



## Full wwPDB EM Validation Report ⓘ

Dec 11, 2022 – 04:40 pm GMT

PDB ID : 6SKF  
EMDB ID : EMD-10223  
Title : Cryo-EM Structure of *T. kodakarensis* 70S ribosome  
Authors : Matzov, D.; Sas-Chen, A.; Thomas, J.M.; Santangelo, T.; Meier, J.L.;  
Schwartz, S.; Shalev-Benami, M.  
Deposited on : 2019-08-15  
Resolution : 2.95 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:

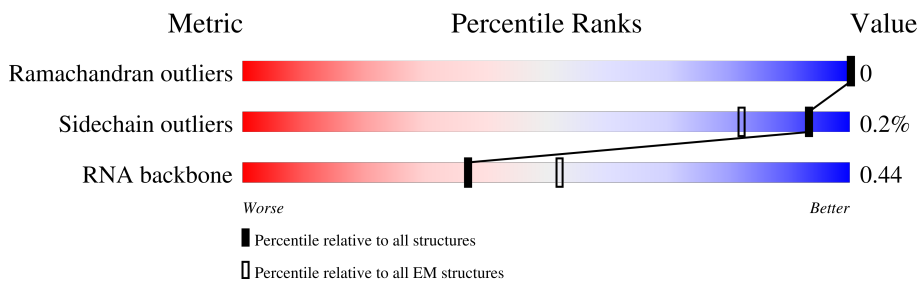
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 2.95 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	Aa	1498	<div style="display: flex; align-items: center;"> <div style="width: 8%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 72%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 24%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">8%      72%      24%      . .</p>
2	Ab	201	<div style="display: flex; align-items: center;"> <div style="width: 25%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 98%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">25%      98%      .</p>
3	Ac	209	<div style="display: flex; align-items: center;"> <div style="width: 71%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 93%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">71%      93%      7%</p>
4	Ad	200	<div style="display: flex; align-items: center;"> <div style="width: 29%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 95%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">29%      95%      5%</p>
5	Ae	180	<div style="display: flex; align-items: center;"> <div style="width: 16%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 97%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 3%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">16%      97%      .</p>
6	Af	243	<div style="display: flex; align-items: center;"> <div style="width: 15%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 99%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">15%      99%      .</p>
7	Ag	235	<div style="display: flex; align-items: center;"> <div style="width: 14%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 95%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">14%      95%      5%</p>
8	Ah	125	<div style="display: flex; align-items: center;"> <div style="width: 58%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 98%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">58%      98%      .</p>

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Mol	Chain	Length	Quality of chain
9	Ai	215	34% 100%
10	Aj	130	10% 99%
11	Ak	130	21% 96%
12	Al	135	44% 99%
13	Am	102	76% 98%
14	An	140	26% 89% 9%
15	Ao	147	14% 97%
16	Ap	149	28% 91% 9%
17	Aq	151	20% 98%
18	Ar	56	43% 96%
19	As	114	18% 95% 5%
20	At	67	90% 96%
21	Au	133	41% 86% 13%
22	Av	150	27% 99%
23	Aw	98	22% 97%
24	Ax	65	34% 94% 6%
25	Ay	70	39% 91% 9%
26	Az	62	21% 89% 11%
27	BA	3037	9% 60% 33%
28	BB	126	20% 73% 25%
29	BC	239	7% 99%
30	BD	346	7% 99%
31	BE	255	100%
32	BF	183	81% 91% 8%
33	BG	184	12% 99%

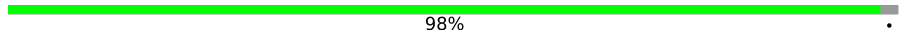
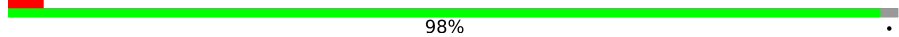

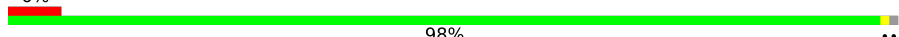
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Mol	Chain	Length	Quality of chain
34	BH	123	36% 98%
34	BI	123	98%
35	BJ	182	10% 92% 8%
36	BK	142	100%
37	BL	141	10% 99%
38	BM	83	25% 96%
38	BN	83	33% 96%
39	BO	148	29% 99%
40	BP	194	99%
41	BQ	201	33% 82% 18%
42	BR	121	98%
43	BS	150	8% 97%
44	BT	77	19% 96%
45	BU	98	98%
46	BV	156	97%
47	BW	86	13% 99%
48	BX	121	7% 99%
49	BY	67	93% 7%
50	BZ	66	27% 89% 9%
51	Ba	155	5% 99%
52	Bb	102	16% 94% 6%
53	Bc	90	12% 99%
54	Bd	125	6% 99%
55	Be	90	7% 98%
56	Bg	86	5% 97%

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Mol	Chain	Length	Quality of chain
57	Bh	63	 98% .
58	Bi	51	 98% .
59	Bj	51	 8% 92% 8% .
60	Bk	37	 97% .
61	Bl	94	 6% 98% ..

## 2 Entry composition

There are 63 unique types of molecules in this entry. The entry contains 161921 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	Aa	1463	31591	14101	5837	10190	1463	0	0

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	Ab	196	1580	1021	272	284	3	0	0

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	Ac	195	1524	973	277	271	3	0	0

- Molecule 4 is a protein called 30S ribosomal protein S3Ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	Ad	190	1550	997	277	273	3	0	0

- Molecule 5 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	Ae	174	1454	912	287	253	2	0	0

- Molecule 6 is a protein called 30S ribosomal protein S4e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	Af	241	1945	1256	348	336	5	0	0

- Molecule 7 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	Ag	223	1753	1107	327	312	7	0	0

- Molecule 8 is a protein called 30S ribosomal protein S6e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	Ah	123	952	599	179	172	2	0	0

- Molecule 9 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	Ai	214	1715	1087	317	303	8	0	0

- Molecule 10 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	Aj	129	1020	662	176	180	2	0	0

- Molecule 11 is a protein called 30S ribosomal protein S8e.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	Ak	125	982	615	198	169	0	0

- Molecule 12 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	Al	133	1054	656	205	188	5	0	0

- Molecule 13 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	Am	100	803	498	154	148	3	0	0

- Molecule 14 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	An	127	Total	C	N	O	S	0	0
			950	586	190	171	3		

- Molecule 15 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Ao	143	Total	C	N	O	S	0	0
			1122	712	216	192	2		

- Molecule 16 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Ap	135	Total	C	N	O	S	0	0
			1090	691	214	181	4		

- Molecule 17 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Aq	149	Total	C	N	O	S	0	0
			1217	776	233	206	2		

- Molecule 18 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Ar	54	Total	C	N	O	S	0	0
			447	284	92	65	6		

- Molecule 19 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	As	108	Total	C	N	O	S	0	0
			879	560	164	152	3		

- Molecule 20 is a protein called 30S ribosomal protein S17e.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	At	64	Total	C	N	O	S	0	0
			538	338	103	95	2		

- Molecule 21 is a protein called 30S ribosomal protein S19.



Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	Au	116	952	608	175	163	6	0	0

- Molecule 22 is a protein called 30S ribosomal protein S19e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	Av	149	1216	788	215	213		0	0

- Molecule 23 is a protein called 30S ribosomal protein S24e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	Aw	95	777	497	131	146	3	0	0

- Molecule 24 is a protein called 30S ribosomal protein S27e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	Ax	61	461	294	83	79	5	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ax	64	GLU	LEU	conflict	UNP Q5JE50

- Molecule 25 is a protein called 30S ribosomal protein S28e.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
25	Ay	64	499	307	99	93	0	0

- Molecule 26 is a protein called Predicted zinc-ribbon RNA-binding protein involved in translation.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	Az	55	426	269	74	75	8	0	0

- Molecule 27 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	N	O	P			S
27	BA	2929	63265	28239	11728	20367	2929	2	0	0

- Molecule 28 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	N	O	P			S
28	BB	125	2678	1191	492	870	125		0	0

- Molecule 29 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	BC	237	1820	1150	356	311	3	0	0

- Molecule 30 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	BD	344	2746	1765	505	469	7	0	0

- Molecule 31 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	BE	255	2026	1286	389	347	4	0	0

- Molecule 32 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	BF	169	1313	821	252	233	7	0	0

- Molecule 33 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	BG	183	1463	942	253	266	2	0	0

- Molecule 34 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BH	121	Total	C	N	O	S	0	0
			928	591	154	180	3		
34	BI	121	Total	C	N	O	S	0	0
			928	591	154	180	3		

- Molecule 35 is a protein called 50S ribosomal protein L10e.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BJ	168	Total	C	N	O	S	0	0
			1378	877	258	236	7		

- Molecule 36 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BK	142	Total	C	N	O	S	0	0
			1146	731	213	198	4		

- Molecule 37 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BL	140	Total	C	N	O	S	0	0
			1055	658	214	180	3		

- Molecule 38 is a protein called 50S ribosomal protein L14e.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BM	81	Total	C	N	O	S	0	0
			610	382	119	108	1		
38	BN	81	Total	C	N	O	S	0	0
			610	382	119	108	1		

- Molecule 39 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BO	148	Total	C	N	O	S	0	0
			1165	742	222	198	3		

- Molecule 40 is a protein called 50S ribosomal protein L15e.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	BP	193	Total	C	N	O	S	0	0
			1582	1010	316	250	6		

- Molecule 41 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	BQ	164	1314	841	243	228	2	0	0

- Molecule 42 is a protein called 50S ribosomal protein L18e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	BR	120	959	601	187	169	2	0	0

- Molecule 43 is a protein called 50S ribosomal protein L19e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	BS	146	1200	753	246	194	7	0	0

- Molecule 44 is a protein called 50S ribosomal protein L18Ae.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
44	BT	74	624	399	113	112	0	0

- Molecule 45 is a protein called 50S ribosomal protein L21e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	BU	96	784	502	158	123	1	0	0

- Molecule 46 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	BV	154	1234	777	242	211	4	0	0

- Molecule 47 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	BW	85	683	438	119	123	3	0	0

- Molecule 48 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	BX	120	991	628	188	170	5	0	0

- Molecule 49 is a protein called 50S ribosomal protein L24e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	BY	62	524	334	99	85	6	0	0

- Molecule 50 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	BZ	60	506	314	98	90	4	0	0

- Molecule 51 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	Ba	154	1242	788	235	214	5	0	0

- Molecule 52 is a protein called 50S ribosomal protein L30e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	Bb	96	730	473	123	133	1	0	0

- Molecule 53 is a protein called 50S ribosomal protein L31e.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
53	Bc	89	721	463	140	118	0	0

- Molecule 54 is a protein called 50S ribosomal protein L32e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	Bd	124	1022	650	208	162	2	0	0

- Molecule 55 is a protein called 50S ribosomal protein L34e.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	Be	89	Total	C	N	O	S	0	0
			728	454	155	110	9		

- Molecule 56 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	Bg	84	Total	C	N	O	S	0	0
			630	392	132	101	5		

- Molecule 57 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	Bh	62	Total	C	N	O	S	0	0
			512	314	118	75	5		

- Molecule 58 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms				AltConf	Trace
58	Bi	50	Total	C	N	O	0	0
			432	276	97	59		

- Molecule 59 is a protein called 50S ribosomal protein L40e.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	Bj	47	Total	C	N	O	S	0	0
			373	233	79	56	5		

- Molecule 60 is a protein called LSU ribosomal protein L41E.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	Bk	36	Total	C	N	O	S	0	0
			345	218	86	39	2		

- Molecule 61 is a protein called 50S ribosomal protein L44e.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	Bl	93	Total	C	N	O	S	0	0
			778	494	160	119	5		

- Molecule 62 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
62	Ag	1	Total 1	Zn 1	0
62	Ar	1	Total 1	Zn 1	0
62	As	1	Total 1	Zn 1	0
62	Ax	1	Total 1	Zn 1	0
62	Az	2	Total 2	Zn 2	0
62	BY	1	Total 1	Zn 1	0
62	Be	1	Total 1	Zn 1	0
62	Bg	1	Total 1	Zn 1	0
62	Bh	1	Total 1	Zn 1	0
62	Bj	1	Total 1	Zn 1	0
62	Bl	1	Total 1	Zn 1	0

- Molecule 63 is water.

Mol	Chain	Residues	Atoms		AltConf
63	Aa	714	Total 714	O 714	0
63	Ab	8	Total 8	O 8	0
63	Ac	10	Total 10	O 10	0
63	Ad	4	Total 4	O 4	0
63	Ae	13	Total 13	O 13	0
63	Af	14	Total 14	O 14	0
63	Ag	14	Total 14	O 14	0
63	Ah	2	Total 2	O 2	0
63	Ai	13	Total 13	O 13	0

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Mol	Chain	Residues	Atoms		AltConf
63	Aj	12	Total 12	O 12	0
63	Ak	8	Total 8	O 8	0
63	Al	7	Total 7	O 7	0
63	Am	2	Total 2	O 2	0
63	An	8	Total 8	O 8	0
63	Ao	10	Total 10	O 10	0
63	Ap	11	Total 11	O 11	0
63	Aq	10	Total 10	O 10	0
63	Ar	2	Total 2	O 2	0
63	As	6	Total 6	O 6	0
63	At	1	Total 1	O 1	0
63	Au	4	Total 4	O 4	0
63	Av	13	Total 13	O 13	0
63	Aw	1	Total 1	O 1	0
63	Ax	3	Total 3	O 3	0
63	Ay	4	Total 4	O 4	0
63	Az	4	Total 4	O 4	0
63	BA	1226	Total 1226	O 1226	0
63	BB	19	Total 19	O 19	0
63	BC	19	Total 19	O 19	0
63	BD	24	Total 24	O 24	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms		AltConf
63	BE	11	Total 11	O 11	0
63	BG	6	Total 6	O 6	0
63	BJ	11	Total 11	O 11	0
63	BK	11	Total 11	O 11	0
63	BL	4	Total 4	O 4	0
63	BM	2	Total 2	O 2	0
63	BN	4	Total 4	O 4	0
63	BO	10	Total 10	O 10	0
63	BP	18	Total 18	O 18	0
63	BQ	7	Total 7	O 7	0
63	BR	8	Total 8	O 8	0
63	BS	7	Total 7	O 7	0
63	BT	3	Total 3	O 3	0
63	BU	7	Total 7	O 7	0
63	BV	7	Total 7	O 7	0
63	BW	4	Total 4	O 4	0
63	BX	6	Total 6	O 6	0
63	BY	3	Total 3	O 3	0
63	BZ	1	Total 1	O 1	0
63	Ba	10	Total 10	O 10	0
63	Bb	1	Total 1	O 1	0

*Continued on next page...*

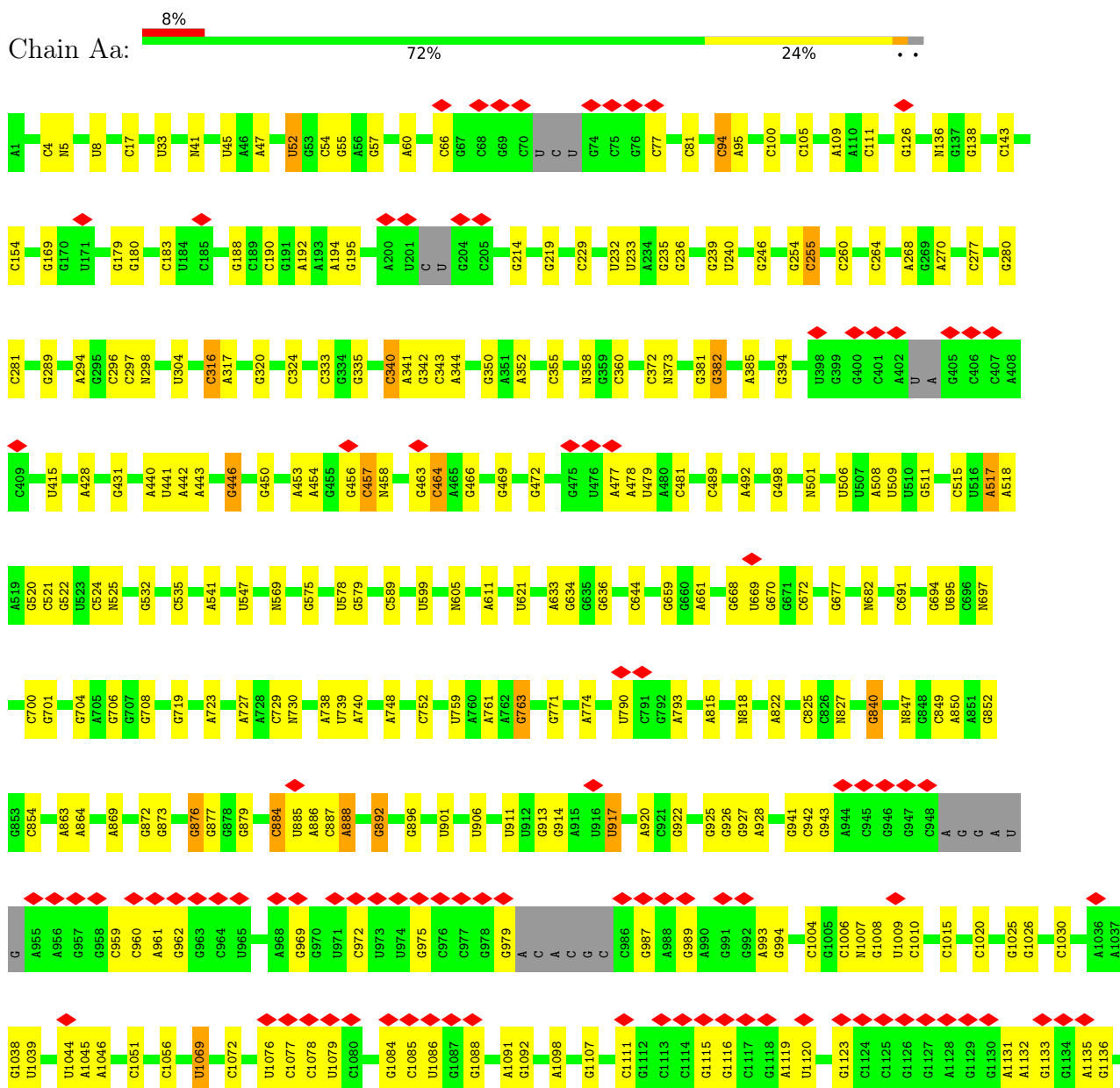
*Continued from previous page...*

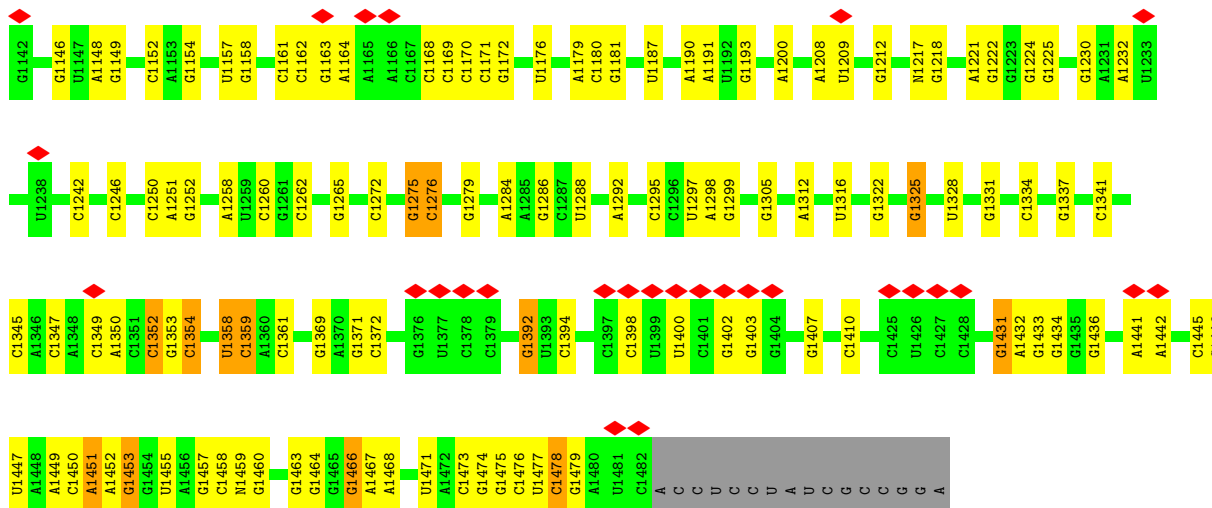
Mol	Chain	Residues	Atoms		AltConf
63	Bc	3	Total 3	O 3	0
63	Bd	5	Total 5	O 5	0
63	Be	3	Total 3	O 3	0
63	Bg	3	Total 3	O 3	0
63	Bh	11	Total 11	O 11	0
63	Bi	2	Total 2	O 2	0
63	Bj	2	Total 2	O 2	0
63	Bk	3	Total 3	O 3	0
63	Bl	8	Total 8	O 8	0

### 3 Residue-property plots

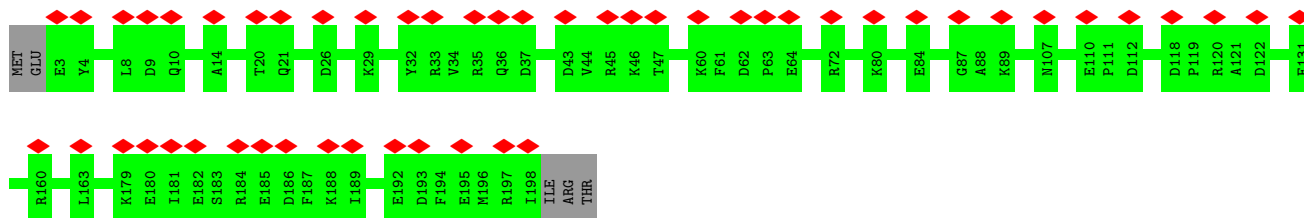
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 16S rRNA

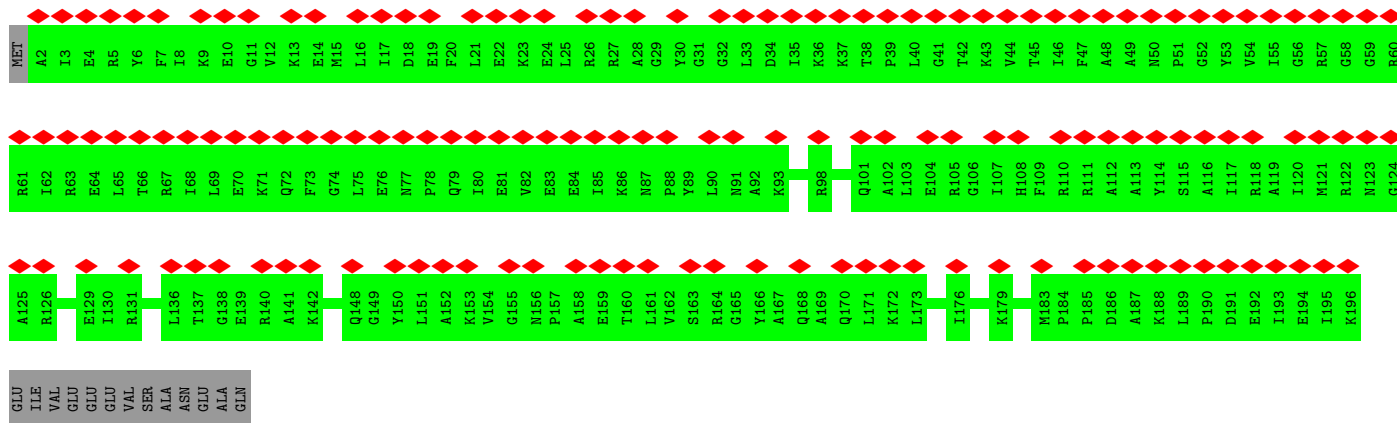
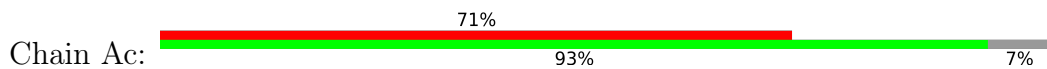




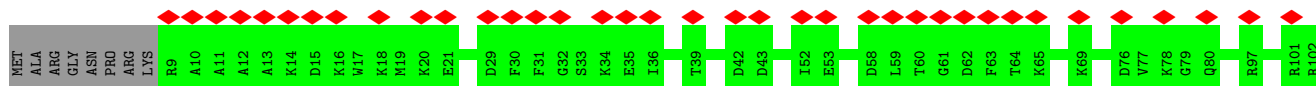
• Molecule 2: 30S ribosomal protein S2

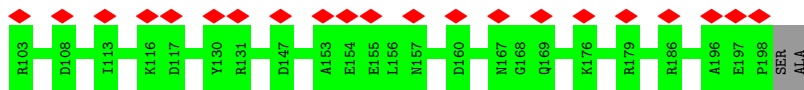


• Molecule 3: 30S ribosomal protein S3

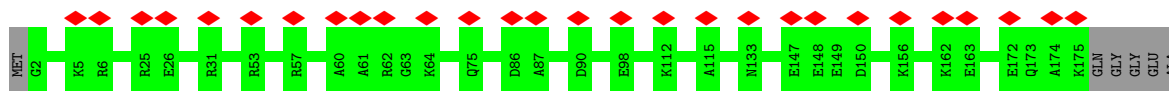


• Molecule 4: 30S ribosomal protein S3Ae

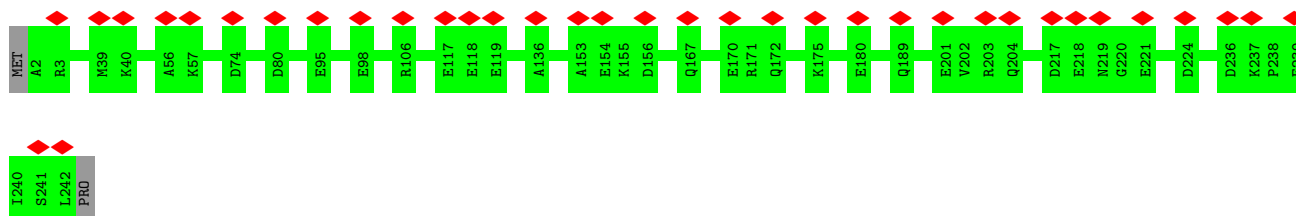




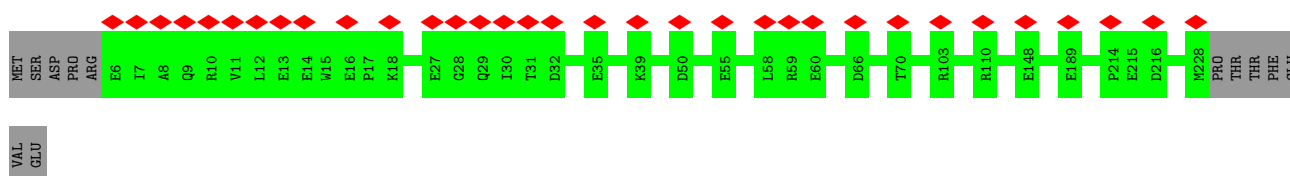
- Molecule 5: 30S ribosomal protein S4



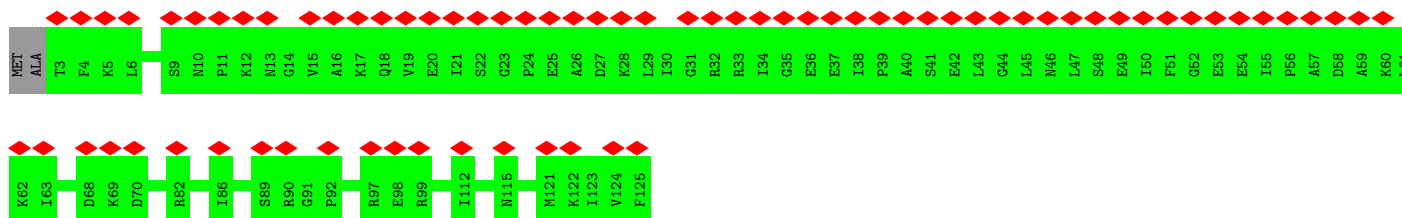
- Molecule 6: 30S ribosomal protein S4e



- Molecule 7: 30S ribosomal protein S5

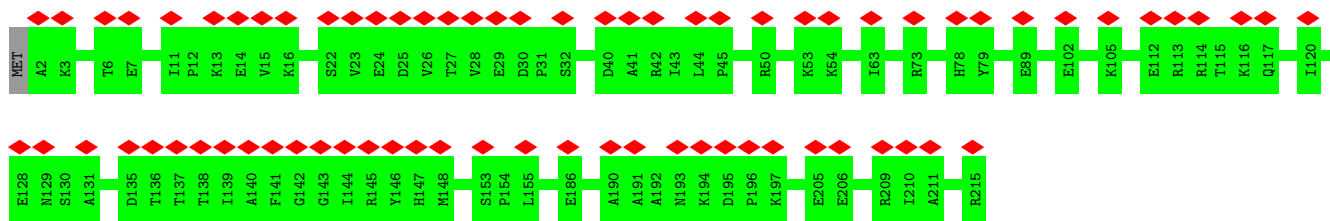


- Molecule 8: 30S ribosomal protein S6e

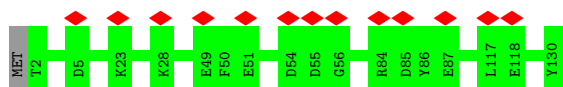


- Molecule 9: 30S ribosomal protein S7

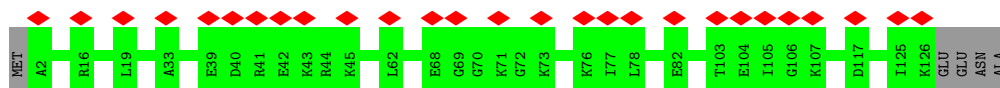




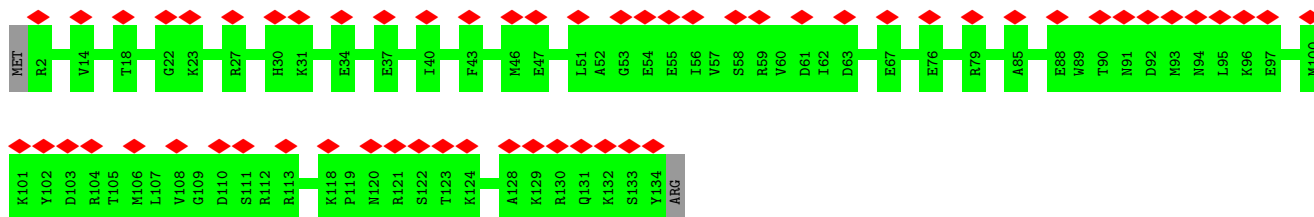
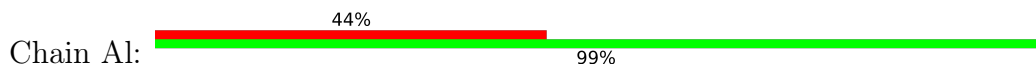
- Molecule 10: 30S ribosomal protein S8



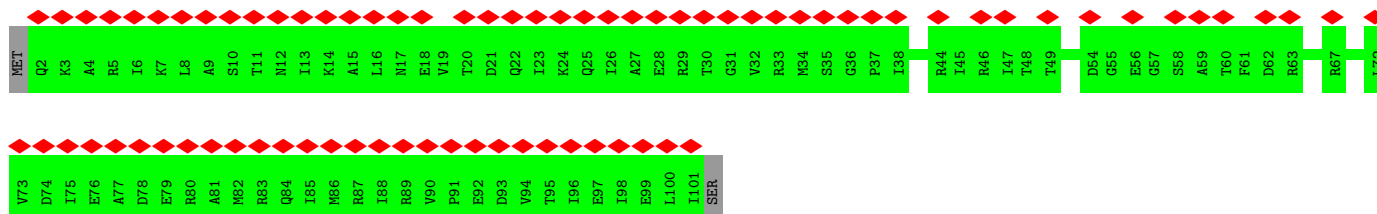
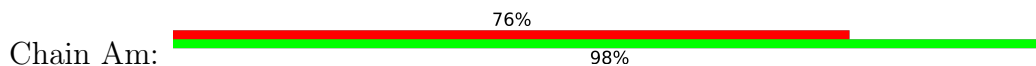
- Molecule 11: 30S ribosomal protein S8e



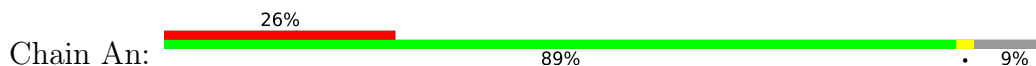
- Molecule 12: 30S ribosomal protein S9

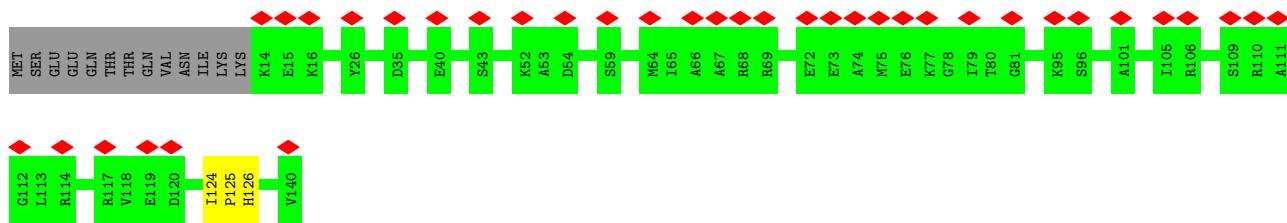


- Molecule 13: 30S ribosomal protein S10

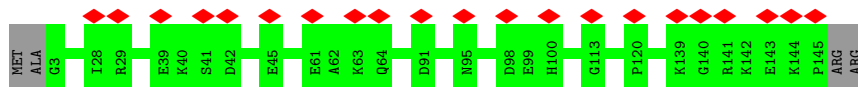


- Molecule 14: 30S ribosomal protein S11

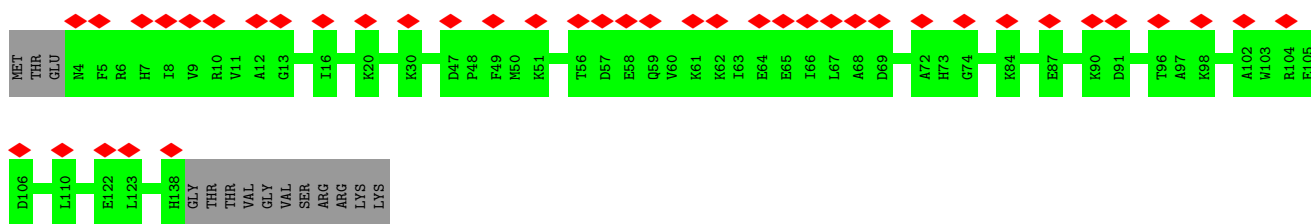




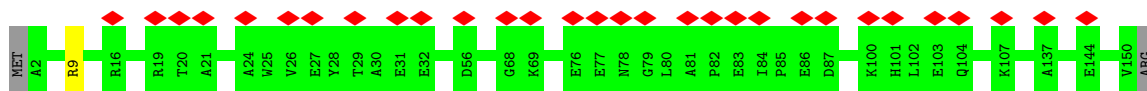
• Molecule 15: 30S ribosomal protein S12



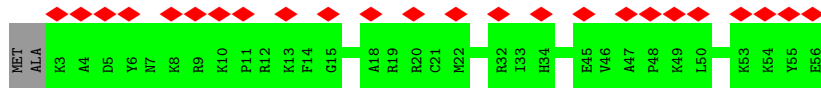
• Molecule 16: 30S ribosomal protein S13



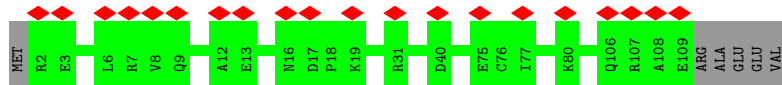
• Molecule 17: 30S ribosomal protein S15



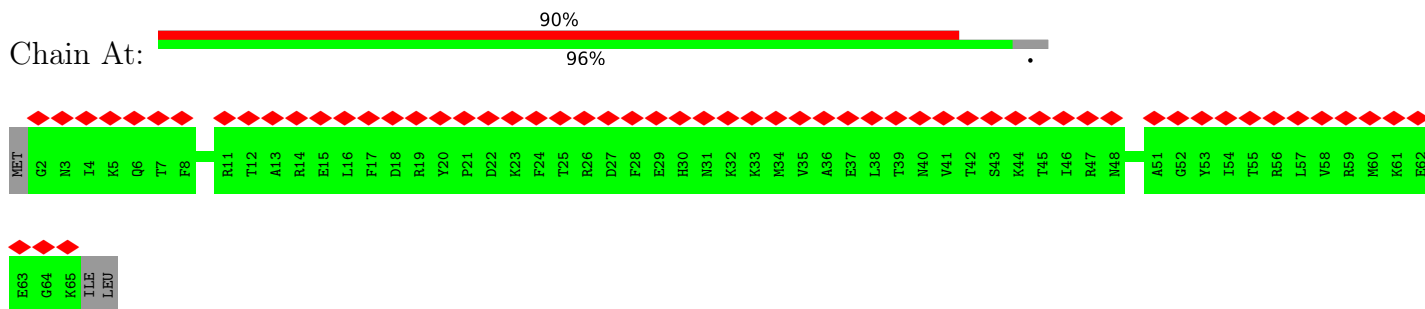
• Molecule 18: 30S ribosomal protein S14 type Z



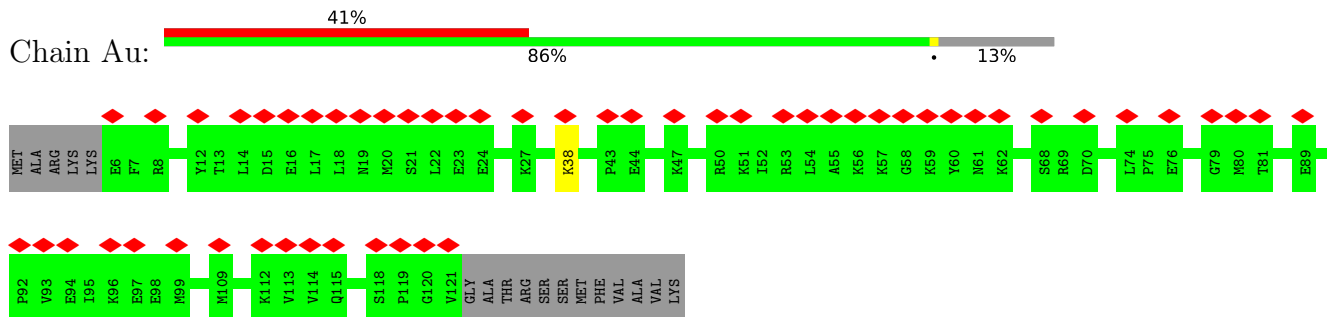
• Molecule 19: 30S ribosomal protein S17



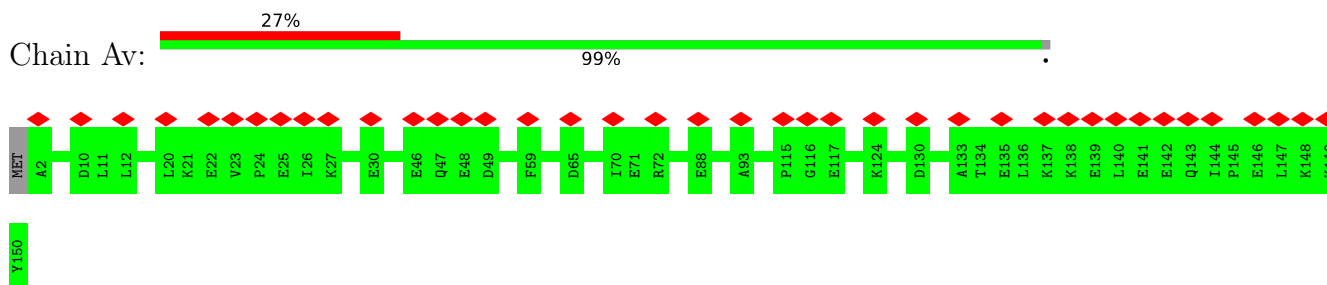
• Molecule 20: 30S ribosomal protein S17e



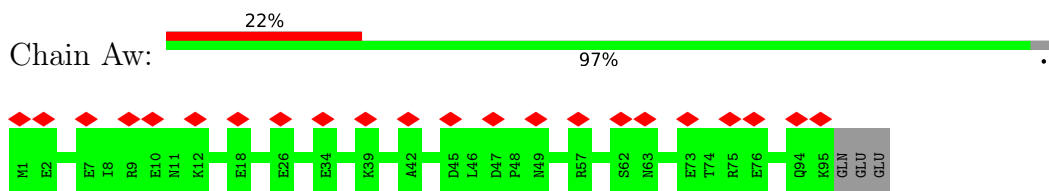
• Molecule 21: 30S ribosomal protein S19



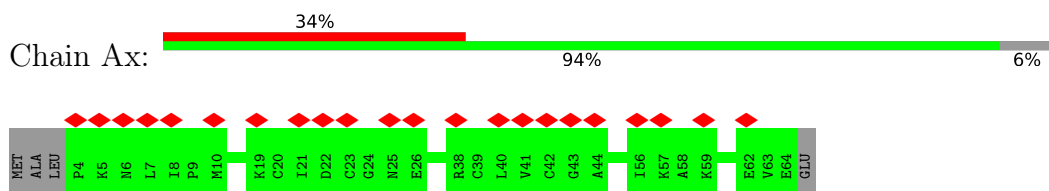
• Molecule 22: 30S ribosomal protein S19e



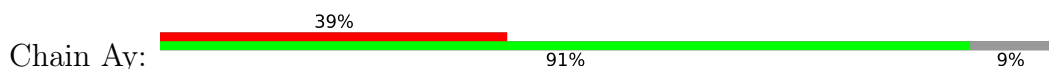
• Molecule 23: 30S ribosomal protein S24e



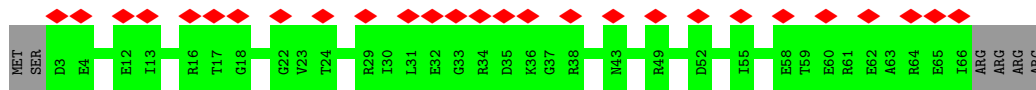
• Molecule 24: 30S ribosomal protein S27e



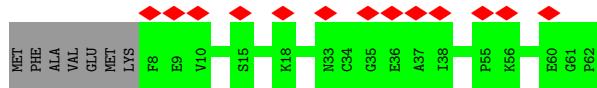
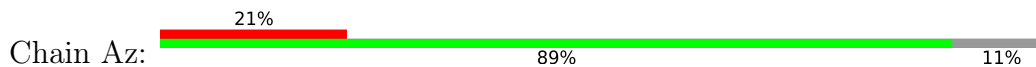
• Molecule 25: 30S ribosomal protein S28e



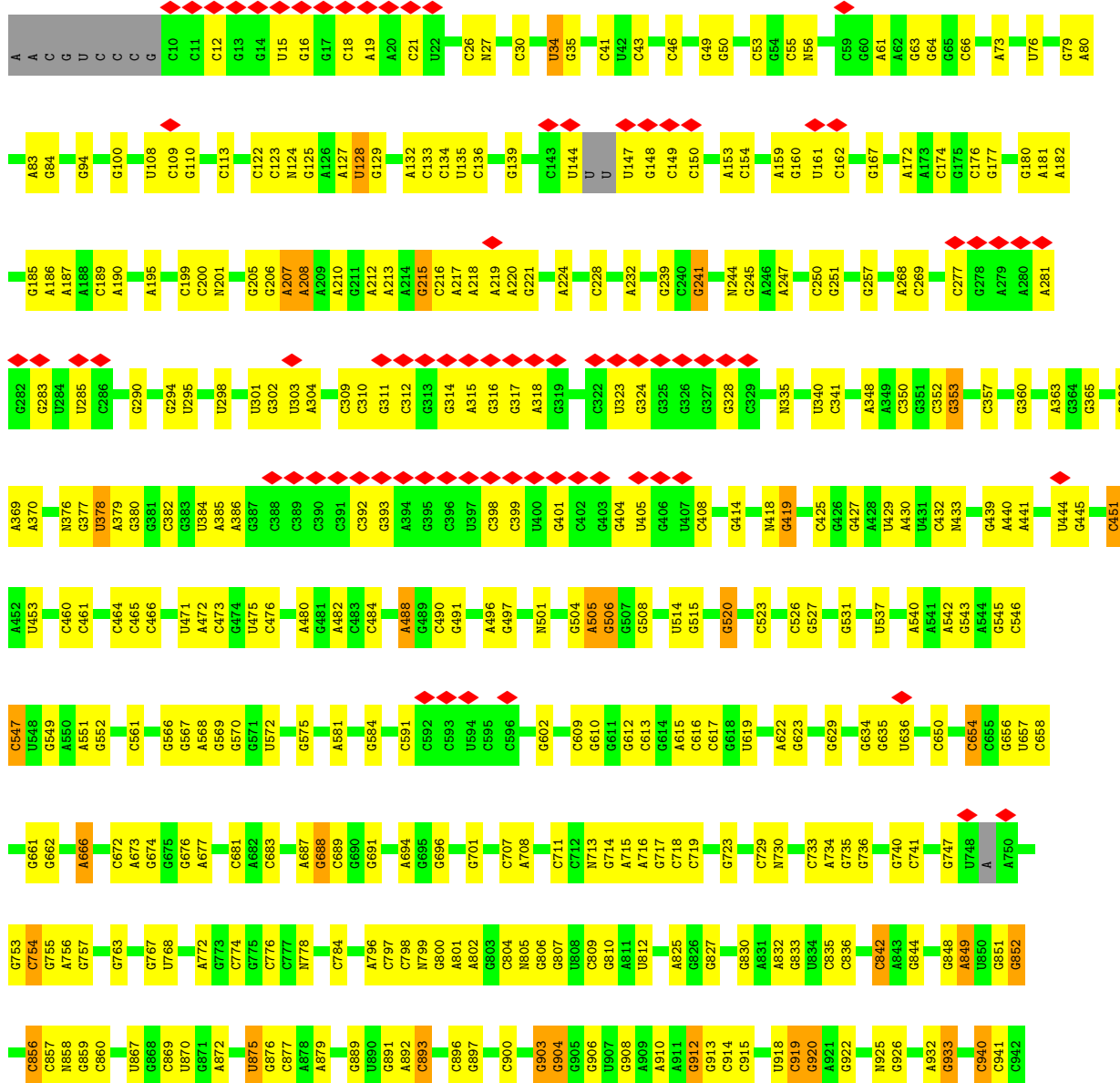


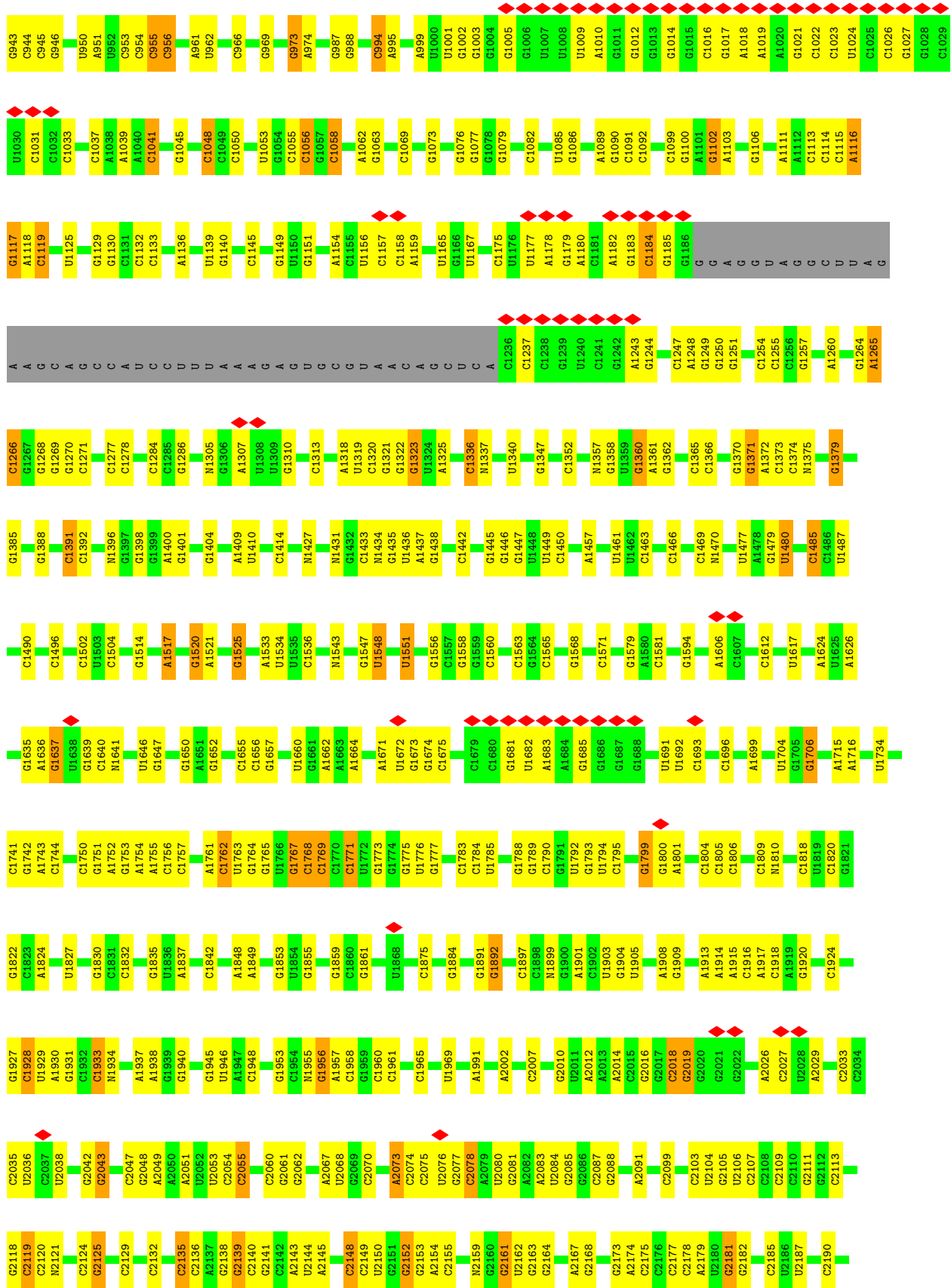


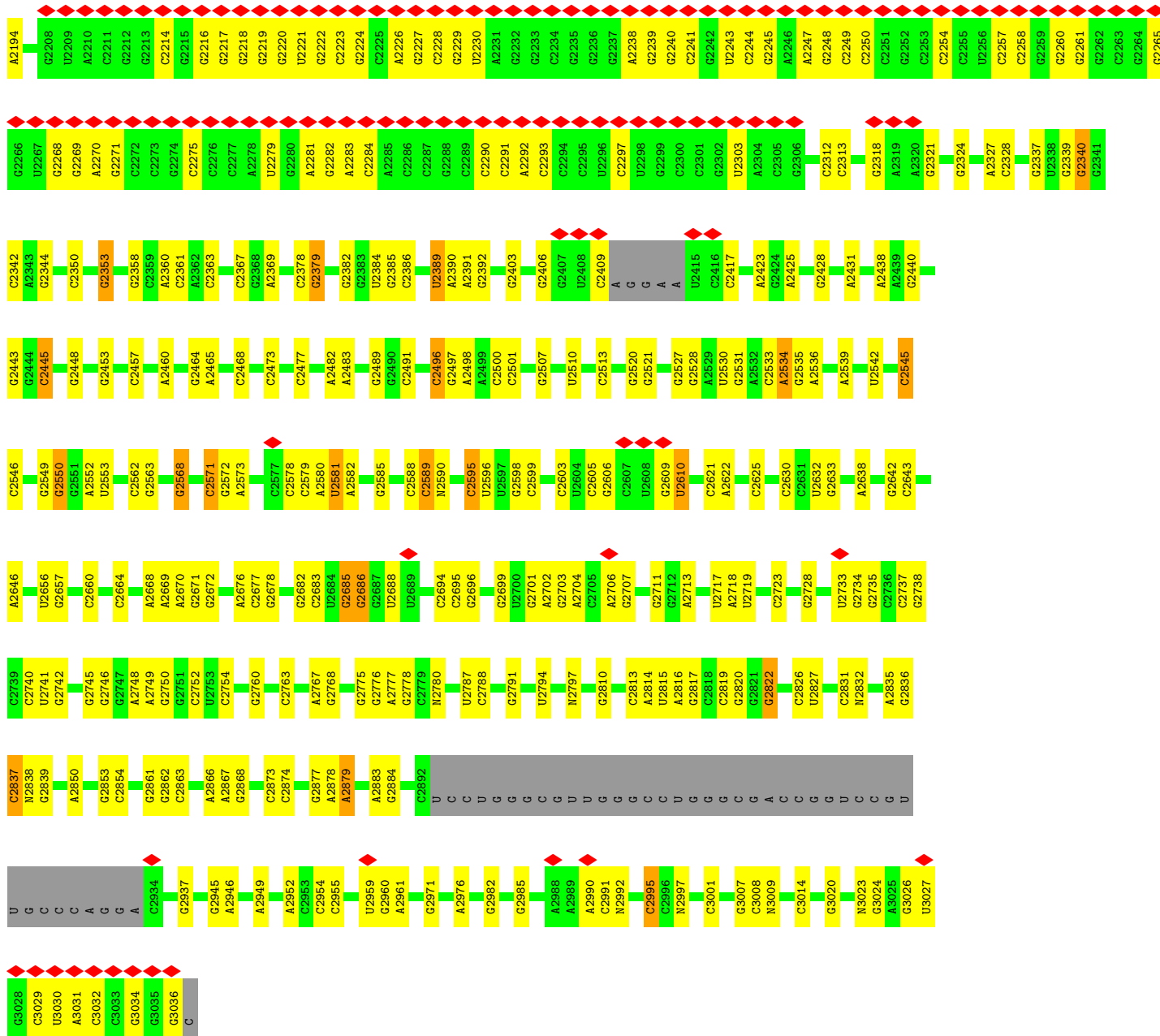
• Molecule 26: Predicted zinc-ribbon RNA-binding protein involved in translation



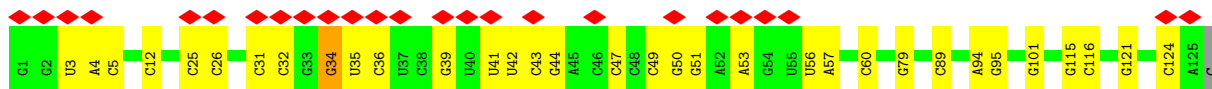
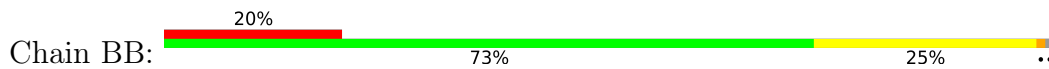
• Molecule 27: 23S rRNA





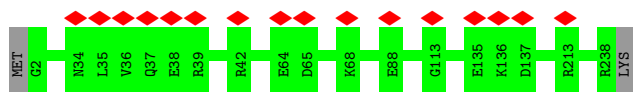


• Molecule 28: 5S rRNA

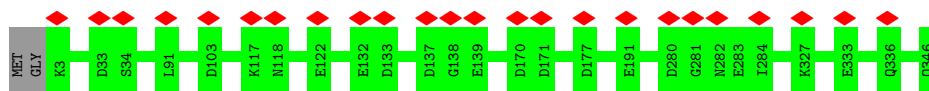


• Molecule 29: 50S ribosomal protein L2

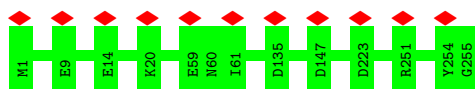




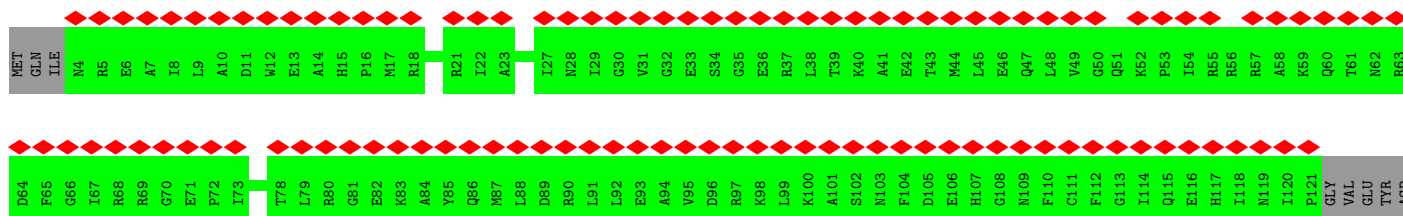
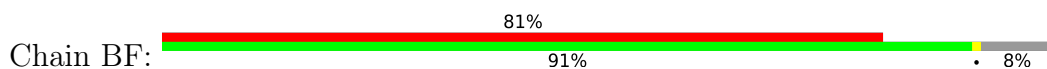
- Molecule 30: 50S ribosomal protein L3



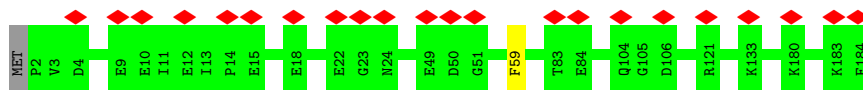
- Molecule 31: 50S ribosomal protein L4



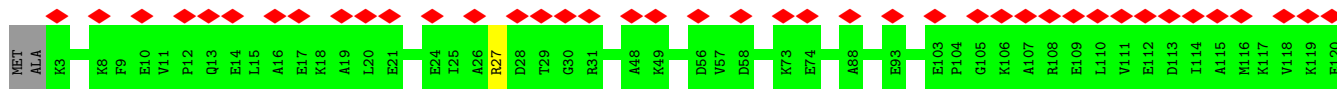
- Molecule 32: 50S ribosomal protein L5



- Molecule 33: 50S ribosomal protein L6



- Molecule 34: 50S ribosomal protein L7Ae

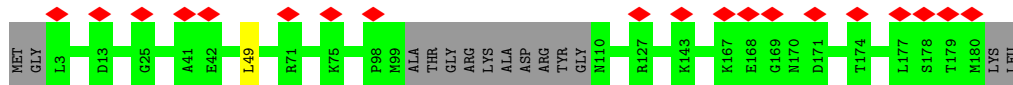
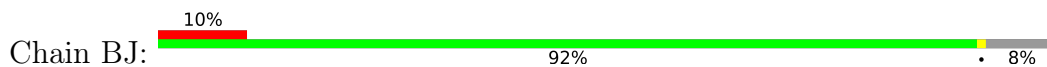




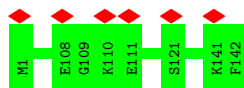
• Molecule 34: 50S ribosomal protein L7Ae



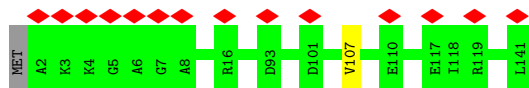
• Molecule 35: 50S ribosomal protein L10e



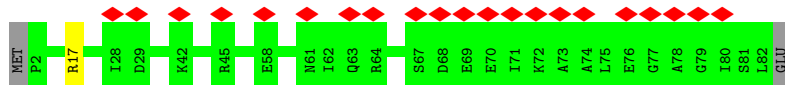
• Molecule 36: 50S ribosomal protein L13



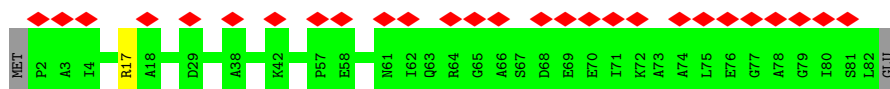
• Molecule 37: 50S ribosomal protein L14



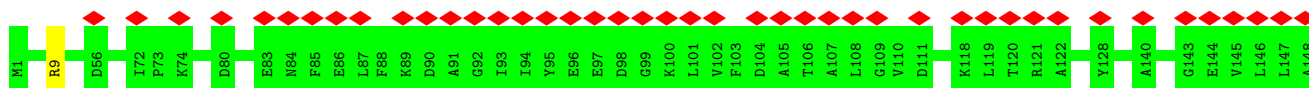
• Molecule 38: 50S ribosomal protein L14e



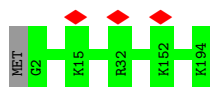
• Molecule 38: 50S ribosomal protein L14e



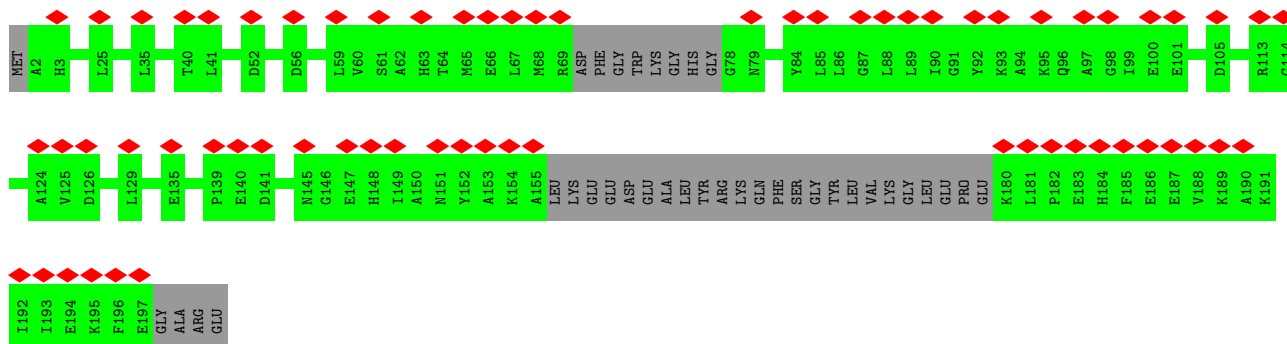
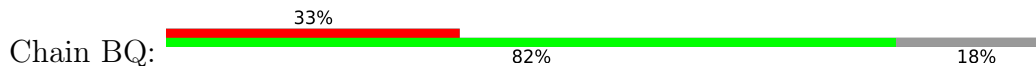
- Molecule 39: 50S ribosomal protein L15



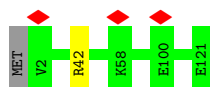
- Molecule 40: 50S ribosomal protein L15e



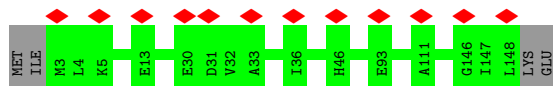
- Molecule 41: 50S ribosomal protein L18



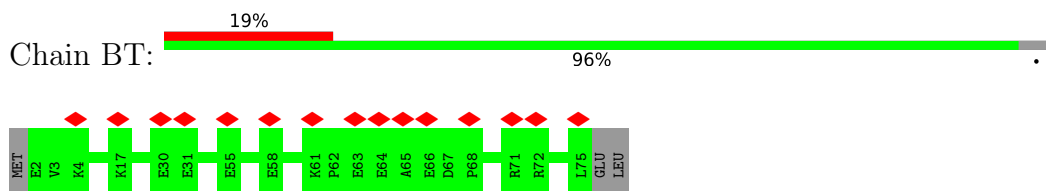
- Molecule 42: 50S ribosomal protein L18e



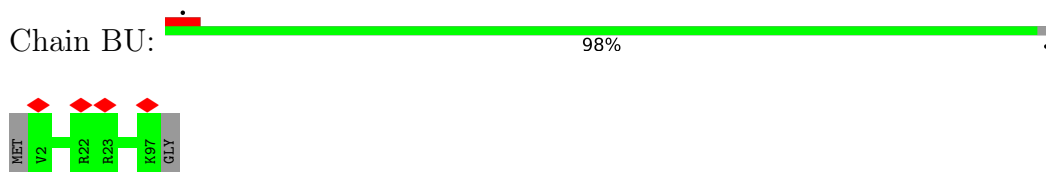
- Molecule 43: 50S ribosomal protein L19e



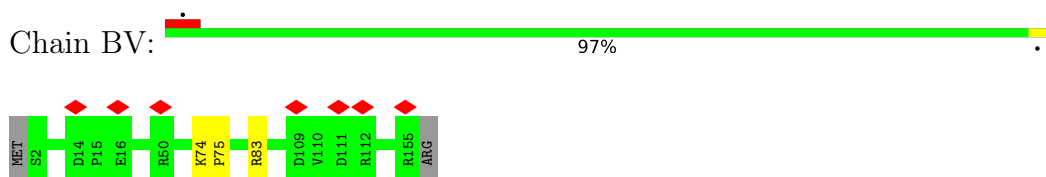
- Molecule 44: 50S ribosomal protein L18Ae



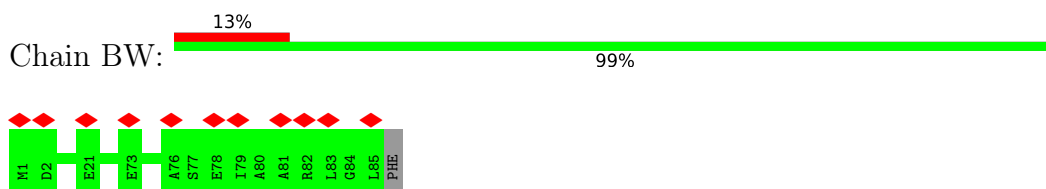
- Molecule 45: 50S ribosomal protein L21e



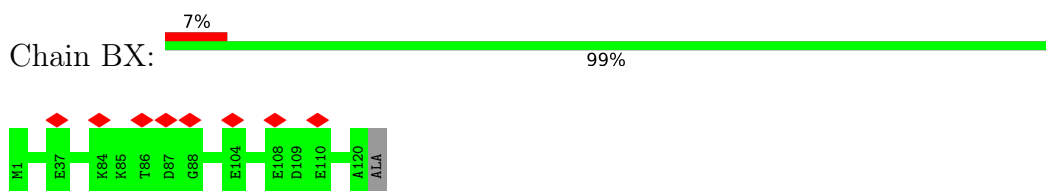
- Molecule 46: 50S ribosomal protein L22



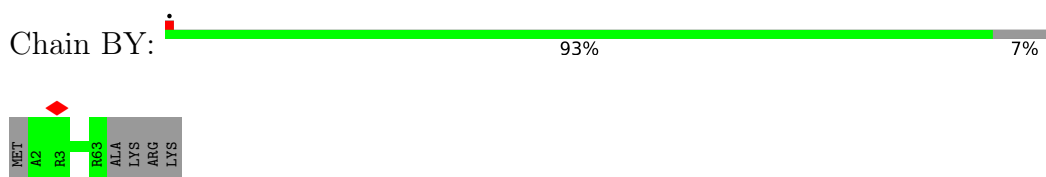
- Molecule 47: 50S ribosomal protein L23



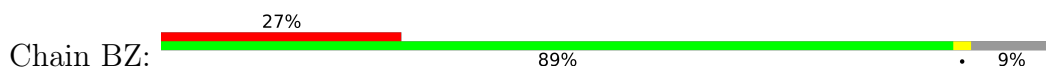
- Molecule 48: 50S ribosomal protein L24

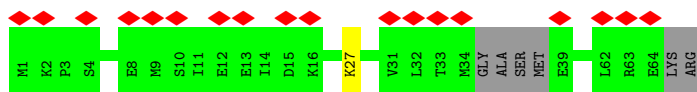


- Molecule 49: 50S ribosomal protein L24e

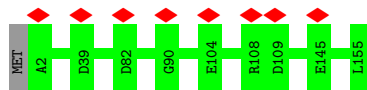


- Molecule 50: 50S ribosomal protein L29





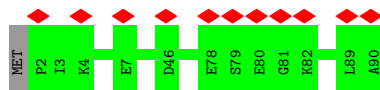
- Molecule 51: 50S ribosomal protein L30



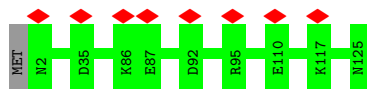
- Molecule 52: 50S ribosomal protein L30e



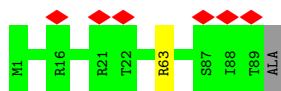
- Molecule 53: 50S ribosomal protein L31e



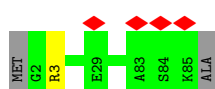
- Molecule 54: 50S ribosomal protein L32e



- Molecule 55: 50S ribosomal protein L34e



- Molecule 56: 50S ribosomal protein L37Ae



- Molecule 57: 50S ribosomal protein L37e

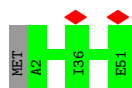


Chain Bh:  98%

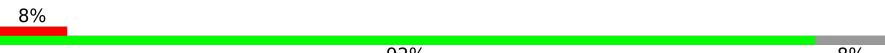


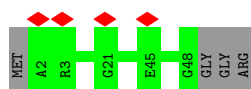
- Molecule 58: 50S ribosomal protein L39e

Chain Bi:  98%



- Molecule 59: 50S ribosomal protein L40e

Chain Bj:  8% 92% 8%



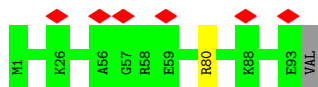
- Molecule 60: LSU ribosomal protein L41E

Chain Bk:  97%



- Molecule 61: 50S ribosomal protein L44e

Chain Bl:  6% 98%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	53737	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 ( $e^-/\text{\AA}^2$ )	34	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	29000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.441	Depositor
Minimum map value	-0.245	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	408.0, 408.0, 408.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, B8T, OMU, LV2, 5MC, LHH, MA6, A2M, 4SU, OMG, 4AC, 6MZ, 2MG, 5MU, OMC

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	Aa	1.19	25/33361 (0.1%)	1.15	100/52003 (0.2%)
2	Ab	0.39	0/1611	0.47	0/2179
3	Ac	0.33	0/1546	0.50	0/2075
4	Ad	0.38	0/1578	0.51	0/2119
5	Ae	0.40	0/1477	0.52	0/1980
6	Af	0.45	0/1991	0.49	0/2688
7	Ag	0.30	0/1779	0.47	0/2396
8	Ah	0.36	0/968	0.51	0/1300
9	Ai	0.37	0/1748	0.48	0/2347
10	Aj	0.43	0/1039	0.51	0/1397
11	Ak	0.42	0/991	0.53	0/1322
12	Al	0.34	0/1068	0.53	0/1430
13	Am	0.31	0/810	0.49	0/1087
14	An	0.61	2/968 (0.2%)	0.58	1/1304 (0.1%)
15	Ao	0.44	0/1139	0.50	0/1518
16	Ap	0.36	0/1113	0.49	0/1500
17	Aq	0.39	0/1241	0.47	0/1667
18	Ar	0.35	0/457	0.48	0/602
19	As	0.29	0/899	0.47	0/1214
20	At	0.30	0/545	0.48	0/725
21	Au	0.37	0/970	0.49	0/1295
22	Av	0.40	0/1249	0.48	0/1687
23	Aw	0.41	0/790	0.50	0/1063
24	Ax	0.26	0/469	0.49	0/633
25	Ay	0.37	0/501	0.52	0/672
26	Az	0.28	0/440	0.44	0/599
27	BA	1.58	139/66981 (0.2%)	1.39	489/104453 (0.5%)
28	BB	1.06	0/2993	1.17	14/4668 (0.3%)
29	BC	0.69	0/1860	0.66	0/2511
30	BD	0.65	0/2815	0.62	0/3795
31	BE	0.63	0/2066	0.61	0/2785
32	BF	0.48	0/1330	0.60	0/1778

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	BG	0.56	0/1490	0.57	0/2006
34	BH	0.46	0/941	0.53	0/1272
34	BI	0.33	0/941	0.50	0/1272
35	BJ	0.61	0/1407	0.63	1/1891 (0.1%)
36	BK	0.67	0/1165	0.68	0/1558
37	BL	0.65	1/1067 (0.1%)	0.62	0/1435
38	BM	0.50	0/614	0.58	0/824
38	BN	0.47	0/614	0.56	0/824
39	BO	0.55	0/1187	0.62	0/1583
40	BP	0.73	0/1621	0.61	0/2163
41	BQ	0.47	0/1342	0.54	0/1804
42	BR	0.58	0/971	0.59	0/1301
43	BS	0.59	0/1216	0.59	0/1607
44	BT	0.58	0/636	0.57	0/852
45	BU	0.62	0/806	0.58	0/1080
46	BV	0.73	2/1259 (0.2%)	0.65	1/1688 (0.1%)
47	BW	0.56	0/690	0.56	0/925
48	BX	0.58	0/1007	0.59	0/1344
49	BY	0.63	0/538	0.54	0/716
50	BZ	0.47	0/506	0.57	0/668
51	Ba	0.61	0/1259	0.63	0/1680
52	Bb	0.47	0/742	0.53	0/1001
53	Bc	0.60	0/736	0.53	0/990
54	Bd	0.66	0/1044	0.60	0/1394
55	Be	0.60	0/746	0.66	0/997
56	Bg	0.63	0/640	0.65	0/855
57	Bh	0.77	0/524	0.66	0/692
58	Bi	0.69	0/441	0.60	0/588
59	Bj	0.55	0/381	0.55	0/505
60	Bk	0.54	0/351	0.67	0/454
61	Bl	0.61	0/796	0.61	0/1056
All	All	1.19	169/166471 (0.1%)	1.11	606/245817 (0.2%)

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
14	An	0	1

All (169) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	BV	75	PRO	N-CA	13.70	1.70	1.47
14	An	125	PRO	N-CA	13.65	1.70	1.47
1	Aa	1463	G	N1-C2	-6.60	1.32	1.37
1	Aa	763	G	N1-C2	-6.49	1.32	1.37
1	Aa	1445	C	C4-C5	-6.41	1.37	1.43
1	Aa	849	C	N1-C6	-6.37	1.33	1.37
27	BA	1806	C	N1-C6	-6.30	1.33	1.37
27	BA	1446	G	C6-N1	-6.28	1.35	1.39
27	BA	1961	C	C4-C5	-6.20	1.38	1.43
27	BA	915	C	C5-C6	-6.14	1.29	1.34
27	BA	2178	C	C4-C5	-6.09	1.38	1.43
27	BA	1958	C	C4-C5	-6.06	1.38	1.43
27	BA	1918	C	N1-C6	-6.00	1.33	1.37
1	Aa	1445	C	N1-C6	-5.99	1.33	1.37
27	BA	2136	C	C4-C5	-5.98	1.38	1.43
1	Aa	887	C	O3'-P	-5.97	1.53	1.61
14	An	124	ILE	C-N	5.97	1.45	1.34
46	BV	74	LYS	C-N	5.96	1.45	1.34
1	Aa	1463	G	C8-N7	-5.96	1.27	1.30
27	BA	232	A	N9-C4	-5.88	1.34	1.37
1	Aa	1474	G	C6-N1	-5.84	1.35	1.39
27	BA	2185	C	C4-C5	-5.81	1.38	1.43
27	BA	2874	C	N1-C6	-5.80	1.33	1.37
27	BA	1757	C	C4-C5	-5.80	1.38	1.43
1	Aa	1445	C	C5-C6	-5.79	1.29	1.34
27	BA	1114	C	C4-C5	-5.77	1.38	1.43
27	BA	1050	C	N1-C6	-5.74	1.33	1.37
1	Aa	1458	C	C5-C6	-5.72	1.29	1.34
27	BA	2643	C	N1-C6	-5.68	1.33	1.37
27	BA	2820	G	C6-N1	-5.68	1.35	1.39
27	BA	689	C	C4-C5	-5.68	1.38	1.43
27	BA	2061	G	N1-C2	-5.66	1.33	1.37
1	Aa	1466	G	C6-N1	-5.65	1.35	1.39
1	Aa	1432	A	N9-C4	-5.64	1.34	1.37
1	Aa	706	G	C6-N1	-5.63	1.35	1.39
1	Aa	1471	U	C4-C5	-5.61	1.38	1.43
27	BA	1805	C	C4-C5	-5.59	1.38	1.43
27	BA	946	G	C6-N1	-5.59	1.35	1.39
27	BA	2621	C	C5-C6	-5.58	1.29	1.34
27	BA	1379	G	C6-N1	-5.56	1.35	1.39
27	BA	900	C	C4-C5	-5.55	1.38	1.43
27	BA	954	C	C4-C5	-5.54	1.38	1.43
27	BA	2062	G	N9-C4	-5.53	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	893	C	C4-C5	-5.52	1.38	1.43
37	BL	107	VAL	C-N	-5.52	1.21	1.34
27	BA	994	C	C4-C5	-5.52	1.38	1.43
27	BA	691	G	C6-N1	-5.52	1.35	1.39
27	BA	2060	C	N1-C6	-5.52	1.33	1.37
27	BA	1784	C	C4-C5	-5.51	1.38	1.43
27	BA	2340	G	C6-N1	-5.50	1.35	1.39
1	Aa	761	A	N9-C4	-5.47	1.34	1.37
27	BA	2111	G	C6-N1	-5.47	1.35	1.39
27	BA	1445	G	C6-N1	-5.47	1.35	1.39
27	BA	2746	G	N1-C2	-5.46	1.33	1.37
27	BA	2012	A	C6-N6	-5.45	1.29	1.33
27	BA	2061	G	C6-N1	-5.45	1.35	1.39
27	BA	241	G	N1-C2	-5.44	1.33	1.37
27	BA	1336	C	N1-C6	-5.44	1.33	1.37
27	BA	941	C	C5-C6	-5.44	1.29	1.34
27	BA	1771	C	C5-C6	-5.44	1.29	1.34
27	BA	1818	C	C5-C6	-5.44	1.29	1.34
27	BA	1806	C	C4-C5	-5.43	1.38	1.43
27	BA	2132	C	C4-C5	-5.42	1.38	1.43
27	BA	46	C	C5-C6	-5.42	1.30	1.34
1	Aa	1466	G	N1-C2	-5.41	1.33	1.37
27	BA	1091	C	C5-C6	-5.41	1.30	1.34
27	BA	807	G	C6-N1	-5.39	1.35	1.39
27	BA	181	A	N7-C5	-5.38	1.36	1.39
27	BA	1805	C	C5-C6	-5.38	1.30	1.34
27	BA	1366	C	C4-C5	-5.38	1.38	1.43
27	BA	1115	C	C5-C6	-5.37	1.30	1.34
27	BA	1938	A	N7-C5	-5.35	1.36	1.39
27	BA	2621	C	N1-C6	-5.34	1.33	1.37
27	BA	484	C	C4-C5	-5.34	1.38	1.43
27	BA	1960	C	C5-C6	-5.34	1.30	1.34
27	BA	784	C	C4-C5	-5.33	1.38	1.43
27	BA	1442	C	C5-C6	-5.33	1.30	1.34
1	Aa	1458	C	N1-C6	-5.32	1.33	1.37
27	BA	2866	A	N9-C4	-5.32	1.34	1.37
27	BA	661	G	N1-C2	-5.30	1.33	1.37
1	Aa	1473	C	C4-C5	-5.29	1.38	1.43
27	BA	1466	C	C4-C5	-5.29	1.38	1.43
27	BA	1775	G	C6-N1	-5.28	1.35	1.39
27	BA	2813	C	N1-C6	-5.28	1.33	1.37
27	BA	711	C	C4-C5	-5.28	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	889	G	C6-N1	-5.28	1.35	1.39
27	BA	915	C	C4-C5	-5.27	1.38	1.43
27	BA	954	C	C5-C6	-5.25	1.30	1.34
27	BA	177	G	C6-N1	-5.25	1.35	1.39
27	BA	2788	C	N1-C6	-5.25	1.33	1.37
27	BA	2087	C	C4-C5	-5.25	1.38	1.43
27	BA	466	C	C5-C6	-5.24	1.30	1.34
27	BA	2621	C	C4-C5	-5.24	1.38	1.43
27	BA	897	G	C6-N1	-5.24	1.35	1.39
27	BA	1374	C	N1-C6	-5.23	1.34	1.37
27	BA	1960	C	C4-C5	-5.23	1.38	1.43
27	BA	859	G	C6-N1	-5.23	1.35	1.39
27	BA	1920	G	C6-N1	-5.22	1.35	1.39
27	BA	1404	G	C6-N1	-5.22	1.35	1.39
27	BA	1277	C	C5-C6	-5.21	1.30	1.34
27	BA	2179	A	C6-N6	-5.21	1.29	1.33
27	BA	961	A	C6-N6	-5.21	1.29	1.33
27	BA	2949	A	C6-N6	-5.21	1.29	1.33
1	Aa	1341	C	N1-C6	-5.20	1.34	1.37
27	BA	1918	C	C5-C6	-5.20	1.30	1.34
27	BA	919	C	C4-C5	-5.19	1.38	1.43
27	BA	2107	C	N1-C6	-5.19	1.34	1.37
27	BA	2161	G	N1-C2	-5.19	1.33	1.37
27	BA	348	A	C6-N6	-5.18	1.29	1.33
27	BA	676	G	C6-N1	-5.18	1.35	1.39
1	Aa	1460	G	C2-N2	-5.18	1.29	1.34
27	BA	1916	C	N3-C4	-5.17	1.30	1.33
27	BA	810	G	C6-N1	-5.17	1.35	1.39
27	BA	182	A	N7-C5	-5.17	1.36	1.39
27	BA	1433	C	C4-C5	-5.16	1.38	1.43
1	Aa	850	A	N7-C5	-5.16	1.36	1.39
27	BA	2185	C	C5-C6	-5.15	1.30	1.34
27	BA	796	A	N9-C4	-5.15	1.34	1.37
27	BA	2350	C	C5-C6	-5.15	1.30	1.34
27	BA	1961	C	C5-C6	-5.14	1.30	1.34
27	BA	2831	C	N1-C6	-5.14	1.34	1.37
27	BA	1365	C	C4-C5	-5.13	1.38	1.43
27	BA	711	C	N1-C6	-5.13	1.34	1.37
27	BA	1913	A	N9-C4	-5.12	1.34	1.37
27	BA	1832	C	C4-C5	-5.12	1.38	1.43
1	Aa	1359	C	N1-C6	-5.12	1.34	1.37
27	BA	1520	G	C8-N7	-5.11	1.27	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	673	A	C6-N6	-5.11	1.29	1.33
27	BA	672	C	N3-C4	-5.10	1.30	1.33
27	BA	1933	C	N1-C6	-5.10	1.34	1.37
27	BA	676	G	C8-N7	-5.09	1.27	1.30
27	BA	1783	C	N1-C6	-5.09	1.34	1.37
27	BA	926	G	C6-N1	-5.09	1.35	1.39
27	BA	941	C	C4-C5	-5.09	1.38	1.43
27	BA	2683	C	C4-C5	-5.09	1.38	1.43
27	BA	1788	G	C6-N1	-5.08	1.35	1.39
27	BA	681	C	C5-C6	-5.08	1.30	1.34
27	BA	2342	C	C5-C6	-5.08	1.30	1.34
27	BA	798	C	C4-N4	-5.08	1.29	1.33
27	BA	920	G	C8-N7	-5.07	1.27	1.30
27	BA	1784	C	N3-C4	-5.07	1.30	1.33
27	BA	174	C	N1-C6	-5.07	1.34	1.37
1	Aa	763	G	N9-C4	-5.07	1.33	1.38
27	BA	2061	G	C2-N2	-5.06	1.29	1.34
27	BA	1401	G	N9-C4	-5.05	1.33	1.38
27	BA	2062	G	C2-N2	-5.05	1.29	1.34
27	BA	2704	A	C6-N6	-5.05	1.29	1.33
27	BA	2361	C	C4-C5	-5.04	1.39	1.43
1	Aa	763	G	C6-N1	-5.04	1.36	1.39
27	BA	2103	C	C4-C5	-5.04	1.39	1.43
27	BA	2549	G	N1-C2	-5.03	1.33	1.37
27	BA	2149	C	C5-C6	-5.03	1.30	1.34
27	BA	123	C	C4-C5	-5.02	1.39	1.43
1	Aa	280	G	C6-N1	-5.02	1.36	1.39
27	BA	914	C	N1-C6	-5.02	1.34	1.37
27	BA	2073	A	C5-C6	-5.02	1.36	1.41
27	BA	656	G	C8-N7	-5.02	1.27	1.30
27	BA	1041	C	C4-C5	-5.02	1.39	1.43
27	BA	1082	C	N1-C6	-5.02	1.34	1.37
27	BA	466	C	N1-C6	-5.01	1.34	1.37
27	BA	908	G	C8-N7	-5.01	1.27	1.30
27	BA	195	A	N9-C4	-5.01	1.34	1.37
27	BA	1114	C	C5-C6	-5.01	1.30	1.34
27	BA	2061	G	N7-C5	-5.01	1.36	1.39
27	BA	2822	G	N1-C2	-5.01	1.33	1.37
27	BA	2091	A	C6-N6	-5.01	1.29	1.33
27	BA	688	G	C8-N7	-5.00	1.27	1.30
27	BA	666	A	C6-N6	-5.00	1.29	1.33
27	BA	1762	C	N1-C6	-5.00	1.34	1.37



All (606) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	BB	31	C	N1-C2-O2	9.66	124.69	118.90
27	BA	2136	C	C2-N1-C1'	8.97	128.67	118.80
27	BA	2187	U	N3-C4-O4	8.57	125.40	119.40
1	Aa	1369	G	N1-C2-N2	-8.51	108.54	116.20
27	BA	1450	C	C2-N1-C1'	8.49	128.14	118.80
27	BA	3029	C	N3-C2-O2	-8.48	115.96	121.90
27	BA	994	C	C5-C4-N4	-8.41	114.31	120.20
27	BA	2312	C	C2-N1-C1'	8.38	128.02	118.80
27	BA	549	G	O4'-C1'-N9	8.32	114.86	108.20
27	BA	1433	C	C2-N1-C1'	8.21	127.83	118.80
27	BA	1433	C	N1-C2-O2	8.13	123.78	118.90
1	Aa	1445	C	C2-N1-C1'	8.09	127.69	118.80
14	An	125	PRO	CA-N-CD	-8.02	100.27	111.50
1	Aa	1445	C	N1-C2-O2	7.98	123.69	118.90
27	BA	2140	C	C5-C4-N4	-7.92	114.66	120.20
27	BA	547	C	N1-C2-O2	7.91	123.65	118.90
1	Aa	1463	G	N3-C2-N2	7.86	125.40	119.90
27	BA	216	C	N3-C4-C5	7.81	125.02	121.90
27	BA	527	G	OP1-P-OP2	7.79	131.29	119.60
27	BA	2062	G	C2-N3-C4	-7.77	108.01	111.90
28	BB	31	C	N3-C2-O2	-7.77	116.46	121.90
27	BA	1916	C	C2-N1-C1'	7.76	127.33	118.80
27	BA	35	G	C2-N3-C4	-7.66	108.07	111.90
46	BV	75	PRO	CA-N-CD	-7.62	100.83	111.50
27	BA	2136	C	C6-N1-C1'	-7.53	111.76	120.80
27	BA	661	G	N1-C2-N2	-7.53	109.43	116.20
1	Aa	281	C	C2-N1-C1'	7.47	127.02	118.80
27	BA	776	C	C2-N1-C1'	7.46	127.01	118.80
27	BA	2826	C	C2-N1-C1'	7.46	127.00	118.80
1	Aa	1445	C	C5-C4-N4	-7.40	115.02	120.20
1	Aa	888	A	O5'-P-OP2	7.39	119.57	110.70
27	BA	1958	C	C2-N1-C1'	7.39	126.93	118.80
1	Aa	700	C	C2-N1-C1'	7.37	126.91	118.80
27	BA	1119	C	C2-N1-C1'	7.33	126.86	118.80
27	BA	2007	C	N1-C2-O2	7.31	123.29	118.90
27	BA	2683	C	C2-N1-C1'	7.31	126.84	118.80
27	BA	1958	C	N1-C2-O2	7.30	123.28	118.90
27	BA	504	G	N7-C8-N9	7.30	116.75	113.10
27	BA	1918	C	C5-C4-N4	-7.29	115.10	120.20
1	Aa	340	C	C5-C4-N4	-7.28	115.10	120.20
27	BA	1958	C	C5-C4-N4	-7.21	115.15	120.20
27	BA	1961	C	N1-C2-O2	7.20	123.22	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BA	2699	G	N3-C4-N9	-7.17	121.70	126.00
27	BA	2683	C	N1-C2-O2	7.13	123.18	118.90
27	BA	2177	C	N1-C2-O2	7.13	123.18	118.90
27	BA	547	C	C2-N1-C1'	7.09	126.60	118.80
27	BA	1358	G	N3-C4-N9	-7.06	121.76	126.00
27	BA	676	G	C2-N3-C4	-7.06	108.37	111.90
27	BA	776	C	N1-C2-O2	7.05	123.13	118.90
27	BA	661	G	C2-N3-C4	-7.04	108.38	111.90
27	BA	2826	C	N1-C2-O2	7.02	123.11	118.90
27	BA	2149	C	C2-N1-C1'	7.02	126.52	118.80
27	BA	2187	U	C5-C4-O4	-7.01	121.69	125.90
27	BA	2061	G	C2-N3-C4	-7.00	108.40	111.90
27	BA	2562	C	N3-C4-C5	6.90	124.66	121.90
27	BA	2190	C	N1-C2-O2	6.88	123.03	118.90
27	BA	2877	G	C2-N3-C4	-6.87	108.47	111.90
27	BA	1928	C	C5-C4-N4	-6.83	115.42	120.20
27	BA	2043	G	O4'-C1'-N9	6.83	113.66	108.20
27	BA	767	G	C6-C5-N7	-6.79	126.33	130.40
1	Aa	1431	G	C2-N3-C4	-6.76	108.52	111.90
27	BA	66	C	N1-C2-O2	6.73	122.94	118.90
1	Aa	1006	C	C2'-C3'-O3'	6.73	124.47	113.70
27	BA	1271	C	C2-N1-C1'	6.72	126.19	118.80
1	Aa	1445	C	C6-N1-C1'	-6.71	112.75	120.80
27	BA	1449	U	C2-N1-C1'	6.71	125.75	117.70
28	BB	31	C	C2-N1-C1'	6.68	126.15	118.80
27	BA	277	C	C2-N1-C1'	6.67	126.13	118.80
1	Aa	1473	C	C5-C4-N4	-6.66	115.54	120.20
1	Aa	1347	C	N1-C2-O2	6.65	122.89	118.90
27	BA	2177	C	C2-N1-C1'	6.61	126.07	118.80
1	Aa	1369	G	N3-C2-N2	6.59	124.52	119.90
27	BA	654	C	N1-C2-O2	6.59	122.86	118.90
1	Aa	1464	G	C5-C6-O6	-6.59	124.64	128.60
27	BA	1450	C	N1-C2-O2	6.58	122.85	118.90
27	BA	2185	C	N1-C2-O2	6.58	122.84	118.90
1	Aa	1069	U	C5-C4-O4	-6.55	121.97	125.90
27	BA	807	G	C2-N3-C4	-6.54	108.63	111.90
27	BA	2136	C	N1-C2-O2	6.54	122.82	118.90
27	BA	2129	C	C5-C4-N4	-6.53	115.63	120.20
1	Aa	1242	C	C2-N1-C1'	6.51	125.97	118.80
35	BJ	49	LEU	CB-CG-CD2	6.51	122.07	111.00
27	BA	1269	G	C8-N9-C4	-6.51	103.80	106.40
27	BA	76	U	C5-C4-O4	-6.50	122.00	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BA	1237	C	N1-C2-O2	6.49	122.80	118.90
27	BA	915	C	N1-C2-O2	6.48	122.79	118.90
27	BA	1777	G	C2-N3-C4	-6.48	108.66	111.90
27	BA	2119	C	N1-C2-O2	6.48	122.79	118.90
27	BA	1767	G	P-O3'-C3'	6.48	127.47	119.70
27	BA	2136	C	C5-C4-N4	-6.47	115.67	120.20
27	BA	1918	C	N3-C4-N4	6.46	122.52	118.00
27	BA	2149	C	N1-C2-O2	6.45	122.77	118.90
27	BA	136	C	N3-C4-C5	6.45	124.48	121.90
1	Aa	1464	G	N1-C6-O6	6.45	123.77	119.90
27	BA	508	G	C2-N3-C4	-6.44	108.68	111.90
1	Aa	297	C	N1-C2-O2	6.44	122.76	118.90
27	BA	767	G	N3-C4-N9	6.40	129.84	126.00
27	BA	2297	C	N1-C2-O2	6.40	122.74	118.90
27	BA	2791	G	C8-N9-C4	-6.39	103.84	106.40
27	BA	955	C	N3-C4-C5	6.36	124.44	121.90
27	BA	689	C	N1-C2-O2	6.35	122.71	118.90
27	BA	973	G	C2-N3-C4	-6.33	108.74	111.90
27	BA	804	C	N1-C2-O2	6.32	122.69	118.90
1	Aa	183	C	N1-C2-O2	6.32	122.69	118.90
27	BA	2007	C	C2-N1-C1'	6.29	125.72	118.80
27	BA	842	C	C5-C4-N4	-6.28	115.81	120.20
27	BA	2695	C	N1-C2-O2	6.28	122.67	118.90
27	BA	2822	G	N1-C2-N2	-6.27	110.56	116.20
27	BA	994	C	N3-C4-N4	6.27	122.39	118.00
27	BA	1048	C	C5-C4-N4	-6.26	115.81	120.20
27	BA	76	U	N3-C4-O4	6.26	123.78	119.40
27	BA	2822	G	C2-N3-C4	-6.25	108.78	111.90
27	BA	1536	C	C2-N1-C1'	6.24	125.67	118.80
27	BA	1433	C	C6-N1-C1'	-6.24	113.32	120.80
1	Aa	481	C	C2-N1-C1'	6.23	125.65	118.80
1	Aa	297	C	C2-N1-C1'	6.23	125.65	118.80
1	Aa	1069	U	N3-C4-O4	6.23	123.76	119.40
27	BA	1903	U	N3-C4-O4	6.22	123.76	119.40
27	BA	2664	C	C2-N1-C1'	6.22	125.64	118.80
27	BA	1116	A	N1-C6-N6	6.22	122.33	118.60
27	BA	2367	C	C6-N1-C2	-6.22	117.81	120.30
27	BA	1401	G	N3-C4-N9	-6.21	122.27	126.00
27	BA	1041	C	C2-N1-C1'	6.21	125.63	118.80
27	BA	1266	C	C5-C4-N4	-6.21	115.86	120.20
27	BA	851	G	C8-N9-C4	-6.20	103.92	106.40
27	BA	918	U	C2-N1-C1'	6.18	125.11	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BA	954	C	N3-C4-C5	6.17	124.37	121.90
27	BA	2350	C	N3-C4-C5	6.16	124.36	121.90
1	Aa	644	C	N1-C2-O2	6.15	122.59	118.90
1	Aa	520	G	P-O3'-C3'	6.15	127.08	119.70
1	Aa	884	C	C2-N1-C1'	6.14	125.56	118.80
27	BA	2118	G	C2-N3-C4	-6.14	108.83	111.90
27	BA	889	G	C2-N3-C4	-6.12	108.84	111.90
27	BA	2297	C	N3-C2-O2	-6.12	117.61	121.90
27	BA	2819	C	N1-C2-O2	6.11	122.57	118.90
1	Aa	1242	C	N1-C2-O2	6.11	122.56	118.90
27	BA	689	C	C2-N1-C1'	6.11	125.52	118.80
27	BA	1365	C	C2-N1-C1'	6.10	125.51	118.80
27	BA	1960	C	N1-C2-O2	6.10	122.56	118.90
27	BA	1365	C	N1-C2-O2	6.10	122.56	118.90
27	BA	1958	C	C6-N1-C1'	-6.10	113.48	120.80
27	BA	1916	C	N1-C2-O2	6.10	122.56	118.90
27	BA	2312	C	N1-C2-O2	6.10	122.56	118.90
1	Aa	281	C	N1-C2-O2	6.10	122.56	118.90
1	Aa	515	C	C2-N1-C1'	6.09	125.50	118.80
27	BA	806	G	C8-N9-C4	-6.09	103.97	106.40
27	BA	661	G	N3-C2-N2	6.08	124.16	119.90
27	BA	1450	C	C6-N1-C1'	-6.08	113.50	120.80
27	BA	1463	C	C5-C4-N4	-6.07	115.95	120.20
1	Aa	1030	C	C2-N1-C1'	6.07	125.48	118.80
1	Aa	515	C	N1-C2-O2	6.07	122.54	118.90
27	BA	2107	C	C2-N1-C1'	6.06	125.46	118.80
27	BA	1114	C	C5-C4-N4	-6.04	115.97	120.20
27	BA	876	G	O4'-C1'-N9	6.04	113.03	108.20
27	BA	953	C	C5-C4-N4	-6.04	115.97	120.20
27	BA	1277	C	C2-N1-C1'	6.03	125.43	118.80
27	BA	2190	C	C2-N1-C1'	6.02	125.42	118.80
27	BA	2826	C	C6-N1-C1'	-6.02	113.58	120.80
27	BA	2140	C	N3-C4-C5	6.01	124.31	121.90
27	BA	2991	C	C2-N1-C1'	6.01	125.41	118.80
27	BA	1237	C	N3-C2-O2	-6.01	117.70	121.90
27	BA	1924	C	C5-C4-N4	-5.99	116.01	120.20
27	BA	1502	C	C5-C4-N4	-5.98	116.02	120.20
27	BA	2854	C	C5-C4-N4	-5.97	116.02	120.20
27	BA	915	C	C2-N1-C1'	5.96	125.36	118.80
27	BA	956	C	C2-N1-C1'	5.96	125.36	118.80
27	BA	1805	C	C5-C4-N4	-5.96	116.03	120.20
1	Aa	1463	G	C4-C5-N7	5.96	113.19	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BA	2837	C	N1-C2-O2	5.95	122.47	118.90
27	BA	1284	C	C2-N1-C1'	5.94	125.33	118.80
27	BA	1769	C	C2-N1-C1'	5.93	125.33	118.80
27	BA	2313	C	C5-C4-N4	-5.93	116.05	120.20
27	BA	809	C	C2-N1-C1'	5.93	125.32	118.80
27	BA	309	C	C2-N1-C1'	5.93	125.32	118.80
27	BA	491	G	C2-N3-C4	-5.93	108.94	111.90
27	BA	1916	C	C6-N1-C2	-5.93	117.93	120.30
28	BB	50	G	N3-C2-N2	5.93	124.05	119.90
27	BA	893	C	C5-C4-N4	-5.92	116.05	120.20
27	BA	277	C	N1-C2-O2	5.92	122.45	118.90
27	BA	2740	C	C2-N1-C1'	5.92	125.31	118.80
1	Aa	700	C	C6-N1-C1'	-5.92	113.70	120.80
27	BA	955	C	C5-C4-N4	-5.91	116.06	120.20
27	BA	189	C	C2-N1-C1'	5.91	125.30	118.80
27	BA	1184	C	N3-C2-O2	-5.91	117.77	121.90
27	BA	1756	C	C2-N1-C1'	5.89	125.28	118.80
27	BA	946	G	C2-N3-C4	-5.89	108.95	111.90
27	BA	1706	G	N7-C8-N9	5.88	116.04	113.10
27	BA	1933	C	N3-C4-C5	5.88	124.25	121.90
27	BA	464	C	C5-C4-N4	-5.88	116.08	120.20
27	BA	1496	C	N1-C2-O2	5.88	122.43	118.90
27	BA	185	G	C8-N9-C4	-5.88	104.05	106.40
27	BA	1370	G	C2-N3-C4	-5.88	108.96	111.90
27	BA	122	C	C2-N1-C1'	5.87	125.26	118.80
27	BA	2185	C	C5-C4-N4	-5.87	116.09	120.20
27	BA	804	C	C2-N1-C1'	5.87	125.26	118.80
27	BA	2185	C	C2-N1-C1'	5.87	125.26	118.80
27	BA	26	C	C2-N1-C1'	5.86	125.25	118.80
27	BA	1655	C	C2-N1-C1'	5.85	125.24	118.80
27	BA	2723	C	N1-C2-O2	5.84	122.41	118.90
27	BA	2685	G	C8-N9-C4	-5.84	104.06	106.40
27	BA	2603	C	C5-C4-N4	-5.84	116.11	120.20
27	BA	956	C	C6-N1-C1'	-5.84	113.79	120.80
27	BA	2477	C	N1-C2-O2	5.82	122.39	118.90
27	BA	2513	C	C2-N1-C1'	5.82	125.20	118.80
27	BA	2534	A	C8-N9-C4	-5.81	103.48	105.80
1	Aa	1369	G	C6-C5-N7	-5.81	126.92	130.40
1	Aa	1394	C	C2-N1-C1'	5.80	125.18	118.80
27	BA	2125	G	C2-N3-C4	-5.80	109.00	111.90
27	BA	1956	G	C2-N3-C4	-5.80	109.00	111.90
27	BA	50	G	C4-N9-C1'	5.80	134.04	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Aa	850	A	N7-C8-N9	5.79	116.69	113.80
27	BA	2312	C	C6-N1-C1'	-5.78	113.86	120.80
27	BA	2339	G	C2-N3-C4	-5.78	109.01	111.90
27	BA	1404	G	C2-N3-C4	-5.76	109.02	111.90
1	Aa	1325	G	N1-C2-N2	-5.76	111.01	116.20
27	BA	1435	G	C2-N3-C4	-5.76	109.02	111.90
27	BA	2837	C	C2-N1-C1'	5.76	125.13	118.80
27	BA	1358	G	N9-C4-C5	5.76	107.70	105.40
27	BA	1278	C	C2-N1-C1'	5.75	125.13	118.80
1	Aa	763	G	C2-N3-C4	-5.74	109.03	111.90
27	BA	2873	C	C2-N1-C1'	5.74	125.12	118.80
27	BA	650	C	C5-C4-N4	-5.74	116.18	120.20
27	BA	1401	G	N3-C4-C5	5.74	131.47	128.60
27	BA	484	C	N1-C2-O2	5.74	122.34	118.90
27	BA	1536	C	N1-C2-O2	5.73	122.34	118.90
27	BA	2177	C	C6-N1-C1'	-5.72	113.93	120.80
27	BA	207	A	C8-N9-C4	-5.72	103.51	105.80
27	BA	918	U	N1-C2-O2	5.72	126.80	122.80
27	BA	520	G	O4'-C1'-N9	5.71	112.77	108.20
27	BA	922	G	N7-C8-N9	5.71	115.96	113.10
27	BA	1520	G	C2-N3-C4	-5.71	109.05	111.90
27	BA	515	G	C2-N3-C4	-5.71	109.05	111.90
28	BB	121	G	C4-N9-C1'	5.70	133.91	126.50
28	BB	121	G	N3-C4-N9	5.70	129.42	126.00
27	BA	1271	C	C6-N1-C1'	-5.68	113.98	120.80
27	BA	1323	G	C2-N3-C4	-5.68	109.06	111.90
27	BA	2181	G	C8-N9-C4	-5.68	104.13	106.40
27	BA	906	G	C8-N9-C4	-5.68	104.13	106.40
1	Aa	691	C	N1-C2-O2	5.68	122.31	118.90
27	BA	1286	G	N7-C8-N9	5.67	115.94	113.10
27	BA	2445	C	C2-N1-C1'	5.67	125.04	118.80
27	BA	962	U	C5-C4-O4	-5.67	122.50	125.90
27	BA	2507	G	C8-N9-C1'	5.67	134.37	127.00
27	BA	2699	G	N3-C4-C5	5.67	131.43	128.60
27	BA	1360	G	N7-C8-N9	5.66	115.93	113.10
27	BA	1100	G	C2-N3-C4	-5.66	109.07	111.90
28	BB	121	G	C6-C5-N7	-5.66	127.00	130.40
27	BA	180	G	N7-C8-N9	5.66	115.93	113.10
27	BA	2473	C	N1-C2-O2	5.66	122.30	118.90
27	BA	2163	G	C2-N3-C4	-5.65	109.07	111.90
27	BA	1804	C	N1-C2-O2	5.65	122.29	118.90
1	Aa	1473	C	N1-C2-O2	5.64	122.29	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BA	741	C	N3-C4-C5	5.64	124.16	121.90
27	BA	2438	A	O4'-C1'-N9	5.64	112.72	108.20
27	BA	2342	C	C2-N1-C1'	5.64	125.00	118.80
27	BA	2500	C	C5-C4-N4	-5.64	116.25	120.20
27	BA	591	C	C5-C4-N4	-5.64	116.25	120.20
27	BA	66	C	C2-N1-C1'	5.63	125.00	118.80
27	BA	427	G	C8-N9-C4	-5.63	104.15	106.40
27	BA	893	C	N1-C2-O2	5.63	122.28	118.90
27	BA	1656	C	C2-N1-C1'	5.63	125.00	118.80
28	BB	60	C	C2-N1-C1'	5.63	125.00	118.80
27	BA	1116	A	C5-C6-N6	-5.63	119.20	123.70
27	BA	2496	C	C5-C4-N4	-5.63	116.26	120.20
27	BA	2879	A	N7-C8-N9	5.63	116.61	113.80
1	Aa	81	C	N1-C2-O2	5.62	122.27	118.90
27	BA	1086	G	C2-N3-C4	-5.62	109.09	111.90
27	BA	2119	C	C2-N1-C1'	5.62	124.98	118.80
27	BA	1830	G	N7-C8-N9	5.62	115.91	113.10
27	BA	1469	C	C2-N1-C1'	5.61	124.97	118.80
1	Aa	316	C	C2-N1-C1'	5.61	124.97	118.80
27	BA	378	U	P-O3'-C3'	5.60	126.42	119.70
27	BA	2135	C	C5-C4-N4	-5.60	116.28	120.20
1	Aa	281	C	C6-N1-C1'	-5.60	114.08	120.80
27	BA	504	G	C5-N7-C8	-5.60	101.50	104.30
27	BA	903	G	N3-C4-N9	-5.60	122.64	126.00
27	BA	1809	C	N1-C2-O2	5.60	122.26	118.90
27	BA	1931	G	N7-C8-N9	5.60	115.90	113.10
1	Aa	763	G	C5-C6-O6	5.59	131.96	128.60
1	Aa	1451	A	O4'-C1'-N9	5.59	112.67	108.20
1	Aa	1463	G	N1-C2-N2	-5.59	111.17	116.20
27	BA	1414	C	C2-N1-C1'	5.58	124.94	118.80
27	BA	177	G	C8-N9-C4	-5.58	104.17	106.40
27	BA	2695	C	C2-N1-C1'	5.58	124.94	118.80
27	BA	128	U	N3-C4-O4	5.57	123.30	119.40
27	BA	473	C	N3-C4-C5	5.57	124.13	121.90
27	BA	2417	C	N3-C4-N4	5.57	121.90	118.00
27	BA	1447	G	C2-N3-C4	-5.56	109.12	111.90
27	BA	2312	C	C6-N1-C2	-5.56	118.08	120.30
27	BA	2363	C	C2-N1-C1'	5.56	124.92	118.80
27	BA	1837	A	C5-N7-C8	-5.56	101.12	103.90
1	Aa	1466	G	N1-C2-N2	-5.55	111.20	116.20
27	BA	915	C	N3-C4-C5	5.55	124.12	121.90
27	BA	185	G	N7-C8-N9	5.55	115.87	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BA	2344	G	C8-N9-C4	-5.55	104.18	106.40
27	BA	2007	C	N3-C2-O2	-5.54	118.02	121.90
1	Aa	1295	C	C2-N1-C1'	5.54	124.90	118.80
1	Aa	515	C	C6-N1-C1'	-5.54	114.15	120.80
27	BA	451	C	C2-N1-C1'	5.54	124.90	118.80
27	BA	1254	C	N1-C2-O2	5.54	122.22	118.90
27	BA	2533	C	C2-N1-C1'	5.54	124.90	118.80
27	BA	2820	G	C2-N3-C4	-5.54	109.13	111.90
27	BA	1325	A	N7-C8-N9	5.54	116.57	113.80
27	BA	1433	C	C5-C4-N4	-5.54	116.32	120.20
27	BA	2290	C	N3-C2-O2	-5.54	118.02	121.90
27	BA	1100	G	N7-C8-N9	5.53	115.86	113.10
27	BA	2599	C	N1-C2-O2	5.53	122.22	118.90
27	BA	2290	C	N1-C2-O2	5.53	122.22	118.90
27	BA	1768	C	O4'-C1'-N1	5.53	112.62	108.20
27	BA	566	G	C2-N3-C4	-5.52	109.14	111.90
27	BA	1358	G	C8-N9-C1'	5.51	134.16	127.00
1	Aa	1450	C	N3-C4-C5	5.50	124.10	121.90
27	BA	2599	C	C2-N1-C1'	5.50	124.85	118.80
27	BA	2874	C	C2-N1-C1'	5.50	124.85	118.80
27	BA	1903	U	C5-C4-O4	-5.50	122.60	125.90
1	Aa	1341	C	N1-C2-O2	5.50	122.20	118.90
27	BA	200	C	C2-N1-C1'	5.49	124.84	118.80
27	BA	2694	C	C5-C4-N4	-5.49	116.36	120.20
27	BA	547	C	N3-C2-O2	-5.48	118.06	121.90
1	Aa	1345	C	C2-N1-C1'	5.48	124.83	118.80
28	BB	34	G	N3-C4-N9	5.47	129.28	126.00
27	BA	1082	C	N1-C2-O2	5.47	122.18	118.90
27	BA	2678	G	N7-C8-N9	5.47	115.84	113.10
1	Aa	520	G	O4'-C1'-N9	-5.47	103.82	108.20
27	BA	2339	G	N1-C2-N2	-5.46	111.28	116.20
27	BA	2342	C	N1-C2-O2	5.46	122.18	118.90
27	BA	2723	C	N3-C2-O2	-5.45	118.08	121.90
1	Aa	264	C	N1-C2-O2	5.45	122.17	118.90
27	BA	1875	C	N1-C2-O2	5.44	122.17	118.90
1	Aa	589	C	N1-C2-O2	5.44	122.16	118.90
1	Aa	343	C	C2-N1-C1'	5.44	124.78	118.80
27	BA	1119	C	C6-N1-C1'	-5.44	114.28	120.80
27	BA	547	C	C5-C4-N4	-5.44	116.39	120.20
1	Aa	763	G	N3-C4-N9	-5.43	122.74	126.00
27	BA	1706	G	N1-C2-N2	-5.43	111.31	116.20
27	BA	1114	C	C2-N1-C1'	5.43	124.77	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BA	1637	G	C2-N3-C4	-5.43	109.18	111.90
27	BA	1469	C	N1-C2-O2	5.43	122.16	118.90
27	BA	2120	C	C2-N1-C1'	5.43	124.77	118.80
27	BA	1117	G	C2-N3-C4	-5.43	109.19	111.90
27	BA	181	A	N7-C8-N9	5.42	116.51	113.80
27	BA	1269	G	N7-C8-N9	5.42	115.81	113.10
27	BA	1534	U	C2-N1-C1'	5.42	124.20	117.70
27	BA	167	G	C8-N9-C4	-5.42	104.23	106.40
27	BA	352	C	N3-C4-C5	5.42	124.07	121.90
27	BA	2711	G	C2-N3-C4	-5.42	109.19	111.90
27	BA	807	G	N7-C8-N9	5.42	115.81	113.10
1	Aa	1463	G	N9-C4-C5	-5.41	103.23	105.40
27	BA	439	G	N1-C2-N2	-5.41	111.33	116.20
27	BA	2125	G	N1-C2-N2	-5.41	111.33	116.20
27	BA	719	C	C2-N1-C1'	5.41	124.75	118.80
27	BA	1948	C	C5-C4-N4	-5.41	116.42	120.20
1	Aa	489	C	C2-N1-C1'	5.40	124.74	118.80
27	BA	1927	G	N3-C4-N9	-5.40	122.76	126.00
27	BA	504	G	C2-N3-C4	-5.40	109.20	111.90
27	BA	1504	C	N1-C2-O2	5.40	122.14	118.90
27	BA	953	C	N3-C4-C5	5.40	124.06	121.90
1	Aa	94	C	P-O3'-C3'	5.39	126.17	119.70
1	Aa	1457	G	C8-N9-C4	-5.39	104.24	106.40
27	BA	784	C	C5-C4-N4	-5.39	116.43	120.20
27	BA	547	C	C6-N1-C1'	-5.39	114.34	120.80
27	BA	933	G	C8-N9-C4	-5.38	104.25	106.40
27	BA	2129	C	C2-N1-C1'	5.38	124.72	118.80
1	Aa	644	C	N3-C2-O2	-5.38	118.13	121.90
27	BA	154	C	C2-N1-C1'	5.38	124.72	118.80
27	BA	2378	C	N1-C2-O2	5.38	122.13	118.90
27	BA	1102	G	N3-C4-N9	-5.38	122.77	126.00
27	BA	1391	C	C2-N1-C1'	5.38	124.71	118.80
27	BA	309	C	C6-N1-C1'	-5.37	114.35	120.80
27	BA	784	C	N3-C4-C5	5.37	124.05	121.90
27	BA	1806	C	C2-N1-C1'	5.37	124.71	118.80
27	BA	2819	C	C2-N1-C1'	5.37	124.70	118.80
27	BA	1056	C	N1-C2-O2	5.37	122.12	118.90
27	BA	1145	C	N1-C2-O2	5.37	122.12	118.90
1	Aa	324	C	N1-C2-O2	5.36	122.12	118.90
1	Aa	873	G	N7-C8-N9	5.36	115.78	113.10
1	Aa	1369	G	C4-N9-C1'	5.36	133.46	126.50
27	BA	441	A	C8-N9-C4	-5.36	103.66	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BA	1514	G	C2-N3-C4	-5.35	109.22	111.90
27	BA	1053	U	C5-C4-O4	-5.35	122.69	125.90
27	BA	1958	C	N3-C4-N4	5.35	121.75	118.00
27	BA	1033	C	C2-N1-C1'	5.35	124.68	118.80
27	BA	1113	C	C5-C4-N4	-5.34	116.46	120.20
27	BA	915	C	C5-C4-N4	-5.34	116.46	120.20
27	BA	79	G	C8-N9-C4	-5.34	104.27	106.40
27	BA	1809	C	C2-N1-C1'	5.34	124.67	118.80
27	BA	2683	C	C6-N1-C1'	-5.34	114.40	120.80
27	BA	2621	C	C5-C4-N4	-5.33	116.47	120.20
1	Aa	887	C	P-O3'-C3'	5.33	126.10	119.70
27	BA	857	C	C2-N1-C1'	5.33	124.67	118.80
27	BA	245	G	N1-C2-N2	-5.33	111.40	116.20
1	Aa	1347	C	C2-N1-C1'	5.33	124.66	118.80
27	BA	776	C	N3-C2-O2	-5.33	118.17	121.90
27	BA	906	G	N7-C8-N9	5.33	115.76	113.10
27	BA	380	G	C2-N3-C4	-5.32	109.24	111.90
27	BA	2664	C	N1-C2-O2	5.32	122.09	118.90
1	Aa	1460	G	C8-N9-C4	-5.31	104.28	106.40
27	BA	1058	C	N1-C2-O2	5.31	122.09	118.90
1	Aa	850	A	C5-N7-C8	-5.30	101.25	103.90
27	BA	2760	G	O4'-C1'-N9	5.30	112.44	108.20
1	Aa	1345	C	N1-C2-O2	5.30	122.08	118.90
27	BA	2694	C	N3-C4-C5	5.30	124.02	121.90
27	BA	1917	A	N7-C8-N9	5.30	116.45	113.80
27	BA	2109	C	C5-C4-N4	-5.29	116.49	120.20
27	BA	2822	G	N7-C8-N9	5.29	115.75	113.10
27	BA	1254	C	C2-N1-C1'	5.29	124.62	118.80
27	BA	1099	C	C2-N1-C1'	5.29	124.61	118.80
27	BA	2668	A	N7-C8-N9	5.29	116.44	113.80
27	BA	2113	C	N3-C4-C5	5.28	124.01	121.90
27	BA	199	C	C2-N1-C1'	5.28	124.61	118.80
27	BA	186	A	C8-N9-C4	-5.28	103.69	105.80
27	BA	1041	C	C5-C4-N4	-5.28	116.50	120.20
27	BA	2132	C	C2-N1-C1'	5.28	124.61	118.80
27	BA	1045	G	C2-N3-C4	-5.28	109.26	111.90
27	BA	1325	A	C8-N9-C4	-5.28	103.69	105.80
1	Aa	1056	C	C2-N1-C1'	5.27	124.60	118.80
27	BA	176	C	C2-N1-C1'	5.27	124.60	118.80
27	BA	2685	G	P-O3'-C3'	5.27	126.03	119.70
27	BA	714	G	C2-N3-C4	-5.27	109.27	111.90
27	BA	806	G	N7-C8-N9	5.27	115.73	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BA	1323	G	N7-C8-N9	5.26	115.73	113.10
27	BA	186	A	N7-C8-N9	5.26	116.43	113.80
27	BA	904	G	C2-N3-C4	-5.26	109.27	111.90
27	BA	1485	C	C5-C4-N4	-5.26	116.52	120.20
27	BA	1938	A	N7-C8-N9	5.26	116.43	113.80
27	BA	2588	C	C2-N1-C1'	5.26	124.58	118.80
27	BA	1612	C	N1-C2-O2	5.26	122.05	118.90
27	BA	2161	G	P-O3'-C3'	5.25	126.00	119.70
27	BA	2664	C	C6-N1-C1'	-5.25	114.50	120.80
27	BA	809	C	N1-C2-O2	5.25	122.05	118.90
27	BA	1931	G	C8-N9-C4	-5.25	104.30	106.40
27	BA	210	A	N7-C8-N9	5.25	116.42	113.80
27	BA	654	C	C2-N1-C1'	5.25	124.57	118.80
27	BA	50	G	C8-N9-C1'	-5.24	120.18	127.00
27	BA	1371	G	C2-N3-C4	-5.24	109.28	111.90
27	BA	2254	C	N3-C2-O2	-5.24	118.23	121.90
27	BA	1271	C	N1-C2-O2	5.24	122.04	118.90
27	BA	2148	C	C2-N1-C1'	5.24	124.56	118.80
1	Aa	316	C	P-O3'-C3'	5.23	125.98	119.70
1	Aa	517	A	N1-C6-N6	-5.23	115.46	118.60
27	BA	1102	G	C2-N3-C4	-5.23	109.28	111.90
27	BA	2087	C	N1-C2-O2	5.23	122.04	118.90
27	BA	2589	C	N1-C2-O2	5.23	122.04	118.90
27	BA	2501	C	C5-C4-N4	-5.23	116.54	120.20
27	BA	2138	G	N7-C8-N9	5.22	115.71	113.10
27	BA	2625	C	C2-N1-C1'	5.22	124.55	118.80
27	BA	1401	G	C2-N3-C4	-5.22	109.29	111.90
27	BA	954	C	C5-C4-N4	-5.22	116.55	120.20
27	BA	1277	C	C6-N1-C1'	-5.22	114.54	120.80
27	BA	2788	C	N3-C4-C5	5.21	123.99	121.90
27	BA	425	C	N3-C4-C5	5.21	123.98	121.90
27	BA	797	C	C5-C4-N4	-5.21	116.55	120.20
27	BA	1114	C	N1-C2-O2	5.21	122.03	118.90
27	BA	719	C	N1-C2-O2	5.21	122.02	118.90
27	BA	2440	G	C4-N9-C1'	5.21	133.27	126.50
27	BA	2873	C	N1-C2-O2	5.21	122.02	118.90
27	BA	2701	G	N7-C8-N9	5.21	115.70	113.10
27	BA	46	C	C2-N1-C1'	5.20	124.52	118.80
27	BA	425	C	C5-C4-N4	-5.20	116.56	120.20
27	BA	876	G	C8-N9-C1'	5.20	133.76	127.00
27	BA	2161	G	C8-N9-C4	-5.20	104.32	106.40
27	BA	1255	C	C2-N1-C1'	5.20	124.52	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	BB	121	G	C8-N9-C1'	-5.20	120.24	127.00
1	Aa	260	C	C2-N1-C1'	5.20	124.52	118.80
27	BA	277	C	C6-N1-C1'	-5.20	114.56	120.80
27	BA	856	C	N1-C2-O2	5.19	122.02	118.90
27	BA	908	G	C2-N3-C4	-5.19	109.30	111.90
27	BA	955	C	C2-N3-C4	-5.19	117.31	119.90
27	BA	1937	A	N7-C8-N9	5.19	116.39	113.80
27	BA	729	C	C2-N1-C1'	5.19	124.51	118.80
27	BA	1784	C	N1-C2-O2	5.19	122.01	118.90
27	BA	2686	G	C4-N9-C1'	5.19	133.24	126.50
1	Aa	1325	G	N3-C2-N2	5.18	123.53	119.90
27	BA	836	C	C2-N1-C1'	5.18	124.50	118.80
27	BA	2431	A	N7-C8-N9	5.18	116.39	113.80
1	Aa	1347	C	N3-C2-O2	-5.18	118.27	121.90
27	BA	241	G	C2-N3-C4	-5.18	109.31	111.90
27	BA	205	G	C5-C6-O6	5.18	131.71	128.60
27	BA	1132	C	C2-N1-C1'	5.18	124.50	118.80
27	BA	1268	G	C8-N9-C4	-5.18	104.33	106.40
27	BA	2668	A	C8-N9-C4	-5.18	103.73	105.80
27	BA	1058	C	C2-N1-C1'	5.18	124.49	118.80
27	BA	1916	C	C6-N1-C1'	-5.18	114.59	120.80
1	Aa	863	A	P-O3'-C3'	5.17	125.90	119.70
27	BA	1073	G	C2-N3-C4	-5.17	109.32	111.90
27	BA	1082	C	C2-N1-C1'	5.17	124.48	118.80
27	BA	199	C	N1-C2-O2	5.17	122.00	118.90
27	BA	2678	G	C8-N9-C4	-5.17	104.33	106.40
27	BA	689	C	C5-C4-N4	-5.16	116.59	120.20
27	BA	1767	G	N7-C8-N9	5.16	115.68	113.10
27	BA	1915	A	N7-C8-N9	5.16	116.38	113.80
27	BA	228	C	N1-C2-O2	5.16	121.99	118.90
27	BA	2683	C	N3-C2-O2	-5.16	118.29	121.90
28	BB	31	C	C6-N1-C2	-5.16	118.24	120.30
27	BA	1938	A	C8-N9-C4	-5.15	103.74	105.80
1	Aa	840	G	C2-N3-C4	-5.15	109.33	111.90
27	BA	523	C	N1-C2-O2	5.15	121.99	118.90
27	BA	1366	C	C2-N1-C1'	5.15	124.47	118.80
27	BA	2699	G	C2-N3-C4	-5.15	109.33	111.90
27	BA	696	G	C2-N3-C4	-5.15	109.33	111.90
27	BA	497	G	N3-C4-N9	-5.15	122.91	126.00
27	BA	1450	C	C6-N1-C2	-5.15	118.24	120.30
1	Aa	1072	C	C2-N1-C1'	5.14	124.46	118.80
27	BA	506	G	C2-N3-C4	-5.14	109.33	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	BB	51	G	N1-C2-N2	-5.14	111.57	116.20
1	Aa	1162	C	N1-C2-O2	5.14	121.98	118.90
27	BA	940	C	C2-N1-C1'	5.14	124.45	118.80
27	BA	2477	C	C5-C4-N4	-5.14	116.60	120.20
1	Aa	1015	C	N3-C4-C5	5.14	123.95	121.90
27	BA	41	C	N3-C4-C5	5.14	123.95	121.90
1	Aa	316	C	N1-C2-O2	5.14	121.98	118.90
1	Aa	1161	C	N1-C2-O2	5.14	121.98	118.90
27	BA	654	C	N3-C2-O2	-5.14	118.31	121.90
27	BA	1783	C	N1-C2-O2	5.13	121.98	118.90
27	BA	1751	G	C2-N3-C4	-5.13	109.34	111.90
27	BA	2344	G	N7-C8-N9	5.13	115.67	113.10
27	BA	1835	G	N1-C2-N2	-5.13	111.59	116.20
27	BA	962	U	N3-C4-O4	5.12	122.99	119.40
1	Aa	1372	C	C2-N1-C1'	5.12	124.44	118.80
27	BA	465	C	N3-C4-C5	5.12	123.95	121.90
27	BA	877	C	C5-C4-N4	-5.12	116.62	120.20
27	BA	2954	C	N3-C4-C5	5.12	123.95	121.90
27	BA	2468	C	C2-N1-C1'	5.12	124.43	118.80
27	BA	1392	C	C5-C4-N4	-5.12	116.62	120.20
1	Aa	154	C	C2-N1-C1'	5.11	124.42	118.80
1	Aa	1392	G	C8-N9-C4	-5.11	104.36	106.40
27	BA	2995	C	C2-N1-C1'	5.11	124.42	118.80
27	BA	208	A	N7-C8-N9	5.11	116.35	113.80
27	BA	772	A	C5-C6-N6	-5.11	119.61	123.70
27	BA	2081	G	C2-N3-C4	-5.11	109.35	111.90
27	BA	776	C	C6-N1-C1'	-5.11	114.67	120.80
27	BA	53	C	C2-N1-C1'	5.10	124.41	118.80
1	Aa	691	C	C2-N1-C1'	5.10	124.41	118.80
1	Aa	1445	C	N3-C2-O2	-5.10	118.33	121.90
27	BA	123	C	C5-C4-N4	-5.10	116.63	120.20
27	BA	1445	G	C2-N3-C4	-5.10	109.35	111.90
27	BA	1765	G	C8-N9-C4	-5.10	104.36	106.40
27	BA	1916	C	C5-C6-N1	5.10	123.55	121.00
27	BA	2874	C	N1-C2-O2	5.10	121.96	118.90
27	BA	830	G	O4'-C1'-N9	5.09	112.28	108.20
27	BA	1450	C	C5-C6-N1	5.09	123.55	121.00
27	BA	2138	G	C8-N9-C4	-5.09	104.36	106.40
1	Aa	105	C	C2-N1-C1'	5.09	124.40	118.80
27	BA	125	G	C2-N3-C4	-5.09	109.35	111.90
27	BA	1092	C	N1-C2-O2	5.09	121.95	118.90
1	Aa	260	C	N1-C2-O2	5.09	121.95	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BA	1352	C	C5-C4-N4	-5.09	116.64	120.20
27	BA	180	G	C2-N3-C4	-5.09	109.36	111.90
27	BA	956	C	N1-C2-O2	5.08	121.95	118.90
27	BA	2141	G	C2-N3-C4	-5.08	109.36	111.90
27	BA	30	C	N1-C2-O2	5.08	121.95	118.90
27	BA	1154	A	C8-N9-C4	-5.08	103.77	105.80
27	BA	2763	C	C2-N1-C1'	5.08	124.39	118.80
27	BA	1744	C	C2-N1-C1'	5.08	124.39	118.80
27	BA	2190	C	C6-N1-C1'	-5.08	114.71	120.80
27	BA	1960	C	C2-N1-C1'	5.08	124.38	118.80
27	BA	2113	C	C5-C4-N4	-5.07	116.65	120.20
27	BA	2361	C	C5-C4-N4	-5.07	116.65	120.20
27	BA	852	G	C2-N3-C4	-5.07	109.37	111.90
27	BA	2254	C	C6-N1-C2	-5.07	118.27	120.30
27	BA	3029	C	N1-C2-O2	5.07	121.94	118.90
27	BA	1579	G	C2-N3-C4	-5.06	109.37	111.90
27	BA	1360	G	C8-N9-C4	-5.06	104.38	106.40
27	BA	3029	C	C6-N1-C2	-5.06	118.28	120.30
28	BB	50	G	N1-C2-N2	-5.06	111.65	116.20
27	BA	1037	C	N3-C4-C5	5.05	123.92	121.90
27	BA	1536	C	C6-N1-C1'	-5.05	114.73	120.80
27	BA	61	A	N7-C8-N9	5.05	116.32	113.80
27	BA	1257	G	N1-C2-N2	-5.05	111.66	116.20
1	Aa	1431	G	N1-C2-N2	-5.05	111.66	116.20
27	BA	1449	U	C6-N1-C1'	-5.05	114.13	121.20
27	BA	1789	G	N3-C2-N2	-5.05	116.37	119.90
27	BA	2062	G	N1-C2-N3	5.05	126.93	123.90
27	BA	2120	C	C6-N1-C1'	-5.05	114.74	120.80
1	Aa	1369	G	N1-C2-N3	5.05	126.93	123.90
27	BA	2312	C	N3-C4-N4	5.05	121.53	118.00
1	Aa	255	C	C2-N1-C1'	5.04	124.34	118.80
27	BA	1257	G	C2-N3-C4	-5.04	109.38	111.90
27	BA	1504	C	C2-N1-C1'	5.04	124.35	118.80
27	BA	2507	G	C4-N9-C1'	-5.04	119.94	126.50
27	BA	1115	C	C2-N1-C1'	5.04	124.34	118.80
1	Aa	1453	G	N3-C4-N9	-5.04	122.98	126.00
27	BA	174	C	C2-N1-C1'	5.04	124.34	118.80
27	BA	245	G	N3-C2-N2	5.03	123.42	119.90
1	Aa	729	C	C2-N1-C1'	5.03	124.33	118.80
27	BA	681	C	C5-C4-N4	-5.02	116.69	120.20
27	BA	1133	C	C2-N1-C1'	5.02	124.33	118.80
1	Aa	81	C	N3-C2-O2	-5.02	118.39	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Aa	1345	C	C6-N1-C1'	-5.02	114.78	120.80
27	BA	2043	G	N3-C4-N9	-5.02	122.99	126.00
27	BA	767	G	N3-C4-C5	-5.02	126.09	128.60
27	BA	2361	C	N1-C2-O2	5.02	121.91	118.90
27	BA	946	G	N1-C2-N2	-5.02	111.69	116.20
28	BB	121	G	C4-C5-N7	5.02	112.81	110.80
1	Aa	1410	C	N1-C2-O2	5.02	121.91	118.90
27	BA	776	C	C6-N1-C2	-5.01	118.30	120.30
27	BA	2139	G	C8-N9-C4	-5.01	104.40	106.40
27	BA	856	C	C2-N1-C1'	5.01	124.31	118.80
27	BA	2078	C	C5-C4-N4	-5.01	116.69	120.20
27	BA	1832	C	C5-C4-N4	-5.00	116.70	120.20
27	BA	2546	C	N1-C2-O2	5.00	121.90	118.90
27	BA	2696	G	N7-C8-N9	5.00	115.60	113.10
1	Aa	316	C	N3-C2-O2	-5.00	118.40	121.90
27	BA	2087	C	C2-N1-C1'	5.00	124.30	118.80
27	BA	2150	U	C5-C6-N1	5.00	125.20	122.70
27	BA	2087	C	C5-C4-N4	-5.00	116.70	120.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	An	126	HIS	Peptide

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

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

## 5.3 Torsion angles [i](#)

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

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

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



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Ab	194/201 (96%)	181 (93%)	13 (7%)	0	100	100
3	Ac	193/209 (92%)	181 (94%)	12 (6%)	0	100	100
4	Ad	188/200 (94%)	172 (92%)	16 (8%)	0	100	100
5	Ae	172/180 (96%)	162 (94%)	10 (6%)	0	100	100
6	Af	239/243 (98%)	222 (93%)	17 (7%)	0	100	100
7	Ag	221/235 (94%)	207 (94%)	14 (6%)	0	100	100
8	Ah	121/125 (97%)	109 (90%)	12 (10%)	0	100	100
9	Ai	212/215 (99%)	200 (94%)	12 (6%)	0	100	100
10	Aj	127/130 (98%)	115 (91%)	12 (9%)	0	100	100
11	Ak	123/130 (95%)	114 (93%)	9 (7%)	0	100	100
12	Al	131/135 (97%)	123 (94%)	8 (6%)	0	100	100
13	Am	98/102 (96%)	90 (92%)	8 (8%)	0	100	100
14	An	125/140 (89%)	120 (96%)	5 (4%)	0	100	100
15	Ao	141/147 (96%)	137 (97%)	4 (3%)	0	100	100
16	Ap	133/149 (89%)	114 (86%)	19 (14%)	0	100	100
17	Aq	147/151 (97%)	141 (96%)	6 (4%)	0	100	100
18	Ar	52/56 (93%)	47 (90%)	5 (10%)	0	100	100
19	As	106/114 (93%)	100 (94%)	6 (6%)	0	100	100
20	At	62/67 (92%)	60 (97%)	2 (3%)	0	100	100
21	Au	114/133 (86%)	108 (95%)	6 (5%)	0	100	100
22	Av	147/150 (98%)	134 (91%)	13 (9%)	0	100	100
23	Aw	93/98 (95%)	89 (96%)	4 (4%)	0	100	100
24	Ax	59/65 (91%)	57 (97%)	2 (3%)	0	100	100
25	Ay	62/70 (89%)	55 (89%)	7 (11%)	0	100	100
26	Az	53/62 (86%)	47 (89%)	6 (11%)	0	100	100
29	BC	235/239 (98%)	209 (89%)	26 (11%)	0	100	100
30	BD	342/346 (99%)	311 (91%)	31 (9%)	0	100	100
31	BE	253/255 (99%)	232 (92%)	21 (8%)	0	100	100
32	BF	165/183 (90%)	136 (82%)	29 (18%)	0	100	100
33	BG	181/184 (98%)	168 (93%)	13 (7%)	0	100	100
34	BH	119/123 (97%)	111 (93%)	8 (7%)	0	100	100
34	BI	119/123 (97%)	106 (89%)	13 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	BJ	164/182 (90%)	149 (91%)	15 (9%)	0	100	100
36	BK	140/142 (99%)	132 (94%)	8 (6%)	0	100	100
37	BL	138/141 (98%)	128 (93%)	10 (7%)	0	100	100
38	BM	79/83 (95%)	72 (91%)	7 (9%)	0	100	100
38	BN	79/83 (95%)	69 (87%)	10 (13%)	0	100	100
39	BO	146/148 (99%)	129 (88%)	17 (12%)	0	100	100
40	BP	191/194 (98%)	178 (93%)	13 (7%)	0	100	100
41	BQ	158/201 (79%)	144 (91%)	14 (9%)	0	100	100
42	BR	118/121 (98%)	106 (90%)	12 (10%)	0	100	100
43	BS	144/150 (96%)	128 (89%)	16 (11%)	0	100	100
44	BT	72/77 (94%)	68 (94%)	4 (6%)	0	100	100
45	BU	94/98 (96%)	88 (94%)	6 (6%)	0	100	100
46	BV	152/156 (97%)	143 (94%)	9 (6%)	0	100	100
47	BW	83/86 (96%)	71 (86%)	12 (14%)	0	100	100
48	BX	118/121 (98%)	111 (94%)	7 (6%)	0	100	100
49	BY	60/67 (90%)	59 (98%)	1 (2%)	0	100	100
50	BZ	56/66 (85%)	54 (96%)	2 (4%)	0	100	100
51	Ba	152/155 (98%)	142 (93%)	10 (7%)	0	100	100
52	Bb	94/102 (92%)	86 (92%)	8 (8%)	0	100	100
53	Bc	87/90 (97%)	84 (97%)	3 (3%)	0	100	100
54	Bd	122/125 (98%)	113 (93%)	9 (7%)	0	100	100
55	Be	87/90 (97%)	77 (88%)	10 (12%)	0	100	100
56	Bg	82/86 (95%)	78 (95%)	4 (5%)	0	100	100
57	Bh	60/63 (95%)	58 (97%)	2 (3%)	0	100	100
58	Bi	48/51 (94%)	43 (90%)	5 (10%)	0	100	100
59	Bj	45/51 (88%)	39 (87%)	6 (13%)	0	100	100
60	Bk	34/37 (92%)	33 (97%)	1 (3%)	0	100	100
61	Bl	91/94 (97%)	88 (97%)	3 (3%)	0	100	100
All	All	7621/8020 (95%)	7028 (92%)	593 (8%)	0	100	100

There are no Ramachandran outliers to report.

### 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	
2	Ab	170/175 (97%)	170 (100%)	0	100	100
3	Ac	154/168 (92%)	154 (100%)	0	100	100
4	Ad	162/169 (96%)	162 (100%)	0	100	100
5	Ae	153/156 (98%)	153 (100%)	0	100	100
6	Af	210/212 (99%)	210 (100%)	0	100	100
7	Ag	185/197 (94%)	185 (100%)	0	100	100
8	Ah	104/105 (99%)	104 (100%)	0	100	100
9	Ai	183/184 (100%)	183 (100%)	0	100	100
10	Aj	106/107 (99%)	106 (100%)	0	100	100
11	Ak	101/105 (96%)	101 (100%)	0	100	100
12	Al	110/112 (98%)	110 (100%)	0	100	100
13	Am	89/91 (98%)	89 (100%)	0	100	100
14	An	94/108 (87%)	94 (100%)	0	100	100
15	Ao	117/120 (98%)	117 (100%)	0	100	100
16	Ap	111/123 (90%)	111 (100%)	0	100	100
17	Aq	129/131 (98%)	128 (99%)	1 (1%)	81	92
18	Ar	45/46 (98%)	45 (100%)	0	100	100
19	As	96/101 (95%)	96 (100%)	0	100	100
20	At	58/61 (95%)	58 (100%)	0	100	100
21	Au	104/117 (89%)	103 (99%)	1 (1%)	76	90
22	Av	125/126 (99%)	125 (100%)	0	100	100
23	Aw	85/88 (97%)	85 (100%)	0	100	100
24	Ax	53/56 (95%)	53 (100%)	0	100	100
25	Ay	53/59 (90%)	53 (100%)	0	100	100
26	Az	49/55 (89%)	49 (100%)	0	100	100
29	BC	185/187 (99%)	185 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	BD	288/289 (100%)	288 (100%)	0	100	100
31	BE	212/212 (100%)	212 (100%)	0	100	100
32	BF	130/155 (84%)	128 (98%)	2 (2%)	65	85
33	BG	158/159 (99%)	157 (99%)	1 (1%)	86	94
34	BH	99/100 (99%)	98 (99%)	1 (1%)	76	90
34	BI	99/100 (99%)	99 (100%)	0	100	100
35	BJ	144/153 (94%)	144 (100%)	0	100	100
36	BK	120/120 (100%)	120 (100%)	0	100	100
37	BL	104/105 (99%)	104 (100%)	0	100	100
38	BM	63/65 (97%)	62 (98%)	1 (2%)	62	84
38	BN	63/65 (97%)	62 (98%)	1 (2%)	62	84
39	BO	116/116 (100%)	115 (99%)	1 (1%)	78	91
40	BP	161/162 (99%)	161 (100%)	0	100	100
41	BQ	138/167 (83%)	138 (100%)	0	100	100
42	BR	101/102 (99%)	100 (99%)	1 (1%)	76	90
43	BS	120/124 (97%)	120 (100%)	0	100	100
44	BT	69/72 (96%)	69 (100%)	0	100	100
45	BU	84/85 (99%)	84 (100%)	0	100	100
46	BV	129/131 (98%)	128 (99%)	1 (1%)	81	92
47	BW	75/76 (99%)	75 (100%)	0	100	100
48	BX	109/109 (100%)	109 (100%)	0	100	100
49	BY	54/58 (93%)	54 (100%)	0	100	100
50	BZ	57/61 (93%)	56 (98%)	1 (2%)	59	82
51	Ba	132/133 (99%)	132 (100%)	0	100	100
52	Bb	76/80 (95%)	76 (100%)	0	100	100
53	Bc	75/76 (99%)	75 (100%)	0	100	100
54	Bd	106/107 (99%)	106 (100%)	0	100	100
55	Be	80/80 (100%)	79 (99%)	1 (1%)	69	87
56	Bg	62/63 (98%)	61 (98%)	1 (2%)	62	84
57	Bh	50/51 (98%)	50 (100%)	0	100	100
58	Bi	45/46 (98%)	45 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
59	Bj	36/38 (95%)	36 (100%)	0	100	100
60	Bk	34/35 (97%)	34 (100%)	0	100	100
61	Bl	83/84 (99%)	82 (99%)	1 (1%)	71	88
All	All	6503/6738 (96%)	6488 (100%)	15 (0%)	93	98

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	Aq	9	ARG
21	Au	38	LYS
32	BF	152	ARG
32	BF	177	LYS
33	BG	59	PHE
34	BH	27	ARG
38	BM	17	ARG
38	BN	17	ARG
39	BO	9	ARG
42	BR	42	ARG
46	BV	83	ARG
50	BZ	27	LYS
55	Be	63	ARG
56	Bg	3	ARG
61	Bl	80	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
2	Ab	104	GLN
13	Am	25	GLN
18	Ar	7	ASN
19	As	29	HIS
30	BD	237	ASN
30	BD	255	GLN
32	BF	161	HIS
38	BN	63	GLN
39	BO	25	HIS
39	BO	45	GLN
42	BR	77	HIS
43	BS	143	GLN
51	Ba	33	HIS

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Mol	Chain	Res	Type
53	Bc	16	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	Aa	1428/1498 (95%)	274 (19%)	0
27	BA	2876/3037 (94%)	668 (23%)	46 (1%)
28	BB	124/126 (98%)	26 (20%)	2 (1%)
All	All	4428/4661 (95%)	968 (21%)	48 (1%)

All (968) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	Aa	4	C
1	Aa	17	C
1	Aa	33	U
1	Aa	45	U
1	Aa	47	A
1	Aa	52	OMU
1	Aa	54	C
1	Aa	55	G
1	Aa	57	G
1	Aa	60	A
1	Aa	66	C
1	Aa	77	C
1	Aa	94	C
1	Aa	95	A
1	Aa	100	C
1	Aa	109	A
1	Aa	111	C
1	Aa	126	G
1	Aa	143	C
1	Aa	169	G
1	Aa	179	G
1	Aa	180	G
1	Aa	188	G
1	Aa	192	A
1	Aa	194	A
1	Aa	195	G
1	Aa	214	G
1	Aa	219	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	Aa	232	U
1	Aa	233	U
1	Aa	235	G
1	Aa	236	G
1	Aa	239	G
1	Aa	254	G
1	Aa	255	C
1	Aa	268	A
1	Aa	270	A
1	Aa	277	C
1	Aa	289	G
1	Aa	294	A
1	Aa	316	C
1	Aa	317	A
1	Aa	333	C
1	Aa	335	G
1	Aa	340	C
1	Aa	341	A
1	Aa	342	G
1	Aa	344	A
1	Aa	350	G
1	Aa	355	C
1	Aa	360	C
1	Aa	372	C
1	Aa	382	OMG
1	Aa	385	A
1	Aa	394	G
1	Aa	415	U
1	Aa	428	A
1	Aa	431	G
1	Aa	440	A
1	Aa	441	U
1	Aa	442	A
1	Aa	443	A
1	Aa	446	OMG
1	Aa	453	A
1	Aa	454	A
1	Aa	456	G
1	Aa	457	5MC
1	Aa	463	G
1	Aa	464	5MC
1	Aa	466	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	Aa	469	G
1	Aa	472	G
1	Aa	477	A
1	Aa	478	A
1	Aa	492	A
1	Aa	506	U
1	Aa	508	A
1	Aa	509	U
1	Aa	511	G
1	Aa	517	A
1	Aa	518	A
1	Aa	521	C
1	Aa	522	G
1	Aa	524	C
1	Aa	541	A
1	Aa	547	U
1	Aa	575	G
1	Aa	578	U
1	Aa	579	G
1	Aa	599	U
1	Aa	611	A
1	Aa	621	U
1	Aa	633	A
1	Aa	634	G
1	Aa	661	A
1	Aa	668	G
1	Aa	669	U
1	Aa	677	G
1	Aa	694	G
1	Aa	695	U
1	Aa	701	G
1	Aa	704	G
1	Aa	708	G
1	Aa	719	G
1	Aa	723	A
1	Aa	727	A
1	Aa	738	A
1	Aa	739	U
1	Aa	740	A
1	Aa	748	A
1	Aa	759	U
1	Aa	763	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	Aa	774	A
1	Aa	790	U
1	Aa	793	A
1	Aa	815	A
1	Aa	822	A
1	Aa	840	G
1	Aa	864	A
1	Aa	869	A
1	Aa	872	G
1	Aa	876	OMG
1	Aa	877	G
1	Aa	879	G
1	Aa	884	C
1	Aa	885	U
1	Aa	886	A
1	Aa	888	A
1	Aa	892	OMG
1	Aa	896	G
1	Aa	901	U
1	Aa	906	U
1	Aa	911	U
1	Aa	914	G
1	Aa	917	5MU
1	Aa	920	A
1	Aa	922	G
1	Aa	925	G
1	Aa	926	G
1	Aa	927	G
1	Aa	928	A
1	Aa	941	G
1	Aa	943	G
1	Aa	959	C
1	Aa	960	C
1	Aa	961	A
1	Aa	962	G
1	Aa	969	G
1	Aa	972	C
1	Aa	975	G
1	Aa	979	G
1	Aa	987	G
1	Aa	989	G
1	Aa	993	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	Aa	1008	G
1	Aa	1009	U
1	Aa	1010	C
1	Aa	1038	G
1	Aa	1039	U
1	Aa	1044	U
1	Aa	1045	A
1	Aa	1046	A
1	Aa	1069	U
1	Aa	1076	U
1	Aa	1077	C
1	Aa	1078	C
1	Aa	1079	U
1	Aa	1084	G
1	Aa	1085	C
1	Aa	1086	U
1	Aa	1088	G
1	Aa	1091	A
1	Aa	1092	G
1	Aa	1098	A
1	Aa	1111	C
1	Aa	1115	G
1	Aa	1116	G
1	Aa	1119	A
1	Aa	1120	U
1	Aa	1123	G
1	Aa	1131	A
1	Aa	1132	A
1	Aa	1133	G
1	Aa	1135	A
1	Aa	1136	G
1	Aa	1146	G
1	Aa	1148	A
1	Aa	1149	G
1	Aa	1152	C
1	Aa	1154	G
1	Aa	1157	U
1	Aa	1158	G
1	Aa	1163	G
1	Aa	1164	A
1	Aa	1168	C
1	Aa	1169	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	Aa	1170	C
1	Aa	1171	C
1	Aa	1172	G
1	Aa	1176	U
1	Aa	1179	A
1	Aa	1180	C
1	Aa	1181	G
1	Aa	1187	U
1	Aa	1190	A
1	Aa	1191	A
1	Aa	1193	G
1	Aa	1200	A
1	Aa	1208	A
1	Aa	1209	U
1	Aa	1212	G
1	Aa	1218	G
1	Aa	1221	A
1	Aa	1222	G
1	Aa	1224	G
1	Aa	1225	G
1	Aa	1230	G
1	Aa	1232	A
1	Aa	1246	C
1	Aa	1250	C
1	Aa	1251	A
1	Aa	1252	G
1	Aa	1258	A
1	Aa	1260	C
1	Aa	1272	C
1	Aa	1275	OMG
1	Aa	1276	5MC
1	Aa	1279	G
1	Aa	1284	A
1	Aa	1286	G
1	Aa	1288	U
1	Aa	1292	A
1	Aa	1297	U
1	Aa	1298	A
1	Aa	1299	G
1	Aa	1305	G
1	Aa	1312	A
1	Aa	1316	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	Aa	1322	G
1	Aa	1325	G
1	Aa	1328	U
1	Aa	1331	G
1	Aa	1334	C
1	Aa	1337	G
1	Aa	1349	C
1	Aa	1350	A
1	Aa	1352	5MC
1	Aa	1353	G
1	Aa	1354	OMC
1	Aa	1358	OMU
1	Aa	1359	C
1	Aa	1371	G
1	Aa	1392	G
1	Aa	1398	C
1	Aa	1400	U
1	Aa	1402	G
1	Aa	1403	G
1	Aa	1407	G
1	Aa	1431	G
1	Aa	1433	G
1	Aa	1436	G
1	Aa	1441	A
1	Aa	1442	A
1	Aa	1446	G
1	Aa	1447	U
1	Aa	1451	A
1	Aa	1452	A
1	Aa	1453	G
1	Aa	1455	U
1	Aa	1466	G
1	Aa	1475	G
1	Aa	1477	U
1	Aa	1478	5MC
1	Aa	1479	G
27	BA	12	C
27	BA	15	U
27	BA	16	G
27	BA	18	C
27	BA	19	A
27	BA	21	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
27	BA	34	OMU
27	BA	43	C
27	BA	49	G
27	BA	55	C
27	BA	73	A
27	BA	80	A
27	BA	83	A
27	BA	84	G
27	BA	94	G
27	BA	100	G
27	BA	108	U
27	BA	109	C
27	BA	110	G
27	BA	113	C
27	BA	127	A
27	BA	128	U
27	BA	129	G
27	BA	132	A
27	BA	133	C
27	BA	135	U
27	BA	139	G
27	BA	144	U
27	BA	148	G
27	BA	149	C
27	BA	150	C
27	BA	153	A
27	BA	159	A
27	BA	160	G
27	BA	161	U
27	BA	162	C
27	BA	172	A
27	BA	187	A
27	BA	190	A
27	BA	206	G
27	BA	207	A
27	BA	208	A
27	BA	213	A
27	BA	215	OMG
27	BA	217	A
27	BA	218	A
27	BA	219	A
27	BA	220	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
27	BA	221	G
27	BA	224	A
27	BA	239	G
27	BA	241	G
27	BA	247	A
27	BA	251	G
27	BA	257	G
27	BA	269	C
27	BA	281	A
27	BA	283	G
27	BA	285	U
27	BA	294	G
27	BA	295	U
27	BA	301	U
27	BA	302	G
27	BA	303	U
27	BA	304	A
27	BA	310	C
27	BA	311	G
27	BA	312	C
27	BA	314	G
27	BA	315	A
27	BA	316	G
27	BA	317	G
27	BA	318	A
27	BA	323	U
27	BA	324	G
27	BA	328	G
27	BA	340	U
27	BA	341	C
27	BA	350	C
27	BA	353	OMG
27	BA	360	G
27	BA	363	A
27	BA	368	G
27	BA	369	A
27	BA	370	A
27	BA	377	G
27	BA	379	A
27	BA	382	C
27	BA	384	U
27	BA	385	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
27	BA	386	A
27	BA	393	G
27	BA	398	C
27	BA	399	C
27	BA	401	G
27	BA	404	G
27	BA	405	U
27	BA	408	C
27	BA	414	G
27	BA	419	OMG
27	BA	429	U
27	BA	430	A
27	BA	432	C
27	BA	440	A
27	BA	444	U
27	BA	445	G
27	BA	451	C
27	BA	460	C
27	BA	461	C
27	BA	472	A
27	BA	475	U
27	BA	476	C
27	BA	480	A
27	BA	482	A
27	BA	488	A2M
27	BA	490	C
27	BA	496	A
27	BA	505	A2M
27	BA	506	G
27	BA	514	U
27	BA	520	G
27	BA	531	G
27	BA	540	A
27	BA	542	A
27	BA	543	G
27	BA	545	G
27	BA	546	C
27	BA	547	C
27	BA	551	A
27	BA	567	G
27	BA	568	A
27	BA	569	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
27	BA	570	G
27	BA	581	A
27	BA	584	G
27	BA	602	G
27	BA	609	C
27	BA	610	G
27	BA	612	G
27	BA	613	C
27	BA	615	A
27	BA	616	C
27	BA	622	A
27	BA	623	G
27	BA	629	G
27	BA	634	G
27	BA	635	G
27	BA	636	U
27	BA	654	C
27	BA	658	C
27	BA	662	G
27	BA	666	A
27	BA	677	A
27	BA	683	C
27	BA	688	G
27	BA	694	A
27	BA	701	G
27	BA	707	C
27	BA	708	A
27	BA	715	A
27	BA	716	A
27	BA	717	G
27	BA	733	C
27	BA	734	A
27	BA	735	G
27	BA	736	G
27	BA	740	G
27	BA	747	G
27	BA	753	G
27	BA	754	OMC
27	BA	755	G
27	BA	757	G
27	BA	774	C
27	BA	801	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
27	BA	802	A
27	BA	812	U
27	BA	827	G
27	BA	832	A
27	BA	835	C
27	BA	842	C
27	BA	844	G
27	BA	848	G
27	BA	849	A2M
27	BA	852	G
27	BA	856	C
27	BA	860	C
27	BA	867	U
27	BA	870	U
27	BA	875	5MU
27	BA	891	G
27	BA	892	A
27	BA	893	C
27	BA	896	C
27	BA	903	G
27	BA	904	G
27	BA	910	A
27	BA	912	OMG
27	BA	913	G
27	BA	919	C
27	BA	920	G
27	BA	933	G
27	BA	940	C
27	BA	943	G
27	BA	945	C
27	BA	950	U
27	BA	951	A
27	BA	955	C
27	BA	956	C
27	BA	966	C
27	BA	969	G
27	BA	974	A
27	BA	988	G
27	BA	994	C
27	BA	995	A
27	BA	999	A
27	BA	1001	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
27	BA	1003	G
27	BA	1005	G
27	BA	1009	U
27	BA	1010	A
27	BA	1012	G
27	BA	1014	G
27	BA	1016	C
27	BA	1017	G
27	BA	1018	A
27	BA	1019	A
27	BA	1021	G
27	BA	1022	C
27	BA	1023	C
27	BA	1024	U
27	BA	1026	C
27	BA	1027	G
27	BA	1031	C
27	BA	1039	A
27	BA	1041	C
27	BA	1048	C
27	BA	1055	C
27	BA	1056	C
27	BA	1058	C
27	BA	1062	A
27	BA	1063	G
27	BA	1069	C
27	BA	1076	G
27	BA	1077	G
27	BA	1079	G
27	BA	1089	A
27	BA	1090	G
27	BA	1102	G
27	BA	1103	A
27	BA	1111	A
27	BA	1116	A
27	BA	1117	G
27	BA	1118	A
27	BA	1119	C
27	BA	1125	U
27	BA	1129	G
27	BA	1130	G
27	BA	1136	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
27	BA	1139	U
27	BA	1140	G
27	BA	1149	G
27	BA	1151	G
27	BA	1156	U
27	BA	1157	C
27	BA	1158	C
27	BA	1159	A
27	BA	1165	U
27	BA	1167	U
27	BA	1175	C
27	BA	1177	U
27	BA	1179	G
27	BA	1180	A
27	BA	1183	G
27	BA	1184	C
27	BA	1185	G
27	BA	1243	A
27	BA	1244	G
27	BA	1247	C
27	BA	1248	A
27	BA	1249	G
27	BA	1250	G
27	BA	1251	G
27	BA	1260	A
27	BA	1264	G
27	BA	1265	A2M
27	BA	1266	C
27	BA	1270	G
27	BA	1307	A
27	BA	1310	G
27	BA	1313	C
27	BA	1318	A
27	BA	1320	C
27	BA	1321	G
27	BA	1322	G
27	BA	1323	G
27	BA	1336	C
27	BA	1347	G
27	BA	1361	A
27	BA	1362	G
27	BA	1371	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
27	BA	1372	A
27	BA	1373	C
27	BA	1379	G
27	BA	1385	G
27	BA	1388	G
27	BA	1391	C
27	BA	1409	A
27	BA	1410	U
27	BA	1436	U
27	BA	1437	A
27	BA	1438	G
27	BA	1457	A
27	BA	1461	U
27	BA	1477	U
27	BA	1479	G
27	BA	1480	OMU
27	BA	1485	C
27	BA	1487	U
27	BA	1490	C
27	BA	1517	A2M
27	BA	1521	A
27	BA	1525	OMG
27	BA	1533	A
27	BA	1547	G
27	BA	1548	5MU
27	BA	1551	OMU
27	BA	1556	G
27	BA	1560	C
27	BA	1563	C
27	BA	1565	C
27	BA	1568	G
27	BA	1571	C
27	BA	1581	C
27	BA	1594	G
27	BA	1606	A
27	BA	1617	U
27	BA	1624	A
27	BA	1626	A
27	BA	1635	G
27	BA	1636	A
27	BA	1637	G
27	BA	1639	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
27	BA	1640	C
27	BA	1646	U
27	BA	1647	G
27	BA	1650	G
27	BA	1652	G
27	BA	1657	G
27	BA	1660	U
27	BA	1662	A
27	BA	1664	A
27	BA	1671	A
27	BA	1672	U
27	BA	1673	G
27	BA	1674	G
27	BA	1675	C
27	BA	1681	G
27	BA	1682	U
27	BA	1683	A
27	BA	1685	G
27	BA	1692	U
27	BA	1693	C
27	BA	1699	A
27	BA	1704	U
27	BA	1706	G
27	BA	1715	A
27	BA	1716	A
27	BA	1734	U
27	BA	1742	G
27	BA	1743	A
27	BA	1752	A
27	BA	1754	A
27	BA	1755	A
27	BA	1761	A
27	BA	1762	C
27	BA	1763	U
27	BA	1764	G
27	BA	1767	G
27	BA	1768	C
27	BA	1769	C
27	BA	1771	C
27	BA	1773	G
27	BA	1785	U
27	BA	1792	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
27	BA	1793	G
27	BA	1794	U
27	BA	1795	C
27	BA	1799	OMG
27	BA	1800	G
27	BA	1801	A
27	BA	1822	G
27	BA	1824	A
27	BA	1827	U
27	BA	1842	C
27	BA	1848	A
27	BA	1849	A
27	BA	1853	G
27	BA	1855	G
27	BA	1859	G
27	BA	1861	G
27	BA	1884	G
27	BA	1891	G
27	BA	1892	OMG
27	BA	1897	C
27	BA	1901	A
27	BA	1904	G
27	BA	1908	A
27	BA	1909	G
27	BA	1914	A
27	BA	1928	C
27	BA	1929	U
27	BA	1930	A
27	BA	1933	C
27	BA	1945	G
27	BA	1946	U
27	BA	1956	G
27	BA	1957	A
27	BA	1991	A
27	BA	2002	A
27	BA	2014	A
27	BA	2018	OMC
27	BA	2019	OMG
27	BA	2026	A
27	BA	2027	C
27	BA	2029	A
27	BA	2033	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
27	BA	2036	U
27	BA	2038	U
27	BA	2042	G
27	BA	2043	G
27	BA	2048	G
27	BA	2049	A
27	BA	2051	A
27	BA	2053	U
27	BA	2054	C
27	BA	2055	5MC
27	BA	2067	A
27	BA	2068	U
27	BA	2073	A
27	BA	2074	C
27	BA	2076	U
27	BA	2077	G
27	BA	2078	C
27	BA	2080	U
27	BA	2083	A
27	BA	2084	U
27	BA	2085	G
27	BA	2088	G
27	BA	2099	C
27	BA	2104	U
27	BA	2105	G
27	BA	2106	U
27	BA	2119	C
27	BA	2125	G
27	BA	2135	C
27	BA	2139	G
27	BA	2143	A
27	BA	2144	U
27	BA	2145	A
27	BA	2148	C
27	BA	2152	OMG
27	BA	2153	G
27	BA	2155	C
27	BA	2162	U
27	BA	2164	G
27	BA	2167	A
27	BA	2173	G
27	BA	2174	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
27	BA	2175	C
27	BA	2181	G
27	BA	2182	G
27	BA	2194	A
27	BA	2214	C
27	BA	2216	G
27	BA	2217	G
27	BA	2218	G
27	BA	2219	G
27	BA	2220	G
27	BA	2221	U
27	BA	2222	G
27	BA	2223	C
27	BA	2224	G
27	BA	2226	A
27	BA	2227	G
27	BA	2228	C
27	BA	2229	G
27	BA	2230	U
27	BA	2238	A
27	BA	2240	G
27	BA	2241	C
27	BA	2243	U
27	BA	2244	C
27	BA	2245	G
27	BA	2247	A
27	BA	2248	G
27	BA	2249	C
27	BA	2250	C
27	BA	2257	C
27	BA	2258	C
27	BA	2260	G
27	BA	2261	G
27	BA	2265	G
27	BA	2269	G
27	BA	2270	A
27	BA	2271	G
27	BA	2275	C
27	BA	2279	U
27	BA	2281	A
27	BA	2282	G
27	BA	2283	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
27	BA	2284	C
27	BA	2291	C
27	BA	2292	A
27	BA	2293	C
27	BA	2303	U
27	BA	2318	G
27	BA	2321	G
27	BA	2327	A
27	BA	2328	C
27	BA	2337	G
27	BA	2340	G
27	BA	2353	OMG
27	BA	2358	G
27	BA	2360	A
27	BA	2369	A
27	BA	2379	OMG
27	BA	2382	G
27	BA	2385	G
27	BA	2386	C
27	BA	2389	OMU
27	BA	2390	A
27	BA	2391	A
27	BA	2392	G
27	BA	2403	G
27	BA	2406	G
27	BA	2409	C
27	BA	2423	A
27	BA	2425	A
27	BA	2428	G
27	BA	2443	G
27	BA	2445	C
27	BA	2448	G
27	BA	2453	G
27	BA	2460	A
27	BA	2464	G
27	BA	2465	A
27	BA	2482	A
27	BA	2483	A
27	BA	2489	G
27	BA	2491	C
27	BA	2497	G
27	BA	2498	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
27	BA	2510	U
27	BA	2520	G
27	BA	2530	U
27	BA	2531	G
27	BA	2534	A
27	BA	2535	G
27	BA	2536	A
27	BA	2539	A
27	BA	2545	OMC
27	BA	2550	OMG
27	BA	2552	A
27	BA	2563	G
27	BA	2568	OMG
27	BA	2572	G
27	BA	2573	A
27	BA	2578	C
27	BA	2579	C
27	BA	2580	A
27	BA	2581	4SU
27	BA	2582	A
27	BA	2585	G
27	BA	2589	C
27	BA	2595	OMC
27	BA	2596	U
27	BA	2598	G
27	BA	2606	G
27	BA	2609	G
27	BA	2610	OMU
27	BA	2622	A
27	BA	2632	U
27	BA	2633	G
27	BA	2638	A
27	BA	2642	G
27	BA	2646	A
27	BA	2660	C
27	BA	2669	A
27	BA	2670	A
27	BA	2671	G
27	BA	2676	A
27	BA	2677	C
27	BA	2682	G
27	BA	2685	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
27	BA	2686	G
27	BA	2703	G
27	BA	2706	A
27	BA	2707	G
27	BA	2713	A
27	BA	2717	U
27	BA	2718	A
27	BA	2719	U
27	BA	2733	U
27	BA	2734	G
27	BA	2735	G
27	BA	2737	C
27	BA	2738	G
27	BA	2741	U
27	BA	2742	G
27	BA	2748	A
27	BA	2749	A
27	BA	2750	G
27	BA	2752	C
27	BA	2754	C
27	BA	2767	A
27	BA	2768	G
27	BA	2775	G
27	BA	2776	G
27	BA	2777	A
27	BA	2778	G
27	BA	2787	U
27	BA	2794	U
27	BA	2810	G
27	BA	2814	A
27	BA	2815	U
27	BA	2816	A
27	BA	2817	G
27	BA	2822	G
27	BA	2827	U
27	BA	2835	A
27	BA	2836	G
27	BA	2837	C
27	BA	2839	G
27	BA	2850	A
27	BA	2853	G
27	BA	2861	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
27	BA	2862	G
27	BA	2867	A
27	BA	2868	G
27	BA	2878	A
27	BA	2879	A
27	BA	2883	A
27	BA	2884	G
27	BA	2937	G
27	BA	2945	G
27	BA	2946	A
27	BA	2952	A
27	BA	2959	U
27	BA	2960	G
27	BA	2961	A
27	BA	2971	G
27	BA	2976	A
27	BA	2982	G
27	BA	2985	G
27	BA	2990	A
27	BA	2995	C
27	BA	3001	C
27	BA	3007	G
27	BA	3008	C
27	BA	3014	C
27	BA	3020	G
27	BA	3024	G
27	BA	3027	U
27	BA	3030	U
27	BA	3031	A
27	BA	3032	C
27	BA	3034	G
27	BA	3036	G
28	BB	4	A
28	BB	5	C
28	BB	12	C
28	BB	25	C
28	BB	26	C
28	BB	32	C
28	BB	34	G
28	BB	35	U
28	BB	36	C
28	BB	39	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
28	BB	41	U
28	BB	42	U
28	BB	43	C
28	BB	44	G
28	BB	47	C
28	BB	49	C
28	BB	53	A
28	BB	57	A
28	BB	79	G
28	BB	89	C
28	BB	94	A
28	BB	95	G
28	BB	101	G
28	BB	115	G
28	BB	116	C
28	BB	124	C

All (48) RNA pucker outliers are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
27	BA	108	U
27	BA	128	U
27	BA	134	C
27	BA	147	U
27	BA	187	A
27	BA	268	A
27	BA	378	U
27	BA	392	C
27	BA	404	G
27	BA	471	U
27	BA	687	A
27	BA	912	OMG
27	BA	973	G
27	BA	987	G
27	BA	1002	G
27	BA	1178	A
27	BA	1182	A
27	BA	1360	G
27	BA	1436	U
27	BA	1520	G
27	BA	1636	A
27	BA	1671	A

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Mol	Chain	Res	Type
27	BA	1673	G
27	BA	1691	U
27	BA	1741	C
27	BA	1753	G
27	BA	1767	G
27	BA	1799	OMG
27	BA	1928	C
27	BA	2053	U
27	BA	2154	A
27	BA	2161	G
27	BA	2173	G
27	BA	2216	G
27	BA	2239	G
27	BA	2268	G
27	BA	2282	G
27	BA	2482	A
27	BA	2496	C
27	BA	2534	A
27	BA	2545	OMC
27	BA	2571	OMC
27	BA	2685	G
27	BA	2836	G
27	BA	2945	G
27	BA	3026	G
28	BB	3	U
28	BB	56	U

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

229 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
27	OMG	BA	1106	27	18,26,27	2.11	7 (38%)	19,38,41	1.42	3 (15%)
1	OMC	Aa	825	1	19,22,23	2.62	7 (36%)	26,31,34	0.86	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	OMU	BA	34	27	19,22,23	2.62	7 (36%)	26,31,34	1.63	4 (15%)
27	4AC	BA	335	27	21,24,25	3.13	9 (42%)	29,34,37	1.14	3 (10%)
1	OMG	Aa	1026	1	18,26,27	2.25	7 (38%)	19,38,41	1.35	4 (21%)
27	B8T	BA	357	27	19,22,23	0.79	0	26,31,34	0.85	1 (3%)
27	4AC	BA	730	27	21,24,25	3.16	10 (47%)	29,34,37	1.37	5 (17%)
27	5MC	BA	2055	27	18,22,23	3.24	7 (38%)	26,32,35	1.11	1 (3%)
1	OMG	Aa	771	1	18,26,27	2.24	7 (38%)	19,38,41	1.37	4 (21%)
27	4AC	BA	27	27	21,24,25	3.17	10 (47%)	29,34,37	1.35	5 (17%)
27	OMC	BA	250	27	19,22,23	2.66	7 (36%)	26,31,34	1.42	5 (19%)
27	4AC	BA	3023	27	21,24,25	3.17	9 (42%)	29,34,37	1.33	7 (24%)
1	4AC	Aa	827	1	21,24,25	3.18	9 (42%)	29,34,37	1.24	4 (13%)
1	4AC	Aa	41	1	21,24,25	3.26	9 (42%)	29,34,37	1.68	5 (17%)
27	A2M	BA	488	27	18,25,26	4.06	8 (44%)	18,36,39	2.96	4 (22%)
1	4AC	Aa	5	1	21,24,25	3.13	10 (47%)	29,34,37	1.64	5 (17%)
27	OMC	BA	2545	27	19,22,23	2.58	7 (36%)	26,31,34	1.29	2 (7%)
1	4AC	Aa	1459	1	21,24,25	2.56	7 (33%)	29,34,37	1.66	8 (27%)
27	OMG	BA	833	27	18,26,27	2.27	8 (44%)	19,38,41	1.71	4 (21%)
27	5MU	BA	2384	27	19,22,23	4.63	7 (36%)	28,32,35	3.73	12 (42%)
27	A2M	BA	872	27	18,25,26	4.15	9 (50%)	18,36,39	3.01	4 (22%)
27	4AC	BA	799	27	21,24,25	2.98	10 (47%)	29,34,37	1.33	3 (10%)
27	OMG	BA	2672	27	18,26,27	2.14	6 (33%)	19,38,41	1.74	4 (21%)
1	5MC	Aa	1352	1	18,22,23	3.42	7 (38%)	26,32,35	1.15	3 (11%)
27	OMC	BA	754	27	19,22,23	2.71	7 (36%)	26,31,34	0.99	0
1	OMG	Aa	636	1	18,26,27	2.31	7 (38%)	19,38,41	1.32	3 (15%)
1	4AC	Aa	136	1	21,24,25	3.33	9 (42%)	29,34,37	1.72	5 (17%)
1	OMC	Aa	1361	27,1	19,22,23	2.56	7 (36%)	26,31,34	0.82	0
27	4AC	BA	1641	27	21,24,25	3.13	9 (42%)	29,34,37	1.25	5 (17%)
27	5MC	BA	2075	27	18,22,23	2.86	7 (38%)	26,32,35	1.02	1 (3%)
27	OMC	BA	2630	27	19,22,23	2.48	7 (36%)	26,31,34	1.10	2 (7%)
1	OMG	Aa	994	1	18,26,27	2.43	8 (44%)	19,38,41	1.45	4 (21%)
27	5MU	BA	298	27	19,22,23	4.46	7 (36%)	28,32,35	3.72	10 (35%)
27	OMC	BA	561	27	19,22,23	2.59	7 (36%)	26,31,34	0.94	1 (3%)
27	5MC	BA	1696	27	18,22,23	3.02	7 (38%)	26,32,35	1.07	2 (7%)
1	4AC	Aa	458	1	21,24,25	1.02	1 (4%)	29,34,37	1.19	3 (10%)
27	OMG	BA	2168	27	18,26,27	2.19	7 (38%)	19,38,41	1.54	6 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	OMU	BA	657	27	19,22,23	2.56	6 (31%)	26,31,34	1.65	6 (23%)
27	4AC	BA	1955	27	21,24,25	2.89	10 (47%)	29,34,37	1.16	4 (13%)
27	4AC	BA	376	27	21,24,25	3.01	9 (42%)	29,34,37	1.32	5 (17%)
27	OMG	BA	2152	27	18,26,27	2.01	5 (27%)	19,38,41	1.53	4 (21%)
27	4AC	BA	1434	27	21,24,25	2.91	10 (47%)	29,34,37	1.70	6 (20%)
27	OMG	BA	365	27	18,26,27	2.04	7 (38%)	19,38,41	1.44	3 (15%)
27	OMG	BA	1892	27	18,26,27	2.12	7 (38%)	19,38,41	1.37	3 (15%)
27	5MC	BA	1965	27	18,22,23	2.86	7 (38%)	26,32,35	1.15	2 (7%)
27	OMU	BA	1776	27	19,22,23	2.71	7 (36%)	26,31,34	1.79	6 (23%)
27	5MU	BA	572	27	19,22,23	4.45	7 (36%)	28,32,35	3.73	12 (42%)
27	OMC	BA	718	27	19,22,23	2.65	7 (36%)	26,31,34	1.30	4 (15%)
1	LV2	Aa	918	1	20,23,24	0.94	0	26,33,36	0.81	0
1	5MC	Aa	1478	1	18,22,23	3.03	7 (38%)	26,32,35	1.48	6 (23%)
1	4AC	Aa	298	1	21,24,25	3.17	9 (42%)	29,34,37	1.61	5 (17%)
27	OMU	BA	1551	27	19,22,23	2.93	7 (36%)	26,31,34	1.77	5 (19%)
27	OMU	BA	2389	27	19,22,23	1.29	3 (15%)	26,31,34	1.84	6 (23%)
27	LHH	BA	2955	27	22,25,26	2.39	5 (22%)	29,35,38	2.00	6 (20%)
27	A2M	BA	2702	27	18,25,26	4.02	9 (50%)	18,36,39	2.59	4 (22%)
27	5MU	BA	2688	27	19,22,23	4.44	7 (36%)	28,32,35	3.70	11 (39%)
1	OMG	Aa	246	1	18,26,27	2.14	7 (38%)	19,38,41	1.36	3 (15%)
1	OMU	Aa	52	1	19,22,23	2.82	7 (36%)	26,31,34	1.62	4 (15%)
27	A2M	BA	756	27	18,25,26	4.21	8 (44%)	18,36,39	2.86	4 (22%)
1	OMU	Aa	240	1	19,22,23	2.88	7 (36%)	26,31,34	1.76	4 (15%)
1	6MZ	Aa	1449	1	18,25,26	0.77	0	16,36,39	1.94	3 (18%)
27	4AC	BA	925	27	21,24,25	1.06	1 (4%)	29,34,37	1.55	6 (20%)
1	4AC	Aa	569	1	21,24,25	3.15	9 (42%)	29,34,37	1.40	5 (17%)
27	5MU	BA	537	27	19,22,23	4.44	7 (36%)	28,32,35	3.88	10 (35%)
1	4AC	Aa	525	1	21,24,25	3.00	10 (47%)	29,34,37	1.88	6 (20%)
1	4AC	Aa	847	1	21,24,25	3.09	10 (47%)	29,34,37	1.19	3 (10%)
27	5MC	BA	944	27	18,22,23	2.92	7 (38%)	26,32,35	1.31	3 (11%)
27	OMU	BA	2542	27	19,22,23	2.70	7 (36%)	26,31,34	1.75	5 (19%)
1	4AC	Aa	682	1	21,24,25	3.23	9 (42%)	29,34,37	1.47	5 (17%)
27	OMG	BA	763	27	18,26,27	2.15	7 (38%)	19,38,41	1.47	4 (21%)
1	OMG	Aa	1434	1	18,26,27	2.16	7 (38%)	19,38,41	1.47	3 (15%)
27	OMG	BA	290	27	18,26,27	2.21	8 (44%)	19,38,41	1.64	4 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	LHH	BA	526	27	22,25,26	2.41	5 (22%)	29,35,38	1.77	7 (24%)
27	A2M	BA	1400	27	18,25,26	4.07	10 (55%)	18,36,39	2.89	4 (22%)
27	OMC	BA	1750	27	19,22,23	2.54	7 (36%)	26,31,34	1.22	5 (19%)
27	OMU	BA	2610	27	19,22,23	3.04	8 (42%)	26,31,34	1.83	4 (15%)
1	5MC	Aa	1276	1	18,22,23	4.83	16 (88%)	26,32,35	1.16	2 (7%)
27	OMG	BA	64	27	18,26,27	2.01	6 (33%)	19,38,41	1.37	3 (15%)
27	OMG	BA	2745	27	18,26,27	2.16	6 (33%)	19,38,41	1.75	4 (21%)
27	OMU	BA	619	27	19,22,23	2.81	7 (36%)	26,31,34	1.79	6 (23%)
1	LHH	Aa	1020	1	22,25,26	2.56	5 (22%)	29,35,38	1.85	8 (27%)
27	OMC	BA	869	27	19,22,23	2.60	7 (36%)	26,31,34	1.06	2 (7%)
1	5MC	Aa	464	1	18,22,23	3.34	7 (38%)	26,32,35	1.22	2 (7%)
1	OMG	Aa	876	1	18,26,27	2.30	8 (44%)	19,38,41	1.37	4 (21%)
27	OMG	BA	215	27	18,26,27	2.27	7 (38%)	19,38,41	1.91	4 (21%)
1	4AC	Aa	730	1	21,24,25	3.06	10 (47%)	29,34,37	1.68	5 (17%)
27	LHH	BA	617	27	22,25,26	2.53	5 (22%)	29,35,38	1.66	6 (20%)
27	4AC	BA	1357	27	21,24,25	3.02	10 (47%)	29,34,37	1.38	6 (20%)
27	4AC	BA	805	27	21,24,25	2.86	10 (47%)	29,34,37	1.40	7 (24%)
1	5MU	Aa	917	1	19,22,23	1.39	4 (21%)	28,32,35	2.22	6 (21%)
27	OMG	BA	2728	27	18,26,27	2.20	6 (33%)	19,38,41	1.58	4 (21%)
1	5MC	Aa	672	1	18,22,23	3.12	7 (38%)	26,32,35	1.20	2 (7%)
1	OMG	Aa	450	1	18,26,27	2.16	7 (38%)	19,38,41	1.30	3 (15%)
27	4AC	BA	418	27	21,24,25	3.20	10 (47%)	29,34,37	1.17	4 (13%)
27	4AC	BA	2780	27	21,24,25	3.13	9 (42%)	29,34,37	1.67	7 (24%)
1	B8T	Aa	1051	1	19,22,23	0.80	0	26,31,34	0.89	1 (3%)
1	MA6	Aa	1468	1	19,26,27	1.34	1 (5%)	18,38,41	3.39	2 (11%)
27	OMG	BA	2019	27	18,26,27	2.41	8 (44%)	19,38,41	1.70	4 (21%)
1	MA6	Aa	1467	1	19,26,27	1.42	3 (15%)	18,38,41	3.19	2 (11%)
1	OMG	Aa	1265	1	18,26,27	2.27	8 (44%)	19,38,41	1.42	3 (15%)
1	5MC	Aa	1004	1	18,22,23	3.24	7 (38%)	26,32,35	1.14	2 (7%)
1	OMG	Aa	138	1	18,26,27	2.27	7 (38%)	19,38,41	1.40	3 (15%)
27	LHH	BA	2457	27	22,25,26	2.52	5 (22%)	29,35,38	2.16	7 (24%)
27	OMG	BA	1398	27	18,26,27	2.09	5 (27%)	19,38,41	1.37	3 (15%)
1	OMG	Aa	498	1	18,26,27	2.23	7 (38%)	19,38,41	1.37	3 (15%)
27	4AC	BA	713	27	21,24,25	3.04	9 (42%)	29,34,37	1.17	2 (6%)
27	4SU	BA	2553	27	18,21,22	3.87	8 (44%)	26,30,33	1.94	5 (19%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	4SU	BA	2581	27	18,21,22	4.00	8 (44%)	26,30,33	2.26	5 (19%)
27	OMG	BA	2324	27	18,26,27	2.19	7 (38%)	19,38,41	1.43	3 (15%)
27	4AC	BA	2797	27	21,24,25	2.96	10 (47%)	29,34,37	1.17	3 (10%)
1	OMC	Aa	296	1	19,22,23	2.62	7 (36%)	26,31,34	0.96	1 (3%)
1	OMG	Aa	320	1	18,26,27	2.25	7 (38%)	19,38,41	1.42	3 (15%)
27	4AC	BA	433	27	21,24,25	3.00	9 (42%)	29,34,37	1.23	3 (10%)
1	4AC	Aa	1217	1	21,24,25	3.44	9 (42%)	29,34,37	1.59	6 (20%)
27	OMC	BA	2595	27	19,22,23	2.57	7 (36%)	26,31,34	1.27	3 (11%)
1	A2M	Aa	352	1	18,25,26	0.94	1 (5%)	18,36,39	1.29	2 (11%)
27	4AC	BA	244	27	21,24,25	2.99	10 (47%)	29,34,37	1.21	4 (13%)
27	OMG	BA	2550	27	18,26,27	2.09	6 (33%)	19,38,41	2.06	6 (31%)
1	2MG	Aa	670	1	18,26,27	2.27	7 (38%)	16,38,41	1.24	2 (12%)
27	OMG	BA	2353	27	18,26,27	2.06	6 (33%)	19,38,41	1.46	4 (21%)
27	OMG	BA	2527	27	18,26,27	2.10	6 (33%)	19,38,41	1.38	3 (15%)
27	4AC	BA	1899	27	21,24,25	2.96	10 (47%)	29,34,37	1.26	4 (13%)
27	4AC	BA	2838	27	21,24,25	3.16	9 (42%)	29,34,37	1.30	4 (13%)
27	5MC	BA	2863	27	18,22,23	3.13	7 (38%)	26,32,35	1.23	4 (15%)
27	OMG	BA	912	27	18,26,27	2.21	7 (38%)	19,38,41	2.02	4 (21%)
27	4AC	BA	124	27	21,24,25	2.91	10 (47%)	29,34,37	1.21	3 (10%)
27	OMG	BA	552	27	18,26,27	2.18	7 (38%)	19,38,41	1.56	5 (26%)
27	4AC	BA	56	27	21,24,25	3.10	9 (42%)	29,34,37	1.35	5 (17%)
1	OMG	Aa	892	1	18,26,27	2.18	7 (38%)	19,38,41	1.35	3 (15%)
1	5MC	Aa	457	1	18,22,23	4.90	15 (83%)	26,32,35	1.12	1 (3%)
27	OMC	BA	2124	27	19,22,23	2.58	7 (36%)	26,31,34	1.08	3 (11%)
1	OMU	Aa	479	1	19,22,23	2.97	8 (42%)	26,31,34	1.69	5 (19%)
1	OMG	Aa	532	1	18,26,27	2.14	7 (38%)	19,38,41	1.37	3 (15%)
27	A2M	BA	1517	27	18,25,26	3.93	7 (38%)	18,36,39	2.89	3 (16%)
1	4AC	Aa	358	1	21,24,25	3.25	9 (42%)	29,34,37	1.60	5 (17%)
27	4AC	BA	2992	27	21,24,25	3.32	10 (47%)	29,34,37	1.39	5 (17%)
1	B8T	Aa	1141	1	19,22,23	0.81	0	26,31,34	0.76	0
27	OMC	BA	2047	27	19,22,23	2.56	7 (36%)	26,31,34	1.06	1 (3%)
1	4AC	Aa	818	1	21,24,25	3.11	10 (47%)	29,34,37	1.57	5 (17%)
1	OMG	Aa	1025	1	18,26,27	2.17	7 (38%)	19,38,41	1.41	3 (15%)
27	4AC	BA	1543	27	21,24,25	3.12	9 (42%)	29,34,37	1.21	4 (13%)
27	5MU	BA	1548	27	19,22,23	4.67	7 (36%)	28,32,35	3.64	10 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	OMU	BA	453	27	19,22,23	2.72	7 (36%)	26,31,34	1.82	5 (19%)
27	4AC	BA	858	27	21,24,25	2.97	10 (47%)	29,34,37	1.65	2 (6%)
27	OMG	BA	1953	27	18,26,27	2.21	7 (38%)	19,38,41	1.73	4 (21%)
27	OMC	BA	1820	27	19,22,23	2.58	7 (36%)	26,31,34	1.29	5 (19%)
27	5MU	BA	1085	27	19,22,23	4.18	7 (36%)	28,32,35	4.37	11 (39%)
1	4AC	Aa	373	1	21,24,25	3.15	9 (42%)	29,34,37	1.45	6 (20%)
1	OMG	Aa	1107	1	18,26,27	2.30	8 (44%)	19,38,41	1.43	4 (21%)
27	OMG	BA	674	27	18,26,27	1.85	6 (33%)	19,38,41	1.69	7 (36%)
27	4AC	BA	2159	27	21,24,25	2.98	10 (47%)	29,34,37	1.32	5 (17%)
27	OMC	BA	2571	27	19,22,23	2.66	7 (36%)	26,31,34	1.28	4 (15%)
1	B8T	Aa	1262	1	19,22,23	0.78	0	26,31,34	0.93	1 (3%)
27	OMU	BA	2656	27	19,22,23	2.65	7 (36%)	26,31,34	1.67	4 (15%)
1	OMU	Aa	304	1	19,22,23	2.87	7 (36%)	26,31,34	1.71	4 (15%)
1	OMG	Aa	852	1	18,26,27	2.09	5 (27%)	19,38,41	1.32	3 (15%)
27	OMG	BA	800	27	18,26,27	1.97	6 (33%)	19,38,41	1.25	4 (21%)
27	4AC	BA	1810	27	21,24,25	3.05	10 (47%)	29,34,37	1.44	5 (17%)
27	A2M	BA	849	27	18,25,26	4.04	8 (44%)	18,36,39	3.29	6 (33%)
27	A2M	BA	879	27	18,25,26	4.12	7 (38%)	18,36,39	2.95	4 (22%)
27	A2M	BA	1265	27	18,25,26	4.19	6 (33%)	18,36,39	3.27	4 (22%)
27	OMU	BA	1340	27	19,22,23	2.65	7 (36%)	26,31,34	1.71	5 (19%)
27	OMG	BA	1525	27	18,26,27	2.23	7 (38%)	19,38,41	1.64	4 (21%)
27	4AC	BA	1305	27	21,24,25	3.31	10 (47%)	29,34,37	1.55	6 (20%)
1	LHH	Aa	229	1	22,25,26	2.50	5 (22%)	29,35,38	1.70	6 (20%)
1	OMU	Aa	1358	1	19,22,23	2.52	7 (36%)	26,31,34	2.31	8 (30%)
27	4AC	BA	1337	27	21,24,25	3.01	10 (47%)	29,34,37	1.18	3 (10%)
27	4AC	BA	1470	27	21,24,25	3.05	9 (42%)	29,34,37	1.55	6 (20%)
27	5MU	BA	875	27	19,22,23	4.58	7 (36%)	28,32,35	3.71	11 (39%)
1	OMG	Aa	1275	1	18,26,27	1.04	1 (5%)	19,38,41	1.08	2 (10%)
1	4AC	Aa	1007	1	21,24,25	1.07	1 (4%)	29,34,37	1.16	4 (13%)
1	4AC	Aa	697	1	21,24,25	3.24	9 (42%)	29,34,37	1.64	6 (20%)
27	OMG	BA	723	27	18,26,27	2.18	8 (44%)	19,38,41	1.82	4 (21%)
27	OMG	BA	2016	27	18,26,27	2.23	6 (33%)	19,38,41	1.59	4 (21%)
27	OMU	BA	1319	27	19,22,23	2.75	7 (36%)	26,31,34	1.70	5 (19%)
1	OMC	Aa	1354	1	19,22,23	2.75	7 (36%)	26,31,34	1.03	2 (7%)
27	OMG	BA	419	27	18,26,27	2.17	5 (27%)	19,38,41	3.64	6 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	OMG	BA	2568	27	18,26,27	1.01	1 (5%)	19,38,41	1.06	2 (10%)
27	4AC	BA	1431	27	21,24,25	3.15	10 (47%)	29,34,37	1.41	6 (20%)
1	OMC	Aa	190	1	19,22,23	2.74	7 (36%)	26,31,34	0.89	0
27	A2M	BA	825	27	18,25,26	4.12	9 (50%)	18,36,39	2.85	3 (16%)
27	OMG	BA	2379	27	18,26,27	2.14	5 (27%)	19,38,41	1.82	4 (21%)
1	5MC	Aa	854	1	18,22,23	2.93	7 (38%)	26,32,35	1.46	5 (19%)
27	4AC	BA	201	27	21,24,25	2.89	10 (47%)	29,34,37	1.65	6 (20%)
27	A2M	BA	932	27	18,25,26	4.18	8 (44%)	18,36,39	2.67	4 (22%)
1	5MC	Aa	1476	1	18,22,23	4.81	15 (83%)	26,32,35	1.20	2 (7%)
27	A2M	BA	212	27	18,25,26	0.89	1 (5%)	18,36,39	1.44	3 (16%)
27	4AC	BA	1396	27	21,24,25	3.07	10 (47%)	29,34,37	1.45	6 (20%)
27	OMG	BA	1940	27	18,26,27	2.05	6 (33%)	19,38,41	1.26	3 (15%)
27	OMC	BA	2018	27	19,22,23	2.36	7 (36%)	26,31,34	1.07	3 (11%)
27	OMG	BA	1799	27	18,26,27	2.33	8 (44%)	19,38,41	1.64	5 (26%)
27	5MC	BA	2035	27	18,22,23	4.78	15 (83%)	26,32,35	1.19	2 (7%)
27	4AC	BA	2997	27	21,24,25	3.17	9 (42%)	29,34,37	1.22	3 (10%)
1	OMU	Aa	8	1	19,22,23	2.73	7 (36%)	26,31,34	1.85	8 (30%)
27	OMG	BA	2528	27	18,26,27	2.31	6 (33%)	19,38,41	1.97	5 (26%)
1	OMC	Aa	535	1	19,22,23	2.71	7 (36%)	26,31,34	0.93	0
27	OMG	BA	2657	27	18,26,27	2.18	7 (38%)	19,38,41	1.49	3 (15%)
1	OMG	Aa	659	1	18,26,27	2.19	8 (44%)	19,38,41	1.35	4 (21%)
27	OMG	BA	353	27	18,26,27	2.44	8 (44%)	19,38,41	1.90	5 (26%)
27	4AC	BA	778	27	21,24,25	3.14	10 (47%)	29,34,37	1.04	2 (6%)
1	5MC	Aa	942	1	18,22,23	3.37	7 (38%)	26,32,35	1.04	2 (7%)
27	OMG	BA	575	27	18,26,27	2.15	7 (38%)	19,38,41	1.42	4 (21%)
27	4AC	BA	1375	27	21,24,25	3.10	10 (47%)	29,34,37	1.32	4 (13%)
1	OMG	Aa	913	1	18,26,27	2.40	8 (44%)	19,38,41	2.05	6 (31%)
27	OMG	BA	2010	27	18,26,27	2.13	6 (33%)	19,38,41	1.40	3 (15%)
27	OMC	BA	1790	27	19,22,23	2.51	7 (36%)	26,31,34	1.12	1 (3%)
27	OMG	BA	1558	27	18,26,27	2.13	7 (38%)	19,38,41	1.54	6 (31%)
27	4AC	BA	3009	27	21,24,25	3.09	10 (47%)	29,34,37	1.22	3 (10%)
27	5MC	BA	2070	27	18,22,23	0.95	2 (11%)	26,32,35	1.20	3 (11%)
1	OMG	Aa	446	1	18,26,27	2.20	7 (38%)	19,38,41	1.40	4 (21%)
1	OMC	Aa	752	1	19,22,23	2.69	7 (36%)	26,31,34	0.98	1 (3%)
27	OMG	BA	63	27	18,26,27	2.13	5 (27%)	19,38,41	1.74	5 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	4AC	BA	501	27	21,24,25	3.05	9 (42%)	29,34,37	1.32	3 (10%)
1	OMG	Aa	382	1	18,26,27	2.18	7 (38%)	19,38,41	1.44	3 (15%)
27	4AC	BA	2590	27	21,24,25	3.04	10 (47%)	29,34,37	1.20	5 (17%)
27	5MU	BA	1905	27	19,22,23	4.46	7 (36%)	28,32,35	3.81	11 (39%)
27	4AC	BA	2832	27	21,24,25	3.03	10 (47%)	29,34,37	1.29	4 (13%)
27	OMU	BA	1969	27	19,22,23	2.75	7 (36%)	26,31,34	1.73	5 (19%)
1	OMG	Aa	381	1	18,26,27	2.22	8 (44%)	19,38,41	1.44	4 (21%)
27	OMU	BA	768	27	19,22,23	2.74	7 (36%)	26,31,34	1.74	4 (15%)
27	OMG	BA	2521	27	18,26,27	2.18	7 (38%)	19,38,41	1.55	3 (15%)
1	4AC	Aa	501	1	21,24,25	3.24	9 (42%)	29,34,37	1.51	5 (17%)
27	OMU	BA	1480	27	19,22,23	2.72	7 (36%)	26,31,34	1.59	4 (15%)
27	4AC	BA	1934	27	21,24,25	2.98	9 (42%)	29,34,37	1.31	4 (13%)
27	4AC	BA	1427	27	21,24,25	2.99	9 (42%)	29,34,37	1.27	4 (13%)
27	A2M	BA	505	27	18,25,26	4.08	8 (44%)	18,36,39	3.44	6 (33%)
27	5MC	BA	2605	27	18,22,23	3.26	7 (38%)	26,32,35	0.90	1 (3%)
27	4AC	BA	2121	27	21,24,25	2.90	10 (47%)	29,34,37	1.33	4 (13%)
1	4AC	Aa	605	1	21,24,25	3.30	9 (42%)	29,34,37	1.91	7 (24%)

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
27	OMG	BA	1106	27	-	0/5/27/28	0/3/3/3
1	OMC	Aa	825	1	-	0/9/27/28	0/2/2/2
27	OMU	BA	34	27	-	1/9/27/28	0/2/2/2
27	4AC	BA	335	27	-	0/11/29/30	0/2/2/2
1	OMG	Aa	1026	1	-	1/5/27/28	0/3/3/3
27	B8T	BA	357	27	-	0/7/27/28	0/2/2/2
27	4AC	BA	730	27	-	0/11/29/30	0/2/2/2
27	5MC	BA	2055	27	-	2/7/25/26	0/2/2/2
1	OMG	Aa	771	1	-	0/5/27/28	0/3/3/3
27	4AC	BA	27	27	-	2/11/29/30	0/2/2/2
27	OMC	BA	250	27	-	0/9/27/28	0/2/2/2
27	4AC	BA	3023	27	-	2/11/29/30	0/2/2/2
1	4AC	Aa	827	1	-	0/11/29/30	0/2/2/2
1	4AC	Aa	41	1	-	2/11/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	A2M	BA	488	27	-	3/5/27/28	0/3/3/3
1	4AC	Aa	5	1	-	4/11/29/30	0/2/2/2
27	OMC	BA	2545	27	-	1/9/27/28	0/2/2/2
1	4AC	Aa	1459	1	-	0/11/29/30	0/2/2/2
27	OMG	BA	833	27	-	0/5/27/28	0/3/3/3
27	5MU	BA	2384	27	-	0/7/25/26	0/2/2/2
27	A2M	BA	872	27	-	0/5/27/28	0/3/3/3
27	4AC	BA	799	27	-	0/11/29/30	0/2/2/2
27	OMG	BA	2672	27	-	0/5/27/28	0/3/3/3
1	5MC	Aa	1352	1	-	2/7/25/26	0/2/2/2
27	OMC	BA	754	27	-	2/9/27/28	0/2/2/2
1	OMG	Aa	636	1	-	2/5/27/28	0/3/3/3
1	4AC	Aa	136	1	-	2/11/29/30	0/2/2/2
1	OMC	Aa	1361	27,1	-	0/9/27/28	0/2/2/2
27	4AC	BA	1641	27	-	2/11/29/30	0/2/2/2
27	5MC	BA	2075	27	-	0/7/25/26	0/2/2/2
27	OMC	BA	2630	27	-	0/9/27/28	0/2/2/2
1	OMG	Aa	994	1	-	1/5/27/28	0/3/3/3
27	5MU	BA	298	27	-	0/7/25/26	0/2/2/2
27	OMC	BA	561	27	-	0/9/27/28	0/2/2/2
27	5MC	BA	1696	27	-	0/7/25/26	0/2/2/2
1	4AC	Aa	458	1	-	6/11/29/30	0/2/2/2
27	OMG	BA	2168	27	-	0/5/27/28	0/3/3/3
27	OMU	BA	657	27	-	1/9/27/28	0/2/2/2
27	4AC	BA	1955	27	-	2/11/29/30	0/2/2/2
27	4AC	BA	376	27	-	0/11/29/30	0/2/2/2
27	OMG	BA	2152	27	-	2/5/27/28	0/3/3/3
27	4AC	BA	1434	27	-	2/11/29/30	0/2/2/2
27	OMG	BA	365	27	-	1/5/27/28	0/3/3/3
27	OMG	BA	1892	27	-	1/5/27/28	0/3/3/3
27	5MC	BA	1965	27	-	0/7/25/26	0/2/2/2
27	OMU	BA	1776	27	-	0/9/27/28	0/2/2/2
27	5MU	BA	572	27	-	0/7/25/26	0/2/2/2
27	OMC	BA	718	27	-	0/9/27/28	0/2/2/2
1	LV2	Aa	918	1	-	0/9/29/30	0/2/2/2
1	5MC	Aa	1478	1	-	3/7/25/26	0/2/2/2
1	4AC	Aa	298	1	-	0/11/29/30	0/2/2/2
27	OMU	BA	1551	27	-	3/9/27/28	0/2/2/2
27	OMU	BA	2389	27	-	2/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LHH	BA	2955	27	-	3/13/31/32	0/2/2/2
27	A2M	BA	2702	27	-	1/5/27/28	0/3/3/3
27	5MU	BA	2688	27	-	0/7/25/26	0/2/2/2
1	OMG	Aa	246	1	-	0/5/27/28	0/3/3/3
1	OMU	Aa	52	1	-	2/9/27/28	0/2/2/2
27	A2M	BA	756	27	-	0/5/27/28	0/3/3/3
1	OMU	Aa	240	1	-	0/9/27/28	0/2/2/2
1	6MZ	Aa	1449	1	-	0/5/27/28	0/3/3/3
27	4AC	BA	925	27	-	2/11/29/30	0/2/2/2
1	4AC	Aa	569	1	-	0/11/29/30	0/2/2/2
27	5MU	BA	537	27	-	0/7/25/26	0/2/2/2
1	4AC	Aa	525	1	-	5/11/29/30	0/2/2/2
1	4AC	Aa	847	1	-	0/11/29/30	0/2/2/2
27	5MC	BA	944	27	-	0/7/25/26	0/2/2/2
27	OMU	BA	2542	27	-	0/9/27/28	0/2/2/2
1	4AC	Aa	682	1	-	0/11/29/30	0/2/2/2
27	OMG	BA	763	27	-	0/5/27/28	0/3/3/3
1	OMG	Aa	1434	1	-	1/5/27/28	0/3/3/3
27	OMG	BA	290	27	-	0/5/27/28	0/3/3/3
27	LHH	BA	526	27	-	1/13/31/32	0/2/2/2
27	A2M	BA	1400	27	-	1/5/27/28	0/3/3/3
27	OMC	BA	1750	27	-	0/9/27/28	0/2/2/2
27	OMU	BA	2610	27	-	3/9/27/28	0/2/2/2
1	5MC	Aa	1276	1	-	2/7/25/26	0/2/2/2
27	OMG	BA	64	27	-	2/5/27/28	0/3/3/3
27	OMG	BA	2745	27	-	0/5/27/28	0/3/3/3
27	OMU	BA	619	27	-	1/9/27/28	0/2/2/2
1	LHH	Aa	1020	1	-	4/13/31/32	0/2/2/2
27	OMC	BA	869	27	-	2/9/27/28	0/2/2/2
1	5MC	Aa	464	1	-	0/7/25/26	0/2/2/2
1	OMG	Aa	876	1	-	2/5/27/28	0/3/3/3
27	OMG	BA	215	27	-	2/5/27/28	0/3/3/3
1	4AC	Aa	730	1	-	2/11/29/30	0/2/2/2
27	LHH	BA	617	27	-	5/13/31/32	0/2/2/2
27	4AC	BA	1357	27	-	0/11/29/30	0/2/2/2
27	4AC	BA	805	27	-	0/11/29/30	0/2/2/2
1	5MU	Aa	917	1	-	2/7/25/26	0/2/2/2
27	OMG	BA	2728	27	-	0/5/27/28	0/3/3/3
1	5MC	Aa	672	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	Aa	450	1	-	0/5/27/28	0/3/3/3
27	4AC	BA	418	27	-	0/11/29/30	0/2/2/2
27	4AC	BA	2780	27	-	0/11/29/30	0/2/2/2
1	B8T	Aa	1051	1	-	0/7/27/28	0/2/2/2
1	MA6	Aa	1468	1	-	2/7/29/30	0/3/3/3
27	OMG	BA	2019	27	-	2/5/27/28	0/3/3/3
1	MA6	Aa	1467	1	-	0/7/29/30	0/3/3/3
1	OMG	Aa	1265	1	-	0/5/27/28	0/3/3/3
1	5MC	Aa	1004	1	-	2/7/25/26	0/2/2/2
1	OMG	Aa	138	1	-	0/5/27/28	0/3/3/3
27	LHH	BA	2457	27	-	4/13/31/32	0/2/2/2
27	OMG	BA	1398	27	-	0/5/27/28	0/3/3/3
1	OMG	Aa	498	1	-	0/5/27/28	0/3/3/3
27	4AC	BA	713	27	-	0/11/29/30	0/2/2/2
27	4SU	BA	2553	27	-	0/7/25/26	0/2/2/2
27	4SU	BA	2581	27	-	2/7/25/26	0/2/2/2
27	OMG	BA	2324	27	-	0/5/27/28	0/3/3/3
27	4AC	BA	2797	27	-	0/11/29/30	0/2/2/2
1	OMC	Aa	296	1	-	0/9/27/28	0/2/2/2
1	OMG	Aa	320	1	-	0/5/27/28	0/3/3/3
27	4AC	BA	433	27	-	0/11/29/30	0/2/2/2
1	4AC	Aa	1217	1	-	4/11/29/30	0/2/2/2
27	OMC	BA	2595	27	-	2/9/27/28	0/2/2/2
1	A2M	Aa	352	1	-	1/5/27/28	0/3/3/3
27	4AC	BA	244	27	-	1/11/29/30	0/2/2/2
27	OMG	BA	2550	27	-	2/5/27/28	0/3/3/3
1	2MG	Aa	670	1	-	0/5/27/28	0/3/3/3
27	OMG	BA	2353	27	-	2/5/27/28	0/3/3/3
27	OMG	BA	2527	27	-	2/5/27/28	0/3/3/3
27	4AC	BA	1899	27	-	0/11/29/30	0/2/2/2
27	4AC	BA	2838	27	-	2/11/29/30	0/2/2/2
27	5MC	BA	2863	27	-	0/7/25/26	0/2/2/2
27	OMG	BA	912	27	-	0/5/27/28	0/3/3/3
27	4AC	BA	124	27	-	0/11/29/30	0/2/2/2
27	OMG	BA	552	27	-	0/5/27/28	0/3/3/3
27	4AC	BA	56	27	-	0/11/29/30	0/2/2/2
1	OMG	Aa	892	1	-	3/5/27/28	0/3/3/3
1	5MC	Aa	457	1	-	2/7/25/26	0/2/2/2
27	OMC	BA	2124	27	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMU	Aa	479	1	-	1/9/27/28	0/2/2/2
1	OMG	Aa	532	1	-	2/5/27/28	0/3/3/3
27	A2M	BA	1517	27	-	1/5/27/28	0/3/3/3
1	4AC	Aa	358	1	-	2/11/29/30	0/2/2/2
27	4AC	BA	2992	27	-	3/11/29/30	0/2/2/2
1	B8T	Aa	1141	1	-	0/7/27/28	0/2/2/2
27	OMC	BA	2047	27	-	0/9/27/28	0/2/2/2
1	4AC	Aa	818	1	-	2/11/29/30	0/2/2/2
1	OMG	Aa	1025	1	-	1/5/27/28	0/3/3/3
27	4AC	BA	1543	27	-	3/11/29/30	0/2/2/2
27	5MU	BA	1548	27	-	2/7/25/26	0/2/2/2
27	OMU	BA	453	27	-	2/9/27/28	0/2/2/2
27	4AC	BA	858	27	-	2/11/29/30	0/2/2/2
27	OMG	BA	1953	27	-	2/5/27/28	0/3/3/3
27	OMC	BA	1820	27	-	0/9/27/28	0/2/2/2
27	5MU	BA	1085	27	-	0/7/25/26	0/2/2/2
1	4AC	Aa	373	1	-	0/11/29/30	0/2/2/2
1	OMG	Aa	1107	1	-	3/5/27/28	0/3/3/3
27	OMG	BA	674	27	-	0/5/27/28	0/3/3/3
27	4AC	BA	2159	27	-	0/11/29/30	0/2/2/2
27	OMC	BA	2571	27	-	2/9/27/28	0/2/2/2
1	B8T	Aa	1262	1	-	0/7/27/28	0/2/2/2
27	OMU	BA	2656	27	-	0/9/27/28	0/2/2/2
1	OMU	Aa	304	1	-	1/9/27/28	0/2/2/2
1	OMG	Aa	852	1	-	0/5/27/28	0/3/3/3
27	OMG	BA	800	27	-	0/5/27/28	0/3/3/3
27	4AC	BA	1810	27	-	2/11/29/30	0/2/2/2
27	A2M	BA	849	27	-	2/5/27/28	0/3/3/3
27	A2M	BA	879	27	-	0/5/27/28	0/3/3/3
27	A2M	BA	1265	27	-	2/5/27/28	0/3/3/3
27	OMU	BA	1340	27	-	0/9/27/28	0/2/2/2
27	OMG	BA	1525	27	-	2/5/27/28	0/3/3/3
27	4AC	BA	1305	27	-	2/11/29/30	0/2/2/2
1	LHH	Aa	229	1	-	3/13/31/32	0/2/2/2
1	OMU	Aa	1358	1	-	3/9/27/28	0/2/2/2
27	4AC	BA	1337	27	-	2/11/29/30	0/2/2/2
27	4AC	BA	1470	27	-	0/11/29/30	0/2/2/2
27	5MU	BA	875	27	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	Aa	1275	1	-	1/5/27/28	0/3/3/3
1	4AC	Aa	1007	1	-	2/11/29/30	0/2/2/2
1	4AC	Aa	697	1	-	4/11/29/30	0/2/2/2
27	OMG	BA	723	27	-	1/5/27/28	0/3/3/3
27	OMG	BA	2016	27	-	0/5/27/28	0/3/3/3
27	OMU	BA	1319	27	-	0/9/27/28	0/2/2/2
1	OMC	Aa	1354	1	-	2/9/27/28	0/2/2/2
27	OMG	BA	419	27	-	2/5/27/28	0/3/3/3
27	OMG	BA	2568	27	-	3/5/27/28	0/3/3/3
27	4AC	BA	1431	27	-	0/11/29/30	0/2/2/2
1	OMC	Aa	190	1	-	2/9/27/28	0/2/2/2
27	A2M	BA	825	27	-	0/5/27/28	0/3/3/3
27	OMG	BA	2379	27	-	3/5/27/28	0/3/3/3
1	5MC	Aa	854	1	-	1/7/25/26	0/2/2/2
27	4AC	BA	201	27	-	2/11/29/30	0/2/2/2
27	A2M	BA	932	27	-	0/5/27/28	0/3/3/3
1	5MC	Aa	1476	1	-	0/7/25/26	0/2/2/2
27	A2M	BA	212	27	-	1/5/27/28	0/3/3/3
27	4AC	BA	1396	27	-	2/11/29/30	0/2/2/2
27	OMG	BA	1940	27	-	2/5/27/28	0/3/3/3
27	OMC	BA	2018	27	-	2/9/27/28	0/2/2/2
27	OMG	BA	1799	27	-	3/5/27/28	0/3/3/3
27	5MC	BA	2035	27	-	0/7/25/26	0/2/2/2
27	4AC	BA	2997	27	-	0/11/29/30	0/2/2/2
1	OMU	Aa	8	1	-	3/9/27/28	0/2/2/2
27	OMG	BA	2528	27	-	0/5/27/28	0/3/3/3
1	OMC	Aa	535	1	-	0/9/27/28	0/2/2/2
27	OMG	BA	2657	27	-	0/5/27/28	0/3/3/3
1	OMG	Aa	659	1	-	0/5/27/28	0/3/3/3
27	OMG	BA	353	27	-	2/5/27/28	0/3/3/3
27	4AC	BA	778	27	-	0/11/29/30	0/2/2/2
1	5MC	Aa	942	1	-	0/7/25/26	0/2/2/2
27	OMG	BA	575	27	-	2/5/27/28	0/3/3/3
27	4AC	BA	1375	27	-	2/11/29/30	0/2/2/2
1	OMG	Aa	913	1	-	2/5/27/28	0/3/3/3
27	OMG	BA	2010	27	-	0/5/27/28	0/3/3/3
27	OMC	BA	1790	27	-	2/9/27/28	0/2/2/2
27	OMG	BA	1558	27	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	4AC	BA	3009	27	-	2/11/29/30	0/2/2/2
27	5MC	BA	2070	27	-	0/7/25/26	0/2/2/2
1	OMG	Aa	446	1	-	2/5/27/28	0/3/3/3
1	OMC	Aa	752	1	-	0/9/27/28	0/2/2/2
27	OMG	BA	63	27	-	0/5/27/28	0/3/3/3
27	4AC	BA	501	27	-	0/11/29/30	0/2/2/2
1	OMG	Aa	382	1	-	2/5/27/28	0/3/3/3
27	4AC	BA	2590	27	-	0/11/29/30	0/2/2/2
27	5MU	BA	1905	27	-	0/7/25/26	0/2/2/2
27	4AC	BA	2832	27	-	1/11/29/30	0/2/2/2
27	OMU	BA	1969	27	-	0/9/27/28	0/2/2/2
1	OMG	Aa	381	1	-	0/5/27/28	0/3/3/3
27	OMU	BA	768	27	-	0/9/27/28	0/2/2/2
27	OMG	BA	2521	27	-	0/5/27/28	0/3/3/3
1	4AC	Aa	501	1	-	0/11/29/30	0/2/2/2
27	OMU	BA	1480	27	-	2/9/27/28	0/2/2/2
27	4AC	BA	1934	27	-	0/11/29/30	0/2/2/2
27	4AC	BA	1427	27	-	0/11/29/30	0/2/2/2
27	A2M	BA	505	27	-	2/5/27/28	0/3/3/3
27	5MC	BA	2605	27	-	0/7/25/26	0/2/2/2
27	4AC	BA	2121	27	-	0/11/29/30	0/2/2/2
1	4AC	Aa	605	1	-	1/11/29/30	0/2/2/2

All (1672) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	1265	A2M	O4'-C1'	14.99	1.62	1.41
27	BA	756	A2M	O4'-C1'	14.76	1.61	1.41
27	BA	932	A2M	O4'-C1'	14.62	1.61	1.41
27	BA	872	A2M	O4'-C1'	14.38	1.61	1.41
27	BA	879	A2M	O4'-C1'	14.34	1.61	1.41
27	BA	849	A2M	O4'-C1'	14.21	1.60	1.41
27	BA	825	A2M	O4'-C1'	14.09	1.60	1.41
27	BA	505	A2M	O4'-C1'	13.96	1.60	1.41
27	BA	488	A2M	O4'-C1'	13.84	1.60	1.41
27	BA	2702	A2M	O4'-C1'	13.72	1.60	1.41
27	BA	1400	A2M	O4'-C1'	13.59	1.60	1.41
27	BA	1517	A2M	O4'-C1'	13.45	1.59	1.41
1	Aa	1476	5MC	C2'-C3'	-10.81	1.23	1.53
1	Aa	1276	5MC	C2'-C3'	-10.79	1.23	1.53
27	BA	1548	5MU	C2-N1	10.67	1.55	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	298	5MU	C2-N1	10.58	1.55	1.38
27	BA	1548	5MU	C6-N1	10.54	1.56	1.38
27	BA	875	5MU	C2-N1	10.51	1.55	1.38
1	Aa	457	5MC	C2'-C3'	-10.49	1.24	1.53
27	BA	2035	5MC	C2'-C3'	-10.37	1.24	1.53
27	BA	537	5MU	C2-N1	10.31	1.55	1.38
27	BA	572	5MU	C2-N1	10.22	1.54	1.38
27	BA	2688	5MU	C2-N1	10.20	1.54	1.38
27	BA	1085	5MU	C2-N1	10.18	1.54	1.38
27	BA	1905	5MU	C2-N1	10.11	1.54	1.38
27	BA	2384	5MU	C2-N1	10.10	1.54	1.38
27	BA	875	5MU	C6-N1	10.05	1.55	1.38
27	BA	2384	5MU	C6-N1	9.92	1.55	1.38
27	BA	2384	5MU	C4-C5	9.52	1.60	1.44
27	BA	298	5MU	C6-N1	9.42	1.54	1.38
27	BA	572	5MU	C6-N1	9.39	1.54	1.38
27	BA	1905	5MU	C6-N1	9.37	1.54	1.38
27	BA	2688	5MU	C6-N1	9.25	1.53	1.38
27	BA	537	5MU	C6-N1	9.25	1.53	1.38
1	Aa	457	5MC	C6-C5	9.12	1.49	1.34
27	BA	1548	5MU	C4-C5	9.00	1.59	1.44
27	BA	2035	5MC	C6-C5	8.90	1.49	1.34
1	Aa	1276	5MC	C6-C5	8.80	1.49	1.34
1	Aa	1020	LHH	O2-C2	8.79	1.40	1.23
27	BA	537	5MU	C4-C5	8.77	1.59	1.44
27	BA	2688	5MU	C4-C5	8.74	1.59	1.44
1	Aa	1476	5MC	C6-C5	8.63	1.48	1.34
27	BA	1905	5MU	C4-C5	8.58	1.59	1.44
27	BA	572	5MU	C4-C5	8.57	1.59	1.44
1	Aa	1352	5MC	C6-C5	8.55	1.48	1.34
27	BA	526	LHH	O2-C2	8.54	1.39	1.23
27	BA	617	LHH	O2-C2	8.53	1.39	1.23
27	BA	2581	4SU	C4-N3	8.53	1.46	1.37
27	BA	2955	LHH	O2-C2	8.53	1.39	1.23
1	Aa	229	LHH	O2-C2	8.53	1.39	1.23
27	BA	875	5MU	C4-C5	8.52	1.58	1.44
27	BA	2457	LHH	O2-C2	8.48	1.39	1.23
1	Aa	942	5MC	C6-C5	8.46	1.48	1.34
27	BA	2055	5MC	C6-C5	8.43	1.48	1.34
27	BA	298	5MU	C4-C5	8.39	1.58	1.44
27	BA	2605	5MC	C6-C5	8.28	1.48	1.34
27	BA	2581	4SU	C2-N1	8.27	1.51	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	875	5MU	C4-N3	-8.26	1.23	1.38
27	BA	2553	4SU	C2-N1	8.25	1.51	1.38
1	Aa	464	5MC	C6-C5	8.22	1.48	1.34
27	BA	1085	5MU	C6-N1	8.13	1.51	1.38
27	BA	2688	5MU	C4-N3	-8.08	1.23	1.38
27	BA	1905	5MU	C4-N3	-8.07	1.23	1.38
27	BA	2384	5MU	C4-N3	-8.01	1.24	1.38
27	BA	572	5MU	C4-N3	-8.00	1.24	1.38
27	BA	537	5MU	C4-N3	-7.93	1.24	1.38
27	BA	1085	5MU	C4-C5	7.89	1.57	1.44
1	Aa	672	5MC	C6-C5	7.81	1.47	1.34
27	BA	1085	5MU	C4-N3	-7.80	1.24	1.38
27	BA	298	5MU	C4-N3	-7.80	1.24	1.38
1	Aa	1004	5MC	C6-C5	7.74	1.47	1.34
1	Aa	1217	4AC	C4-N3	7.57	1.46	1.32
27	BA	2863	5MC	C6-C5	7.55	1.47	1.34
27	BA	2553	4SU	C4-N3	7.48	1.45	1.37
27	BA	1548	5MU	C4-N3	-7.48	1.25	1.38
1	Aa	1478	5MC	C6-C5	7.46	1.46	1.34
27	BA	2610	OMU	C2-N1	7.39	1.50	1.38
27	BA	1400	A2M	O4'-C4'	-7.31	1.28	1.45
27	BA	2992	4AC	C4-N3	7.22	1.45	1.32
27	BA	1696	5MC	C6-C5	7.17	1.46	1.34
27	BA	1305	4AC	C4-N3	7.13	1.45	1.32
27	BA	1551	OMU	C2-N1	7.11	1.49	1.38
1	Aa	358	4AC	C4-N3	7.11	1.45	1.32
1	Aa	605	4AC	C4-N3	7.07	1.45	1.32
1	Aa	697	4AC	C4-N3	7.07	1.45	1.32
1	Aa	682	4AC	C4-N3	7.07	1.45	1.32
27	BA	2702	A2M	O4'-C4'	-7.06	1.29	1.45
1	Aa	136	4AC	C4-N3	7.06	1.45	1.32
1	Aa	501	4AC	C4-N3	7.05	1.45	1.32
27	BA	505	A2M	O4'-C4'	-7.04	1.29	1.45
27	BA	825	A2M	O4'-C4'	-7.04	1.29	1.45
27	BA	1431	4AC	C4-N3	7.03	1.45	1.32
1	Aa	479	OMU	C2-N3	6.98	1.50	1.38
27	BA	2997	4AC	C4-N3	6.96	1.44	1.32
27	BA	418	4AC	C4-N3	6.94	1.44	1.32
1	Aa	298	4AC	C4-N3	6.94	1.44	1.32
27	BA	730	4AC	C4-N3	6.93	1.44	1.32
27	BA	2838	4AC	C4-N3	6.92	1.44	1.32
1	Aa	479	OMU	C2-N1	6.92	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	3023	4AC	C4-N3	6.92	1.44	1.32
1	Aa	41	4AC	C4-N3	6.90	1.44	1.32
27	BA	778	4AC	C4-N3	6.88	1.44	1.32
27	BA	488	A2M	O4'-C4'	-6.88	1.29	1.45
1	Aa	847	4AC	C4-N3	6.86	1.44	1.32
27	BA	27	4AC	C4-N3	6.84	1.44	1.32
27	BA	1337	4AC	C4-N3	6.84	1.44	1.32
1	Aa	818	4AC	C4-N3	6.84	1.44	1.32
27	BA	872	A2M	O4'-C4'	-6.83	1.29	1.45
27	BA	1934	4AC	C4-N3	6.83	1.44	1.32
27	BA	1375	4AC	C4-N3	6.81	1.44	1.32
1	Aa	373	4AC	C4-N3	6.80	1.44	1.32
27	BA	56	4AC	C4-N3	6.80	1.44	1.32
27	BA	433	4AC	C4-N3	6.80	1.44	1.32
27	BA	858	4AC	C4-N3	6.80	1.44	1.32
27	BA	1517	A2M	O4'-C4'	-6.79	1.29	1.45
27	BA	944	5MC	C6-C5	6.79	1.45	1.34
27	BA	1810	4AC	C4-N3	6.79	1.44	1.32
1	Aa	240	OMU	C2-N1	6.79	1.49	1.38
1	Aa	5	4AC	C4-N3	6.78	1.44	1.32
1	Aa	827	4AC	C4-N3	6.77	1.44	1.32
27	BA	2075	5MC	C6-C5	6.77	1.45	1.34
27	BA	1396	4AC	C4-N3	6.75	1.44	1.32
27	BA	2159	4AC	C4-N3	6.74	1.44	1.32
27	BA	2832	4AC	C4-N3	6.74	1.44	1.32
1	Aa	569	4AC	C4-N3	6.73	1.44	1.32
27	BA	932	A2M	O4'-C4'	-6.73	1.30	1.45
27	BA	1543	4AC	C4-N3	6.72	1.44	1.32
27	BA	376	4AC	C4-N3	6.72	1.44	1.32
27	BA	1357	4AC	C4-N3	6.72	1.44	1.32
27	BA	3009	4AC	C4-N3	6.71	1.44	1.32
27	BA	2780	4AC	C4-N3	6.71	1.44	1.32
27	BA	335	4AC	C4-N3	6.69	1.44	1.32
27	BA	501	4AC	C4-N3	6.69	1.44	1.32
1	Aa	854	5MC	C6-C5	6.69	1.45	1.34
1	Aa	304	OMU	C2-N1	6.68	1.49	1.38
27	BA	2610	OMU	C2-N3	6.67	1.49	1.38
27	BA	1899	4AC	C4-N3	6.67	1.44	1.32
27	BA	1641	4AC	C4-N3	6.66	1.44	1.32
27	BA	244	4AC	C4-N3	6.66	1.44	1.32
27	BA	756	A2M	O4'-C4'	-6.64	1.30	1.45
27	BA	619	OMU	C2-N1	6.63	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Aa	730	4AC	C4-N3	6.61	1.44	1.32
1	Aa	52	OMU	C2-N1	6.60	1.49	1.38
27	BA	799	4AC	C4-N3	6.58	1.44	1.32
27	BA	1470	4AC	C4-N3	6.55	1.44	1.32
27	BA	879	A2M	O4'-C4'	-6.54	1.30	1.45
27	BA	1965	5MC	C6-C5	6.54	1.45	1.34
27	BA	2581	4SU	C2-N3	6.48	1.49	1.38
1	Aa	1352	5MC	C4-N3	6.48	1.45	1.34
27	BA	2590	4AC	C4-N3	6.48	1.44	1.32
27	BA	1265	A2M	O4'-C4'	-6.48	1.30	1.45
27	BA	849	A2M	O4'-C4'	-6.48	1.30	1.45
1	Aa	304	OMU	C2-N3	6.45	1.49	1.38
27	BA	1969	OMU	C2-N1	6.45	1.48	1.38
1	Aa	525	4AC	C4-N3	6.45	1.44	1.32
27	BA	1427	4AC	C4-N3	6.43	1.44	1.32
27	BA	1776	OMU	C2-N1	6.43	1.48	1.38
27	BA	768	OMU	C2-N1	6.42	1.48	1.38
27	BA	2121	4AC	C4-N3	6.40	1.43	1.32
27	BA	1319	OMU	C2-N1	6.40	1.48	1.38
1	Aa	240	OMU	C2-N3	6.39	1.49	1.38
27	BA	2797	4AC	C4-N3	6.39	1.43	1.32
1	Aa	457	5MC	C4-N3	6.38	1.44	1.34
27	BA	713	4AC	C4-N3	6.38	1.43	1.32
27	BA	1319	OMU	C2-N3	6.36	1.49	1.38
1	Aa	8	OMU	C2-N1	6.35	1.48	1.38
27	BA	1955	4AC	C4-N3	6.31	1.43	1.32
27	BA	1551	OMU	C2-N3	6.29	1.49	1.38
1	Aa	1004	5MC	C4-N3	6.29	1.44	1.34
27	BA	2553	4SU	C2-N3	6.29	1.49	1.38
1	Aa	1476	5MC	C4-N3	6.27	1.44	1.34
1	Aa	41	4AC	C6-C5	6.25	1.49	1.35
27	BA	619	OMU	C2-N3	6.25	1.49	1.38
27	BA	453	OMU	C2-N1	6.25	1.48	1.38
1	Aa	1276	5MC	C4-N3	6.24	1.44	1.34
1	Aa	52	OMU	C2-N3	6.24	1.49	1.38
27	BA	1434	4AC	C4-N3	6.23	1.43	1.32
1	Aa	942	5MC	C4-N3	6.22	1.44	1.34
1	Aa	136	4AC	C6-C5	6.22	1.49	1.35
27	BA	805	4AC	C4-N3	6.22	1.43	1.32
27	BA	201	4AC	C4-N3	6.22	1.43	1.32
1	Aa	847	4AC	C6-C5	6.21	1.49	1.35
27	BA	2992	4AC	C6-C5	6.21	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	2605	5MC	C4-N3	6.21	1.44	1.34
1	Aa	464	5MC	C4-N3	6.20	1.44	1.34
1	Aa	358	4AC	C6-C5	6.19	1.49	1.35
27	BA	2542	OMU	C2-N1	6.15	1.48	1.38
27	BA	2035	5MC	C4-N3	6.15	1.44	1.34
27	BA	657	OMU	C2-N1	6.14	1.48	1.38
27	BA	1480	OMU	C2-N1	6.13	1.48	1.38
27	BA	1305	4AC	C6-C5	6.12	1.49	1.35
1	Aa	1217	4AC	C6-C5	6.09	1.49	1.35
27	BA	768	OMU	C2-N3	6.09	1.48	1.38
1	Aa	818	4AC	C6-C5	6.09	1.49	1.35
27	BA	1340	OMU	C2-N1	6.09	1.48	1.38
27	BA	2863	5MC	C4-N3	6.08	1.44	1.34
1	Aa	1354	OMC	C2-N3	6.06	1.48	1.36
27	BA	2997	4AC	C6-C5	6.06	1.49	1.35
1	Aa	5	4AC	C6-C5	6.06	1.49	1.35
27	BA	1969	OMU	C2-N3	6.05	1.48	1.38
1	Aa	457	5MC	C2-N3	6.04	1.48	1.36
27	BA	3009	4AC	C6-C5	6.04	1.49	1.35
27	BA	869	OMC	C2-N3	6.04	1.48	1.36
27	BA	418	4AC	C6-C5	6.00	1.49	1.35
1	Aa	535	OMC	C2-N3	5.98	1.48	1.36
27	BA	124	4AC	C4-N3	5.97	1.43	1.32
27	BA	2542	OMU	C2-N3	5.96	1.48	1.38
1	Aa	464	5MC	C2-N3	5.96	1.48	1.36
1	Aa	1352	5MC	C2-N3	5.96	1.48	1.36
1	Aa	8	OMU	C2-N3	5.94	1.48	1.38
27	BA	2656	OMU	C2-N3	5.94	1.48	1.38
1	Aa	827	4AC	C6-C5	5.93	1.48	1.35
27	BA	2581	4SU	C5-C4	5.93	1.50	1.42
27	BA	1696	5MC	C4-N3	5.93	1.44	1.34
27	BA	2553	4SU	C6-C5	5.92	1.48	1.35
27	BA	453	OMU	C2-N3	5.92	1.48	1.38
1	Aa	501	4AC	C6-C5	5.92	1.48	1.35
1	Aa	697	4AC	C6-C5	5.91	1.48	1.35
1	Aa	682	4AC	C6-C5	5.90	1.48	1.35
27	BA	2035	5MC	C2-N3	5.90	1.48	1.36
1	Aa	373	4AC	C6-C5	5.90	1.48	1.35
1	Aa	569	4AC	C6-C5	5.89	1.48	1.35
27	BA	1480	OMU	C2-N3	5.89	1.48	1.38
27	BA	56	4AC	C6-C5	5.88	1.48	1.35
1	Aa	942	5MC	C2-N3	5.88	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Aa	605	4AC	C7-N4	5.87	1.48	1.37
1	Aa	1476	5MC	C2-N3	5.86	1.48	1.36
27	BA	2581	4SU	C6-C5	5.85	1.48	1.35
27	BA	2656	OMU	C2-N1	5.84	1.47	1.38
1	Aa	1276	5MC	C2-N3	5.84	1.48	1.36
1	Aa	752	OMC	C2-N3	5.83	1.48	1.36
27	BA	1641	4AC	C6-C5	5.82	1.48	1.35
1	Aa	854	5MC	C4-N3	5.81	1.44	1.34
1	Aa	730	4AC	C6-C5	5.81	1.48	1.35
27	BA	1820	OMC	C2-N3	5.80	1.48	1.36
27	BA	730	4AC	C6-C5	5.80	1.48	1.35
1	Aa	1459	4AC	C4-N3	5.79	1.42	1.32
1	Aa	190	OMC	C2-N3	5.79	1.48	1.36
27	BA	1375	4AC	C6-C5	5.78	1.48	1.35
27	BA	2055	5MC	C4-N3	5.77	1.43	1.34
27	BA	353	OMG	C2-N3	5.77	1.47	1.33
27	BA	754	OMC	C2-N3	5.77	1.48	1.36
1	Aa	1004	5MC	C2-N3	5.76	1.48	1.36
27	BA	501	4AC	C6-C5	5.75	1.48	1.35
27	BA	3023	4AC	C6-C5	5.74	1.48	1.35
1	Aa	672	5MC	C4-N3	5.74	1.43	1.34
1	Aa	605	4AC	C6-C5	5.74	1.48	1.35
27	BA	250	OMC	C2-N3	5.73	1.48	1.36
27	BA	1396	4AC	C7-N4	5.72	1.47	1.37
1	Aa	136	4AC	C7-N4	5.72	1.47	1.37
1	Aa	298	4AC	C7-N4	5.71	1.47	1.37
27	BA	335	4AC	C6-C5	5.71	1.48	1.35
27	BA	2590	4AC	C6-C5	5.71	1.48	1.35
27	BA	1340	OMU	C2-N3	5.70	1.48	1.38
27	BA	713	4AC	C6-C5	5.70	1.48	1.35
27	BA	2528	OMG	C2-N3	5.69	1.47	1.33
27	BA	1776	OMU	C2-N3	5.69	1.48	1.38
27	BA	34	OMU	C2-N1	5.69	1.47	1.38
27	BA	1431	4AC	C7-N4	5.68	1.47	1.37
27	BA	2553	4SU	C5-C4	5.68	1.49	1.42
27	BA	718	OMC	C2-N3	5.67	1.47	1.36
1	Aa	697	4AC	C7-N4	5.66	1.47	1.37
1	Aa	825	OMC	C2-N3	5.65	1.47	1.36
1	Aa	1361	OMC	C2-N3	5.65	1.47	1.36
27	BA	27	4AC	C6-C5	5.64	1.48	1.35
27	BA	778	4AC	C6-C5	5.64	1.48	1.35
27	BA	858	4AC	C6-C5	5.64	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	2832	4AC	C6-C5	5.64	1.48	1.35
27	BA	1470	4AC	C6-C5	5.63	1.48	1.35
27	BA	2838	4AC	C6-C5	5.61	1.48	1.35
27	BA	1305	4AC	C7-N4	5.61	1.47	1.37
27	BA	1750	OMC	C2-N3	5.60	1.47	1.36
1	Aa	41	4AC	C7-N4	5.59	1.47	1.37
27	BA	1543	4AC	C6-C5	5.59	1.48	1.35
27	BA	2075	5MC	C4-N3	5.59	1.43	1.34
27	BA	2610	OMU	C6-C5	5.58	1.48	1.35
27	BA	2780	4AC	C7-N4	5.58	1.47	1.37
1	Aa	358	4AC	C7-N4	5.58	1.47	1.37
1	Aa	525	4AC	C6-C5	5.57	1.48	1.35
1	Aa	1217	4AC	C7-N4	5.57	1.47	1.37
1	Aa	854	5MC	C2-N3	5.56	1.47	1.36
27	BA	1337	4AC	C6-C5	5.56	1.48	1.35
27	BA	418	4AC	C7-N4	5.55	1.47	1.37
27	BA	657	OMU	C2-N3	5.54	1.47	1.38
1	Aa	298	4AC	C6-C5	5.54	1.47	1.35
27	BA	2838	4AC	C7-N4	5.54	1.47	1.37
27	BA	1548	5MU	C6-C5	5.53	1.43	1.34
27	BA	2780	4AC	C6-C5	5.53	1.47	1.35
27	BA	34	OMU	C2-N3	5.53	1.47	1.38
1	Aa	569	4AC	C7-N4	5.52	1.47	1.37
27	BA	1543	4AC	C7-N4	5.51	1.47	1.37
1	Aa	994	OMG	C2-N3	5.50	1.46	1.33
1	Aa	1358	OMU	C2-N1	5.50	1.47	1.38
1	Aa	827	4AC	C7-N4	5.48	1.47	1.37
27	BA	1427	4AC	C6-C5	5.48	1.47	1.35
1	Aa	913	OMG	C2-N3	5.48	1.46	1.33
27	BA	3023	4AC	C7-N4	5.47	1.47	1.37
27	BA	2384	5MU	C6-C5	5.47	1.43	1.34
27	BA	27	4AC	C7-N4	5.47	1.47	1.37
1	Aa	296	OMC	C2-N3	5.46	1.47	1.36
27	BA	1357	4AC	C6-C5	5.46	1.47	1.35
27	BA	2992	4AC	C7-N4	5.46	1.47	1.37
27	BA	561	OMC	C2-N3	5.46	1.47	1.36
1	Aa	190	OMC	C6-C5	5.46	1.47	1.35
1	Aa	636	OMG	C2-N3	5.44	1.46	1.33
1	Aa	501	4AC	C7-N4	5.43	1.47	1.37
27	BA	2545	OMC	C2-N3	5.43	1.47	1.36
27	BA	1551	OMU	C6-C5	5.43	1.47	1.35
27	BA	201	4AC	C6-C5	5.41	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Aa	672	5MC	C2-N3	5.41	1.47	1.36
27	BA	2124	OMC	C2-N3	5.41	1.47	1.36
1	Aa	682	4AC	C7-N4	5.40	1.47	1.37
27	BA	2630	OMC	C2-N3	5.40	1.47	1.36
27	BA	2797	4AC	C6-C5	5.40	1.47	1.35
27	BA	2457	LHH	C7-N4	5.39	1.47	1.37
27	BA	2159	4AC	C6-C5	5.38	1.47	1.35
27	BA	376	4AC	C6-C5	5.37	1.47	1.35
27	BA	805	4AC	C7-N4	5.37	1.47	1.37
27	BA	1434	4AC	C6-C5	5.36	1.47	1.35
27	BA	2019	OMG	C2-N3	5.35	1.46	1.33
27	BA	2055	5MC	C2-N3	5.35	1.47	1.36
27	BA	2571	OMC	C2-N3	5.34	1.47	1.36
1	Aa	752	OMC	C6-C5	5.34	1.47	1.35
1	Aa	1217	4AC	C2-N3	5.34	1.47	1.36
27	BA	244	4AC	C6-C5	5.34	1.47	1.35
27	BA	1790	OMC	C2-N3	5.31	1.47	1.36
27	BA	2863	5MC	C2-N3	5.31	1.47	1.36
1	Aa	1478	5MC	C4-N3	5.30	1.43	1.34
1	Aa	876	OMG	C2-N3	5.30	1.46	1.33
27	BA	1955	4AC	C6-C5	5.30	1.47	1.35
27	BA	1375	4AC	C7-N4	5.30	1.47	1.37
27	BA	2595	OMC	C2-N3	5.29	1.47	1.36
1	Aa	1361	OMC	C6-C5	5.29	1.47	1.35
27	BA	1810	4AC	C6-C5	5.29	1.47	1.35
1	Aa	1358	OMU	C2-N3	5.29	1.47	1.38
27	BA	730	4AC	C7-N4	5.29	1.47	1.37
1	Aa	240	OMU	C6-C5	5.28	1.47	1.35
1	Aa	535	OMC	C6-C5	5.28	1.47	1.35
1	Aa	373	4AC	C7-N4	5.27	1.47	1.37
27	BA	124	4AC	C7-N4	5.27	1.46	1.37
27	BA	1810	4AC	C7-N4	5.26	1.46	1.37
1	Aa	296	OMC	C6-C5	5.26	1.47	1.35
1	Aa	1478	5MC	C2-N3	5.26	1.47	1.36
27	BA	215	OMG	C2-N3	5.26	1.46	1.33
27	BA	124	4AC	C6-C5	5.26	1.47	1.35
27	BA	335	4AC	C7-N4	5.26	1.46	1.37
27	BA	799	4AC	C6-C5	5.25	1.47	1.35
27	BA	1396	4AC	C6-C5	5.25	1.47	1.35
27	BA	2121	4AC	C6-C5	5.23	1.47	1.35
27	BA	1431	4AC	C6-C5	5.22	1.47	1.35
27	BA	2571	OMC	C6-C5	5.22	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	1899	4AC	C6-C5	5.22	1.47	1.35
1	Aa	818	4AC	C7-N4	5.21	1.46	1.37
27	BA	778	4AC	C7-N4	5.21	1.46	1.37
27	BA	1965	5MC	C4-N3	5.20	1.42	1.34
27	BA	799	4AC	C7-N4	5.20	1.46	1.37
27	BA	1899	4AC	C7-N4	5.19	1.46	1.37
27	BA	2018	OMC	C2-N3	5.19	1.46	1.36
1	Aa	479	OMU	C6-C5	5.18	1.47	1.35
27	BA	1696	5MC	C2-N3	5.18	1.46	1.36
1	Aa	1217	4AC	C4-N4	5.18	1.47	1.39
27	BA	433	4AC	C7-N4	5.18	1.46	1.37
27	BA	1470	4AC	C7-N4	5.17	1.46	1.37
27	BA	2159	4AC	C7-N4	5.17	1.46	1.37
27	BA	2075	5MC	C2-N3	5.17	1.46	1.36
1	Aa	1107	OMG	C2-N3	5.17	1.45	1.33
27	BA	944	5MC	C2-N3	5.16	1.46	1.36
1	Aa	320	OMG	C2-N3	5.16	1.45	1.33
1	Aa	304	OMU	C6-C5	5.16	1.47	1.35
1	Aa	138	OMG	C2-N3	5.16	1.45	1.33
27	BA	201	4AC	C7-N4	5.15	1.46	1.37
27	BA	3009	4AC	C7-N4	5.14	1.46	1.37
27	BA	244	4AC	C7-N4	5.14	1.46	1.37
27	BA	2521	OMG	C2-N3	5.14	1.45	1.33
27	BA	2047	OMC	C6-C5	5.13	1.47	1.35
27	BA	2797	4AC	C7-N4	5.13	1.46	1.37
1	Aa	825	OMC	C6-C5	5.13	1.47	1.35
27	BA	713	4AC	C7-N4	5.12	1.46	1.37
27	BA	1641	4AC	C7-N4	5.11	1.46	1.37
1	Aa	1354	OMC	C6-C5	5.11	1.46	1.35
1	Aa	52	OMU	C6-C5	5.10	1.46	1.35
27	BA	944	5MC	C4-N3	5.10	1.42	1.34
27	BA	1357	4AC	C7-N4	5.10	1.46	1.37
1	Aa	1265	OMG	C2-N3	5.08	1.45	1.33
1	Aa	8	OMU	C6-C5	5.08	1.46	1.35
27	BA	1427	4AC	C7-N4	5.07	1.46	1.37
27	BA	1434	4AC	C7-N4	5.07	1.46	1.37
27	BA	2016	OMG	C2-N3	5.07	1.45	1.33
1	Aa	771	OMG	C2-N3	5.06	1.45	1.33
27	BA	2605	5MC	C2-N3	5.06	1.46	1.36
27	BA	2832	4AC	C7-N4	5.05	1.46	1.37
27	BA	754	OMC	C6-C5	5.05	1.46	1.35
27	BA	2590	4AC	C7-N4	5.05	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Aa	730	4AC	C7-N4	5.04	1.46	1.37
27	BA	619	OMU	C6-C5	5.04	1.46	1.35
1	Aa	1026	OMG	C2-N3	5.04	1.45	1.33
27	BA	2047	OMC	C2-N3	5.04	1.46	1.36
27	BA	63	OMG	C2-N3	5.02	1.45	1.33
1	Aa	605	4AC	C2-N3	5.02	1.46	1.36
27	BA	2997	4AC	C7-N4	5.02	1.46	1.37
27	BA	250	OMC	C6-C5	5.01	1.46	1.35
27	BA	2780	4AC	C2-N1	5.00	1.50	1.40
27	BA	1953	OMG	C2-N3	5.00	1.45	1.33
27	BA	376	4AC	C7-N4	4.99	1.46	1.37
27	BA	2545	OMC	C6-C5	4.99	1.46	1.35
1	Aa	5	4AC	C7-N4	4.99	1.46	1.37
27	BA	1934	4AC	C6-C5	4.99	1.46	1.35
27	BA	2992	4AC	C2-N3	4.97	1.46	1.36
27	BA	912	OMG	C2-N3	4.97	1.45	1.33
1	Aa	498	OMG	C2-N3	4.97	1.45	1.33
27	BA	501	4AC	C7-N4	4.97	1.46	1.37
27	BA	1934	4AC	C7-N4	4.97	1.46	1.37
27	BA	833	OMG	C2-N3	4.97	1.45	1.33
27	BA	1305	4AC	C2-N3	4.96	1.46	1.36
1	Aa	670	2MG	C2-N2	4.96	1.44	1.33
27	BA	433	4AC	C6-C5	4.94	1.46	1.35
27	BA	2780	4AC	C2-N3	4.93	1.46	1.36
27	BA	3023	4AC	C2-N3	4.92	1.46	1.36
27	BA	754	OMC	C4-N3	4.92	1.44	1.34
1	Aa	41	4AC	C2-N1	4.92	1.50	1.40
1	Aa	381	OMG	C2-N3	4.92	1.45	1.33
27	BA	1480	OMU	C6-C5	4.91	1.46	1.35
27	BA	353	OMG	C4-N3	4.91	1.49	1.37
27	BA	561	OMC	C6-C5	4.91	1.46	1.35
27	BA	526	LHH	C7-N4	4.91	1.46	1.37
27	BA	2657	OMG	C2-N3	4.90	1.45	1.33
1	Aa	136	4AC	C2-N3	4.90	1.46	1.36
27	BA	1892	OMG	C2-N3	4.90	1.45	1.33
27	BA	1543	4AC	C2-N3	4.89	1.46	1.36
27	BA	730	4AC	C2-N1	4.89	1.50	1.40
27	BA	2992	4AC	C2-N1	4.89	1.50	1.40
1	Aa	525	4AC	C7-N4	4.89	1.46	1.37
1	Aa	373	4AC	C2-N3	4.89	1.46	1.36
1	Aa	682	4AC	C2-N3	4.89	1.46	1.36
27	BA	2838	4AC	C2-N3	4.89	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Aa	1020	LHH	C7-N4	4.89	1.46	1.37
27	BA	2595	OMC	C6-C5	4.89	1.46	1.35
1	Aa	136	4AC	C2-N1	4.89	1.50	1.40
1	Aa	382	OMG	C2-N3	4.88	1.45	1.33
27	BA	1969	OMU	C6-C5	4.88	1.46	1.35
1	Aa	446	OMG	C2-N3	4.88	1.45	1.33
1	Aa	450	OMG	C2-N3	4.88	1.45	1.33
27	BA	718	OMC	C4-N3	4.87	1.44	1.34
27	BA	2728	OMG	C2-N3	4.87	1.45	1.33
1	Aa	298	4AC	C2-N3	4.87	1.46	1.36
1	Aa	1217	4AC	C2-N1	4.87	1.50	1.40
27	BA	1965	5MC	C2-N3	4.86	1.46	1.36
27	BA	1750	OMC	C6-C5	4.86	1.46	1.35
27	BA	778	4AC	C2-N1	4.86	1.50	1.40
1	Aa	659	OMG	C2-N3	4.86	1.45	1.33
27	BA	1337	4AC	C7-N4	4.85	1.46	1.37
27	BA	1641	4AC	C2-N1	4.85	1.50	1.40
27	BA	56	4AC	C7-N4	4.85	1.46	1.37
27	BA	1810	4AC	C2-N3	4.85	1.46	1.36
1	Aa	827	4AC	C2-N3	4.85	1.46	1.36
27	BA	2324	OMG	C2-N3	4.84	1.45	1.33
27	BA	453	OMU	C6-C5	4.84	1.46	1.35
27	BA	2019	OMG	C4-N3	4.84	1.49	1.37
27	BA	2124	OMC	C6-C5	4.84	1.46	1.35
27	BA	2997	4AC	C2-N3	4.84	1.46	1.36
1	Aa	246	OMG	C2-N3	4.83	1.44	1.33
27	BA	2838	4AC	C2-N1	4.83	1.50	1.40
27	BA	718	OMC	C6-C5	4.83	1.46	1.35
1	Aa	358	4AC	C2-N3	4.82	1.46	1.36
1	Aa	373	4AC	C2-N1	4.82	1.50	1.40
27	BA	376	4AC	C2-N3	4.82	1.46	1.36
27	BA	335	4AC	C2-N1	4.82	1.50	1.40
1	Aa	1025	OMG	C2-N3	4.81	1.44	1.33
27	BA	1799	OMG	C2-N3	4.81	1.44	1.33
27	BA	250	OMC	C4-N3	4.81	1.44	1.34
27	BA	2672	OMG	C2-N3	4.80	1.44	1.33
27	BA	1955	4AC	C7-N4	4.80	1.46	1.37
27	BA	2379	OMG	C2-N3	4.79	1.44	1.33
27	BA	290	OMG	C2-N3	4.79	1.44	1.33
27	BA	869	OMC	C4-N3	4.79	1.44	1.34
1	Aa	605	4AC	C2-N1	4.78	1.50	1.40
27	BA	56	4AC	C2-N3	4.78	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Aa	682	4AC	C2-N1	4.78	1.50	1.40
27	BA	2353	OMG	C2-N3	4.78	1.44	1.33
1	Aa	1354	OMC	C4-N3	4.78	1.44	1.34
27	BA	27	4AC	C2-N3	4.78	1.46	1.36
27	BA	2528	OMG	C4-N3	4.77	1.48	1.37
1	Aa	994	OMG	C4-N3	4.77	1.48	1.37
27	BA	1398	OMG	C2-N3	4.77	1.44	1.33
27	BA	805	4AC	C6-C5	4.76	1.46	1.35
27	BA	869	OMC	C6-C5	4.75	1.46	1.35
27	BA	1799	OMG	C6-N1	4.75	1.44	1.37
1	Aa	501	4AC	C2-N1	4.75	1.50	1.40
27	BA	617	LHH	C7-N4	4.74	1.46	1.37
27	BA	298	5MU	C6-C5	4.74	1.42	1.34
1	Aa	569	4AC	C2-N3	4.74	1.46	1.36
27	BA	572	5MU	C6-C5	4.74	1.42	1.34
1	Aa	892	OMG	C2-N3	4.74	1.44	1.33
27	BA	2688	5MU	C6-C5	4.73	1.42	1.34
1	Aa	1434	OMG	C2-N3	4.73	1.44	1.33
27	BA	34	OMU	C6-C5	4.73	1.46	1.35
27	BA	27	4AC	C2-N1	4.73	1.50	1.40
1	Aa	697	4AC	C2-N1	4.72	1.50	1.40
27	BA	1525	OMG	C2-N3	4.72	1.44	1.33
27	BA	1790	OMC	C6-C5	4.72	1.46	1.35
1	Aa	229	LHH	C7-N4	4.72	1.45	1.37
27	BA	2010	OMG	C2-N3	4.71	1.44	1.33
1	Aa	697	4AC	C2-N3	4.71	1.45	1.36
27	BA	1106	OMG	C2-N3	4.70	1.44	1.33
1	Aa	605	4AC	C4-N4	4.70	1.46	1.39
27	BA	418	4AC	C2-N3	4.70	1.45	1.36
27	BA	433	4AC	C2-N3	4.70	1.45	1.36
1	Aa	501	4AC	C2-N3	4.69	1.45	1.36
27	BA	1396	4AC	C2-N3	4.69	1.45	1.36
1	Aa	913	OMG	C4-N3	4.68	1.48	1.37
27	BA	2550	OMG	C2-N3	4.68	1.44	1.33
1	Aa	535	OMC	C4-N3	4.68	1.43	1.34
27	BA	2527	OMG	C2-N3	4.68	1.44	1.33
1	Aa	670	2MG	C4-N3	4.68	1.48	1.37
27	BA	713	4AC	C2-N3	4.67	1.45	1.36
1	Aa	525	4AC	C2-N1	4.67	1.50	1.40
27	BA	1431	4AC	C2-N1	4.67	1.50	1.40
1	Aa	5	4AC	C2-N3	4.67	1.45	1.36
1	Aa	1459	4AC	C6-C5	4.66	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Aa	847	4AC	C7-N4	4.66	1.45	1.37
1	Aa	752	OMC	C4-N3	4.66	1.43	1.34
27	BA	1305	4AC	C4-N4	4.66	1.46	1.39
27	BA	433	4AC	C2-N1	4.65	1.50	1.40
27	BA	2745	OMG	C2-N3	4.65	1.44	1.33
1	Aa	525	4AC	C2-N3	4.65	1.45	1.36
27	BA	1776	OMU	C6-C5	4.65	1.45	1.35
27	BA	1431	4AC	C2-N3	4.65	1.45	1.36
27	BA	1810	4AC	C2-N1	4.64	1.50	1.40
27	BA	723	OMG	C2-N3	4.64	1.44	1.33
1	Aa	852	OMG	C2-N3	4.64	1.44	1.33
27	BA	1375	4AC	C2-N3	4.63	1.45	1.36
27	BA	1470	4AC	C2-N1	4.63	1.50	1.40
1	Aa	532	OMG	C2-N3	4.63	1.44	1.33
27	BA	2553	4SU	C4-S4	-4.62	1.59	1.68
27	BA	2630	OMC	C6-C5	4.62	1.45	1.35
27	BA	335	4AC	C2-N3	4.62	1.45	1.36
27	BA	1934	4AC	C2-N3	4.62	1.45	1.36
27	BA	768	OMU	C6-C5	4.62	1.45	1.35
27	BA	418	4AC	C2-N1	4.61	1.50	1.40
1	Aa	1217	4AC	CM7-C7	4.61	1.60	1.50
27	BA	3009	4AC	C2-N1	4.61	1.50	1.40
1	Aa	298	4AC	C2-N1	4.61	1.50	1.40
27	BA	2595	OMC	C2-N1	4.61	1.50	1.40
27	BA	858	4AC	C2-N3	4.61	1.45	1.36
27	BA	537	5MU	C6-C5	4.60	1.42	1.34
1	Aa	190	OMC	C4-N3	4.60	1.43	1.34
27	BA	376	4AC	C2-N1	4.60	1.50	1.40
1	Aa	457	5MC	C6-N1	4.60	1.45	1.38
1	Aa	358	4AC	C2-N1	4.60	1.50	1.40
27	BA	2997	4AC	C2-N1	4.59	1.50	1.40
27	BA	2121	4AC	C7-N4	4.59	1.45	1.37
27	BA	1340	OMU	C6-C5	4.59	1.45	1.35
27	BA	875	5MU	C6-C5	4.59	1.42	1.34
27	BA	1396	4AC	C2-N1	4.59	1.49	1.40
27	BA	1319	OMU	C6-C5	4.59	1.45	1.35
27	BA	799	4AC	C2-N3	4.59	1.45	1.36
1	Aa	818	4AC	C2-N3	4.58	1.45	1.36
1	Aa	457	5MC	O4'-C1'	-4.58	1.31	1.42
27	BA	244	4AC	C2-N3	4.58	1.45	1.36
1	Aa	41	4AC	C2-N3	4.57	1.45	1.36
27	BA	778	4AC	C2-N3	4.57	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	3009	4AC	C2-N3	4.57	1.45	1.36
27	BA	1357	4AC	C2-N1	4.57	1.49	1.40
27	BA	1820	OMC	C4-N3	4.56	1.43	1.34
27	BA	3023	4AC	C2-N1	4.56	1.49	1.40
27	BA	552	OMG	C2-N3	4.56	1.44	1.33
27	BA	1337	4AC	C2-N3	4.56	1.45	1.36
1	Aa	136	4AC	C4-N4	4.56	1.46	1.39
1	Aa	818	4AC	C2-N1	4.55	1.49	1.40
1	Aa	697	4AC	C4-N4	4.55	1.46	1.39
1	Aa	825	OMC	C4-N3	4.55	1.43	1.34
27	BA	730	4AC	C2-N3	4.55	1.45	1.36
27	BA	713	4AC	C2-N1	4.55	1.49	1.40
1	Aa	5	4AC	C2-N1	4.55	1.49	1.40
27	BA	1427	4AC	C2-N1	4.55	1.49	1.40
27	BA	1470	4AC	C2-N3	4.54	1.45	1.36
1	Aa	1107	OMG	C4-N3	4.54	1.48	1.37
27	BA	2016	OMG	C4-N3	4.54	1.48	1.37
1	Aa	636	OMG	C4-N3	4.53	1.48	1.37
27	BA	2832	4AC	C2-N3	4.53	1.45	1.36
1	Aa	847	4AC	C2-N1	4.53	1.49	1.40
1	Aa	569	4AC	C2-N1	4.52	1.49	1.40
27	BA	2992	4AC	C4-N4	4.52	1.46	1.39
1	Aa	847	4AC	C2-N3	4.52	1.45	1.36
27	BA	1934	4AC	C2-N1	4.51	1.49	1.40
27	BA	1525	OMG	C4-N3	4.51	1.48	1.37
27	BA	63	OMG	C4-N3	4.51	1.48	1.37
27	BA	2955	LHH	C7-N4	4.51	1.45	1.37
27	BA	501	4AC	C2-N3	4.51	1.45	1.36
1	Aa	1476	5MC	O4'-C1'	-4.50	1.31	1.42
27	BA	1790	OMC	C4-N3	4.50	1.43	1.34
27	BA	1899	4AC	C2-N1	4.50	1.49	1.40
1	Aa	876	OMG	C4-N3	4.50	1.48	1.37
27	BA	365	OMG	C2-N3	4.50	1.44	1.33
27	BA	2571	OMC	C4-N3	4.49	1.43	1.34
27	BA	1641	4AC	C2-N3	4.48	1.45	1.36
27	BA	1899	4AC	C2-N3	4.48	1.45	1.36
27	BA	1305	4AC	C2-N1	4.48	1.49	1.40
1	Aa	730	4AC	C2-N3	4.48	1.45	1.36
27	BA	2035	5MC	O4'-C1'	-4.47	1.31	1.42
1	Aa	138	OMG	C4-N3	4.47	1.48	1.37
1	Aa	1276	5MC	O4'-C1'	-4.47	1.31	1.42
27	BA	2159	4AC	C2-N3	4.47	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	56	4AC	C2-N1	4.46	1.49	1.40
27	BA	2542	OMU	C6-C5	4.46	1.45	1.35
27	BA	1905	5MU	C6-C5	4.46	1.41	1.34
27	BA	244	4AC	C2-N1	4.45	1.49	1.40
27	BA	501	4AC	C2-N1	4.45	1.49	1.40
27	BA	1940	OMG	C2-N3	4.45	1.44	1.33
27	BA	2521	OMG	C4-N3	4.44	1.48	1.37
1	Aa	827	4AC	C2-N1	4.43	1.49	1.40
1	Aa	1276	5MC	C6-N1	4.43	1.45	1.38
1	Aa	1358	OMU	C6-C5	4.43	1.45	1.35
27	BA	2656	OMU	C6-C5	4.43	1.45	1.35
1	Aa	320	OMG	C4-N3	4.43	1.48	1.37
1	Aa	1361	OMC	C4-N3	4.43	1.43	1.34
1	Aa	1265	OMG	C4-N3	4.43	1.48	1.37
27	BA	1427	4AC	C2-N3	4.42	1.45	1.36
27	BA	2168	OMG	C2-N3	4.42	1.43	1.33
27	BA	2124	OMC	C4-N3	4.42	1.43	1.34
27	BA	1375	4AC	C2-N1	4.42	1.49	1.40
27	BA	1357	4AC	C2-N3	4.41	1.45	1.36
1	Aa	190	OMC	C4-N4	4.41	1.44	1.33
1	Aa	682	4AC	C4-N4	4.41	1.46	1.39
1	Aa	730	4AC	C4-N4	4.41	1.46	1.39
1	Aa	1026	OMG	C4-N3	4.41	1.48	1.37
1	Aa	1476	5MC	C6-N1	4.40	1.45	1.38
27	BA	2590	4AC	C2-N1	4.39	1.49	1.40
27	BA	561	OMC	C4-N3	4.39	1.43	1.34
1	Aa	771	OMG	C4-N3	4.39	1.48	1.37
27	BA	250	OMC	C4-N4	4.39	1.44	1.33
27	BA	124	4AC	C2-N3	4.38	1.45	1.36
27	BA	2581	4SU	C4-S4	-4.38	1.60	1.68
27	BA	2571	OMC	C4-N4	4.38	1.44	1.33
27	BA	1543	4AC	C2-N1	4.38	1.49	1.40
27	BA	763	OMG	C2-N3	4.37	1.43	1.33
27	BA	2797	4AC	C2-N1	4.37	1.49	1.40
27	BA	2121	4AC	C2-N1	4.37	1.49	1.40
27	BA	1434	4AC	C2-N3	4.37	1.45	1.36
27	BA	858	4AC	C2-N1	4.36	1.49	1.40
27	BA	2832	4AC	C2-N1	4.36	1.49	1.40
27	BA	2018	OMC	C6-C5	4.35	1.45	1.35
27	BA	1750	OMC	C4-N3	4.35	1.43	1.34
27	BA	718	OMC	C2-N1	4.35	1.49	1.40
27	BA	2152	OMG	C2-N3	4.34	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Aa	296	OMC	C4-N3	4.34	1.43	1.34
1	Aa	41	4AC	C4-N4	4.33	1.46	1.39
27	BA	575	OMG	C2-N3	4.33	1.43	1.33
1	Aa	1354	OMC	C4-N4	4.33	1.44	1.33
27	BA	1953	OMG	C4-N3	4.33	1.47	1.37
27	BA	419	OMG	O6-C6	-4.33	1.14	1.23
1	Aa	381	OMG	C4-N3	4.33	1.47	1.37
27	BA	2035	5MC	C6-N1	4.32	1.45	1.38
27	BA	944	5MC	C6-N1	4.32	1.45	1.38
27	BA	657	OMU	C6-C5	4.32	1.45	1.35
1	Aa	1354	OMC	C2-N1	4.31	1.49	1.40
27	BA	723	OMG	C4-N3	4.31	1.47	1.37
27	BA	2121	4AC	C2-N3	4.31	1.45	1.36
27	BA	805	4AC	C2-N3	4.31	1.45	1.36
27	BA	2324	OMG	C4-N3	4.30	1.47	1.37
27	BA	2595	OMC	C4-N3	4.30	1.43	1.34
27	BA	2545	OMC	C4-N3	4.30	1.43	1.34
27	BA	858	4AC	C7-N4	4.30	1.45	1.37
27	BA	2672	OMG	C4-N3	4.30	1.47	1.37
27	BA	2630	OMC	C4-N3	4.30	1.43	1.34
27	BA	1820	OMC	C6-C5	4.29	1.45	1.35
27	BA	1337	4AC	C2-N1	4.29	1.49	1.40
1	Aa	501	4AC	CM7-C7	4.29	1.59	1.50
1	Aa	498	OMG	C4-N3	4.29	1.47	1.37
1	Aa	535	OMC	C4-N4	4.28	1.44	1.33
1	Aa	659	OMG	C4-N3	4.26	1.47	1.37
1	Aa	892	OMG	C4-N3	4.26	1.47	1.37
27	BA	800	OMG	C2-N3	4.26	1.43	1.33
27	BA	833	OMG	C4-N3	4.26	1.47	1.37
27	BA	763	OMG	C4-N3	4.25	1.47	1.37
27	BA	2379	OMG	C4-N3	4.25	1.47	1.37
27	BA	799	4AC	C2-N1	4.25	1.49	1.40
1	Aa	1276	5MC	C4-N4	4.25	1.45	1.34
1	Aa	5	4AC	C4-N4	4.25	1.45	1.39
27	BA	1375	4AC	CM7-C7	4.25	1.59	1.50
27	BA	2124	OMC	C2-N1	4.24	1.49	1.40
27	BA	2797	4AC	CM7-C7	4.24	1.59	1.50
27	BA	124	4AC	C2-N1	4.24	1.49	1.40
27	BA	2590	4AC	C2-N3	4.24	1.44	1.36
1	Aa	852	OMG	C4-N3	4.23	1.47	1.37
1	Aa	457	5MC	C4-N4	4.22	1.45	1.34
27	BA	2159	4AC	C2-N1	4.22	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Aa	1459	4AC	C2-N1	4.22	1.49	1.40
27	BA	2035	5MC	C2-N1	4.22	1.49	1.40
27	BA	201	4AC	C2-N3	4.21	1.44	1.36
27	BA	1955	4AC	C2-N3	4.21	1.44	1.36
1	Aa	1476	5MC	C4-N4	4.21	1.45	1.34
1	Aa	457	5MC	C2-N1	4.21	1.49	1.40
27	BA	1398	OMG	C4-N3	4.20	1.47	1.37
27	BA	805	4AC	C2-N1	4.20	1.49	1.40
1	Aa	501	4AC	C4-N4	4.19	1.45	1.39
27	BA	1434	4AC	C2-N1	4.19	1.49	1.40
1	Aa	1352	5MC	C2-N1	4.19	1.49	1.40
27	BA	2571	OMC	C2-N1	4.19	1.49	1.40
27	BA	250	OMC	C2-N1	4.19	1.49	1.40
1	Aa	457	5MC	C2'-C1'	4.19	1.66	1.53
1	Aa	450	OMG	C4-N3	4.18	1.47	1.37
1	Aa	827	4AC	CM7-C7	4.18	1.59	1.50
27	BA	2010	OMG	C4-N3	4.18	1.47	1.37
27	BA	2657	OMG	C4-N3	4.18	1.47	1.37
1	Aa	446	OMG	C4-N3	4.17	1.47	1.37
1	Aa	358	4AC	C4-N4	4.17	1.45	1.39
27	BA	1305	4AC	CM7-C7	4.17	1.59	1.50
27	BA	2047	OMC	C4-N3	4.16	1.42	1.34
27	BA	335	4AC	CM7-C7	4.16	1.59	1.50
1	Aa	752	OMC	C2-N1	4.15	1.49	1.40
1	Aa	730	4AC	C2-N1	4.15	1.49	1.40
27	BA	1955	4AC	CM7-C7	4.15	1.59	1.50
1	Aa	1020	LHH	C4-N4	4.15	1.45	1.39
27	BA	2728	OMG	C4-N3	4.14	1.47	1.37
27	BA	552	OMG	C4-N3	4.14	1.47	1.37
1	Aa	190	OMC	C2-N1	4.13	1.48	1.40
27	BA	2527	OMG	C4-N3	4.13	1.47	1.37
27	BA	2550	OMG	C4-N3	4.13	1.47	1.37
1	Aa	818	4AC	C4-N4	4.13	1.45	1.39
27	BA	1427	4AC	CM7-C7	4.13	1.59	1.50
27	BA	1558	OMG	C2-N3	4.13	1.43	1.33
1	Aa	296	OMC	C2-N1	4.12	1.48	1.40
1	Aa	605	4AC	CM7-C7	4.12	1.59	1.50
1	Aa	1478	5MC	C2-N1	4.12	1.48	1.40
1	Aa	1025	OMG	C4-N3	4.12	1.47	1.37
27	BA	418	4AC	CM7-C7	4.12	1.59	1.50
1	Aa	464	5MC	C2-N1	4.11	1.48	1.40
27	BA	1810	4AC	CM7-C7	4.11	1.59	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Aa	382	OMG	C4-N3	4.11	1.47	1.37
27	BA	2047	OMC	C4-N4	4.11	1.43	1.33
27	BA	290	OMG	C4-N3	4.11	1.47	1.37
27	BA	2797	4AC	C2-N3	4.11	1.44	1.36
1	Aa	825	OMC	C4-N4	4.10	1.43	1.33
1	Aa	942	5MC	C4-N4	4.10	1.44	1.34
1	Aa	752	OMC	C4-N4	4.10	1.43	1.33
27	BA	2605	5MC	C2-N1	4.10	1.48	1.40
27	BA	2035	5MC	C4-N4	4.09	1.44	1.34
27	BA	1940	OMG	C4-N3	4.09	1.47	1.37
27	BA	2832	4AC	CM7-C7	4.09	1.59	1.50
1	Aa	246	OMG	C4-N3	4.09	1.47	1.37
27	BA	2838	4AC	CM7-C7	4.09	1.59	1.50
27	BA	2590	4AC	CM7-C7	4.09	1.59	1.50
1	Aa	942	5MC	C6-N1	4.09	1.45	1.38
27	BA	730	4AC	CM7-C7	4.08	1.59	1.50
27	BA	1641	4AC	CM7-C7	4.08	1.59	1.50
27	BA	1892	OMG	C4-N3	4.08	1.47	1.37
27	BA	799	4AC	CM7-C7	4.08	1.59	1.50
27	BA	64	OMG	C2-N3	4.07	1.43	1.33
1	Aa	136	4AC	CM7-C7	4.07	1.59	1.50
27	BA	501	4AC	C4-N4	4.07	1.45	1.39
27	BA	778	4AC	CM7-C7	4.07	1.59	1.50
27	BA	754	OMC	C2-N1	4.07	1.48	1.40
27	BA	27	4AC	CM7-C7	4.07	1.59	1.50
27	BA	1820	OMC	C2-N1	4.06	1.48	1.40
27	BA	2997	4AC	CM7-C7	4.06	1.59	1.50
27	BA	419	OMG	C2-N3	4.05	1.43	1.33
27	BA	2047	OMC	C2-N1	4.05	1.48	1.40
27	BA	2152	OMG	C4-N3	4.05	1.47	1.37
1	Aa	296	OMC	C4-N4	4.05	1.43	1.33
27	BA	27	4AC	C4-N4	4.04	1.45	1.39
1	Aa	827	4AC	C4-N4	4.04	1.45	1.39
1	Aa	1459	4AC	C7-N4	4.04	1.44	1.37
27	BA	2035	5MC	C2'-C1'	4.04	1.66	1.53
1	Aa	1434	OMG	C4-N3	4.04	1.47	1.37
27	BA	2168	OMG	C4-N3	4.03	1.47	1.37
27	BA	617	LHH	C4-N4	4.03	1.45	1.39
27	BA	1543	4AC	CM7-C7	4.03	1.58	1.50
1	Aa	479	OMU	C4-N3	4.03	1.45	1.38
1	Aa	1276	5MC	C2'-C1'	4.03	1.66	1.53
27	BA	2353	OMG	C4-N3	4.03	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Aa	1459	4AC	C2-N3	4.03	1.44	1.36
27	BA	912	OMG	C4-N3	4.02	1.47	1.37
27	BA	713	4AC	CM7-C7	4.02	1.58	1.50
27	BA	1558	OMG	C4-N3	4.02	1.47	1.37
27	BA	1820	OMC	C4-N4	4.02	1.43	1.33
1	Aa	457	5MC	C5'-C4'	-4.02	1.39	1.51
27	BA	201	4AC	C2-N1	4.02	1.48	1.40
27	BA	2055	5MC	C6-N1	4.02	1.44	1.38
27	BA	3023	4AC	CM7-C7	4.01	1.58	1.50
1	Aa	464	5MC	C6-N1	4.01	1.44	1.38
27	BA	561	OMC	C4-N4	4.01	1.43	1.33
1	Aa	569	4AC	C4-N4	4.01	1.45	1.39
27	BA	778	4AC	C4-N4	4.00	1.45	1.39
1	Aa	1004	5MC	C4-N4	4.00	1.44	1.34
27	BA	1431	4AC	CM7-C7	4.00	1.58	1.50
27	BA	1431	4AC	C4-N4	4.00	1.45	1.39
1	Aa	1352	5MC	C4-N4	4.00	1.44	1.34
27	BA	1396	4AC	CM7-C7	4.00	1.58	1.50
27	BA	2992	4AC	CM7-C7	3.99	1.58	1.50
1	Aa	535	OMC	C2-N1	3.99	1.48	1.40
27	BA	718	OMC	C4-N4	3.99	1.43	1.33
1	Aa	373	4AC	C4-N4	3.99	1.45	1.39
27	BA	215	OMG	C4-N3	3.98	1.47	1.37
1	Aa	1276	5MC	C2-N1	3.98	1.48	1.40
27	BA	1337	4AC	CM7-C7	3.98	1.58	1.50
27	BA	433	4AC	CM7-C7	3.97	1.58	1.50
1	Aa	1276	5MC	C5'-C4'	-3.96	1.39	1.51
1	Aa	1352	5MC	C6-N1	3.96	1.44	1.38
27	BA	1955	4AC	C2-N1	3.96	1.48	1.40
27	BA	3009	4AC	CM7-C7	3.95	1.58	1.50
1	Aa	994	OMG	C2-N2	3.95	1.43	1.34
27	BA	869	OMC	C2-N1	3.95	1.48	1.40
27	BA	2630	OMC	C2-N1	3.95	1.48	1.40
27	BA	2121	4AC	CM7-C7	3.94	1.58	1.50
27	BA	858	4AC	CM7-C7	3.94	1.58	1.50
27	BA	1750	OMC	C2-N1	3.94	1.48	1.40
27	BA	56	4AC	CM7-C7	3.93	1.58	1.50
27	BA	2605	5MC	C6-N1	3.93	1.44	1.38
27	BA	754	OMC	C4-N4	3.93	1.43	1.33
27	BA	1790	OMC	C2-N1	3.93	1.48	1.40
1	Aa	229	LHH	C4-N4	3.92	1.45	1.39
27	BA	1934	4AC	CM7-C7	3.92	1.58	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	2745	OMG	C4-N3	3.92	1.46	1.37
1	Aa	532	OMG	C4-N3	3.91	1.46	1.37
27	BA	805	4AC	CM7-C7	3.91	1.58	1.50
27	BA	1357	4AC	CM7-C7	3.91	1.58	1.50
1	Aa	1004	5MC	C2-N1	3.91	1.48	1.40
27	BA	2545	OMC	C4-N4	3.90	1.43	1.33
1	Aa	1476	5MC	C5'-C4'	-3.90	1.39	1.51
27	BA	575	OMG	C4-N3	3.90	1.46	1.37
1	Aa	682	4AC	CM7-C7	3.89	1.58	1.50
27	BA	2780	4AC	CM7-C7	3.89	1.58	1.50
1	Aa	298	4AC	C4-N4	3.89	1.45	1.39
27	BA	730	4AC	C4-N4	3.89	1.45	1.39
27	BA	561	OMC	C2-N1	3.88	1.48	1.40
27	BA	1106	OMG	C4-N3	3.88	1.46	1.37
27	BA	1470	4AC	CM7-C7	3.88	1.58	1.50
1	Aa	825	OMC	C2-N1	3.88	1.48	1.40
27	BA	3023	4AC	C4-N4	3.87	1.45	1.39
1	Aa	304	OMU	C4-N3	3.87	1.45	1.38
27	BA	419	OMG	C2-N1	3.86	1.47	1.37
1	Aa	942	5MC	C2-N1	3.86	1.48	1.40
27	BA	419	OMG	C4-N3	3.86	1.46	1.37
27	BA	944	5MC	C2-N1	3.86	1.48	1.40
27	BA	56	4AC	C4-N4	3.86	1.45	1.39
27	BA	124	4AC	CM7-C7	3.86	1.58	1.50
27	BA	418	4AC	C4-N4	3.86	1.45	1.39
1	Aa	1476	5MC	C2'-C1'	3.86	1.65	1.53
27	BA	1750	OMC	C4-N4	3.86	1.43	1.33
27	BA	2018	OMC	C4-N3	3.85	1.42	1.34
27	BA	2997	4AC	C4-N4	3.85	1.45	1.39
1	Aa	464	5MC	C4-N4	3.85	1.44	1.34
27	BA	768	OMU	C4-N3	3.84	1.45	1.38
27	BA	453	OMU	C4-N3	3.83	1.45	1.38
27	BA	1905	5MU	O4-C4	-3.83	1.16	1.23
27	BA	2863	5MC	C2-N1	3.83	1.48	1.40
1	Aa	41	4AC	CM7-C7	3.82	1.58	1.50
27	BA	1319	OMU	C4-N3	3.82	1.45	1.38
1	Aa	569	4AC	CM7-C7	3.81	1.58	1.50
27	BA	201	4AC	CM7-C7	3.81	1.58	1.50
1	Aa	847	4AC	CM7-C7	3.81	1.58	1.50
27	BA	1790	OMC	C4-N4	3.81	1.42	1.33
27	BA	2055	5MC	C2-N1	3.81	1.48	1.40
1	Aa	240	OMU	C4-N3	3.81	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Aa	298	4AC	CM7-C7	3.80	1.58	1.50
1	Aa	1476	5MC	C2-N1	3.80	1.48	1.40
1	Aa	672	5MC	C2-N1	3.79	1.48	1.40
27	BA	2590	4AC	C4-N4	3.79	1.45	1.39
27	BA	1551	OMU	C4-N3	3.79	1.45	1.38
27	BA	800	OMG	C4-N3	3.79	1.46	1.37
27	BA	1641	4AC	C4-N4	3.79	1.45	1.39
27	BA	2035	5MC	C5'-C4'	-3.79	1.39	1.51
1	Aa	525	4AC	CM7-C7	3.79	1.58	1.50
27	BA	2124	OMC	C4-N4	3.78	1.42	1.33
1	Aa	1004	5MC	C6-N1	3.78	1.44	1.38
27	BA	244	4AC	CM7-C7	3.78	1.58	1.50
27	BA	1799	OMG	C2-N2	3.77	1.43	1.34
1	Aa	670	2MG	C2-N1	3.77	1.42	1.36
27	BA	763	OMG	C6-N1	3.76	1.43	1.37
27	BA	1558	OMG	C6-N1	3.75	1.43	1.37
27	BA	1899	4AC	CM7-C7	3.75	1.58	1.50
27	BA	2595	OMC	C4-N4	3.75	1.42	1.33
27	BA	1965	5MC	C2-N1	3.74	1.48	1.40
27	BA	619	OMU	C4-N3	3.74	1.45	1.38
27	BA	376	4AC	CM7-C7	3.74	1.58	1.50
27	BA	575	OMG	C6-N1	3.74	1.43	1.37
27	BA	365	OMG	C4-N3	3.72	1.46	1.37
1	Aa	373	4AC	CM7-C7	3.72	1.58	1.50
27	BA	2542	OMU	C4-N3	3.71	1.45	1.38
1	Aa	52	OMU	C4-N3	3.71	1.45	1.38
27	BA	713	4AC	C4-N4	3.71	1.45	1.39
1	Aa	1361	OMC	C2-N1	3.70	1.48	1.40
27	BA	1776	OMU	O4-C4	-3.70	1.17	1.24
27	BA	2159	4AC	CM7-C7	3.70	1.58	1.50
27	BA	2610	OMU	C4-N3	3.70	1.45	1.38
27	BA	2457	LHH	C4-N4	3.69	1.45	1.39
27	BA	1470	4AC	C4-N4	3.69	1.45	1.39
1	Aa	847	4AC	C4-N4	3.68	1.45	1.39
1	Aa	358	4AC	CM7-C7	3.68	1.58	1.50
1	Aa	854	5MC	C4-N4	3.68	1.43	1.34
27	BA	353	OMG	C2-N2	3.68	1.42	1.34
27	BA	552	OMG	C6-N1	3.67	1.43	1.37
1	Aa	1026	OMG	C2-N2	3.66	1.42	1.34
1	Aa	1467	MA6	C5-C4	-3.66	1.31	1.40
27	BA	2863	5MC	C4-N4	3.66	1.43	1.34
27	BA	501	4AC	CM7-C7	3.66	1.58	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	335	4AC	C4-N4	3.66	1.45	1.39
27	BA	2055	5MC	C4-N4	3.65	1.43	1.34
27	BA	1543	4AC	C4-N4	3.64	1.45	1.39
1	Aa	697	4AC	CM7-C7	3.64	1.58	1.50
27	BA	2838	4AC	C4-N4	3.64	1.45	1.39
27	BA	2780	4AC	C4-N4	3.64	1.45	1.39
27	BA	1799	OMG	C4-N3	3.64	1.46	1.37
27	BA	617	LHH	C2-N3	3.62	1.43	1.36
27	BA	1434	4AC	CM7-C7	3.60	1.58	1.50
27	BA	34	OMU	O4-C4	-3.59	1.17	1.24
1	Aa	457	5MC	O3'-C3'	3.58	1.51	1.43
27	BA	674	OMG	C2-N3	3.58	1.41	1.33
27	BA	1696	5MC	C2-N1	3.58	1.47	1.40
27	BA	1340	OMU	O4-C4	-3.57	1.17	1.24
27	BA	64	OMG	C4-N3	3.57	1.46	1.37
27	BA	419	OMG	C2-N2	3.56	1.42	1.34
1	Aa	1020	LHH	C2-N3	3.56	1.43	1.36
27	BA	2018	OMC	C2-N1	3.55	1.47	1.40
27	BA	1400	A2M	C5-C4	-3.54	1.31	1.40
27	BA	572	5MU	O4-C4	-3.54	1.16	1.23
1	Aa	913	OMG	C2-N2	3.54	1.42	1.34
1	Aa	1358	OMU	O4-C4	-3.53	1.17	1.24
27	BA	875	5MU	O4-C4	-3.53	1.16	1.23
27	BA	215	OMG	O6-C6	-3.53	1.16	1.23
27	BA	1969	OMU	O4-C4	-3.53	1.17	1.24
1	Aa	1361	OMC	C4-N4	3.52	1.42	1.33
1	Aa	5	4AC	CM7-C7	3.52	1.57	1.50
27	BA	2168	OMG	C2-N2	3.52	1.42	1.34
27	BA	657	OMU	O4-C4	-3.52	1.17	1.24
27	BA	1696	5MC	C4-N4	3.52	1.43	1.34
27	BA	2545	OMC	C2-N1	3.51	1.47	1.40
27	BA	2019	OMG	C2-N2	3.51	1.42	1.34
27	BA	1965	5MC	C4-N4	3.50	1.43	1.34
27	BA	674	OMG	C4-N3	3.49	1.45	1.37
27	BA	2863	5MC	C6-N1	3.49	1.44	1.38
27	BA	1480	OMU	C4-N3	3.49	1.44	1.38
1	Aa	854	5MC	C2-N1	3.49	1.47	1.40
1	Aa	229	LHH	C2-N3	3.49	1.43	1.36
27	BA	2745	OMG	O6-C6	-3.49	1.16	1.23
1	Aa	672	5MC	C4-N4	3.49	1.43	1.34
27	BA	244	4AC	C4-N4	3.48	1.44	1.39
27	BA	1434	4AC	C4-N4	3.48	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	2035	5MC	O3'-C3'	3.47	1.51	1.43
27	BA	505	A2M	C5-C4	-3.47	1.31	1.40
1	Aa	672	5MC	C6-N1	3.47	1.44	1.38
1	Aa	1265	OMG	C2-N2	3.47	1.42	1.34
27	BA	2550	OMG	O6-C6	-3.47	1.16	1.23
27	BA	2656	OMU	C4-N3	3.46	1.44	1.38
1	Aa	876	OMG	C2-N2	3.46	1.42	1.34
27	BA	2728	OMG	C2-N2	3.46	1.42	1.34
27	BA	1357	4AC	C4-N4	3.45	1.44	1.39
27	BA	1965	5MC	O2-C2	-3.44	1.17	1.23
27	BA	2545	OMC	O2-C2	-3.44	1.17	1.23
27	BA	215	OMG	C2-N2	3.44	1.42	1.34
27	BA	912	OMG	O6-C6	-3.44	1.16	1.23
1	Aa	1478	5MC	C4-N4	3.44	1.43	1.34
1	Aa	381	OMG	C2-N2	3.44	1.42	1.34
27	BA	912	OMG	C5-C4	-3.44	1.34	1.43
27	BA	2018	OMC	O2-C2	-3.43	1.17	1.23
1	Aa	636	OMG	C2-N2	3.43	1.42	1.34
1	Aa	138	OMG	C2-N2	3.43	1.42	1.34
1	Aa	1476	5MC	O2-C2	-3.43	1.17	1.23
1	Aa	771	OMG	C2-N2	3.43	1.42	1.34
27	BA	1480	OMU	O4-C4	-3.42	1.17	1.24
27	BA	2605	5MC	C4-N4	3.42	1.43	1.34
1	Aa	1478	5MC	C6-N1	3.42	1.43	1.38
27	BA	2542	OMU	O4-C4	-3.41	1.17	1.24
27	BA	1696	5MC	C6-N1	3.41	1.43	1.38
27	BA	1340	OMU	C4-N3	3.41	1.44	1.38
1	Aa	136	4AC	C5-C4	3.41	1.48	1.40
27	BA	1305	4AC	C5-C4	3.40	1.48	1.40
27	BA	2018	OMC	C4-N4	3.40	1.41	1.33
27	BA	2152	OMG	C5-C4	-3.40	1.34	1.43
27	BA	1085	5MU	O2-C2	-3.40	1.16	1.23
27	BA	833	OMG	C2-N2	3.39	1.42	1.34
27	BA	869	OMC	C4-N4	3.39	1.41	1.33
27	BA	1969	OMU	C4-N3	3.39	1.44	1.38
27	BA	2379	OMG	O6-C6	-3.39	1.16	1.23
27	BA	2457	LHH	C2-N3	3.39	1.43	1.36
27	BA	3009	4AC	C4-N4	3.38	1.44	1.39
27	BA	2075	5MC	C2-N1	3.38	1.47	1.40
1	Aa	659	OMG	C2-N2	3.38	1.42	1.34
27	BA	1085	5MU	O4-C4	-3.37	1.17	1.23
27	BA	1965	5MC	C6-N1	3.37	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	754	OMC	O2-C2	-3.37	1.17	1.23
27	BA	298	5MU	O4-C4	-3.37	1.17	1.23
1	Aa	498	OMG	C2-N2	3.37	1.42	1.34
27	BA	2550	OMG	C5-C4	-3.36	1.34	1.43
27	BA	1337	4AC	C4-N4	3.35	1.44	1.39
27	BA	526	LHH	C2-N3	3.35	1.43	1.36
27	BA	453	OMU	O4-C4	-3.35	1.18	1.24
1	Aa	1107	OMG	C2-N2	3.35	1.42	1.34
1	Aa	8	OMU	O4-C4	-3.35	1.18	1.24
27	BA	825	A2M	C5-C4	-3.35	1.32	1.40
27	BA	2630	OMC	O2-C2	-3.35	1.17	1.23
1	Aa	1358	OMU	C4-N3	3.34	1.44	1.38
27	BA	537	5MU	O4-C4	-3.34	1.17	1.23
27	BA	2672	OMG	O6-C6	-3.34	1.16	1.23
27	BA	2832	4AC	C4-N4	3.34	1.44	1.39
1	Aa	1476	5MC	O3'-C3'	3.34	1.50	1.43
27	BA	1396	4AC	C4-N4	3.34	1.44	1.39
27	BA	2610	OMU	O4-C4	-3.33	1.18	1.24
1	Aa	1276	5MC	O3'-C3'	3.33	1.50	1.43
27	BA	799	4AC	C4-N4	3.31	1.44	1.39
27	BA	2992	4AC	C5-C4	3.29	1.47	1.40
27	BA	1375	4AC	C4-N4	3.29	1.44	1.39
1	Aa	446	OMG	C2-N2	3.29	1.42	1.34
27	BA	2728	OMG	C5-C4	-3.29	1.34	1.43
27	BA	1319	OMU	O4-C4	-3.28	1.18	1.24
27	BA	2168	OMG	C6-N1	3.28	1.42	1.37
27	BA	2047	OMC	O2-C2	-3.28	1.17	1.23
1	Aa	358	4AC	C5-C4	3.28	1.47	1.40
1	Aa	994	OMG	C6-N1	3.28	1.42	1.37
27	BA	1810	4AC	C4-N4	3.28	1.44	1.39
27	BA	2528	OMG	C2-N2	3.28	1.42	1.34
27	BA	124	4AC	C4-N4	3.27	1.44	1.39
1	Aa	41	4AC	C5-C4	3.26	1.47	1.40
27	BA	1820	OMC	O2-C2	-3.26	1.17	1.23
1	Aa	852	OMG	O6-C6	-3.26	1.16	1.23
27	BA	1517	A2M	C5-C4	-3.26	1.32	1.40
27	BA	1551	OMU	O4-C4	-3.25	1.18	1.24
27	BA	619	OMU	O4-C4	-3.25	1.18	1.24
1	Aa	320	OMG	C2-N2	3.25	1.41	1.34
27	BA	2745	OMG	C5-C4	-3.25	1.34	1.43
27	BA	2159	4AC	C4-N4	3.25	1.44	1.39
27	BA	1696	5MC	O2-C2	-3.25	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Aa	892	OMG	C2-N2	3.24	1.41	1.34
27	BA	2010	OMG	C2-N2	3.24	1.41	1.34
1	Aa	1025	OMG	C2-N2	3.24	1.41	1.34
27	BA	488	A2M	C5-C4	-3.24	1.32	1.40
27	BA	1905	5MU	O2-C2	-3.24	1.17	1.23
27	BA	2055	5MC	O2-C2	-3.24	1.17	1.23
27	BA	561	OMC	O2-C2	-3.24	1.17	1.23
27	BA	2672	OMG	C5-C4	-3.24	1.34	1.43
27	BA	215	OMG	C5-C4	-3.24	1.34	1.43
27	BA	2656	OMU	O4-C4	-3.23	1.18	1.24
1	Aa	672	5MC	O2-C2	-3.23	1.17	1.23
27	BA	1934	4AC	C4-N4	3.23	1.44	1.39
27	BA	2324	OMG	C2-N2	3.23	1.41	1.34
27	BA	2384	5MU	O4-C4	-3.23	1.17	1.23
27	BA	1953	OMG	C5-C4	-3.23	1.34	1.43
27	BA	1899	4AC	C4-N4	3.22	1.44	1.39
27	BA	34	OMU	C4-N3	3.22	1.44	1.38
27	BA	2657	OMG	C2-N2	3.22	1.41	1.34
27	BA	1398	OMG	O6-C6	-3.22	1.16	1.23
27	BA	34	OMU	O2-C2	-3.22	1.17	1.23
1	Aa	1459	4AC	O7-C7	-3.22	1.16	1.23
27	BA	2955	LHH	C2-N3	3.22	1.42	1.36
27	BA	2152	OMG	O6-C6	-3.21	1.16	1.23
1	Aa	854	5MC	O2-C2	-3.21	1.17	1.23
27	BA	575	OMG	C2-N2	3.21	1.41	1.34
1	Aa	240	OMU	O4-C4	-3.20	1.18	1.24
27	BA	433	4AC	C4-N4	3.20	1.44	1.39
27	BA	2075	5MC	O2-C2	-3.19	1.17	1.23
27	BA	2630	OMC	C4-N4	3.19	1.41	1.33
27	BA	872	A2M	C5-C4	-3.19	1.32	1.40
27	BA	849	A2M	C5-C4	-3.19	1.32	1.40
27	BA	201	4AC	C4-N4	3.19	1.44	1.39
1	Aa	1107	OMG	C6-N1	3.19	1.42	1.37
27	BA	2688	5MU	O4-C4	-3.18	1.17	1.23
27	BA	64	OMG	C2-N2	3.18	1.41	1.34
27	BA	1750	OMC	O2-C2	-3.17	1.17	1.23
27	BA	2075	5MC	C4-N4	3.17	1.42	1.34
27	BA	2528	OMG	O6-C6	-3.17	1.16	1.23
1	Aa	1478	5MC	O2-C2	-3.17	1.17	1.23
27	BA	833	OMG	O6-C6	-3.16	1.16	1.23
27	BA	756	A2M	C5-C4	-3.16	1.32	1.40
1	Aa	450	OMG	C2-N2	3.16	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	2553	4SU	O2-C2	-3.16	1.17	1.23
27	BA	1790	OMC	O2-C2	-3.16	1.17	1.23
1	Aa	304	OMU	O4-C4	-3.16	1.18	1.24
27	BA	2527	OMG	C5-C4	-3.15	1.35	1.43
27	BA	1525	OMG	C5-C4	-3.15	1.35	1.43
27	BA	2797	4AC	C4-N4	3.15	1.44	1.39
1	Aa	296	OMC	O2-C2	-3.14	1.17	1.23
27	BA	2702	A2M	C5-C4	-3.14	1.32	1.40
27	BA	2605	5MC	O2-C2	-3.14	1.17	1.23
27	BA	858	4AC	C4-N4	3.14	1.44	1.39
1	Aa	52	OMU	O4-C4	-3.13	1.18	1.24
27	BA	2016	OMG	O6-C6	-3.13	1.16	1.23
27	BA	2656	OMU	O2-C2	-3.13	1.17	1.23
27	BA	932	A2M	C5-C4	-3.13	1.32	1.40
1	Aa	532	OMG	C5-C4	-3.13	1.35	1.43
27	BA	778	4AC	C5-C4	3.13	1.47	1.40
1	Aa	1468	MA6	C5-C4	-3.13	1.32	1.40
27	BA	879	A2M	O5'-C5'	-3.13	1.37	1.44
27	BA	2121	4AC	C4-N4	3.13	1.44	1.39
27	BA	723	OMG	C5-C4	-3.13	1.35	1.43
27	BA	1548	5MU	O4-C4	-3.12	1.17	1.23
27	BA	290	OMG	C5-C4	-3.12	1.35	1.43
1	Aa	682	4AC	C5-C4	3.11	1.47	1.40
27	BA	2016	OMG	C2-N2	3.11	1.41	1.34
1	Aa	382	OMG	C2-N2	3.11	1.41	1.34
27	BA	2379	OMG	C5-C4	-3.10	1.35	1.43
27	BA	768	OMU	O4-C4	-3.10	1.18	1.24
27	BA	1776	OMU	C4-N3	3.10	1.44	1.38
27	BA	932	A2M	O3'-C3'	-3.10	1.35	1.43
27	BA	1953	OMG	O6-C6	-3.10	1.17	1.23
1	Aa	1025	OMG	C5-C4	-3.09	1.35	1.43
27	BA	944	5MC	O2-C2	-3.09	1.18	1.23
1	Aa	525	4AC	C4-N4	3.09	1.44	1.39
27	BA	376	4AC	C4-N4	3.09	1.44	1.39
27	BA	290	OMG	C2-N2	3.09	1.41	1.34
27	BA	2016	OMG	C5-C4	-3.09	1.35	1.43
27	BA	2010	OMG	C5-C4	-3.08	1.35	1.43
27	BA	552	OMG	C5-C4	-3.08	1.35	1.43
27	BA	1427	4AC	C4-N4	3.08	1.44	1.39
27	BA	64	OMG	C5-C4	-3.08	1.35	1.43
27	BA	805	4AC	C4-N4	3.08	1.44	1.39
1	Aa	532	OMG	C2-N2	3.08	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Aa	8	OMU	C4-N3	3.07	1.44	1.38
1	Aa	190	OMC	O2-C2	-3.07	1.18	1.23
27	BA	335	4AC	C5-C4	3.07	1.47	1.40
27	BA	2542	OMU	O2-C2	-3.07	1.17	1.23
27	BA	418	4AC	C5-C4	3.07	1.47	1.40
27	BA	1525	OMG	O6-C6	-3.06	1.17	1.23
1	Aa	913	OMG	C6-N1	3.06	1.42	1.37
1	Aa	1276	5MC	O2-C2	-3.06	1.18	1.23
1	Aa	5	4AC	C5-C4	3.06	1.47	1.40
27	BA	2745	OMG	C2-N2	3.06	1.41	1.34
27	BA	2075	5MC	C6-N1	3.06	1.43	1.38
1	Aa	464	5MC	O2-C2	-3.05	1.18	1.23
1	Aa	1358	OMU	O2-C2	-3.05	1.17	1.23
1	Aa	1434	OMG	C2-N2	3.05	1.41	1.34
27	BA	290	OMG	O6-C6	-3.05	1.17	1.23
1	Aa	1434	OMG	C5-C4	-3.05	1.35	1.43
1	Aa	479	OMU	O4-C4	-3.05	1.18	1.24
27	BA	756	A2M	O5'-C5'	-3.04	1.37	1.44
27	BA	526	LHH	C4-N4	3.04	1.44	1.39
27	BA	1085	5MU	C6-C5	3.04	1.39	1.34
27	BA	657	OMU	O2-C2	-3.04	1.17	1.23
27	BA	912	OMG	C2-N2	3.04	1.41	1.34
1	Aa	825	OMC	O2-C2	-3.04	1.18	1.23
27	BA	250	OMC	O2-C2	-3.04	1.18	1.23
1	Aa	852	OMG	C5-C4	-3.03	1.35	1.43
1	Aa	569	4AC	C5-C4	3.03	1.47	1.40
1	Aa	697	4AC	C5-C4	3.03	1.47	1.40
27	BA	1340	OMU	O2-C2	-3.03	1.17	1.23
27	BA	1776	OMU	O2-C2	-3.03	1.17	1.23
27	BA	2728	OMG	O6-C6	-3.03	1.17	1.23
27	BA	298	5MU	O2-C2	-3.03	1.17	1.23
27	BA	2863	5MC	O2-C2	-3.02	1.18	1.23
27	BA	2124	OMC	O2-C2	-3.02	1.18	1.23
27	BA	869	OMC	O2-C2	-3.01	1.18	1.23
1	Aa	246	OMG	C2-N2	3.01	1.41	1.34
27	BA	833	OMG	C5-C4	-3.01	1.35	1.43
27	BA	2657	OMG	C5-C4	-3.01	1.35	1.43
27	BA	2955	LHH	C4-N4	3.01	1.44	1.39
27	BA	2545	OMC	C6-N1	3.00	1.45	1.38
27	BA	825	A2M	O3'-C3'	-3.00	1.35	1.43
1	Aa	1217	4AC	C5-C4	3.00	1.47	1.40
27	BA	1641	4AC	C5-C4	3.00	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	2035	5MC	C3'-C4'	3.00	1.60	1.53
27	BA	944	5MC	C4-N4	2.99	1.41	1.34
27	BA	2595	OMC	O2-C2	-2.99	1.18	1.23
27	BA	2527	OMG	O6-C6	-2.99	1.17	1.23
27	BA	2568	OMG	C6-N1	-2.99	1.33	1.37
27	BA	1799	OMG	C5-C4	-2.99	1.35	1.43
27	BA	1892	OMG	C2-N2	2.98	1.41	1.34
27	BA	365	OMG	C5-C4	-2.98	1.35	1.43
27	BA	674	OMG	C5-C4	-2.98	1.35	1.43
1	Aa	525	4AC	C5-C4	2.98	1.47	1.40
27	BA	2997	4AC	C5-C4	2.98	1.47	1.40
27	BA	63	OMG	O6-C6	-2.97	1.17	1.23
27	BA	1480	OMU	O2-C2	-2.97	1.17	1.23
1	Aa	827	4AC	C5-C4	2.97	1.47	1.40
1	Aa	446	OMG	C5-C4	-2.97	1.35	1.43
27	BA	365	OMG	C2-N2	2.97	1.41	1.34
27	BA	2528	OMG	C5-C4	-2.97	1.35	1.43
27	BA	552	OMG	C5-C6	2.97	1.53	1.47
1	Aa	1354	OMC	O2-C2	-2.97	1.18	1.23
27	BA	2590	4AC	C5-C4	2.96	1.47	1.40
1	Aa	298	4AC	C5-C4	2.96	1.47	1.40
1	Aa	535	OMC	O2-C2	-2.96	1.18	1.23
27	BA	56	4AC	C5-C4	2.96	1.47	1.40
27	BA	763	OMG	C2-N2	2.96	1.41	1.34
1	Aa	605	4AC	C5-C4	2.95	1.47	1.40
1	Aa	942	5MC	O2-C2	-2.95	1.18	1.23
27	BA	879	A2M	C5-C4	-2.95	1.33	1.40
27	BA	1940	OMG	C2-N2	2.95	1.41	1.34
1	Aa	752	OMC	O2-C2	-2.95	1.18	1.23
1	Aa	892	OMG	C5-C4	-2.95	1.35	1.43
27	BA	63	OMG	C2-N2	2.95	1.41	1.34
1	Aa	818	4AC	C5-C4	2.94	1.47	1.40
27	BA	1558	OMG	C2-N2	2.94	1.41	1.34
27	BA	2571	OMC	O2-C2	-2.94	1.18	1.23
27	BA	723	OMG	O6-C6	-2.93	1.17	1.23
27	BA	1940	OMG	O6-C6	-2.93	1.17	1.23
1	Aa	730	4AC	C5-C4	2.93	1.47	1.40
27	BA	2384	5MU	O2-C2	-2.93	1.17	1.23
1	Aa	457	5MC	C3'-C4'	2.93	1.60	1.53
1	Aa	382	OMG	C5-C4	-2.93	1.35	1.43
27	BA	2324	OMG	C5-C4	-2.93	1.35	1.43
27	BA	1955	4AC	C4-N4	2.93	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	1398	OMG	C5-C4	-2.92	1.35	1.43
27	BA	1265	A2M	C5-C4	-2.92	1.33	1.40
27	BA	488	A2M	O2'-C2'	2.91	1.50	1.42
1	Aa	246	OMG	C5-C4	-2.91	1.35	1.43
1	Aa	1352	5MC	O2-C2	-2.91	1.18	1.23
1	Aa	501	4AC	C5-C4	2.91	1.47	1.40
1	Aa	1004	5MC	O2-C2	-2.91	1.18	1.23
27	BA	1431	4AC	C5-C4	2.90	1.47	1.40
1	Aa	818	4AC	CM7-C7	2.90	1.56	1.50
27	BA	1525	OMG	C2-N2	2.90	1.41	1.34
27	BA	2019	OMG	O6-C6	-2.90	1.17	1.23
27	BA	2521	OMG	C5-C4	-2.89	1.35	1.43
27	BA	1969	OMU	O2-C2	-2.89	1.17	1.23
1	Aa	381	OMG	O6-C6	-2.89	1.17	1.23
1	Aa	8	OMU	O2-C2	-2.89	1.17	1.23
1	Aa	498	OMG	C5-C4	-2.88	1.35	1.43
27	BA	1106	OMG	O6-C6	-2.88	1.17	1.23
27	BA	64	OMG	O6-C6	-2.88	1.17	1.23
27	BA	1940	OMG	C5-C4	-2.88	1.35	1.43
1	Aa	636	OMG	C6-N1	2.87	1.42	1.37
27	BA	537	5MU	O2-C2	-2.87	1.17	1.23
27	BA	875	5MU	O2-C2	-2.86	1.17	1.23
27	BA	575	OMG	C5-C6	2.86	1.53	1.47
27	BA	63	OMG	C5-C4	-2.86	1.35	1.43
27	BA	1106	OMG	C5-C4	-2.86	1.35	1.43
1	Aa	457	5MC	O2-C2	-2.86	1.18	1.23
1	Aa	1025	OMG	O6-C6	-2.85	1.17	1.23
1	Aa	771	OMG	C5-C4	-2.85	1.35	1.43
27	BA	572	5MU	O2-C2	-2.85	1.17	1.23
27	BA	3023	4AC	C5-C4	2.85	1.46	1.40
1	Aa	381	OMG	C5-C4	-2.85	1.35	1.43
27	BA	1106	OMG	C2-N2	2.85	1.41	1.34
1	Aa	320	OMG	O6-C6	-2.85	1.17	1.23
27	BA	2527	OMG	C2-N2	2.84	1.41	1.34
27	BA	2010	OMG	O6-C6	-2.84	1.17	1.23
1	Aa	1265	OMG	C5-C4	-2.84	1.35	1.43
27	BA	657	OMU	C4-N3	2.83	1.43	1.38
27	BA	718	OMC	O2-C2	-2.83	1.18	1.23
27	BA	1400	A2M	O3'-C3'	-2.83	1.36	1.43
1	Aa	498	OMG	C6-N1	2.83	1.42	1.37
27	BA	2035	5MC	O2-C2	-2.83	1.18	1.23
27	BA	1106	OMG	C6-N1	2.83	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	501	4AC	O7-C7	-2.83	1.16	1.23
1	Aa	382	OMG	C6-N1	2.82	1.42	1.37
27	BA	2019	OMG	C5-C4	-2.82	1.35	1.43
27	BA	800	OMG	C5-C4	-2.82	1.35	1.43
1	Aa	532	OMG	C6-N1	2.81	1.42	1.37
27	BA	353	OMG	O6-C6	-2.81	1.17	1.23
27	BA	879	A2M	O3'-C3'	-2.81	1.36	1.43
1	Aa	876	OMG	O6-C6	-2.81	1.17	1.23
27	BA	1548	5MU	O2-C2	-2.81	1.17	1.23
27	BA	1543	4AC	C5-C4	2.81	1.46	1.40
1	Aa	771	OMG	O6-C6	-2.81	1.17	1.23
27	BA	376	4AC	O7-C7	-2.81	1.16	1.23
1	Aa	917	5MU	C4-N3	-2.81	1.33	1.38
27	BA	1955	4AC	O7-C7	-2.81	1.16	1.23
1	Aa	670	2MG	C5-C4	-2.80	1.35	1.43
27	BA	2521	OMG	O6-C6	-2.80	1.17	1.23
27	BA	763	OMG	C5-C4	-2.80	1.35	1.43
27	BA	453	OMU	O2-C2	-2.80	1.17	1.23
27	BA	2610	OMU	C6-N1	2.80	1.44	1.38
27	BA	488	A2M	O3'-C3'	-2.80	1.36	1.43
1	Aa	1434	OMG	C6-N1	2.80	1.42	1.37
27	BA	2581	4SU	O2-C2	-2.80	1.17	1.23
27	BA	1892	OMG	O6-C6	-2.80	1.17	1.23
1	Aa	532	OMG	O6-C6	-2.80	1.17	1.23
1	Aa	1007	4AC	C4-N4	-2.80	1.35	1.39
27	BA	730	4AC	C5-C4	2.80	1.46	1.40
1	Aa	913	OMG	C5-C4	-2.79	1.36	1.43
1	Aa	138	OMG	O6-C6	-2.79	1.17	1.23
27	BA	713	4AC	C5-C4	2.79	1.46	1.40
27	BA	353	OMG	C5-C4	-2.79	1.36	1.43
27	BA	1427	4AC	O7-C7	-2.78	1.16	1.23
1	Aa	847	4AC	O7-C7	-2.78	1.16	1.23
27	BA	2780	4AC	C5-C4	2.78	1.46	1.40
27	BA	800	OMG	O6-C6	-2.78	1.17	1.23
1	Aa	138	OMG	C6-N1	2.78	1.42	1.37
1	Aa	1361	OMC	O2-C2	-2.78	1.18	1.23
27	BA	365	OMG	O6-C6	-2.78	1.17	1.23
1	Aa	1026	OMG	C5-C4	-2.78	1.36	1.43
27	BA	575	OMG	C5-C4	-2.77	1.36	1.43
27	BA	1551	OMU	O2-C2	-2.77	1.18	1.23
27	BA	2168	OMG	C5-C4	-2.77	1.36	1.43
1	Aa	913	OMG	O6-C6	-2.77	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Aa	1265	OMG	C6-N1	2.77	1.42	1.37
1	Aa	446	OMG	O6-C6	-2.77	1.17	1.23
1	Aa	876	OMG	C5-C4	-2.77	1.36	1.43
27	BA	2159	4AC	O7-C7	-2.77	1.17	1.23
27	BA	723	OMG	C5-C6	2.76	1.53	1.47
27	BA	1398	OMG	C2-N2	2.76	1.40	1.34
1	Aa	373	4AC	C5-C4	2.76	1.46	1.40
27	BA	1375	4AC	C5-C4	2.76	1.46	1.40
1	Aa	892	OMG	C6-N1	2.76	1.42	1.37
27	BA	925	4AC	C4-N4	-2.76	1.35	1.39
1	Aa	450	OMG	C5-C4	-2.76	1.36	1.43
27	BA	2379	OMG	C2-N2	2.76	1.40	1.34
27	BA	2688	5MU	O2-C2	-2.76	1.18	1.23
27	BA	858	4AC	C5-C4	2.75	1.46	1.40
1	Aa	1434	OMG	O6-C6	-2.75	1.17	1.23
27	BA	2353	OMG	O6-C6	-2.75	1.17	1.23
27	BA	2121	4AC	C5-C4	2.75	1.46	1.40
27	BA	1934	4AC	O7-C7	-2.74	1.17	1.23
27	BA	505	A2M	O5'-C5'	-2.74	1.38	1.44
27	BA	825	A2M	O5'-C5'	-2.74	1.38	1.44
1	Aa	1476	5MC	C3'-C4'	2.74	1.60	1.53
1	Aa	730	4AC	CM7-C7	2.74	1.56	1.50
1	Aa	450	OMG	O6-C6	-2.74	1.17	1.23
27	BA	2353	OMG	C2-N2	2.74	1.40	1.34
27	BA	2838	4AC	C5-C4	2.73	1.46	1.40
27	BA	2168	OMG	C5-C6	2.73	1.53	1.47
27	BA	1319	OMU	O2-C2	-2.73	1.18	1.23
27	BA	1892	OMG	C5-C4	-2.73	1.36	1.43
1	Aa	847	4AC	C5-C4	2.72	1.46	1.40
1	Aa	659	OMG	C5-C4	-2.72	1.36	1.43
27	BA	2657	OMG	O6-C6	-2.72	1.17	1.23
1	Aa	1265	OMG	O6-C6	-2.72	1.17	1.23
27	BA	2124	OMC	C6-N1	2.72	1.44	1.38
1	Aa	382	OMG	O6-C6	-2.72	1.17	1.23
1	Aa	730	4AC	O7-C7	-2.72	1.17	1.23
1	Aa	1276	5MC	C3'-C4'	2.71	1.59	1.53
27	BA	290	OMG	C5-C6	2.71	1.52	1.47
27	BA	2121	4AC	O7-C7	-2.71	1.17	1.23
27	BA	932	A2M	C6-N6	2.71	1.43	1.34
27	BA	1641	4AC	O7-C7	-2.71	1.17	1.23
27	BA	756	A2M	O3'-C3'	-2.71	1.36	1.43
27	BA	849	A2M	C6-N6	2.71	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	2353	OMG	C5-C4	-2.71	1.36	1.43
27	BA	1953	OMG	C2-N2	2.71	1.40	1.34
1	Aa	1275	OMG	C6-N1	-2.70	1.33	1.37
27	BA	2521	OMG	C2-N2	2.70	1.40	1.34
1	Aa	994	OMG	C5-C6	2.70	1.52	1.47
1	Aa	876	OMG	C6-N1	2.70	1.41	1.37
27	BA	1517	A2M	C6-N6	2.70	1.43	1.34
27	BA	872	A2M	O3'-C3'	-2.70	1.36	1.43
27	BA	2019	OMG	C6-N1	2.70	1.41	1.37
1	Aa	138	OMG	C5-C4	-2.69	1.36	1.43
1	Aa	1026	OMG	O6-C6	-2.69	1.17	1.23
1	Aa	659	OMG	C6-N1	2.69	1.41	1.37
1	Aa	320	OMG	C5-C4	-2.69	1.36	1.43
1	Aa	246	OMG	O6-C6	-2.69	1.17	1.23
27	BA	723	OMG	C2-N2	2.68	1.40	1.34
27	BA	1558	OMG	C5-C4	-2.68	1.36	1.43
1	Aa	457	5MC	O4'-C4'	2.68	1.51	1.45
27	BA	2324	OMG	O6-C6	-2.68	1.17	1.23
27	BA	2019	OMG	C5-C6	2.68	1.52	1.47
1	Aa	498	OMG	O6-C6	-2.68	1.17	1.23
1	Aa	190	OMC	C6-N1	2.68	1.44	1.38
1	Aa	298	4AC	O7-C7	-2.68	1.17	1.23
27	BA	768	OMU	O2-C2	-2.67	1.18	1.23
27	BA	27	4AC	C5-C4	2.67	1.46	1.40
1	Aa	659	OMG	O6-C6	-2.67	1.17	1.23
27	BA	1558	OMG	C5-C6	2.67	1.52	1.47
27	BA	1400	A2M	O2'-C2'	2.66	1.49	1.42
27	BA	879	A2M	C6-N6	2.66	1.43	1.34
27	BA	1357	4AC	C5-C4	2.65	1.46	1.40
27	BA	1955	4AC	C5-C4	2.65	1.46	1.40
1	Aa	246	OMG	C6-N1	2.65	1.41	1.37
27	BA	872	A2M	O5'-C5'	-2.65	1.38	1.44
27	BA	1470	4AC	O7-C7	-2.65	1.17	1.23
1	Aa	1107	OMG	C5-C6	2.64	1.52	1.47
1	Aa	670	2MG	O6-C6	-2.64	1.17	1.23
27	BA	1265	A2M	C6-N6	2.64	1.43	1.34
27	BA	1375	4AC	O7-C7	-2.64	1.17	1.23
27	BA	1934	4AC	C5-C4	2.64	1.46	1.40
1	Aa	636	OMG	C5-C6	2.63	1.52	1.47
1	Aa	670	2MG	C6-N1	2.63	1.41	1.37
27	BA	64	OMG	C6-N1	2.63	1.41	1.37
27	BA	674	OMG	C5-C6	2.63	1.52	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	2702	A2M	O2'-C2'	2.63	1.49	1.42
1	Aa	917	5MU	C6-C5	2.63	1.38	1.34
1	Aa	52	OMU	O2-C2	-2.62	1.18	1.23
1	Aa	450	OMG	C6-N1	2.62	1.41	1.37
1	Aa	5	4AC	O7-C7	-2.62	1.17	1.23
27	BA	1525	OMG	C6-N1	2.62	1.41	1.37
1	Aa	1476	5MC	O4'-C4'	2.62	1.50	1.45
27	BA	244	4AC	O7-C7	-2.62	1.17	1.23
27	BA	833	OMG	C2-N1	2.61	1.44	1.37
1	Aa	1107	OMG	C5-C4	-2.61	1.36	1.43
1	Aa	1026	OMG	C6-N1	2.61	1.41	1.37
1	Aa	304	OMU	O2-C2	-2.61	1.18	1.23
27	BA	2571	OMC	C6-N1	2.61	1.44	1.38
1	Aa	320	OMG	C5-C6	2.61	1.52	1.47
27	BA	674	OMG	C6-N1	2.60	1.41	1.37
27	BA	2353	OMG	C6-N1	2.60	1.41	1.37
1	Aa	479	OMU	C6-N1	2.60	1.44	1.38
27	BA	1265	A2M	O2'-C2'	2.60	1.49	1.42
27	BA	2997	4AC	O7-C7	-2.60	1.17	1.23
27	BA	2672	OMG	C2-N2	2.60	1.40	1.34
27	BA	718	OMC	C6-N1	2.60	1.44	1.38
27	BA	3009	4AC	C5-C4	2.60	1.46	1.40
27	BA	756	A2M	C6-N6	2.60	1.43	1.34
27	BA	619	OMU	O2-C2	-2.59	1.18	1.23
1	Aa	240	OMU	O2-C2	-2.59	1.18	1.23
27	BA	730	4AC	O7-C7	-2.59	1.17	1.23
27	BA	1434	4AC	O7-C7	-2.59	1.17	1.23
1	Aa	373	4AC	O7-C7	-2.59	1.17	1.23
27	BA	2832	4AC	O7-C7	-2.59	1.17	1.23
27	BA	488	A2M	C6-N6	2.59	1.43	1.34
27	BA	2035	5MC	O4'-C4'	2.59	1.50	1.45
1	Aa	636	OMG	O6-C6	-2.59	1.18	1.23
1	Aa	670	2MG	C5-C6	2.59	1.52	1.47
27	BA	2797	4AC	C5-C4	2.59	1.46	1.40
27	BA	3009	4AC	O7-C7	-2.58	1.17	1.23
27	BA	2702	A2M	C6-N6	2.58	1.43	1.34
27	BA	376	4AC	C5-C4	2.58	1.46	1.40
27	BA	1357	4AC	O7-C7	-2.58	1.17	1.23
27	BA	56	4AC	O7-C7	-2.58	1.17	1.23
1	Aa	852	OMG	C2-N2	2.57	1.40	1.34
27	BA	1899	4AC	O7-C7	-2.57	1.17	1.23
1	Aa	501	4AC	O7-C7	-2.57	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Aa	1276	5MC	O4'-C4'	2.57	1.50	1.45
1	Aa	296	OMC	C6-N1	2.57	1.44	1.38
1	Aa	771	OMG	C6-N1	2.57	1.41	1.37
27	BA	2389	OMU	C4-N3	-2.57	1.34	1.38
1	Aa	752	OMC	C6-N1	2.56	1.44	1.38
27	BA	754	OMC	C6-N1	2.56	1.44	1.38
1	Aa	636	OMG	C5-C4	-2.56	1.36	1.43
1	Aa	1434	OMG	C5-C6	2.56	1.52	1.47
1	Aa	381	OMG	C6-N1	2.55	1.41	1.37
27	BA	2324	OMG	C5-C6	2.55	1.52	1.47
27	BA	858	4AC	O7-C7	-2.55	1.17	1.23
1	Aa	605	4AC	O7-C7	-2.55	1.17	1.23
27	BA	879	A2M	O2'-C2'	2.54	1.49	1.42
27	BA	1396	4AC	C5-C4	2.54	1.46	1.40
1	Aa	446	OMG	C6-N1	2.54	1.41	1.37
27	BA	1427	4AC	C5-C4	2.54	1.46	1.40
27	BA	1337	4AC	O7-C7	-2.53	1.17	1.23
27	BA	800	OMG	C2-N2	2.53	1.40	1.34
27	BA	353	OMG	C2-N1	2.53	1.43	1.37
1	Aa	569	4AC	O7-C7	-2.53	1.17	1.23
27	BA	2702	A2M	O3'-C3'	-2.53	1.37	1.43
27	BA	2550	OMG	C2-N2	2.53	1.40	1.34
27	BA	2745	OMG	C5-C6	2.52	1.52	1.47
27	BA	723	OMG	C6-N1	2.52	1.41	1.37
1	Aa	994	OMG	C5-C4	-2.52	1.36	1.43
1	Aa	304	OMU	C6-N1	2.52	1.44	1.38
27	BA	335	4AC	O7-C7	-2.52	1.17	1.23
1	Aa	892	OMG	O6-C6	-2.52	1.18	1.23
27	BA	505	A2M	C6-N6	2.52	1.43	1.34
27	BA	833	OMG	C5-C6	2.51	1.52	1.47
1	Aa	1107	OMG	O6-C6	-2.51	1.18	1.23
27	BA	501	4AC	C5-C4	2.51	1.46	1.40
1	Aa	535	OMC	C6-N1	2.51	1.44	1.38
27	BA	2672	OMG	C5-C6	2.51	1.52	1.47
27	BA	3023	4AC	O7-C7	-2.50	1.17	1.23
27	BA	2832	4AC	C5-C4	2.50	1.46	1.40
27	BA	1470	4AC	C5-C4	2.50	1.46	1.40
27	BA	799	4AC	C5-C4	2.50	1.46	1.40
27	BA	1810	4AC	O7-C7	-2.50	1.17	1.23
1	Aa	994	OMG	O6-C6	-2.50	1.18	1.23
27	BA	2070	5MC	C6-N1	-2.50	1.33	1.38
1	Aa	52	OMU	C6-N1	2.50	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	2780	4AC	O7-C7	-2.49	1.17	1.23
27	BA	2797	4AC	O7-C7	-2.49	1.17	1.23
27	BA	1265	A2M	O3'-C3'	-2.49	1.37	1.43
1	Aa	458	4AC	C4-N4	-2.48	1.36	1.39
27	BA	2610	OMU	O2-C2	-2.48	1.18	1.23
27	BA	552	OMG	C2-N2	2.48	1.40	1.34
1	Aa	240	OMU	C6-N1	2.48	1.44	1.38
27	BA	124	4AC	O7-C7	-2.47	1.17	1.23
1	Aa	682	4AC	O7-C7	-2.47	1.17	1.23
27	BA	1551	OMU	C6-N1	2.47	1.43	1.38
27	BA	763	OMG	C5-C6	2.47	1.52	1.47
1	Aa	1025	OMG	C6-N1	2.46	1.41	1.37
1	Aa	320	OMG	C6-N1	2.46	1.41	1.37
27	BA	713	4AC	O7-C7	-2.46	1.17	1.23
27	BA	778	4AC	O7-C7	-2.45	1.17	1.23
1	Aa	1354	OMC	C6-N1	2.45	1.43	1.38
27	BA	433	4AC	O7-C7	-2.45	1.17	1.23
27	BA	1776	OMU	C6-N1	2.45	1.43	1.38
27	BA	2590	4AC	O7-C7	-2.45	1.17	1.23
27	BA	2728	OMG	C5-C6	2.45	1.52	1.47
27	BA	433	4AC	C5-C4	2.45	1.46	1.40
27	BA	805	4AC	O7-C7	-2.44	1.17	1.23
1	Aa	1265	OMG	C5-C6	2.44	1.52	1.47
1	Aa	358	4AC	O7-C7	-2.43	1.17	1.23
27	BA	1337	4AC	C5-C4	2.43	1.46	1.40
27	BA	201	4AC	O7-C7	-2.42	1.17	1.23
27	BA	2630	OMC	C6-N1	2.42	1.43	1.38
27	BA	2838	4AC	O7-C7	-2.42	1.17	1.23
27	BA	505	A2M	C4-N3	-2.42	1.32	1.35
27	BA	2152	OMG	C2-N2	2.42	1.40	1.34
1	Aa	1217	4AC	O7-C7	-2.42	1.17	1.23
1	Aa	913	OMG	C5-C6	2.41	1.52	1.47
27	BA	1517	A2M	O3'-C3'	-2.41	1.37	1.43
1	Aa	1361	OMC	C6-N1	2.41	1.43	1.38
27	BA	619	OMU	C6-N1	2.41	1.43	1.38
27	BA	2595	OMC	C6-N1	2.41	1.43	1.38
27	BA	932	A2M	O5'-C5'	-2.40	1.38	1.44
1	Aa	659	OMG	C5-C6	2.40	1.52	1.47
27	BA	800	OMG	C5-C6	2.40	1.52	1.47
27	BA	34	OMU	C6-N1	2.40	1.43	1.38
27	BA	825	A2M	O2'-C2'	2.40	1.48	1.42
1	Aa	532	OMG	C5-C6	2.39	1.52	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Aa	138	OMG	C5-C6	2.39	1.52	1.47
1	Aa	854	5MC	C6-N1	2.39	1.42	1.38
1	Aa	917	5MU	C2-N3	-2.39	1.33	1.38
1	Aa	450	OMG	C5-C6	2.39	1.52	1.47
27	BA	1558	OMG	O6-C6	-2.39	1.18	1.23
27	BA	1820	OMC	C6-N1	2.39	1.43	1.38
27	BA	2047	OMC	C6-N1	2.38	1.43	1.38
27	BA	215	OMG	C2-N1	2.38	1.43	1.37
27	BA	2553	4SU	C6-N1	2.37	1.43	1.38
27	BA	2168	OMG	O6-C6	-2.37	1.18	1.23
1	Aa	827	4AC	O7-C7	-2.37	1.17	1.23
1	Aa	917	5MU	C6-N1	-2.37	1.34	1.38
27	BA	1396	4AC	O7-C7	-2.36	1.17	1.23
27	BA	1431	4AC	O7-C7	-2.36	1.17	1.23
1	Aa	479	OMU	O2-C2	-2.36	1.18	1.23
1	Aa	246	OMG	C5-C6	2.36	1.52	1.47
1	Aa	825	OMC	C6-N1	2.36	1.43	1.38
1	Aa	818	4AC	O7-C7	-2.36	1.17	1.23
27	BA	201	4AC	C5-C4	2.36	1.45	1.40
27	BA	2010	OMG	C5-C6	2.35	1.52	1.47
27	BA	2992	4AC	O7-C7	-2.35	1.17	1.23
27	BA	1892	OMG	C6-N1	2.35	1.41	1.37
27	BA	27	4AC	O7-C7	-2.35	1.17	1.23
27	BA	1810	4AC	C5-C4	2.35	1.45	1.40
27	BA	1525	OMG	C5-C6	2.35	1.52	1.47
27	BA	1400	A2M	C6-C5	-2.35	1.34	1.43
27	BA	2657	OMG	C6-N1	2.35	1.41	1.37
27	BA	1543	4AC	O7-C7	-2.35	1.17	1.23
1	Aa	525	4AC	O7-C7	-2.35	1.17	1.23
27	BA	244	4AC	C5-C4	2.35	1.45	1.40
27	BA	849	A2M	O2'-C2'	2.34	1.48	1.42
27	BA	1431	4AC	O2-C2	-2.34	1.19	1.23
27	BA	872	A2M	C6-N6	2.34	1.42	1.34
27	BA	768	OMU	C6-N1	2.34	1.43	1.38
1	Aa	498	OMG	C5-C6	2.34	1.52	1.47
27	BA	1480	OMU	C6-N1	2.34	1.43	1.38
27	BA	799	4AC	O7-C7	-2.34	1.18	1.23
1	Aa	913	OMG	C2-N1	2.33	1.43	1.37
27	BA	2016	OMG	C5-C6	2.33	1.52	1.47
27	BA	2389	OMU	C2-N3	-2.33	1.33	1.38
27	BA	353	OMG	C6-N1	2.33	1.41	1.37
1	Aa	876	OMG	C5-C6	2.33	1.52	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Aa	8	OMU	C6-N1	2.33	1.43	1.38
27	BA	2324	OMG	C6-N1	2.33	1.41	1.37
1	Aa	1459	4AC	O2-C2	-2.32	1.19	1.23
27	BA	418	4AC	O7-C7	-2.32	1.18	1.23
27	BA	805	4AC	C5-C4	2.32	1.45	1.40
27	BA	290	OMG	C6-N1	2.32	1.41	1.37
27	BA	2590	4AC	O2-C2	-2.32	1.19	1.23
27	BA	2035	5MC	O2'-C2'	2.32	1.48	1.43
1	Aa	994	OMG	C2-N1	2.32	1.43	1.37
27	BA	869	OMC	C6-N1	2.31	1.43	1.38
27	BA	2019	OMG	C2-N1	2.31	1.43	1.37
27	BA	561	OMC	C6-N1	2.31	1.43	1.38
1	Aa	457	5MC	O2'-C2'	2.31	1.48	1.43
27	BA	365	OMG	C6-N1	2.31	1.41	1.37
27	BA	1940	OMG	C6-N1	2.30	1.41	1.37
1	Aa	697	4AC	O7-C7	-2.30	1.18	1.23
27	BA	2542	OMU	C6-N1	2.30	1.43	1.38
1	Aa	892	OMG	C5-C6	2.30	1.52	1.47
27	BA	1517	A2M	O2'-C2'	2.30	1.48	1.42
27	BA	1400	A2M	O5'-C5'	-2.30	1.39	1.44
27	BA	674	OMG	O6-C6	-2.29	1.18	1.23
27	BA	1899	4AC	C5-C4	2.29	1.45	1.40
27	BA	124	4AC	O2-C2	-2.29	1.19	1.23
27	BA	2070	5MC	C6-C5	2.28	1.38	1.34
27	BA	1305	4AC	O7-C7	-2.28	1.18	1.23
27	BA	2159	4AC	O2-C2	-2.28	1.19	1.23
27	BA	488	A2M	O5'-C5'	-2.27	1.39	1.44
27	BA	1892	OMG	C5-C6	2.27	1.52	1.47
1	Aa	382	OMG	C5-C6	2.27	1.52	1.47
27	BA	1969	OMU	C6-N1	2.26	1.43	1.38
27	BA	2527	OMG	C6-N1	2.25	1.41	1.37
27	BA	505	A2M	O3'-C3'	-2.25	1.37	1.43
27	BA	763	OMG	O6-C6	-2.25	1.18	1.23
27	BA	872	A2M	C6-C5	-2.25	1.34	1.43
27	BA	1375	4AC	O2-C2	-2.24	1.19	1.23
27	BA	2389	OMU	C5-C4	-2.24	1.38	1.43
1	Aa	1026	OMG	C5-C6	2.24	1.52	1.47
1	Aa	446	OMG	C5-C6	2.24	1.52	1.47
27	BA	1799	OMG	C5-C6	2.24	1.51	1.47
27	BA	2656	OMU	C6-N1	2.23	1.43	1.38
27	BA	1434	4AC	C5-C4	2.23	1.45	1.40
1	Aa	41	4AC	O7-C7	-2.23	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	124	4AC	C5-C4	2.23	1.45	1.40
27	BA	932	A2M	O2'-C2'	2.21	1.48	1.42
27	BA	2657	OMG	C5-C6	2.21	1.51	1.47
1	Aa	1025	OMG	C5-C6	2.21	1.51	1.47
1	Aa	352	A2M	C5-C4	2.21	1.46	1.40
27	BA	799	4AC	O2-C2	-2.20	1.19	1.23
1	Aa	136	4AC	O7-C7	-2.20	1.18	1.23
27	BA	365	OMG	C5-C6	2.20	1.51	1.47
27	BA	872	A2M	O2'-C2'	2.19	1.48	1.42
27	BA	805	4AC	O2-C2	-2.19	1.19	1.23
1	Aa	771	OMG	C5-C6	2.19	1.51	1.47
1	Aa	525	4AC	O2-C2	-2.19	1.19	1.23
1	Aa	479	OMU	C5-C4	2.19	1.48	1.43
27	BA	201	4AC	O2-C2	-2.18	1.19	1.23
27	BA	290	OMG	C2-N1	2.18	1.43	1.37
1	Aa	1107	OMG	C2-N1	2.18	1.43	1.37
27	BA	1106	OMG	C5-C6	2.18	1.51	1.47
27	BA	1953	OMG	C5-C6	2.18	1.51	1.47
27	BA	1434	4AC	O2-C2	-2.18	1.19	1.23
27	BA	825	A2M	C6-C5	-2.18	1.35	1.43
27	BA	2521	OMG	C5-C6	2.17	1.51	1.47
27	BA	2550	OMG	C5-C6	2.17	1.51	1.47
27	BA	2581	4SU	C6-N1	2.17	1.43	1.38
27	BA	872	A2M	C5-N7	-2.17	1.31	1.39
27	BA	849	A2M	O5'-C5'	-2.17	1.39	1.44
27	BA	505	A2M	C5-N7	-2.17	1.31	1.39
1	Aa	381	OMG	C5-C6	2.16	1.51	1.47
1	Aa	1276	5MC	O2'-C2'	2.16	1.48	1.43
27	BA	1396	4AC	O2-C2	-2.16	1.19	1.23
27	BA	1400	A2M	C8-N7	-2.15	1.30	1.34
27	BA	575	OMG	O6-C6	-2.15	1.18	1.23
1	Aa	730	4AC	O2-C2	-2.15	1.19	1.23
27	BA	2018	OMC	C6-N1	2.14	1.43	1.38
27	BA	617	LHH	O7-C7	-2.14	1.18	1.23
27	BA	723	OMG	C2-N1	2.14	1.43	1.37
27	BA	212	A2M	C5-C4	2.14	1.46	1.40
27	BA	912	OMG	C2-N1	2.14	1.43	1.37
27	BA	756	A2M	O2'-C2'	2.14	1.48	1.42
27	BA	526	LHH	O7-C7	-2.14	1.18	1.23
27	BA	1400	A2M	C5-N7	-2.14	1.32	1.39
27	BA	2702	A2M	C6-C5	-2.14	1.35	1.43
27	BA	912	OMG	C5-C6	2.13	1.51	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	2955	LHH	O7-C7	-2.13	1.18	1.23
27	BA	1400	A2M	C6-N6	2.13	1.41	1.34
27	BA	1790	OMC	C6-N1	2.12	1.43	1.38
27	BA	833	OMG	C6-N1	2.12	1.41	1.37
27	BA	244	4AC	O2-C2	-2.12	1.19	1.23
1	Aa	1476	5MC	O2'-C2'	2.12	1.48	1.43
27	BA	2832	4AC	O2-C2	-2.12	1.19	1.23
27	BA	825	A2M	C6-N6	2.12	1.41	1.34
27	BA	849	A2M	O3'-C3'	-2.11	1.38	1.43
27	BA	1953	OMG	C2-N1	2.11	1.42	1.37
1	Aa	876	OMG	C2-N1	2.11	1.42	1.37
27	BA	1319	OMU	C6-N1	2.10	1.43	1.38
27	BA	2702	A2M	C5-N7	-2.10	1.32	1.39
27	BA	858	4AC	O2-C2	-2.10	1.19	1.23
27	BA	353	OMG	C5-C6	2.10	1.51	1.47
27	BA	1305	4AC	C6-N1	2.09	1.43	1.38
27	BA	1899	4AC	O2-C2	-2.09	1.19	1.23
1	Aa	1467	MA6	C4-N3	-2.09	1.32	1.35
27	BA	2457	LHH	O7-C7	-2.08	1.18	1.23
27	BA	1955	4AC	O2-C2	-2.07	1.19	1.23
27	BA	3009	4AC	O2-C2	-2.07	1.19	1.23
27	BA	1750	OMC	C6-N1	2.07	1.43	1.38
1	Aa	1467	MA6	C5-N7	-2.07	1.32	1.39
27	BA	1799	OMG	O6-C6	-2.07	1.19	1.23
27	BA	2121	4AC	O2-C2	-2.07	1.19	1.23
27	BA	730	4AC	O2-C2	-2.07	1.19	1.23
1	Aa	381	OMG	C2-N1	2.07	1.42	1.37
1	Aa	5	4AC	O2-C2	-2.07	1.19	1.23
27	BA	1357	4AC	O2-C2	-2.07	1.19	1.23
27	BA	27	4AC	O2-C2	-2.07	1.19	1.23
1	Aa	1020	LHH	O7-C7	-2.06	1.18	1.23
27	BA	453	OMU	C6-N1	2.06	1.42	1.38
27	BA	1340	OMU	C6-N1	2.05	1.42	1.38
1	Aa	1358	OMU	C6-N1	2.05	1.42	1.38
27	BA	215	OMG	C5-C6	2.05	1.51	1.47
27	BA	1810	4AC	O2-C2	-2.05	1.19	1.23
27	BA	932	A2M	C5-N7	-2.05	1.32	1.39
27	BA	418	4AC	O2-C2	-2.05	1.19	1.23
27	BA	825	A2M	C5-N7	-2.05	1.32	1.39
27	BA	2521	OMG	C6-N1	2.04	1.40	1.37
27	BA	756	A2M	C5-N7	-2.04	1.32	1.39
27	BA	2159	4AC	C5-C4	2.04	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Aa	1276	5MC	O5'-C5'	-2.04	1.39	1.44
27	BA	552	OMG	C2-N1	2.04	1.42	1.37
27	BA	2797	4AC	O2-C2	-2.03	1.19	1.23
27	BA	849	A2M	C5-N7	-2.03	1.32	1.39
1	Aa	847	4AC	O2-C2	-2.03	1.19	1.23
1	Aa	229	LHH	O7-C7	-2.03	1.18	1.23
27	BA	2702	A2M	O5'-C5'	-2.03	1.39	1.44
27	BA	778	4AC	C6-N1	2.02	1.42	1.38
27	BA	2528	OMG	C5-C6	2.02	1.51	1.47
27	BA	250	OMC	C6-N1	2.02	1.42	1.38
27	BA	1799	OMG	C2-N1	2.02	1.42	1.37
27	BA	2610	OMU	C5-C4	2.01	1.48	1.43
27	BA	2992	4AC	C6-N1	2.01	1.42	1.38
1	Aa	659	OMG	C2-N1	2.01	1.42	1.37
1	Aa	1265	OMG	C2-N1	2.01	1.42	1.37
27	BA	1517	A2M	O5'-C5'	-2.01	1.39	1.44
1	Aa	818	4AC	O2-C2	-2.01	1.20	1.23
27	BA	1337	4AC	O2-C2	-2.00	1.20	1.23
27	BA	488	A2M	C5-N7	-2.00	1.32	1.39

All (955) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Aa	1468	MA6	N1-C6-N6	-13.10	103.27	117.06
27	BA	1905	5MU	C5-C4-N3	12.43	125.92	115.31
27	BA	537	5MU	C5-C4-N3	12.41	125.90	115.31
1	Aa	1467	MA6	N1-C6-N6	-12.33	104.08	117.06
27	BA	1548	5MU	C5-C4-N3	12.23	125.75	115.31
27	BA	572	5MU	C5-C4-N3	12.21	125.73	115.31
27	BA	875	5MU	C5-C4-N3	12.16	125.69	115.31
27	BA	2384	5MU	C5-C4-N3	11.97	125.53	115.31
27	BA	298	5MU	C5-C4-N3	11.66	125.26	115.31
27	BA	2688	5MU	C5-C4-N3	11.34	124.99	115.31
27	BA	1085	5MU	C5-C6-N1	-10.38	112.67	123.34
27	BA	505	A2M	C5-C6-N6	10.33	136.05	120.35
27	BA	1265	A2M	C5-C6-N6	10.11	135.72	120.35
27	BA	1085	5MU	C5-C4-N3	10.06	123.90	115.31
27	BA	849	A2M	C5-C6-N6	9.70	135.10	120.35
27	BA	1085	5MU	C5M-C5-C6	-9.63	109.99	122.85
27	BA	2688	5MU	C5-C6-N1	-9.37	113.70	123.34
27	BA	879	A2M	C5-C6-N6	8.96	133.96	120.35
27	BA	1548	5MU	C5-C6-N1	-8.94	114.14	123.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BA	875	5MU	C5-C6-N1	-8.93	114.15	123.34
27	BA	298	5MU	C5-C6-N1	-8.92	114.16	123.34
27	BA	488	A2M	C5-C6-N6	8.88	133.85	120.35
27	BA	872	A2M	C5-C6-N6	8.87	133.83	120.35
27	BA	2384	5MU	C5-C6-N1	-8.76	114.32	123.34
27	BA	756	A2M	C5-C6-N6	8.63	133.47	120.35
27	BA	1517	A2M	C5-C6-N6	8.50	133.27	120.35
27	BA	537	5MU	C5-C6-N1	-8.45	114.65	123.34
27	BA	825	A2M	C5-C6-N6	8.29	132.95	120.35
27	BA	1400	A2M	C5-C6-N6	8.28	132.94	120.35
27	BA	419	OMG	O6-C6-N1	-8.05	111.14	120.65
27	BA	1085	5MU	C5M-C5-C4	8.02	127.59	118.77
27	BA	1905	5MU	C5-C6-N1	-7.99	115.12	123.34
27	BA	419	OMG	C2-N1-C6	-7.82	110.70	125.10
27	BA	572	5MU	C5-C6-N1	-7.81	115.31	123.34
27	BA	932	A2M	C5-C6-N6	7.77	132.16	120.35
27	BA	2457	LHH	CM7-C7-N4	7.76	128.72	115.29
27	BA	2702	A2M	C5-C6-N6	7.62	131.93	120.35
27	BA	537	5MU	C5M-C5-C4	7.62	127.15	118.77
27	BA	2581	4SU	C4-N3-C2	-7.57	119.98	127.34
27	BA	1265	A2M	N6-C6-N1	-7.49	103.03	118.57
27	BA	1905	5MU	C5M-C5-C4	7.46	126.98	118.77
27	BA	505	A2M	N6-C6-N1	-7.20	103.62	118.57
27	BA	419	OMG	C5-C6-N1	7.12	126.52	113.95
27	BA	849	A2M	N6-C6-N1	-6.72	104.64	118.57
27	BA	2553	4SU	C4-N3-C2	-6.60	120.92	127.34
27	BA	872	A2M	N6-C6-N1	-6.55	104.98	118.57
27	BA	572	5MU	C5M-C5-C4	6.53	125.95	118.77
27	BA	879	A2M	N6-C6-N1	-6.44	105.21	118.57
27	BA	488	A2M	N6-C6-N1	-6.38	105.34	118.57
27	BA	2384	5MU	C5M-C5-C4	6.32	125.73	118.77
27	BA	537	5MU	C5M-C5-C6	-6.31	114.42	122.85
27	BA	419	OMG	N2-C2-N3	-6.28	107.51	119.74
1	Aa	1449	6MZ	C2-N1-C6	6.20	121.91	116.59
1	Aa	1358	OMU	C4-N3-C2	-6.19	118.42	126.58
27	BA	825	A2M	N6-C6-N1	-6.18	105.74	118.57
27	BA	1400	A2M	N6-C6-N1	-6.14	105.83	118.57
1	Aa	136	4AC	CM7-C7-N4	6.09	125.83	115.29
27	BA	756	A2M	N6-C6-N1	-6.05	106.01	118.57
27	BA	1517	A2M	N6-C6-N1	-6.01	106.11	118.57
1	Aa	41	4AC	CM7-C7-N4	5.99	125.66	115.29
27	BA	2955	LHH	CM7-C7-N4	5.96	125.60	115.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BA	298	5MU	O4-C4-C5	-5.95	118.00	124.90
27	BA	1905	5MU	C5M-C5-C6	-5.92	114.94	122.85
27	BA	858	4AC	CM7-C7-N4	5.90	125.49	115.29
1	Aa	358	4AC	CM7-C7-N4	5.88	125.47	115.29
27	BA	2688	5MU	C5M-C5-C6	-5.85	115.03	122.85
1	Aa	5	4AC	CM7-C7-N4	5.84	125.39	115.29
27	BA	572	5MU	O4-C4-C5	-5.79	118.19	124.90
27	BA	1085	5MU	O4-C4-C5	-5.78	118.20	124.90
27	BA	1434	4AC	CM7-C7-N4	5.78	125.29	115.29
1	Aa	697	4AC	CM7-C7-N4	5.71	125.17	115.29
1	Aa	525	4AC	N4-C4-N3	5.71	123.43	113.85
27	BA	1305	4AC	CM7-C7-N4	5.71	125.16	115.29
27	BA	201	4AC	CM7-C7-N4	5.70	125.15	115.29
27	BA	1085	5MU	C4-N3-C2	-5.62	120.07	127.35
27	BA	617	LHH	CM7-C7-N4	5.60	124.99	115.29
27	BA	2688	5MU	C5M-C5-C4	5.60	124.93	118.77
27	BA	2702	A2M	N6-C6-N1	-5.59	106.97	118.57
27	BA	932	A2M	N6-C6-N1	-5.54	107.08	118.57
1	Aa	229	LHH	CM7-C7-N4	5.47	124.75	115.29
27	BA	2384	5MU	C5M-C5-C6	-5.44	115.58	122.85
27	BA	2610	OMU	C4-N3-C2	-5.43	119.42	126.58
1	Aa	818	4AC	CM7-C7-N4	5.42	124.66	115.29
1	Aa	917	5MU	C4-N3-C2	-5.40	120.36	127.35
27	BA	875	5MU	O4-C4-C5	-5.39	118.65	124.90
27	BA	1400	A2M	N3-C2-N1	-5.39	120.25	128.68
27	BA	875	5MU	C5M-C5-C4	5.35	124.66	118.77
1	Aa	730	4AC	CM7-C7-N4	5.30	124.46	115.29
27	BA	572	5MU	C5M-C5-C6	-5.30	115.78	122.85
27	BA	768	OMU	C4-N3-C2	-5.29	119.60	126.58
27	BA	2656	OMU	C4-N3-C2	-5.28	119.61	126.58
27	BA	1548	5MU	O4-C4-C5	-5.25	118.81	124.90
1	Aa	917	5MU	N3-C2-N1	5.24	121.85	114.89
27	BA	1085	5MU	C6-C5-C4	5.24	122.41	118.03
1	Aa	479	OMU	C4-N3-C2	-5.23	119.69	126.58
27	BA	1517	A2M	N3-C2-N1	-5.20	120.55	128.68
1	Aa	1468	MA6	N3-C2-N1	-5.17	120.60	128.68
1	Aa	304	OMU	C4-N3-C2	-5.16	119.77	126.58
27	BA	537	5MU	O4-C4-C5	-5.16	118.92	124.90
27	BA	619	OMU	C4-N3-C2	-5.14	119.80	126.58
1	Aa	1020	LHH	CM7-C7-N4	5.12	124.15	115.29
27	BA	875	5MU	C5M-C5-C6	-5.11	116.02	122.85
27	BA	2581	4SU	C5-C4-N3	5.10	119.42	114.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Aa	240	OMU	C4-N3-C2	-5.09	119.86	126.58
27	BA	1319	OMU	C4-N3-C2	-5.09	119.86	126.58
27	BA	849	A2M	N3-C2-N1	-5.09	120.73	128.68
27	BA	825	A2M	N3-C2-N1	-5.07	120.75	128.68
27	BA	1548	5MU	C4-N3-C2	-4.98	120.91	127.35
27	BA	298	5MU	C5M-C5-C6	-4.95	116.24	122.85
27	BA	1340	OMU	C4-N3-C2	-4.94	120.07	126.58
27	BA	453	OMU	C4-N3-C2	-4.93	120.08	126.58
27	BA	2688	5MU	C4-N3-C2	-4.88	121.03	127.35
27	BA	1085	5MU	N3-C2-N1	4.88	121.37	114.89
1	Aa	8	OMU	C4-N3-C2	-4.87	120.15	126.58
1	Aa	1467	MA6	N3-C2-N1	-4.86	121.08	128.68
27	BA	1551	OMU	C4-N3-C2	-4.85	120.19	126.58
27	BA	872	A2M	N3-C2-N1	-4.84	121.11	128.68
27	BA	298	5MU	C4-N3-C2	-4.84	121.09	127.35
27	BA	2384	5MU	N3-C2-N1	4.84	121.31	114.89
27	BA	298	5MU	C5M-C5-C4	4.84	124.09	118.77
27	BA	2384	5MU	C4-N3-C2	-4.83	121.10	127.35
1	Aa	52	OMU	C4-N3-C2	-4.82	120.22	126.58
27	BA	34	OMU	C4-N3-C2	-4.80	120.25	126.58
1	Aa	605	4AC	CM7-C7-N4	4.80	123.59	115.29
27	BA	1905	5MU	O4-C4-C5	-4.73	119.41	124.90
27	BA	1548	5MU	N3-C2-N1	4.72	121.16	114.89
27	BA	2702	A2M	N3-C2-N1	-4.72	121.31	128.68
27	BA	932	A2M	N3-C2-N1	-4.71	121.31	128.68
27	BA	2542	OMU	C4-N3-C2	-4.71	120.37	126.58
27	BA	1969	OMU	C4-N3-C2	-4.70	120.38	126.58
27	BA	1776	OMU	C4-N3-C2	-4.70	120.38	126.58
27	BA	1548	5MU	C5M-C5-C4	4.69	123.93	118.77
27	BA	912	OMG	C5-C6-N1	4.69	122.22	113.95
1	Aa	1358	OMU	N3-C2-N1	4.68	121.10	114.89
27	BA	2528	OMG	C5-C6-N1	4.68	122.21	113.95
27	BA	1480	OMU	C4-N3-C2	-4.65	120.44	126.58
1	Aa	917	5MU	C5-C4-N3	4.65	119.28	115.31
27	BA	756	A2M	N3-C2-N1	-4.64	121.42	128.68
27	BA	2688	5MU	O4-C4-C5	-4.63	119.53	124.90
27	BA	1265	A2M	N3-C2-N1	-4.63	121.44	128.68
27	BA	1085	5MU	C1'-N1-C2	4.61	125.91	117.57
1	Aa	1217	4AC	N4-C4-N3	4.60	121.58	113.85
27	BA	879	A2M	N3-C2-N1	-4.58	121.51	128.68
27	BA	353	OMG	C5-C6-N1	4.56	122.01	113.95
27	BA	537	5MU	C4-N3-C2	-4.55	121.46	127.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Aa	605	4AC	N4-C4-N3	4.54	121.48	113.85
27	BA	2379	OMG	O6-C6-N1	-4.53	115.30	120.65
1	Aa	525	4AC	CM7-C7-N4	4.49	123.06	115.29
27	BA	912	OMG	O6-C6-N1	-4.47	115.36	120.65
27	BA	215	OMG	C5-C6-N1	4.46	121.83	113.95
27	BA	505	A2M	N3-C2-N1	-4.45	121.72	128.68
27	BA	298	5MU	N3-C2-N1	4.45	120.79	114.89
27	BA	1548	5MU	C5M-C5-C6	-4.45	116.91	122.85
27	BA	572	5MU	C4-N3-C2	-4.44	121.60	127.35
27	BA	875	5MU	C4-N3-C2	-4.41	121.64	127.35
27	BA	2389	OMU	C4-N3-C2	-4.38	120.80	126.58
27	BA	2688	5MU	N3-C2-N1	4.38	120.70	114.89
27	BA	2581	4SU	C5-C4-S4	-4.37	118.83	124.47
1	Aa	8	OMU	N3-C2-N1	4.36	120.68	114.89
27	BA	1905	5MU	C4-N3-C2	-4.35	121.72	127.35
27	BA	1953	OMG	C5-C6-N1	4.34	121.62	113.95
1	Aa	917	5MU	O4-C4-C5	-4.33	119.88	124.90
27	BA	2379	OMG	C5-C6-N1	4.32	121.57	113.95
27	BA	63	OMG	C5-C6-N1	4.31	121.56	113.95
27	BA	488	A2M	N3-C2-N1	-4.26	122.03	128.68
27	BA	215	OMG	O6-C6-N1	-4.25	115.63	120.65
27	BA	912	OMG	C2-N1-C6	-4.21	117.34	125.10
27	BA	2550	OMG	C5-C6-N1	4.21	121.38	113.95
27	BA	419	OMG	N2-C2-N1	4.19	125.64	116.71
27	BA	2019	OMG	C5-C6-N1	4.17	121.32	113.95
27	BA	2159	4AC	N4-C4-N3	4.16	120.83	113.85
1	Aa	682	4AC	N4-C4-N3	4.11	120.75	113.85
27	BA	858	4AC	O7-C7-N4	-4.10	115.18	121.82
27	BA	2955	LHH	O3'-C3'-C2'	4.08	122.76	111.17
27	BA	2780	4AC	N4-C4-N3	4.08	120.70	113.85
27	BA	1810	4AC	N4-C4-N3	4.07	120.69	113.85
27	BA	833	OMG	C5-C6-N1	4.06	121.12	113.95
27	BA	2610	OMU	N3-C2-N1	4.05	120.27	114.89
27	BA	526	LHH	N4-C4-N3	4.03	120.62	113.85
1	Aa	913	OMG	O3'-C3'-C2'	4.03	122.61	111.17
27	BA	2553	4SU	N3-C2-N1	4.02	120.22	114.89
27	BA	2656	OMU	N3-C2-N1	4.02	120.22	114.89
1	Aa	1459	4AC	N4-C4-N3	4.02	120.59	113.85
27	BA	833	OMG	C2-N1-C6	-4.01	117.72	125.10
27	BA	1776	OMU	N3-C2-N1	4.00	120.20	114.89
27	BA	1085	5MU	C1'-N1-C6	-3.97	114.51	121.12
27	BA	2992	4AC	N4-C4-N3	3.97	120.52	113.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BA	572	5MU	N3-C2-N1	3.97	120.16	114.89
1	Aa	240	OMU	N3-C2-N1	3.96	120.15	114.89
27	BA	2672	OMG	C5-C6-N1	3.96	120.94	113.95
1	Aa	298	4AC	N4-C4-N3	3.96	120.50	113.85
27	BA	768	OMU	N3-C2-N1	3.96	120.14	114.89
1	Aa	298	4AC	CM7-C7-N4	3.94	122.11	115.29
27	BA	298	5MU	C1'-N1-C2	3.91	124.64	117.57
1	Aa	373	4AC	N4-C4-N3	3.91	120.41	113.85
27	BA	290	OMG	C2-N1-C6	-3.90	117.92	125.10
27	BA	2745	OMG	C5-C6-N1	3.89	120.83	113.95
1	Aa	501	4AC	N4-C4-N3	3.89	120.38	113.85
27	BA	1525	OMG	C5-C6-N1	3.88	120.80	113.95
27	BA	2457	LHH	O7-C7-N4	-3.88	115.54	121.82
27	BA	657	OMU	C1'-N1-C2	3.88	124.59	117.57
27	BA	723	OMG	CM2-O2'-C2'	-3.87	104.38	114.52
27	BA	215	OMG	C2-N1-C6	-3.86	117.99	125.10
27	BA	2672	OMG	O6-C6-N1	-3.86	116.09	120.65
27	BA	2672	OMG	C2-N1-C6	-3.85	118.00	125.10
27	BA	2016	OMG	C5-C6-N1	3.85	120.75	113.95
27	BA	290	OMG	C5-C6-N1	3.85	120.74	113.95
1	Aa	913	OMG	C5-C6-N1	3.83	120.71	113.95
1	Aa	917	5MU	C5-C6-N1	-3.83	119.40	123.34
27	BA	2528	OMG	O6-C6-N1	-3.83	116.13	120.65
27	BA	1551	OMU	N3-C2-N1	3.80	119.94	114.89
27	BA	2550	OMG	C2-N1-C6	-3.80	118.11	125.10
27	BA	2019	OMG	C2-N1-C6	-3.79	118.12	125.10
27	BA	526	LHH	CM7-C7-N4	3.79	121.85	115.29
27	BA	657	OMU	C4-N3-C2	-3.79	121.58	126.58
27	BA	2389	OMU	C5-C4-N3	3.78	120.50	114.84
27	BA	925	4AC	CM7-C7-N4	3.78	121.83	115.29
27	BA	2955	LHH	O3'-C3'-C4'	3.76	121.92	111.05
27	BA	27	4AC	N4-C4-N3	3.76	120.16	113.85
27	BA	1905	5MU	C1'-N1-C2	3.75	124.36	117.57
27	BA	453	OMU	O4-C4-C5	-3.74	118.58	125.16
1	Aa	605	4AC	O7-C7-CM7	-3.74	115.12	122.06
27	BA	501	4AC	N4-C4-N3	3.74	120.12	113.85
1	Aa	913	OMG	O3'-C3'-C4'	3.73	121.84	111.05
27	BA	1396	4AC	N4-C4-N3	3.73	120.11	113.85
27	BA	2389	OMU	N3-C2-N1	3.72	119.83	114.89
27	BA	537	5MU	N3-C2-N1	3.72	119.83	114.89
27	BA	2545	OMC	O3'-C3'-C2'	3.72	121.73	111.17
27	BA	2055	5MC	C5-C6-N1	-3.71	119.53	123.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BA	2070	5MC	C5-C6-N1	-3.70	119.53	123.34
27	BA	875	5MU	N3-C2-N1	3.68	119.77	114.89
27	BA	1905	5MU	N3-C2-N1	3.68	119.77	114.89
27	BA	1431	4AC	N4-C4-N3	3.67	120.02	113.85
27	BA	2581	4SU	N3-C2-N1	3.67	119.76	114.89
1	Aa	304	OMU	N3-C2-N1	3.67	119.76	114.89
27	BA	1953	OMG	C2-N1-C6	-3.67	118.34	125.10
1	Aa	730	4AC	C6-C5-C4	3.66	121.44	116.96
1	Aa	854	5MC	C5-C6-N1	-3.65	119.58	123.34
27	BA	2550	OMG	O6-C6-N1	-3.65	116.34	120.65
27	BA	2384	5MU	O4-C4-C5	-3.65	120.67	124.90
1	Aa	1358	OMU	O3'-C3'-C4'	3.64	121.59	111.05
27	BA	2075	5MC	C5-C6-N1	-3.64	119.59	123.34
27	BA	2542	OMU	N3-C2-N1	3.63	119.71	114.89
27	BA	2457	LHH	C6-C5-C4	3.63	121.40	116.96
27	BA	572	5MU	C1'-N1-C2	3.62	124.13	117.57
27	BA	2553	4SU	C5-C4-N3	3.62	118.05	114.69
27	BA	1470	4AC	N4-C4-N3	3.62	119.93	113.85
1	Aa	913	OMG	C2-N1-C6	-3.62	118.44	125.10
27	BA	2838	4AC	N4-C4-N3	3.61	119.91	113.85
27	BA	2728	OMG	C5-C6-N1	3.60	120.31	113.95
1	Aa	1478	5MC	C5-C6-N1	-3.59	119.64	123.34
27	BA	1357	4AC	N4-C4-N3	3.59	119.87	113.85
1	Aa	1358	OMU	O3'-C3'-C2'	3.59	121.35	111.17
27	BA	2521	OMG	C2-N1-C6	-3.58	118.51	125.10
1	Aa	569	4AC	N4-C4-N3	3.58	119.86	113.85
27	BA	1969	OMU	N3-C2-N1	3.57	119.63	114.89
27	BA	869	OMC	C5-C4-N4	-3.56	114.97	120.57
1	Aa	605	4AC	C6-C5-C4	3.55	121.30	116.96
1	Aa	464	5MC	CM5-C5-C6	-3.54	118.12	122.85
27	BA	56	4AC	O3'-C3'-C4'	3.54	121.29	111.05
27	BA	2745	OMG	C2-N1-C6	-3.53	118.59	125.10
27	BA	2016	OMG	C2-N1-C6	-3.53	118.60	125.10
27	BA	2542	OMU	O4-C4-C5	-3.53	118.95	125.16
27	BA	619	OMU	N3-C2-N1	3.53	119.57	114.89
27	BA	799	4AC	N4-C4-N3	3.51	119.75	113.85
27	BA	723	OMG	C2-N1-C6	-3.51	118.63	125.10
27	BA	2521	OMG	C5-C6-N1	3.50	120.14	113.95
27	BA	2745	OMG	O6-C6-N1	-3.50	116.52	120.65
27	BA	2152	OMG	C5-C6-N1	3.49	120.11	113.95
27	BA	718	OMC	C5-C4-N4	-3.48	115.10	120.57
27	BA	376	4AC	N4-C4-N3	3.48	119.69	113.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Aa	1004	5MC	CM5-C5-C6	-3.47	118.21	122.85
27	BA	1899	4AC	N4-C4-N3	3.47	119.68	113.85
27	BA	1375	4AC	N4-C4-N3	3.47	119.67	113.85
1	Aa	525	4AC	C5-C4-N4	-3.46	116.90	122.92
27	BA	925	4AC	C6-C5-C4	3.46	121.20	116.96
1	Aa	479	OMU	N3-C2-N1	3.46	119.49	114.89
27	BA	2610	OMU	C5-C4-N3	3.46	120.02	114.84
1	Aa	298	4AC	O7-C7-CM7	-3.45	115.66	122.06
1	Aa	52	OMU	N3-C2-N1	3.43	119.44	114.89
27	BA	552	OMG	C2-N1-C6	-3.41	118.82	125.10
27	BA	2379	OMG	C2-N1-C6	-3.41	118.82	125.10
27	BA	1398	OMG	C5-C6-N1	3.41	119.97	113.95
27	BA	2457	LHH	O7-C7-CM7	-3.40	115.73	122.06
27	BA	537	5MU	C1'-N1-C2	3.40	123.73	117.57
27	BA	723	OMG	C5-C6-N1	3.40	119.96	113.95
27	BA	2010	OMG	C5-C6-N1	3.40	119.95	113.95
27	BA	2657	OMG	C5-C6-N1	3.40	119.95	113.95
27	BA	34	OMU	N3-C2-N1	3.39	119.38	114.89
27	BA	944	5MC	CM5-C5-C6	-3.38	118.33	122.85
27	BA	1340	OMU	O4-C4-C5	-3.38	119.22	125.16
1	Aa	501	4AC	CM7-C7-N4	3.38	121.14	115.29
27	BA	2832	4AC	N4-C4-N3	3.38	119.52	113.85
1	Aa	1358	OMU	C5-C4-N3	3.38	119.89	114.84
1	Aa	994	OMG	C5-C6-N1	3.37	119.89	113.95
27	BA	2728	OMG	C2-N1-C6	-3.36	118.91	125.10
27	BA	1525	OMG	C2-N1-C6	-3.35	118.93	125.10
1	Aa	1020	LHH	C6-C5-C4	3.35	121.05	116.96
27	BA	619	OMU	C5-C4-N3	3.34	119.84	114.84
27	BA	34	OMU	C5-C4-N3	3.34	119.83	114.84
1	Aa	827	4AC	N4-C4-N3	3.33	119.44	113.85
27	BA	3023	4AC	N4-C4-N3	3.33	119.44	113.85
27	BA	2550	OMG	O3'-C3'-C4'	3.32	120.65	111.05
27	BA	212	A2M	N3-C2-N1	-3.32	123.49	128.68
1	Aa	229	LHH	C6-C5-C4	3.32	121.02	116.96
27	BA	453	OMU	N3-C2-N1	3.31	119.28	114.89
27	BA	433	4AC	N4-C4-N3	3.31	119.41	113.85
1	Aa	479	OMU	C5-C4-N3	3.31	119.78	114.84
1	Aa	1020	LHH	N4-C4-N3	3.30	119.40	113.85
27	BA	1810	4AC	C6-C5-C4	3.30	121.00	116.96
27	BA	1319	OMU	N3-C2-N1	3.30	119.27	114.89
27	BA	2384	5MU	O4-C4-N3	-3.30	113.80	120.12
1	Aa	876	OMG	C5-C6-N1	3.29	119.77	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BA	526	LHH	O7-C7-CM7	-3.29	115.94	122.06
1	Aa	8	OMU	CM2-O2'-C2'	-3.29	105.89	114.52
27	BA	1470	4AC	O3'-C3'-C4'	3.29	120.56	111.05
1	Aa	672	5MC	C5-C6-N1	-3.29	119.95	123.34
1	Aa	1265	OMG	C5-C6-N1	3.29	119.76	113.95
27	BA	1340	OMU	N3-C2-N1	3.28	119.25	114.89
1	Aa	381	OMG	C5-C6-N1	3.28	119.75	113.95
1	Aa	1478	5MC	C5-C4-N4	-3.28	116.57	121.48
1	Aa	457	5MC	C5-C6-N1	-3.28	119.97	123.34
27	BA	2780	4AC	CM7-C7-N4	3.28	120.96	115.29
27	BA	2528	OMG	C2-N1-C6	-3.28	119.07	125.10
1	Aa	240	OMU	O4-C4-C5	-3.27	119.40	125.16
1	Aa	1217	4AC	C6-C5-C4	3.27	120.96	116.96
1	Aa	304	OMU	C5-C4-N3	3.27	119.73	114.84
27	BA	1969	OMU	O4-C4-C5	-3.26	119.42	125.16
1	Aa	730	4AC	O7-C7-CM7	-3.26	116.01	122.06
27	BA	730	4AC	N4-C4-N3	3.25	119.31	113.85
1	Aa	1358	OMU	O4-C4-C5	-3.25	119.44	125.16
27	BA	2035	5MC	C5-C6-N1	-3.25	120.00	123.34
27	BA	2527	OMG	C5-C6-N1	3.24	119.67	113.95
27	BA	1340	OMU	C5-C4-N3	3.23	119.68	114.84
27	BA	1551	OMU	O4-C4-C5	-3.23	119.47	125.16
27	BA	1337	4AC	N4-C4-N3	3.23	119.28	113.85
27	BA	453	OMU	C5-C4-N3	3.23	119.67	114.84
27	BA	2324	OMG	C5-C6-N1	3.22	119.64	113.95
27	BA	501	4AC	C6-C5-C4	3.21	120.89	116.96
27	BA	2863	5MC	C1'-N1-C6	-3.21	115.77	121.12
27	BA	2997	4AC	N4-C4-N3	3.21	119.24	113.85
27	BA	2528	OMG	N2-C2-N3	3.20	125.96	119.74
27	BA	244	4AC	N4-C4-N3	3.19	119.21	113.85
1	Aa	352	A2M	N3-C2-N1	-3.19	123.69	128.68
27	BA	2780	4AC	C6-C5-C4	3.19	120.86	116.96
27	BA	1319	OMU	O4-C4-C5	-3.18	119.56	125.16
1	Aa	138	OMG	C5-C6-N1	3.18	119.57	113.95
27	BA	2550	OMG	O3'-C3'-C2'	3.18	120.20	111.17
27	BA	2389	OMU	O4-C4-C5	-3.18	119.57	125.16
1	Aa	304	OMU	O4-C4-C5	-3.18	119.57	125.16
27	BA	1934	4AC	N4-C4-N3	3.18	119.18	113.85
27	BA	1398	OMG	C2-N1-C6	-3.18	119.25	125.10
27	BA	713	4AC	N4-C4-N3	3.17	119.18	113.85
1	Aa	569	4AC	CM7-C7-N4	3.17	120.77	115.29
1	Aa	1020	LHH	O4'-C1'-N1	3.16	115.59	108.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BA	27	4AC	C6-C5-C4	3.16	120.83	116.96
27	BA	63	OMG	O6-C6-N1	-3.16	116.92	120.65
1	Aa	501	4AC	C6-C5-C4	3.16	120.82	116.96
1	Aa	320	OMG	C5-C6-N1	3.15	119.52	113.95
27	BA	1480	OMU	N3-C2-N1	3.15	119.07	114.89
1	Aa	1459	4AC	O7-C7-CM7	-3.15	116.21	122.06
27	BA	2657	OMG	C2-N1-C6	-3.15	119.30	125.10
1	Aa	446	OMG	C5-C6-N1	3.14	119.50	113.95
1	Aa	1459	4AC	C1'-N1-C2	3.14	125.42	118.42
27	BA	805	4AC	N4-C4-N3	3.13	119.11	113.85
27	BA	849	A2M	C3'-C2'-C1'	3.13	108.77	102.89
27	BA	1480	OMU	C5-C4-N3	3.13	119.52	114.84
1	Aa	854	5MC	CM5-C5-C6	-3.12	118.68	122.85
1	Aa	1449	6MZ	N3-C2-N1	-3.12	123.80	128.68
1	Aa	240	OMU	C5-C4-N3	3.12	119.51	114.84
1	Aa	1434	OMG	C5-C6-N1	3.12	119.46	113.95
27	BA	2955	LHH	C6-C5-C4	3.11	120.77	116.96
1	Aa	670	2MG	C5-C6-N1	3.11	119.44	113.95
1	Aa	1276	5MC	C5-C6-N1	-3.11	120.14	123.34
1	Aa	771	OMG	C5-C6-N1	3.11	119.44	113.95
1	Aa	636	OMG	C5-C6-N1	3.10	119.43	113.95
27	BA	56	4AC	O3'-C3'-C2'	3.10	121.86	111.82
1	Aa	847	4AC	N4-C4-N3	3.10	119.05	113.85
1	Aa	52	OMU	C5-C4-N3	3.10	119.47	114.84
1	Aa	525	4AC	C6-C5-C4	3.10	120.75	116.96
1	Aa	229	LHH	N4-C4-N3	3.09	119.04	113.85
27	BA	1470	4AC	O3'-C3'-C2'	3.09	121.82	111.82
27	BA	2353	OMG	O3'-C3'-C4'	3.09	119.99	111.05
27	BA	657	OMU	N3-C2-N1	3.09	118.99	114.89
1	Aa	1026	OMG	C5-C6-N1	3.09	119.41	113.95
1	Aa	682	4AC	CM7-C7-N4	3.09	120.64	115.29
27	BA	768	OMU	O4-C4-C5	-3.09	119.73	125.16
27	BA	617	LHH	C6-C5-C4	3.09	120.74	116.96
1	Aa	382	OMG	C5-C6-N1	3.08	119.40	113.95
1	Aa	659	OMG	C5-C6-N1	3.08	119.39	113.95
27	BA	250	OMC	N4-C4-N3	3.07	123.36	117.97
1	Aa	298	4AC	C6-C5-C4	3.07	120.72	116.96
27	BA	1319	OMU	C5-C4-N3	3.07	119.44	114.84
27	BA	2656	OMU	C5-C4-N3	3.07	119.43	114.84
1	Aa	697	4AC	C6-C5-C4	3.07	120.71	116.96
1	Aa	358	4AC	O7-C7-CM7	-3.07	116.36	122.06
27	BA	1427	4AC	N4-C4-N3	3.06	118.99	113.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BA	1434	4AC	C6-C5-C4	3.05	120.70	116.96
27	BA	768	OMU	C5-C4-N3	3.05	119.40	114.84
27	BA	2152	OMG	C2-N1-C6	-3.05	119.48	125.10
27	BA	2545	OMC	O3'-C3'-C4'	3.05	119.86	111.05
27	BA	674	OMG	C2-N1-C6	-3.05	119.49	125.10
27	BA	2121	4AC	CM7-C7-N4	3.04	120.54	115.29
27	BA	1799	OMG	O6-C6-C5	-3.03	118.45	124.37
1	Aa	1025	OMG	C5-C6-N1	3.03	119.31	113.95
27	BA	365	OMG	C5-C6-N1	3.03	119.30	113.95
1	Aa	892	OMG	C5-C6-N1	3.03	119.30	113.95
27	BA	1969	OMU	C5-C4-N3	3.03	119.37	114.84
1	Aa	498	OMG	C5-C6-N1	3.03	119.30	113.95
1	Aa	464	5MC	C5-C6-N1	-3.03	120.22	123.34
27	BA	1641	4AC	N4-C4-N3	3.02	118.93	113.85
1	Aa	1476	5MC	C5-C6-N1	-3.02	120.23	123.34
1	Aa	382	OMG	C2-N1-C6	-3.02	119.53	125.10
27	BA	526	LHH	C1'-N1-C2	3.02	125.16	118.42
27	BA	1558	OMG	O6-C6-C5	-3.02	118.48	124.37
1	Aa	818	4AC	O7-C7-CM7	-3.02	116.46	122.06
27	BA	619	OMU	O4-C4-C5	-3.01	119.86	125.16
27	BA	657	OMU	O4-C4-C5	-3.01	119.86	125.16
27	BA	1543	4AC	N4-C4-N3	3.01	118.90	113.85
27	BA	944	5MC	C5-C6-N1	-3.01	120.24	123.34
1	Aa	1265	OMG	C2-N1-C6	-3.00	119.58	125.10
1	Aa	636	OMG	C2-N1-C6	-2.99	119.58	125.10
1	Aa	876	OMG	C2-N1-C6	-2.99	119.58	125.10
27	BA	526	LHH	C6-C5-C4	2.99	120.62	116.96
27	BA	718	OMC	N4-C4-N3	2.99	123.22	117.97
1	Aa	569	4AC	C6-C5-C4	2.99	120.62	116.96
1	Aa	682	4AC	C6-C5-C4	2.99	120.62	116.96
1	Aa	479	OMU	O4-C4-C5	-2.99	119.90	125.16
27	BA	1480	OMU	O4-C4-C5	-2.98	119.91	125.16
1	Aa	450	OMG	C5-C6-N1	2.98	119.22	113.95
27	BA	1551	OMU	C5-C4-N3	2.98	119.30	114.84
27	BA	124	4AC	N4-C4-N3	2.97	118.84	113.85
27	BA	1905	5MU	C1'-N1-C6	-2.97	116.18	121.12
27	BA	2610	OMU	O4-C4-C5	-2.97	119.94	125.16
1	Aa	697	4AC	O7-C7-CM7	-2.97	116.55	122.06
27	BA	353	OMG	C2-N1-C6	-2.97	119.64	125.10
1	Aa	320	OMG	C2-N1-C6	-2.96	119.64	125.10
1	Aa	1449	6MZ	C4-C5-N7	-2.96	106.31	109.40
27	BA	2384	5MU	O2-C2-N1	-2.96	118.85	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BA	2047	OMC	O2-C2-N3	-2.96	117.52	122.33
27	BA	298	5MU	C1'-N1-C6	-2.96	116.20	121.12
1	Aa	246	OMG	C5-C6-N1	2.95	119.17	113.95
27	BA	849	A2M	C2'-C3'-C4'	-2.95	95.58	101.99
27	BA	1776	OMU	O4-C4-C5	-2.95	119.97	125.16
27	BA	1799	OMG	N2-C2-N1	2.95	122.99	116.71
1	Aa	1434	OMG	C2-N1-C6	-2.95	119.67	125.10
27	BA	730	4AC	CM7-C7-N4	2.95	120.39	115.29
1	Aa	605	4AC	C5-C4-N3	-2.95	117.85	122.59
1	Aa	52	OMU	O4-C4-C5	-2.94	119.98	125.16
1	Aa	1107	OMG	C5-C6-N1	2.94	119.14	113.95
27	BA	1776	OMU	C5-C4-N3	2.93	119.23	114.84
27	BA	2571	OMC	O2-C2-N3	-2.93	117.56	122.33
27	BA	1892	OMG	C2-N1-C6	-2.93	119.70	125.10
1	Aa	1217	4AC	CM7-C7-N4	2.93	120.36	115.29
1	Aa	1217	4AC	C5-C4-N3	-2.93	117.88	122.59
1	Aa	446	OMG	C2-N1-C6	-2.92	119.72	125.10
27	BA	2955	LHH	O7-C7-N4	-2.92	117.09	121.82
1	Aa	41	4AC	O7-C7-CM7	-2.91	116.65	122.06
1	Aa	373	4AC	C6-C5-C4	2.91	120.52	116.96
27	BA	1375	4AC	CM7-C7-N4	2.91	120.32	115.29
27	BA	201	4AC	C6-C5-C4	2.90	120.51	116.96
1	Aa	532	OMG	C5-C6-N1	2.90	119.08	113.95
1	Aa	1459	4AC	C1'-N1-C6	-2.90	114.52	120.84
27	BA	2010	OMG	C2-N1-C6	-2.90	119.76	125.10
27	BA	212	A2M	C4-C5-N7	-2.90	106.38	109.40
1	Aa	994	OMG	C2-N1-C6	-2.90	119.77	125.10
27	BA	1955	4AC	C6-C5-C4	2.89	120.50	116.96
1	Aa	458	4AC	C6-C5-C4	2.89	120.50	116.96
27	BA	1892	OMG	C5-C6-N1	2.89	119.06	113.95
27	BA	2553	4SU	C5-C4-S4	-2.89	120.74	124.47
27	BA	1470	4AC	C6-C5-C4	2.88	120.49	116.96
27	BA	2168	OMG	C8-N7-C5	2.88	108.48	102.99
27	BA	2780	4AC	O7-C7-CM7	-2.88	116.70	122.06
1	Aa	450	OMG	C2-N1-C6	-2.88	119.80	125.10
27	BA	713	4AC	C6-C5-C4	2.88	120.48	116.96
1	Aa	730	4AC	C5-C4-N3	-2.87	117.97	122.59
27	BA	2016	OMG	C8-N7-C5	2.87	108.45	102.99
27	BA	2581	4SU	O2-C2-N1	-2.87	118.97	122.79
27	BA	2324	OMG	C2-N1-C6	-2.86	119.82	125.10
27	BA	763	OMG	N2-C2-N1	2.86	122.80	116.71
27	BA	124	4AC	C6-C5-C4	2.86	120.46	116.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Aa	136	4AC	O7-C7-CM7	-2.86	116.75	122.06
27	BA	1305	4AC	O7-C7-N4	-2.86	117.19	121.82
27	BA	1696	5MC	C5-C6-N1	-2.86	120.40	123.34
27	BA	505	A2M	C1'-N9-C4	-2.86	121.62	126.64
27	BA	1396	4AC	C1'-N1-C2	2.85	124.78	118.42
27	BA	1776	OMU	C1'-N1-C2	2.85	122.73	117.57
27	BA	1934	4AC	CM7-C7-N4	2.85	120.22	115.29
27	BA	1905	5MU	O4-C4-N3	-2.84	114.67	120.12
27	BA	552	OMG	C8-N7-C5	2.84	108.40	102.99
27	BA	56	4AC	N4-C4-N3	2.84	118.62	113.85
27	BA	875	5MU	C1'-N1-C2	2.84	122.71	117.57
1	Aa	136	4AC	C6-C5-C4	2.84	120.43	116.96
27	BA	730	4AC	C6-C5-C4	2.84	120.43	116.96
1	Aa	659	OMG	C2-N1-C6	-2.83	119.88	125.10
1	Aa	381	OMG	C2-N1-C6	-2.83	119.89	125.10
27	BA	537	5MU	C1'-N1-C6	-2.83	116.42	121.12
27	BA	1799	OMG	C2-N1-C6	-2.82	119.90	125.10
27	BA	3009	4AC	N4-C4-N3	2.82	118.59	113.85
27	BA	552	OMG	O6-C6-C5	-2.82	118.86	124.37
27	BA	2780	4AC	C1'-N1-C2	2.82	124.72	118.42
27	BA	2527	OMG	C2-N1-C6	-2.81	119.92	125.10
1	Aa	1004	5MC	C5-C6-N1	-2.81	120.44	123.34
27	BA	453	OMU	C1'-N1-C2	2.81	122.66	117.57
1	Aa	827	4AC	C6-C5-C4	2.81	120.40	116.96
27	BA	2992	4AC	C6-C5-C4	2.81	120.40	116.96
1	Aa	852	OMG	C5-C6-N1	2.81	118.91	113.95
27	BA	1434	4AC	O7-C7-N4	-2.80	117.28	121.82
27	BA	2353	OMG	O3'-C3'-C2'	2.79	119.10	111.17
1	Aa	942	5MC	CM5-C5-C6	-2.79	119.12	122.85
27	BA	723	OMG	C8-N7-C5	2.79	108.30	102.99
1	Aa	1478	5MC	C1'-N1-C6	-2.78	116.49	121.12
1	Aa	229	LHH	O7-C7-CM7	-2.78	116.89	122.06
1	Aa	892	OMG	C2-N1-C6	-2.78	119.98	125.10
27	BA	799	4AC	C6-C5-C4	2.78	120.36	116.96
27	BA	805	4AC	CM7-C7-N4	2.78	120.10	115.29
27	BA	1953	OMG	O6-C6-N1	-2.77	117.38	120.65
1	Aa	1358	OMU	O2-C2-N1	-2.76	119.11	122.79
27	BA	376	4AC	CM7-C7-N4	2.76	120.07	115.29
27	BA	2542	OMU	C5-C4-N3	2.76	118.97	114.84
27	BA	1955	4AC	CM7-C7-N4	2.76	120.06	115.29
27	BA	2168	OMG	N2-C2-N1	2.76	122.58	116.71
27	BA	1750	OMC	C1'-N1-C2	2.76	124.57	118.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BA	1558	OMG	O6-C6-N1	2.75	123.90	120.65
1	Aa	498	OMG	C2-N1-C6	-2.75	120.03	125.10
1	Aa	1107	OMG	C2-N1-C6	-2.75	120.03	125.10
1	Aa	913	OMG	C8-N7-C5	2.75	108.23	102.99
27	BA	2019	OMG	C8-N7-C5	2.75	108.23	102.99
1	Aa	246	OMG	C2-N1-C6	-2.75	120.04	125.10
27	BA	418	4AC	N4-C4-N3	2.74	118.45	113.85
1	Aa	771	OMG	C2-N1-C6	-2.74	120.06	125.10
27	BA	1106	OMG	C2-N1-C6	-2.73	120.06	125.10
27	BA	1525	OMG	C8-N7-C5	2.73	108.20	102.99
27	BA	1431	4AC	C6-C5-C4	2.73	120.30	116.96
1	Aa	138	OMG	C2-N1-C6	-2.73	120.07	125.10
27	BA	353	OMG	O6-C6-N1	-2.73	117.43	120.65
1	Aa	41	4AC	C6-C5-C4	2.73	120.30	116.96
1	Aa	1217	4AC	C1'-N1-C2	2.72	124.50	118.42
27	BA	617	LHH	N4-C4-N3	2.72	118.41	113.85
27	BA	1357	4AC	CM7-C7-N4	2.72	119.99	115.29
27	BA	2595	OMC	O2-C2-N3	-2.72	117.91	122.33
1	Aa	5	4AC	O7-C7-CM7	-2.72	117.01	122.06
27	BA	34	OMU	O4-C4-C5	-2.71	120.39	125.16
1	Aa	136	4AC	O7-C7-N4	-2.71	117.42	121.82
1	Aa	1007	4AC	C6-C5-C4	2.71	120.28	116.96
27	BA	617	LHH	O7-C7-CM7	-2.71	117.02	122.06
1	Aa	1352	5MC	C5-C6-N1	-2.71	120.55	123.34
1	Aa	917	5MU	O2-C2-N1	-2.71	119.19	122.79
27	BA	2688	5MU	O2-C2-N1	-2.71	119.19	122.79
27	BA	201	4AC	O7-C7-N4	-2.71	117.44	121.82
1	Aa	1026	OMG	C2-N1-C6	-2.70	120.12	125.10
27	BA	1641	4AC	C6-C5-C4	2.70	120.26	116.96
27	BA	619	OMU	CM2-O2'-C2'	2.70	121.60	114.52
27	BA	2728	OMG	O6-C6-N1	-2.69	117.47	120.65
27	BA	1969	OMU	C1'-N1-C2	2.68	122.43	117.57
27	BA	353	OMG	N1-C2-N3	-2.68	118.31	123.32
27	BA	1820	OMC	N4-C4-N3	2.68	122.67	117.97
27	BA	1965	5MC	C5-C6-N1	-2.68	120.58	123.34
27	BA	1955	4AC	N4-C4-N3	2.67	118.34	113.85
27	BA	1427	4AC	CM7-C7-N4	2.67	119.91	115.29
1	Aa	352	A2M	C4-C5-N7	-2.67	106.62	109.40
27	BA	869	OMC	N4-C4-N3	2.67	122.65	117.97
27	BA	2688	5MU	C1'-N1-C2	2.67	122.40	117.57
1	Aa	818	4AC	C6-C5-C4	2.67	120.22	116.96
27	BA	63	OMG	N1-C2-N3	-2.66	118.34	123.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BA	1820	OMC	C1'-N1-C2	2.66	124.36	118.42
27	BA	1427	4AC	C6-C5-C4	2.66	120.22	116.96
1	Aa	373	4AC	CM7-C7-N4	2.66	119.89	115.29
27	BA	944	5MC	O2-C2-N3	-2.66	118.01	122.33
27	BA	2838	4AC	CM7-C7-N4	2.66	119.89	115.29
27	BA	2863	5MC	CM5-C5-C6	-2.66	119.30	122.85
27	BA	2595	OMC	C1'-N1-C6	-2.65	115.05	120.84
27	BA	2152	OMG	C8-N7-C5	2.65	108.05	102.99
1	Aa	1020	LHH	C5-C4-N3	-2.65	118.32	122.59
27	BA	2605	5MC	CM5-C5-C6	-2.65	119.31	122.85
27	BA	290	OMG	C8-N7-C5	2.65	108.04	102.99
27	BA	1434	4AC	N4-C4-N3	2.65	118.30	113.85
27	BA	674	OMG	C8-N7-C5	2.65	108.04	102.99
1	Aa	569	4AC	O7-C7-CM7	-2.65	117.14	122.06
27	BA	2542	OMU	C1'-N1-C2	2.65	122.36	117.57
1	Aa	942	5MC	C5-C6-N1	-2.64	120.62	123.34
27	BA	674	OMG	N2-C2-N1	2.64	122.33	116.71
1	Aa	532	OMG	C2-N1-C6	-2.63	120.25	125.10
27	BA	3023	4AC	CM7-C7-N4	2.62	119.82	115.29
1	Aa	1352	5MC	CM5-C5-C6	-2.61	119.36	122.85
27	BA	526	LHH	C1'-N1-C6	-2.61	115.15	120.84
1	Aa	1459	4AC	O7-C7-N4	2.61	126.04	121.82
27	BA	2457	LHH	C5-C4-N3	-2.61	118.39	122.59
1	Aa	5	4AC	O7-C7-N4	-2.61	117.59	121.82
1	Aa	852	OMG	C2-N1-C6	-2.60	120.30	125.10
27	BA	1551	OMU	C1'-N1-C2	2.60	122.28	117.57
27	BA	335	4AC	CM7-C7-N4	2.60	119.79	115.29
27	BA	365	OMG	C2-N1-C6	-2.60	120.31	125.10
27	BA	290	OMG	O6-C6-N1	-2.58	117.60	120.65
27	BA	1799	OMG	C5-C6-N1	2.58	118.51	113.95
27	BA	1396	4AC	C1'-N1-C6	-2.58	115.22	120.84
27	BA	2571	OMC	O3'-C3'-C2'	2.58	118.49	111.17
27	BA	763	OMG	C8-N7-C5	2.58	107.90	102.99
27	BA	537	5MU	O4-C4-N3	-2.58	115.18	120.12
27	BA	1337	4AC	C6-C5-C4	2.58	120.11	116.96
27	BA	1940	OMG	C5-C6-N1	2.58	118.50	113.95
1	Aa	682	4AC	O7-C7-CM7	-2.57	117.28	122.06
1	Aa	854	5MC	C5-C4-N4	-2.57	117.63	121.48
1	Aa	8	OMU	C5-C4-N3	2.57	118.68	114.84
1	Aa	1020	LHH	O7-C7-CM7	-2.57	117.29	122.06
27	BA	1396	4AC	O7-C7-CM7	-2.57	117.29	122.06
27	BA	2457	LHH	O4'-C4'-C5'	2.56	117.80	109.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Aa	1459	4AC	C5-C4-N4	-2.56	118.48	122.92
27	BA	2955	LHH	O7-C7-CM7	-2.56	117.31	122.06
27	BA	1265	A2M	C3'-C2'-C1'	2.55	107.68	102.89
27	BA	488	A2M	C3'-C2'-C1'	2.55	107.67	102.89
27	BA	2121	4AC	C6-C5-C4	2.55	120.08	116.96
1	Aa	41	4AC	O7-C7-N4	-2.55	117.69	121.82
27	BA	617	LHH	C5-C4-N3	-2.54	118.50	122.59
27	BA	2997	4AC	CM7-C7-N4	2.54	119.69	115.29
27	BA	1319	OMU	C1'-N1-C2	2.54	122.17	117.57
27	BA	575	OMG	N2-C2-N1	2.54	122.12	116.71
27	BA	215	OMG	C8-N7-C5	2.54	107.82	102.99
27	BA	1543	4AC	C1'-N1-C2	2.54	124.08	118.42
27	BA	778	4AC	N4-C4-N3	2.53	118.10	113.85
1	Aa	847	4AC	CM7-C7-N4	2.53	119.67	115.29
27	BA	572	5MU	C1'-N1-C6	-2.53	116.92	121.12
27	BA	2018	OMC	C1'-N1-C6	-2.52	115.34	120.84
1	Aa	605	4AC	C5'-C4'-C3'	2.52	124.64	115.18
1	Aa	501	4AC	C5-C4-N3	-2.52	118.54	122.59
27	BA	1820	OMC	C5-C4-N4	-2.52	116.61	120.57
27	BA	925	4AC	C5-C4-N3	-2.51	118.55	122.59
27	BA	1810	4AC	CM7-C7-N4	2.51	119.64	115.29
27	BA	2797	4AC	N4-C4-N3	2.51	118.07	113.85
27	BA	805	4AC	C6-C5-C4	2.51	120.03	116.96
27	BA	64	OMG	C5-C6-N1	2.51	118.38	113.95
27	BA	1431	4AC	CM7-C7-N4	2.50	119.62	115.29
27	BA	1641	4AC	CM7-C7-N4	2.50	119.62	115.29
1	Aa	818	4AC	C5-C4-N3	-2.50	118.57	122.59
27	BA	201	4AC	O7-C7-CM7	-2.50	117.42	122.06
1	Aa	229	LHH	C5-C4-N3	-2.50	118.57	122.59
27	BA	2568	OMG	C8-N7-C5	2.49	107.74	102.99
1	Aa	1265	OMG	C8-N7-C5	2.49	107.74	102.99
27	BA	1434	4AC	O7-C7-CM7	-2.49	117.43	122.06
27	BA	1106	OMG	C5-C6-N1	2.49	118.35	113.95
1	Aa	5	4AC	C5-C4-N3	-2.49	118.59	122.59
27	BA	250	OMC	O2-C2-N3	-2.49	118.29	122.33
27	BA	2019	OMG	O6-C6-N1	-2.49	117.71	120.65
27	BA	805	4AC	O7-C7-CM7	-2.48	117.44	122.06
27	BA	674	OMG	CM2-O2'-C2'	-2.48	108.02	114.52
27	BA	201	4AC	C5-C4-N3	-2.48	118.61	122.59
1	Aa	5	4AC	C6-C5-C4	2.48	119.99	116.96
1	Aa	827	4AC	CM7-C7-N4	2.47	119.57	115.29
1	Aa	1107	OMG	C8-N7-C5	2.47	107.70	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BA	1396	4AC	CM7-C7-N4	2.47	119.57	115.29
1	Aa	358	4AC	C6-C5-C4	2.47	119.98	116.96
27	BA	2832	4AC	C6-C5-C4	2.47	119.98	116.96
27	BA	912	OMG	C8-N7-C5	2.47	107.69	102.99
1	Aa	458	4AC	N4-C4-N3	2.47	117.99	113.85
27	BA	3023	4AC	C1'-N1-C2	2.46	123.91	118.42
27	BA	879	A2M	O5'-C5'-C4'	2.46	117.36	108.99
27	BA	244	4AC	C6-C5-C4	2.46	119.97	116.96
27	BA	805	4AC	C1'-N1-C2	2.46	123.90	118.42
27	BA	2630	OMC	C5-C4-N4	-2.46	116.71	120.57
27	BA	2527	OMG	C8-N7-C5	2.46	107.67	102.99
27	BA	833	OMG	O6-C6-N1	-2.45	117.75	120.65
27	BA	1431	4AC	O7-C7-CM7	-2.45	117.50	122.06
1	Aa	994	OMG	C8-N7-C5	2.45	107.66	102.99
1	Aa	501	4AC	O7-C7-CM7	-2.45	117.51	122.06
27	BA	552	OMG	O6-C6-N1	2.45	123.54	120.65
27	BA	2832	4AC	CM7-C7-N4	2.45	119.53	115.29
27	BA	2568	OMG	C5-C6-N1	2.45	118.27	113.95
1	Aa	605	4AC	O4'-C4'-C5'	2.45	117.42	109.37
27	BA	1548	5MU	O4-C4-N3	-2.44	115.44	120.12
1	Aa	1478	5MC	N4-C4-N3	2.44	122.93	118.48
27	BA	2992	4AC	C5-C4-N3	-2.44	118.67	122.59
1	Aa	697	4AC	C5-C4-N3	-2.43	118.68	122.59
27	BA	2152	OMG	O6-C6-N1	-2.43	117.78	120.65
1	Aa	1025	OMG	C2-N1-C6	-2.43	120.62	125.10
27	BA	2688	5MU	O4-C4-N3	-2.43	115.47	120.12
27	BA	1357	4AC	O7-C7-CM7	-2.43	117.55	122.06
1	Aa	672	5MC	C5-C4-N4	-2.42	117.85	121.48
27	BA	1400	A2M	C1'-N9-C4	-2.42	122.38	126.64
27	BA	353	OMG	C8-N7-C5	2.42	107.59	102.99
1	Aa	847	4AC	C6-C5-C4	2.42	119.92	116.96
1	Aa	136	4AC	C5-C4-N3	-2.41	118.71	122.59
27	BA	2159	4AC	C6-C5-C4	2.41	119.91	116.96
1	Aa	532	OMG	C8-N7-C5	2.41	107.58	102.99
27	BA	335	4AC	N4-C4-N3	2.41	117.90	113.85
27	BA	2016	OMG	O6-C6-N1	-2.41	117.81	120.65
27	BA	1776	OMU	C6-N1-C2	-2.41	117.91	120.99
1	Aa	1051	B8T	C6-C5-C4	2.41	119.91	116.96
27	BA	2521	OMG	C8-N7-C5	2.41	107.57	102.99
27	BA	27	4AC	CM7-C7-N4	2.41	119.45	115.29
27	BA	418	4AC	CM7-C7-N4	2.41	119.45	115.29
27	BA	2124	OMC	C5-C4-N4	-2.40	116.79	120.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BA	1558	OMG	C2-N1-C6	-2.40	120.67	125.10
27	BA	419	OMG	C8-N7-C5	2.40	107.56	102.99
27	BA	2688	5MU	C6-C5-C4	2.40	120.04	118.03
27	BA	800	OMG	C5-C6-N1	2.40	118.18	113.95
27	BA	1357	4AC	C1'-N1-C2	2.40	123.77	118.42
27	BA	1934	4AC	C6-C5-C4	2.39	119.89	116.96
27	BA	674	OMG	N2-C2-N3	-2.39	115.08	119.74
1	Aa	1459	4AC	O2-C2-N3	-2.39	118.44	122.33
1	Aa	41	4AC	C5-C4-N3	-2.39	118.75	122.59
27	BA	1396	4AC	C6-C5-C4	2.39	119.88	116.96
27	BA	2324	OMG	C8-N7-C5	2.38	107.53	102.99
27	BA	925	4AC	O2'-C2'-C3'	-2.38	104.12	111.82
27	BA	657	OMU	C5-C4-N3	2.38	118.40	114.84
1	Aa	458	4AC	C5-C4-N3	-2.38	118.77	122.59
27	BA	932	A2M	C3'-C2'-C1'	2.38	107.36	102.89
27	BA	925	4AC	N4-C4-N3	2.38	117.84	113.85
27	BA	1305	4AC	O7-C7-CM7	-2.37	117.65	122.06
1	Aa	8	OMU	O4-C4-C5	-2.37	120.98	125.16
1	Aa	525	4AC	O2-C2-N3	-2.37	118.47	122.33
27	BA	1548	5MU	C6-N1-C2	-2.37	118.89	121.30
27	BA	2797	4AC	C6-C5-C4	2.37	119.86	116.96
27	BA	1375	4AC	C6-C5-C4	2.37	119.86	116.96
27	BA	1470	4AC	CM7-C7-N4	2.37	119.39	115.29
27	BA	617	LHH	O7-C7-N4	-2.36	117.99	121.82
27	BA	2672	OMG	C8-N7-C5	2.36	107.49	102.99
1	Aa	1478	5MC	C1'-N1-C2	2.36	123.68	118.42
27	BA	2018	OMC	C1'-N1-C2	2.36	123.68	118.42
1	Aa	246	OMG	C8-N7-C5	2.35	107.48	102.99
1	Aa	1275	OMG	C5-C6-N1	2.35	118.11	113.95
27	BA	376	4AC	C1'-N1-C2	2.35	123.67	118.42
27	BA	2657	OMG	C8-N7-C5	2.35	107.47	102.99
27	BA	800	OMG	C2-N1-C6	-2.35	120.77	125.10
1	Aa	373	4AC	C1'-N1-C2	2.35	123.66	118.42
27	BA	1750	OMC	C5-C4-N4	-2.35	116.88	120.57
27	BA	365	OMG	N2-C2-N1	2.34	121.70	116.71
27	BA	505	A2M	C3'-C2'-C1'	2.34	107.29	102.89
27	BA	1305	4AC	C5-C4-N3	-2.34	118.83	122.59
1	Aa	670	2MG	C8-N7-C5	2.34	107.45	102.99
27	BA	2590	4AC	N4-C4-N3	2.34	117.78	113.85
27	BA	2838	4AC	C6-C5-C4	2.33	119.82	116.96
27	BA	2728	OMG	C8-N7-C5	2.33	107.43	102.99
27	BA	3023	4AC	C6-C5-C4	2.33	119.81	116.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BA	418	4AC	C6-C5-C4	2.33	119.81	116.96
1	Aa	682	4AC	C5-C4-N3	-2.32	118.85	122.59
27	BA	1750	OMC	N4-C4-N3	2.32	122.05	117.97
27	BA	124	4AC	C5-C4-N3	-2.32	118.85	122.59
27	BA	1558	OMG	C8-N7-C5	2.32	107.42	102.99
27	BA	875	5MU	O4-C4-N3	-2.32	115.66	120.12
27	BA	2590	4AC	C6-C5-C4	2.32	119.80	116.96
27	BA	572	5MU	C6-N1-C2	-2.32	118.95	121.30
27	BA	2595	OMC	C1'-N1-C2	2.31	123.59	118.42
27	BA	2992	4AC	CM7-C7-N4	2.31	119.30	115.29
27	BA	1357	4AC	C6-C5-C4	2.31	119.79	116.96
1	Aa	382	OMG	C8-N7-C5	2.31	107.39	102.99
27	BA	1375	4AC	O7-C7-CM7	-2.31	117.77	122.06
1	Aa	498	OMG	C8-N7-C5	2.31	107.38	102.99
1	Aa	1352	5MC	C1'-N1-C6	-2.31	117.29	121.12
27	BA	2457	LHH	C5'-C4'-C3'	2.30	123.81	115.18
27	BA	1820	OMC	O2-C2-N3	-2.30	118.59	122.33
27	BA	925	4AC	O7-C7-CM7	-2.30	117.79	122.06
27	BA	250	OMC	C5-C4-N4	-2.29	116.97	120.57
1	Aa	1434	OMG	C8-N7-C5	2.29	107.36	102.99
27	BA	2997	4AC	C6-C5-C4	2.29	119.77	116.96
27	BA	1431	4AC	C1'-N1-C2	2.29	123.53	118.42
1	Aa	479	OMU	O2-C2-N1	-2.29	119.74	122.79
1	Aa	320	OMG	C8-N7-C5	2.29	107.35	102.99
27	BA	575	OMG	C2-N1-C6	-2.29	120.89	125.10
27	BA	2745	OMG	C8-N7-C5	2.28	107.34	102.99
1	Aa	876	OMG	C8-N7-C5	2.28	107.34	102.99
1	Aa	1107	OMG	CM2-O2'-C2'	2.28	120.52	114.52
27	BA	2121	4AC	N4-C4-N3	2.28	117.69	113.85
27	BA	2780	4AC	C5-C4-N3	-2.28	118.92	122.59
27	BA	2353	OMG	C2-N1-C6	-2.28	120.90	125.10
1	Aa	446	OMG	C8-N7-C5	2.28	107.33	102.99
27	BA	2838	4AC	O7-C7-CM7	-2.28	117.82	122.06
27	BA	833	OMG	C8-N7-C5	2.28	107.33	102.99
27	BA	1940	OMG	C2-N1-C6	-2.28	120.90	125.10
1	Aa	697	4AC	N4-C4-N3	2.27	117.67	113.85
27	BA	1434	4AC	C5-C4-N3	-2.27	118.94	122.59
27	BA	575	OMG	C8-N7-C5	2.27	107.32	102.99
27	BA	376	4AC	O7-C7-CM7	-2.27	117.84	122.06
27	BA	64	OMG	C2-N1-C6	-2.27	120.92	125.10
27	BA	1548	5MU	O2-C2-N1	-2.26	119.78	122.79
27	BA	1934	4AC	O7-C7-CM7	-2.26	117.86	122.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BA	1899	4AC	C6-C5-C4	2.26	119.73	116.96
1	Aa	1025	OMG	C8-N7-C5	2.26	107.30	102.99
27	BA	2550	OMG	C8-N7-C5	2.26	107.29	102.99
27	BA	3009	4AC	CM7-C7-N4	2.26	119.19	115.29
1	Aa	358	4AC	O7-C7-N4	-2.26	118.17	121.82
27	BA	1431	4AC	C5-C4-N3	-2.26	118.96	122.59
27	BA	1965	5MC	O2-C2-N3	-2.25	118.66	122.33
1	Aa	138	OMG	C8-N7-C5	2.25	107.28	102.99
27	BA	27	4AC	C5-C4-N3	-2.25	118.97	122.59
27	BA	298	5MU	C6-N1-C2	-2.25	119.02	121.30
27	BA	718	OMC	O2-C2-N3	-2.25	118.67	122.33
1	Aa	373	4AC	O7-C7-CM7	-2.25	117.88	122.06
27	BA	575	OMG	O6-C6-C5	-2.25	119.98	124.37
27	BA	335	4AC	C6-C5-C4	2.25	119.71	116.96
27	BA	1892	OMG	C8-N7-C5	2.25	107.27	102.99
1	Aa	1276	5MC	CM5-C5-C6	-2.25	119.85	122.85
27	BA	2384	5MU	O4'-C4'-C5'	2.25	116.76	109.37
27	BA	63	OMG	C2-N1-C6	-2.24	120.97	125.10
27	BA	2797	4AC	CM7-C7-N4	2.24	119.17	115.29
27	BA	875	5MU	O2-C2-N1	-2.24	119.81	122.79
1	Aa	358	4AC	C5-C4-N3	-2.24	118.99	122.59
27	BA	501	4AC	C5-C4-N3	-2.24	118.99	122.59
27	BA	2590	4AC	O2-C2-N3	-2.24	118.69	122.33
27	BA	805	4AC	C1'-N1-C6	-2.23	115.97	120.84
27	BA	2384	5MU	C6-N1-C2	-2.23	119.04	121.30
27	BA	1106	OMG	O6-C6-C5	-2.23	120.01	124.37
27	BA	2389	OMU	O3'-C3'-C4'	-2.23	104.60	111.05
1	Aa	1007	4AC	C2'-C1'-N1	-2.23	106.91	113.22
27	BA	2590	4AC	C5-C4-N3	-2.23	119.01	122.59
27	BA	1790	OMC	CM2-O2'-C2'	-2.23	108.68	114.52
27	BA	2571	OMC	O2-C2-N1	2.22	123.48	118.89
27	BA	357	B8T	C6-C5-C4	2.22	119.68	116.96
1	Aa	1459	4AC	C6-C5-C4	2.22	119.67	116.96
27	BA	433	4AC	CM7-C7-N4	2.22	119.13	115.29
1	Aa	1262	B8T	C6-C5-C4	2.22	119.67	116.96
1	Aa	1275	OMG	C8-N7-C5	2.22	107.21	102.99
27	BA	63	OMG	C8-N7-C5	2.21	107.21	102.99
27	BA	778	4AC	CM7-C7-N4	2.20	119.11	115.29
27	BA	505	A2M	O2'-C2'-C1'	-2.20	104.72	109.09
27	BA	1525	OMG	O6-C6-N1	-2.20	118.05	120.65
27	BA	212	A2M	O2'-C2'-C1'	2.20	113.45	109.09
27	BA	27	4AC	O7-C7-CM7	-2.20	117.97	122.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Aa	373	4AC	C5-C4-N3	-2.20	119.06	122.59
27	BA	2010	OMG	C8-N7-C5	2.19	107.17	102.99
1	Aa	913	OMG	O6-C6-C5	-2.19	120.09	124.37
1	Aa	697	4AC	O7-C7-N4	-2.19	118.28	121.82
27	BA	657	OMU	C6-N1-C2	-2.19	118.20	120.99
27	BA	1558	OMG	N2-C2-N1	2.18	121.36	116.71
27	BA	849	A2M	O4'-C1'-C2'	-2.18	102.80	106.59
27	BA	572	5MU	O2-C2-N1	-2.18	119.89	122.79
27	BA	1470	4AC	O7-C7-CM7	-2.18	118.01	122.06
1	Aa	659	OMG	C8-N7-C5	2.18	107.14	102.99
27	BA	619	OMU	C1'-N1-C2	2.17	121.50	117.57
27	BA	756	A2M	C3'-C2'-C1'	2.17	106.97	102.89
27	BA	2124	OMC	O2-C2-N3	-2.17	118.80	122.33
27	BA	2389	OMU	O2'-C2'-C1'	2.17	113.31	109.08
27	BA	2168	OMG	O6-C6-C5	-2.16	120.15	124.37
27	BA	526	LHH	O2-C2-N3	-2.16	118.82	122.33
1	Aa	854	5MC	N4-C4-N3	2.16	122.41	118.48
27	BA	1810	4AC	O7-C7-CM7	-2.16	118.05	122.06
1	Aa	1026	OMG	C8-N7-C5	2.16	107.10	102.99
1	Aa	730	4AC	N4-C4-N3	2.16	117.47	113.85
1	Aa	1476	5MC	CM5-C5-C6	-2.15	119.97	122.85
1	Aa	525	4AC	O7-C7-CM7	-2.15	118.06	122.06
27	BA	2528	OMG	C8-N7-C5	2.15	107.09	102.99
27	BA	799	4AC	CM7-C7-N4	2.15	119.02	115.29
27	BA	872	A2M	C3'-C2'-C1'	2.15	106.93	102.89
27	BA	244	4AC	C1'-N1-C2	2.15	123.22	118.42
27	BA	2590	4AC	CM7-C7-N4	2.15	119.01	115.29
27	BA	56	4AC	C6-C5-C4	2.15	119.59	116.96
27	BA	1543	4AC	C6-C5-C4	2.15	119.59	116.96
1	Aa	296	OMC	O2-C2-N3	-2.15	118.84	122.33
1	Aa	298	4AC	C5-C4-N3	-2.15	119.14	122.59
1	Aa	1026	OMG	O6-C6-C5	-2.14	120.19	124.37
1	Aa	229	LHH	O7-C7-N4	-2.14	118.36	121.82
27	BA	2702	A2M	C3'-C2'-C1'	2.14	106.90	102.89
27	BA	1750	OMC	C1'-N1-C6	-2.13	116.19	120.84
27	BA	800	OMG	C8-N7-C5	2.13	107.05	102.99
1	Aa	771	OMG	C8-N7-C5	2.13	107.05	102.99
27	BA	763	OMG	O6-C6-C5	-2.13	120.21	124.37
27	BA	1750	OMC	O2-C2-N3	-2.13	118.88	122.33
27	BA	244	4AC	C5-C4-N3	-2.12	119.18	122.59
27	BA	805	4AC	C5-C4-N3	-2.12	119.18	122.59
1	Aa	892	OMG	C8-N7-C5	2.12	107.03	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Aa	827	4AC	C5-C4-N3	-2.12	119.19	122.59
27	BA	376	4AC	C6-C5-C4	2.12	119.55	116.96
1	Aa	569	4AC	C5-C4-N3	-2.12	119.19	122.59
27	BA	2571	OMC	O3'-C3'-C4'	2.12	117.17	111.05
27	BA	2630	OMC	O2-C2-N3	-2.12	118.89	122.33
1	Aa	771	OMG	O6-C6-C5	-2.12	120.24	124.37
1	Aa	1478	5MC	O2-C2-N3	-2.11	118.89	122.33
27	BA	1641	4AC	O2-C2-N3	-2.11	118.89	122.33
1	Aa	636	OMG	C8-N7-C5	2.11	107.01	102.99
27	BA	800	OMG	N2-C2-N1	2.11	121.20	116.71
27	BA	2168	OMG	C2-N1-C6	-2.11	121.22	125.10
27	BA	572	5MU	O4-C4-N3	-2.11	116.08	120.12
1	Aa	1007	4AC	N4-C4-N3	2.10	117.38	113.85
27	BA	1305	4AC	C6-C5-C4	2.10	119.53	116.96
27	BA	1543	4AC	C1'-N1-C6	-2.10	116.27	120.84
27	BA	2379	OMG	C8-N7-C5	2.10	106.98	102.99
1	Aa	876	OMG	O6-C6-C5	-2.10	120.28	124.37
27	BA	2353	OMG	C5-C6-N1	2.09	117.65	113.95
27	BA	1305	4AC	N4-C4-N3	2.09	117.36	113.85
27	BA	2159	4AC	O7-C7-CM7	-2.09	118.18	122.06
27	BA	56	4AC	C5-C4-N3	-2.09	119.23	122.59
27	BA	1427	4AC	O7-C7-CM7	-2.09	118.18	122.06
27	BA	1357	4AC	C1'-N1-C6	-2.09	116.29	120.84
27	BA	1641	4AC	C5-C4-N3	-2.09	119.23	122.59
1	Aa	381	OMG	C8-N7-C5	2.09	106.97	102.99
27	BA	561	OMC	O2-C2-N3	-2.08	118.94	122.33
27	BA	250	OMC	C1'-N1-C2	2.08	123.07	118.42
27	BA	1398	OMG	C8-N7-C5	2.08	106.95	102.99
27	BA	1810	4AC	C5-C4-N3	-2.08	119.25	122.59
27	BA	674	OMG	C5-C6-N1	2.08	117.62	113.95
27	BA	674	OMG	O6-C6-C5	-2.08	120.32	124.37
27	BA	1558	OMG	C5-C6-N1	2.08	117.62	113.95
1	Aa	1354	OMC	N4-C4-N3	2.07	121.61	117.97
27	BA	2168	OMG	CM2-O2'-C2'	-2.07	109.10	114.52
27	BA	552	OMG	C5-C6-N1	2.07	117.60	113.95
27	BA	1696	5MC	CM5-C5-C6	-2.07	120.09	122.85
1	Aa	752	OMC	C5-C4-N4	-2.06	117.33	120.57
27	BA	418	4AC	C5-C4-N3	-2.06	119.27	122.59
27	BA	1085	5MU	O2-C2-N1	-2.06	120.05	122.79
27	BA	2121	4AC	O7-C7-CM7	-2.06	118.23	122.06
27	BA	1899	4AC	CM7-C7-N4	2.06	118.86	115.29
1	Aa	1020	LHH	C2'-C1'-N1	2.06	118.22	114.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BA	763	OMG	C5-C6-N1	2.06	117.59	113.95
27	BA	2832	4AC	C1'-N1-C2	2.06	123.01	118.42
27	BA	1953	OMG	C8-N7-C5	2.06	106.91	102.99
27	BA	2656	OMU	O4-C4-C5	-2.06	121.55	125.16
27	BA	1340	OMU	C1'-N1-C2	2.05	121.29	117.57
27	BA	2168	OMG	C5-C6-N1	2.05	117.57	113.95
27	BA	2863	5MC	O2-C2-N3	-2.05	119.00	122.33
27	BA	2780	4AC	C1'-N1-C6	-2.05	116.38	120.84
27	BA	718	OMC	O2-C2-N1	2.05	123.12	118.89
27	BA	2018	OMC	O2-C2-N3	-2.05	119.00	122.33
27	BA	2124	OMC	C1'-N1-C2	2.05	122.98	118.42
1	Aa	8	OMU	C6-N1-C2	-2.04	118.38	120.99
27	BA	2035	5MC	CM5-C5-C6	-2.04	120.12	122.85
1	Aa	994	OMG	O6-C6-C5	-2.04	120.38	124.37
27	BA	3023	4AC	O7-C7-CM7	-2.04	118.27	122.06
1	Aa	854	5MC	C1'-N1-C6	-2.04	117.73	121.12
27	BA	64	OMG	O6-C6-C5	-2.04	120.39	124.37
27	BA	1899	4AC	O7-C7-CM7	-2.04	118.27	122.06
1	Aa	450	OMG	C8-N7-C5	2.04	106.88	102.99
1	Aa	818	4AC	N4-C4-N3	2.04	117.28	113.85
1	Aa	852	OMG	C8-N7-C5	2.04	106.87	102.99
27	BA	2553	4SU	O2-C2-N1	-2.04	120.08	122.79
27	BA	3009	4AC	C5-C4-N3	-2.04	119.32	122.59
27	BA	2384	5MU	C5'-C4'-C3'	2.04	122.81	115.18
27	BA	2863	5MC	C1'-N1-C2	2.04	122.96	118.42
27	BA	2070	5MC	C2'-C1'-N1	-2.03	107.45	113.22
27	BA	3023	4AC	C1'-N1-C6	-2.03	116.41	120.84
27	BA	201	4AC	N4-C4-N3	2.03	117.27	113.85
27	BA	1337	4AC	CM7-C7-N4	2.03	118.81	115.29
27	BA	2070	5MC	C5-C4-N3	-2.03	119.48	121.67
27	BA	730	4AC	O7-C7-CM7	-2.03	118.28	122.06
27	BA	730	4AC	O2-C2-N3	-2.03	119.03	122.33
27	BA	3023	4AC	C5-C4-N3	-2.03	119.33	122.59
27	BA	1799	OMG	O6-C6-N1	2.03	123.04	120.65
27	BA	1940	OMG	O6-C6-C5	-2.03	120.42	124.37
27	BA	1955	4AC	C5-C4-N3	-2.03	119.33	122.59
27	BA	875	5MU	O2'-C2'-C3'	2.02	118.37	111.82
27	BA	433	4AC	C6-C5-C4	2.02	119.44	116.96
27	BA	2159	4AC	CM7-C7-N4	2.02	118.79	115.29
1	Aa	1358	OMU	C1'-N1-C6	2.02	125.25	120.84
27	BA	1820	OMC	C1'-N1-C6	-2.02	116.44	120.84
1	Aa	381	OMG	O6-C6-C5	-2.02	120.43	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Aa	1007	4AC	C5-C4-N3	-2.02	119.35	122.59
1	Aa	446	OMG	O6-C6-C5	-2.01	120.44	124.37
1	Aa	1020	LHH	O7-C7-N4	-2.01	118.56	121.82
1	Aa	1217	4AC	C1'-N1-C6	-2.01	116.45	120.84
27	BA	250	OMC	C6-C5-C4	2.01	120.75	117.50
27	BA	2159	4AC	C5-C4-N4	-2.01	119.43	122.92
27	BA	2992	4AC	C1'-N1-C2	2.01	122.91	118.42
1	Aa	659	OMG	O6-C6-C5	-2.01	120.45	124.37
27	BA	1905	5MU	O2-C2-N1	-2.01	120.12	122.79
1	Aa	1354	OMC	C5-C4-N4	-2.00	117.42	120.57
1	Aa	8	OMU	O2-C2-N1	-2.00	120.13	122.79
1	Aa	8	OMU	O2'-C2'-C1'	2.00	112.98	109.08

There are no chirality outliers.

All (235) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	Aa	52	OMU	C3'-C4'-C5'-O5'
1	Aa	52	OMU	O4'-C4'-C5'-O5'
1	Aa	352	A2M	C1'-C2'-O2'-CM'
1	Aa	382	OMG	O4'-C4'-C5'-O5'
1	Aa	446	OMG	O4'-C4'-C5'-O5'
1	Aa	446	OMG	C3'-C4'-C5'-O5'
1	Aa	458	4AC	O7-C7-N4-C4
1	Aa	458	4AC	CM7-C7-N4-C4
1	Aa	525	4AC	O4'-C1'-N1-C2
1	Aa	525	4AC	O4'-C1'-N1-C6
1	Aa	876	OMG	O4'-C4'-C5'-O5'
1	Aa	876	OMG	C3'-C4'-C5'-O5'
1	Aa	917	5MU	C3'-C4'-C5'-O5'
1	Aa	917	5MU	O4'-C4'-C5'-O5'
1	Aa	1107	OMG	C3'-C2'-O2'-CM2
1	Aa	1217	4AC	C3'-C4'-C5'-O5'
1	Aa	1275	OMG	C1'-C2'-O2'-CM2
1	Aa	1352	5MC	O4'-C4'-C5'-O5'
1	Aa	1352	5MC	C3'-C4'-C5'-O5'
1	Aa	1354	OMC	C3'-C4'-C5'-O5'
1	Aa	1354	OMC	O4'-C4'-C5'-O5'
1	Aa	1358	OMU	O4'-C4'-C5'-O5'
1	Aa	1468	MA6	O4'-C4'-C5'-O5'
27	BA	27	4AC	O4'-C4'-C5'-O5'
27	BA	27	4AC	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
27	BA	34	OMU	C1'-C2'-O2'-CM2
27	BA	212	A2M	C1'-C2'-O2'-CM'
27	BA	215	OMG	O4'-C4'-C5'-O5'
27	BA	353	OMG	O4'-C4'-C5'-O5'
27	BA	353	OMG	C3'-C4'-C5'-O5'
27	BA	488	A2M	C3'-C2'-O2'-CM'
27	BA	619	OMU	C1'-C2'-O2'-CM2
27	BA	657	OMU	C1'-C2'-O2'-CM2
27	BA	754	OMC	C3'-C4'-C5'-O5'
27	BA	849	A2M	C3'-C4'-C5'-O5'
27	BA	1480	OMU	O4'-C4'-C5'-O5'
27	BA	1517	A2M	C3'-C2'-O2'-CM'
27	BA	1525	OMG	O4'-C4'-C5'-O5'
27	BA	1525	OMG	C3'-C4'-C5'-O5'
27	BA	1543	4AC	C3'-C4'-C5'-O5'
27	BA	1548	5MU	C3'-C4'-C5'-O5'
27	BA	1551	OMU	C1'-C2'-O2'-CM2
27	BA	2018	OMC	O4'-C4'-C5'-O5'
27	BA	2019	OMG	C3'-C4'-C5'-O5'
27	BA	2055	5MC	O4'-C4'-C5'-O5'
27	BA	2152	OMG	O4'-C4'-C5'-O5'
27	BA	2152	OMG	C3'-C4'-C5'-O5'
27	BA	2353	OMG	O4'-C4'-C5'-O5'
27	BA	2353	OMG	C3'-C4'-C5'-O5'
27	BA	2389	OMU	C3'-C4'-C5'-O5'
27	BA	2457	LHH	C3'-C4'-C5'-O5'
27	BA	2457	LHH	O4'-C4'-C5'-O5'
27	BA	2550	OMG	O4'-C4'-C5'-O5'
27	BA	2568	OMG	C3'-C4'-C5'-O5'
27	BA	2581	4SU	O4'-C4'-C5'-O5'
27	BA	2838	4AC	C3'-C4'-C5'-O5'
27	BA	2955	LHH	C1'-C2'-O2'-C1
27	BA	2992	4AC	O4'-C4'-C5'-O5'
27	BA	2992	4AC	C3'-C4'-C5'-O5'
27	BA	3023	4AC	O4'-C4'-C5'-O5'
1	Aa	382	OMG	C3'-C4'-C5'-O5'
1	Aa	457	5MC	O4'-C4'-C5'-O5'
1	Aa	457	5MC	C3'-C4'-C5'-O5'
1	Aa	458	4AC	O4'-C4'-C5'-O5'
1	Aa	532	OMG	O4'-C4'-C5'-O5'
1	Aa	532	OMG	C3'-C4'-C5'-O5'
1	Aa	892	OMG	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	Aa	892	OMG	C3'-C4'-C5'-O5'
1	Aa	1007	4AC	O4'-C4'-C5'-O5'
1	Aa	1276	5MC	C3'-C4'-C5'-O5'
1	Aa	1358	OMU	C3'-C4'-C5'-O5'
1	Aa	1468	MA6	C3'-C4'-C5'-O5'
27	BA	64	OMG	C3'-C4'-C5'-O5'
27	BA	215	OMG	C3'-C4'-C5'-O5'
27	BA	419	OMG	O4'-C4'-C5'-O5'
27	BA	875	5MU	C3'-C4'-C5'-O5'
27	BA	875	5MU	O4'-C4'-C5'-O5'
27	BA	1375	4AC	O4'-C4'-C5'-O5'
27	BA	1480	OMU	C3'-C4'-C5'-O5'
27	BA	1543	4AC	O4'-C4'-C5'-O5'
27	BA	1810	4AC	O4'-C4'-C5'-O5'
27	BA	1940	OMG	O4'-C4'-C5'-O5'
27	BA	1955	4AC	O4'-C4'-C5'-O5'
27	BA	2018	OMC	C3'-C4'-C5'-O5'
27	BA	2019	OMG	O4'-C4'-C5'-O5'
27	BA	2055	5MC	C3'-C4'-C5'-O5'
27	BA	2379	OMG	O4'-C4'-C5'-O5'
27	BA	2379	OMG	C3'-C4'-C5'-O5'
27	BA	2550	OMG	C3'-C4'-C5'-O5'
27	BA	2581	4SU	C3'-C4'-C5'-O5'
27	BA	2595	OMC	O4'-C4'-C5'-O5'
27	BA	2610	OMU	C3'-C4'-C5'-O5'
27	BA	3023	4AC	C3'-C4'-C5'-O5'
1	Aa	697	4AC	O4'-C4'-C5'-O5'
1	Aa	1004	5MC	O4'-C4'-C5'-O5'
1	Aa	1007	4AC	C3'-C4'-C5'-O5'
27	BA	64	OMG	O4'-C4'-C5'-O5'
27	BA	419	OMG	C3'-C4'-C5'-O5'
27	BA	488	A2M	O4'-C4'-C5'-O5'
27	BA	754	OMC	O4'-C4'-C5'-O5'
27	BA	849	A2M	O4'-C4'-C5'-O5'
27	BA	1265	A2M	O4'-C4'-C5'-O5'
27	BA	1337	4AC	O4'-C4'-C5'-O5'
27	BA	1375	4AC	C3'-C4'-C5'-O5'
27	BA	1396	4AC	O4'-C4'-C5'-O5'
27	BA	1548	5MU	O4'-C4'-C5'-O5'
27	BA	1810	4AC	C3'-C4'-C5'-O5'
27	BA	1940	OMG	C3'-C4'-C5'-O5'
27	BA	1953	OMG	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
27	BA	1955	4AC	C3'-C4'-C5'-O5'
27	BA	2389	OMU	O4'-C4'-C5'-O5'
27	BA	2527	OMG	O4'-C4'-C5'-O5'
27	BA	2595	OMC	C3'-C4'-C5'-O5'
27	BA	2610	OMU	O4'-C4'-C5'-O5'
27	BA	2838	4AC	O4'-C4'-C5'-O5'
1	Aa	458	4AC	C3'-C4'-C5'-O5'
27	BA	1953	OMG	O4'-C4'-C5'-O5'
27	BA	2568	OMG	O4'-C4'-C5'-O5'
1	Aa	1004	5MC	C3'-C4'-C5'-O5'
1	Aa	1107	OMG	C3'-C4'-C5'-O5'
1	Aa	1217	4AC	O4'-C4'-C5'-O5'
27	BA	575	OMG	C3'-C4'-C5'-O5'
27	BA	1265	A2M	C3'-C4'-C5'-O5'
27	BA	1396	4AC	C3'-C4'-C5'-O5'
1	Aa	605	4AC	O4'-C4'-C5'-O5'
1	Aa	697	4AC	C3'-C4'-C5'-O5'
1	Aa	913	OMG	C3'-C4'-C5'-O5'
27	BA	575	OMG	O4'-C4'-C5'-O5'
27	BA	2527	OMG	C3'-C4'-C5'-O5'
1	Aa	5	4AC	O4'-C4'-C5'-O5'
1	Aa	1107	OMG	O4'-C4'-C5'-O5'
27	BA	1337	4AC	C3'-C4'-C5'-O5'
27	BA	3009	4AC	O4'-C4'-C5'-O5'
27	BA	505	A2M	O4'-C4'-C5'-O5'
27	BA	1790	OMC	O4'-C4'-C5'-O5'
27	BA	617	LHH	O4'-C4'-C5'-O5'
27	BA	869	OMC	O4'-C4'-C5'-O5'
1	Aa	5	4AC	O7-C7-N4-C4
1	Aa	5	4AC	CM7-C7-N4-C4
1	Aa	41	4AC	O7-C7-N4-C4
1	Aa	41	4AC	CM7-C7-N4-C4
1	Aa	136	4AC	O7-C7-N4-C4
1	Aa	136	4AC	CM7-C7-N4-C4
1	Aa	229	LHH	CM7-C7-N4-C4
1	Aa	229	LHH	O7-C7-N4-C4
1	Aa	358	4AC	O7-C7-N4-C4
1	Aa	358	4AC	CM7-C7-N4-C4
1	Aa	525	4AC	O7-C7-N4-C4
1	Aa	525	4AC	CM7-C7-N4-C4
1	Aa	697	4AC	O7-C7-N4-C4
1	Aa	697	4AC	CM7-C7-N4-C4

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Mol	Chain	Res	Type	Atoms
1	Aa	730	4AC	O7-C7-N4-C4
1	Aa	730	4AC	CM7-C7-N4-C4
1	Aa	818	4AC	O7-C7-N4-C4
1	Aa	818	4AC	CM7-C7-N4-C4
1	Aa	1020	LHH	CM7-C7-N4-C4
1	Aa	1020	LHH	O7-C7-N4-C4
27	BA	201	4AC	O7-C7-N4-C4
27	BA	201	4AC	CM7-C7-N4-C4
27	BA	617	LHH	CM7-C7-N4-C4
27	BA	617	LHH	O7-C7-N4-C4
27	BA	858	4AC	O7-C7-N4-C4
27	BA	858	4AC	CM7-C7-N4-C4
27	BA	925	4AC	O7-C7-N4-C4
27	BA	925	4AC	CM7-C7-N4-C4
27	BA	1305	4AC	O7-C7-N4-C4
27	BA	1305	4AC	CM7-C7-N4-C4
27	BA	1434	4AC	O7-C7-N4-C4
27	BA	1434	4AC	CM7-C7-N4-C4
27	BA	2457	LHH	CM7-C7-N4-C4
27	BA	2457	LHH	O7-C7-N4-C4
27	BA	2955	LHH	CM7-C7-N4-C4
27	BA	2955	LHH	O7-C7-N4-C4
1	Aa	190	OMC	O4'-C4'-C5'-O5'
1	Aa	636	OMG	O4'-C4'-C5'-O5'
27	BA	453	OMU	O4'-C4'-C5'-O5'
27	BA	2571	OMC	C3'-C4'-C5'-O5'
27	BA	2568	OMG	C1'-C2'-O2'-CM2
1	Aa	1478	5MC	O4'-C1'-N1-C6
1	Aa	994	OMG	C4'-C5'-O5'-P
1	Aa	913	OMG	O4'-C4'-C5'-O5'
1	Aa	1276	5MC	O4'-C4'-C5'-O5'
1	Aa	892	OMG	C3'-C2'-O2'-CM2
1	Aa	458	4AC	N3-C4-N4-C7
1	Aa	458	4AC	C5-C4-N4-C7
1	Aa	525	4AC	N3-C4-N4-C7
27	BA	2379	OMG	C4'-C5'-O5'-P
27	BA	1641	4AC	O4'-C4'-C5'-O5'
27	BA	1641	4AC	C3'-C4'-C5'-O5'
27	BA	1799	OMG	O4'-C4'-C5'-O5'
27	BA	2571	OMC	O4'-C4'-C5'-O5'
1	Aa	1478	5MC	O4'-C1'-N1-C2
27	BA	2545	OMC	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
1	Aa	479	OMU	C3'-C2'-O2'-CM2
27	BA	617	LHH	C3'-C2'-O2'-C1
27	BA	1799	OMG	C3'-C2'-O2'-CM2
27	BA	2702	A2M	C3'-C2'-O2'-CM'
27	BA	488	A2M	C3'-C4'-C5'-O5'
27	BA	1892	OMG	C3'-C4'-C5'-O5'
1	Aa	1025	OMG	C4'-C5'-O5'-P
27	BA	505	A2M	C3'-C2'-O2'-CM'
27	BA	1400	A2M	C3'-C2'-O2'-CM'
1	Aa	1217	4AC	C2'-C1'-N1-C6
27	BA	365	OMG	O4'-C4'-C5'-O5'
1	Aa	5	4AC	C3'-C4'-C5'-O5'
1	Aa	1026	OMG	O4'-C4'-C5'-O5'
27	BA	244	4AC	O4'-C4'-C5'-O5'
27	BA	1790	OMC	C3'-C4'-C5'-O5'
27	BA	1799	OMG	C3'-C4'-C5'-O5'
27	BA	2832	4AC	O4'-C4'-C5'-O5'
27	BA	3009	4AC	C3'-C4'-C5'-O5'
1	Aa	1217	4AC	C2'-C1'-N1-C2
27	BA	1551	OMU	C2'-C1'-N1-C2
1	Aa	1434	OMG	O4'-C4'-C5'-O5'
1	Aa	304	OMU	C2'-C1'-N1-C2
1	Aa	1358	OMU	C2'-C1'-N1-C2
27	BA	2610	OMU	C2'-C1'-N1-C2
27	BA	453	OMU	C3'-C4'-C5'-O5'
27	BA	617	LHH	C3'-C4'-C5'-O5'
27	BA	869	OMC	C3'-C4'-C5'-O5'
1	Aa	1478	5MC	C2'-C1'-N1-C2
27	BA	2992	4AC	C2'-C1'-N1-C2
27	BA	723	OMG	C4'-C5'-O5'-P
1	Aa	8	OMU	O4'-C4'-C5'-O5'
1	Aa	190	OMC	C3'-C4'-C5'-O5'
1	Aa	636	OMG	C3'-C4'-C5'-O5'
1	Aa	8	OMU	C2'-C1'-N1-C6
1	Aa	229	LHH	N3-C4-N4-C7
1	Aa	1020	LHH	C5-C4-N4-C7
1	Aa	1020	LHH	N3-C4-N4-C7
27	BA	526	LHH	N3-C4-N4-C7
27	BA	1543	4AC	C2'-C1'-N1-C2
27	BA	1551	OMU	C4'-C5'-O5'-P
1	Aa	8	OMU	O4'-C1'-N1-C6
1	Aa	854	5MC	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 12 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.

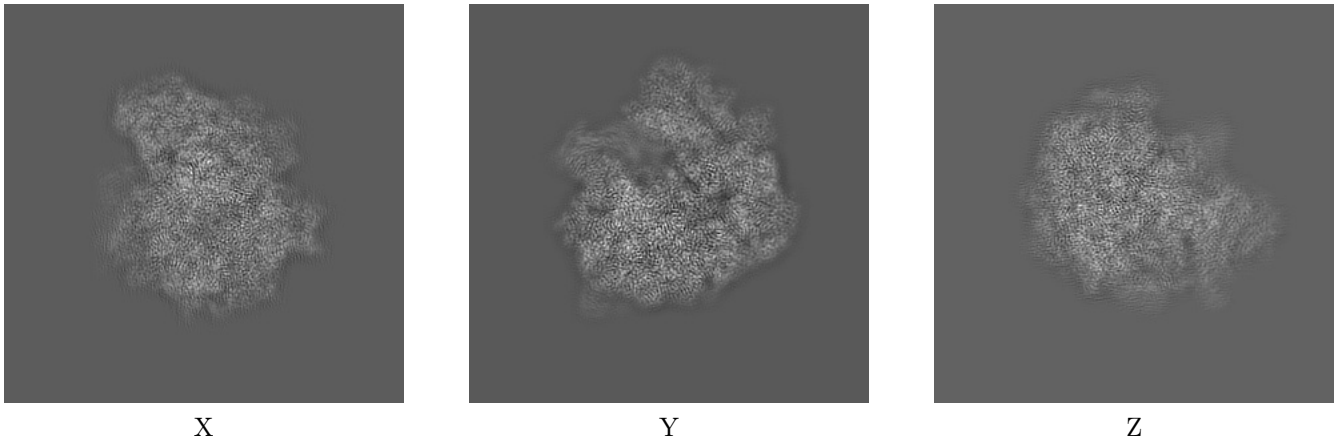
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10223. 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](#)

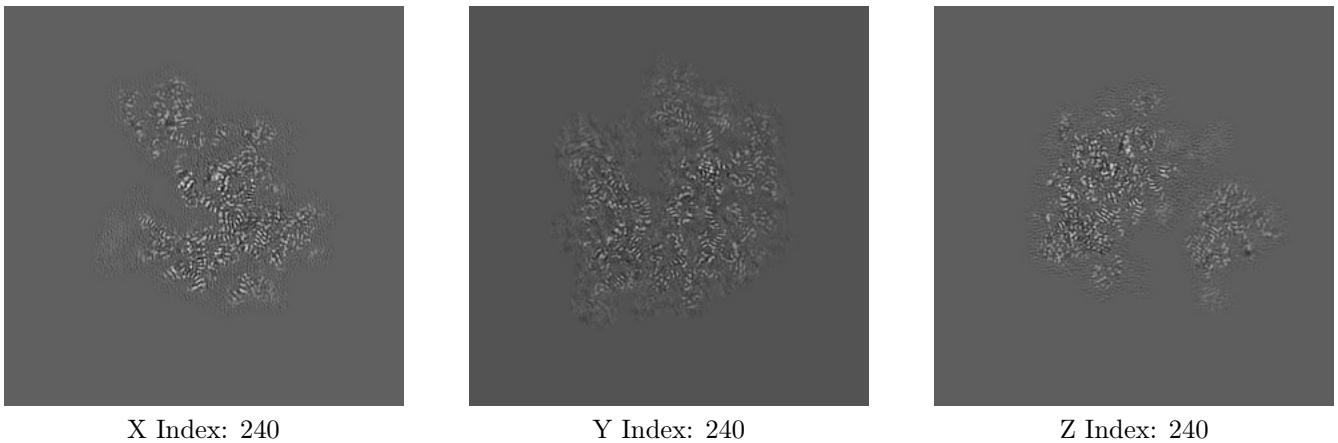
#### 6.1.1 Primary map



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

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

#### 6.2.1 Primary map

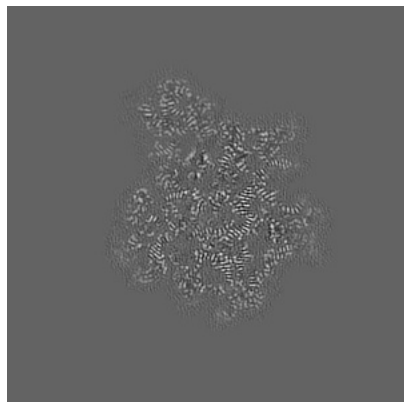




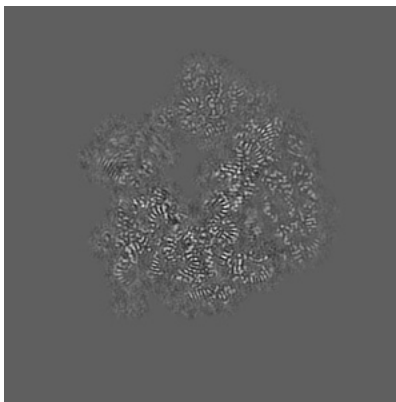
The images above show central slices of the map in three orthogonal directions.

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

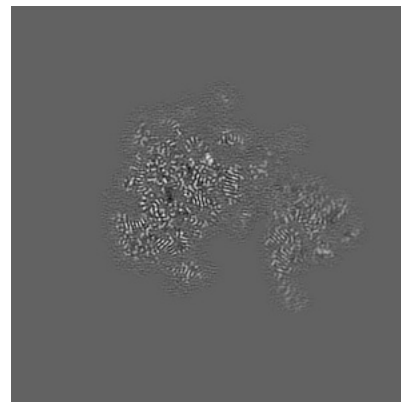
### 6.3.1 Primary map



X Index: 213



Y Index: 224

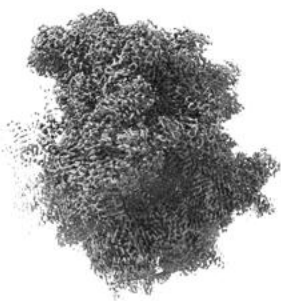


Z Index: 247

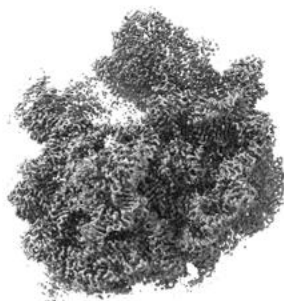
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

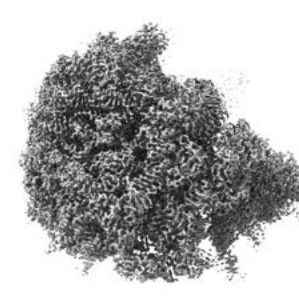
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

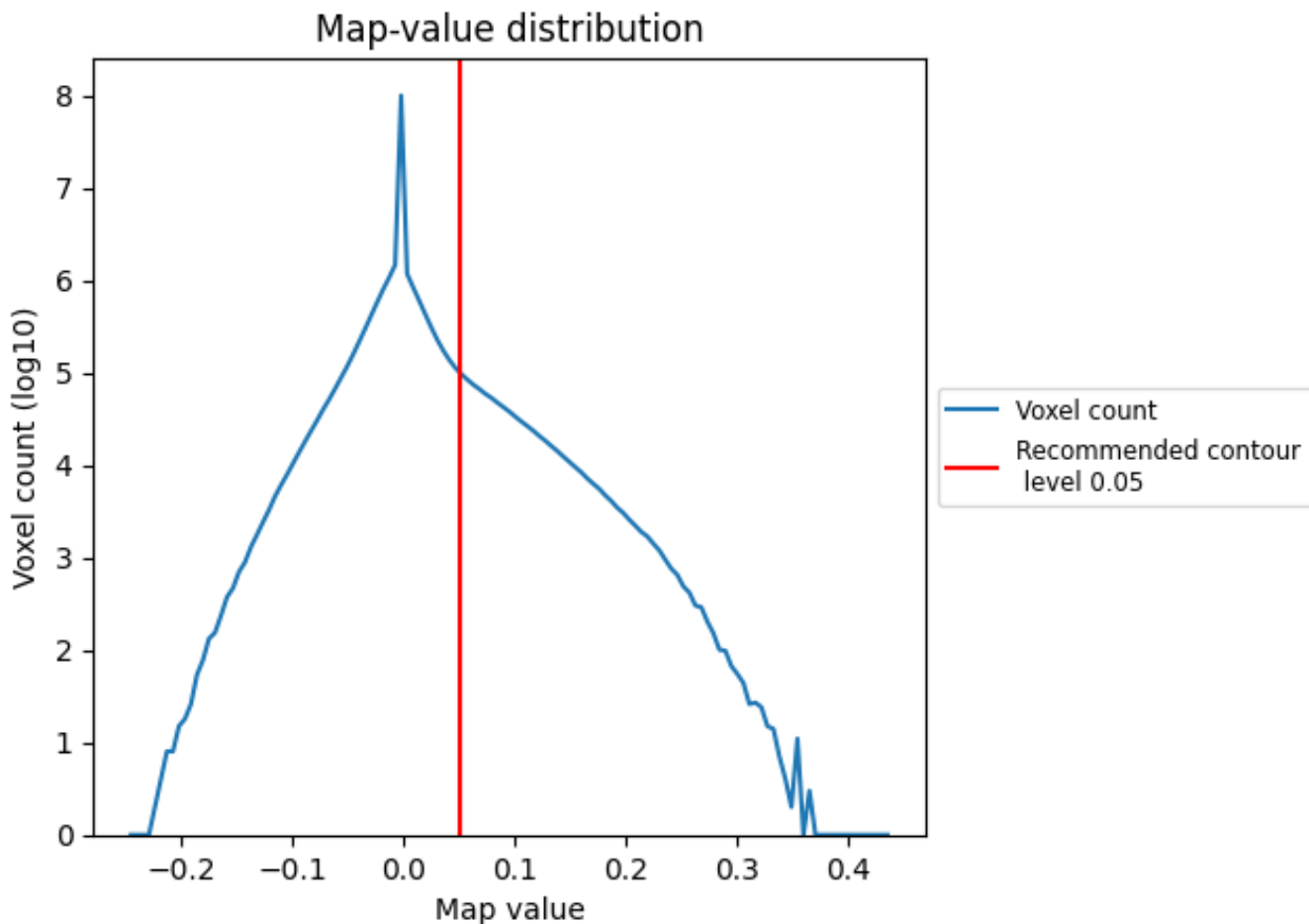
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

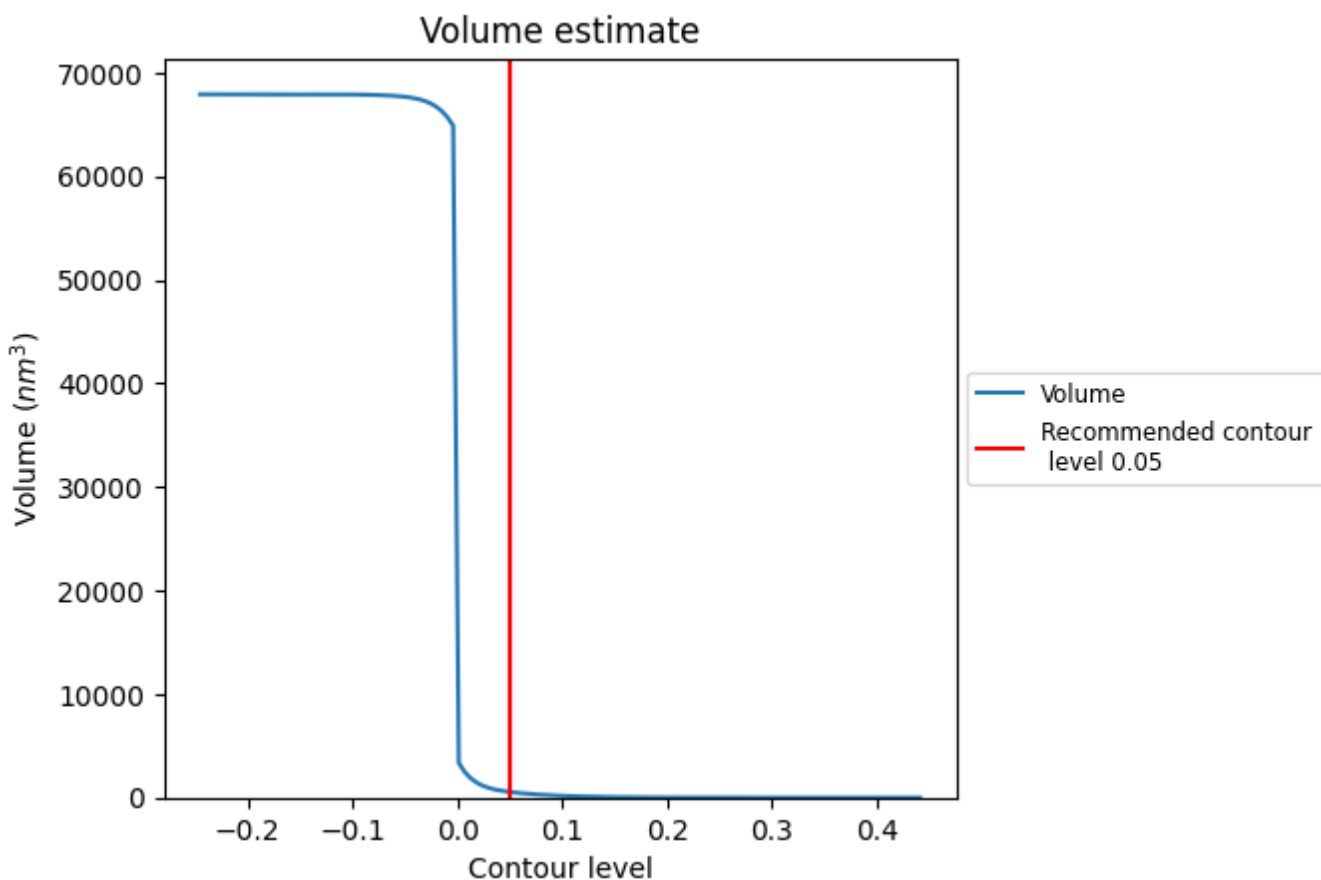
This section contains the results of statistical analysis of the map.

### 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.

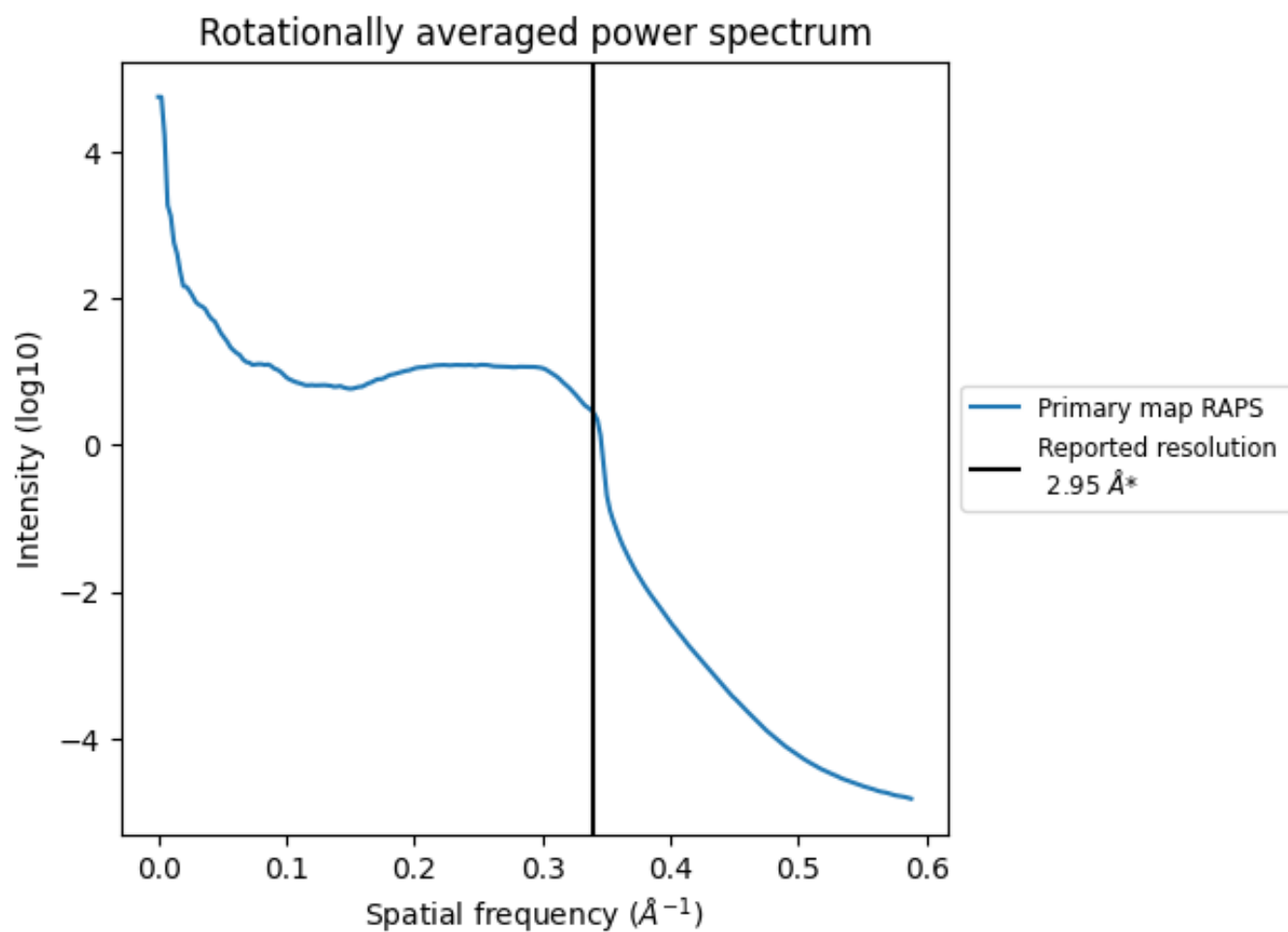
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 541 nm<sup>3</sup>; this corresponds to an approximate mass of 488 kDa.

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

### 7.3 Rotationally averaged power spectrum [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.339 \text{\AA}^{-1}$

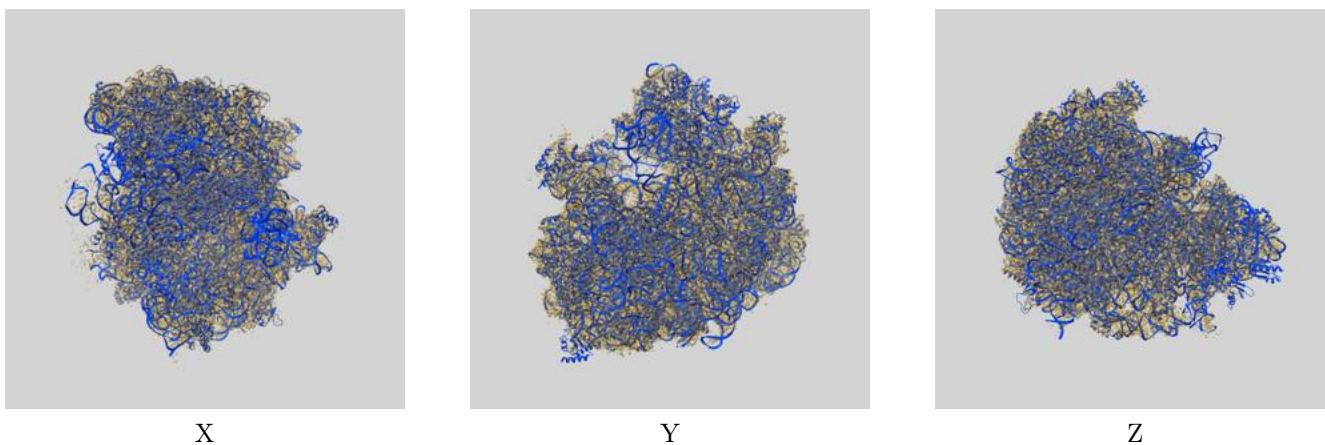
## 8 Fourier-Shell correlation

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

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

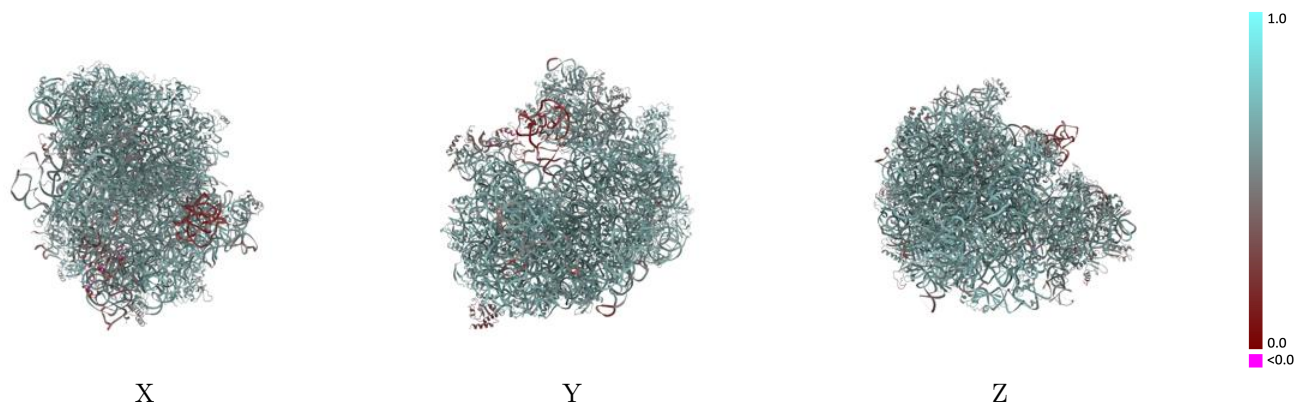
This section contains information regarding the fit between EMDB map EMD-10223 and PDB model 6SKF. Per-residue inclusion information can be found in section 3 on page 19.

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



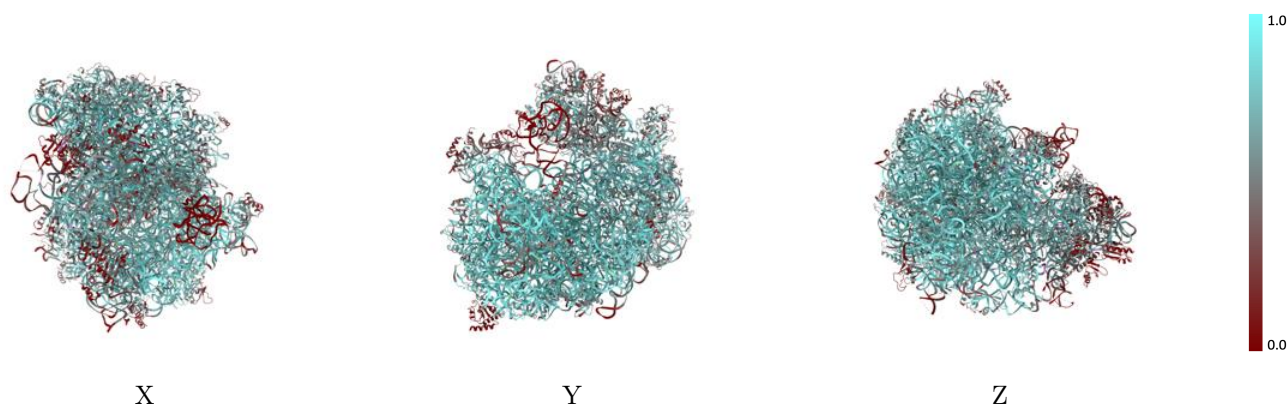
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

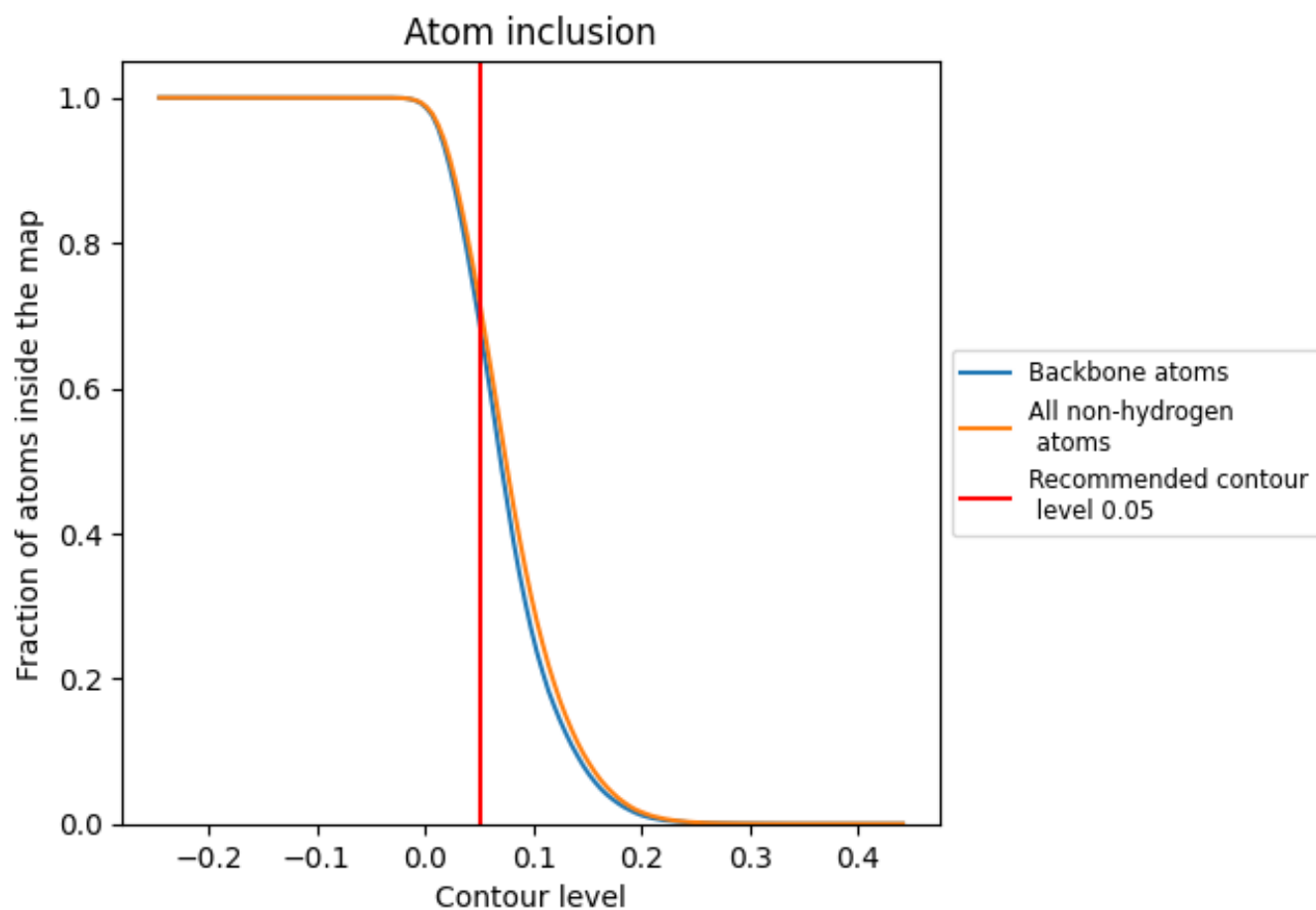
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.05).









































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 72% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7215	 0.5970
Aa	 0.7524	 0.6120
Ab	 0.5250	 0.5890
Ac	 0.2443	 0.5210
Ad	 0.5153	 0.5720
Ae	 0.6273	 0.5960
Af	 0.6610	 0.6140
Ag	 0.6510	 0.6090
Ah	 0.3634	 0.5600
Ai	 0.4982	 0.5560
Aj	 0.6690	 0.6090
Ak	 0.6118	 0.5980
Al	 0.4230	 0.5680
Am	 0.2059	 0.5180
An	 0.5507	 0.5760
Ao	 0.5925	 0.6110
Ap	 0.5276	 0.5540
Aq	 0.6230	 0.5870
Ar	 0.4592	 0.5780
As	 0.6273	 0.6170
At	 0.1596	 0.4910
Au	 0.4605	 0.5730
Av	 0.5554	 0.5690
Aw	 0.5728	 0.5920
Ax	 0.5000	 0.5810
Ay	 0.4372	 0.5440
Az	 0.5823	 0.6170
BA	 0.8212	 0.6050
BB	 0.6120	 0.5320
BC	 0.7767	 0.6200
BD	 0.7812	 0.6230
BE	 0.7630	 0.6170
BF	 0.1558	 0.3000
BG	 0.6630	 0.5920
BH	 0.5049	 0.5590



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Chain	Atom inclusion	Q-score
BI	 0.0623	 0.3640
BJ	 0.7314	 0.6020
BK	 0.7457	 0.6140
BL	 0.7414	 0.6150
BM	 0.5943	 0.5770
BN	 0.5421	 0.5580
BO	 0.6002	 0.5700
BP	 0.8302	 0.6350
BQ	 0.4813	 0.5340
BR	 0.7481	 0.6110
BS	 0.7238	 0.5990
BT	 0.6149	 0.5890
BU	 0.8013	 0.6300
BV	 0.7831	 0.6250
BW	 0.6841	 0.5900
BX	 0.7409	 0.6110
BY	 0.8095	 0.6270
BZ	 0.5617	 0.5550
Ba	 0.7606	 0.6100
Bb	 0.6198	 0.5610
Bc	 0.7112	 0.5980
Bd	 0.7668	 0.6230
Be	 0.7388	 0.6080
Bg	 0.7508	 0.6160
Bh	 0.8755	 0.6460
Bi	 0.7913	 0.6290
Bj	 0.7472	 0.6170
Bk	 0.8899	 0.6250
Bl	 0.7299	 0.6170