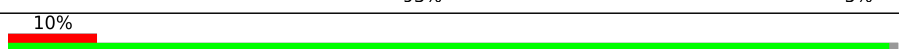
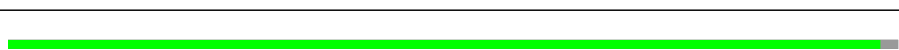
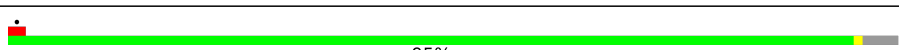



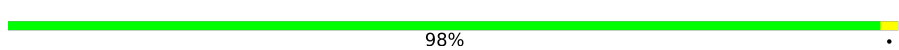
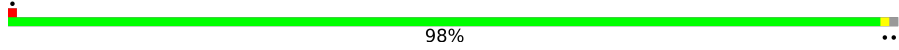
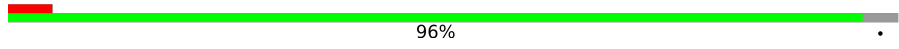
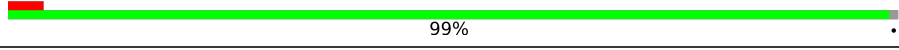
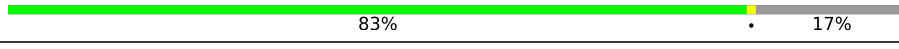
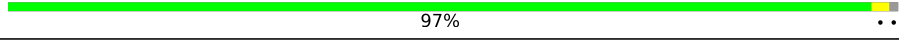


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	2	5070	
3	3	534	
4	5	120	
5	6	245	
6	8	156	
7	A	217	
8	B	403	

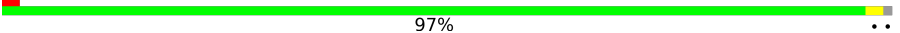



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Mol	Chain	Length	Quality of chain
9	C	159	
10	D	427	
11	E	115	
12	F	117	
13	G	266	
14	H	123	
15	I	192	
16	J	214	
17	K	105	
18	L	148	
19	M	97	
20	N	178	
21	O	70	
22	P	51	
23	Q	211	
24	R	128	
25	S	215	
26	T	125	
27	U	204	
28	V	203	
29	W	106	
30	X	92	
31	Y	184	
32	Z	188	
33	a	196	

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Mol	Chain	Length	Quality of chain
34	b	176	 98%
35	c	160	 97%
36	d	128	 9% 76% 21%
37	e	140	 92% 7%
38	f	157	 39% 61%
39	g	156	 74% 25%
40	h	145	 87% 10%
41	i	136	 99%
42	l	137	 87% 9%
43	m	257	 93%
44	r	297	 7% 98%
45	t	135	 93% 5%
46	u	110	 95% 5%
47	v	288	 10% 78% 18%
48	w	248	 90% 9%

## 2 Entry composition

There are 49 unique types of molecules in this entry. The entry contains 139464 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	66	Total	C	N	O	S	0	0
			555	347	111	89	8		

- Molecule 2 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	3532	Total	C	N	O	P	0	0
			75841	33834	13861	24615	3531		

- Molecule 3 is a protein called 60S ribosomal export protein NMD3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	254	Total	C	N	O	S	0	0
			2043	1297	357	372	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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 4 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	120	Total	C	N	O	P	0	0
			2558	1141	456	842	119		

- Molecule 5 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	220	Total	C	N	O	S	0	0
			1672	1040	288	333	11		

- Molecule 6 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	8	156	Total	C	N	O	P	0	0
			3314	1480	585	1094	155		

- Molecule 7 is a protein called 60S ribosomal protein L10a.

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

- Molecule 8 is a protein called 60S ribosomal protein L3.

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

- Molecule 9 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	97	Total	C	N	O	S	0	0
			788	489	172	123	4		

- Molecule 10 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	358	Total	C	N	O	S	0	0
			2850	1794	569	473	14		

- Molecule 11 is a protein called 60S ribosomal protein L30.

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

- Molecule 12 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	114	Total	C	N	O	S	0	0
			906	566	187	147	6		

- Molecule 13 is a protein called 60S ribosomal protein L7a.

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

- Molecule 14 is a protein called 60S ribosomal protein L35.

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

- Molecule 15 is a protein called 60S ribosomal protein L9.

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

- Molecule 16 is a protein called 60S ribosomal protein L10-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	J	154	Total	C	N	O	S	0	0
			1249	795	233	212	9		

- 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	176	Total	C	N	O	S	0	0
			1410	888	263	253	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	O	69	Total	C	N	O	S	0	0
			569	366	103	99	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	203	Total	C	N	O	S	0	0
			1640	1027	341	268	4		

- Molecule 24 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	R	47	Total	C	N	O	S	0	0
			387	237	83	61	6		

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

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

- Molecule 26 is a protein called 60S ribosomal protein L31.

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

- Molecule 27 is a protein called 60S ribosomal protein L15.

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

- Molecule 28 is a protein called 60S ribosomal protein L13a.

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

- Molecule 29 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	W	102	Total	C	N	O	S	1	0
			842	527	174	135	6		

- Molecule 30 is a protein called 60S ribosomal protein L37a.

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

- Molecule 31 is a protein called 60S ribosomal protein L17.

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

- Molecule 32 is a protein called 60S ribosomal protein L18.

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

- Molecule 33 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	a	153	Total	C	N	O	S	0	0
			1281	799	276	197	9		

- Molecule 34 is a protein called 60S ribosomal protein L18a.

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

- Molecule 35 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	c	159	Total	C	N	O	S	0	0
			1298	823	252	217	6		

- Molecule 36 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	d	101	Total	C	N	O	S	0	0
			825	529	144	150	2		

- Molecule 37 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	e	130	Total	C	N	O	S	0	0
			973	615	183	170	5		

- Molecule 38 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	f	61	Total	C	N	O	S	0	0
			515	330	100	82	3		

- Molecule 39 is a protein called 60S ribosomal protein L23a.

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

- Molecule 40 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	h	131	Total	C	N	O	S	0	0
			1093	686	221	183	3		

- Molecule 41 is a protein called 60S ribosomal protein L27.

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

- Molecule 42 is a protein called 60S ribosomal protein L28.

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

- Molecule 43 is a protein called 60S ribosomal protein L8.

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

- Molecule 44 is a protein called 60S ribosomal protein L5.

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

- Molecule 45 is a protein called 60S ribosomal protein L32.

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

- Molecule 46 is a protein called 60S ribosomal protein L35a.

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

- Molecule 47 is a protein called 60S ribosomal protein L6.

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

- Molecule 48 is a protein called 60S ribosomal protein L7.

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

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

Mol	Chain	Residues	Atoms		AltConf
49	2	245	Total	Mg	0
			245	245	
49	5	3	Total	Mg	0
			3	3	
49	B	1	Total	Mg	0
			1	1	

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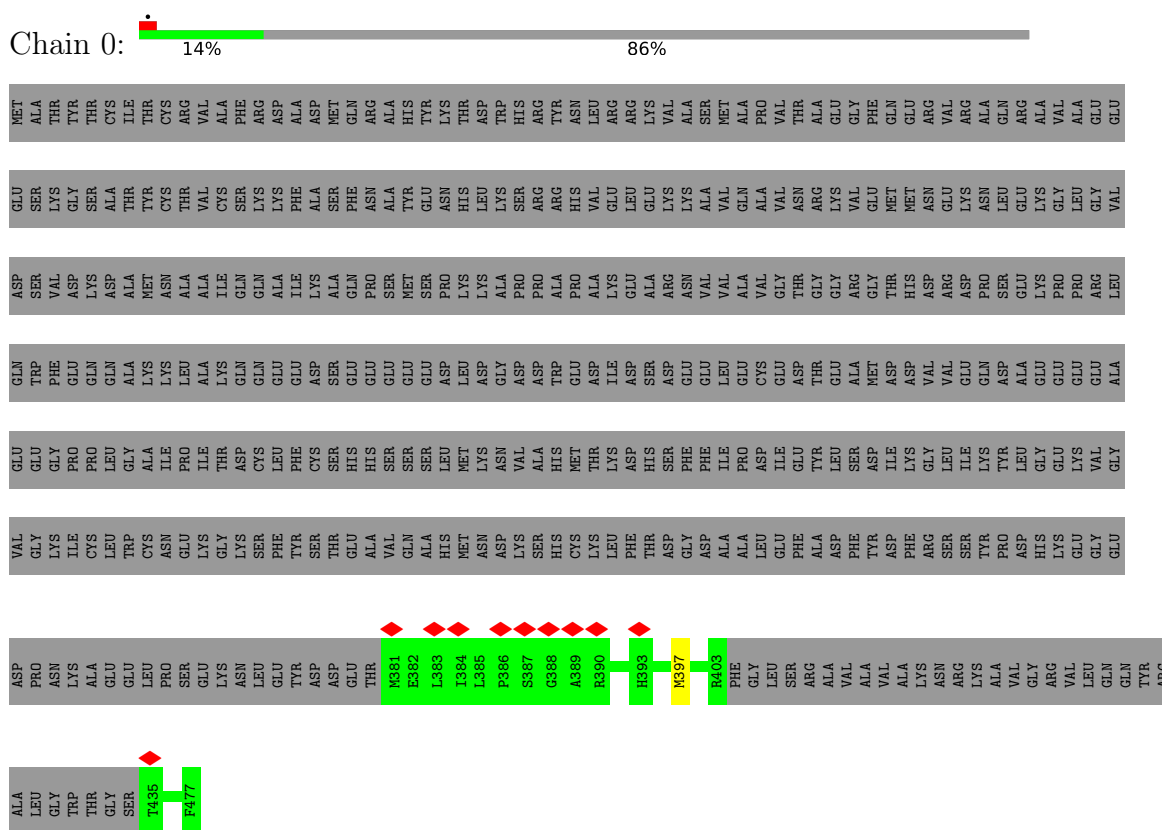
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Mol	Chain	Residues	Atoms		AltConf
49	F	1	Total 1	Mg 1	0
49	m	1	Total 1	Mg 1	0

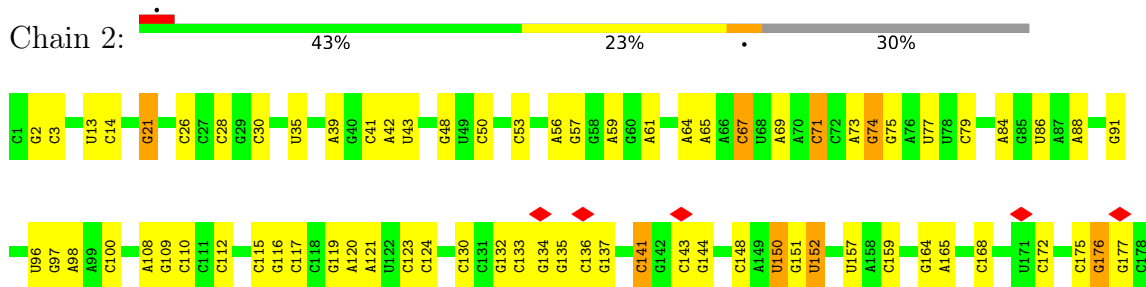
### 3 Residue-property plots

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

#### • Molecule 1: Zinc finger protein 622



#### • Molecule 2: 28S rRNA

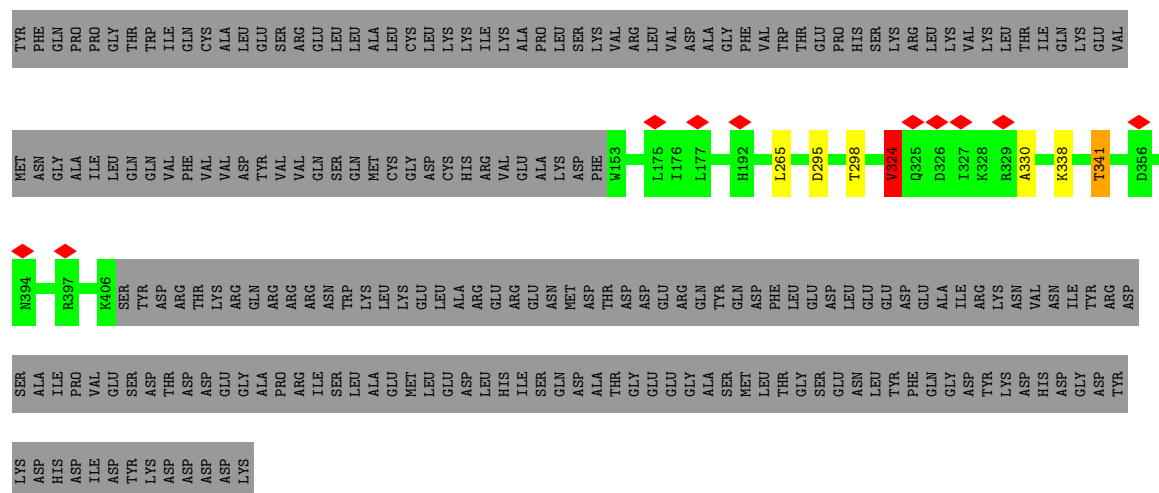




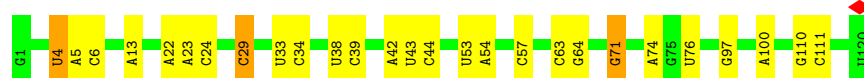
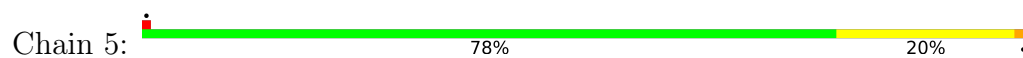




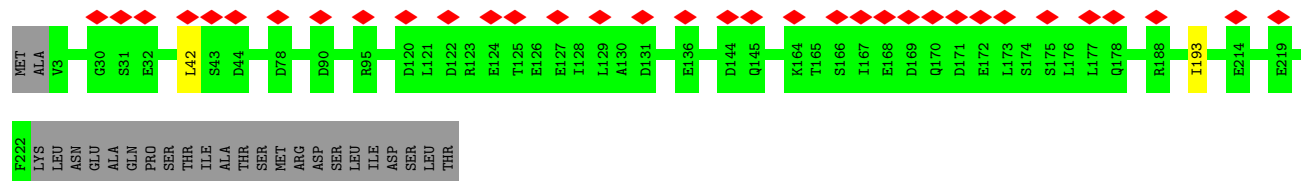
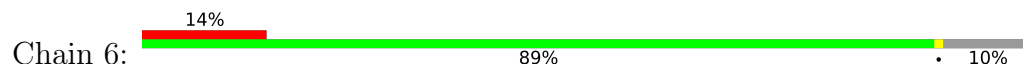




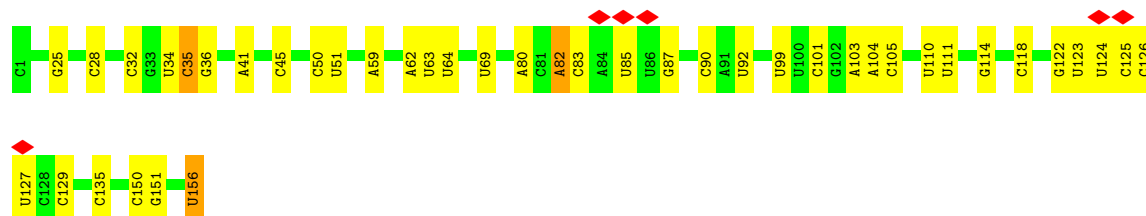
- Molecule 4: 5S rRNA



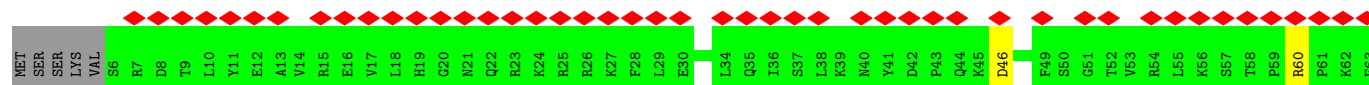
- Molecule 5: Eukaryotic translation initiation factor 6

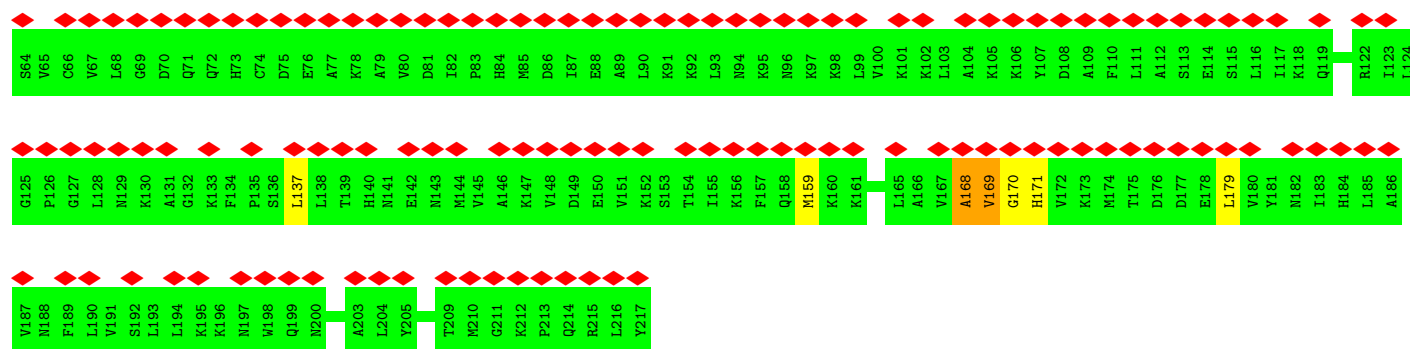


- Molecule 6: 5.8S rRNA



- Molecule 7: 60S ribosomal protein L10a





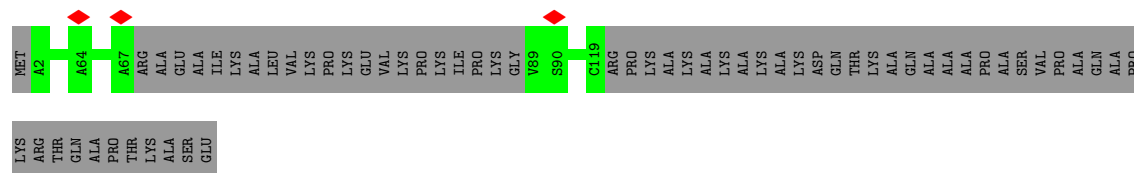
• Molecule 8: 60S ribosomal protein L3

Chain B:  99%




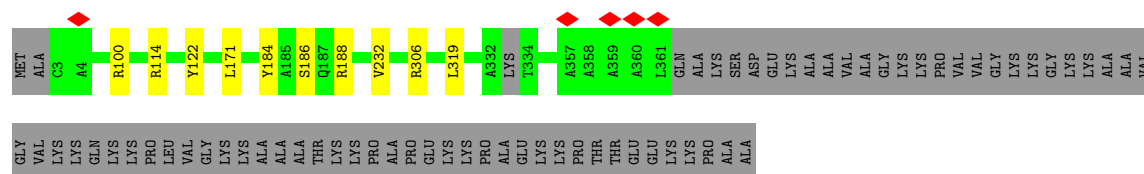
• Molecule 9: 60S ribosomal protein L29

Chain C:  61%




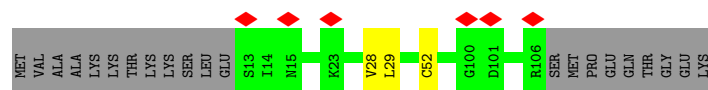
• Molecule 10: 60S ribosomal protein L4

Chain D:  81%



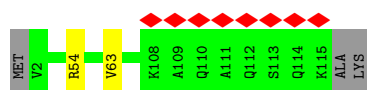
• Molecule 11: 60S ribosomal protein L30

Chain E:  5%

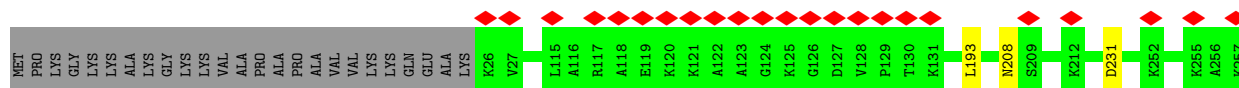
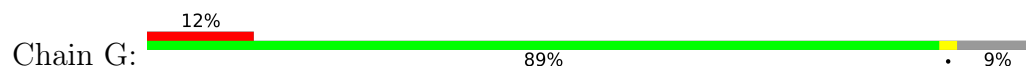


• Molecule 12: 60S ribosomal protein L34

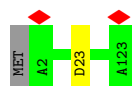
Chain F:  7%



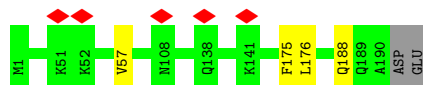
- Molecule 13: 60S ribosomal protein L7a



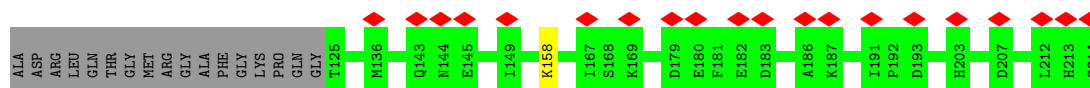
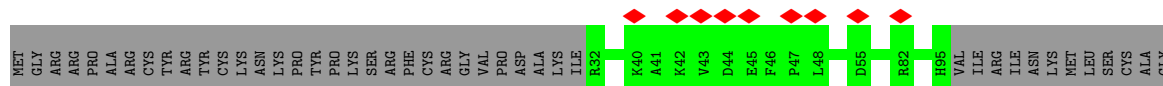
- Molecule 14: 60S ribosomal protein L35



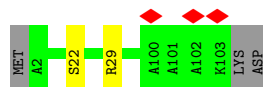
- Molecule 15: 60S ribosomal protein L9



- Molecule 16: 60S ribosomal protein L10-like

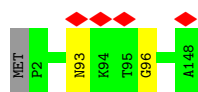


- Molecule 17: 60S ribosomal protein L36




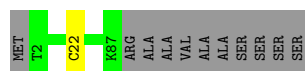
- Molecule 18: 60S ribosomal protein L27a

Chain L:  98% ..




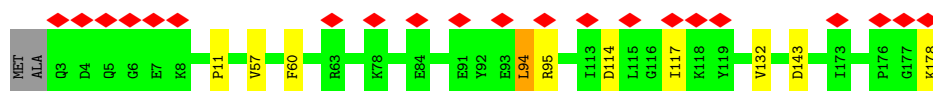
- Molecule 19: 60S ribosomal protein L37

Chain M:  88% . 11%



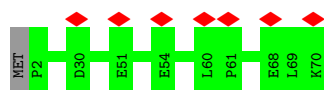
- Molecule 20: 60S ribosomal protein L11

Chain N:  12% 93% 5% ..

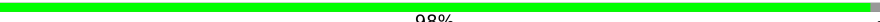


- Molecule 21: 60S ribosomal protein L38

Chain O:  10% 99% .



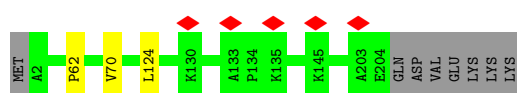
- Molecule 22: 60S ribosomal protein L39

Chain P:  98% .



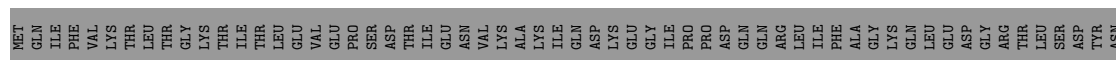
- Molecule 23: 60S ribosomal protein L13

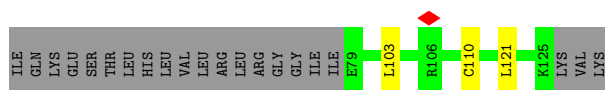
Chain Q:  95% ..



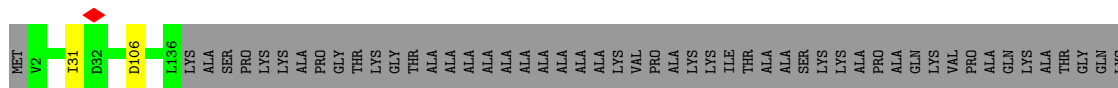
- Molecule 24: Ubiquitin-60S ribosomal protein L40

Chain R:  34% . 63%

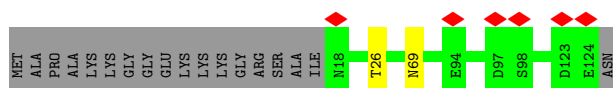
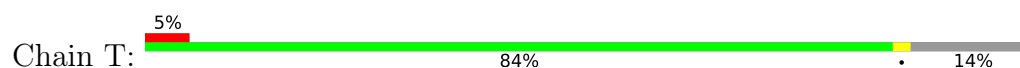




- Molecule 25: 60S ribosomal protein L14



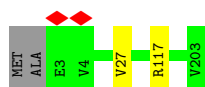
- Molecule 26: 60S ribosomal protein L31



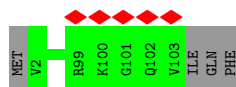
- Molecule 27: 60S ribosomal protein L15



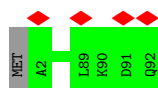
- Molecule 28: 60S ribosomal protein L13a




- Molecule 29: 60S ribosomal protein L36a

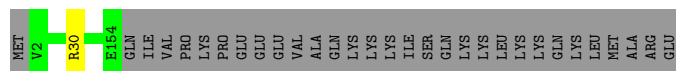


- Molecule 30: 60S ribosomal protein L37a



- Molecule 31: 60S ribosomal protein L17

Chain Y:  83% 17%




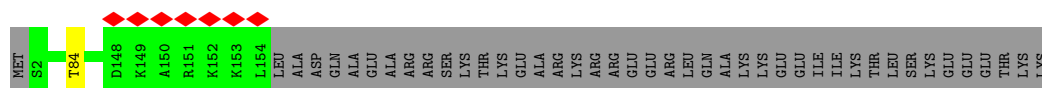
- Molecule 32: 60S ribosomal protein L18

Chain Z:  97% ..



- Molecule 33: 60S ribosomal protein L19

Chain a:  78% 22%



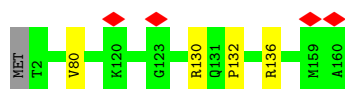
- Molecule 34: 60S ribosomal protein L18a

Chain b:  98% ..




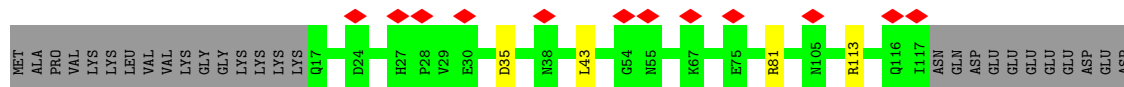
- Molecule 35: 60S ribosomal protein L21

Chain c:  97% ..



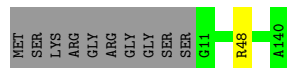
- Molecule 36: 60S ribosomal protein L22

Chain d:  9% 76% 21%

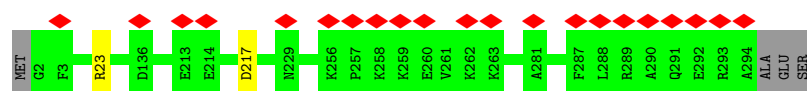


- Molecule 37: 60S ribosomal protein L23

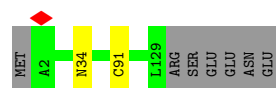
Chain e:  92% 7%



- Molecule 44: 60S ribosomal protein L5




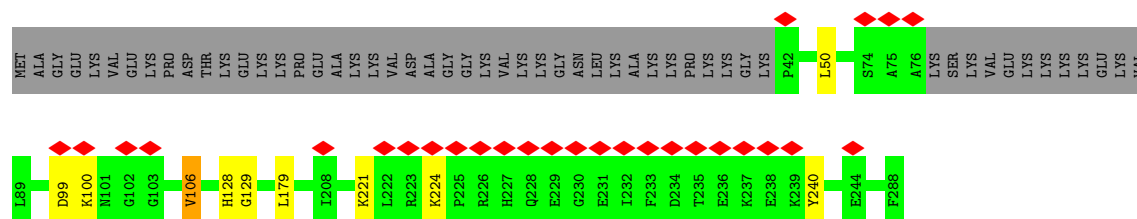
- Chain t:  93% • 5%



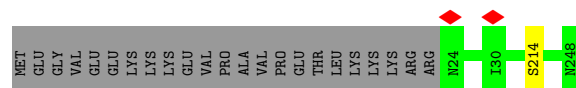
- Chain u:  95% 5%



- Chain v: 



- Chain w:  90% 9%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	21707	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	0.454	Depositor
Minimum map value	-0.178	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.065	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: OMU, A2M, OMG, OMC, B8K, PSU, M7A, 6MZ, MHG, UR3, 2MG, 1MA, I4U, BGH, E6G, B9B, 5MU, B8H, MG, B8W, P4U, 5MC, E7G, B9H, B8T, B8Q, 7MG, P7G

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	0/563	0.59	0/742
2	2	1.68	62/82280 (0.1%)	1.37	1037/128277 (0.8%)
3	3	0.49	0/2086	0.67	1/2820 (0.0%)
4	5	1.23	0/2858	1.22	24/4455 (0.5%)
5	6	0.46	0/1696	0.67	1/2309 (0.0%)
6	8	1.45	2/3701 (0.1%)	1.26	33/5766 (0.6%)
7	A	0.46	2/1736 (0.1%)	0.81	5/2328 (0.2%)
8	B	0.67	0/3315	0.70	2/4435 (0.0%)
9	C	0.50	0/800	0.63	0/1055
10	D	0.73	1/2903 (0.0%)	0.70	3/3899 (0.1%)
11	E	0.56	0/742	0.72	1/996 (0.1%)
12	F	0.67	1/916 (0.1%)	0.64	0/1220
13	G	0.60	0/1960	0.70	2/2637 (0.1%)
14	H	0.60	0/1023	0.61	0/1351
15	I	0.59	0/1537	0.69	0/2066
16	J	0.39	0/1278	0.63	1/1708 (0.1%)
17	K	0.54	0/843	0.69	1/1115 (0.1%)
18	L	0.71	0/1191	0.69	0/1591
19	M	0.75	0/720	0.73	0/952
20	N	0.51	1/1433 (0.1%)	0.70	0/1915
21	O	0.55	0/575	0.65	0/761
22	P	0.67	0/454	0.65	0/599
23	Q	0.65	0/1671	0.68	1/2237 (0.0%)
24	R	0.52	1/393 (0.3%)	0.70	0/521
25	S	0.58	0/1133	0.63	0/1516
26	T	0.67	0/903	0.66	0/1216
27	U	0.76	0/1746	0.66	0/2338
28	V	0.68	0/1682	0.64	0/2250
29	W	0.69	0/858	0.66	0/1131
30	X	0.64	0/718	0.63	0/953
31	Y	0.71	0/1268	0.65	0/1701

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	Z	0.74	1/1537 (0.1%)	0.71	0/2052
33	a	0.59	0/1297	0.63	0/1716
34	b	0.72	0/1493	0.61	0/2003
35	c	0.65	0/1326	0.66	0/1770
36	d	0.47	0/839	0.73	1/1126 (0.1%)
37	e	0.62	0/987	0.64	0/1324
38	f	0.64	0/528	0.59	0/703
39	g	0.61	0/975	0.64	0/1312
40	h	0.69	0/1110	0.65	0/1477
41	i	0.63	0/1130	0.61	0/1507
42	l	0.68	0/1017	0.62	0/1364
43	m	0.73	1/1936 (0.1%)	0.73	1/2596 (0.0%)
44	r	1.43	3/2428 (0.1%)	0.91	4/3252 (0.1%)
45	t	0.74	0/1071	0.65	0/1429
46	u	0.76	0/895	0.72	1/1198 (0.1%)
47	v	0.55	0/1935	0.71	2/2596 (0.1%)
48	w	0.69	1/1916 (0.1%)	0.68	0/2553
All	All	1.36	76/147402 (0.1%)	1.17	1121/216838 (0.5%)

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
3	3	0	4
7	A	0	3
11	E	0	1
13	G	0	1
15	I	0	2
18	L	0	1
20	N	0	1
34	b	0	1
35	c	0	3
42	l	0	2
43	m	0	1
45	t	0	2
46	u	0	2
47	v	0	1
All	All	0	25

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	4280	A	N3-C4	148.71	2.24	1.34
2	2	4280	A	C6-N1	129.88	2.26	1.35
2	2	4280	A	N1-C2	98.61	2.23	1.34
2	2	4280	A	C2-N3	95.13	2.19	1.33
2	2	4280	A	C5-C4	93.78	2.04	1.38
2	2	4280	A	C5-C6	79.47	2.12	1.41
44	r	23	ARG	CD-NE	61.74	2.51	1.46
44	r	23	ARG	NE-CZ	16.26	1.54	1.33
7	A	170	GLY	CA-C	7.14	1.63	1.51
2	2	4764	A	N9-C4	-7.11	1.33	1.37
10	D	186	SER	CA-CB	-6.93	1.42	1.52
2	2	2465	C	N1-C6	-6.62	1.33	1.37
2	2	4281	A	N7-C5	-6.37	1.35	1.39
2	2	1577	G	C2-N3	-6.35	1.27	1.32
2	2	1663	C	N1-C6	-6.22	1.33	1.37
2	2	2333	G	C2-N3	-6.17	1.27	1.32
2	2	1340	C	C4-C5	-6.16	1.38	1.43
2	2	686	A	N9-C4	-6.09	1.34	1.37
2	2	41	C	C4-C5	-6.06	1.38	1.43
44	r	23	ARG	CG-CD	6.06	1.67	1.51
32	Z	148	VAL	CB-CG1	-5.99	1.40	1.52
2	2	1340	C	N1-C6	-5.89	1.33	1.37
12	F	63	VAL	CB-CG1	-5.88	1.40	1.52
2	2	3646	A	N7-C5	-5.84	1.35	1.39
2	2	2783	A	N9-C4	-5.83	1.34	1.37
2	2	2283	G	C5-C4	-5.78	1.34	1.38
2	2	4303	C	N3-C4	-5.76	1.29	1.33
43	m	169	VAL	CB-CG1	-5.73	1.40	1.52
48	w	214	SER	C-N	-5.67	1.21	1.34
2	2	21	G	C2-N3	-5.64	1.28	1.32
7	A	170	GLY	N-CA	5.61	1.54	1.46
6	8	36	G	C5-C4	-5.60	1.34	1.38
2	2	2333	G	C2-N2	-5.58	1.28	1.34
24	R	110	CYS	CB-SG	5.57	1.91	1.82
2	2	372	A	C5-C4	-5.53	1.34	1.38
2	2	3775	A	N7-C5	-5.50	1.35	1.39
2	2	1908	A	N9-C4	-5.50	1.34	1.37
2	2	2506	G	C2-N3	-5.45	1.28	1.32
2	2	2409	U	C2-O2	-5.45	1.17	1.22
2	2	3637	U	C2-N3	-5.42	1.33	1.37
2	2	1852	U	C2-N3	-5.41	1.33	1.37
2	2	1498	G	C2-N3	-5.41	1.28	1.32
2	2	2409	U	N3-C4	-5.40	1.33	1.38

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*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	3656	A	N9-C4	-5.36	1.34	1.37
2	2	1645	C	N3-C4	-5.34	1.30	1.33
2	2	4281	A	N3-C4	-5.33	1.31	1.34
6	8	104	A	C5-C4	-5.32	1.35	1.38
2	2	1520	C	C4-C5	-5.29	1.38	1.43
2	2	1914	C	N1-C6	-5.21	1.34	1.37
2	2	2278	G	C8-N7	-5.20	1.27	1.30
2	2	4281	A	N9-C4	-5.20	1.34	1.37
2	2	4242	U	C2-N3	-5.20	1.34	1.37
2	2	1928	C	N1-C2	5.19	1.45	1.40
2	2	1495	G	C6-N1	-5.19	1.35	1.39
2	2	1684	A	N9-C4	-5.19	1.34	1.37
2	2	1674	C	C4-C5	-5.17	1.38	1.43
2	2	2639	U	C2-N3	-5.17	1.34	1.37
2	2	2349	A	C5-C4	-5.16	1.35	1.38
2	2	3652	A	N7-C5	-5.16	1.36	1.39
2	2	1396	G	N7-C5	-5.13	1.36	1.39
2	2	2333	G	N3-C4	-5.13	1.31	1.35
2	2	1663	C	C4-C5	-5.13	1.38	1.43
2	2	3852	A	N7-C5	-5.10	1.36	1.39
2	2	2806	A	C5-C4	-5.09	1.35	1.38
2	2	1335	G	C8-N7	-5.08	1.27	1.30
2	2	74	G	C8-N7	-5.05	1.27	1.30
2	2	1347	G	N9-C8	-5.05	1.34	1.37
2	2	2347	A	N9-C4	-5.04	1.34	1.37
2	2	4538	G	C8-N7	-5.04	1.27	1.30
20	N	132	VAL	CB-CG1	-5.04	1.42	1.52
2	2	97	G	C5-C4	-5.03	1.34	1.38
2	2	1531	U	C2-N3	-5.02	1.34	1.37
2	2	2465	C	C4-C5	-5.02	1.39	1.43
2	2	2427	G	C6-N1	-5.01	1.36	1.39
2	2	374	G	C5-C4	-5.01	1.34	1.38
2	2	375	G	C5-C4	-5.01	1.34	1.38

All (1121) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	4280	A	N1-C2-N3	-64.44	97.08	129.30
2	2	4280	A	C2-N3-C4	49.77	135.48	110.60
2	2	4280	A	N7-C8-N9	28.07	127.84	113.80
2	2	4280	A	C6-N1-C2	27.68	135.21	118.60
44	r	23	ARG	CD-NE-CZ	27.05	161.47	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	4280	A	C4-C5-N7	-25.19	98.11	110.70
2	2	4280	A	N3-C4-N9	21.24	144.39	127.40
44	r	23	ARG	NE-CZ-NH1	20.37	130.48	120.30
2	2	4280	A	N9-C4-C5	-16.23	99.31	105.80
2	2	340	C	N1-C2-O2	15.08	127.95	118.90
2	2	4280	A	N3-C4-C5	-15.06	116.26	126.80
2	2	516	C	N1-C2-O2	14.10	127.36	118.90
2	2	485	C	C2-N1-C1'	14.08	134.29	118.80
2	2	180	C	C6-N1-C2	-13.44	114.92	120.30
2	2	340	C	C2-N1-C1'	13.09	133.19	118.80
2	2	340	C	N3-C2-O2	-12.36	113.25	121.90
2	2	4117	U	N3-C2-O2	-12.03	113.78	122.20
2	2	516	C	C2-N1-C1'	11.68	131.65	118.80
2	2	417	G	O4'-C1'-N9	11.54	117.43	108.20
2	2	4601	U	C5-C6-N1	11.22	128.31	122.70
2	2	662	C	C6-N1-C2	-11.14	115.84	120.30
2	2	4280	A	C6-C5-N7	11.07	140.05	132.30
2	2	753	C	N1-C2-O2	10.92	125.45	118.90
44	r	23	ARG	NE-CZ-NH2	-10.85	114.88	120.30
2	2	4775	C	N1-C2-O2	10.82	125.39	118.90
2	2	485	C	C6-N1-C1'	-10.79	107.85	120.80
2	2	4117	U	N1-C2-O2	10.63	130.24	122.80
2	2	4281	A	N7-C8-N9	10.61	119.11	113.80
2	2	4420	U	N1-C2-O2	10.55	130.18	122.80
2	2	1183	C	N1-C2-O2	10.49	125.19	118.90
2	2	1928	C	N1-C2-O2	10.43	125.16	118.90
2	2	753	C	N3-C2-O2	-10.34	114.66	121.90
2	2	4945	G	C5-C6-O6	-10.27	122.44	128.60
2	2	516	C	N3-C2-O2	-10.26	114.72	121.90
2	2	1183	C	C2-N1-C1'	10.16	129.98	118.80
2	2	493	G	N9-C4-C5	10.11	109.45	105.40
2	2	485	C	N1-C2-O2	10.10	124.96	118.90
2	2	1928	C	N3-C2-O2	-10.10	114.83	121.90
2	2	100	C	C2-N1-C1'	10.03	129.83	118.80
2	2	1340	C	C5-C6-N1	9.79	125.90	121.00
2	2	2409	U	N3-C2-O2	-9.76	115.37	122.20
2	2	115	C	C2-N1-C1'	9.70	129.47	118.80
2	2	3741	C	N3-C2-O2	-9.65	115.14	121.90
2	2	4775	C	N3-C2-O2	-9.60	115.18	121.90
2	2	2319	C	C6-N1-C2	-9.58	116.47	120.30
2	2	2409	U	N1-C2-N3	9.58	120.65	114.90
2	2	4895	C	N1-C2-O2	9.52	124.61	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	4420	U	N3-C2-O2	-9.51	115.54	122.20
2	2	4280	A	C4-C5-C6	9.50	121.75	117.00
2	2	643	C	N1-C2-O2	9.47	124.58	118.90
2	2	340	C	C6-N1-C1'	-9.37	109.55	120.80
2	2	493	G	N3-C2-N2	-9.26	113.42	119.90
2	2	220	C	N1-C2-O2	9.23	124.44	118.90
2	2	753	C	C2-N1-C1'	9.18	128.89	118.80
2	2	4557	U	N3-C2-O2	-9.17	115.78	122.20
2	2	925	C	C5-C6-N1	9.14	125.57	121.00
2	2	4990	C	C2-N1-C1'	9.13	128.85	118.80
2	2	2260	C	N3-C2-O2	-9.11	115.53	121.90
2	2	4891	G	N1-C6-O6	-9.08	114.45	119.90
2	2	4303	C	N3-C2-O2	-9.05	115.56	121.90
2	2	4281	A	C5-N7-C8	-8.98	99.41	103.90
2	2	1705	G	C8-N9-C4	-8.98	102.81	106.40
2	2	4193	C	C6-N1-C2	-8.88	116.75	120.30
6	8	111	U	N1-C2-O2	8.88	129.01	122.80
6	8	111	U	C2-N1-C1'	8.87	128.34	117.70
2	2	4420	U	C2-N1-C1'	8.86	128.33	117.70
10	D	319	LEU	CA-CB-CG	8.86	135.67	115.30
2	2	4557	U	C2-N1-C1'	8.81	128.27	117.70
17	K	22	SER	C-N-CA	8.78	143.65	121.70
2	2	4990	C	N1-C2-O2	8.77	124.16	118.90
2	2	4601	U	C2-N1-C1'	8.74	128.19	117.70
2	2	4280	A	C5-N7-C8	8.73	108.27	103.90
2	2	2260	C	N1-C2-O2	8.73	124.14	118.90
2	2	2783	A	C6-N1-C2	8.72	123.83	118.60
2	2	925	C	N1-C2-O2	8.71	124.12	118.90
2	2	1197	C	C6-N1-C2	-8.68	116.83	120.30
2	2	77	U	N3-C2-O2	-8.67	116.13	122.20
2	2	925	C	C6-N1-C2	-8.67	116.83	120.30
2	2	1241	C	C2-N1-C1'	8.65	128.31	118.80
2	2	1243	C	N1-C2-O2	8.64	124.08	118.90
2	2	264	C	C6-N1-C2	-8.62	116.85	120.30
2	2	2580	U	N3-C2-O2	-8.61	116.17	122.20
6	8	51	U	N1-C2-O2	8.60	128.82	122.80
2	2	904	C	N1-C2-O2	8.60	124.06	118.90
2	2	3710	G	O4'-C1'-N9	8.60	115.08	108.20
2	2	4926	C	C2-N1-C1'	8.60	128.25	118.80
2	2	3741	C	N1-C2-O2	8.58	124.05	118.90
2	2	4926	C	N1-C2-O2	8.50	124.00	118.90
2	2	1192	C	N1-C2-O2	8.49	123.99	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	100	C	N1-C2-O2	8.47	123.98	118.90
2	2	180	C	C5-C6-N1	8.46	125.23	121.00
2	2	704	C	N1-C2-O2	8.41	123.94	118.90
2	2	1705	G	C4-N9-C1'	8.40	137.43	126.50
2	2	907	C	N3-C2-O2	-8.34	116.06	121.90
2	2	493	G	C4-C5-N7	-8.31	107.48	110.80
6	8	51	U	N3-C2-O2	-8.30	116.39	122.20
2	2	516	C	C6-N1-C1'	-8.30	110.84	120.80
2	2	4895	C	C2-N1-C1'	8.30	127.93	118.80
2	2	4945	G	C4-C5-N7	8.29	114.12	110.80
2	2	1705	G	N3-C4-C5	-8.24	124.48	128.60
6	8	64	U	N3-C2-O2	-8.24	116.43	122.20
2	2	1663	C	C5-C6-N1	8.24	125.12	121.00
2	2	1703	C	N1-C2-O2	8.22	123.83	118.90
2	2	4914	C	C6-N1-C2	-8.21	117.02	120.30
2	2	4775	C	C2-N1-C1'	8.19	127.81	118.80
2	2	4662	C	C6-N1-C2	-8.17	117.03	120.30
2	2	449	C	N1-C2-O2	8.16	123.80	118.90
2	2	5016	A	N7-C8-N9	8.16	117.88	113.80
2	2	1662	C	C6-N1-C2	-8.15	117.04	120.30
7	A	170	GLY	O-C-N	-8.15	109.66	122.70
2	2	643	C	C2-N1-C1'	8.14	127.75	118.80
2	2	643	C	C6-N1-C2	-8.12	117.05	120.30
2	2	2303	C	C6-N1-C1'	8.12	130.55	120.80
2	2	2478	C	C6-N1-C2	-8.10	117.06	120.30
2	2	4280	A	C5-C6-N1	-8.10	113.65	117.70
2	2	493	G	N3-C4-N9	-8.09	121.14	126.00
2	2	2303	C	N3-C4-N4	-8.09	112.34	118.00
2	2	3911	C	C5-C6-N1	8.07	125.04	121.00
2	2	988	C	C2-N1-C1'	8.03	127.63	118.80
2	2	1183	C	N3-C2-O2	-8.00	116.30	121.90
2	2	41	C	C6-N1-C2	-8.00	117.10	120.30
2	2	3911	C	C6-N1-C2	-8.00	117.10	120.30
2	2	3637	U	N3-C2-O2	-7.98	116.62	122.20
2	2	4758	U	N3-C2-O2	-7.95	116.64	122.20
2	2	3775	A	O4'-C1'-N9	7.90	114.52	108.20
2	2	4557	U	N1-C2-O2	7.89	128.32	122.80
2	2	3866	C	C5-C6-N1	7.89	124.94	121.00
6	8	111	U	N3-C2-O2	-7.88	116.68	122.20
2	2	2528	G	C4-N9-C1'	7.84	136.70	126.50
2	2	340	C	C6-N1-C2	-7.83	117.17	120.30
2	2	2262	G	C4-N9-C1'	7.78	136.62	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	662	C	C5-C6-N1	7.78	124.89	121.00
2	2	5030	U	C5-C6-N1	7.75	126.57	122.70
2	2	4730	C	C6-N1-C2	-7.74	117.20	120.30
2	2	988	C	C6-N1-C2	-7.74	117.20	120.30
2	2	2850	A	C8-N9-C4	-7.73	102.71	105.80
2	2	4398	C	N1-C2-O2	7.73	123.54	118.90
2	2	2478	C	N1-C2-O2	7.73	123.54	118.90
2	2	1241	C	N1-C2-O2	7.72	123.53	118.90
6	8	129	C	N3-C2-O2	-7.71	116.50	121.90
2	2	704	C	C2-N1-C1'	7.70	127.27	118.80
2	2	3866	C	C6-N1-C2	-7.70	117.22	120.30
2	2	1405	C	N1-C2-O2	7.70	123.52	118.90
2	2	4281	A	C8-N9-C4	-7.67	102.73	105.80
2	2	256	G	N3-C4-N9	-7.67	121.40	126.00
2	2	4739	C	C6-N1-C2	-7.63	117.25	120.30
2	2	753	C	C6-N1-C2	-7.63	117.25	120.30
2	2	1241	C	C6-N1-C2	-7.63	117.25	120.30
2	2	2499	C	C6-N1-C2	-7.61	117.26	120.30
2	2	1666	C	C6-N1-C2	-7.61	117.26	120.30
2	2	228	C	C6-N1-C2	-7.60	117.26	120.30
2	2	1607	C	C6-N1-C2	-7.60	117.26	120.30
2	2	2505	C	N1-C2-O2	7.59	123.45	118.90
2	2	256	G	C4-N9-C1'	-7.59	116.64	126.50
2	2	4928	C	N1-C2-O2	7.55	123.43	118.90
2	2	2580	U	N1-C2-O2	7.54	128.08	122.80
2	2	4137	C	C6-N1-C2	-7.52	117.29	120.30
2	2	4926	C	N3-C2-O2	-7.52	116.64	121.90
2	2	963	G	C4-N9-C1'	7.51	136.26	126.50
2	2	2303	C	C5-C4-N4	7.51	125.46	120.20
2	2	4471	U	N3-C2-O2	-7.48	116.96	122.20
2	2	3655	C	C6-N1-C2	-7.48	117.31	120.30
2	2	141	C	C2-N1-C1'	7.48	127.02	118.80
2	2	4281	A	C2-N3-C4	-7.47	106.86	110.60
2	2	1915	C	N3-C2-O2	-7.46	116.67	121.90
2	2	35	U	N3-C2-O2	-7.45	116.99	122.20
2	2	4682	U	C2-N1-C1'	7.43	126.62	117.70
2	2	3915	U	N3-C2-O2	-7.43	117.00	122.20
2	2	4476	C	N1-C2-O2	7.41	123.35	118.90
2	2	493	G	C6-C5-N7	7.41	134.84	130.40
2	2	1243	C	C2-N1-C1'	7.40	126.94	118.80
2	2	485	C	C5-C6-N1	7.39	124.70	121.00
2	2	1183	C	C6-N1-C1'	-7.37	111.95	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	4758	U	N1-C2-O2	7.37	127.96	122.80
2	2	2710	C	C2-N1-C1'	7.37	126.90	118.80
2	2	988	C	C5-C6-N1	7.35	124.68	121.00
2	2	2494	U	C2-N1-C1'	7.35	126.53	117.70
2	2	4138	C	C6-N1-C2	-7.35	117.36	120.30
2	2	100	C	N3-C2-O2	-7.33	116.77	121.90
2	2	655	C	N3-C2-O2	-7.33	116.77	121.90
2	2	4601	U	C6-N1-C2	-7.32	116.61	121.00
2	2	2409	U	C6-N1-C2	-7.31	116.61	121.00
2	2	1598	C	N1-C2-O2	7.31	123.28	118.90
2	2	4139	G	N7-C8-N9	7.31	116.75	113.10
6	8	32	C	C6-N1-C2	-7.30	117.38	120.30
2	2	53	C	C6-N1-C2	-7.30	117.38	120.30
2	2	2362	U	N3-C2-O2	-7.28	117.10	122.20
2	2	2820	C	N1-C2-O2	7.25	123.25	118.90
2	2	4476	C	C2-N1-C1'	7.24	126.77	118.80
2	2	4758	U	C2-N1-C1'	7.21	126.36	117.70
2	2	3773	U	C2-N1-C1'	7.21	126.36	117.70
2	2	4926	C	C6-N1-C2	-7.20	117.42	120.30
8	B	141	ASP	CB-CG-OD1	7.20	124.78	118.30
2	2	1250	C	C6-N1-C2	-7.19	117.42	120.30
2	2	643	C	N3-C2-O2	-7.19	116.87	121.90
44	r	23	ARG	CG-CD-NE	7.18	126.89	111.80
2	2	1848	C	C6-N1-C2	-7.17	117.43	120.30
2	2	1893	C	C5-C6-N1	7.17	124.58	121.00
2	2	1702	C	C2-N1-C1'	7.16	126.67	118.80
2	2	516	C	C6-N1-C2	-7.14	117.44	120.30
2	2	4902	C	C2-N1-C1'	7.14	126.65	118.80
2	2	4895	C	N3-C2-O2	-7.12	116.91	121.90
2	2	4928	C	N3-C2-O2	-7.12	116.91	121.90
2	2	2627	C	C5-C6-N1	7.12	124.56	121.00
2	2	5016	A	C8-N9-C4	-7.11	102.96	105.80
2	2	1821	G	N3-C4-C5	-7.10	125.05	128.60
2	2	4342	C	C5-C6-N1	7.10	124.55	121.00
2	2	1674	C	C5-C6-N1	7.10	124.55	121.00
4	5	34	C	N1-C2-O2	7.10	123.16	118.90
2	2	1628	C	C6-N1-C2	-7.10	117.46	120.30
2	2	4303	C	C6-N1-C2	-7.10	117.46	120.30
2	2	115	C	N1-C2-O2	7.09	123.15	118.90
2	2	4772	C	N1-C2-O2	7.09	123.15	118.90
2	2	1050	C	C5-C6-N1	7.09	124.54	121.00
2	2	505	G	N3-C4-N9	7.08	130.25	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	170	GLY	C-N-CA	7.08	139.39	121.70
2	2	673	C	N1-C2-O2	7.07	123.14	118.90
2	2	1731	C	C6-N1-C2	-7.07	117.47	120.30
2	2	988	C	N1-C2-O2	7.07	123.14	118.90
2	2	4990	C	C5-C6-N1	7.06	124.53	121.00
2	2	1082	C	P-O3'-C3'	7.06	128.17	119.70
6	8	64	U	N1-C2-O2	7.06	127.74	122.80
2	2	2760	G	P-O3'-C3'	7.04	128.15	119.70
2	2	1243	C	C5-C6-N1	7.04	124.52	121.00
2	2	643	C	C5-C6-N1	7.04	124.52	121.00
2	2	4302	U	N3-C2-O2	-7.03	117.28	122.20
2	2	4229	U	N1-C2-O2	7.03	127.72	122.80
2	2	513	U	C2-N1-C1'	7.03	126.13	117.70
2	2	2580	U	C2-N1-C1'	7.03	126.13	117.70
2	2	504	G	C4-N9-C1'	7.03	135.63	126.50
2	2	1703	C	N3-C2-O2	-7.02	116.98	121.90
2	2	449	C	N3-C2-O2	-7.01	116.99	121.90
2	2	100	C	C6-N1-C1'	-7.01	112.39	120.80
2	2	4920	C	N1-C2-O2	6.99	123.10	118.90
2	2	220	C	N3-C2-O2	-6.99	117.01	121.90
2	2	4945	G	N9-C4-C5	-6.98	102.61	105.40
2	2	4350	C	C6-N1-C2	-6.98	117.51	120.30
2	2	4945	G	N1-C6-O6	6.98	124.09	119.90
2	2	4682	U	N1-C2-O2	6.98	127.68	122.80
2	2	4476	C	N3-C2-O2	-6.97	117.02	121.90
2	2	4258	C	C5-C6-N1	6.96	124.48	121.00
2	2	3636	C	C6-N1-C2	-6.96	117.52	120.30
2	2	4258	C	C6-N1-C2	-6.96	117.52	120.30
2	2	2262	G	N3-C4-C5	-6.95	125.12	128.60
2	2	2362	U	N1-C2-O2	6.95	127.67	122.80
4	5	34	C	N3-C2-O2	-6.95	117.04	121.90
2	2	2528	G	N3-C4-N9	6.94	130.17	126.00
2	2	3840	U	N3-C2-O2	-6.92	117.35	122.20
2	2	1405	C	C5-C6-N1	6.92	124.46	121.00
2	2	1597	G	O4'-C1'-N9	6.92	113.73	108.20
2	2	96	U	N3-C2-O2	-6.91	117.37	122.20
2	2	1243	C	C6-N1-C2	-6.90	117.54	120.30
2	2	112	C	C2-N1-C1'	6.89	126.39	118.80
2	2	4945	G	N3-C4-N9	6.88	130.13	126.00
2	2	904	C	N3-C2-O2	-6.88	117.09	121.90
2	2	1313	C	C6-N1-C2	-6.87	117.55	120.30
2	2	2482	C	C6-N1-C2	-6.87	117.55	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1893	C	C2-N1-C1'	6.86	126.35	118.80
2	2	1552	G	O4'-C1'-N9	6.86	113.69	108.20
2	2	4117	U	C2-N1-C1'	6.86	125.93	117.70
2	2	1190	C	C6-N1-C2	-6.85	117.56	120.30
2	2	2426	U	N3-C2-O2	-6.85	117.40	122.20
2	2	4193	C	C5-C6-N1	6.85	124.43	121.00
2	2	256	G	C8-N9-C1'	6.85	135.91	127.00
16	J	158	LYS	C-N-CA	6.85	138.82	121.70
2	2	4775	C	C6-N1-C2	-6.84	117.56	120.30
2	2	2482	C	C5-C6-N1	6.84	124.42	121.00
2	2	513	U	C5-C6-N1	6.83	126.11	122.70
2	2	2675	G	P-O3'-C3'	6.83	127.90	119.70
2	2	505	G	C4-N9-C1'	6.83	135.37	126.50
2	2	1190	C	C5-C6-N1	6.82	124.41	121.00
2	2	4303	C	C2-N1-C1'	6.81	126.30	118.80
2	2	148	C	C6-N1-C2	-6.81	117.58	120.30
2	2	2494	U	N1-C2-O2	6.80	127.56	122.80
2	2	516	C	C5-C6-N1	6.79	124.39	121.00
2	2	2593	C	C6-N1-C2	-6.79	117.59	120.30
2	2	4674	C	C6-N1-C2	-6.78	117.59	120.30
2	2	914	U	P-O3'-C3'	6.78	127.84	119.70
2	2	181	C	C2-N1-C1'	-6.77	111.35	118.80
2	2	925	C	N3-C2-O2	-6.77	117.16	121.90
2	2	4914	C	C5-C6-N1	6.76	124.38	121.00
2	2	2814	C	N1-C2-O2	6.76	122.95	118.90
2	2	4229	U	N3-C2-O2	-6.75	117.47	122.20
2	2	26	C	C6-N1-C2	-6.75	117.60	120.30
2	2	115	C	C6-N1-C1'	-6.75	112.70	120.80
2	2	3693	U	N3-C2-O2	-6.74	117.48	122.20
2	2	2410	C	C2-N1-C1'	6.74	126.21	118.80
2	2	2499	C	N1-C2-O2	6.73	122.94	118.90
2	2	4137	C	C5-C6-N1	6.73	124.36	121.00
2	2	2528	G	N3-C4-C5	-6.72	125.24	128.60
2	2	1367	C	C2-N1-C1'	6.71	126.19	118.80
2	2	4342	C	C6-N1-C2	-6.71	117.61	120.30
2	2	1665	C	C6-N1-C2	-6.70	117.62	120.30
2	2	3693	U	N1-C2-O2	6.70	127.49	122.80
2	2	1598	C	N3-C2-O2	-6.70	117.21	121.90
2	2	2262	G	N3-C4-N9	6.69	130.02	126.00
2	2	2491	C	N3-C2-O2	-6.69	117.22	121.90
2	2	4730	C	C2-N3-C4	6.69	123.25	119.90
2	2	1702	C	C6-N1-C2	-6.68	117.63	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	4945	G	C6-C5-N7	-6.68	126.39	130.40
2	2	4109	G	N3-C4-C5	-6.67	125.27	128.60
2	2	4109	G	N3-C4-N9	6.67	130.00	126.00
2	2	2603	C	C6-N1-C2	-6.66	117.64	120.30
2	2	672	C	C5-C6-N1	6.66	124.33	121.00
2	2	1402	C	N1-C2-O2	6.66	122.89	118.90
2	2	96	U	N1-C2-O2	6.66	127.46	122.80
2	2	1367	C	N1-C2-O2	6.66	122.89	118.90
2	2	4429	C	C5-C6-N1	6.65	124.32	121.00
2	2	4928	C	C2-N1-C1'	6.64	126.10	118.80
2	2	2303	C	C6-N1-C2	-6.63	117.65	120.30
2	2	1705	G	N7-C8-N9	6.63	116.41	113.10
2	2	4426	C	C2-N1-C1'	6.62	126.08	118.80
2	2	5016	A	C5-N7-C8	-6.62	100.59	103.90
2	2	4682	U	N3-C2-O2	-6.60	117.58	122.20
2	2	5052	C	C6-N1-C2	-6.60	117.66	120.30
2	2	1367	C	N3-C2-O2	-6.60	117.28	121.90
2	2	1535	C	C6-N1-C2	-6.60	117.66	120.30
2	2	1577	G	N1-C6-O6	-6.60	115.94	119.90
2	2	489	C	N1-C2-O2	6.59	122.86	118.90
2	2	2319	C	C5-C6-N1	6.59	124.30	121.00
2	2	2333	G	N3-C2-N2	-6.59	115.29	119.90
2	2	1540	C	C6-N1-C2	-6.58	117.67	120.30
2	2	2494	U	N3-C2-O2	-6.58	117.60	122.20
2	2	3775	A	N7-C8-N9	6.58	117.09	113.80
2	2	4241	C	C5-C6-N1	6.57	124.29	121.00
2	2	4429	C	C6-N1-C2	-6.57	117.67	120.30
6	8	32	C	N3-C2-O2	-6.56	117.31	121.90
2	2	686	A	N3-C4-N9	-6.56	122.16	127.40
2	2	3685	C	C6-N1-C2	-6.56	117.68	120.30
2	2	504	G	C2-N3-C4	6.54	115.17	111.90
2	2	337	U	N3-C2-O2	-6.54	117.62	122.20
2	2	1578	U	C5-C6-N1	6.54	125.97	122.70
8	B	360	LEU	CA-CB-CG	6.54	130.34	115.30
2	2	2073	C	C6-N1-C2	-6.53	117.69	120.30
2	2	2035	C	C6-N1-C2	-6.53	117.69	120.30
2	2	141	C	N1-C2-O2	6.52	122.81	118.90
2	2	904	C	C2-N1-C1'	6.52	125.97	118.80
2	2	4891	G	C5-C6-O6	6.50	132.50	128.60
2	2	1674	C	C6-N1-C2	-6.50	117.70	120.30
4	5	71	G	C8-N9-C1'	-6.50	118.56	127.00
2	2	493	G	C8-N9-C1'	6.49	135.44	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	4341	C	C6-N1-C2	-6.49	117.70	120.30
2	2	5052	C	C5-C6-N1	6.49	124.24	121.00
2	2	3650	C	C6-N1-C2	-6.49	117.71	120.30
2	2	4557	U	C6-N1-C1'	-6.48	112.13	121.20
2	2	1665	C	C5-C6-N1	6.48	124.24	121.00
2	2	2303	C	C2-N1-C1'	-6.48	111.67	118.80
2	2	2505	C	N3-C2-O2	-6.48	117.37	121.90
2	2	4709	U	N3-C2-O2	-6.47	117.67	122.20
2	2	4241	C	N1-C2-O2	6.47	122.78	118.90
2	2	4923	C	C6-N1-C2	-6.47	117.71	120.30
2	2	1906	U	N1-C2-O2	6.47	127.33	122.80
2	2	3772	U	N3-C2-O2	-6.46	117.68	122.20
2	2	2478	C	C5-C6-N1	6.46	124.23	121.00
2	2	1178	G	C4-N9-C1'	6.45	134.89	126.50
2	2	4880	C	N1-C2-O2	6.45	122.77	118.90
2	2	2526	C	C6-N1-C2	-6.45	117.72	120.30
2	2	3920	U	N3-C2-O2	-6.45	117.69	122.20
2	2	100	C	C6-N1-C2	-6.45	117.72	120.30
2	2	1340	C	C6-N1-C2	-6.44	117.72	120.30
2	2	1821	G	C4-N9-C1'	6.44	134.88	126.50
2	2	2096	G	N3-C4-N9	6.44	129.86	126.00
2	2	2506	G	N3-C2-N2	-6.43	115.40	119.90
2	2	4730	C	C5-C6-N1	6.43	124.22	121.00
2	2	2478	C	N3-C2-O2	-6.43	117.40	121.90
2	2	1216	C	C2-N1-C1'	6.43	125.87	118.80
2	2	1663	C	C6-N1-C2	-6.42	117.73	120.30
2	2	4662	C	N3-C2-O2	-6.42	117.41	121.90
2	2	4426	C	C5-C6-N1	6.41	124.20	121.00
2	2	1494	U	N3-C2-O2	-6.41	117.72	122.20
2	2	2528	G	C8-N9-C1'	-6.41	118.67	127.00
2	2	2802	C	C5-C6-N1	6.41	124.20	121.00
2	2	3775	A	C5-N7-C8	-6.40	100.70	103.90
2	2	468	U	C5-C6-N1	6.40	125.90	122.70
4	5	71	G	C4-N9-C1'	6.40	134.82	126.50
2	2	2262	G	C8-N9-C1'	-6.39	118.69	127.00
2	2	2333	G	C5-C6-O6	6.39	132.43	128.60
2	2	2410	C	N1-C2-O2	6.39	122.73	118.90
2	2	2096	G	C4-N9-C1'	6.39	134.80	126.50
2	2	1816	C	C6-N1-C2	-6.39	117.75	120.30
2	2	4350	C	C5-C6-N1	6.39	124.19	121.00
6	8	28	C	C6-N1-C2	-6.38	117.75	120.30
2	2	1197	C	C5-C6-N1	6.38	124.19	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	112	C	C6-N1-C2	-6.38	117.75	120.30
2	2	2033	A	P-O3'-C3'	6.38	127.36	119.70
2	2	2652	G	N3-C4-N9	-6.38	122.17	126.00
2	2	4206	C	C5-C6-N1	6.37	124.19	121.00
2	2	4206	C	C6-N1-C2	-6.37	117.75	120.30
2	2	4743	G	N3-C4-N9	-6.37	122.18	126.00
2	2	1241	C	N3-C2-O2	-6.37	117.44	121.90
2	2	4990	C	C6-N1-C2	-6.37	117.75	120.30
2	2	2667	C	N1-C2-O2	6.36	122.72	118.90
2	2	4337	C	C6-N1-C2	-6.36	117.75	120.30
2	2	3696	C	C6-N1-C2	-6.36	117.75	120.30
2	2	4888	U	N1-C2-O2	6.36	127.25	122.80
2	2	673	C	C2-N1-C1'	6.35	125.78	118.80
2	2	4583	C	O4'-C1'-N1	6.35	113.28	108.20
2	2	4601	U	N1-C2-O2	6.35	127.25	122.80
2	2	175	C	C6-N1-C2	-6.34	117.76	120.30
2	2	485	C	C6-N1-C2	-6.34	117.76	120.30
2	2	4709	U	N1-C2-O2	6.34	127.24	122.80
2	2	3926	C	C6-N1-C2	-6.34	117.76	120.30
2	2	504	G	N3-C4-N9	6.33	129.80	126.00
2	2	2250	C	N1-C2-O2	6.33	122.70	118.90
2	2	704	C	N3-C2-O2	-6.32	117.47	121.90
2	2	4928	C	C6-N1-C2	-6.32	117.77	120.30
2	2	4118	U	N3-C2-O2	-6.32	117.78	122.20
2	2	3930	U	C5-C6-N1	6.32	125.86	122.70
4	5	71	G	N3-C4-N9	6.32	129.79	126.00
2	2	3895	G	N1-C6-O6	-6.32	116.11	119.90
2	2	28	C	C6-N1-C2	-6.31	117.78	120.30
2	2	2410	C	C5-C6-N1	6.31	124.16	121.00
2	2	4746	C	C2-N1-C1'	6.31	125.74	118.80
7	A	170	GLY	N-CA-C	6.31	128.87	113.10
2	2	974	C	C6-N1-C2	-6.31	117.78	120.30
2	2	4626	A	O4'-C1'-N9	6.30	113.24	108.20
2	2	1241	C	C5-C6-N1	6.30	124.15	121.00
2	2	1663	C	C2-N1-C1'	6.30	125.73	118.80
2	2	963	G	C8-N9-C1'	-6.30	118.82	127.00
2	2	4119	C	N1-C2-O2	6.29	122.68	118.90
2	2	1183	C	C6-N1-C2	-6.29	117.78	120.30
2	2	4138	C	C5-C6-N1	6.29	124.15	121.00
2	2	4303	C	N1-C2-O2	6.29	122.67	118.90
2	2	1620	U	N3-C2-O2	-6.28	117.80	122.20
2	2	1915	C	C2-N1-C1'	6.28	125.71	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	4887	C	C5-C6-N1	6.28	124.14	121.00
6	8	111	U	C6-N1-C1'	-6.26	112.43	121.20
2	2	936	C	N1-C2-O2	6.26	122.66	118.90
2	2	504	G	C8-N9-C1'	-6.26	118.87	127.00
2	2	2653	C	C6-N1-C2	-6.26	117.80	120.30
2	2	35	U	N1-C2-O2	6.25	127.18	122.80
2	2	168	C	C6-N1-C2	-6.25	117.80	120.30
4	5	111	C	C6-N1-C2	-6.24	117.80	120.30
2	2	1245	C	C2-N1-C1'	6.24	125.67	118.80
2	2	673	C	C5-C6-N1	6.23	124.12	121.00
2	2	4452	U	N3-C2-O2	-6.23	117.84	122.20
2	2	1301	C	C6-N1-C2	-6.23	117.81	120.30
2	2	2260	C	C6-N1-C2	-6.22	117.81	120.30
2	2	489	C	C2-N1-C1'	6.22	125.64	118.80
2	2	4990	C	C6-N1-C1'	-6.22	113.34	120.80
2	2	4864	U	N1-C2-O2	6.21	127.15	122.80
2	2	4990	C	N3-C2-O2	-6.21	117.56	121.90
2	2	2096	G	N3-C4-C5	-6.21	125.50	128.60
2	2	1216	C	N1-C2-O2	6.20	122.62	118.90
2	2	3920	U	N1-C2-O2	6.20	127.14	122.80
2	2	4902	C	N1-C2-O2	6.19	122.62	118.90
2	2	2532	C	C5-C6-N1	6.19	124.09	121.00
2	2	1275	G	O4'-C1'-N9	6.18	113.15	108.20
2	2	2690	C	C6-N1-C2	-6.18	117.83	120.30
2	2	1183	C	C5-C6-N1	6.18	124.09	121.00
2	2	115	C	C6-N1-C2	-6.18	117.83	120.30
2	2	969	C	C2-N1-C1'	6.18	125.59	118.80
2	2	4709	U	C2-N1-C1'	6.17	125.11	117.70
2	2	4302	U	N1-C2-O2	6.17	127.12	122.80
2	2	2499	C	C2-N1-C1'	6.17	125.59	118.80
2	2	3641	U	C4-C5-C6	6.17	123.40	119.70
2	2	1364	U	N3-C2-O2	-6.17	117.88	122.20
2	2	1442	C	C4-C5-C6	6.17	120.48	117.40
2	2	4772	C	N3-C2-O2	-6.16	117.59	121.90
2	2	2478	C	C2-N1-C1'	6.16	125.57	118.80
2	2	2260	C	C2-N1-C1'	6.15	125.57	118.80
2	2	505	G	C8-N9-C1'	-6.15	119.00	127.00
10	D	171	LEU	CA-CB-CG	6.15	129.44	115.30
2	2	4103	C	C6-N1-C2	-6.14	117.84	120.30
2	2	4471	U	N1-C2-O2	6.13	127.09	122.80
2	2	115	C	C5-C6-N1	6.13	124.06	121.00
2	2	453	G	N3-C2-N2	-6.12	115.61	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1191	C	N3-C2-O2	-6.12	117.61	121.90
2	2	2710	C	N3-C2-O2	-6.12	117.61	121.90
2	2	5028	G	N3-C4-C5	-6.12	125.54	128.60
2	2	1702	C	C5-C6-N1	6.11	124.06	121.00
2	2	2303	C	N3-C2-O2	-6.11	117.62	121.90
2	2	485	C	N3-C2-O2	-6.10	117.63	121.90
2	2	2036	C	C5-C6-N1	6.09	124.05	121.00
2	2	412	G	C4-C5-N7	6.08	113.23	110.80
2	2	972	C	N1-C2-O2	6.08	122.55	118.90
2	2	2255	C	C2-N1-C1'	6.07	125.48	118.80
2	2	4337	C	C5-C6-N1	6.07	124.04	121.00
2	2	4745	G	C4-C5-N7	6.07	113.23	110.80
2	2	4969	C	C6-N1-C2	-6.07	117.87	120.30
2	2	242	U	N3-C2-O2	-6.07	117.95	122.20
2	2	2107	C	N3-C2-O2	-6.06	117.66	121.90
2	2	1705	G	N3-C2-N2	-6.06	115.66	119.90
2	2	3912	U	N3-C2-O2	-6.05	117.96	122.20
2	2	2281	U	C2-N1-C1'	6.05	124.96	117.70
2	2	1404	G	N3-C4-C5	-6.05	125.58	128.60
2	2	4461	C	C6-N1-C2	-6.05	117.88	120.30
6	8	99	U	N3-C2-O2	-6.05	117.97	122.20
2	2	2409	U	C4-C5-C6	6.05	123.33	119.70
2	2	4771	C	C5-C6-N1	6.05	124.02	121.00
2	2	1308	C	C5-C6-N1	6.04	124.02	121.00
2	2	1717	C	N1-C2-O2	6.04	122.52	118.90
2	2	1377	G	C4-C5-N7	6.04	113.21	110.80
2	2	1579	C	C5-C6-N1	6.04	124.02	121.00
2	2	4864	U	C2-N1-C1'	6.04	124.94	117.70
2	2	1088	C	C6-N1-C2	-6.03	117.89	120.30
2	2	2627	C	C2-N1-C1'	6.03	125.43	118.80
2	2	3601	C	C6-N1-C2	-6.03	117.89	120.30
2	2	4600	G	P-O3'-C3'	6.03	126.93	119.70
4	5	111	C	C5-C6-N1	6.03	124.01	121.00
2	2	1192	C	N3-C2-O2	-6.02	117.69	121.90
2	2	4272	G	N9-C4-C5	-6.02	102.99	105.40
2	2	1309	C	C5-C6-N1	6.02	124.01	121.00
2	2	4199	C	N1-C2-O2	6.02	122.51	118.90
2	2	4703	U	N3-C2-O2	-6.02	117.99	122.20
2	2	4549	G	C4-C5-N7	6.01	113.21	110.80
2	2	250	C	N1-C2-O2	6.01	122.51	118.90
2	2	504	G	N3-C4-C5	-6.00	125.60	128.60
2	2	907	C	N1-C2-O2	6.00	122.50	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1242	G	C4-N9-C1'	6.00	134.29	126.50
2	2	1428	U	C5-C6-N1	5.99	125.70	122.70
2	2	2850	A	N7-C8-N9	5.99	116.80	113.80
2	2	1367	C	C6-N1-C2	-5.99	117.90	120.30
2	2	50	C	C6-N1-C2	-5.99	117.91	120.30
4	5	39	C	C6-N1-C2	-5.99	117.90	120.30
2	2	4215	C	N3-C2-O2	-5.99	117.71	121.90
2	2	1352	C	C6-N1-C2	-5.98	117.91	120.30
2	2	936	C	C2-N1-C1'	5.96	125.36	118.80
2	2	1556	C	C6-N1-C2	-5.96	117.92	120.30
2	2	2627	C	N1-C2-O2	5.96	122.48	118.90
2	2	686	A	N3-C4-C5	5.96	130.97	126.80
2	2	1468	C	C6-N1-C2	-5.95	117.92	120.30
2	2	2333	G	N1-C2-N3	5.95	127.47	123.90
2	2	3641	U	C5-C6-N1	-5.95	119.73	122.70
2	2	2526	C	C5-C6-N1	5.95	123.97	121.00
2	2	185	C	N1-C2-O2	5.94	122.47	118.90
2	2	264	C	C6-N1-C1'	5.94	127.93	120.80
2	2	2489	C	C6-N1-C2	-5.94	117.92	120.30
2	2	2627	C	C6-N1-C2	-5.94	117.92	120.30
2	2	3772	U	C2-N1-C1'	5.94	124.83	117.70
2	2	4281	A	O4'-C1'-N9	5.94	112.95	108.20
2	2	1494	U	N1-C2-O2	5.93	126.95	122.80
2	2	4592	C	C6-N1-C2	-5.93	117.93	120.30
2	2	4502	C	N3-C2-O2	-5.93	117.75	121.90
2	2	4109	G	C4-N9-C1'	5.92	134.20	126.50
2	2	2416	G	P-O3'-C3'	5.92	126.80	119.70
4	5	39	C	N1-C2-O2	5.92	122.45	118.90
2	2	406	C	P-O3'-C3'	5.92	126.80	119.70
2	2	115	C	N3-C2-O2	-5.91	117.76	121.90
2	2	4490	C	C5-C6-N1	5.91	123.95	121.00
2	2	4913	G	P-O3'-C3'	5.91	126.79	119.70
2	2	4887	C	N1-C2-O2	5.91	122.44	118.90
2	2	367	C	C6-N1-C2	-5.91	117.94	120.30
2	2	963	G	N3-C4-N9	5.90	129.54	126.00
4	5	4	U	N1-C2-O2	5.90	126.93	122.80
2	2	453	G	C2-N3-C4	5.89	114.85	111.90
2	2	112	C	C5-C6-N1	5.89	123.95	121.00
2	2	3866	C	C2-N3-C4	5.89	122.84	119.90
2	2	460	C	C5-C6-N1	5.89	123.94	121.00
2	2	2439	G	C4-N9-C1'	5.89	134.15	126.50
2	2	252	C	C5-C6-N1	5.88	123.94	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1182	C	N1-C2-O2	5.88	122.43	118.90
2	2	1884	C	N1-C2-O2	5.88	122.43	118.90
2	2	4887	C	C6-N1-C2	-5.88	117.95	120.30
2	2	5021	C	C6-N1-C2	-5.88	117.95	120.30
2	2	1541	C	C6-N1-C2	-5.88	117.95	120.30
2	2	4344	U	C5-C6-N1	5.88	125.64	122.70
4	5	29	C	N1-C2-O2	5.88	122.43	118.90
2	2	406	C	C6-N1-C2	-5.88	117.95	120.30
2	2	1579	C	C6-N1-C2	-5.87	117.95	120.30
2	2	971	U	C2-N1-C1'	5.87	124.75	117.70
2	2	2337	C	C6-N1-C2	-5.87	117.95	120.30
2	2	4502	C	N1-C2-O2	5.87	122.42	118.90
2	2	1258	G	N7-C8-N9	5.87	116.03	113.10
2	2	2409	U	C5-C4-O4	5.86	129.42	125.90
2	2	1308	C	C6-N1-C2	-5.86	117.95	120.30
2	2	4888	U	N3-C2-O2	-5.86	118.10	122.20
2	2	282	C	N3-C2-O2	-5.86	117.80	121.90
2	2	2081	C	C6-N1-C2	-5.86	117.96	120.30
2	2	3673	C	P-O3'-C3'	5.86	126.73	119.70
2	2	5050	C	C2-N1-C1'	5.86	125.24	118.80
2	2	2410	C	C6-N1-C2	-5.84	117.96	120.30
2	2	4420	U	C6-N1-C1'	-5.84	113.02	121.20
2	2	4568	A	N1-C6-N6	-5.84	115.09	118.60
2	2	256	G	C6-C5-N7	5.84	133.90	130.40
2	2	4490	C	C6-N1-C2	-5.84	117.96	120.30
2	2	141	C	C6-N1-C1'	-5.84	113.79	120.80
2	2	2710	C	N1-C2-O2	5.84	122.40	118.90
2	2	5052	C	C2-N1-C1'	5.84	125.22	118.80
2	2	1777	C	C5-C6-N1	5.83	123.92	121.00
2	2	2710	C	C6-N1-C2	-5.83	117.97	120.30
2	2	3882	C	C6-N1-C2	-5.83	117.97	120.30
2	2	3672	G	N3-C4-N9	5.83	129.50	126.00
2	2	673	C	C6-N1-C2	-5.82	117.97	120.30
2	2	2814	C	N3-C2-O2	-5.82	117.82	121.90
2	2	753	C	C6-N1-C1'	-5.82	113.82	120.80
2	2	1093	C	N1-C2-O2	5.81	122.39	118.90
2	2	473	C	C5-C6-N1	5.81	123.91	121.00
2	2	4895	C	C6-N1-C2	-5.81	117.98	120.30
2	2	1182	C	C2-N1-C1'	5.81	125.19	118.80
2	2	1530	G	N1-C6-O6	-5.81	116.42	119.90
2	2	4426	C	N1-C2-O2	5.81	122.38	118.90
2	2	4113	U	O4'-C1'-N1	5.81	112.84	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	4392	G	N1-C6-O6	-5.81	116.42	119.90
2	2	468	U	C6-N1-C2	-5.80	117.52	121.00
2	2	972	C	N3-C2-O2	-5.80	117.84	121.90
2	2	4771	C	C6-N1-C2	-5.80	117.98	120.30
2	2	2351	C	C2-N1-C1'	5.80	125.17	118.80
2	2	2319	C	O5'-P-OP2	-5.79	100.48	105.70
2	2	2802	C	C6-N1-C2	-5.79	117.98	120.30
2	2	2347	A	O4'-C1'-N9	-5.79	103.57	108.20
2	2	4254	G	N3-C4-C5	-5.79	125.70	128.60
2	2	71	C	C6-N1-C1'	5.79	127.75	120.80
2	2	1702	C	N1-C2-O2	5.79	122.37	118.90
2	2	1404	G	C2-N3-C4	5.79	114.79	111.90
2	2	2048	U	N1-C2-O2	5.79	126.85	122.80
2	2	4396	A	N1-C2-N3	-5.79	126.41	129.30
2	2	367	C	C5-C6-N1	5.79	123.89	121.00
2	2	1731	C	C2-N1-C1'	5.79	125.17	118.80
2	2	2362	U	C2-N1-C1'	5.78	124.64	117.70
2	2	969	C	N1-C2-O2	5.78	122.37	118.90
2	2	2103	G	N3-C4-N9	5.78	129.47	126.00
2	2	4299	U	N3-C2-O2	-5.78	118.15	122.20
2	2	1644	C	C6-N1-C2	-5.78	117.99	120.30
2	2	41	C	C5-C6-N1	5.78	123.89	121.00
2	2	4281	A	N1-C2-N3	5.77	132.19	129.30
2	2	505	G	N3-C4-C5	-5.76	125.72	128.60
3	3	324	VAL	CA-CB-CG2	5.76	119.54	110.90
2	2	1472	C	C6-N1-C2	-5.76	118.00	120.30
2	2	1188	C	C5-C6-N1	5.75	123.88	121.00
2	2	1188	C	C6-N1-C2	-5.75	118.00	120.30
2	2	4540	C	C6-N1-C2	-5.75	118.00	120.30
2	2	2048	U	N3-C2-O2	-5.75	118.17	122.20
2	2	2084	C	P-O3'-C3'	5.75	126.60	119.70
2	2	148	C	C5-C6-N1	5.75	123.87	121.00
6	8	118	C	N1-C2-O2	5.75	122.35	118.90
2	2	264	C	C5-C6-N1	5.74	123.87	121.00
2	2	657	C	C5-C6-N1	5.74	123.87	121.00
2	2	2653	C	C2-N1-C1'	5.74	125.11	118.80
2	2	4288	C	C6-N1-C2	-5.74	118.00	120.30
4	5	4	U	N3-C2-O2	-5.74	118.18	122.20
2	2	757	G	C5-C6-O6	5.74	132.04	128.60
2	2	2528	G	C6-C5-N7	-5.74	126.96	130.40
2	2	4864	U	N3-C2-O2	-5.74	118.19	122.20
2	2	963	G	N3-C4-C5	-5.73	125.73	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	4549	G	C6-C5-N7	-5.73	126.96	130.40
2	2	1821	G	N3-C4-N9	5.73	129.44	126.00
2	2	2684	C	C6-N1-C2	-5.72	118.01	120.30
2	2	1893	C	C6-N1-C2	-5.72	118.01	120.30
2	2	2031	C	C6-N1-C2	-5.71	118.01	120.30
2	2	2489	C	C5-C6-N1	5.71	123.86	121.00
2	2	2850	A	C4-N9-C1'	5.71	136.58	126.30
2	2	2499	C	N3-C2-O2	-5.71	117.90	121.90
4	5	29	C	C2-N1-C1'	5.71	125.08	118.80
6	8	156	U	N3-C2-O2	-5.71	118.20	122.20
2	2	2036	C	C6-N1-C2	-5.71	118.02	120.30
2	2	340	C	C5-C6-N1	5.71	123.86	121.00
2	2	1821	G	C2-N3-C4	5.71	114.75	111.90
2	2	1928	C	C2-N1-C1'	5.71	125.08	118.80
2	2	100	C	O4'-C1'-N1	5.70	112.76	108.20
2	2	469	C	C4-C5-C6	5.70	120.25	117.40
2	2	1725	U	N3-C2-O2	-5.70	118.21	122.20
2	2	3939	G	N3-C4-C5	-5.70	125.75	128.60
2	2	4137	C	C2-N1-C1'	5.70	125.08	118.80
2	2	504	G	P-O3'-C3'	5.70	126.54	119.70
2	2	505	G	C6-C5-N7	-5.70	126.98	130.40
2	2	4138	C	C2-N1-C1'	5.70	125.07	118.80
2	2	4980	C	C6-N1-C2	-5.70	118.02	120.30
5	6	42	LEU	CA-CB-CG	5.70	128.40	115.30
2	2	4201	G	C4-N9-C1'	5.69	133.90	126.50
13	G	265	LEU	CA-CB-CG	5.69	128.38	115.30
2	2	86	U	N1-C2-O2	5.69	126.78	122.80
2	2	3802	U	C2-N1-C1'	5.69	124.53	117.70
2	2	4918	C	C6-N1-C2	-5.69	118.03	120.30
2	2	176	G	C4-N9-C1'	5.69	133.89	126.50
2	2	130	C	C5-C6-N1	5.68	123.84	121.00
2	2	1928	C	C6-N1-C2	-5.68	118.03	120.30
2	2	365	U	C5-C6-N1	5.67	125.54	122.70
2	2	716	C	C6-N1-C2	-5.67	118.03	120.30
2	2	4138	C	N1-C2-O2	5.67	122.30	118.90
2	2	4559	A	C6-N1-C2	5.67	122.00	118.60
2	2	453	G	N3-C4-C5	-5.67	125.76	128.60
2	2	4452	U	N1-C2-O2	5.67	126.77	122.80
2	2	1847	C	C5-C6-N1	5.67	123.83	121.00
2	2	1912	G	C4-N9-C1'	5.67	133.86	126.50
2	2	513	U	C6-N1-C2	-5.66	117.60	121.00
6	8	156	U	N1-C2-O2	5.66	126.76	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	2495	U	N3-C2-O2	-5.66	118.24	122.20
2	2	3688	U	N3-C2-O2	-5.66	118.24	122.20
2	2	3680	U	N3-C2-O2	-5.66	118.24	122.20
2	2	1820	C	C6-N1-C2	-5.66	118.04	120.30
6	8	92	U	N3-C2-O2	-5.66	118.24	122.20
2	2	1216	C	N3-C2-O2	-5.65	117.94	121.90
2	2	28	C	C5-C6-N1	5.65	123.82	121.00
2	2	115	C	O4'-C1'-N1	5.65	112.72	108.20
2	2	1705	G	C8-N9-C1'	-5.65	119.66	127.00
2	2	365	U	C2-N1-C1'	5.65	124.47	117.70
2	2	1275	G	N3-C4-N9	-5.64	122.61	126.00
2	2	2532	C	N1-C2-O2	5.64	122.29	118.90
2	2	3882	C	C2-N1-C1'	5.64	125.01	118.80
2	2	1275	G	C8-N9-C1'	5.64	134.33	127.00
2	2	4980	C	C5-C6-N1	5.64	123.82	121.00
2	2	2820	C	N3-C2-O2	-5.63	117.96	121.90
2	2	4895	C	C5-C6-N1	5.63	123.82	121.00
2	2	4215	C	C6-N1-C2	-5.63	118.05	120.30
2	2	152	U	N3-C2-O2	-5.63	118.26	122.20
2	2	1483	C	N1-C2-O2	5.63	122.28	118.90
2	2	2783	A	C5-C6-N1	-5.63	114.89	117.70
2	2	4215	C	N1-C2-O2	5.62	122.28	118.90
2	2	3808	C	N3-C2-O2	-5.62	117.96	121.90
2	2	488	G	C6-C5-N7	-5.62	127.03	130.40
2	2	5004	C	C5-C6-N1	5.62	123.81	121.00
2	2	250	C	C2-N1-C1'	5.62	124.98	118.80
2	2	1189	G	N3-C4-C5	-5.62	125.79	128.60
2	2	2532	C	C2-N1-C1'	5.62	124.98	118.80
2	2	1245	C	N1-C2-O2	5.62	122.27	118.90
2	2	704	C	C6-N1-C1'	-5.61	114.06	120.80
2	2	3926	C	N1-C2-O2	5.61	122.27	118.90
2	2	1203	G	N3-C4-N9	5.61	129.37	126.00
2	2	1648	C	C6-N1-C2	-5.61	118.06	120.30
2	2	417	G	N1-C6-O6	-5.61	116.54	119.90
2	2	4565	C	N1-C2-O2	5.61	122.26	118.90
2	2	4752	U	N1-C2-O2	5.61	126.72	122.80
2	2	4667	C	C5-C6-N1	5.61	123.80	121.00
2	2	2407	G	O4'-C1'-N9	5.60	112.68	108.20
2	2	1792	U	N3-C2-O2	-5.60	118.28	122.20
2	2	4895	C	C6-N1-C1'	-5.59	114.09	120.80
2	2	4109	G	C2-N3-C4	5.58	114.69	111.90
2	2	2096	G	C8-N9-C1'	-5.58	119.75	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1662	C	C5-C6-N1	5.58	123.79	121.00
2	2	1687	U	N3-C2-O2	-5.57	118.30	122.20
2	2	4930	C	C6-N1-C2	-5.57	118.07	120.30
2	2	4254	G	N3-C4-N9	5.57	129.34	126.00
2	2	2762	G	C8-N9-C4	-5.57	104.17	106.40
2	2	4920	C	C2-N1-C1'	5.56	124.92	118.80
2	2	412	G	O4'-C1'-N9	5.56	112.65	108.20
2	2	2783	A	N1-C2-N3	-5.56	126.52	129.30
2	2	4243	C	C2-N1-C1'	5.56	124.92	118.80
2	2	3641	U	N1-C2-N3	5.56	118.24	114.90
6	8	99	U	N1-C2-O2	5.56	126.69	122.80
2	2	1458	C	C6-N1-C2	-5.56	118.08	120.30
4	5	39	C	C2-N1-C1'	5.56	124.91	118.80
2	2	1458	C	N3-C2-O2	-5.55	118.01	121.90
2	2	4133	C	C5-C6-N1	5.55	123.77	121.00
6	8	32	C	N1-C2-O2	5.54	122.23	118.90
2	2	436	C	N1-C2-O2	5.54	122.22	118.90
2	2	4973	U	N1-C2-O2	5.54	126.68	122.80
2	2	662	C	N3-C2-O2	-5.54	118.02	121.90
2	2	1384	C	C6-N1-C2	-5.54	118.08	120.30
2	2	4678	G	P-O3'-C3'	5.54	126.35	119.70
6	8	99	U	C2-N1-C1'	5.54	124.34	117.70
2	2	1796	U	N3-C2-O2	-5.54	118.33	122.20
2	2	4902	C	C6-N1-C1'	-5.54	114.16	120.80
2	2	77	U	N1-C2-O2	5.53	126.67	122.80
2	2	985	C	C2-N1-C1'	5.53	124.88	118.80
2	2	1731	C	C5-C6-N1	5.53	123.77	121.00
2	2	1929	A	C4-N9-C1'	5.53	136.25	126.30
2	2	4504	C	C6-N1-C2	-5.53	118.09	120.30
2	2	4674	C	C5-C6-N1	5.52	123.76	121.00
2	2	4283	G	C8-N9-C1'	-5.52	119.82	127.00
2	2	4682	U	C5-C6-N1	5.52	125.46	122.70
2	2	1214	C	N1-C2-O2	5.52	122.21	118.90
2	2	1346	C	C5-C6-N1	5.52	123.76	121.00
2	2	1632	A	C2-N3-C4	5.52	113.36	110.60
2	2	1050	C	C6-N1-C2	-5.52	118.09	120.30
2	2	1304	C	C6-N1-C2	-5.52	118.09	120.30
2	2	2867	C	C2-N1-C1'	5.52	124.87	118.80
2	2	4926	C	C5-C6-N1	5.51	123.76	121.00
2	2	1364	U	C2-N3-C4	-5.50	123.70	127.00
23	Q	124	LEU	CA-CB-CG	5.50	127.96	115.30
2	2	188	G	C4-N9-C1'	5.50	133.66	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1789	C	C6-N1-C2	-5.50	118.10	120.30
2	2	4094	G	N3-C4-C5	-5.50	125.85	128.60
2	2	2351	C	N1-C2-O2	5.49	122.19	118.90
2	2	2078	C	C6-N1-C2	-5.49	118.11	120.30
2	2	4703	U	N1-C2-O2	5.49	126.64	122.80
2	2	4743	G	C8-N9-C1'	5.49	134.13	127.00
2	2	1633	G	O5'-P-OP1	-5.48	100.76	105.70
2	2	86	U	C2-N1-C1'	5.48	124.28	117.70
2	2	1190	C	N1-C2-O2	5.48	122.19	118.90
2	2	493	G	N1-C2-N2	5.48	121.13	116.20
2	2	188	G	N3-C4-N9	5.47	129.28	126.00
2	2	1275	G	C4-N9-C1'	-5.47	119.38	126.50
2	2	1397	A	O5'-P-OP1	-5.47	100.77	105.70
46	u	105	LEU	CA-CB-CG	5.47	127.89	115.30
2	2	412	G	C5-N7-C8	-5.47	101.56	104.30
2	2	3870	C	C5-C6-N1	5.47	123.73	121.00
2	2	1249	C	N1-C2-O2	5.47	122.18	118.90
2	2	1353	G	P-O3'-C3'	5.47	126.26	119.70
2	2	1477	C	C2-N1-C1'	5.47	124.81	118.80
6	8	101	C	C2-N1-C1'	5.47	124.81	118.80
2	2	2397	G	O4'-C1'-N9	5.46	112.57	108.20
2	2	4601	U	N3-C2-O2	-5.46	118.38	122.20
2	2	1469	C	C5-C6-N1	5.46	123.73	121.00
2	2	2303	C	N1-C2-N3	5.45	123.02	119.20
2	2	100	C	C5-C6-N1	5.45	123.72	121.00
2	2	1191	C	C6-N1-C2	-5.45	118.12	120.30
2	2	4926	C	C6-N1-C1'	-5.45	114.26	120.80
2	2	26	C	C5-C6-N1	5.45	123.72	121.00
2	2	2593	C	C5-C6-N1	5.45	123.72	121.00
2	2	4230	C	C6-N1-C2	-5.45	118.12	120.30
2	2	1402	C	N3-C2-O2	-5.44	118.09	121.90
2	2	123	C	C6-N1-C2	-5.44	118.12	120.30
2	2	995	C	C6-N1-C2	-5.44	118.12	120.30
2	2	1381	U	N1-C2-O2	5.44	126.61	122.80
2	2	4137	C	N1-C2-O2	5.44	122.16	118.90
2	2	3838	U	N3-C2-O2	-5.44	118.39	122.20
2	2	228	C	C5-C6-N1	5.43	123.72	121.00
2	2	2351	C	C5-C6-N1	5.43	123.72	121.00
2	2	294	G	N3-C4-N9	5.43	129.26	126.00
2	2	1203	G	C6-C5-N7	-5.43	127.14	130.40
2	2	1924	C	C6-N1-C2	-5.43	118.13	120.30
2	2	2250	C	N3-C2-O2	-5.43	118.10	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	152	U	C2-N1-C1'	5.43	124.21	117.70
2	2	4283	G	C4-N9-C1'	5.43	133.55	126.50
2	2	2333	G	N1-C6-O6	-5.42	116.65	119.90
2	2	3870	C	C2-N1-C1'	5.42	124.76	118.80
2	2	1275	G	C6-C5-N7	5.42	133.65	130.40
2	2	1192	C	C2-N1-C1'	5.42	124.76	118.80
2	2	1236	C	C5-C6-N1	5.42	123.71	121.00
2	2	4289	U	N3-C2-O2	-5.42	118.41	122.20
2	2	124	C	C6-N1-C2	-5.41	118.13	120.30
2	2	1093	C	C2-N1-C1'	5.41	124.75	118.80
2	2	4528	G	N3-C4-N9	5.41	129.25	126.00
47	v	99	ASP	N-CA-C	-5.41	96.39	111.00
7	A	168	ALA	CA-C-N	-5.41	105.30	117.20
2	2	4945	G	C8-N9-C1'	-5.41	119.97	127.00
36	d	43	LEU	CA-CB-CG	5.41	127.73	115.30
2	2	1241	C	C6-N1-C1'	-5.40	114.31	120.80
2	2	4712	C	C6-N1-C2	-5.40	118.14	120.30
2	2	3930	U	C2-N1-C1'	5.40	124.18	117.70
2	2	264	C	C2-N3-C4	5.40	122.60	119.90
2	2	123	C	C5-C6-N1	5.40	123.70	121.00
2	2	672	C	C6-N1-C2	-5.40	118.14	120.30
2	2	1178	G	C8-N9-C1'	-5.40	119.98	127.00
2	2	1912	G	C8-N9-C1'	-5.40	119.98	127.00
2	2	2544	G	C4-N9-C1'	5.40	133.51	126.50
6	8	135	C	C6-N1-C2	-5.40	118.14	120.30
2	2	1731	C	N1-C2-O2	5.39	122.14	118.90
2	2	4738	C	C6-N1-C2	-5.39	118.14	120.30
2	2	3893	C	C6-N1-C2	-5.39	118.14	120.30
2	2	1406	G	N7-C8-N9	5.39	115.79	113.10
2	2	1541	C	C5-C6-N1	5.39	123.69	121.00
2	2	3926	C	N3-C2-O2	-5.39	118.13	121.90
2	2	4171	C	N1-C2-O2	5.39	122.13	118.90
2	2	2540	C	C6-N1-C2	-5.38	118.15	120.30
2	2	408	A	P-O3'-C3'	5.38	126.16	119.70
2	2	2439	G	C8-N9-C1'	-5.38	120.01	127.00
2	2	4508	C	C6-N1-C2	-5.38	118.15	120.30
2	2	4193	C	C2-N1-C1'	5.38	124.71	118.80
2	2	4241	C	C2-N1-C1'	5.38	124.71	118.80
2	2	977	C	C2-N1-C1'	5.37	124.71	118.80
2	2	3851	U	N1-C2-O2	5.37	126.56	122.80
2	2	1816	C	C2-N1-C1'	5.37	124.70	118.80
2	2	1182	C	N3-C2-O2	-5.36	118.15	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1269	G	C4-N9-C1'	-5.36	119.53	126.50
2	2	1483	C	N3-C2-O2	-5.36	118.15	121.90
2	2	2319	C	P-O3'-C3'	5.36	126.14	119.70
2	2	4887	C	C2-N1-C1'	5.36	124.70	118.80
2	2	1242	G	N3-C4-N9	5.36	129.22	126.00
43	m	55	GLY	C-N-CA	5.36	135.09	121.70
2	2	1381	U	N3-C2-O2	-5.35	118.45	122.20
2	2	2667	C	N3-C2-O2	-5.35	118.16	121.90
13	G	193	LEU	CA-CB-CG	5.35	127.60	115.30
2	2	57	G	N1-C6-O6	-5.34	116.69	119.90
2	2	180	C	N3-C2-O2	-5.34	118.16	121.90
6	8	82	A	C2-N3-C4	5.34	113.27	110.60
2	2	4340	U	N3-C2-O2	-5.34	118.46	122.20
2	2	493	G	C8-N9-C4	-5.34	104.26	106.40
2	2	152	U	N1-C2-O2	5.34	126.54	122.80
2	2	337	U	N1-C2-O2	5.34	126.53	122.80
2	2	1893	C	N1-C2-O2	5.34	122.10	118.90
6	8	51	U	C2-N1-C1'	5.34	124.10	117.70
2	2	3775	A	C4-C5-N7	5.33	113.36	110.70
6	8	45	C	C6-N1-C2	-5.33	118.17	120.30
2	2	504	G	OP1-P-O3'	5.33	116.93	105.20
2	2	1577	G	C5-C6-O6	5.33	131.80	128.60
2	2	4861	G	C5-C6-O6	5.33	131.80	128.60
2	2	2701	U	N1-C2-O2	5.32	126.53	122.80
2	2	4365	C	N1-C2-O2	5.32	122.09	118.90
2	2	1576	G	N3-C4-C5	-5.32	125.94	128.60
2	2	4476	C	C6-N1-C1'	-5.32	114.42	120.80
2	2	2491	C	C6-N1-C1'	5.31	127.18	120.80
2	2	3838	U	N1-C2-O2	5.31	126.52	122.80
2	2	4699	U	OP1-P-O3'	5.31	116.89	105.20
2	2	1820	C	C5-C6-N1	5.31	123.65	121.00
2	2	2337	C	C5-C6-N1	5.31	123.65	121.00
2	2	1735	U	N3-C2-O2	-5.30	118.49	122.20
2	2	4613	C	N1-C2-O2	5.30	122.08	118.90
2	2	3634	G	N1-C6-O6	-5.30	116.72	119.90
2	2	5028	G	N3-C4-N9	5.30	129.18	126.00
47	v	50	LEU	CA-CB-CG	5.30	127.50	115.30
2	2	468	U	N3-C4-O4	5.30	123.11	119.40
2	2	2652	G	N3-C4-C5	5.30	131.25	128.60
2	2	43	U	N3-C2-O2	-5.30	118.49	122.20
2	2	2856	C	C2-N1-C1'	5.30	124.63	118.80
2	2	4281	A	C6-C5-N7	-5.30	128.59	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	2716	C	C6-N1-C2	-5.30	118.18	120.30
11	E	29	LEU	CA-CB-CG	5.30	127.48	115.30
2	2	3926	C	C2-N1-C1'	5.29	124.62	118.80
2	2	3778	U	C2-N1-C1'	5.29	124.05	117.70
2	2	4452	U	C6-N1-C2	-5.29	117.82	121.00
2	2	1243	C	N3-C2-O2	-5.29	118.20	121.90
2	2	4764	A	C6-N1-C2	5.29	121.77	118.60
2	2	4639	G	C2-N3-C4	5.29	114.54	111.90
2	2	2849	A	C2-N3-C4	5.28	113.24	110.60
2	2	220	C	C2-N1-C1'	5.28	124.61	118.80
2	2	86	U	N3-C2-O2	-5.28	118.50	122.20
2	2	188	G	N3-C4-C5	-5.28	125.96	128.60
2	2	4416	G	C4-N9-C1'	5.27	133.36	126.50
2	2	1705	G	N3-C4-N9	5.27	129.16	126.00
2	2	4281	A	C4-C5-N7	5.27	113.33	110.70
2	2	2319	C	C2'-C3'-O3'	5.27	122.13	113.70
2	2	4375	C	C6-N1-C2	-5.27	118.19	120.30
2	2	4981	G	C4-N9-C1'	5.27	133.35	126.50
2	2	4969	C	C5-C6-N1	5.26	123.63	121.00
2	2	4973	U	N3-C2-O2	-5.26	118.52	122.20
2	2	4559	A	N1-C2-N3	-5.26	126.67	129.30
2	2	455	C	C6-N1-C2	-5.26	118.19	120.30
2	2	1402	C	C2-N1-C1'	5.26	124.59	118.80
2	2	4561	C	C2-N1-C1'	5.26	124.59	118.80
4	5	6	C	C6-N1-C2	-5.26	118.20	120.30
2	2	4902	C	C5-C6-N1	5.26	123.63	121.00
2	2	1469	C	C6-N1-C2	-5.26	118.20	120.30
2	2	179	G	N3-C4-N9	5.25	129.15	126.00
2	2	1275	G	N9-C4-C5	5.25	107.50	105.40
2	2	179	G	C4-N9-C1'	5.25	133.33	126.50
2	2	3841	C	C6-N1-C2	-5.25	118.20	120.30
2	2	4547	C	P-O3'-C3'	5.25	126.00	119.70
2	2	4709	U	C6-N1-C2	-5.25	117.85	121.00
2	2	4280	A	C5-C6-N6	5.25	127.90	123.70
2	2	663	G	N3-C4-N9	5.25	129.15	126.00
2	2	1339	U	N3-C2-O2	-5.25	118.53	122.20
2	2	1248	C	C5-C6-N1	5.24	123.62	121.00
2	2	3688	U	N1-C2-O2	5.24	126.47	122.80
4	5	43	U	N1-C2-O2	5.24	126.47	122.80
2	2	2304	U	N3-C2-O2	-5.24	118.53	122.20
2	2	4094	G	N3-C4-N9	5.24	129.14	126.00
2	2	3685	C	C5-C6-N1	5.24	123.62	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	180	C	C6-N1-C1'	5.23	127.08	120.80
2	2	322	C	N1-C2-O2	5.23	122.04	118.90
2	2	390	C	C5-C6-N1	5.23	123.62	121.00
2	2	2447	U	N3-C2-O2	-5.23	118.54	122.20
2	2	2701	U	N3-C2-O2	-5.23	118.54	122.20
2	2	972	C	C6-N1-C2	-5.23	118.21	120.30
2	2	4229	U	C2-N1-C1'	5.22	123.97	117.70
2	2	3	C	C5-C6-N1	5.22	123.61	121.00
2	2	2843	U	N3-C2-O2	-5.22	118.55	122.20
2	2	4738	C	C5-C6-N1	5.22	123.61	121.00
2	2	130	C	C6-N1-C2	-5.22	118.21	120.30
6	8	35	C	C5-C6-N1	5.22	123.61	121.00
6	8	50	C	C6-N1-C2	-5.22	118.21	120.30
2	2	2867	C	N1-C2-O2	5.21	122.03	118.90
2	2	79	C	C6-N1-C2	-5.21	118.22	120.30
2	2	1203	G	N9-C4-C5	-5.21	103.32	105.40
2	2	1881	C	OP2-P-O3'	5.21	116.67	105.20
2	2	2257	C	C6-N1-C2	-5.21	118.22	120.30
2	2	4723	A	C2-N3-C4	5.21	113.20	110.60
2	2	1640	C	C6-N1-C2	-5.20	118.22	120.30
2	2	3696	C	C5-C6-N1	5.20	123.60	121.00
4	5	24	C	N1-C2-O2	5.20	122.02	118.90
2	2	1191	C	C5-C6-N1	5.20	123.60	121.00
2	2	1735	U	N1-C2-O2	5.20	126.44	122.80
6	8	122	G	C5-C6-O6	5.20	131.72	128.60
2	2	61	A	N7-C8-N9	5.20	116.40	113.80
2	2	4139	G	C6-C5-N7	-5.20	127.28	130.40
2	2	662	C	N1-C2-O2	5.20	122.02	118.90
2	2	204	U	N1-C2-O2	5.20	126.44	122.80
2	2	1468	C	C5-C6-N1	5.19	123.60	121.00
2	2	1476	C	C6-N1-C2	-5.19	118.22	120.30
2	2	2528	G	N7-C8-N9	5.19	115.69	113.10
2	2	2258	C	N3-C2-O2	-5.19	118.27	121.90
2	2	4118	U	N1-C2-O2	5.19	126.43	122.80
2	2	1632	A	C4-N9-C1'	5.19	135.63	126.30
2	2	3840	U	N1-C2-O2	5.18	126.43	122.80
2	2	686	A	C2-N3-C4	-5.18	108.01	110.60
2	2	2652	G	C4-N9-C1'	-5.18	119.77	126.50
6	8	129	C	N1-C2-O2	5.18	122.01	118.90
2	2	175	C	N1-C2-O2	5.17	122.00	118.90
2	2	256	G	N3-C4-C5	5.17	131.19	128.60
2	2	906	C	N1-C2-O2	5.17	122.00	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	3882	C	C5-C6-N1	5.17	123.59	121.00
2	2	971	U	N1-C2-O2	5.17	126.42	122.80
2	2	1250	C	C5-C6-N1	5.17	123.59	121.00
2	2	1377	G	C6-C5-N7	-5.17	127.30	130.40
2	2	4365	C	N3-C2-O2	-5.17	118.28	121.90
2	2	294	G	C5-C6-O6	-5.16	125.50	128.60
2	2	4709	U	C5-C6-N1	5.16	125.28	122.70
2	2	2652	G	C8-N9-C1'	5.16	133.71	127.00
2	2	4967	A	N9-C4-C5	-5.16	103.74	105.80
2	2	1405	C	C6-N1-C2	-5.15	118.24	120.30
2	2	1178	G	N3-C4-C5	-5.15	126.02	128.60
2	2	1267	C	N3-C2-O2	-5.15	118.30	121.90
2	2	4775	C	C6-N1-C1'	-5.15	114.62	120.80
2	2	1258	G	C4-N9-C1'	5.15	133.19	126.50
2	2	1853	G	C4-N9-C1'	5.15	133.19	126.50
2	2	3853	U	N3-C2-O2	-5.15	118.60	122.20
2	2	3649	A	N7-C8-N9	5.15	116.37	113.80
2	2	3863	C	C6-N1-C2	-5.14	118.24	120.30
2	2	513	U	N3-C2-O2	-5.14	118.60	122.20
2	2	963	G	C2-N3-C4	5.13	114.47	111.90
4	5	43	U	N3-C2-O2	-5.13	118.61	122.20
2	2	4201	G	N3-C4-N9	5.13	129.08	126.00
2	2	1236	C	C2-N1-C1'	5.13	124.44	118.80
2	2	1580	C	C6-N1-C2	-5.13	118.25	120.30
2	2	2103	G	C4-N9-C1'	5.13	133.16	126.50
2	2	4133	C	C6-N1-C2	-5.13	118.25	120.30
2	2	4139	G	C5-N7-C8	-5.12	101.74	104.30
2	2	4918	C	C2-N1-C1'	5.12	124.44	118.80
2	2	983	C	C6-N1-C2	-5.12	118.25	120.30
2	2	4862	G	N3-C2-N2	5.12	123.49	119.90
2	2	2072	C	C5-C6-N1	5.12	123.56	121.00
2	2	512	U	C2-N1-C1'	5.12	123.84	117.70
2	2	2257	C	C2-N1-C1'	5.12	124.43	118.80
2	2	1294	A	O4'-C1'-N9	5.11	112.29	108.20
2	2	2499	C	C5-C6-N1	5.11	123.56	121.00
2	2	4752	U	N3-C2-O2	-5.11	118.62	122.20
2	2	350	C	C6-N1-C2	-5.11	118.25	120.30
2	2	1856	C	C6-N1-C2	-5.11	118.26	120.30
2	2	181	C	C6-N1-C1'	5.10	126.92	120.80
2	2	1477	C	C5-C6-N1	5.10	123.55	121.00
2	2	1777	C	C2-N1-C1'	5.10	124.41	118.80
2	2	4698	C	C6-N1-C2	-5.10	118.26	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	8	122	G	N1-C6-O6	-5.10	116.84	119.90
2	2	2799	G	C4-C5-N7	5.10	112.84	110.80
2	2	164	G	N3-C4-N9	5.09	129.06	126.00
2	2	977	C	N1-C2-O2	5.09	121.96	118.90
2	2	3667	C	C6-N1-C2	-5.09	118.26	120.30
2	2	4272	G	C8-N9-C1'	-5.09	120.38	127.00
2	2	2856	C	C6-N1-C2	-5.09	118.26	120.30
2	2	1615	C	C6-N1-C2	-5.09	118.26	120.30
2	2	3631	U	N3-C2-O2	-5.09	118.64	122.20
4	5	76	U	C2-N1-C1'	5.09	123.81	117.70
2	2	507	G	C8-N9-C1'	-5.09	120.39	127.00
2	2	936	C	N3-C2-O2	-5.09	118.34	121.90
2	2	1358	G	C8-N9-C4	-5.09	104.36	106.40
4	5	57	C	C6-N1-C2	-5.09	118.27	120.30
2	2	3602	C	C5-C6-N1	5.08	123.54	121.00
2	2	3853	U	C2-N1-C1'	5.08	123.80	117.70
2	2	3892	U	N1-C2-O2	5.08	126.36	122.80
2	2	4416	G	N3-C4-N9	5.08	129.05	126.00
2	2	1720	C	C5-C6-N1	5.08	123.54	121.00
2	2	513	U	N1-C2-O2	5.08	126.36	122.80
6	8	92	U	N1-C2-O2	5.08	126.36	122.80
2	2	2544	G	N3-C4-N9	5.08	129.05	126.00
2	2	266	C	N1-C2-O2	5.08	121.95	118.90
2	2	3778	U	N1-C2-O2	5.07	126.35	122.80
2	2	4117	U	C5-C4-O4	5.07	128.94	125.90
2	2	4503	A	C2-N3-C4	5.07	113.14	110.60
2	2	4766	C	C5-C6-N1	5.07	123.54	121.00
7	A	179	LEU	CA-CB-CG	5.07	126.97	115.30
10	D	100	ARG	CG-CD-NE	-5.07	101.15	111.80
2	2	459	C	C5-C6-N1	5.07	123.54	121.00
2	2	686	A	C4-C5-C6	-5.07	114.47	117.00
2	2	2819	U	N3-C2-O2	-5.07	118.65	122.20
2	2	4528	G	C4-N9-C1'	5.07	133.09	126.50
4	5	4	U	C2-N1-C1'	5.07	123.78	117.70
2	2	209	U	O4'-C1'-N1	5.07	112.25	108.20
4	5	57	C	C5-C6-N1	5.07	123.53	121.00
2	2	1702	C	N3-C2-O2	-5.07	118.35	121.90
2	2	2803	U	N1-C2-O2	5.07	126.34	122.80
2	2	4961	G	N3-C4-N9	5.07	129.04	126.00
2	2	453	G	C4-N9-C1'	5.06	133.08	126.50
2	2	1406	G	C8-N9-C4	-5.06	104.38	106.40
2	2	1578	U	N1-C2-O2	5.06	126.34	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1847	C	C6-N1-C2	-5.06	118.28	120.30
2	2	2084	C	OP2-P-O3'	5.06	116.33	105.20
2	2	1236	C	N1-C2-O2	5.06	121.94	118.90
2	2	2351	C	C6-N1-C2	-5.05	118.28	120.30
2	2	3812	C	C6-N1-C2	-5.05	118.28	120.30
2	2	4698	C	N1-C2-O2	5.05	121.93	118.90
2	2	1906	U	N3-C2-O2	-5.05	118.66	122.20
2	2	4360	U	N1-C2-O2	5.05	126.34	122.80
2	2	3851	U	N3-C2-O2	-5.05	118.67	122.20
2	2	4138	C	N3-C2-O2	-5.05	118.36	121.90
2	2	209	U	N3-C2-O2	-5.05	118.67	122.20
2	2	2392	C	C6-N1-C2	-5.05	118.28	120.30
2	2	3694	U	C2-N1-C1'	5.05	123.76	117.70
2	2	4080	C	C6-N1-C2	-5.04	118.28	120.30
2	2	4905	C	C5-C6-N1	5.04	123.52	121.00
2	2	3775	A	C6-C5-N7	-5.04	128.77	132.30
2	2	1512	G	N1-C6-O6	-5.04	116.88	119.90
2	2	512	U	N1-C2-O2	5.04	126.33	122.80
2	2	1577	G	N3-C2-N2	-5.04	116.37	119.90
2	2	14	C	C6-N1-C2	-5.04	118.29	120.30
2	2	2491	C	C2-N1-C1'	-5.04	113.26	118.80
6	8	90	C	C5-C6-N1	5.04	123.52	121.00
2	2	1293	G	N3-C4-C5	-5.03	126.08	128.60
2	2	4766	C	C6-N1-C2	-5.03	118.29	120.30
2	2	4975	G	O4'-C1'-N9	5.03	112.23	108.20
6	8	41	A	O5'-P-OP1	-5.03	101.17	105.70
2	2	2416	G	C8-N9-C4	-5.03	104.39	106.40
2	2	4945	G	C4-N9-C1'	5.03	133.04	126.50
2	2	1705	G	C6-N1-C2	-5.03	122.08	125.10
2	2	3778	U	C5-C6-N1	5.03	125.22	122.70
2	2	4905	C	C6-N1-C2	-5.03	118.29	120.30
2	2	4939	C	N1-C2-O2	5.03	121.92	118.90
2	2	290	U	C5-C6-N1	5.03	125.21	122.70
2	2	2856	C	N1-C2-O2	5.03	121.92	118.90
4	5	44	C	N1-C2-O2	5.03	121.92	118.90
4	5	34	C	C6-N1-C2	-5.03	118.29	120.30
2	2	2059	C	C6-N1-C2	-5.02	118.29	120.30
2	2	4201	G	C8-N9-C1'	-5.02	120.47	127.00
2	2	67	C	C5-C6-N1	5.02	123.51	121.00
2	2	2603	C	C5-C6-N1	5.02	123.51	121.00
2	2	2675	G	OP2-P-O3'	5.02	116.25	105.20
2	2	4162	C	N3-C2-O2	-5.02	118.39	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1535	C	C5-C6-N1	5.02	123.51	121.00
2	2	3606	U	C2-N1-C1'	5.02	123.72	117.70
2	2	1178	G	N3-C4-N9	5.02	129.01	126.00
2	2	150	U	C4-C5-C6	-5.01	116.69	119.70
2	2	436	C	N3-C2-O2	-5.01	118.39	121.90
2	2	2491	C	N3-C4-N4	-5.01	114.49	118.00
2	2	4420	U	C5-C6-N1	5.01	125.21	122.70
2	2	4764	A	N3-C4-C5	5.01	130.31	126.80
2	2	4937	C	C5-C6-N1	5.01	123.51	121.00
2	2	1405	C	N3-C2-O2	-5.01	118.39	121.90
2	2	2067	C	N3-C2-O2	-5.01	118.39	121.90
2	2	2491	C	C5-C4-N4	5.01	123.71	120.20
2	2	4243	C	C6-N1-C2	-5.01	118.30	120.30
2	2	1911	C	C6-N1-C2	-5.01	118.30	120.30
2	2	2589	C	C6-N1-C2	-5.01	118.30	120.30
2	2	4482	U	N3-C2-O2	-5.01	118.69	122.20
2	2	4994	G	C4-N9-C1'	5.01	133.01	126.50
2	2	3826	C	C6-N1-C2	-5.01	118.30	120.30
2	2	4352	U	N3-C2-O2	-5.01	118.69	122.20
2	2	4951	G	N3-C4-N9	5.01	129.00	126.00
2	2	333	U	N3-C2-O2	-5.01	118.70	122.20
2	2	4461	C	C5-C6-N1	5.00	123.50	121.00
2	2	654	C	C6-N1-C2	-5.00	118.30	120.30
2	2	4201	G	N3-C4-C5	-5.00	126.10	128.60

There are no chirality outliers.

All (25) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	3	324	VAL	Peptide
3	3	330	ALA	Peptide
3	3	338	LYS	Peptide
3	3	341	THR	Peptide
7	A	159	MET	Peptide
7	A	168	ALA	Mainchain
7	A	46	ASP	Peptide
11	E	52	CYS	Peptide
13	G	208	ASN	Peptide
15	I	175	PHE	Peptide
15	I	188	GLN	Peptide
18	L	93	ASN	Peptide
20	N	94	LEU	Peptide

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Mol	Chain	Res	Type	Group
34	b	5	GLY	Peptide
35	c	132	PRO	Peptide
35	c	136	ARG	Peptide
35	c	80	VAL	Peptide
42	l	122	LYS	Peptide
42	l	20	ARG	Peptide
43	m	54	ARG	Peptide
45	t	34	ASN	Peptide
45	t	91	CYS	Peptide
46	u	103	VAL	Peptide
46	u	106	TYR	Peptide
47	v	129	GLY	Peptide

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

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

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	62/477 (13%)	58 (94%)	3 (5%)	1 (2%)	8	31
3	3	252/534 (47%)	220 (87%)	32 (13%)	0	100	100
5	6	218/245 (89%)	205 (94%)	13 (6%)	0	100	100
7	A	210/217 (97%)	179 (85%)	29 (14%)	2 (1%)	13	42
8	B	401/403 (100%)	380 (95%)	21 (5%)	0	100	100
9	C	93/159 (58%)	88 (95%)	5 (5%)	0	100	100
10	D	354/427 (83%)	327 (92%)	26 (7%)	1 (0%)	37	68
11	E	92/115 (80%)	87 (95%)	5 (5%)	0	100	100
12	F	112/117 (96%)	109 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	G	239/266 (90%)	225 (94%)	14 (6%)	0	100	100
14	H	120/123 (98%)	116 (97%)	4 (3%)	0	100	100
15	I	188/192 (98%)	173 (92%)	14 (7%)	1 (0%)	25	58
16	J	150/214 (70%)	135 (90%)	15 (10%)	0	100	100
17	K	100/105 (95%)	93 (93%)	7 (7%)	0	100	100
18	L	145/148 (98%)	133 (92%)	11 (8%)	1 (1%)	19	51
19	M	84/97 (87%)	79 (94%)	5 (6%)	0	100	100
20	N	174/178 (98%)	143 (82%)	29 (17%)	2 (1%)	12	39
21	O	67/70 (96%)	62 (92%)	5 (8%)	0	100	100
22	P	48/51 (94%)	44 (92%)	4 (8%)	0	100	100
23	Q	201/211 (95%)	184 (92%)	16 (8%)	1 (0%)	25	58
24	R	45/128 (35%)	38 (84%)	7 (16%)	0	100	100
25	S	133/215 (62%)	126 (95%)	7 (5%)	0	100	100
26	T	105/125 (84%)	98 (93%)	7 (7%)	0	100	100
27	U	201/204 (98%)	191 (95%)	9 (4%)	1 (0%)	25	58
28	V	199/203 (98%)	195 (98%)	4 (2%)	0	100	100
29	W	101/106 (95%)	93 (92%)	8 (8%)	0	100	100
30	X	89/92 (97%)	84 (94%)	5 (6%)	0	100	100
31	Y	151/184 (82%)	140 (93%)	11 (7%)	0	100	100
32	Z	185/188 (98%)	177 (96%)	8 (4%)	0	100	100
33	a	151/196 (77%)	145 (96%)	6 (4%)	0	100	100
34	b	173/176 (98%)	163 (94%)	9 (5%)	1 (1%)	22	53
35	c	157/160 (98%)	146 (93%)	11 (7%)	0	100	100
36	d	99/128 (77%)	87 (88%)	12 (12%)	0	100	100
37	e	128/140 (91%)	120 (94%)	8 (6%)	0	100	100
38	f	59/157 (38%)	57 (97%)	2 (3%)	0	100	100
39	g	115/156 (74%)	108 (94%)	7 (6%)	0	100	100
40	h	129/145 (89%)	120 (93%)	9 (7%)	0	100	100
41	i	133/136 (98%)	115 (86%)	18 (14%)	0	100	100
42	l	123/137 (90%)	111 (90%)	12 (10%)	0	100	100
43	m	246/257 (96%)	221 (90%)	24 (10%)	1 (0%)	30	63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	r	291/297 (98%)	267 (92%)	24 (8%)	0	100	100
45	t	126/135 (93%)	116 (92%)	10 (8%)	0	100	100
46	u	107/110 (97%)	100 (94%)	5 (5%)	2 (2%)	6	27
47	v	231/288 (80%)	209 (90%)	20 (9%)	2 (1%)	14	45
48	w	224/248 (90%)	208 (93%)	16 (7%)	0	100	100
All	All	7011/8660 (81%)	6475 (92%)	520 (7%)	16 (0%)	45	74

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	A	171	HIS
15	I	176	LEU
7	A	169	VAL
46	u	80	ASN
47	v	179	LEU
27	U	84	PRO
47	v	106	VAL
1	0	397	MET
18	L	96	GLY
20	N	11	PRO
20	N	117	ILE
46	u	107	PRO
10	D	232	VAL
43	m	55	GLY
34	b	155	PRO
23	Q	62	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	58/404 (14%)	58 (100%)	0	100	100
3	3	234/485 (48%)	229 (98%)	5 (2%)	48	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	6	190/213 (89%)	189 (100%)	1 (0%)	86	92
7	A	191/196 (97%)	188 (98%)	3 (2%)	58	79
8	B	349/349 (100%)	346 (99%)	3 (1%)	75	88
9	C	80/126 (64%)	80 (100%)	0	100	100
10	D	298/348 (86%)	293 (98%)	5 (2%)	56	78
11	E	79/97 (81%)	78 (99%)	1 (1%)	65	82
12	F	98/100 (98%)	97 (99%)	1 (1%)	73	86
13	G	203/223 (91%)	202 (100%)	1 (0%)	86	92
14	H	109/110 (99%)	108 (99%)	1 (1%)	75	88
15	I	169/171 (99%)	168 (99%)	1 (1%)	84	91
16	J	133/181 (74%)	133 (100%)	0	100	100
17	K	86/89 (97%)	85 (99%)	1 (1%)	67	83
18	L	120/121 (99%)	120 (100%)	0	100	100
19	M	73/80 (91%)	72 (99%)	1 (1%)	62	81
20	N	148/149 (99%)	141 (95%)	7 (5%)	22	52
21	O	64/65 (98%)	64 (100%)	0	100	100
22	P	47/48 (98%)	47 (100%)	0	100	100
23	Q	169/177 (96%)	168 (99%)	1 (1%)	84	91
24	R	43/116 (37%)	41 (95%)	2 (5%)	22	52
25	S	115/161 (71%)	113 (98%)	2 (2%)	56	78
26	T	98/110 (89%)	96 (98%)	2 (2%)	50	74
27	U	171/172 (99%)	168 (98%)	3 (2%)	54	76
28	V	173/174 (99%)	171 (99%)	2 (1%)	67	83
29	W	91/94 (97%)	91 (100%)	0	100	100
30	X	74/75 (99%)	74 (100%)	0	100	100
31	Y	134/163 (82%)	133 (99%)	1 (1%)	81	90
32	Z	164/165 (99%)	161 (98%)	3 (2%)	54	76
33	a	137/175 (78%)	136 (99%)	1 (1%)	81	90
34	b	156/157 (99%)	155 (99%)	1 (1%)	84	91
35	c	139/140 (99%)	138 (99%)	1 (1%)	81	90
36	d	91/115 (79%)	88 (97%)	3 (3%)	33	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	e	100/107 (94%)	99 (99%)	1 (1%)	73	86
38	f	54/126 (43%)	54 (100%)	0	100	100
39	g	105/133 (79%)	103 (98%)	2 (2%)	52	75
40	h	122/135 (90%)	117 (96%)	5 (4%)	26	57
41	i	117/118 (99%)	116 (99%)	1 (1%)	75	88
42	l	109/121 (90%)	105 (96%)	4 (4%)	29	59
43	m	190/199 (96%)	185 (97%)	5 (3%)	41	68
44	r	246/250 (98%)	245 (100%)	1 (0%)	89	94
45	t	114/121 (94%)	114 (100%)	0	100	100
46	u	88/89 (99%)	88 (100%)	0	100	100
47	v	208/252 (82%)	202 (97%)	6 (3%)	37	65
48	w	195/215 (91%)	195 (100%)	0	100	100
All	All	6132/7415 (83%)	6054 (99%)	78 (1%)	64	82

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	3	265	LEU
3	3	295	ASP
3	3	298	THR
3	3	324	VAL
3	3	341	THR
5	6	193	ILE
7	A	60	ARG
7	A	137	LEU
7	A	169	VAL
8	B	329	ASP
8	B	341[A]	LYS
8	B	341[B]	LYS
10	D	114	ARG
10	D	122	TYR
10	D	184	TYR
10	D	188	ARG
10	D	306	ARG
11	E	28	VAL
12	F	54	ARG
13	G	231	ASP
14	H	23	ASP

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Mol	Chain	Res	Type
15	I	57	VAL
17	K	29	ARG
19	M	22	CYS
20	N	57	VAL
20	N	60	PHE
20	N	94	LEU
20	N	95	ARG
20	N	114	ASP
20	N	143	ASP
20	N	178	LYS
23	Q	70	VAL
24	R	103	LEU
24	R	121	LEU
25	S	31	ILE
25	S	106	ASP
26	T	26	THR
26	T	69	ASN
27	U	38	ARG
27	U	99	GLN
27	U	174	LEU
28	V	27	VAL
28	V	117	ARG
31	Y	30	ARG
32	Z	28	LEU
32	Z	42	THR
32	Z	184	ARG
33	a	84	THR
34	b	90	THR
35	c	130	ARG
36	d	35	ASP
36	d	81	ARG
36	d	113	ARG
37	e	48	ARG
39	g	95	THR
39	g	127	LEU
40	h	10	ASP
40	h	55	VAL
40	h	74	TYR
40	h	78	TYR
40	h	84	ARG
41	i	112	ARG
42	l	27	THR

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Mol	Chain	Res	Type
42	l	49	VAL
42	l	63	VAL
42	l	105	ASP
43	m	3	ARG
43	m	30	ARG
43	m	68	ARG
43	m	84	THR
43	m	247	ARG
44	r	217	ASP
47	v	100	LYS
47	v	106	VAL
47	v	128	HIS
47	v	221	LYS
47	v	224	LYS
47	v	240	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
3	3	183	GLN
3	3	192	HIS
3	3	232	HIS
3	3	358	GLN
3	3	370	ASN
3	3	382	ASN
5	6	66	ASN
5	6	75	ASN
5	6	82	GLN
5	6	83	HIS
5	6	118	HIS
7	A	22	GLN
7	A	84	HIS
7	A	94	ASN
8	B	3	HIS
8	B	42	HIS
8	B	302	ASN
9	C	60	ASN
13	G	85	GLN
13	G	141	ASN
13	G	227	ASN
15	I	78	GLN
15	I	116	ASN

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Mol	Chain	Res	Type
16	J	213	HIS
18	L	66	ASN
20	N	3	GLN
20	N	42	GLN
20	N	46	GLN
20	N	98	ASN
21	O	28	ASN
23	Q	87	HIS
23	Q	149	GLN
23	Q	159	ASN
24	R	90	ASN
25	S	48	GLN
27	U	196	ASN
29	W	19	GLN
29	W	102	GLN
30	X	56	HIS
31	Y	25	HIS
31	Y	28	ASN
31	Y	34	GLN
31	Y	93	HIS
31	Y	97	ASN
31	Y	116	HIS
32	Z	44	ASN
32	Z	160	HIS
33	a	7	GLN
33	a	75	HIS
34	b	77	ASN
35	c	144	ASN
36	d	94	ASN
36	d	116	GLN
38	f	59	HIS
39	g	151	ASN
41	i	40	HIS
42	l	6	GLN
43	m	132	ASN
43	m	162	ASN
44	r	225	GLN
45	t	117	GLN
47	v	250	GLN
47	v	268	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	2	3489/5070 (68%)	896 (25%)	27 (0%)
4	5	119/120 (99%)	18 (15%)	0
6	8	155/156 (99%)	24 (15%)	0
All	All	3763/5346 (70%)	938 (24%)	27 (0%)

All (938) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	2	2	G
2	2	13	U
2	2	21	G
2	2	30	C
2	2	39	A
2	2	42	A
2	2	48	G
2	2	56	A
2	2	59	A
2	2	64	A
2	2	65	A
2	2	67	C
2	2	69	A
2	2	71	C
2	2	73	A
2	2	74	G
2	2	75	G
2	2	84	A
2	2	88	A
2	2	91	G
2	2	98	A
2	2	108	A
2	2	109	G
2	2	110	C
2	2	116	G
2	2	117	C
2	2	119	G
2	2	120	A
2	2	121	A
2	2	132	G
2	2	133	C
2	2	134	G
2	2	135	G
2	2	136	C
2	2	137	G

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Mol	Chain	Res	Type
2	2	141	C
2	2	143	C
2	2	144	G
2	2	150	U
2	2	151	G
2	2	152	U
2	2	157	U
2	2	159	C
2	2	165	A
2	2	172	C
2	2	176	G
2	2	177	G
2	2	180	C
2	2	181	C
2	2	183	C
2	2	184	U
2	2	185	C
2	2	186	G
2	2	188	G
2	2	189	G
2	2	200	U
2	2	216	C
2	2	218	A
2	2	220	C
2	2	233	U
2	2	234	G
2	2	254	G
2	2	255	C
2	2	256	G
2	2	257	C
2	2	258	G
2	2	259	C
2	2	261	G
2	2	265	C
2	2	266	C
2	2	276	C
2	2	277	G
2	2	278	G
2	2	279	A
2	2	280	G
2	2	297	U
2	2	305	A

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Mol	Chain	Res	Type
2	2	306	A
2	2	315	G
2	2	316	U
2	2	318	A
2	2	326	C
2	2	340	C
2	2	353	A
2	2	363	A
2	2	372	A
2	2	377	A
2	2	379	G
2	2	383	A
2	2	387	G
2	2	396	A
2	2	398	A2M
2	2	407	A
2	2	408	A
2	2	409	G
2	2	410	A
2	2	412	G
2	2	413	G
2	2	449	C
2	2	450	G
2	2	452	A
2	2	453	G
2	2	454	U
2	2	457	G
2	2	461	G
2	2	462	G
2	2	464	G
2	2	465	G
2	2	467	U
2	2	472	C
2	2	473	C
2	2	479	G
2	2	483	G
2	2	484	U
2	2	485	C
2	2	486	C
2	2	489	C
2	2	493	G
2	2	494	U

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Mol	Chain	Res	Type
2	2	497	G
2	2	498	C
2	2	500	G
2	2	501	C
2	2	502	C
2	2	503	C
2	2	504	G
2	2	505	G
2	2	507	G
2	2	509	A
2	2	510	U
2	2	511	C
2	2	512	U
2	2	513	U
2	2	514	U
2	2	515	C
2	2	517	C
2	2	518	G
2	2	519	C
2	2	643	C
2	2	644	G
2	2	645	G
2	2	646	G
2	2	653	U
2	2	654	C
2	2	656	C
2	2	657	C
2	2	659	G
2	2	661	C
2	2	665	C
2	2	666	G
2	2	667	A
2	2	668	C
2	2	670	G
2	2	674	G
2	2	682	G
2	2	685	C
2	2	686	A
2	2	687	U
2	2	692	A
2	2	695	G
2	2	696	C

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Mol	Chain	Res	Type
2	2	697	G
2	2	703	G
2	2	704	C
2	2	708	G
2	2	718	C
2	2	730	G
2	2	731	G
2	2	738	C
2	2	739	G
2	2	742	G
2	2	746	A
2	2	748	G
2	2	751	G
2	2	757	G
2	2	904	C
2	2	905	C
2	2	913	U
2	2	914	U
2	2	915	A
2	2	917	A
2	2	918	G
2	2	923	C
2	2	924	C
2	2	926	G
2	2	932	A
2	2	933	G
2	2	935	A
2	2	936	C
2	2	941	C
2	2	943	A
2	2	944	A
2	2	945	U
2	2	946	C
2	2	959	G
2	2	960	A
2	2	961	G
2	2	962	C
2	2	965	G
2	2	966	A
2	2	967	C
2	2	970	G
2	2	971	U

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Mol	Chain	Res	Type
2	2	977	C
2	2	982	U
2	2	984	C
2	2	988	C
2	2	989	U
2	2	990	C
2	2	991	C
2	2	992	C
2	2	993	G
2	2	995	C
2	2	996	G
2	2	1048	G
2	2	1049	C
2	2	1050	C
2	2	1051	G
2	2	1069	G
2	2	1070	G
2	2	1072	C
2	2	1073	G
2	2	1083	U
2	2	1094	G
2	2	1100	U
2	2	1168	G
2	2	1171	G
2	2	1172	C
2	2	1173	G
2	2	1175	A
2	2	1178	G
2	2	1179	U
2	2	1180	C
2	2	1181	C
2	2	1182	C
2	2	1183	C
2	2	1184	A
2	2	1190	C
2	2	1198	G
2	2	1200	G
2	2	1202	C
2	2	1203	G
2	2	1210	C
2	2	1211	G
2	2	1214	C

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Mol	Chain	Res	Type
2	2	1215	C
2	2	1216	C
2	2	1217	G
2	2	1222	A
2	2	1241	C
2	2	1242	G
2	2	1243	C
2	2	1246	G
2	2	1249	C
2	2	1252	C
2	2	1253	G
2	2	1255	A
2	2	1256	G
2	2	1257	A
2	2	1258	G
2	2	1259	G
2	2	1266	G
2	2	1267	C
2	2	1269	G
2	2	1270	A
2	2	1271	G
2	2	1272	C
2	2	1273	G
2	2	1275	G
2	2	1277	G
2	2	1280	C
2	2	1284	G
2	2	1287	G
2	2	1293	G
2	2	1294	A
2	2	1295	C
2	2	1300	G
2	2	1301	C
2	2	1303	A
2	2	1304	C
2	2	1314	C
2	2	1316	OMG
2	2	1326	A2M
2	2	1337	A
2	2	1354	A
2	2	1356	U
2	2	1358	G

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Mol	Chain	Res	Type
2	2	1359	G
2	2	1365	C
2	2	1367	C
2	2	1370	G
2	2	1377	G
2	2	1378	C
2	2	1379	C
2	2	1382	G
2	2	1387	A
2	2	1393	G
2	2	1394	G
2	2	1398	A
2	2	1399	G
2	2	1400	G
2	2	1403	G
2	2	1407	C
2	2	1408	G
2	2	1409	C
2	2	1410	U
2	2	1412	G
2	2	1415	G
2	2	1420	A
2	2	1425	G
2	2	1438	U
2	2	1442	C
2	2	1443	A
2	2	1444	G
2	2	1445	U
2	2	1447	C
2	2	1452	A
2	2	1473	U
2	2	1480	C
2	2	1482	G
2	2	1483	C
2	2	1497	A
2	2	1498	G
2	2	1501	C
2	2	1502	G
2	2	1514	U
2	2	1525	A
2	2	1534	A2M
2	2	1537	A

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Mol	Chain	Res	Type
2	2	1547	A
2	2	1566	C
2	2	1578	U
2	2	1586	G
2	2	1591	U
2	2	1596	U
2	2	1597	G
2	2	1621	A
2	2	1624	G
2	2	1625	OMG
2	2	1631	A
2	2	1633	G
2	2	1634	A
2	2	1637	A
2	2	1638	A
2	2	1640	C
2	2	1641	G
2	2	1642	A
2	2	1654	G
2	2	1661	C
2	2	1663	C
2	2	1676	C
2	2	1677	PSU
2	2	1678	C
2	2	1679	A
2	2	1680	G
2	2	1694	C
2	2	1696	C
2	2	1697	G
2	2	1699	A
2	2	1700	G
2	2	1701	A
2	2	1704	C
2	2	1705	G
2	2	1715	C
2	2	1716	G
2	2	1717	C
2	2	1719	A
2	2	1726	U
2	2	1731	C
2	2	1734	G
2	2	1740	C

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Mol	Chain	Res	Type
2	2	1742	A
2	2	1750	G
2	2	1753	G
2	2	1781	U
2	2	1785	C
2	2	1787	A
2	2	1804	A
2	2	1810	G
2	2	1815	G
2	2	1817	U
2	2	1821	G
2	2	1822	U
2	2	1834	U
2	2	1836	G
2	2	1837	A
2	2	1842	G
2	2	1843	A
2	2	1855	G
2	2	1867	A
2	2	1869	G
2	2	1881	C
2	2	1882	U
2	2	1888	A
2	2	1892	A
2	2	1897	A
2	2	1915	C
2	2	1917	A
2	2	1918	U
2	2	1919	G
2	2	1920	C
2	2	1922	G
2	2	1930	U
2	2	1931	C
2	2	1935	C
2	2	1939	A
2	2	1947	U
2	2	1948	G
2	2	1949	U
2	2	1951	G
2	2	1958	A
2	2	1959	U
2	2	1960	A

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Mol	Chain	Res	Type
2	2	1961	G
2	2	1962	A
2	2	1963	C
2	2	1964	A
2	2	1965	G
2	2	2024	G
2	2	2025	A
2	2	2026	A
2	2	2033	A
2	2	2034	G
2	2	2046	G
2	2	2048	U
2	2	2055	G
2	2	2056	G
2	2	2069	A
2	2	2071	A
2	2	2084	C
2	2	2085	G
2	2	2091	C
2	2	2093	A
2	2	2094	G
2	2	2095	A
2	2	2096	G
2	2	2097	U
2	2	2098	G
2	2	2100	A
2	2	2102	G
2	2	2103	G
2	2	2104	G
2	2	2106	G
2	2	2108	G
2	2	2111	G
2	2	2112	G
2	2	2113	C
2	2	2250	C
2	2	2252	G
2	2	2253	A
2	2	2254	G
2	2	2256	C
2	2	2258	C
2	2	2268	A
2	2	2269	C

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Mol	Chain	Res	Type
2	2	2277	C
2	2	2280	G
2	2	2289	C
2	2	2300	A
2	2	2301	G
2	2	2306	G
2	2	2313	A
2	2	2320	G
2	2	2333	G
2	2	2348	G
2	2	2351	C
2	2	2357	G
2	2	2364	OMG
2	2	2369	U
2	2	2382	A
2	2	2389	A
2	2	2395	A
2	2	2398	U
2	2	2401	A2M
2	2	2402	G
2	2	2409	U
2	2	2417	A
2	2	2422	OMC
2	2	2425	U
2	2	2426	U
2	2	2436	U
2	2	2437	C
2	2	2441	C
2	2	2447	U
2	2	2450	G
2	2	2453	A
2	2	2460	A
2	2	2464	C
2	2	2465	C
2	2	2471	G
2	2	2472	A
2	2	2474	G
2	2	2475	G
2	2	2476	G
2	2	2478	C
2	2	2484	A
2	2	2487	G

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Mol	Chain	Res	Type
2	2	2488	C
2	2	2489	C
2	2	2490	U
2	2	2491	C
2	2	2492	C
2	2	2493	G
2	2	2494	U
2	2	2503	G
2	2	2504	C
2	2	2505	C
2	2	2506	G
2	2	2511	A
2	2	2513	A
2	2	2519	U
2	2	2520	C
2	2	2525	U
2	2	2526	C
2	2	2529	A
2	2	2537	A
2	2	2544	G
2	2	2546	G
2	2	2547	G
2	2	2553	A
2	2	2560	C
2	2	2566	G
2	2	2567	G
2	2	2573	A
2	2	2577	C
2	2	2583	C
2	2	2586	G
2	2	2587	A
2	2	2589	C
2	2	2592	U
2	2	2596	G
2	2	2601	A
2	2	2618	G
2	2	2623	A
2	2	2627	C
2	2	2653	C
2	2	2662	G
2	2	2663	G
2	2	2664	G

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Mol	Chain	Res	Type
2	2	2669	C
2	2	2670	C
2	2	2675	G
2	2	2676	A
2	2	2686	G
2	2	2687	U
2	2	2694	G
2	2	2695	A
2	2	2696	A
2	2	2706	G
2	2	2707	U
2	2	2708	U
2	2	2709	C
2	2	2710	C
2	2	2711	G
2	2	2719	C
2	2	2723	U
2	2	2725	A
2	2	2726	G
2	2	2739	C
2	2	2742	G
2	2	2743	A
2	2	2756	G
2	2	2761	U
2	2	2763	U
2	2	2764	A
2	2	2768	C
2	2	2769	U
2	2	2770	C
2	2	2788	U
2	2	2790	U
2	2	2794	C
2	2	2806	A
2	2	2814	C
2	2	2815	A
2	2	2819	U
2	2	2826	U
2	2	2827	G
2	2	2829	U
2	2	2835	A
2	2	2838	G
2	2	2842	G

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Mol	Chain	Res	Type
2	2	2846	G
2	2	2848	G
2	2	2855	G
2	2	2856	C
2	2	2857	A
2	2	2867	C
2	2	2875	C
2	2	2877	G
2	2	2885	A
2	2	2897	G
2	2	2900	U
2	2	2902	G
2	2	3604	A
2	2	3605	C
2	2	3606	U
2	2	3615	G
2	2	3618	C
2	2	3626	G
2	2	3635	A
2	2	3644	U
2	2	3648	A
2	2	3649	A
2	2	3662	A
2	2	3664	G
2	2	3667	C
2	2	3672	G
2	2	3673	C
2	2	3674	G
2	2	3680	U
2	2	3691	G
2	2	3710	G
2	2	3711	A
2	2	3713	U
2	2	3714	G
2	2	3728	A
2	2	3729	PSU
2	2	3734	U
2	2	3735	G
2	2	3736	A
2	2	3748	A
2	2	3774	A
2	2	3776	G

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Mol	Chain	Res	Type
2	2	3777	G
2	2	3778	U
2	2	3783	A
2	2	3784	A
2	2	3785	A2M
2	2	3786	U
2	2	3802	U
2	2	3810	C
2	2	3811	G
2	2	3812	C
2	2	3813	A
2	2	3814	U
2	2	3817	A
2	2	3818	U
2	2	3819	G
2	2	3823	G
2	2	3838	U
2	2	3840	U
2	2	3867	A2M
2	2	3868	G
2	2	3871	A
2	2	3876	A
2	2	3877	A
2	2	3878	C
2	2	3879	G
2	2	3892	U
2	2	3898	G
2	2	3901	A
2	2	3902	A
2	2	3906	A
2	2	3907	G
2	2	3908	A
2	2	3915	U
2	2	3916	G
2	2	3925	U
2	2	3926	C
2	2	3938	G
2	2	3939	G
2	2	3941	G
2	2	4076	G
2	2	4084	G
2	2	4086	G

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Mol	Chain	Res	Type
2	2	4095	G
2	2	4097	G
2	2	4101	C
2	2	4104	G
2	2	4105	A
2	2	4106	G
2	2	4107	G
2	2	4110	C
2	2	4111	U
2	2	4112	C
2	2	4113	U
2	2	4114	C
2	2	4115	G
2	2	4116	C
2	2	4117	U
2	2	4119	C
2	2	4120	U
2	2	4122	G
2	2	4133	C
2	2	4140	C
2	2	4141	G
2	2	4142	C
2	2	4143	G
2	2	4146	G
2	2	4147	G
2	2	4150	G
2	2	4151	G
2	2	4160	C
2	2	4162	C
2	2	4163	U
2	2	4168	G
2	2	4170	A
2	2	4177	C
2	2	4183	G
2	2	4184	G
2	2	4191	G
2	2	4193	C
2	2	4195	G
2	2	4201	G
2	2	4212	A
2	2	4215	C
2	2	4221	C

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Mol	Chain	Res	Type
2	2	4222	G
2	2	4225	G
2	2	4228	G
2	2	4229	U
2	2	4233	A
2	2	4237	C
2	2	4249	G
2	2	4251	A
2	2	4254	G
2	2	4257	A
2	2	4268	A
2	2	4271	A
2	2	4273	A
2	2	4281	A
2	2	4282	A
2	2	4297	G
2	2	4304	A
2	2	4305	G
2	2	4312	U
2	2	4314	C
2	2	4319	C
2	2	4329	G
2	2	4330	G
2	2	4332	C
2	2	4348	A
2	2	4349	C
2	2	4350	C
2	2	4372	U
2	2	4373	G
2	2	4376	A
2	2	4377	G
2	2	4378	A
2	2	4379	A
2	2	4381	A
2	2	4386	C
2	2	4387	C
2	2	4391	G
2	2	4394	A
2	2	4405	G
2	2	4415	1MA
2	2	4418	G
2	2	4421	C

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Mol	Chain	Res	Type
2	2	4422	A
2	2	4424	A
2	2	4426	C
2	2	4429	C
2	2	4437	U
2	2	4438	U
2	2	4444	C
2	2	4448	G
2	2	4449	A
2	2	4464	A
2	2	4466	C
2	2	4475	G
2	2	4488	A
2	2	4500	PSU
2	2	4502	C
2	2	4510	A
2	2	4512	U
2	2	4513	A
2	2	4518	A
2	2	4519	C
2	2	4524	G
2	2	4528	G
2	2	4530	UR3
2	2	4531	PSU
2	2	4532	U
2	2	4545	G
2	2	4548	A
2	2	4549	G
2	2	4560	C
2	2	4567	G
2	2	4570	G
2	2	4573	G
2	2	4575	G
2	2	4589	A
2	2	4590	A
2	2	4600	G
2	2	4601	U
2	2	4606	G
2	2	4617	G
2	2	4635	A
2	2	4636	PSU
2	2	4637	OMG

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Mol	Chain	Res	Type
2	2	4647	G
2	2	4656	A
2	2	4657	U
2	2	4670	C
2	2	4677	U
2	2	4679	G
2	2	4694	G
2	2	4695	C
2	2	4700	A
2	2	4704	C
2	2	4708	A
2	2	4709	U
2	2	4720	C
2	2	4729	A
2	2	4731	G
2	2	4732	G
2	2	4733	C
2	2	4734	A
2	2	4735	G
2	2	4740	G
2	2	4741	C
2	2	4742	G
2	2	4745	G
2	2	4751	G
2	2	4754	G
2	2	4757	C
2	2	4759	C
2	2	4761	G
2	2	4764	A
2	2	4765	G
2	2	4771	C
2	2	4773	C
2	2	4774	C
2	2	4775	C
2	2	4776	G
2	2	4859	C
2	2	4861	G
2	2	4862	G
2	2	4870	OMG
2	2	4871	C
2	2	4875	G
2	2	4876	U

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Mol	Chain	Res	Type
2	2	4880	C
2	2	4881	U
2	2	4882	U
2	2	4883	C
2	2	4886	C
2	2	4889	G
2	2	4895	C
2	2	4896	G
2	2	4897	G
2	2	4898	G
2	2	4899	G
2	2	4900	C
2	2	4901	G
2	2	4910	G
2	2	4911	A
2	2	4912	G
2	2	4914	C
2	2	4919	G
2	2	4920	C
2	2	4922	C
2	2	4924	C
2	2	4927	G
2	2	4928	C
2	2	4931	G
2	2	4935	C
2	2	4937	C
2	2	4941	G
2	2	4943	A
2	2	4949	G
2	2	4955	A
2	2	4960	G
2	2	4961	G
2	2	4963	G
2	2	4966	A
2	2	4975	G
2	2	4976	U
2	2	4980	C
2	2	4985	U
2	2	4988	U
2	2	4989	U
2	2	4990	C
2	2	4991	U

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Mol	Chain	Res	Type
2	2	5013	C
2	2	5014	A
2	2	5017	G
2	2	5020	G
2	2	5022	U
2	2	5023	C
2	2	5024	C
2	2	5025	C
2	2	5028	G
2	2	5029	C
2	2	5030	U
2	2	5031	G
2	2	5034	A
2	2	5041	G
2	2	5050	C
2	2	5053	U
2	2	5054	C
2	2	5055	G
2	2	5058	A
2	2	5061	A
2	2	5069	U
4	5	4	U
4	5	5	A
4	5	13	A
4	5	22	A
4	5	23	A
4	5	29	C
4	5	33	U
4	5	38	U
4	5	42	A
4	5	53	U
4	5	54	A
4	5	63	C
4	5	64	G
4	5	71	G
4	5	74	A
4	5	97	G
4	5	100	A
4	5	110	G
6	8	25	G
6	8	34	U
6	8	35	C

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Mol	Chain	Res	Type
6	8	59	A
6	8	62	A
6	8	63	U
6	8	69	U
6	8	80	A
6	8	82	A
6	8	83	C
6	8	85	U
6	8	87	G
6	8	103	A
6	8	105	C
6	8	110	U
6	8	114	G
6	8	123	U
6	8	124	U
6	8	125	C
6	8	126	C
6	8	127	U
6	8	150	C
6	8	151	G
6	8	156	U

All (27) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	2	150	U
2	2	406	C
2	2	408	A
2	2	504	G
2	2	730	G
2	2	914	U
2	2	1082	C
2	2	1353	G
2	2	1625	OMG
2	2	1930	U
2	2	2033	A
2	2	2084	C
2	2	2319	C
2	2	2416	G
2	2	2587	A
2	2	2675	G
2	2	2760	G

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Mol	Chain	Res	Type
2	2	3614	G
2	2	3673	C
2	2	4378	A
2	2	4547	C
2	2	4548	A
2	2	4600	G
2	2	4678	G
2	2	4699	U
2	2	4913	G
2	2	5022	U

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

99 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	$\# Z  > 2$
2	A2M	2	1534	49,2	18,25,26	4.17	8 (44%)	18,36,39	2.98	3 (16%)
2	E7G	2	2297	2	24,27,28	3.40	11 (45%)	30,40,43	2.25	11 (36%)
2	OMG	2	3792	2	18,26,27	2.31	6 (33%)	19,38,41	1.48	4 (21%)
2	5MU	2	4083	2	19,22,23	4.49	7 (36%)	28,32,35	3.87	9 (32%)
2	A2M	2	4571	2	18,25,26	4.20	9 (50%)	18,36,39	2.79	3 (16%)
2	OMC	2	3869	2	19,22,23	2.63	7 (36%)	26,31,34	0.72	0
2	OMC	2	3887	2	19,22,23	2.70	7 (36%)	26,31,34	0.97	0
2	OMG	2	2364	2	18,26,27	2.17	6 (33%)	19,38,41	1.65	4 (21%)
2	A2M	2	3723	2,17	18,25,26	4.22	6 (33%)	18,36,39	3.21	3 (16%)
2	PSU	2	3729	2	18,21,22	1.04	1 (5%)	22,30,33	1.81	4 (18%)
2	B8K	2	4690	2	24,28,29	4.42	15 (62%)	30,42,45	2.86	13 (43%)
2	5MC	2	4447	2	18,22,23	3.20	7 (38%)	26,32,35	1.67	5 (19%)
2	B9B	2	2754	2,41	21,28,29	5.61	8 (38%)	23,40,43	2.47	6 (26%)
2	OMG	2	1883	2	18,26,27	2.17	6 (33%)	19,38,41	1.90	5 (26%)
2	A2M	2	2401	2	18,25,26	4.16	9 (50%)	18,36,39	2.76	3 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	OMC	2	3701	49,2	19,22,23	2.49	7 (36%)	26,31,34	0.83	0
2	A2M	2	1524	2	18,25,26	4.04	7 (38%)	18,36,39	3.13	4 (22%)
2	A2M	2	1326	2	18,25,26	4.06	7 (38%)	18,36,39	3.46	3 (16%)
2	A2M	2	1871	2	18,25,26	4.24	8 (44%)	18,36,39	2.99	4 (22%)
2	PSU	2	4636	2	18,21,22	1.27	3 (16%)	22,30,33	2.21	6 (27%)
2	1MA	2	1322	49,2	16,25,26	3.51	5 (31%)	18,37,40	1.86	3 (16%)
2	OMC	2	2861	2	19,22,23	2.75	7 (36%)	26,31,34	0.75	1 (3%)
2	OMC	2	2365	49,2	19,22,23	2.62	7 (36%)	26,31,34	0.86	1 (3%)
2	B8W	2	4129	2	18,26,27	6.07	8 (44%)	21,38,41	2.91	10 (47%)
2	PSU	2	4442	2	18,21,22	1.08	1 (5%)	22,30,33	1.77	4 (18%)
2	B8W	2	2380	2	18,26,27	6.11	8 (44%)	21,38,41	2.38	7 (33%)
2	MHG	2	4371	2	29,32,33	3.62	12 (41%)	34,46,49	2.59	12 (35%)
2	2MG	2	1517	2	18,26,27	2.13	6 (33%)	16,38,41	1.85	5 (31%)
2	P4U	2	1348	2	21,24,25	3.33	8 (38%)	27,33,36	1.13	1 (3%)
2	BGH	2	3899	2	25,29,30	3.97	16 (64%)	31,43,46	2.38	13 (41%)
2	I4U	2	1659	49,2	21,24,25	4.49	15 (71%)	27,34,37	1.80	7 (25%)
2	PSU	2	1677	2	18,21,22	1.40	3 (16%)	22,30,33	2.06	5 (22%)
2	OMG	2	4637	2	18,26,27	2.23	6 (33%)	19,38,41	1.59	4 (21%)
2	5MC	2	4335	2	18,22,23	3.18	7 (38%)	26,32,35	1.27	1 (3%)
2	PSU	2	4531	2	18,21,22	0.96	1 (5%)	22,30,33	1.77	4 (18%)
2	A2M	2	4523	49,2	18,25,26	3.99	8 (44%)	18,36,39	3.19	5 (27%)
2	OMC	2	3909	2	19,22,23	2.85	8 (42%)	26,31,34	1.46	4 (15%)
2	PSU	2	4403	2	18,21,22	1.05	1 (5%)	22,30,33	1.89	5 (22%)
2	PSU	2	4293	2	18,21,22	1.21	2 (11%)	22,30,33	1.94	4 (18%)
2	OMC	2	2422	49,2	19,22,23	2.69	7 (36%)	26,31,34	1.03	1 (3%)
2	B8W	2	4185	2	18,26,27	6.41	8 (44%)	21,38,41	2.52	7 (33%)
2	B8T	2	4671	2	19,22,23	3.13	8 (42%)	26,31,34	1.06	2 (7%)
2	P7G	2	3880	2	24,28,29	3.97	11 (45%)	27,41,44	2.12	3 (11%)
2	B9B	2	237	2	21,28,29	5.67	9 (42%)	23,40,43	2.41	6 (26%)
2	7MG	2	2522	2,12	22,26,27	3.13	10 (45%)	29,39,42	2.07	10 (34%)
2	B8H	2	1860	2	19,22,23	6.81	7 (36%)	22,32,35	2.48	5 (22%)
2	OMG	2	373	2,19	18,26,27	2.25	7 (38%)	19,38,41	1.76	5 (26%)
2	I4U	2	4194	2	21,24,25	4.65	16 (76%)	27,34,37	1.63	7 (25%)
2	B8T	2	4483	2	19,22,23	3.39	8 (42%)	26,31,34	0.87	2 (7%)
2	OMG	2	1316	49,2	18,26,27	2.24	6 (33%)	19,38,41	1.81	4 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	PSU	2	2508	2	18,21,22	1.09	2 (11%)	22,30,33	1.86	4 (18%)
2	A2M	2	3718	2	18,25,26	4.25	7 (38%)	18,36,39	2.99	3 (16%)
2	UR3	2	4597	2	19,22,23	2.53	6 (31%)	26,32,35	1.32	4 (15%)
2	P7G	2	1909	2	24,28,29	4.18	11 (45%)	27,41,44	1.91	5 (18%)
2	A2M	2	3867	2	18,25,26	3.98	6 (33%)	18,36,39	2.97	4 (22%)
2	OMG	2	1625	49,2	18,26,27	2.25	7 (38%)	19,38,41	1.53	4 (21%)
2	OMG	2	4870	2	18,26,27	2.35	8 (44%)	19,38,41	1.61	4 (21%)
2	2MG	2	729	2,34	18,26,27	2.37	6 (33%)	16,38,41	1.63	3 (18%)
2	7MG	2	4550	2	22,26,27	2.99	10 (45%)	29,39,42	1.96	9 (31%)
2	OMG	2	2050	2	18,26,27	2.18	5 (27%)	19,38,41	1.63	5 (26%)
2	OMC	2	4536	2	19,22,23	2.60	7 (36%)	26,31,34	0.99	0
2	2MG	2	978	2	18,26,27	2.35	7 (38%)	16,38,41	1.42	4 (25%)
2	B8H	2	4296	2	19,22,23	6.90	6 (31%)	22,32,35	2.50	5 (22%)
2	6MZ	2	4220	2	18,25,26	1.92	4 (22%)	16,36,39	3.52	3 (18%)
2	OMG	2	4370	2,29	18,26,27	2.28	7 (38%)	19,38,41	1.63	5 (26%)
2	UR3	2	1866	2	19,22,23	2.77	5 (26%)	26,32,35	1.68	5 (19%)
2	OMG	2	2773	2	18,26,27	2.34	8 (44%)	19,38,41	1.66	4 (21%)
2	PSU	2	4450	49,2	18,21,22	1.06	2 (11%)	22,30,33	1.91	4 (18%)
2	B9H	2	2786	49,2	20,25,26	2.68	5 (25%)	22,35,38	3.46	7 (31%)
2	B9B	2	1574	2	21,28,29	5.63	9 (42%)	23,40,43	2.31	4 (17%)
2	PSU	2	4628	2	18,21,22	1.15	2 (11%)	22,30,33	1.89	5 (22%)
2	OMG	2	4623	2	18,26,27	2.22	6 (33%)	19,38,41	1.67	4 (21%)
2	OMU	2	4620	2	19,22,23	2.64	7 (36%)	26,31,34	1.84	5 (19%)
2	PSU	2	1582	2	18,21,22	1.18	3 (16%)	22,30,33	1.78	3 (13%)
2	OMG	2	1522	2	18,26,27	2.22	7 (38%)	19,38,41	1.51	3 (15%)
2	B8Q	2	1456	2	17,22,23	2.79	5 (29%)	22,32,35	2.35	6 (27%)
2	A2M	2	2363	49,2	18,25,26	4.09	9 (50%)	18,36,39	3.03	3 (16%)
2	B8K	2	3897	2	24,28,29	4.12	16 (66%)	30,42,45	2.59	13 (43%)
2	B8W	2	4472	2	18,26,27	6.21	8 (44%)	21,38,41	2.50	8 (38%)
2	A2M	2	398	2	18,25,26	4.22	7 (38%)	18,36,39	2.96	3 (16%)
2	OMG	2	4196	49,2	18,26,27	2.33	8 (44%)	19,38,41	1.46	3 (15%)
2	PSU	2	3715	2	18,21,22	1.02	1 (5%)	22,30,33	1.72	4 (18%)
2	UR3	2	4530	2	19,22,23	2.84	6 (31%)	26,32,35	1.55	4 (15%)
2	E6G	2	4355	2	20,27,28	5.95	9 (45%)	22,39,42	2.74	9 (40%)
2	M7A	2	4564	2	20,25,26	1.91	4 (20%)	28,37,40	3.95	7 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	5MC	2	3782	49,2	18,22,23	3.12	7 (38%)	26,32,35	1.22	3 (11%)
2	E7G	2	1797	2	24,27,28	3.57	11 (45%)	30,40,43	2.27	9 (30%)
2	A2M	2	3825	2	18,25,26	4.08	7 (38%)	18,36,39	3.04	3 (16%)
2	PSU	2	4500	2	18,21,22	1.19	3 (16%)	22,30,33	2.00	5 (22%)
2	2MG	2	4872	28,2,25	18,26,27	2.76	7 (38%)	16,38,41	1.62	3 (18%)
2	OMC	2	2804	2	19,22,23	2.56	7 (36%)	26,31,34	0.76	0
2	OMG	2	2424	49,2	18,26,27	2.27	7 (38%)	19,38,41	1.47	3 (15%)
2	7MG	2	1605	2	22,26,27	3.12	10 (45%)	29,39,42	2.08	8 (27%)
2	OMU	2	4306	2	19,22,23	2.68	7 (36%)	26,31,34	1.85	5 (19%)
2	A2M	2	3785	2	18,25,26	3.90	9 (50%)	18,36,39	3.04	3 (16%)
2	PSU	2	1683	2	18,21,22	1.24	2 (11%)	22,30,33	1.79	5 (22%)
2	OMG	2	4494	2	18,26,27	2.29	6 (33%)	19,38,41	1.57	5 (26%)
2	B8W	2	4529	49,2,3	18,26,27	6.03	7 (38%)	21,38,41	3.20	9 (42%)
2	1MA	2	4415	2	16,25,26	3.97	4 (25%)	18,37,40	1.72	3 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A2M	2	1534	49,2	-	2/5/27/28	0/3/3/3
2	E7G	2	2297	2	-	1/9/39/40	0/3/3/3
2	OMG	2	3792	2	-	0/5/27/28	0/3/3/3
2	5MU	2	4083	2	-	0/7/25/26	0/2/2/2
2	A2M	2	4571	2	-	0/5/27/28	0/3/3/3
2	OMC	2	3869	2	-	0/9/27/28	0/2/2/2
2	OMC	2	3887	2	-	1/9/27/28	0/2/2/2
2	OMG	2	2364	2	-	2/5/27/28	0/3/3/3
2	A2M	2	3723	2,17	-	0/5/27/28	0/3/3/3
2	PSU	2	3729	2	-	2/7/25/26	0/2/2/2
2	B8K	2	4690	2	-	0/11/41/42	0/3/3/3
2	5MC	2	4447	2	-	3/7/25/26	0/2/2/2
2	B9B	2	2754	2,41	-	4/7/29/30	0/3/3/3
2	OMG	2	1883	2	-	2/5/27/28	0/3/3/3
2	A2M	2	2401	2	-	2/5/27/28	0/3/3/3
2	OMC	2	3701	49,2	-	4/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A2M	2	1524	2	-	0/5/27/28	0/3/3/3
2	A2M	2	1326	2	-	0/5/27/28	0/3/3/3
2	A2M	2	1871	2	-	0/5/27/28	0/3/3/3
2	PSU	2	4636	2	-	5/7/25/26	0/2/2/2
2	1MA	2	1322	49,2	-	0/3/25/26	0/3/3/3
2	OMC	2	2861	2	-	1/9/27/28	0/2/2/2
2	OMC	2	2365	49,2	-	0/9/27/28	0/2/2/2
2	B8W	2	4129	2	-	2/5/27/28	0/3/3/3
2	PSU	2	4442	2	-	0/7/25/26	0/2/2/2
2	B8W	2	2380	2	-	4/5/27/28	0/3/3/3
2	MHG	2	4371	2	-	7/16/46/47	0/3/3/3
2	2MG	2	1517	2	-	0/5/27/28	0/3/3/3
2	P4U	2	1348	2	-	2/10/29/30	0/2/2/2
2	BGH	2	3899	2	-	2/13/43/44	0/3/3/3
2	I4U	2	1659	49,2	-	1/9/29/30	0/2/2/2
2	PSU	2	1677	2	-	5/7/25/26	0/2/2/2
2	OMG	2	4637	2	-	2/5/27/28	0/3/3/3
2	5MC	2	4335	2	-	0/7/25/26	0/2/2/2
2	PSU	2	4531	2	-	0/7/25/26	0/2/2/2
2	A2M	2	4523	49,2	-	0/5/27/28	0/3/3/3
2	OMC	2	3909	2	-	1/9/27/28	0/2/2/2
2	PSU	2	4403	2	-	2/7/25/26	0/2/2/2
2	PSU	2	4293	2	-	0/7/25/26	0/2/2/2
2	OMC	2	2422	49,2	-	2/9/27/28	0/2/2/2
2	B8W	2	4185	2	-	3/5/27/28	0/3/3/3
2	B8T	2	4671	2	-	0/7/27/28	0/2/2/2
2	P7G	2	3880	2	-	5/10/40/41	0/3/3/3
2	B9B	2	237	2	-	6/7/29/30	0/3/3/3
2	7MG	2	2522	2,12	-	0/7/37/38	0/3/3/3
2	B8H	2	1860	2	-	2/7/25/26	0/2/2/2
2	OMG	2	373	2,19	-	0/5/27/28	0/3/3/3
2	I4U	2	4194	2	-	4/9/29/30	0/2/2/2
2	B8T	2	4483	2	-	0/7/27/28	0/2/2/2
2	OMG	2	1316	49,2	-	2/5/27/28	0/3/3/3
2	PSU	2	2508	2	-	0/7/25/26	0/2/2/2
2	A2M	2	3718	2	-	0/5/27/28	0/3/3/3
2	UR3	2	4597	2	-	0/7/25/26	0/2/2/2
2	P7G	2	1909	2	-	1/10/40/41	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A2M	2	3867	2	-	2/5/27/28	0/3/3/3
2	OMG	2	1625	49,2	-	2/5/27/28	0/3/3/3
2	OMG	2	4870	2	-	3/5/27/28	0/3/3/3
2	2MG	2	729	2,34	-	1/5/27/28	0/3/3/3
2	7MG	2	4550	2	-	0/7/37/38	0/3/3/3
2	OMG	2	2050	2	-	0/5/27/28	0/3/3/3
2	OMC	2	4536	2	-	1/9/27/28	0/2/2/2
2	2MG	2	978	2	-	0/5/27/28	0/3/3/3
2	B8H	2	4296	2	-	4/7/25/26	0/2/2/2
2	6MZ	2	4220	2	-	0/5/27/28	0/3/3/3
2	OMG	2	4370	2,29	-	0/5/27/28	0/3/3/3
2	UR3	2	1866	2	-	0/7/25/26	0/2/2/2
2	OMG	2	2773	2	-	1/5/27/28	0/3/3/3
2	PSU	2	4450	49,2	-	1/7/25/26	0/2/2/2
2	B9H	2	2786	49,2	-	2/12/47/48	0/2/2/2
2	B9B	2	1574	2	-	3/7/29/30	0/3/3/3
2	PSU	2	4628	2	-	0/7/25/26	0/2/2/2
2	OMG	2	4623	2	-	0/5/27/28	0/3/3/3
2	OMU	2	4620	2	-	0/9/27/28	0/2/2/2
2	PSU	2	1582	2	-	0/7/25/26	0/2/2/2
2	OMG	2	1522	2	-	0/5/27/28	0/3/3/3
2	B8Q	2	1456	2	-	0/7/42/43	0/2/2/2
2	A2M	2	2363	49,2	-	0/5/27/28	0/3/3/3
2	B8K	2	3897	2	-	3/11/41/42	0/3/3/3
2	B8W	2	4472	2	-	2/5/27/28	0/3/3/3
2	A2M	2	398	2	-	2/5/27/28	0/3/3/3
2	OMG	2	4196	49,2	-	1/5/27/28	0/3/3/3
2	PSU	2	3715	2	-	0/7/25/26	0/2/2/2
2	UR3	2	4530	2	-	2/7/25/26	0/2/2/2
2	E6G	2	4355	2	-	4/6/28/29	0/3/3/3
2	M7A	2	4564	2	-	0/7/37/38	0/3/3/3
2	5MC	2	3782	49,2	-	0/7/25/26	0/2/2/2
2	E7G	2	1797	2	-	3/9/39/40	0/3/3/3
2	A2M	2	3825	2	-	0/5/27/28	0/3/3/3
2	PSU	2	4500	2	-	5/7/25/26	0/2/2/2
2	2MG	2	4872	28,2,25	-	2/5/27/28	0/3/3/3
2	OMC	2	2804	2	-	0/9/27/28	0/2/2/2
2	OMG	2	2424	49,2	-	0/5/27/28	0/3/3/3
2	7MG	2	1605	2	-	0/7/37/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMU	2	4306	2	-	0/9/27/28	0/2/2/2
2	A2M	2	3785	2	-	2/5/27/28	0/3/3/3
2	PSU	2	1683	2	-	1/7/25/26	0/2/2/2
2	OMG	2	4494	2	-	1/5/27/28	0/3/3/3
2	B8W	2	4529	49,2,3	-	2/5/27/28	0/3/3/3
2	1MA	2	4415	2	-	2/3/25/26	0/3/3/3

All (691) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	4185	B8W	O4'-C1'	17.66	1.65	1.41
2	2	4472	B8W	O4'-C1'	17.39	1.65	1.41
2	2	2380	B8W	O4'-C1'	17.36	1.65	1.41
2	2	4129	B8W	O4'-C1'	17.34	1.65	1.41
2	2	4296	B8H	C6-C5	-17.27	1.10	1.34
2	2	4355	E6G	C2'-C1'	-17.13	1.27	1.53
2	2	1860	B8H	C6-C5	-16.93	1.11	1.34
2	2	237	B9B	C2'-C1'	-16.78	1.28	1.53
2	2	4185	B8W	C2'-C1'	-16.78	1.28	1.53
2	2	4529	B8W	O4'-C1'	16.75	1.64	1.41
2	2	4296	B8H	C4-N3	-16.58	1.08	1.38
2	2	1574	B9B	C2'-C1'	-16.29	1.29	1.53
2	2	1860	B8H	C4-N3	-16.15	1.08	1.38
2	2	2754	B9B	C2'-C1'	-16.08	1.29	1.53
2	2	4472	B8W	C2'-C1'	-15.84	1.29	1.53
2	2	3723	A2M	O4'-C1'	15.13	1.62	1.41
2	2	4355	E6G	O4'-C1'	15.04	1.62	1.41
2	2	2380	B8W	C2'-C1'	-15.00	1.31	1.53
2	2	1871	A2M	O4'-C1'	14.99	1.62	1.41
2	2	2754	B9B	O4'-C1'	14.90	1.61	1.41
2	2	4129	B8W	C2'-C1'	-14.89	1.31	1.53
2	2	3718	A2M	O4'-C1'	14.78	1.61	1.41
2	2	4529	B8W	C2'-C1'	-14.76	1.31	1.53
2	2	398	A2M	O4'-C1'	14.73	1.61	1.41
2	2	1574	B9B	O4'-C1'	14.61	1.61	1.41
2	2	1534	A2M	O4'-C1'	14.52	1.61	1.41
2	2	2401	A2M	O4'-C1'	14.35	1.61	1.41
2	2	4415	1MA	C2-N3	14.33	1.46	1.29
2	2	4571	A2M	O4'-C1'	14.29	1.61	1.41
2	2	237	B9B	O4'-C1'	14.25	1.61	1.41
2	2	3825	A2M	O4'-C1'	13.96	1.60	1.41
2	2	1326	A2M	O4'-C1'	13.72	1.60	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1524	A2M	O4'-C1'	13.72	1.60	1.41
2	2	2363	A2M	O4'-C1'	13.55	1.60	1.41
2	2	3867	A2M	O4'-C1'	13.41	1.59	1.41
2	2	4523	A2M	O4'-C1'	13.29	1.59	1.41
2	2	3785	A2M	O4'-C1'	13.16	1.59	1.41
2	2	4296	B8H	C4-C5	12.71	1.80	1.44
2	2	1860	B8H	C4-C5	12.67	1.80	1.44
2	2	1322	1MA	C2-N3	12.30	1.43	1.29
2	2	1909	P7G	C8-N9	12.19	1.52	1.46
2	2	3880	P7G	C8-N9	11.98	1.52	1.46
2	2	4296	B8H	C6-N1	11.63	1.65	1.36
2	2	1860	B8H	C6-N1	11.62	1.65	1.36
2	2	1659	I4U	C3'-C2'	-10.70	1.24	1.53
2	2	4690	B8K	C3'-C4'	-10.41	1.26	1.53
2	2	4194	I4U	C3'-C2'	-10.40	1.24	1.53
2	2	3897	B8K	C3'-C4'	-10.35	1.26	1.53
2	2	3899	BGH	C3'-C4'	-10.30	1.26	1.53
2	2	4690	B8K	O4'-C4'	10.14	1.67	1.45
2	2	4083	5MU	C6-N1	9.93	1.55	1.38
2	2	3897	B8K	O4'-C4'	9.89	1.67	1.45
2	2	1348	P4U	C4-N3	9.75	1.44	1.31
2	2	4083	5MU	C2-N1	9.40	1.53	1.38
2	2	1797	E7G	C8-N9	9.30	1.51	1.46
2	2	1909	P7G	C5-N7	8.98	1.45	1.35
2	2	4529	B8W	C2-N2	8.91	1.51	1.33
2	2	4447	5MC	C6-C5	8.89	1.49	1.34
2	2	4194	I4U	C4-N3	8.88	1.42	1.31
2	2	237	B9B	O4'-C4'	-8.80	1.25	1.45
2	2	3899	BGH	O4'-C4'	8.73	1.64	1.45
2	2	4355	E6G	O4'-C4'	-8.52	1.26	1.45
2	2	4083	5MU	C4-C5	8.32	1.58	1.44
2	2	1659	I4U	C4-N3	8.22	1.42	1.31
2	2	1574	B9B	O4'-C4'	-8.21	1.26	1.45
2	2	2786	B9H	C2-N3	8.19	1.47	1.37
2	2	4083	5MU	C4-N3	-8.18	1.23	1.38
2	2	4371	MHG	C8-N9	8.17	1.50	1.46
2	2	2297	E7G	C8-N9	8.10	1.50	1.46
2	2	1659	I4U	O4'-C4'	-8.10	1.26	1.45
2	2	1797	E7G	C5-N7	8.09	1.44	1.35
2	2	4335	5MC	C6-C5	8.07	1.47	1.34
2	2	4129	B8W	C2-N2	8.02	1.49	1.33
2	2	2297	E7G	C5-N7	7.97	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	4194	I4U	O4'-C4'	-7.93	1.27	1.45
2	2	2380	B8W	C2-N2	7.90	1.49	1.33
2	2	4371	MHG	C5-N7	7.89	1.44	1.35
2	2	4472	B8W	C2-N2	7.89	1.49	1.33
2	2	4185	B8W	C2-N2	7.83	1.49	1.33
2	2	1456	B8Q	C6-C5	7.82	1.50	1.33
2	2	2754	B9B	O4'-C4'	-7.82	1.27	1.45
2	2	3782	5MC	C6-C5	7.79	1.47	1.34
2	2	3880	P7G	C5-N7	7.69	1.44	1.35
2	2	2522	7MG	C5-N7	7.58	1.44	1.35
2	2	2363	A2M	O4'-C4'	-7.49	1.28	1.45
2	2	4371	MHG	C2-N3	7.43	1.46	1.31
2	2	1605	7MG	C5-N7	7.34	1.44	1.35
2	2	4523	A2M	O4'-C4'	-7.32	1.28	1.45
2	2	4571	A2M	O4'-C4'	-7.25	1.28	1.45
2	2	1524	A2M	O4'-C4'	-7.25	1.28	1.45
2	2	4530	UR3	C2-N1	7.21	1.48	1.38
2	2	1326	A2M	O4'-C4'	-7.01	1.29	1.45
2	2	3867	A2M	O4'-C4'	-7.00	1.29	1.45
2	2	1456	B8Q	C2-N3	6.98	1.47	1.35
2	2	4872	2MG	C2-N2	6.96	1.48	1.33
2	2	4550	7MG	C5-N7	6.96	1.43	1.35
2	2	4483	B8T	C2-N3	6.95	1.50	1.36
2	2	398	A2M	O4'-C4'	-6.92	1.29	1.45
2	2	3718	A2M	O4'-C4'	-6.91	1.29	1.45
2	2	3825	A2M	O4'-C4'	-6.89	1.29	1.45
2	2	2401	A2M	O4'-C4'	-6.80	1.29	1.45
2	2	1534	A2M	O4'-C4'	-6.76	1.29	1.45
2	2	1866	UR3	C2-N1	6.66	1.48	1.38
2	2	3785	A2M	O4'-C4'	-6.64	1.30	1.45
2	2	1866	UR3	C6-C5	6.62	1.50	1.35
2	2	2754	B9B	O6-C6	6.60	1.40	1.35
2	2	1909	P7G	C4-N3	6.54	1.49	1.37
2	2	4194	I4U	C6-C5	6.52	1.50	1.35
2	2	4530	UR3	C6-C5	6.51	1.50	1.35
2	2	1871	A2M	O4'-C4'	-6.50	1.30	1.45
2	2	4483	B8T	C6-C5	6.50	1.50	1.35
2	2	1605	7MG	C8-N9	6.50	1.49	1.46
2	2	4483	B8T	C4-N3	6.50	1.44	1.32
2	2	3880	P7G	C4-N3	6.50	1.49	1.37
2	2	4671	B8T	C6-C5	6.45	1.50	1.35
2	2	4550	7MG	C8-N9	6.32	1.49	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	3723	A2M	O4'-C4'	-6.30	1.30	1.45
2	2	4671	B8T	C2-N3	6.26	1.49	1.36
2	2	2522	7MG	C8-N9	6.21	1.49	1.46
2	2	4355	E6G	O6-C6	6.15	1.40	1.35
2	2	1659	I4U	C6-C5	6.13	1.49	1.35
2	2	1348	P4U	C2-N3	6.09	1.48	1.36
2	2	4597	UR3	C6-C5	6.07	1.49	1.35
2	2	4371	MHG	C8-N7	6.04	1.51	1.45
2	2	3897	B8K	O4'-C1'	-6.02	1.27	1.42
2	2	4483	B8T	C4-N4	6.00	1.48	1.35
2	2	4690	B8K	C8-N9	5.99	1.49	1.46
2	2	4220	6MZ	C6-N6	5.98	1.44	1.35
2	2	4620	OMU	C2-N3	5.95	1.48	1.38
2	2	4690	B8K	C2-N3	5.94	1.47	1.33
2	2	1574	B9B	O6-C6	5.93	1.40	1.35
2	2	4306	OMU	C2-N1	5.87	1.47	1.38
2	2	4529	B8W	O4'-C4'	-5.87	1.31	1.45
2	2	237	B9B	O6-C6	5.86	1.40	1.35
2	2	4371	MHG	C4-N9	5.82	1.44	1.37
2	2	4335	5MC	C4-N3	5.81	1.44	1.34
2	2	4306	OMU	C2-N3	5.77	1.48	1.38
2	2	2422	OMC	C2-N3	5.76	1.48	1.36
2	2	3909	OMC	C6-C5	5.73	1.48	1.35
2	2	4671	B8T	C4-N3	5.72	1.42	1.32
2	2	2380	B8W	O4'-C4'	-5.72	1.32	1.45
2	2	3887	OMC	C2-N3	5.70	1.47	1.36
2	2	4472	B8W	O4'-C4'	-5.69	1.32	1.45
2	2	4597	UR3	C2-N1	5.69	1.46	1.38
2	2	3782	5MC	C2-N3	5.68	1.47	1.36
2	2	2861	OMC	C2-N3	5.68	1.47	1.36
2	2	2365	OMC	C2-N3	5.67	1.47	1.36
2	2	4129	B8W	O4'-C4'	-5.66	1.32	1.45
2	2	729	2MG	C2-N2	5.65	1.46	1.33
2	2	729	2MG	C4-N3	5.61	1.51	1.37
2	2	4083	5MU	C6-C5	5.60	1.43	1.34
2	2	2861	OMC	C6-C5	5.60	1.48	1.35
2	2	4185	B8W	O4'-C4'	-5.57	1.32	1.45
2	2	2786	B9H	C6-C5	5.57	1.45	1.33
2	2	3869	OMC	C2-N3	5.56	1.47	1.36
2	2	3887	OMC	C6-C5	5.55	1.48	1.35
2	2	4371	MHG	C2-N2	5.55	1.45	1.33
2	2	3909	OMC	C2-N3	5.53	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	4690	B8K	O4'-C1'	-5.51	1.28	1.42
2	2	3869	OMC	C6-C5	5.48	1.47	1.35
2	2	237	B9B	C2-N2	5.47	1.44	1.33
2	2	4371	MHG	C4-N3	5.46	1.47	1.34
2	2	4671	B8T	C4-N4	5.46	1.47	1.35
2	2	1909	P7G	C2-N2	5.45	1.47	1.34
2	2	2422	OMC	C6-C5	5.43	1.47	1.35
2	2	4185	B8W	O3'-C3'	-5.40	1.30	1.43
2	2	3701	OMC	C6-C5	5.39	1.47	1.35
2	2	1348	P4U	C6-C5	5.39	1.47	1.35
2	2	3782	5MC	C4-N3	5.37	1.43	1.34
2	2	4620	OMU	C2-N1	5.30	1.46	1.38
2	2	1866	UR3	C2-N3	5.30	1.49	1.39
2	2	4690	B8K	O2'-C2'	-5.27	1.30	1.43
2	2	2804	OMC	C2-N3	5.27	1.47	1.36
2	2	4872	2MG	C4-N3	5.25	1.50	1.37
2	2	4335	5MC	C2-N3	5.23	1.47	1.36
2	2	3880	P7G	C2-N2	5.21	1.46	1.34
2	2	2365	OMC	C6-C5	5.21	1.47	1.35
2	2	1574	B9B	C2-N2	5.20	1.44	1.33
2	2	4536	OMC	C2-N3	5.19	1.46	1.36
2	2	2804	OMC	C6-C5	5.19	1.47	1.35
2	2	3701	OMC	C2-N3	5.18	1.46	1.36
2	2	3792	OMG	C2-N3	5.18	1.45	1.33
2	2	4194	I4U	C2-N3	5.17	1.46	1.36
2	2	4355	E6G	C2-N2	5.15	1.44	1.33
2	2	4536	OMC	C6-C5	5.14	1.47	1.35
2	2	3899	BGH	C8-N9	5.13	1.48	1.46
2	2	1659	I4U	C2-N3	5.12	1.46	1.36
2	2	978	2MG	C2-N2	5.09	1.44	1.33
2	2	2786	B9H	C2-N1	5.09	1.45	1.38
2	2	3899	BGH	O4'-C1'	-5.08	1.30	1.42
2	2	2297	E7G	C4-N3	5.08	1.46	1.34
2	2	4447	5MC	C4-N3	5.07	1.42	1.34
2	2	1797	E7G	C2-N3	5.05	1.45	1.33
2	2	4620	OMU	C6-C5	5.04	1.46	1.35
2	2	1909	P7G	C2-N1	5.03	1.45	1.33
2	2	1797	E7G	C4-N3	5.03	1.46	1.34
2	2	4870	OMG	C2-N3	5.01	1.45	1.33
2	2	3897	B8K	C2-N3	5.00	1.45	1.33
2	2	4530	UR3	C2-N3	4.99	1.48	1.39
2	2	4306	OMU	C6-C5	4.98	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	2754	B9B	C2-N2	4.95	1.43	1.33
2	2	4690	B8K	C4-N3	4.95	1.46	1.34
2	2	1605	7MG	C2-N3	4.93	1.45	1.33
2	2	2522	7MG	C4-N3	4.92	1.46	1.34
2	2	2522	7MG	C2-N3	4.91	1.45	1.33
2	2	1625	OMG	C2-N3	4.90	1.45	1.33
2	2	4196	OMG	C2-N3	4.90	1.45	1.33
2	2	2773	OMG	C2-N3	4.89	1.45	1.33
2	2	4623	OMG	C2-N3	4.87	1.45	1.33
2	2	4371	MHG	C2-N1	4.86	1.44	1.36
2	2	4872	2MG	C2-N1	4.86	1.44	1.36
2	2	1605	7MG	C4-N3	4.85	1.45	1.34
2	2	4597	UR3	C2-N3	4.84	1.48	1.39
2	2	1797	E7G	C8-N7	4.83	1.50	1.45
2	2	3897	B8K	O2'-C2'	-4.82	1.31	1.43
2	2	4550	7MG	C2-N3	4.81	1.44	1.33
2	2	4494	OMG	C2-N3	4.78	1.44	1.33
2	2	2424	OMG	C2-N3	4.75	1.44	1.33
2	2	2050	OMG	C2-N3	4.75	1.44	1.33
2	2	4415	1MA	C2-N1	4.74	1.44	1.35
2	2	4564	M7A	C4-N9	4.73	1.47	1.38
2	2	4536	OMC	C4-N4	4.71	1.45	1.33
2	2	4129	B8W	O3'-C3'	-4.71	1.31	1.43
2	2	1909	P7G	C4-N9	4.71	1.42	1.35
2	2	4194	I4U	C1'-N1	-4.71	1.34	1.47
2	2	4550	7MG	C4-N3	4.71	1.45	1.34
2	2	2297	E7G	C2-N3	4.68	1.44	1.33
2	2	4564	M7A	C6-N6	4.68	1.45	1.34
2	2	1348	P4U	O4-C4	4.67	1.40	1.35
2	2	2297	E7G	C8-N7	4.65	1.50	1.45
2	2	2297	E7G	C2-N2	4.64	1.45	1.34
2	2	3909	OMC	C4-N4	4.64	1.44	1.33
2	2	2861	OMC	C4-N4	4.63	1.44	1.33
2	2	4447	5MC	C2-N3	4.62	1.45	1.36
2	2	1797	E7G	C2-N2	4.62	1.45	1.34
2	2	3887	OMC	C4-N4	4.60	1.44	1.33
2	2	978	2MG	C4-N3	4.59	1.48	1.37
2	2	4370	OMG	C2-N3	4.59	1.44	1.33
2	2	4472	B8W	O3'-C3'	-4.58	1.32	1.43
2	2	4637	OMG	C2-N3	4.57	1.44	1.33
2	2	3899	BGH	C2-N3	4.55	1.44	1.33
2	2	1316	OMG	C2-N3	4.55	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1659	I4U	C1'-N1	-4.51	1.34	1.47
2	2	1522	OMG	C2-N3	4.50	1.44	1.33
2	2	978	2MG	C2-N1	4.48	1.43	1.36
2	2	2380	B8W	O3'-C3'	-4.47	1.32	1.43
2	2	4196	OMG	C4-N3	4.47	1.48	1.37
2	2	3869	OMC	C4-N4	4.47	1.44	1.33
2	2	4690	B8K	C4-N9	4.45	1.42	1.37
2	2	3899	BGH	C4-N3	4.44	1.44	1.34
2	2	3909	OMC	C2-N1	4.43	1.49	1.40
2	2	4494	OMG	C4-N3	4.43	1.48	1.37
2	2	1517	2MG	C2-N2	4.41	1.43	1.33
2	2	1909	P7G	O6-C6	-4.39	1.16	1.23
2	2	373	OMG	C2-N3	4.39	1.43	1.33
2	2	2522	7MG	C2-N2	4.39	1.44	1.34
2	2	3792	OMG	C4-N3	4.38	1.48	1.37
2	2	3899	BGH	O2'-C2'	-4.37	1.31	1.42
2	2	2364	OMG	C2-N3	4.36	1.43	1.33
2	2	3897	B8K	C4-N3	4.36	1.44	1.34
2	2	373	OMG	C4-N3	4.35	1.47	1.37
2	2	4870	OMG	C4-N3	4.34	1.47	1.37
2	2	2050	OMG	C4-N3	4.32	1.47	1.37
2	2	4194	I4U	C3'-C4'	4.32	1.64	1.53
2	2	2365	OMC	C4-N3	4.31	1.43	1.34
2	2	2422	OMC	C4-N4	4.30	1.44	1.33
2	2	4637	OMG	C4-N3	4.29	1.47	1.37
2	2	2424	OMG	C4-N3	4.29	1.47	1.37
2	2	4529	B8W	O3'-C3'	-4.28	1.32	1.43
2	2	3880	P7G	C2-N1	4.26	1.43	1.33
2	2	2804	OMC	C4-N4	4.26	1.43	1.33
2	2	4623	OMG	C4-N3	4.25	1.47	1.37
2	2	3701	OMC	C4-N4	4.23	1.43	1.33
2	2	1625	OMG	C4-N3	4.23	1.47	1.37
2	2	4536	OMC	C4-N3	4.22	1.43	1.34
2	2	1517	2MG	C4-N3	4.22	1.47	1.37
2	2	3869	OMC	C4-N3	4.21	1.43	1.34
2	2	4550	7MG	C2-N2	4.21	1.44	1.34
2	2	2773	OMG	C4-N3	4.20	1.47	1.37
2	2	2422	OMC	C2-N1	4.20	1.49	1.40
2	2	1605	7MG	C2-N2	4.18	1.44	1.34
2	2	3880	P7G	O6-C6	-4.18	1.17	1.23
2	2	3909	OMC	O2-C2	-4.18	1.16	1.23
2	2	1883	OMG	C2-N3	4.17	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	3899	BGH	C2-N2	4.17	1.44	1.34
2	2	2365	OMC	C4-N4	4.16	1.43	1.33
2	2	3909	OMC	C4-N3	4.16	1.42	1.34
2	2	2522	7MG	C4-N9	4.15	1.42	1.37
2	2	1522	OMG	C4-N3	4.14	1.47	1.37
2	2	4447	5MC	C4-N4	4.13	1.44	1.34
2	2	3887	OMC	C4-N3	4.12	1.42	1.34
2	2	2861	OMC	C4-N3	4.10	1.42	1.34
2	2	3880	P7G	C4-N9	4.09	1.41	1.35
2	2	4370	OMG	C4-N3	4.08	1.47	1.37
2	2	4690	B8K	O6-C6	-4.08	1.15	1.23
2	2	2804	OMC	C4-N3	4.05	1.42	1.34
2	2	2297	E7G	C4-N9	4.04	1.42	1.37
2	2	2364	OMG	C4-N3	4.03	1.47	1.37
2	2	3782	5MC	C2-N1	4.00	1.48	1.40
2	2	1316	OMG	C4-N3	3.98	1.47	1.37
2	2	1797	E7G	C4-N9	3.97	1.42	1.37
2	2	3880	P7G	C8-N7	3.97	1.49	1.45
2	2	4483	B8T	C2-N1	3.95	1.48	1.40
2	2	1659	I4U	O2-C2	-3.95	1.16	1.23
2	2	4447	5MC	O2-C2	-3.95	1.16	1.23
2	2	1860	B8H	C2-N3	3.95	1.45	1.38
2	2	2861	OMC	C2-N1	3.92	1.48	1.40
2	2	1348	P4U	C5-C4	3.91	1.48	1.43
2	2	1605	7MG	C4-N9	3.90	1.42	1.37
2	2	2422	OMC	C4-N3	3.89	1.42	1.34
2	2	1316	OMG	C5-C4	-3.86	1.33	1.43
2	2	4335	5MC	C4-N4	3.86	1.44	1.34
2	2	3782	5MC	C4-N4	3.84	1.44	1.34
2	2	4415	1MA	C4-N3	3.84	1.49	1.37
2	2	3897	B8K	O6-C6	-3.82	1.16	1.23
2	2	2364	OMG	C5-C4	-3.82	1.33	1.43
2	2	2773	OMG	C2-N2	3.82	1.43	1.34
2	2	2754	B9B	O2'-C2'	3.80	1.51	1.43
2	2	4306	OMU	O4-C4	-3.78	1.17	1.24
2	2	1883	OMG	C4-N3	3.78	1.46	1.37
2	2	2365	OMC	C2-N1	3.77	1.48	1.40
2	2	1659	I4U	O4'-C1'	3.76	1.50	1.42
2	2	4447	5MC	C6-N1	3.76	1.44	1.38
2	2	1322	1MA	C5-C4	-3.75	1.33	1.43
2	2	237	B9B	O3'-C3'	-3.73	1.34	1.43
2	2	4296	B8H	C2-N3	3.72	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	3701	OMC	C4-N3	3.71	1.42	1.34
2	2	1326	A2M	C5-C4	-3.70	1.31	1.40
2	2	3785	A2M	C5-C4	-3.70	1.31	1.40
2	2	4637	OMG	C5-C4	-3.69	1.33	1.43
2	2	1883	OMG	C5-C4	-3.69	1.33	1.43
2	2	4690	B8K	C2-N2	3.68	1.43	1.34
2	2	4671	B8T	C2-N1	3.68	1.48	1.40
2	2	1659	I4U	C2-N1	3.67	1.48	1.40
2	2	4335	5MC	C6-N1	3.67	1.44	1.38
2	2	3792	OMG	C2-N2	3.66	1.42	1.34
2	2	1909	P7G	C6-N1	3.65	1.44	1.38
2	2	4620	OMU	C4-N3	3.65	1.45	1.38
2	2	373	OMG	C5-C4	-3.63	1.33	1.43
2	2	1574	B9B	C5-C4	-3.62	1.31	1.40
2	2	4355	E6G	O3'-C3'	-3.61	1.34	1.43
2	2	4194	I4U	O2-C2	-3.59	1.17	1.23
2	2	1574	B9B	O3'-C3'	-3.57	1.34	1.43
2	2	1909	P7G	C2-N3	3.57	1.46	1.37
2	2	3867	A2M	C5-C4	-3.57	1.31	1.40
2	2	1534	A2M	C5-C4	-3.56	1.31	1.40
2	2	4690	B8K	C5-N7	3.56	1.45	1.39
2	2	1522	OMG	C5-C4	-3.55	1.34	1.43
2	2	4083	5MU	O4-C4	-3.55	1.16	1.23
2	2	1348	P4U	C6-N1	3.54	1.46	1.38
2	2	2050	OMG	C5-C4	-3.53	1.34	1.43
2	2	3899	BGH	O6-C6	-3.53	1.16	1.23
2	2	1625	OMG	C2-N2	3.52	1.42	1.34
2	2	4494	OMG	C2-N2	3.52	1.42	1.34
2	2	4870	OMG	C2-N2	3.52	1.42	1.34
2	2	4194	I4U	C5-C4	3.52	1.47	1.43
2	2	1517	2MG	C5-C4	-3.51	1.34	1.43
2	2	1316	OMG	O6-C6	-3.51	1.16	1.23
2	2	2401	A2M	C5-C4	-3.51	1.31	1.40
2	2	2424	OMG	C2-N2	3.51	1.42	1.34
2	2	4370	OMG	C2-N2	3.51	1.42	1.34
2	2	4536	OMC	O2-C2	-3.51	1.17	1.23
2	2	1797	E7G	C2-N1	3.51	1.46	1.37
2	2	4194	I4U	C2-N1	3.50	1.47	1.40
2	2	1326	A2M	O3'-C3'	-3.50	1.34	1.43
2	2	4483	B8T	C5-C4	3.49	1.48	1.40
2	2	3897	B8K	C5-N7	3.49	1.45	1.39
2	2	4623	OMG	C2-N2	3.49	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1883	OMG	C2-N2	3.47	1.42	1.34
2	2	4335	5MC	O2-C2	-3.47	1.17	1.23
2	2	4196	OMG	C2-N2	3.46	1.42	1.34
2	2	4870	OMG	C6-N1	3.46	1.43	1.37
2	2	1316	OMG	C2-N2	3.45	1.42	1.34
2	2	3867	A2M	O3'-C3'	-3.45	1.34	1.43
2	2	4355	E6G	C5-C4	-3.44	1.31	1.40
2	2	2050	OMG	C2-N2	3.44	1.42	1.34
2	2	1524	A2M	O3'-C3'	-3.44	1.34	1.43
2	2	3899	BGH	C71-N7	3.43	1.47	1.39
2	2	4370	OMG	C5-C4	-3.43	1.34	1.43
2	2	4623	OMG	C5-C4	-3.42	1.34	1.43
2	2	3880	P7G	C2-N3	3.42	1.46	1.37
2	2	4523	A2M	C5-C4	-3.42	1.31	1.40
2	2	3718	A2M	C5-C4	-3.42	1.31	1.40
2	2	398	A2M	C5-C4	-3.41	1.31	1.40
2	2	4083	5MU	O2-C2	-3.40	1.16	1.23
2	2	3718	A2M	O3'-C3'	-3.39	1.35	1.43
2	2	2424	OMG	C5-C4	-3.39	1.34	1.43
2	2	1871	A2M	O3'-C3'	-3.38	1.35	1.43
2	2	4550	7MG	O6-C6	-3.38	1.17	1.23
2	2	1677	PSU	C6-C5	3.38	1.39	1.35
2	2	1909	P7G	C5-C4	3.38	1.44	1.37
2	2	3897	B8K	C5-C6	3.37	1.52	1.43
2	2	4872	2MG	C6-N1	3.37	1.42	1.37
2	2	1574	B9B	O2'-C2'	3.37	1.50	1.43
2	2	4671	B8T	O2-C2	-3.36	1.17	1.23
2	2	3899	BGH	C5-N7	3.36	1.45	1.39
2	2	2364	OMG	C2-N2	3.35	1.42	1.34
2	2	3887	OMC	C2-N1	3.34	1.47	1.40
2	2	4335	5MC	C2-N1	3.33	1.47	1.40
2	2	1522	OMG	C2-N2	3.33	1.42	1.34
2	2	4196	OMG	C6-N1	3.33	1.42	1.37
2	2	4194	I4U	O4'-C1'	3.33	1.49	1.42
2	2	373	OMG	C2-N2	3.33	1.42	1.34
2	2	2363	A2M	C5-C4	-3.32	1.32	1.40
2	2	2861	OMC	O2-C2	-3.32	1.17	1.23
2	2	1605	7MG	O6-C6	-3.32	1.17	1.23
2	2	2804	OMC	C2-N1	3.31	1.47	1.40
2	2	3782	5MC	C6-N1	3.31	1.43	1.38
2	2	2754	B9B	C5-C4	-3.31	1.32	1.40
2	2	4530	UR3	C6-N1	3.30	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	4690	B8K	C5-C6	3.30	1.52	1.43
2	2	4494	OMG	C5-C4	-3.30	1.34	1.43
2	2	4371	MHG	C5-C6	3.29	1.52	1.43
2	2	2804	OMC	O2-C2	-3.29	1.17	1.23
2	2	3792	OMG	C5-C4	-3.28	1.34	1.43
2	2	4483	B8T	O2-C2	-3.28	1.17	1.23
2	2	3869	OMC	O2-C2	-3.27	1.17	1.23
2	2	4637	OMG	C2-N2	3.26	1.42	1.34
2	2	2522	7MG	O6-C6	-3.25	1.17	1.23
2	2	1625	OMG	C5-C4	-3.25	1.34	1.43
2	2	3880	P7G	C6-N1	3.25	1.43	1.38
2	2	4220	6MZ	C5-C4	-3.25	1.32	1.40
2	2	1871	A2M	C5-C4	-3.24	1.32	1.40
2	2	4620	OMU	O2-C2	-3.24	1.17	1.23
2	2	2050	OMG	O6-C6	-3.24	1.16	1.23
2	2	4571	A2M	O3'-C3'	-3.24	1.35	1.43
2	2	729	2MG	C2-N1	3.23	1.41	1.36
2	2	398	A2M	O3'-C3'	-3.23	1.35	1.43
2	2	1517	2MG	C2-N1	3.23	1.41	1.36
2	2	3723	A2M	C5-C4	-3.22	1.32	1.40
2	2	3825	A2M	C5-C4	-3.22	1.32	1.40
2	2	3887	OMC	O2-C2	-3.21	1.17	1.23
2	2	4872	2MG	C5-C4	-3.21	1.34	1.43
2	2	4571	A2M	C5-C4	-3.21	1.32	1.40
2	2	4550	7MG	C4-N9	3.21	1.41	1.37
2	2	3825	A2M	O3'-C3'	-3.19	1.35	1.43
2	2	4194	I4U	O4-C4	3.18	1.41	1.35
2	2	4620	OMU	O4-C4	-3.18	1.18	1.24
2	2	4536	OMC	C2-N1	3.17	1.46	1.40
2	2	3897	B8K	C2-N2	3.16	1.41	1.34
2	2	2773	OMG	C5-C4	-3.16	1.35	1.43
2	2	1524	A2M	C5-C4	-3.16	1.32	1.40
2	2	4870	OMG	C5-C4	-3.15	1.35	1.43
2	2	2297	E7G	C2-N1	3.15	1.45	1.37
2	2	3880	P7G	C5-C4	3.14	1.43	1.37
2	2	2365	OMC	O2-C2	-3.14	1.17	1.23
2	2	4370	OMG	C6-N1	3.14	1.42	1.37
2	2	2364	OMG	O6-C6	-3.14	1.16	1.23
2	2	2773	OMG	C6-N1	3.12	1.42	1.37
2	2	3701	OMC	C2-N1	3.12	1.46	1.40
2	2	2363	A2M	O3'-C3'	-3.11	1.35	1.43
2	2	4306	OMU	C4-N3	3.11	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	2422	OMC	O2-C2	-3.11	1.17	1.23
2	2	1659	I4U	C3'-C4'	3.11	1.60	1.53
2	2	3897	B8K	C8-N9	3.10	1.47	1.46
2	2	4306	OMU	O2-C2	-3.10	1.17	1.23
2	2	4671	B8T	C5-C4	3.10	1.47	1.40
2	2	1348	P4U	C2-N1	3.10	1.46	1.40
2	2	4196	OMG	C5-C6	3.09	1.53	1.47
2	2	1659	I4U	O4-C4	3.09	1.41	1.35
2	2	237	B9B	O2'-C2'	3.08	1.50	1.43
2	2	4194	I4U	O2'-C2'	3.07	1.50	1.43
2	2	4494	OMG	C6-N1	3.07	1.42	1.37
2	2	1322	1MA	C2-N1	3.07	1.41	1.35
2	2	237	B9B	C5-C4	-3.07	1.32	1.40
2	2	1522	OMG	O6-C6	-3.06	1.17	1.23
2	2	1883	OMG	O6-C6	-3.06	1.17	1.23
2	2	2424	OMG	C6-N1	3.05	1.42	1.37
2	2	4523	A2M	O3'-C3'	-3.05	1.35	1.43
2	2	3887	OMC	C6-N1	3.04	1.45	1.38
2	2	1866	UR3	C6-N1	3.04	1.45	1.38
2	2	4637	OMG	O6-C6	-3.03	1.17	1.23
2	2	3897	B8K	C4-N9	3.03	1.41	1.37
2	2	3869	OMC	C2-N1	3.03	1.46	1.40
2	2	1883	OMG	C6-N1	3.03	1.42	1.37
2	2	1322	1MA	C4-N3	3.00	1.46	1.37
2	2	4370	OMG	O6-C6	-3.00	1.17	1.23
2	2	1625	OMG	O6-C6	-3.00	1.17	1.23
2	2	978	2MG	C6-N1	3.00	1.42	1.37
2	2	4564	M7A	C5-N7	2.99	1.46	1.39
2	2	4185	B8W	C5-C4	-2.99	1.33	1.40
2	2	4571	A2M	C6-N6	2.98	1.44	1.34
2	2	4597	UR3	C6-N1	2.97	1.45	1.38
2	2	1797	E7G	C5-C6	2.97	1.51	1.43
2	2	3723	A2M	C6-N6	2.96	1.44	1.34
2	2	4483	B8T	C6-N1	2.96	1.45	1.38
2	2	3723	A2M	O3'-C3'	-2.96	1.36	1.43
2	2	2401	A2M	O3'-C3'	-2.96	1.36	1.43
2	2	3899	BGH	C2-N1	2.95	1.45	1.37
2	2	3897	B8K	C2-N1	2.95	1.45	1.37
2	2	2773	OMG	O6-C6	-2.94	1.17	1.23
2	2	1797	E7G	O6-C6	-2.93	1.18	1.23
2	2	373	OMG	C6-N1	2.92	1.42	1.37
2	2	4623	OMG	O6-C6	-2.91	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1605	7MG	C2-N1	2.91	1.44	1.37
2	2	3792	OMG	C6-N1	2.91	1.42	1.37
2	2	2297	E7G	O6-C6	-2.90	1.18	1.23
2	2	4296	B8H	O4-C4	-2.89	1.18	1.23
2	2	2522	7MG	C2-N1	2.89	1.44	1.37
2	2	4870	OMG	O6-C6	-2.89	1.17	1.23
2	2	2861	OMC	C6-N1	2.88	1.44	1.38
2	2	3782	5MC	O2-C2	-2.87	1.18	1.23
2	2	1909	P7G	C8-N7	2.86	1.48	1.45
2	2	2297	E7G	C5-C6	2.85	1.50	1.43
2	2	4494	OMG	O6-C6	-2.85	1.17	1.23
2	2	4442	PSU	C6-C5	2.84	1.38	1.35
2	2	4523	A2M	C6-N6	2.83	1.44	1.34
2	2	373	OMG	O6-C6	-2.83	1.17	1.23
2	2	1517	2MG	O6-C6	-2.83	1.17	1.23
2	2	1456	B8Q	C2-N1	2.83	1.42	1.38
2	2	2786	B9H	O2-C2	-2.82	1.17	1.22
2	2	2424	OMG	O6-C6	-2.82	1.17	1.23
2	2	1605	7MG	C5-C6	2.81	1.50	1.43
2	2	3701	OMC	O2-C2	-2.80	1.18	1.23
2	2	2380	B8W	C5-C4	-2.79	1.33	1.40
2	2	4355	E6G	O2'-C2'	2.79	1.49	1.43
2	2	3715	PSU	C6-C5	2.79	1.38	1.35
2	2	398	A2M	C6-N6	2.79	1.44	1.34
2	2	3792	OMG	O6-C6	-2.78	1.17	1.23
2	2	3825	A2M	C6-N6	2.78	1.44	1.34
2	2	2297	E7G	C6-N1	2.77	1.44	1.38
2	2	3909	OMC	C6-N1	2.77	1.44	1.38
2	2	4531	PSU	C6-C5	2.77	1.38	1.35
2	2	3899	BGH	C5-C6	2.76	1.50	1.43
2	2	2401	A2M	C6-N6	2.75	1.44	1.34
2	2	3867	A2M	C6-N6	2.75	1.44	1.34
2	2	4371	MHG	O6-C6	-2.75	1.18	1.23
2	2	3785	A2M	O2'-C2'	2.75	1.49	1.42
2	2	4371	MHG	C72-C71	2.74	1.58	1.52
2	2	2754	B9B	O3'-C3'	-2.73	1.36	1.43
2	2	4550	7MG	C5-C6	2.73	1.50	1.43
2	2	3718	A2M	C6-N6	2.72	1.44	1.34
2	2	4355	E6G	O5'-C5'	-2.72	1.38	1.44
2	2	978	2MG	C5-C4	-2.71	1.36	1.43
2	2	4196	OMG	C5-C4	-2.70	1.36	1.43
2	2	1517	2MG	C6-N1	2.70	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	4371	MHG	C6-N1	2.70	1.43	1.38
2	2	4500	PSU	C4-C5	-2.70	1.36	1.44
2	2	1524	A2M	C6-N6	2.70	1.43	1.34
2	2	4447	5MC	C2-N1	2.70	1.45	1.40
2	2	1659	I4U	C5-C4	2.69	1.46	1.43
2	2	1534	A2M	O3'-C3'	-2.69	1.36	1.43
2	2	1871	A2M	C6-N6	2.69	1.43	1.34
2	2	1534	A2M	C6-N6	2.68	1.43	1.34
2	2	1326	A2M	C6-N6	2.66	1.43	1.34
2	2	2422	OMC	C6-N1	2.66	1.44	1.38
2	2	3785	A2M	C6-N6	2.65	1.43	1.34
2	2	4872	2MG	O6-C6	-2.65	1.17	1.23
2	2	729	2MG	C5-C4	-2.64	1.36	1.43
2	2	4637	OMG	C6-N1	2.64	1.41	1.37
2	2	3825	A2M	O5'-C5'	-2.63	1.38	1.44
2	2	3869	OMC	C6-N1	2.63	1.44	1.38
2	2	4690	B8K	C2-N1	2.63	1.44	1.37
2	2	4636	PSU	C6-C5	2.62	1.38	1.35
2	2	3701	OMC	C6-N1	2.62	1.44	1.38
2	2	1348	P4U	O2-C2	-2.62	1.18	1.23
2	2	1659	I4U	O2'-C2'	2.61	1.49	1.43
2	2	4194	I4U	C6-N1	2.61	1.44	1.38
2	2	1797	E7G	C6-N1	2.61	1.43	1.38
2	2	4370	OMG	C5-C6	2.61	1.52	1.47
2	2	3899	BGH	C6-N1	2.60	1.43	1.38
2	2	2365	OMC	C6-N1	2.60	1.44	1.38
2	2	4129	B8W	O2'-C2'	2.60	1.49	1.43
2	2	2380	B8W	O2'-C2'	2.58	1.49	1.43
2	2	4690	B8K	C71-N7	2.58	1.45	1.39
2	2	4550	7MG	C2-N1	2.58	1.44	1.37
2	2	4194	I4U	O5'-C5'	-2.58	1.38	1.44
2	2	4472	B8W	C8-N7	-2.55	1.30	1.34
2	2	4293	PSU	C6-C5	2.55	1.38	1.35
2	2	2522	7MG	C5-C6	2.54	1.50	1.43
2	2	1860	B8H	O4-C4	-2.54	1.18	1.23
2	2	4196	OMG	O6-C6	-2.53	1.18	1.23
2	2	4529	B8W	O2'-C2'	2.53	1.48	1.43
2	2	1860	B8H	C2-N1	-2.53	1.33	1.38
2	2	3897	B8K	C6-N1	2.52	1.43	1.38
2	2	237	B9B	O5'-C5'	-2.52	1.38	1.44
2	2	2363	A2M	C6-N6	2.51	1.43	1.34
2	2	2804	OMC	C6-N1	2.51	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	4571	A2M	O2'-C2'	2.51	1.49	1.42
2	2	2773	OMG	C5-C6	2.51	1.52	1.47
2	2	1683	PSU	C4-C5	-2.51	1.37	1.44
2	2	1625	OMG	C6-N1	2.50	1.41	1.37
2	2	4415	1MA	C5-C4	-2.49	1.36	1.43
2	2	2363	A2M	O5'-C5'	-2.49	1.38	1.44
2	2	4597	UR3	O2-C2	-2.49	1.18	1.22
2	2	3825	A2M	O2'-C2'	2.49	1.49	1.42
2	2	1582	PSU	C6-C5	2.49	1.38	1.35
2	2	978	2MG	O6-C6	-2.48	1.18	1.23
2	2	3899	BGH	C4-N9	2.48	1.40	1.37
2	2	3785	A2M	O3'-C3'	-2.47	1.37	1.43
2	2	2363	A2M	O2'-C2'	2.46	1.48	1.42
2	2	729	2MG	O6-C6	-2.45	1.18	1.23
2	2	4536	OMC	C6-N1	2.45	1.43	1.38
2	2	4671	B8T	C6-N1	2.44	1.43	1.38
2	2	1871	A2M	O5'-C5'	-2.44	1.38	1.44
2	2	1522	OMG	C6-N1	2.43	1.41	1.37
2	2	978	2MG	C5-C6	2.42	1.52	1.47
2	2	4690	B8K	O3'-C3'	2.40	1.48	1.43
2	2	398	A2M	O2'-C2'	2.39	1.48	1.42
2	2	4500	PSU	O4'-C1'	-2.38	1.40	1.43
2	2	4636	PSU	C4-C5	-2.38	1.37	1.44
2	2	4870	OMG	C5-C6	2.38	1.52	1.47
2	2	4129	B8W	C8-N7	-2.36	1.30	1.34
2	2	1866	UR3	O2-C2	-2.35	1.18	1.22
2	2	3897	B8K	O3'-C3'	2.35	1.48	1.43
2	2	1871	A2M	O2'-C2'	2.35	1.48	1.42
2	2	4403	PSU	C6-C5	2.35	1.38	1.35
2	2	4472	B8W	C5-C4	-2.33	1.34	1.40
2	2	4564	M7A	C5-C6	-2.32	1.34	1.40
2	2	1524	A2M	O5'-C5'	-2.32	1.39	1.44
2	2	1534	A2M	O5'-C5'	-2.32	1.39	1.44
2	2	1605	7MG	C6-N1	2.32	1.43	1.38
2	2	4450	PSU	C6-C5	2.32	1.38	1.35
2	2	4523	A2M	O2'-C2'	2.32	1.48	1.42
2	2	2786	B9H	C6-N1	2.31	1.43	1.38
2	2	4571	A2M	O5'-C5'	-2.31	1.39	1.44
2	2	3909	OMC	C5-C4	2.30	1.48	1.42
2	2	4523	A2M	O5'-C5'	-2.30	1.39	1.44
2	2	1326	A2M	O5'-C5'	-2.30	1.39	1.44
2	2	3729	PSU	C4-C5	-2.29	1.37	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1677	PSU	O4'-C1'	-2.29	1.40	1.43
2	2	4196	OMG	C2-N1	2.29	1.43	1.37
2	2	3897	B8K	C71-N7	2.28	1.44	1.39
2	2	1582	PSU	C4-C5	-2.28	1.37	1.44
2	2	4628	PSU	O4'-C1'	-2.28	1.40	1.43
2	2	3785	A2M	O5'-C5'	-2.28	1.39	1.44
2	2	2380	B8W	C3'-C2'	2.28	1.59	1.53
2	2	1659	I4U	C6-N1	2.27	1.43	1.38
2	2	729	2MG	C5-C6	2.27	1.52	1.47
2	2	4636	PSU	O4'-C1'	-2.26	1.40	1.43
2	2	373	OMG	C5-C6	2.25	1.52	1.47
2	2	2401	A2M	O2'-C2'	2.25	1.48	1.42
2	2	398	A2M	O5'-C5'	-2.24	1.39	1.44
2	2	2522	7MG	C6-N1	2.24	1.43	1.38
2	2	1522	OMG	C5-C6	2.23	1.51	1.47
2	2	1456	B8Q	C6-N1	2.23	1.43	1.38
2	2	1677	PSU	C4-C5	-2.22	1.37	1.44
2	2	4185	B8W	C8-N7	-2.21	1.30	1.34
2	2	4472	B8W	O2'-C2'	2.20	1.48	1.43
2	2	3899	BGH	O5'-C5'	-2.20	1.39	1.44
2	2	2401	A2M	O5'-C5'	-2.19	1.39	1.44
2	2	4529	B8W	C5-C4	-2.19	1.35	1.40
2	2	2363	A2M	C5-N7	-2.18	1.31	1.39
2	2	1524	A2M	O2'-C2'	2.18	1.48	1.42
2	2	1322	1MA	CM1-N1	-2.17	1.42	1.46
2	2	1326	A2M	O2'-C2'	2.17	1.48	1.42
2	2	2401	A2M	C6-C5	-2.17	1.35	1.43
2	2	4450	PSU	C4-C5	-2.17	1.38	1.44
2	2	4623	OMG	C6-N1	2.16	1.41	1.37
2	2	4530	UR3	O2-C2	-2.16	1.18	1.22
2	2	2401	A2M	C5-N7	-2.15	1.31	1.39
2	2	3723	A2M	O2'-C2'	2.15	1.48	1.42
2	2	2363	A2M	C6-C5	-2.15	1.35	1.43
2	2	2364	OMG	C6-N1	2.14	1.41	1.37
2	2	4571	A2M	C5-N7	-2.14	1.32	1.39
2	2	1625	OMG	C5-C6	2.13	1.51	1.47
2	2	2773	OMG	C2-N1	2.13	1.42	1.37
2	2	1534	A2M	C6-C5	-2.13	1.35	1.43
2	2	4870	OMG	C2-N1	2.12	1.42	1.37
2	2	4220	6MZ	C2-N3	2.12	1.35	1.32
2	2	4872	2MG	C5-C6	2.11	1.51	1.47
2	2	2508	PSU	C4-C5	-2.11	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	4550	7MG	C6-N1	2.11	1.42	1.38
2	2	4293	PSU	C4-C5	-2.10	1.38	1.44
2	2	3718	A2M	O5'-C5'	-2.10	1.39	1.44
2	2	1456	B8Q	O2-C2	-2.09	1.18	1.22
2	2	4523	A2M	C6-C5	-2.09	1.35	1.43
2	2	4620	OMU	C6-N1	2.09	1.43	1.38
2	2	4185	B8W	O2'-C2'	2.09	1.47	1.43
2	2	1316	OMG	C6-N1	2.09	1.41	1.37
2	2	4571	A2M	C2-N3	2.08	1.35	1.32
2	2	1659	I4U	O5'-C5'	-2.05	1.39	1.44
2	2	1683	PSU	C4-N3	-2.05	1.35	1.38
2	2	1534	A2M	C5-N7	-2.05	1.32	1.39
2	2	4597	UR3	C3U-N3	-2.05	1.43	1.47
2	2	4129	B8W	C5-C4	-2.05	1.35	1.40
2	2	4500	PSU	C6-C5	2.05	1.37	1.35
2	2	4530	UR3	O4-C4	-2.05	1.19	1.23
2	2	3718	A2M	C4-N3	-2.04	1.32	1.35
2	2	4306	OMU	C6-N1	2.03	1.42	1.38
2	2	1582	PSU	O4'-C1'	-2.03	1.41	1.43
2	2	1574	B9B	C5-N7	-2.03	1.32	1.39
2	2	4220	6MZ	C5-N7	-2.03	1.32	1.39
2	2	3785	A2M	C6-C5	-2.03	1.35	1.43
2	2	2424	OMG	C5-C6	2.02	1.51	1.47
2	2	2508	PSU	C6-C5	2.01	1.37	1.35
2	2	1871	A2M	C6-C5	-2.01	1.35	1.43
2	2	3785	A2M	C5-N7	-2.01	1.32	1.39
2	2	4194	I4U	O3'-C3'	2.01	1.47	1.43
2	2	3867	A2M	C6-C5	-2.00	1.35	1.43
2	2	4628	PSU	C4-C5	-2.00	1.38	1.44

All (468) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	4564	M7A	C5-C6-N6	13.21	146.30	123.74
2	2	4083	5MU	C5-C4-N3	12.42	125.91	115.31
2	2	4220	6MZ	C1'-N9-C4	-12.33	104.98	126.64
2	2	4564	M7A	N6-C6-N1	-11.53	93.09	118.35
2	2	2786	B9H	C31-N3-C2	10.39	130.20	117.21
2	2	4083	5MU	C5-C6-N1	-10.36	112.68	123.34
2	2	1326	A2M	C5-C6-N6	9.80	135.24	120.35
2	2	3723	A2M	C5-C6-N6	9.40	134.63	120.35
2	2	3825	A2M	C5-C6-N6	9.28	134.45	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	2363	A2M	C5-C6-N6	9.06	134.13	120.35
2	2	3718	A2M	C5-C6-N6	9.02	134.06	120.35
2	2	1524	A2M	C5-C6-N6	9.01	134.05	120.35
2	2	4523	A2M	C5-C6-N6	8.88	133.85	120.35
2	2	3880	P7G	C4-C5-N7	8.76	111.29	106.67
2	2	1871	A2M	C5-C6-N6	8.63	133.47	120.35
2	2	1534	A2M	C5-C6-N6	8.63	133.47	120.35
2	2	2786	B9H	C6-N1-C2	-8.52	114.16	121.79
2	2	3867	A2M	C5-C6-N6	8.36	133.06	120.35
2	2	398	A2M	C5-C6-N6	8.35	133.04	120.35
2	2	3785	A2M	C5-C6-N6	8.11	132.68	120.35
2	2	4571	A2M	C5-C6-N6	8.05	132.58	120.35
2	2	2401	A2M	C5-C6-N6	7.96	132.45	120.35
2	2	2754	B9B	O6-C6-N1	-7.76	113.42	120.12
2	2	1909	P7G	C4-C5-N7	7.62	110.69	106.67
2	2	1326	A2M	N6-C6-N1	-7.37	103.27	118.57
2	2	4296	B8H	C4-N3-C2	-7.30	117.90	127.35
2	2	4690	B8K	C72-C71-N7	7.21	129.70	118.86
2	2	4371	MHG	C2-N3-C4	7.07	120.80	112.04
2	2	4529	B8W	N3-C2-N1	-7.06	117.81	127.22
2	2	4529	B8W	C2-N3-C4	6.83	123.16	115.36
2	2	4083	5MU	O4-C4-C5	-6.82	116.99	124.90
2	2	1326	A2M	N3-C2-N1	-6.80	118.05	128.68
2	2	4129	B8W	O6-C6-C5	6.74	125.65	116.01
2	2	3723	A2M	N6-C6-N1	-6.73	104.61	118.57
2	2	1860	B8H	C4-N3-C2	-6.67	118.72	127.35
2	2	237	B9B	O6-C6-N1	-6.66	114.37	120.12
2	2	3785	A2M	N3-C2-N1	-6.60	118.36	128.68
2	2	4564	M7A	N3-C4-N9	6.54	135.13	126.87
2	2	1574	B9B	O6-C6-N1	-6.52	114.50	120.12
2	2	1524	A2M	N6-C6-N1	-6.52	105.05	118.57
2	2	1860	B8H	N3-C2-N1	6.45	122.11	115.14
2	2	3718	A2M	N6-C6-N1	-6.39	105.32	118.57
2	2	4564	M7A	N3-C2-N1	-6.38	118.62	128.60
2	2	4523	A2M	N3-C2-N1	-6.38	118.71	128.68
2	2	2363	A2M	N6-C6-N1	-6.36	105.38	118.57
2	2	3825	A2M	N6-C6-N1	-6.33	105.44	118.57
2	2	4690	B8K	C5-C6-N1	6.29	122.07	110.99
2	2	3785	A2M	N6-C6-N1	-6.24	105.62	118.57
2	2	398	A2M	N3-C2-N1	-6.17	119.03	128.68
2	2	1534	A2M	N6-C6-N1	-6.17	105.78	118.57
2	2	398	A2M	N6-C6-N1	-6.15	105.81	118.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1871	A2M	N3-C2-N1	-6.14	119.09	128.68
2	2	1534	A2M	N3-C2-N1	-6.07	119.19	128.68
2	2	3897	B8K	C5-C6-N1	6.07	121.68	110.99
2	2	1871	A2M	N6-C6-N1	-6.03	106.06	118.57
2	2	4523	A2M	N6-C6-N1	-6.02	106.08	118.57
2	2	3867	A2M	N6-C6-N1	-6.01	106.10	118.57
2	2	3723	A2M	N3-C2-N1	-6.00	119.30	128.68
2	2	1322	1MA	N1-C2-N3	-5.94	119.09	126.02
2	2	1456	B8Q	N3-C2-N1	5.94	124.11	117.13
2	2	4220	6MZ	N3-C2-N1	-5.91	119.44	128.68
2	2	3867	A2M	N3-C2-N1	-5.89	119.48	128.68
2	2	4636	PSU	N1-C2-N3	5.85	121.75	115.13
2	2	4472	B8W	N3-C2-N1	-5.78	119.51	127.22
2	2	2401	A2M	N3-C2-N1	-5.77	119.65	128.68
2	2	4690	B8K	C4-C5-N7	5.74	110.02	104.91
2	2	1524	A2M	N3-C2-N1	-5.72	119.73	128.68
2	2	4083	5MU	C4-N3-C2	-5.71	119.96	127.35
2	2	2363	A2M	N3-C2-N1	-5.67	119.82	128.68
2	2	4571	A2M	N3-C2-N1	-5.64	119.86	128.68
2	2	2786	B9H	C32-C31-N3	5.64	124.24	112.47
2	2	2401	A2M	N6-C6-N1	-5.60	106.96	118.57
2	2	237	B9B	N3-C2-N1	-5.59	119.77	127.22
2	2	3718	A2M	N3-C2-N1	-5.58	119.96	128.68
2	2	4529	B8W	O6-C6-C5	5.54	123.93	116.01
2	2	2297	E7G	C5-C6-N1	5.54	120.75	110.99
2	2	4571	A2M	N6-C6-N1	-5.53	107.09	118.57
2	2	4450	PSU	C4-N3-C2	-5.50	118.42	126.34
2	2	4129	B8W	N3-C2-N1	-5.49	119.90	127.22
2	2	4296	B8H	N3-C2-N1	5.48	121.07	115.14
2	2	4185	B8W	N3-C2-N1	-5.47	119.93	127.22
2	2	4371	MHG	C5-C6-N1	5.45	120.60	110.99
2	2	4306	OMU	C4-N3-C2	-5.45	119.39	126.58
2	2	4083	5MU	N3-C2-N1	5.43	122.10	114.89
2	2	4129	B8W	N2-C2-N3	5.42	126.62	117.79
2	2	1456	B8Q	C31-N3-C4	5.40	122.39	114.25
2	2	4636	PSU	C4-N3-C2	-5.38	118.59	126.34
2	2	2522	7MG	C5-C6-N1	5.38	120.47	110.99
2	2	4355	E6G	N2-C2-N3	5.36	126.52	117.79
2	2	1797	E7G	C4-C5-N7	5.35	109.67	104.91
2	2	3899	BGH	C5-C6-N1	5.34	120.40	110.99
2	2	4355	E6G	N3-C2-N1	-5.33	120.11	127.22
2	2	1677	PSU	C4-N3-C2	-5.33	118.66	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	4628	PSU	N1-C2-N3	5.30	121.13	115.13
2	2	1677	PSU	N1-C2-N3	5.27	121.10	115.13
2	2	4293	PSU	N1-C2-N3	5.26	121.09	115.13
2	2	4355	E6G	C2-N3-C4	5.24	121.34	115.36
2	2	3825	A2M	N3-C2-N1	-5.24	120.49	128.68
2	2	4371	MHG	C4-C5-N7	5.22	109.55	104.91
2	2	4620	OMU	C4-N3-C2	-5.19	119.73	126.58
2	2	2754	B9B	N3-C2-N1	-5.16	120.33	127.22
2	2	4415	1MA	N1-C2-N3	-5.16	120.01	126.02
2	2	1605	7MG	C5-C6-N1	5.14	120.06	110.99
2	2	1797	E7G	C5-C6-N1	5.11	120.00	110.99
2	2	1574	B9B	N3-C2-N1	-5.10	120.42	127.22
2	2	4185	B8W	C2-N3-C4	5.06	121.14	115.36
2	2	2297	E7G	C2-N3-C4	5.06	121.31	112.30
2	2	4447	5MC	C5-C6-N1	-5.05	118.15	123.34
2	2	4371	MHG	C72-C71-N7	5.04	117.37	112.41
2	2	3899	BGH	C72-C71-N7	5.03	126.43	118.86
2	2	4550	7MG	C5-C6-N1	5.02	119.84	110.99
2	2	4529	B8W	C4-C5-N7	-5.00	104.19	109.40
2	2	3897	B8K	C72-C71-N7	4.98	126.35	118.86
2	2	4500	PSU	C4-N3-C2	-4.96	119.19	126.34
2	2	4185	B8W	O6-C6-N1	4.95	125.89	119.03
2	2	1659	I4U	C5-C4-N3	-4.92	117.42	124.91
2	2	2508	PSU	N1-C2-N3	4.91	120.70	115.13
2	2	2380	B8W	N3-C2-N1	-4.91	120.68	127.22
2	2	4293	PSU	C4-N3-C2	-4.90	119.28	126.34
2	2	4403	PSU	N1-C2-N3	4.87	120.64	115.13
2	2	2297	E7G	C4-C5-N7	4.85	109.23	104.91
2	2	2754	B9B	C2-N3-C4	4.85	120.90	115.36
2	2	4531	PSU	N1-C2-N3	4.84	120.62	115.13
2	2	237	B9B	C2-N3-C4	4.82	120.86	115.36
2	2	2380	B8W	O6-C6-N1	4.81	125.70	119.03
2	2	4450	PSU	N1-C2-N3	4.77	120.54	115.13
2	2	4403	PSU	C4-N3-C2	-4.74	119.51	126.34
2	2	1797	E7G	C2-N3-C4	4.71	120.69	112.30
2	2	1582	PSU	N1-C2-N3	4.70	120.45	115.13
2	2	4442	PSU	N1-C2-N3	4.68	120.44	115.13
2	2	4355	E6G	O6-C6-N1	4.68	124.17	120.12
2	2	1582	PSU	C4-N3-C2	-4.68	119.59	126.34
2	2	1860	B8H	O2-C2-N1	-4.66	117.62	122.87
2	2	3899	BGH	C4-C5-N7	4.65	109.05	104.91
2	2	3909	OMC	O2-C2-N3	-4.60	114.85	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1683	PSU	C4-N3-C2	-4.58	119.74	126.34
2	2	2508	PSU	C4-N3-C2	-4.57	119.76	126.34
2	2	3729	PSU	C4-N3-C2	-4.55	119.78	126.34
2	2	4628	PSU	C4-N3-C2	-4.53	119.81	126.34
2	2	1866	UR3	C4-N3-C2	-4.52	120.31	124.56
2	2	3897	B8K	C4-C5-N7	4.50	108.92	104.91
2	2	3729	PSU	N1-C2-N3	4.48	120.20	115.13
2	2	4472	B8W	C2-N3-C4	4.48	120.47	115.36
2	2	4185	B8W	N2-C2-N3	4.46	125.06	117.79
2	2	4371	MHG	C5-C4-N3	-4.44	119.66	128.13
2	2	4690	B8K	C2-N3-C4	4.44	120.21	112.30
2	2	2522	7MG	C2-N3-C4	4.42	120.18	112.30
2	2	4550	7MG	C2-N3-C4	4.39	120.12	112.30
2	2	4531	PSU	C4-N3-C2	-4.39	120.02	126.34
2	2	3897	B8K	C2-N3-C4	4.37	120.08	112.30
2	2	4500	PSU	N1-C2-N3	4.37	120.08	115.13
2	2	3715	PSU	N1-C2-N3	4.32	120.03	115.13
2	2	2380	B8W	N2-C2-N3	4.32	124.83	117.79
2	2	4442	PSU	C4-N3-C2	-4.32	120.12	126.34
2	2	4194	I4U	C5-C4-N3	-4.31	118.35	124.91
2	2	4371	MHG	C2-N1-C6	-4.31	119.52	124.48
2	2	1683	PSU	N1-C2-N3	4.31	120.01	115.13
2	2	4620	OMU	N3-C2-N1	4.29	120.58	114.89
2	2	3899	BGH	C2-N3-C4	4.28	119.92	112.30
2	2	1316	OMG	C5-C6-N1	4.28	121.50	113.95
2	2	4083	5MU	O2-C2-N1	-4.25	117.13	122.79
2	2	4472	B8W	N2-C2-N3	4.22	124.67	117.79
2	2	4355	E6G	O4'-C4'-C3'	-4.21	96.78	105.11
2	2	4415	1MA	C5-C6-N1	4.16	120.11	113.90
2	2	2050	OMG	C5-C6-N1	4.15	121.29	113.95
2	2	4296	B8H	C5-C4-N3	4.15	125.97	116.58
2	2	729	2MG	CM2-N2-C2	-4.13	114.73	123.86
2	2	4690	B8K	N9-C8-N7	4.13	108.87	103.33
2	2	1866	UR3	C6-N1-C2	-4.11	118.10	121.79
2	2	1517	2MG	C5-C6-N1	4.09	121.18	113.95
2	2	1456	B8Q	O2-C2-N3	-4.08	116.95	122.95
2	2	4529	B8W	C3'-C2'-C1'	4.08	107.12	100.98
2	2	1574	B9B	C2-N3-C4	4.05	119.98	115.36
2	2	1605	7MG	C2-N3-C4	4.05	119.51	112.30
2	2	4623	OMG	C5-C6-N1	4.02	121.05	113.95
2	2	1797	E7G	C5-C4-N3	-4.01	120.48	128.13
2	2	4530	UR3	C1'-N1-C2	4.00	123.75	116.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1574	B9B	C1'-N9-C4	-4.00	119.61	126.64
2	2	1883	OMG	C5-C6-N1	4.00	121.01	113.95
2	2	3897	B8K	C5-C4-N9	3.95	111.47	106.35
2	2	1524	A2M	O4'-C4'-C3'	-3.94	97.31	105.11
2	2	2364	OMG	C5-C6-N1	3.94	120.91	113.95
2	2	4306	OMU	C5-C4-N3	3.91	120.68	114.84
2	2	4872	2MG	C5-C6-N1	3.90	120.83	113.95
2	2	2380	B8W	C3'-C2'-C1'	3.89	106.83	100.98
2	2	4530	UR3	C4-N3-C2	-3.88	120.91	124.56
2	2	4472	B8W	O6-C6-N1	3.87	124.39	119.03
2	2	2773	OMG	C5-C6-N1	3.86	120.77	113.95
2	2	4335	5MC	C5-C6-N1	-3.84	119.39	123.34
2	2	1348	P4U	C5-C4-N3	-3.84	119.07	124.91
2	2	4870	OMG	C5-C6-N1	3.82	120.69	113.95
2	2	2786	B9H	O3'-C3'-C2'	3.80	121.95	111.17
2	2	4597	UR3	C4-N3-C2	-3.79	121.00	124.56
2	2	1797	E7G	C5-C4-N9	3.78	111.25	106.35
2	2	1605	7MG	C5-C4-N3	-3.78	120.93	128.13
2	2	2297	E7G	C5-C4-N3	-3.77	120.94	128.13
2	2	2380	B8W	C2-N3-C4	3.77	119.66	115.36
2	2	4447	5MC	C1'-N1-C6	3.77	127.40	121.12
2	2	4500	PSU	C6-C5-C4	3.77	120.83	118.20
2	2	1883	OMG	C2-N1-C6	-3.74	118.22	125.10
2	2	4371	MHG	C5-C4-N9	3.74	111.20	106.35
2	2	3897	B8K	N9-C8-N7	3.73	108.33	103.33
2	2	4690	B8K	C5-C4-N9	3.72	111.18	106.35
2	2	3715	PSU	C4-N3-C2	-3.71	120.99	126.34
2	2	3715	PSU	C6-N1-C2	-3.69	118.91	122.68
2	2	1883	OMG	O6-C6-C5	-3.69	117.16	124.37
2	2	4129	B8W	C2-N3-C4	3.69	119.57	115.36
2	2	1322	1MA	C5-C6-N1	3.67	119.38	113.90
2	2	4129	B8W	C2-N1-C6	3.67	121.98	116.08
2	2	1625	OMG	C5-C6-N1	3.66	120.42	113.95
2	2	4564	M7A	C2-N3-C4	3.65	120.37	111.75
2	2	373	OMG	C5-C6-N1	3.64	120.38	113.95
2	2	1456	B8Q	C31-N3-C2	3.64	123.07	117.79
2	2	4370	OMG	C5-C6-N1	3.62	120.35	113.95
2	2	2424	OMG	C5-C6-N1	3.62	120.35	113.95
2	2	1909	P7G	N9-C8-N7	3.61	108.54	103.38
2	2	1605	7MG	N9-C8-N7	3.60	108.53	103.38
2	2	3792	OMG	C5-C6-N1	3.60	120.31	113.95
2	2	4494	OMG	C5-C6-N1	3.59	120.28	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	2522	7MG	C5-C4-N3	-3.59	121.30	128.13
2	2	4637	OMG	C5-C6-N1	3.57	120.25	113.95
2	2	4306	OMU	N3-C2-N1	3.57	119.63	114.89
2	2	1522	OMG	C5-C6-N1	3.56	120.24	113.95
2	2	4550	7MG	C5-C4-N9	3.55	110.96	106.35
2	2	1316	OMG	C2-N1-C6	-3.52	118.61	125.10
2	2	3880	P7G	N2-C2-N3	3.50	124.16	116.71
2	2	1517	2MG	CM2-N2-C2	-3.50	116.14	123.86
2	2	4597	UR3	C6-N1-C2	-3.48	118.67	121.79
2	2	4550	7MG	C5-C4-N3	-3.45	121.55	128.13
2	2	2297	E7G	C5-C4-N9	3.45	110.83	106.35
2	2	729	2MG	C5-C6-N1	3.44	120.02	113.95
2	2	1605	7MG	C5-C4-N9	3.43	110.80	106.35
2	2	4129	B8W	C4-C5-N7	-3.39	105.86	109.40
2	2	1517	2MG	O6-C6-C5	-3.39	117.75	124.37
2	2	237	B9B	C3'-C2'-C1'	3.39	106.08	100.98
2	2	1605	7MG	C4-C5-N7	3.38	110.23	105.53
2	2	4529	B8W	C2-N1-C6	3.37	121.50	116.08
2	2	4472	B8W	C2-N1-C6	3.37	121.48	116.08
2	2	4870	OMG	C2-N1-C6	-3.35	118.93	125.10
2	2	1866	UR3	O2-C2-N3	-3.34	116.63	121.34
2	2	1860	B8H	C5-C4-N3	3.32	124.10	116.58
2	2	3899	BGH	C5-C4-N9	3.32	110.66	106.35
2	2	2773	OMG	C2-N1-C6	-3.30	119.02	125.10
2	2	4690	B8K	C5-C4-N3	-3.30	121.84	128.13
2	2	978	2MG	C5-C6-N1	3.29	119.75	113.95
2	2	1456	B8Q	C6-N1-C2	-3.28	118.85	121.79
2	2	4636	PSU	O2-C2-N1	-3.28	119.18	122.79
2	2	2364	OMG	C2-N1-C6	-3.28	119.07	125.10
2	2	3899	BGH	N9-C8-N7	3.25	107.70	103.33
2	2	4083	5MU	C5M-C5-C6	-3.25	118.51	122.85
2	2	4530	UR3	O2-C2-N3	-3.24	116.77	121.34
2	2	3909	OMC	C1'-N1-C2	3.23	125.62	118.42
2	2	4623	OMG	C2-N1-C6	-3.22	119.16	125.10
2	2	3782	5MC	C5-C6-N1	-3.22	120.02	123.34
2	2	3897	B8K	C6-C5-C4	-3.21	115.99	122.62
2	2	3729	PSU	O2-C2-N1	-3.21	119.26	122.79
2	2	4442	PSU	C6-N1-C2	-3.20	119.41	122.68
2	2	2522	7MG	C5-C4-N9	3.20	110.50	106.35
2	2	4196	OMG	C5-C6-N1	3.17	119.55	113.95
2	2	1625	OMG	C2-N1-C6	-3.17	119.27	125.10
2	2	4637	OMG	C2-N1-C6	-3.14	119.32	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1866	UR3	C1'-N1-C2	3.13	122.27	116.99
2	2	373	OMG	C8-N7-C5	3.12	108.94	102.99
2	2	4306	OMU	O4-C4-C5	-3.12	119.67	125.16
2	2	3897	B8K	C2-N1-C6	-3.12	119.42	125.10
2	2	3782	5MC	CM5-C5-C6	-3.11	118.69	122.85
2	2	2422	OMC	O2-C2-N3	-3.09	117.30	122.33
2	2	4523	A2M	O4'-C4'-C3'	-3.09	99.00	105.11
2	2	2522	7MG	C4-C5-N7	3.07	109.79	105.53
2	2	4690	B8K	C6-C5-C4	-3.06	116.31	122.62
2	2	373	OMG	C2-N1-C6	-3.06	119.47	125.10
2	2	4531	PSU	O2-C2-N1	-3.05	119.43	122.79
2	2	3792	OMG	C2-N1-C6	-3.04	119.49	125.10
2	2	3729	PSU	C6-N1-C2	-3.04	119.58	122.68
2	2	4620	OMU	O4-C4-C5	-3.01	119.86	125.16
2	2	4370	OMG	C2-N1-C6	-3.01	119.56	125.10
2	2	1456	B8Q	C1'-N1-C2	3.01	122.07	116.99
2	2	4628	PSU	C6-N1-C2	-3.01	119.61	122.68
2	2	4872	2MG	O6-C6-C5	-3.00	118.50	124.37
2	2	4620	OMU	O2-C2-N1	-3.00	118.80	122.79
2	2	4196	OMG	C2-N1-C6	-2.98	119.61	125.10
2	2	3899	BGH	C5-C4-N3	-2.98	122.45	128.13
2	2	2050	OMG	C2-N1-C6	-2.97	119.63	125.10
2	2	2424	OMG	C2-N1-C6	-2.97	119.63	125.10
2	2	4296	B8H	O2-C2-N1	-2.97	119.53	122.87
2	2	4620	OMU	C5-C4-N3	2.96	119.27	114.84
2	2	4494	OMG	C2-N1-C6	-2.95	119.67	125.10
2	2	1797	E7G	N9-C8-N7	2.94	107.58	103.38
2	2	1605	7MG	C2-N1-C6	-2.92	119.77	125.10
2	2	4296	B8H	O4-C4-N3	-2.92	114.53	120.12
2	2	2786	B9H	O2-C2-N1	-2.89	115.95	122.72
2	2	4293	PSU	O2-C2-N1	-2.89	119.61	122.79
2	2	4564	M7A	C71-N7-C5	-2.88	112.95	124.01
2	2	1677	PSU	O2-C2-N1	-2.87	119.63	122.79
2	2	4636	PSU	C6-C5-C4	2.85	120.19	118.20
2	2	4194	I4U	C3'-C2'-C1'	2.85	106.84	101.43
2	2	4636	PSU	C6-N1-C2	-2.83	119.79	122.68
2	2	2508	PSU	C6-N1-C2	-2.83	119.79	122.68
2	2	1522	OMG	C2-N1-C6	-2.82	119.91	125.10
2	2	3715	PSU	O2-C2-N1	-2.80	119.71	122.79
2	2	1659	I4U	O4'-C4'-C3'	-2.80	99.58	105.11
2	2	4872	2MG	C8-N7-C5	2.79	108.31	102.99
2	2	2364	OMG	C8-N7-C5	2.78	108.30	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1316	OMG	C8-N7-C5	2.78	108.29	102.99
2	2	3897	B8K	C5-C4-N3	-2.78	122.83	128.13
2	2	2773	OMG	C8-N7-C5	2.78	108.28	102.99
2	2	2508	PSU	O2-C2-N1	-2.78	119.73	122.79
2	2	1866	UR3	C3U-N3-C4	2.77	121.85	117.89
2	2	4531	PSU	C6-N1-C2	-2.76	119.86	122.68
2	2	3880	P7G	N9-C8-N7	2.75	107.32	103.38
2	2	978	2MG	CM2-N2-C2	-2.75	117.78	123.86
2	2	3899	BGH	C6-C5-C4	-2.75	116.95	122.62
2	2	4355	E6G	O4'-C1'-C2'	-2.75	102.91	106.93
2	2	2297	E7G	C2-N1-C6	-2.74	120.10	125.10
2	2	4671	B8T	C6-C5-C4	2.74	120.31	116.96
2	2	4370	OMG	C8-N7-C5	2.73	108.20	102.99
2	2	2786	B9H	O3'-C3'-C4'	2.73	118.95	111.05
2	2	4293	PSU	C6-N1-C2	-2.73	119.89	122.68
2	2	2786	B9H	C1'-N1-C6	2.72	126.78	120.84
2	2	3897	B8K	N2-C2-N1	2.72	122.51	116.71
2	2	4472	B8W	C5-C6-N1	-2.70	118.12	123.26
2	2	1659	I4U	O2-C2-N3	-2.70	117.95	122.33
2	2	2522	7MG	O6-C6-C5	-2.69	120.94	127.54
2	2	1883	OMG	N2-C2-N1	2.69	122.44	116.71
2	2	1797	E7G	C2-N1-C6	-2.69	120.20	125.10
2	2	3899	BGH	O4'-C1'-N9	-2.68	105.64	109.30
2	2	4220	6MZ	C2-N1-C6	2.68	118.89	116.59
2	2	237	B9B	N2-C2-N3	2.67	122.15	117.79
2	2	1659	I4U	O4'-C1'-C2'	-2.67	100.83	106.64
2	2	3867	A2M	C3'-C2'-C1'	2.66	107.90	102.89
2	2	4690	B8K	C2-N1-C6	-2.62	120.32	125.10
2	2	4637	OMG	C8-N7-C5	2.62	107.97	102.99
2	2	4415	1MA	C8-N7-C5	2.61	107.97	102.99
2	2	2297	E7G	O6-C6-C5	-2.61	121.14	127.54
2	2	4370	OMG	N2-C2-N1	2.61	122.27	116.71
2	2	4196	OMG	C8-N7-C5	2.60	107.95	102.99
2	2	2050	OMG	O6-C6-C5	-2.60	119.30	124.37
2	2	4564	M7A	C5-C4-N3	-2.59	120.53	126.62
2	2	1322	1MA	C8-N7-C5	2.59	107.92	102.99
2	2	4550	7MG	C4-C5-N7	2.59	109.12	105.53
2	2	2522	7MG	C2-N1-C6	-2.58	120.40	125.10
2	2	4628	PSU	O2-C2-N1	-2.57	119.96	122.79
2	2	1683	PSU	C6-N1-C2	-2.57	120.06	122.68
2	2	1909	P7G	C71-N7-C5	2.56	130.59	124.52
2	2	4371	MHG	N9-C8-N7	2.55	107.03	103.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	4403	PSU	O2-C2-N1	-2.55	119.98	122.79
2	2	4447	5MC	N1-C2-N3	2.54	123.44	118.81
2	2	1625	OMG	O6-C6-C5	-2.54	119.41	124.37
2	2	4083	5MU	C5M-C5-C4	2.54	121.56	118.77
2	2	4870	OMG	O6-C6-C5	-2.52	119.44	124.37
2	2	4129	B8W	C3'-C2'-C1'	2.52	104.77	100.98
2	2	2754	B9B	C3'-C2'-C1'	2.52	104.77	100.98
2	2	1582	PSU	C6-N1-C2	-2.52	120.11	122.68
2	2	2754	B9B	C1'-N9-C4	-2.52	122.22	126.64
2	2	3899	BGH	C2-N1-C6	-2.51	120.51	125.10
2	2	4306	OMU	C1'-N1-C2	2.51	122.12	117.57
2	2	1605	7MG	O6-C6-C5	-2.51	121.38	127.54
2	2	4637	OMG	O6-C6-C5	-2.51	119.47	124.37
2	2	4355	E6G	N2-C2-N1	-2.50	113.36	117.25
2	2	3792	OMG	O6-C6-C5	-2.49	119.51	124.37
2	2	4129	B8W	O6-C6-N1	-2.48	115.59	119.03
2	2	1883	OMG	C8-N7-C5	2.48	107.71	102.99
2	2	3897	B8K	O3'-C3'-C2'	-2.47	103.83	111.82
2	2	1522	OMG	C8-N7-C5	2.47	107.70	102.99
2	2	1316	OMG	O6-C6-C5	-2.46	119.56	124.37
2	2	4194	I4U	C5'-C4'-C3'	-2.46	105.96	115.18
2	2	4623	OMG	C8-N7-C5	2.46	107.68	102.99
2	2	4371	MHG	N9-C4-N3	2.45	129.12	125.47
2	2	978	2MG	O6-C6-C5	-2.44	119.61	124.37
2	2	4530	UR3	C6-N1-C2	-2.44	119.60	121.79
2	2	1677	PSU	C6-N1-C2	-2.43	120.19	122.68
2	2	4403	PSU	C6-N1-C2	-2.43	120.19	122.68
2	2	4129	B8W	N2-C2-N1	-2.43	113.47	117.25
2	2	2424	OMG	O6-C6-C5	-2.39	119.70	124.37
2	2	4447	5MC	O2-C2-N3	-2.39	118.45	122.33
2	2	1797	E7G	C8-N7-C71	2.39	126.18	120.50
2	2	4529	B8W	N2-C2-N1	2.37	120.93	117.25
2	2	4129	B8W	C5-C6-N1	-2.36	118.76	123.26
2	2	1625	OMG	C8-N7-C5	2.36	107.49	102.99
2	2	2297	E7G	N1-C2-N3	-2.36	118.92	123.32
2	2	4371	MHG	N1-C2-N3	-2.36	120.31	123.95
2	2	4185	B8W	O4'-C1'-C2'	-2.35	103.50	106.93
2	2	2050	OMG	C8-N7-C5	2.34	107.46	102.99
2	2	1871	A2M	O4'-C4'-C3'	-2.34	100.49	105.11
2	2	2522	7MG	N9-C8-N7	2.34	106.72	103.38
2	2	1517	2MG	C8-N7-C5	2.34	107.44	102.99
2	2	1659	I4U	C6-N1-C2	-2.34	116.44	120.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	3897	B8K	O6-C6-C5	-2.34	121.81	127.54
2	2	4194	I4U	C2-N3-C4	2.33	123.01	117.44
2	2	4690	B8K	O6-C6-C5	-2.33	121.83	127.54
2	2	4494	OMG	C8-N7-C5	2.33	107.42	102.99
2	2	4194	I4U	O4'-C1'-C2'	-2.33	101.57	106.64
2	2	4597	UR3	C1'-N1-C2	2.32	120.91	116.99
2	2	4483	B8T	C6-C5-C4	2.32	119.80	116.96
2	2	4623	OMG	O6-C6-C5	-2.31	119.86	124.37
2	2	978	2MG	C8-N7-C5	2.29	107.36	102.99
2	2	4870	OMG	C8-N7-C5	2.29	107.36	102.99
2	2	4494	OMG	O6-C6-C5	-2.28	119.92	124.37
2	2	3899	BGH	O4'-C4'-C3'	-2.28	100.61	105.11
2	2	2380	B8W	C2-N1-C6	2.27	119.73	116.08
2	2	4083	5MU	C6-C5-C4	2.27	119.93	118.03
2	2	2297	E7G	C6-C5-C4	-2.26	117.96	122.62
2	2	4494	OMG	CM2-O2'-C2'	-2.26	108.61	114.52
2	2	4550	7MG	O6-C6-C5	-2.24	122.04	127.54
2	2	4371	MHG	O6-C6-C5	-2.23	122.06	127.54
2	2	4500	PSU	C5-C6-N1	-2.23	118.76	122.11
2	2	4472	B8W	C2'-C3'-C4'	-2.23	98.31	102.64
2	2	1517	2MG	C3'-C2'-C1'	2.23	104.33	100.98
2	2	4550	7MG	C6-C5-C4	-2.22	118.03	122.62
2	2	4690	B8K	C5'-C4'-C3'	-2.22	106.85	115.18
2	2	3792	OMG	C8-N7-C5	2.22	107.21	102.99
2	2	2297	E7G	N2-C2-N1	2.22	121.43	116.71
2	2	237	B9B	C2-N1-C6	2.21	119.64	116.08
2	2	4371	MHG	C21-N2-C2	-2.20	119.00	123.86
2	2	1659	I4U	C2-N3-C4	2.20	122.69	117.44
2	2	4185	B8W	O4'-C4'-C3'	-2.20	100.77	105.11
2	2	3899	BGH	C3'-C2'-C1'	-2.19	98.77	102.89
2	2	3909	OMC	C6-N1-C2	-2.19	116.70	120.49
2	2	1860	B8H	O4-C4-N3	-2.18	115.93	120.12
2	2	4690	B8K	N1-C2-N3	-2.18	119.25	123.32
2	2	3897	B8K	O4'-C1'-C2'	-2.18	101.89	106.64
2	2	4447	5MC	C1'-N1-C2	-2.17	113.57	118.42
2	2	4550	7MG	C2-N1-C6	-2.16	121.16	125.10
2	2	4355	E6G	C2-N1-C6	2.16	119.55	116.08
2	2	4550	7MG	N1-C2-N3	-2.16	119.30	123.32
2	2	1797	E7G	O6-C6-C5	-2.16	122.25	127.54
2	2	2522	7MG	C6-C5-C4	-2.14	118.21	122.62
2	2	4194	I4U	O4-C41-C43	2.14	112.82	107.14
2	2	4529	B8W	N2-C2-N3	2.13	121.26	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	4636	PSU	O4'-C1'-C2'	2.13	108.15	105.14
2	2	2773	OMG	O6-C6-C5	-2.12	120.23	124.37
2	2	4403	PSU	O4'-C1'-C2'	2.12	108.13	105.14
2	2	2364	OMG	O6-C6-C5	-2.10	120.26	124.37
2	2	4628	PSU	O4'-C1'-C2'	2.10	108.11	105.14
2	2	2050	OMG	N1-C2-N3	-2.10	119.40	123.32
2	2	3782	5MC	O2-C2-N3	-2.10	118.92	122.33
2	2	1909	P7G	N2-C2-N3	2.09	121.17	116.71
2	2	4690	B8K	O6-C6-N1	-2.09	116.10	120.12
2	2	729	2MG	C8-N7-C5	2.09	106.97	102.99
2	2	2522	7MG	N1-C2-N3	-2.09	119.43	123.32
2	2	373	OMG	N2-C2-N1	2.08	121.14	116.71
2	2	1909	P7G	C5-C4-N3	-2.08	120.33	124.00
2	2	4370	OMG	O6-C6-C5	-2.08	120.31	124.37
2	2	4523	A2M	O3'-C3'-C2'	2.07	117.05	111.17
2	2	4671	B8T	C41-N4-C4	-2.07	118.41	122.45
2	2	2861	OMC	O2-C2-N3	-2.06	118.97	122.33
2	2	3909	OMC	N1-C2-N3	2.06	122.56	118.81
2	2	4185	B8W	C2-N1-C6	2.06	119.39	116.08
2	2	4597	UR3	C3U-N3-C2	2.06	120.92	117.31
2	2	4500	PSU	O4-C4-C5	-2.04	118.70	124.05
2	2	4529	B8W	C5'-C4'-C3'	-2.04	107.54	115.18
2	2	2365	OMC	O2-C2-N3	-2.04	119.02	122.33
2	2	4450	PSU	O2-C2-N1	-2.04	120.55	122.79
2	2	1677	PSU	C6-C5-C4	2.04	119.62	118.20
2	2	1683	PSU	C5-C4-N3	2.03	121.17	116.58
2	2	2297	E7G	C8-N7-C71	2.03	125.32	120.50
2	2	2754	B9B	C4-C5-N7	-2.03	107.29	109.40
2	2	1659	I4U	C43-C41-C42	-2.02	102.70	113.47
2	2	4442	PSU	O2-C2-N1	-2.02	120.56	122.79
2	2	1683	PSU	O4-C4-N3	-2.02	116.24	120.12
2	2	3899	BGH	O6-C6-C5	-2.02	122.59	127.54
2	2	4355	E6G	C4-C5-N7	-2.02	107.30	109.40
2	2	373	OMG	O6-C6-C5	-2.02	120.44	124.37
2	2	4450	PSU	C5-C4-N3	2.02	121.14	116.58
2	2	4483	B8T	O2-C2-N3	-2.01	119.06	122.33
2	2	4194	I4U	O2-C2-N3	-2.01	119.07	122.33
2	2	4472	B8W	O4'-C1'-C2'	-2.01	104.00	106.93
2	2	2380	B8W	C5-C6-N1	-2.00	119.45	123.26

There are no chirality outliers.

All (134) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	2	237	B9B	C5-C6-O6-C61
2	2	237	B9B	N1-C6-O6-C61
2	2	237	B9B	C3'-C4'-C5'-O5'
2	2	237	B9B	C62-C61-O6-C6
2	2	398	A2M	O4'-C4'-C5'-O5'
2	2	1348	P4U	N3-C4-O4-C41
2	2	1574	B9B	C5-C6-O6-C61
2	2	1574	B9B	N1-C6-O6-C61
2	2	1677	PSU	C2'-C1'-C5-C4
2	2	1677	PSU	C3'-C4'-C5'-O5'
2	2	1677	PSU	O4'-C4'-C5'-O5'
2	2	1797	E7G	O4'-C4'-C5'-O5'
2	2	1860	B8H	O4'-C4'-C5'-O5'
2	2	2364	OMG	O4'-C4'-C5'-O5'
2	2	2380	B8W	C5-C6-O6-C61
2	2	2380	B8W	N1-C6-O6-C61
2	2	2380	B8W	O4'-C4'-C5'-O5'
2	2	2401	A2M	C3'-C4'-C5'-O5'
2	2	2754	B9B	C5-C6-O6-C61
2	2	2754	B9B	N1-C6-O6-C61
2	2	2786	B9H	C32-C31-N3-C2
2	2	2786	B9H	C32-C31-N3-C4
2	2	3701	OMC	C2'-C1'-N1-C2
2	2	3701	OMC	C2'-C1'-N1-C6
2	2	3785	A2M	C3'-C4'-C5'-O5'
2	2	3867	A2M	C3'-C4'-C5'-O5'
2	2	3899	BGH	O4'-C4'-C5'-O5'
2	2	4129	B8W	C5-C6-O6-C61
2	2	4129	B8W	N1-C6-O6-C61
2	2	4185	B8W	C5-C6-O6-C61
2	2	4185	B8W	N1-C6-O6-C61
2	2	4194	I4U	C3'-C4'-C5'-O5'
2	2	4194	I4U	O4'-C4'-C5'-O5'
2	2	4196	OMG	C1'-C2'-O2'-CM2
2	2	4355	E6G	C5-C6-O6-C61
2	2	4355	E6G	N1-C6-O6-C61
2	2	4403	PSU	O4'-C1'-C5-C4
2	2	4403	PSU	O4'-C1'-C5-C6
2	2	4415	1MA	O4'-C4'-C5'-O5'
2	2	4415	1MA	C3'-C4'-C5'-O5'
2	2	4472	B8W	C5-C6-O6-C61
2	2	4472	B8W	N1-C6-O6-C61
2	2	4500	PSU	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	2	4500	PSU	O4'-C4'-C5'-O5'
2	2	4529	B8W	C5-C6-O6-C61
2	2	4529	B8W	N1-C6-O6-C61
2	2	4530	UR3	C3'-C4'-C5'-O5'
2	2	4636	PSU	C2'-C1'-C5-C4
2	2	4636	PSU	O4'-C1'-C5-C6
2	2	4636	PSU	C3'-C4'-C5'-O5'
2	2	4636	PSU	O4'-C4'-C5'-O5'
2	2	4637	OMG	O4'-C4'-C5'-O5'
2	2	4637	OMG	C3'-C4'-C5'-O5'
2	2	4870	OMG	O4'-C4'-C5'-O5'
2	2	4870	OMG	C3'-C4'-C5'-O5'
2	2	237	B9B	O4'-C4'-C5'-O5'
2	2	1316	OMG	O4'-C4'-C5'-O5'
2	2	1316	OMG	C3'-C4'-C5'-O5'
2	2	1797	E7G	C3'-C4'-C5'-O5'
2	2	1860	B8H	C3'-C4'-C5'-O5'
2	2	1883	OMG	C3'-C4'-C5'-O5'
2	2	2364	OMG	C3'-C4'-C5'-O5'
2	2	2380	B8W	C3'-C4'-C5'-O5'
2	2	2401	A2M	O4'-C4'-C5'-O5'
2	2	3729	PSU	C3'-C4'-C5'-O5'
2	2	3729	PSU	O4'-C4'-C5'-O5'
2	2	3785	A2M	O4'-C4'-C5'-O5'
2	2	3867	A2M	O4'-C4'-C5'-O5'
2	2	3880	P7G	C3'-C4'-C5'-O5'
2	2	3880	P7G	O4'-C4'-C5'-O5'
2	2	3897	B8K	O4'-C4'-C5'-O5'
2	2	4371	MHG	O4'-C4'-C5'-O5'
2	2	4530	UR3	O4'-C4'-C5'-O5'
2	2	3880	P7G	N7-C71-C72-C73
2	2	237	B9B	O6-C61-C62-C63
2	2	398	A2M	C3'-C4'-C5'-O5'
2	2	1659	I4U	O4'-C4'-C5'-O5'
2	2	2422	OMC	O4'-C4'-C5'-O5'
2	2	3897	B8K	C3'-C4'-C5'-O5'
2	2	4296	B8H	C3'-C4'-C5'-O5'
2	2	4371	MHG	C72-C71-N7-C8
2	2	1883	OMG	O4'-C4'-C5'-O5'
2	2	3899	BGH	C3'-C4'-C5'-O5'
2	2	1348	P4U	O4-C41-C42-C43
2	2	2422	OMC	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	2	4371	MHG	C3'-C4'-C5'-O5'
2	2	2754	B9B	O6-C61-C62-C63
2	2	1625	OMG	C3'-C4'-C5'-O5'
2	2	4185	B8W	O4'-C4'-C5'-O5'
2	2	4296	B8H	O4'-C4'-C5'-O5'
2	2	3880	P7G	C72-C71-N7-C8
2	2	4872	2MG	O4'-C4'-C5'-O5'
2	2	1534	A2M	C4'-C5'-O5'-P
2	2	1909	P7G	N7-C71-C72-C73
2	2	4371	MHG	C2'-C1'-N9-C8
2	2	1574	B9B	O6-C61-C62-C63
2	2	1797	E7G	C72-C71-N7-C8
2	2	4870	OMG	C4'-C5'-O5'-P
2	2	4494	OMG	C3'-C2'-O2'-CM2
2	2	1625	OMG	O4'-C4'-C5'-O5'
2	2	4371	MHG	C71-C72-C73-C75
2	2	3701	OMC	O4'-C1'-N1-C6
2	2	4355	E6G	C62-C61-O6-C6
2	2	4500	PSU	C4'-C5'-O5'-P
2	2	4872	2MG	C3'-C4'-C5'-O5'
2	2	4536	OMC	C3'-C2'-O2'-CM2
2	2	3887	OMC	C4'-C5'-O5'-P
2	2	2297	E7G	C72-C71-N7-C8
2	2	3701	OMC	O4'-C1'-N1-C2
2	2	1677	PSU	O4'-C1'-C5-C4
2	2	2754	B9B	C62-C61-O6-C6
2	2	4296	B8H	O4'-C1'-C5-C4
2	2	4500	PSU	O4'-C1'-C5-C4
2	2	4636	PSU	O4'-C1'-C5-C4
2	2	3897	B8K	C4'-C5'-O5'-P
2	2	4447	5MC	O4'-C1'-N1-C6
2	2	1534	A2M	O4'-C4'-C5'-O5'
2	2	4447	5MC	C2'-C1'-N1-C6
2	2	729	2MG	O4'-C4'-C5'-O5'
2	2	3880	P7G	C72-C71-N7-C5
2	2	4371	MHG	C72-C71-N7-C5
2	2	4355	E6G	O4'-C4'-C5'-O5'
2	2	2861	OMC	C1'-C2'-O2'-CM2
2	2	4371	MHG	O4'-C1'-N9-C8
2	2	3909	OMC	C2'-C1'-N1-C2
2	2	1677	PSU	O4'-C1'-C5-C6
2	2	4296	B8H	O4'-C1'-C5-C6

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Mol	Chain	Res	Type	Atoms
2	2	4450	PSU	O4'-C1'-C5-C6
2	2	4500	PSU	O4'-C1'-C5-C6
2	2	1683	PSU	O4'-C4'-C5'-O5'
2	2	2773	OMG	O4'-C4'-C5'-O5'
2	2	4447	5MC	O4'-C4'-C5'-O5'
2	2	4194	I4U	C42-C41-O4-C4
2	2	4194	I4U	C43-C41-O4-C4

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 251 ligands modelled in this entry, 251 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 [i](#)

There are no chain breaks in this entry.

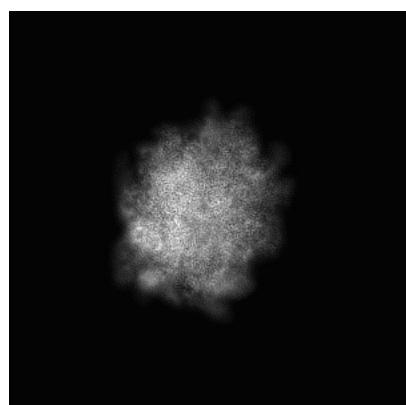
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0948. These allow visual inspection of the internal detail of the map and identification of artifacts.

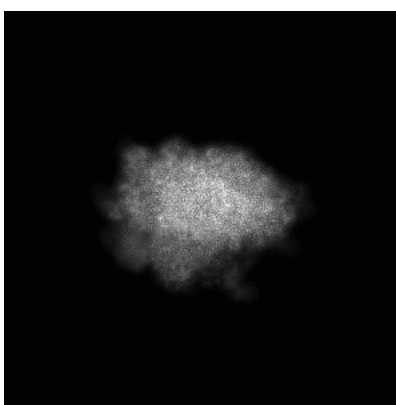
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

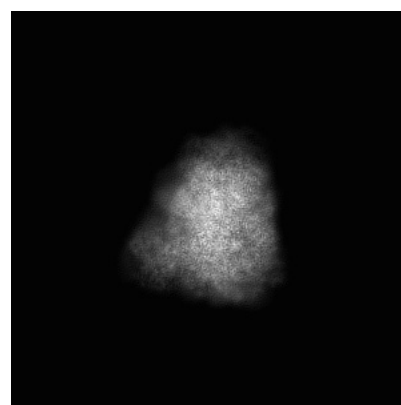
#### 6.1.1 Primary map



X



Y

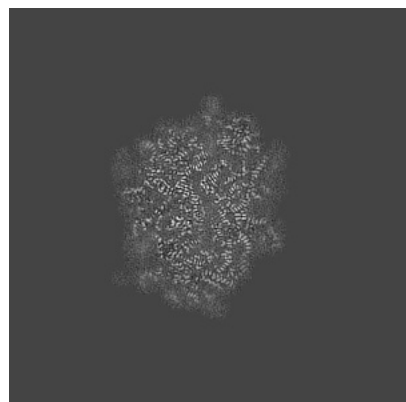


Z

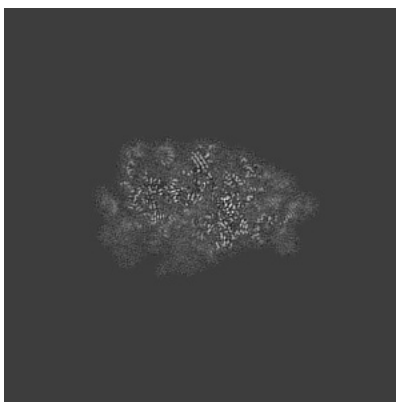
The images above show the map projected in three orthogonal directions.

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

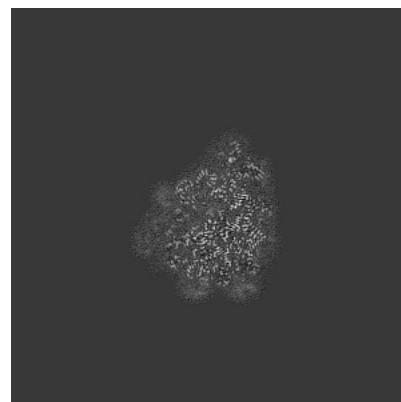
#### 6.2.1 Primary map



X Index: 240



Y Index: 240

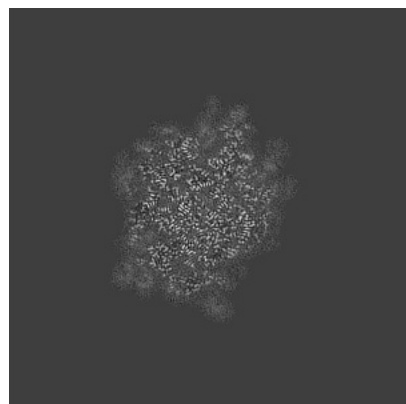


Z Index: 240

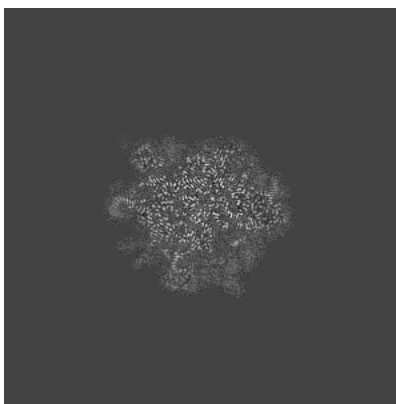
The images above show central slices of the map in three orthogonal directions.

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

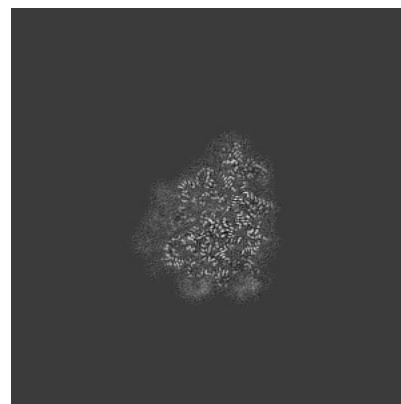
### 6.3.1 Primary map



X Index: 253



Y Index: 200

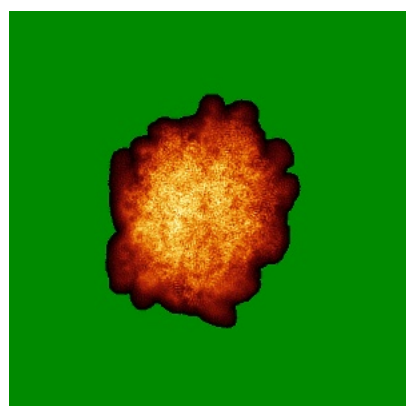


Z Index: 237

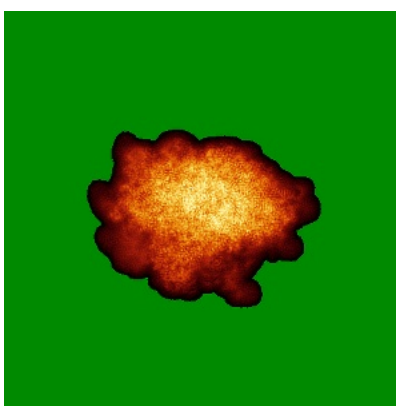
The images above show the largest variance slices of the map in three orthogonal directions.

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

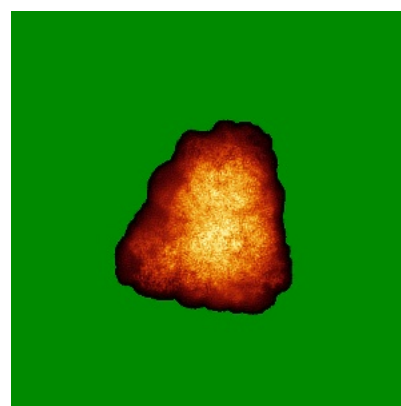
### 6.4.1 Primary map



X



Y

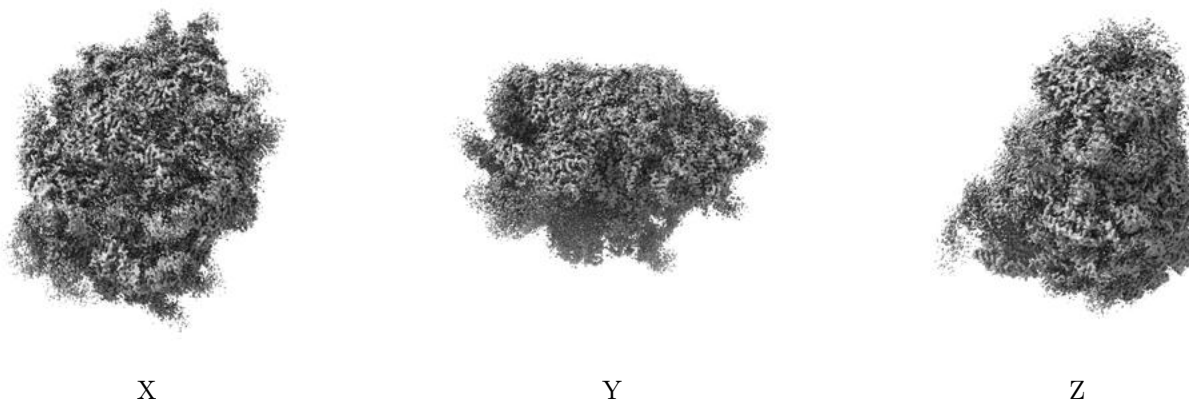


Z

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 0.065. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

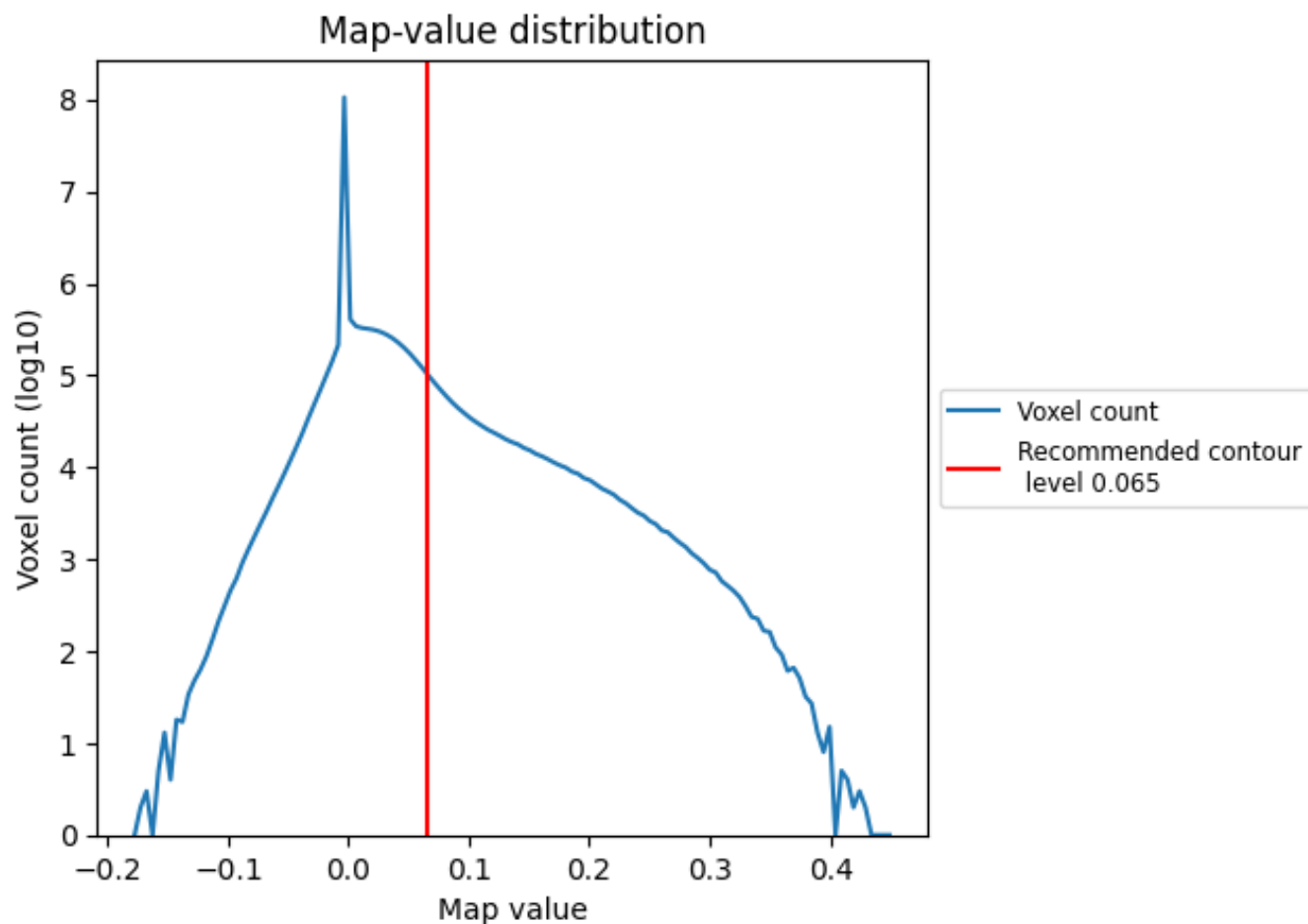
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

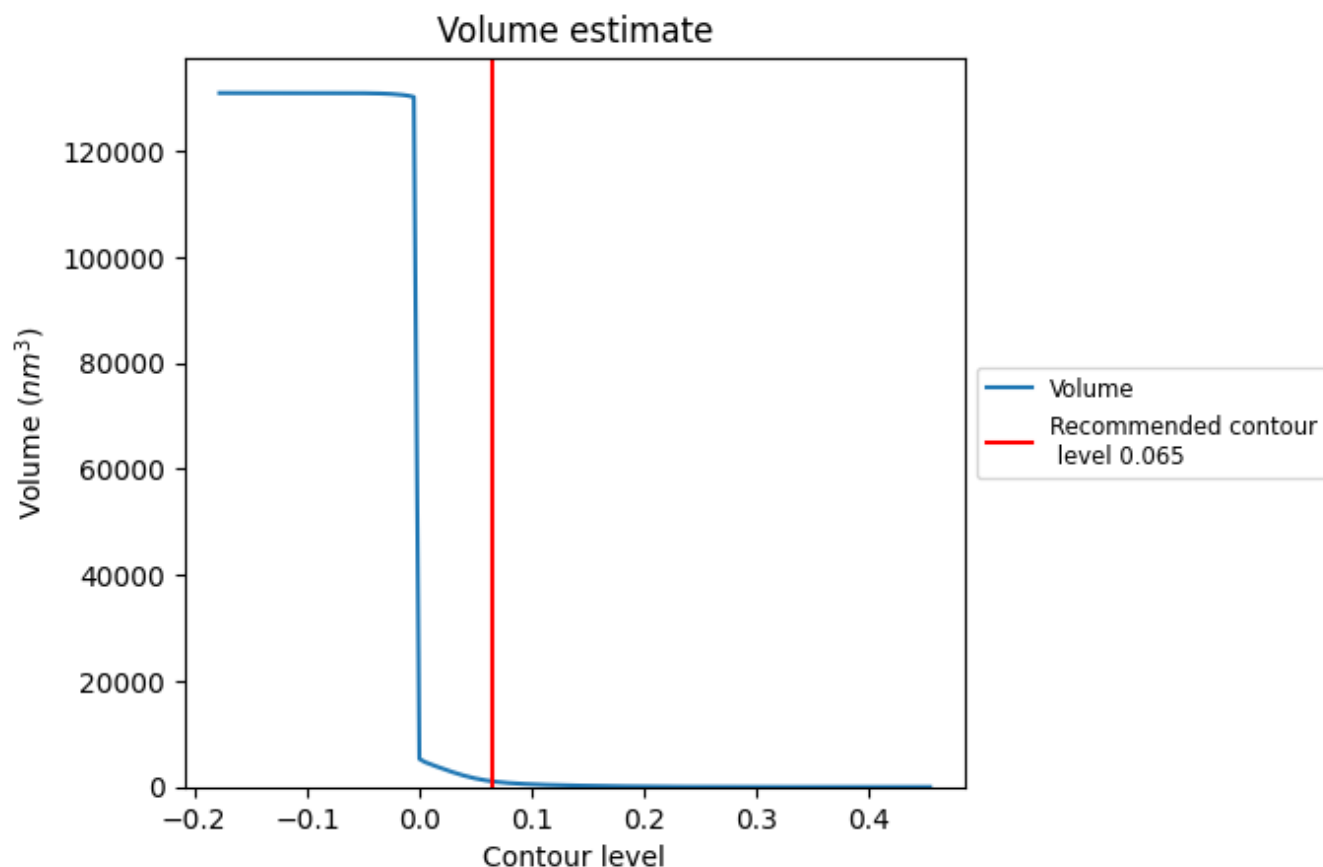
This section contains the results of statistical analysis of the map.

### 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.

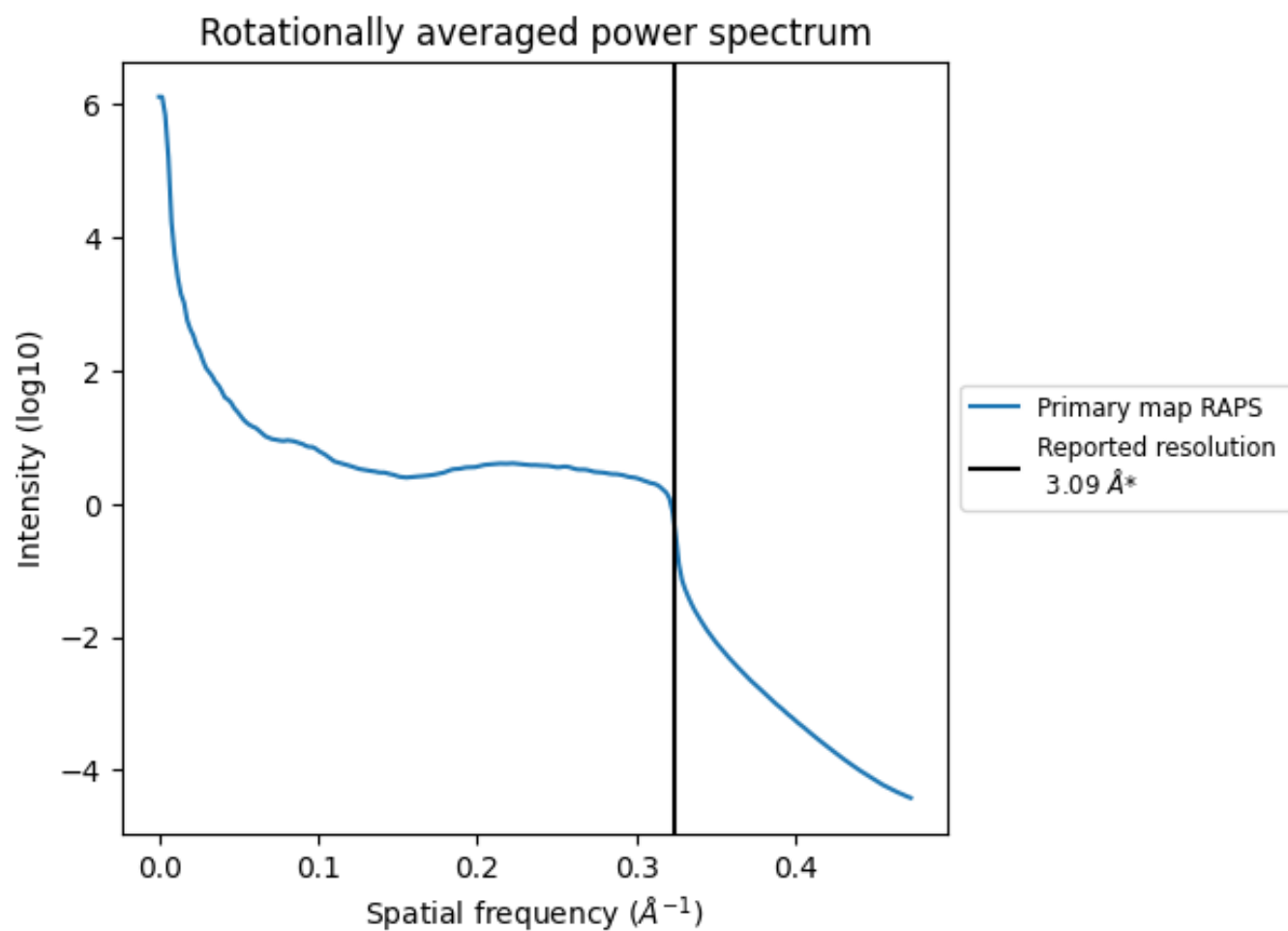
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1059  $\text{nm}^3$ ; this corresponds to an approximate mass of 957 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 0.324 Å<sup>-1</sup>

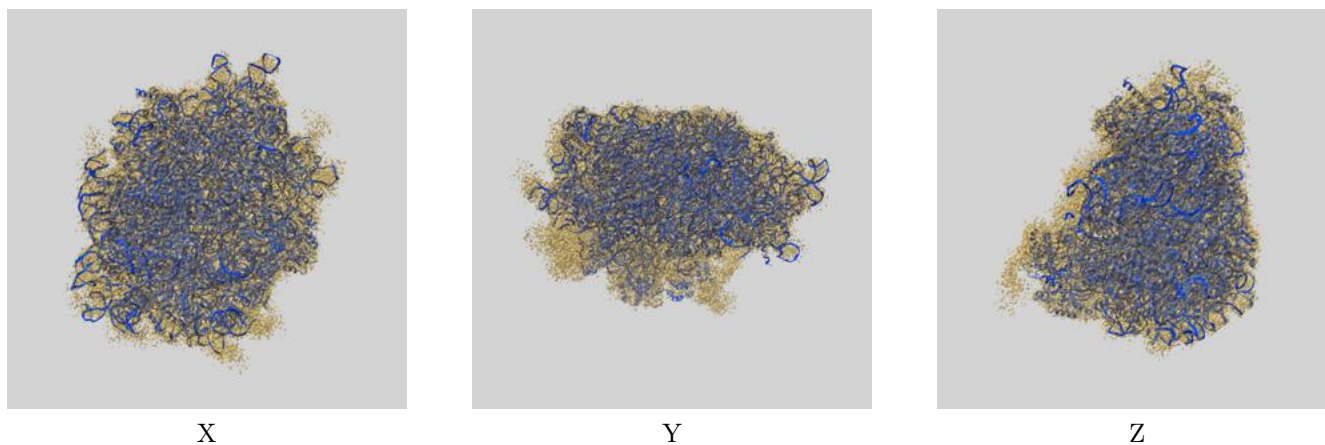
## 8 Fourier-Shell correlation

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

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

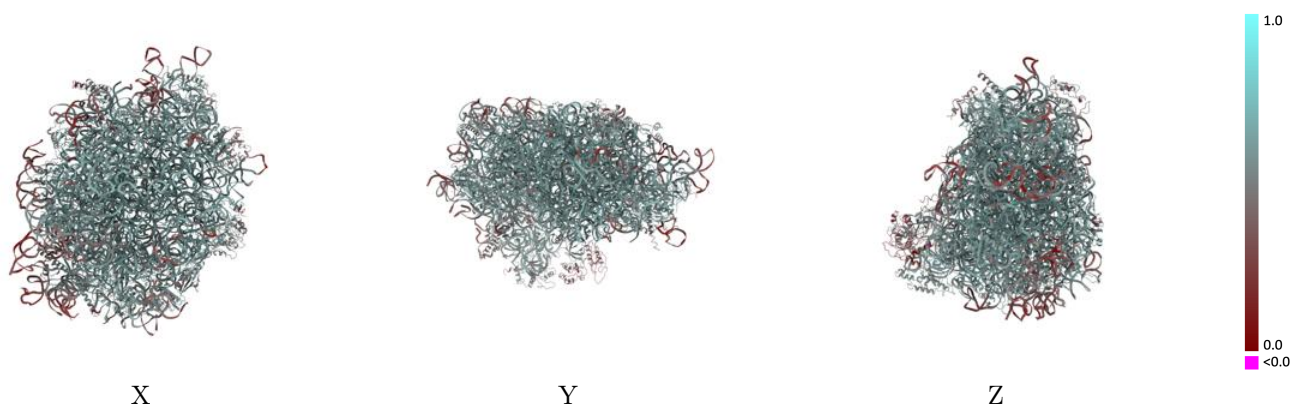
This section contains information regarding the fit between EMDB map EMD-0948 and PDB model 6LQM. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

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



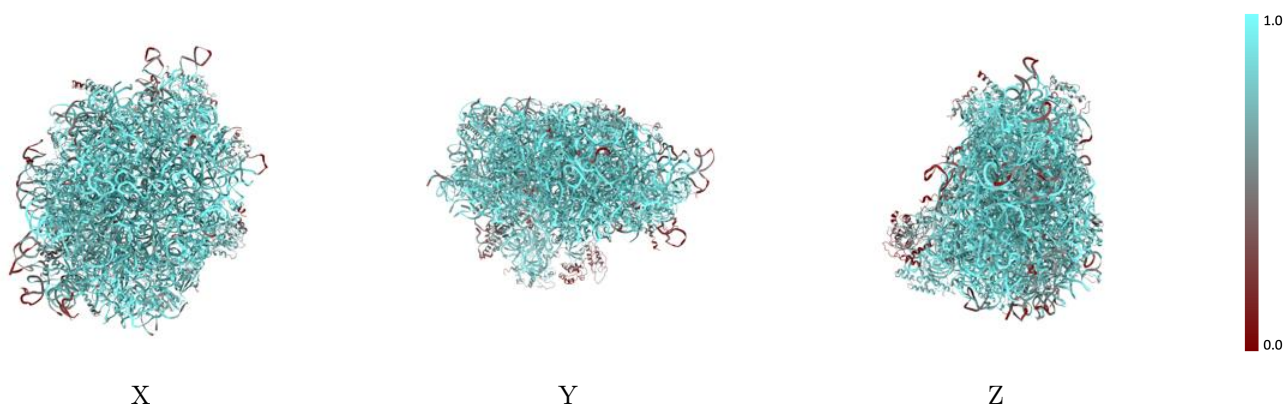
The images above show the 3D surface view of the map at the recommended contour level 0.065 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



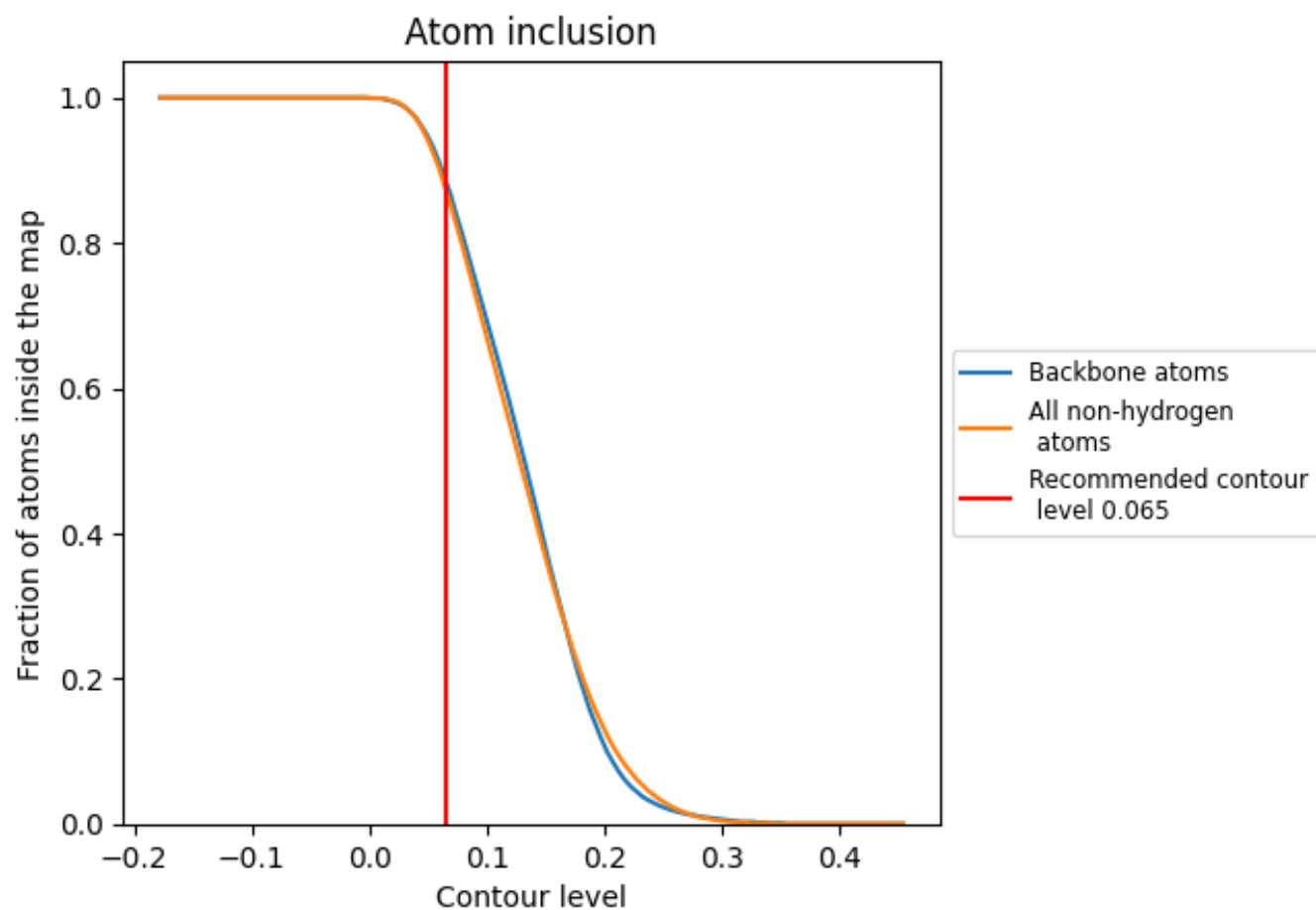
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.065).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 87% 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 (0.065) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8740	 0.5550
0	 0.6940	 0.4930
2	 0.8960	 0.5500
3	 0.7860	 0.5210
5	 0.9680	 0.5760
6	 0.6390	 0.5010
8	 0.9410	 0.5780
A	 0.2160	 0.2790
B	 0.8900	 0.5820
C	 0.8310	 0.5450
D	 0.9170	 0.5940
E	 0.7940	 0.5460
F	 0.8640	 0.5830
G	 0.7790	 0.5390
H	 0.8710	 0.5760
I	 0.8480	 0.5630
J	 0.6120	 0.5000
K	 0.8330	 0.5590
L	 0.9210	 0.6080
M	 0.9580	 0.6070
N	 0.6900	 0.4850
O	 0.7160	 0.5330
P	 0.9550	 0.5950
Q	 0.8780	 0.5790
R	 0.7610	 0.5280
S	 0.8930	 0.5770
T	 0.8480	 0.5760
U	 0.9720	 0.6150
V	 0.9150	 0.5950
W	 0.8820	 0.5730
X	 0.8610	 0.5810
Y	 0.9240	 0.6020
Z	 0.9520	 0.6100
a	 0.8660	 0.5700
b	 0.9420	 0.6010



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Chain	Atom inclusion	Q-score
c	 0.8910	 0.5740
d	 0.6690	 0.4730
e	 0.9000	 0.5900
f	 0.8910	 0.5800
g	 0.8840	 0.5840
h	 0.8980	 0.5910
i	 0.8330	 0.5650
l	 0.9120	 0.5920
m	 0.9320	 0.6000
r	 0.7920	 0.5380
t	 0.9460	 0.6070
u	 0.9500	 0.6130
v	 0.7810	 0.5310
w	 0.9140	 0.5870