



Full wwPDB EM Validation Report ⓘ

Apr 16, 2024 – 10:09 am BST

PDB ID : 8A98
EMDB ID : EMD-15272
Title : CRYO-EM STRUCTURE OF LEISHMANIA MAJOR 80S RIBOSOME :
snoRNA MUTANT
Authors : Rajan, K.S.; Yonath, A.; Bashan, A.
Deposited on : 2022-06-28
Resolution : 2.46 Å (reported)
Based on initial models : 6AZ3, 6AZ1, 5T2A

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev92
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 : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

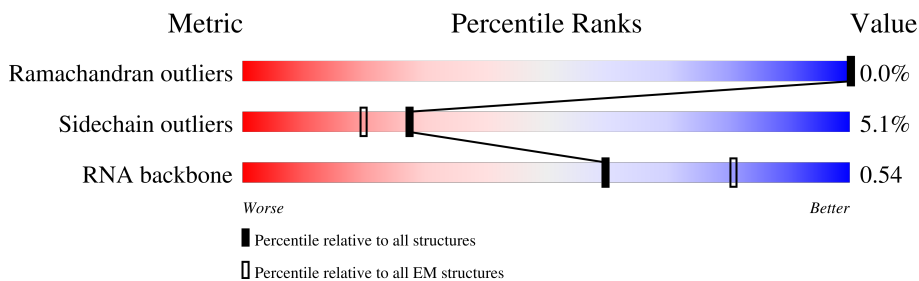
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.46 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	SW	152	
2	SZ	137	
3	SY	164	
4	SX	161	
5	SV	143	
6	SU	173	
7	ST	151	
8	SS	57	
9	SR	153	





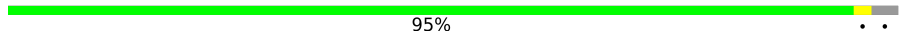





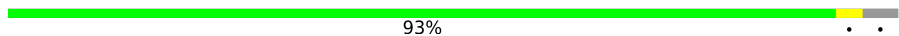


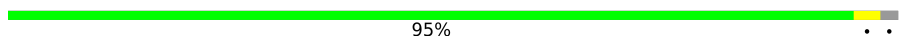


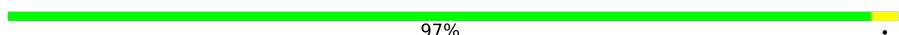
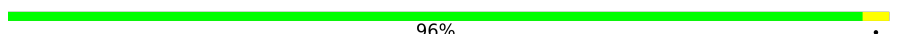

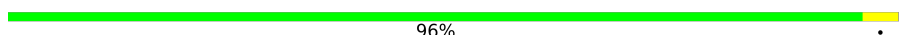

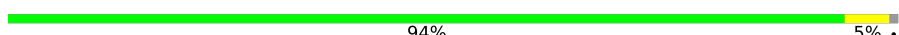



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Mol	Chain	Length	Quality of chain
10	SB	246	80% 5% 15%
11	SC	219	93% . .
12	SD	190	95% . .
13	SE	273	93% . 5%
14	SK	220	80% . 18%
15	S4	19	68% 32%
16	Sg	312	87% 9% .
17	Sa	120	54% 5% 41%
18	Sc	86	90% 8% .
19	Se	66	76% . 21%
20	S1	2204	58% 18% . 22%
21	SQ	141	20% 80%
22	SP	143	94% 5% .
23	SO	144	90% . 6%
24	SN	168	55% 5% 40%
25	Sd	87	69% 6% 25%
26	SM	116	84% . 12%
27	SL	149	95% . .
28	SJ	130	96% . .
29	SI	200	95% 5%
30	SH	190	94% . .
31	SG	249	91% . 6%
32	SF	265	80% . 17%
33	SA	264	80% 6% 15%
34	Sb	112	88% . 11%

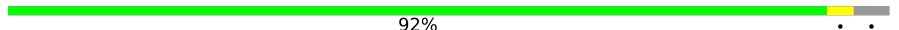


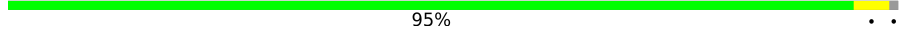




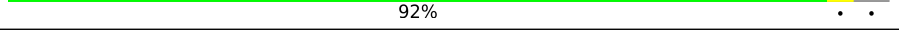




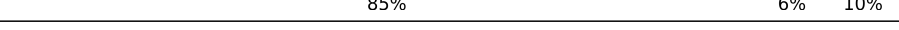

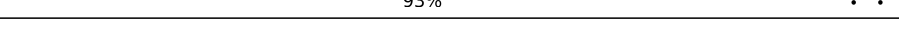


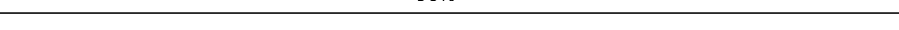


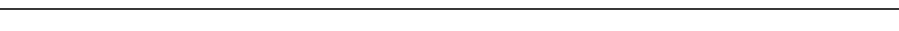


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Mol	Chain	Length	Quality of chain
35	Sh	235	 34% 6% 60%
36	f	133	 90% 8%
37	d	104	 83% 13%
38	c	252	 88% 10%
39	a	127	 95%
40	b	70	 91% 6%
41	1	1782	 67% 20% 11%
42	2	1526	 49% 18% 31%
43	4	183	 79% 21%
44	7	171	 74% 18% 6%
45	B	419	 93%
46	8	123	 82% 14%
47	5	135	 59% 19% 18%
48	A	260	 95%
49	O	305	 80% 17%
50	G	264	 86% 12%
51	H	222	 97%
52	M	204	 96%
53	I	220	 90% 7%
54	P	198	 96%
55	Q	254	 71% 26%
56	R	179	 94% 5%
57	E	190	 91% 7%
58	6	73	 53% 41%
59	T	166	 91% 8%

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Mol	Chain	Length	Quality of chain
60	S	159	92% 
61	K	175	83%  5% 13%
62	D	188	81%  15%
63	L	145	95%  ..
64	Y	134	94%  ..
65	Z	147	92%  5%
66	F	195	70%  27%
67	h	168	70%  5% 25%
68	g	144	92%  ..
69	J	139	88%  5% 7%
70	V	145	79%  19%
71	W	143	80%  17%
72	U	129	79%  8% 13%
73	i	105	85%  6% 10%
74	p	106	84%  7% 9%
75	o	92	93%  ..
76	X	124	51%  48%
77	k	83	82%  6% 12%
78	l	51	96%  ..
79	n	34	88%  9% .
80	C	373	94%  ..
81	3	216	52%  19% . 25%
82	e	188	84%  7% . 8%
83	j	83	93%  ..

2 Entry composition

There are 88 unique types of molecules in this entry. The entry contains 197779 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Putative 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	SW	105	787	506	152	125	4	0	0

- Molecule 2 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	SZ	122	967	620	184	160	3	1	0

- Molecule 3 is a protein called Putative 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	SY	83	604	371	110	119	4	0	0

- Molecule 4 is a protein called 40S ribosomal protein S19-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	SX	139	1071	682	204	181	4	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SX	37	SER	THR	conflict	UNP E9AEE8

- Molecule 5 is a protein called Putative 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	SV	113	843	535	159	145	4	0	0

- Molecule 6 is a protein called Putative 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	SU	148	1170	739	235	191	5	0	0

- Molecule 7 is a protein called Putative 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	ST	141	1145	723	228	186	8	0	0

- Molecule 8 is a protein called Putative ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	SS	55	428	265	87	72	4	0	0

- Molecule 9 is a protein called Putative 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	SR	119	892	567	167	154	4	0	0

- Molecule 10 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	SB	209	1643	1046	297	288	12	2	0

- Molecule 11 is a protein called Putative 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	SC	212	1619	1028	296	282	13	2	0

- Molecule 12 is a protein called Putative 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	SD	182	1513	951	308	246	8	1	0

- Molecule 13 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	SE	260	2056	1304	396	347	9	2	0

- Molecule 14 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	SK	180	1424	895	300	227	2	0	0

- Molecule 15 is a RNA chain called E-site_tRNA_chain_S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
15	S4	19	404	181	76	129	18	0	0

- Molecule 16 is a protein called Small ribosomal subunit protein RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	Sg	300	2251	1415	399	424	13	0	0

- Molecule 17 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	Sa	71	541	345	93	100	3	0	0

- Molecule 18 is a protein called Putative 40S ribosomal protein S27-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	Sc	84	638	396	123	111	8	0	0

- Molecule 19 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	Se	52	404	253	87	63	1	0	0

- Molecule 20 is a RNA chain called SSU_rRNA_chain_S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
20	S1	1727	36928	16523	6655	12024	1726	0	0

- Molecule 21 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	SQ	28	179	111	33	33	2	0	0

- Molecule 22 is a protein called Putative 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	SP	142	1115	704	222	186	3	3	0

- Molecule 23 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	SO	136	1012	625	197	182	8	1	0

- Molecule 24 is a protein called Putative 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	SN	101	813	521	143	142	7	0	0

- Molecule 25 is a protein called Putative 40S ribosomal protein S33.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	Sd	65	466	286	94	82	4	0	0

- Molecule 26 is a protein called Putative ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	SM	102	811	506	149	154	2	1	0

- Molecule 27 is a protein called Putative 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	SL	143	Total	C	N	O	S	0	0
			1130	727	209	191	3		

- Molecule 28 is a protein called Putative 40S ribosomal protein S15A.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	SJ	129	Total	C	N	O	S	0	0
			1014	643	188	175	8		

- Molecule 29 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	SI	200	Total	C	N	O	S	0	0
			1613	1026	307	272	8		

- Molecule 30 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	SH	184	Total	C	N	O	S	0	0
			1437	894	277	259	7		

- Molecule 31 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	SG	233	Total	C	N	O	S	1	0
			1809	1131	370	305	3		

- Molecule 32 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	SF	220	Total	C	N	O	S	0	0
			1656	1063	299	284	10		

- Molecule 33 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	SA	225	Total	C	N	O	S	2	0
			1834	1148	353	322	11		

- Molecule 34 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Sb	100	Total	C	N	O	S	0	0
			779	484	162	126	7		

- Molecule 35 is a protein called Putative RNA binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Sh	94	Total	C	N	O	S	0	0
			657	406	125	124	2		

- Molecule 36 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	f	122	Total	C	N	O	S	0	0
			988	621	196	167	4		

- Molecule 37 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	d	90	Total	C	N	O	S	0	0
			625	388	114	118	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	c	227	Total	C	N	O	S	0	0
			1779	1134	340	294	11		

- Molecule 39 is a protein called Putative 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	a	123	Total	C	N	O	S	0	0
			955	597	199	157	2		

- Molecule 40 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	b	66	Total	C	N	O	0	0
			520	318	120	82		

- Molecule 41 is a RNA chain called LSUa_rRNA_chain_1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
41	1	1579	33802	15099	6193	10932	1578	0	0

- Molecule 42 is a RNA chain called LSub_rRNA_chain_2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
42	2	1047	22358	10009	4022	7280	1047	0	0

- Molecule 43 is a RNA chain called SR2_chain_4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
43	4	183	3906	1742	706	1275	183	0	0

- Molecule 44 is a RNA chain called 5.8S_rRNA_chain_7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
44	7	160	3399	1520	599	1121	159	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
7	87	U	A	conflict	GB 1207899567

- Molecule 45 is a protein called Putative ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	B	402	3200	2019	636	532	13	7	0

- Molecule 46 is a RNA chain called 5S_rRNA_chain_8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
46	8	118	2511	1123	448	822	118	0	0

- Molecule 47 is a RNA chain called SR4_chain_5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
47	5	111	2373	1058	431	773	111	0	0

- Molecule 48 is a protein called Putative 60S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	A	255	1973	1229	407	326	11	5	0

- Molecule 49 is a protein called Putative 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	O	252	1970	1259	373	333	5	3	0

- Molecule 50 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	G	233	1850	1160	370	313	7	2	0

- Molecule 51 is a protein called Putative 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	H	221	1771	1121	352	291	7	1	0

- Molecule 52 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	M	203	1714	1080	362	264	8	0	0

- Molecule 53 is a protein called eL13_chain_I.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	I	205	1593	993	318	274	8	0	0

- Molecule 54 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	P	197	1539	968	307	258	6	0	0

- Molecule 55 is a protein called Putative 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	Q	189	1482	916	319	241	6	0	0

- Molecule 56 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	R	178	1447	921	277	244	5	0	0

- Molecule 57 is a protein called Putative 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	E	186	1439	911	267	255	6	0	0

- Molecule 58 is a RNA chain called SR6_chain_6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
58	6	71	1484	663	267	483	71	0	0

- Molecule 59 is a protein called Putative 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
59	T	153	1233	770	244	208	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
60	S	152	1203	764	236	200	3	0	0

- Molecule 61 is a protein called Putative 40S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
61	K	153	1193	746	234	206	7	0	0

- Molecule 62 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
62	D	159	1140	723	212	197	8	0	0

- Molecule 63 is a protein called Putative 60S ribosomal protein L27A/L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
63	L	144	1124	707	226	185	6	0	0

- Molecule 64 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
64	Y	132	1046	667	211	165	3	1	0

- Molecule 65 is a protein called Putative 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
65	Z	139	1052	642	221	184	5	0	0

- Molecule 66 is a protein called Putative 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
66	F	142	1045	665	194	184	2	0	0

- Molecule 67 is a protein called Putative 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
67	h	126	1016	626	222	162	6	1	0

- Molecule 68 is a protein called Putative ribosomal protein l35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	g	138	Total	C	N	O	S	0	0
			1101	684	233	179	5		

- Molecule 69 is a protein called Putative 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	J	129	Total	C	N	O	S	0	0
			968	614	183	165	6		

- Molecule 70 is a protein called Putative 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	V	118	Total	C	N	O	S	0	0
			939	595	176	165	3		

- Molecule 71 is a protein called Putative 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	W	118	Total	C	N	O	S	0	0
			948	591	197	156	4		

- Molecule 72 is a protein called Putative 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	U	112	Total	C	N	O	S	0	0
			879	572	154	151	2		

- Molecule 73 is a protein called Putative 60S Ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	i	95	Total	C	N	O	S	0	0
			738	467	148	121	2		

- Molecule 74 is a protein called Putative 60S ribosomal protein L44.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	p	96	Total	C	N	O	S	0	0
			722	460	144	116	2		

- Molecule 75 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	o	90	Total	C	N	O	S	0	0
			696	432	144	114	6		

- Molecule 76 is a protein called Putative ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	X	65	Total	C	N	O	S	0	0
			553	362	106	81	4		

- Molecule 77 is a protein called Putative ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	k	73	Total	C	N	O	S	0	0
			546	342	104	97	3		

- Molecule 78 is a protein called Putative 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	l	50	Total	C	N	O	S	0	0
			440	285	91	63	1		

- Molecule 79 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	n	33	Total	C	N	O	S	0	0
			259	161	60	37	1		

- Molecule 80 is a protein called Putative ribosomal protein L1a.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	C	366	Total	C	N	O	S	0	0
			2797	1745	554	483	15		

- Molecule 81 is a RNA chain called SR1_chain_3.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	3	161	Total	C	N	O	P	0	0
			3419	1529	596	1133	161		

- Molecule 82 is a protein called Putative 60S ribosomal subunit protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	e	173	Total	C	N	O	S	0	0
			1298	821	254	220	3		

- Molecule 83 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	j	80	Total	C	N	O	S	0	0
			662	403	151	102	6		

- Molecule 84 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
84	SS	1	Total	Mg	0
			1	1	
84	S1	23	Total	Mg	0
			23	23	
84	SL	1	Total	Mg	0
			1	1	
84	1	61	Total	Mg	0
			61	61	
84	2	31	Total	Mg	0
			31	31	
84	4	3	Total	Mg	0
			3	3	
84	7	4	Total	Mg	0
			4	4	
84	8	1	Total	Mg	0
			1	1	
84	5	1	Total	Mg	0
			1	1	
84	6	1	Total	Mg	0
			1	1	
84	T	1	Total	Mg	0
			1	1	
84	J	1	Total	Mg	0
			1	1	
84	3	1	Total	Mg	0
			1	1	

- Molecule 85 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
85	Sc	1	Total 1	Zn 1	0
85	Sb	1	Total 1	Zn 1	0
85	o	1	Total 1	Zn 1	0
85	j	1	Total 1	Zn 1	0

- Molecule 86 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
86	1	5	Total 5	Na 5	0
86	2	3	Total 3	Na 3	0

- Molecule 87 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
87	1	2	Total 2	K 2	0

- Molecule 88 is water.

Mol	Chain	Residues	Atoms		AltConf
88	SZ	1	Total 1	O 1	0
88	SY	1	Total 1	O 1	0
88	SX	7	Total 7	O 7	0
88	ST	5	Total 5	O 5	0
88	SS	1	Total 1	O 1	0
88	SR	2	Total 2	O 2	0
88	SB	3	Total 3	O 3	0
88	SC	1	Total 1	O 1	0

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Mol	Chain	Residues	Atoms		AltConf
88	SD	1	Total 1	O 1	0
88	SE	1	Total 1	O 1	0
88	SK	1	Total 1	O 1	0
88	S4	1	Total 1	O 1	0
88	Sg	3	Total 3	O 3	0
88	Sa	1	Total 1	O 1	0
88	Sc	2	Total 2	O 2	0
88	S1	237	Total 237	O 237	0
88	SP	3	Total 3	O 3	0
88	SO	2	Total 2	O 2	0
88	SN	3	Total 3	O 3	0
88	Sd	1	Total 1	O 1	0
88	SH	4	Total 4	O 4	0
88	SF	2	Total 2	O 2	0
88	Sb	2	Total 2	O 2	0
88	f	16	Total 16	O 16	0
88	d	3	Total 3	O 3	0
88	c	4	Total 4	O 4	0
88	a	3	Total 3	O 3	0
88	1	918	Total 918	O 918	0
88	2	536	Total 536	O 536	0

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Mol	Chain	Residues	Atoms		AltConf
88	4	73	Total 73	O 73	0
88	7	85	Total 85	O 85	0
88	B	29	Total 29	O 29	0
88	8	17	Total 17	O 17	0
88	5	37	Total 37	O 37	0
88	A	30	Total 30	O 30	0
88	G	4	Total 4	O 4	0
88	H	9	Total 9	O 9	0
88	M	28	Total 28	O 28	0
88	I	21	Total 21	O 21	0
88	P	12	Total 12	O 12	0
88	Q	6	Total 6	O 6	0
88	R	1	Total 1	O 1	0
88	E	1	Total 1	O 1	0
88	6	3	Total 3	O 3	0
88	T	14	Total 14	O 14	0
88	S	4	Total 4	O 4	0
88	K	1	Total 1	O 1	0
88	L	17	Total 17	O 17	0
88	h	12	Total 12	O 12	0
88	g	9	Total 9	O 9	0

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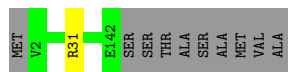
Mol	Chain	Residues	Atoms		AltConf
88	J	1	Total 1	O 1	0
88	V	6	Total 6	O 6	0
88	W	2	Total 2	O 2	0
88	i	1	Total 1	O 1	0
88	p	13	Total 13	O 13	0
88	o	2	Total 2	O 2	0
88	X	2	Total 2	O 2	0
88	k	2	Total 2	O 2	0
88	l	6	Total 6	O 6	0
88	C	21	Total 21	O 21	0
88	3	31	Total 31	O 31	0
88	e	9	Total 9	O 9	0
88	j	13	Total 13	O 13	0

Chain SU:  83% 14%



• Molecule 7: Putative 40S ribosomal protein S13

Chain ST:  93% 7%




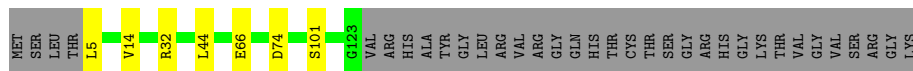
• Molecule 8: Putative ribosomal protein S29

Chain SS:  93%




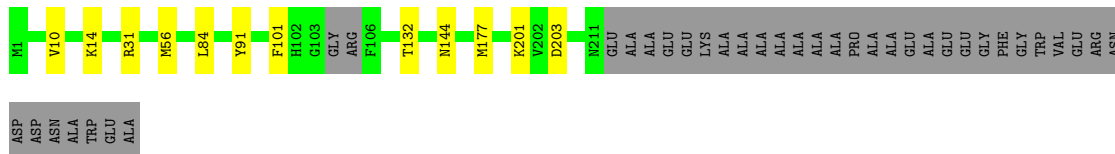
• Molecule 9: Putative 40S ribosomal protein S18

Chain SR:  73% 5% 22%



• Molecule 10: 40S ribosomal protein SA

Chain SB:  80% 5% 15%



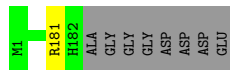
• Molecule 11: Putative 40S ribosomal protein S3

Chain SC:  93%



• Molecule 12: Putative 40S ribosomal protein S9

Chain SD:  95%




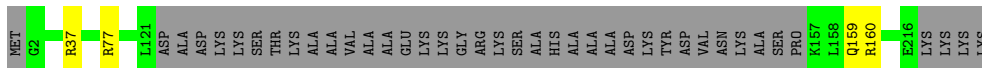
- Molecule 13: 40S ribosomal protein S4

Chain SE:  93% • 5%



- Molecule 14: 40S ribosomal protein S8

Chain SK:  80% • 18%




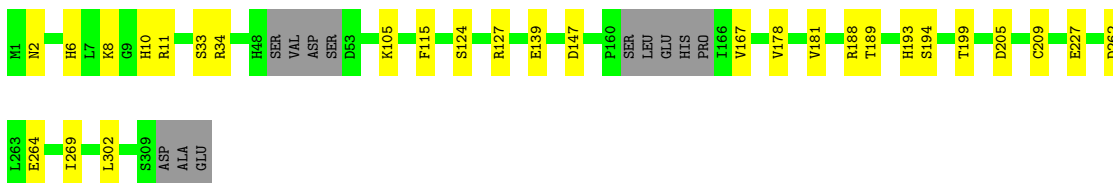
- Molecule 15: E-site_tRNA_chain_S4

Chain S4:  68% 32%



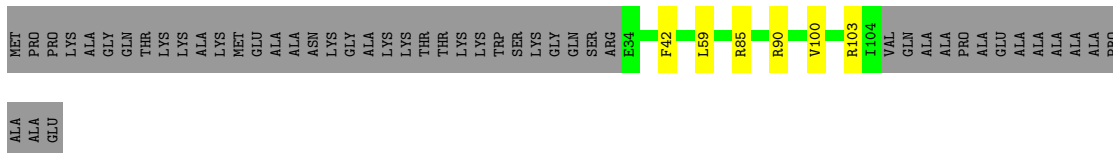
- Molecule 16: Small ribosomal subunit protein RACK1

Chain Sg:  87% 9% •




- Molecule 17: 40S ribosomal protein S25

Chain Sa:  54% 5% 41%

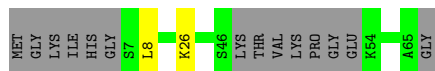
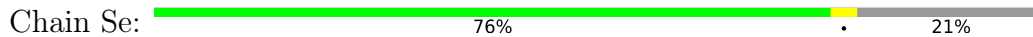


- Molecule 18: Putative 40S ribosomal protein S27-1

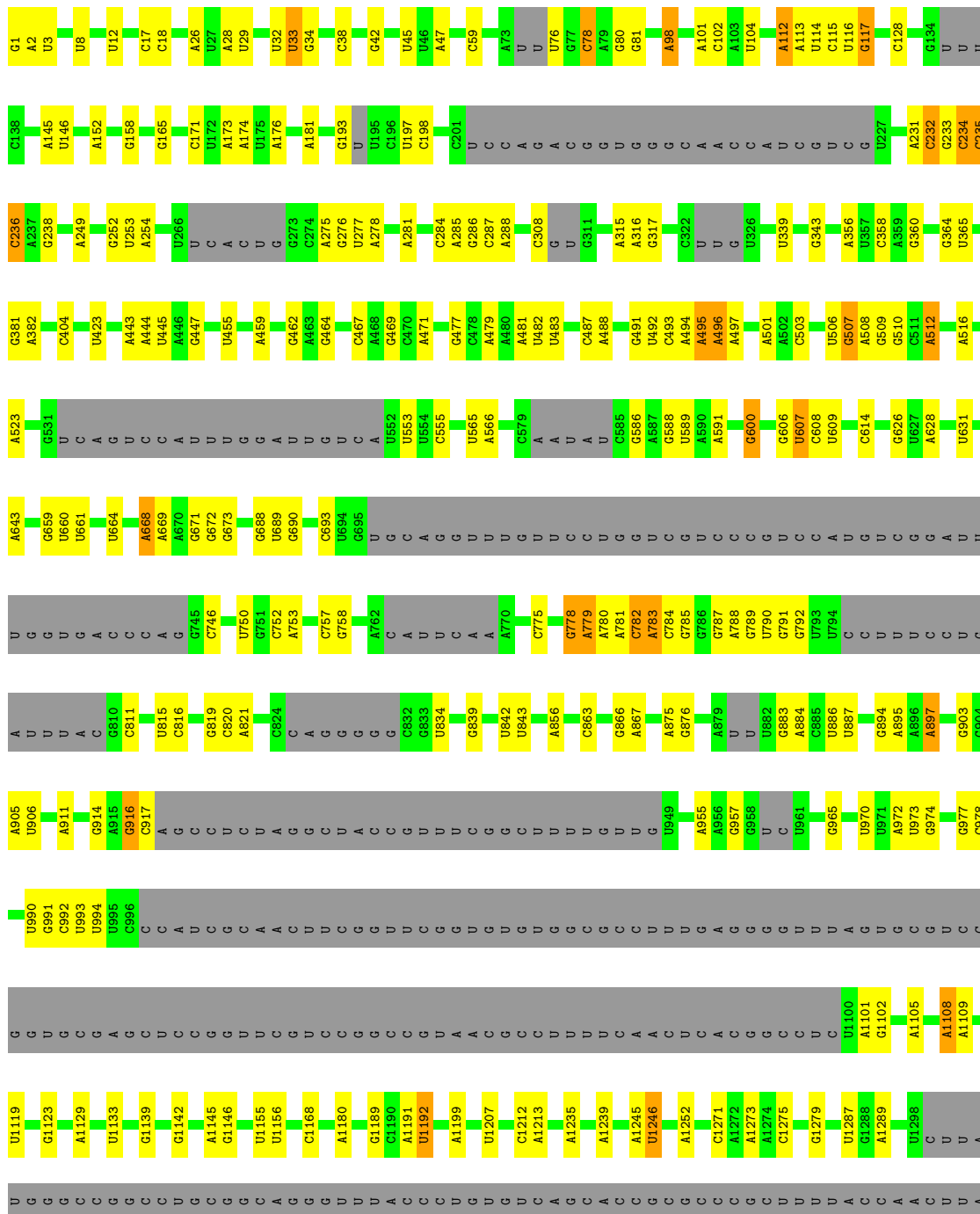
Chain Sc:  90% 8% •

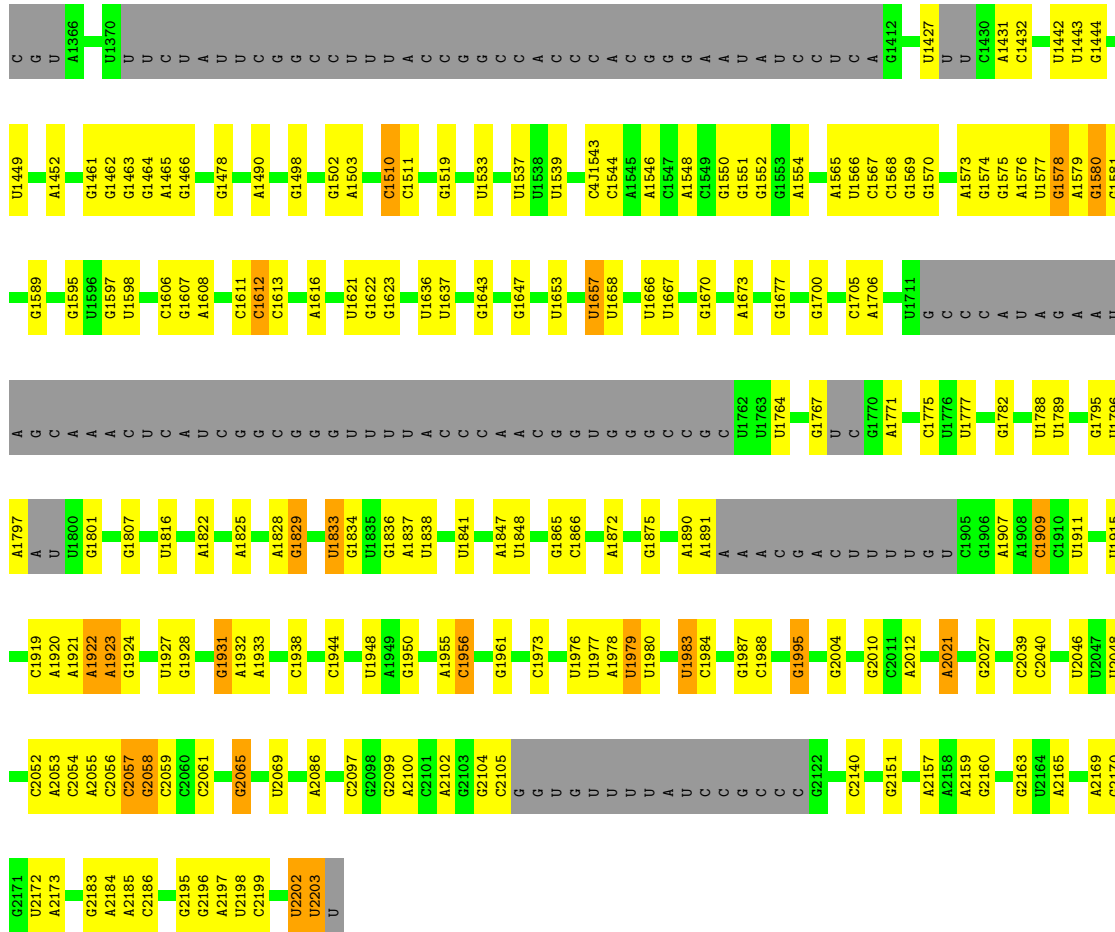


- Molecule 19: 40S ribosomal protein S30

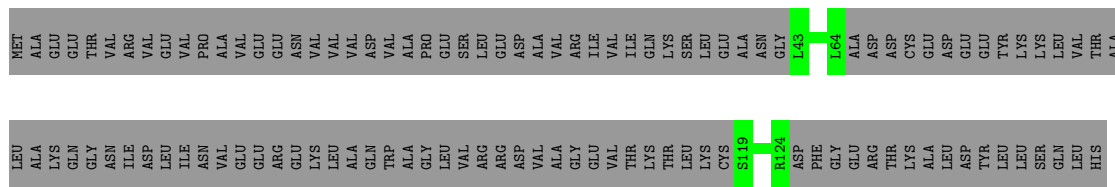


● Molecule 20: SSU_rRNA_chain_S1





• Molecule 21: 40S ribosomal protein S12



• Molecule 22: Putative 40S ribosomal protein S23



• Molecule 23: 40S ribosomal protein S14

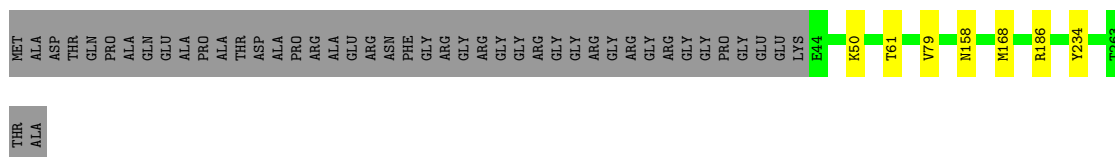
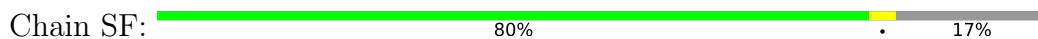




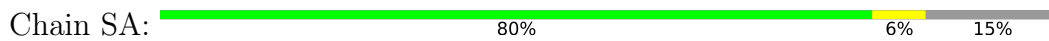
- Molecule 31: 40S ribosomal protein S6



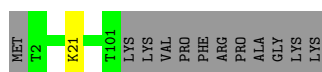
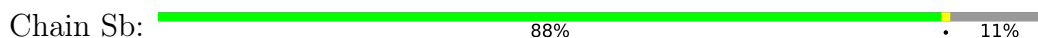
- Molecule 32: 40S ribosomal protein S2



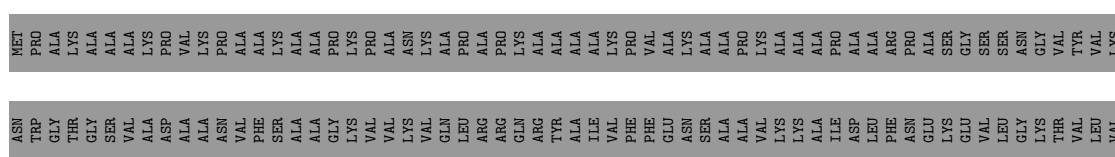
- Molecule 33: 40S ribosomal protein S3a



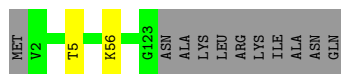
- Molecule 34: 40S ribosomal protein S26



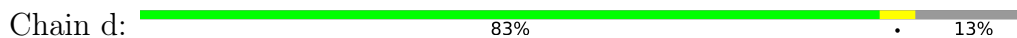
- Molecule 35: Putative RNA binding protein



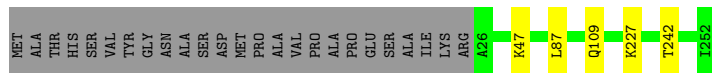
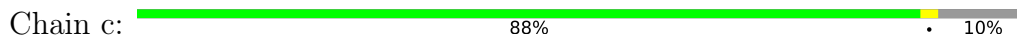
• Molecule 36: 60S ribosomal protein L32



• Molecule 37: 60S ribosomal protein L30



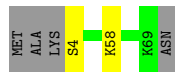
• Molecule 38: Putative 60S ribosomal protein L7



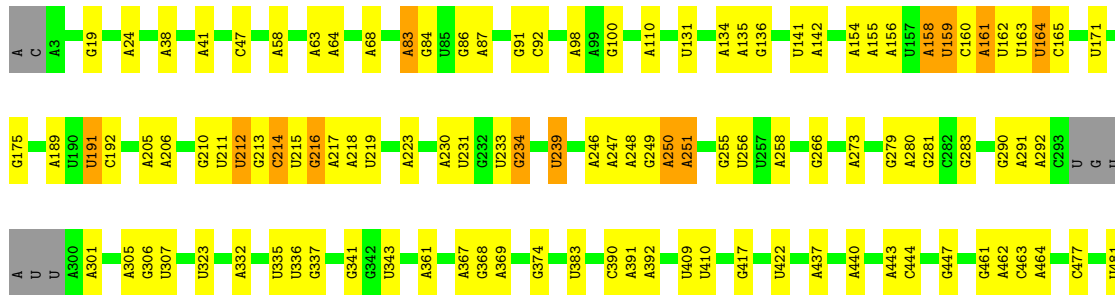
• Molecule 39: Putative 60S ribosomal protein L35

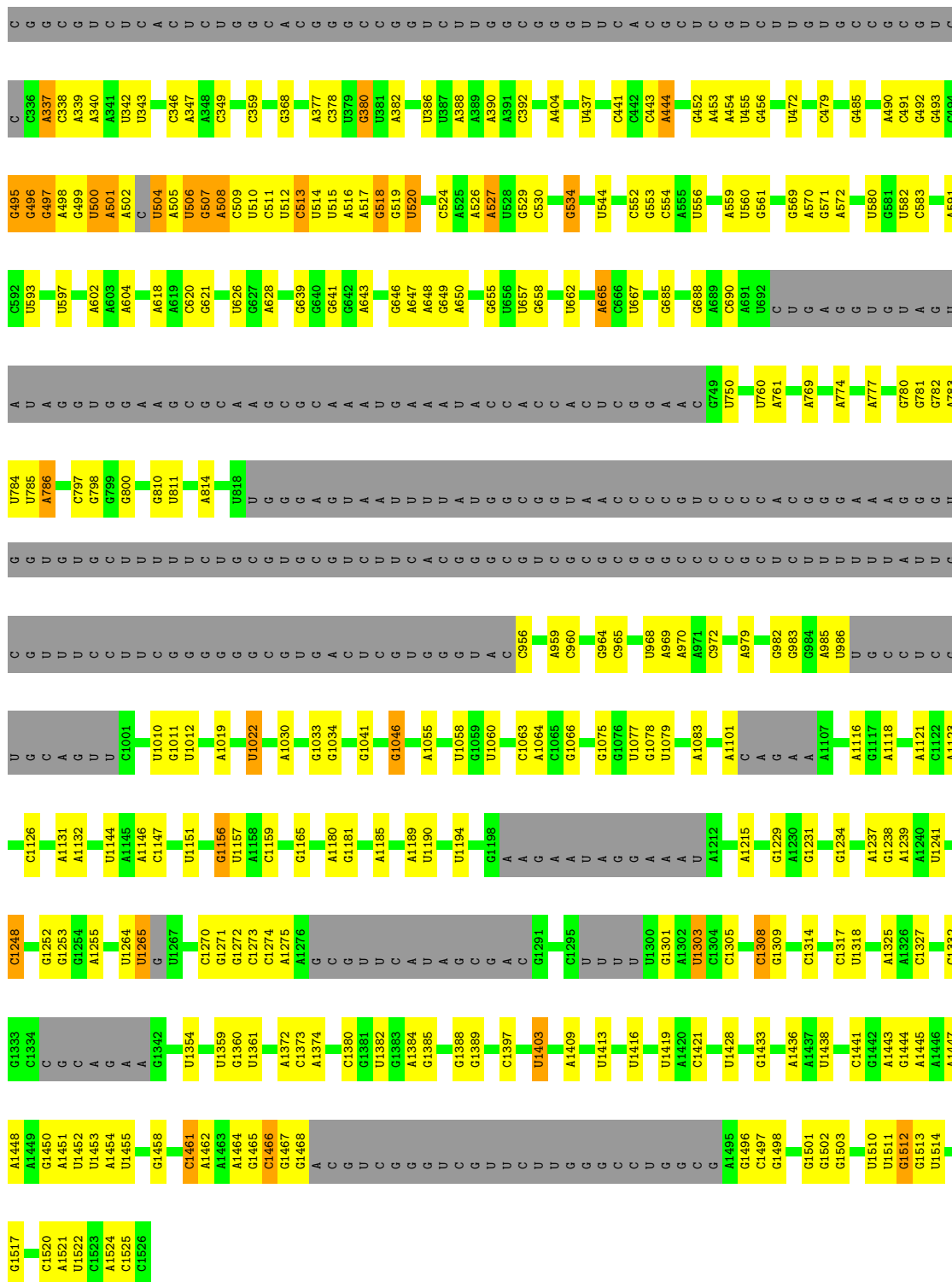


• Molecule 40: 60S ribosomal protein L29

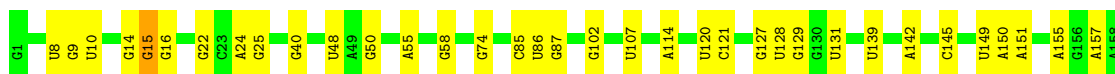


• Molecule 41: LSUa_rRNA_chain_1



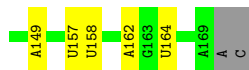
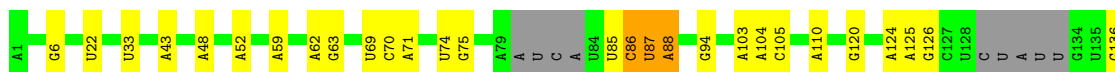


• Molecule 43: SR2_chain_4





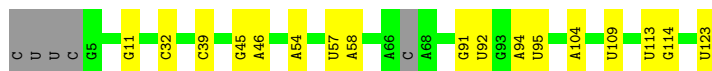
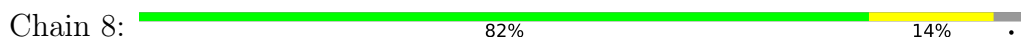
• Molecule 44: 5.8S_rRNA_chain_7



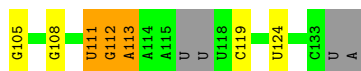
• Molecule 45: Putative ribosomal protein L3



• Molecule 46: 5S_rRNA_chain_8



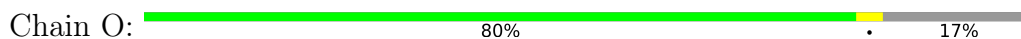
• Molecule 47: SR4_chain_5



• Molecule 48: Putative 60S ribosomal protein L2



• Molecule 49: Putative 60S ribosomal protein L5




- Molecule 56: 60S ribosomal protein L18a

Chain R:  94% 5%



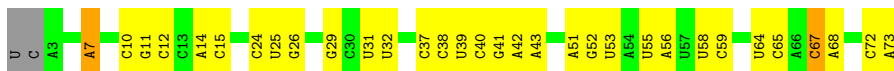
- Molecule 57: Putative 60S ribosomal protein L9

Chain E:  91% 7%



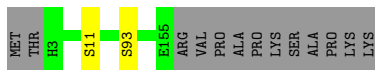
- Molecule 58: SR6_chain_6

Chain 6:  53% 41%




- Molecule 59: Putative 60S ribosomal protein L17

Chain T:  91% 8%




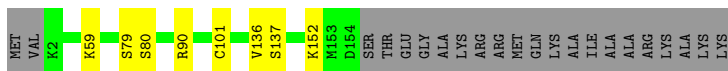
- Molecule 60: Putative 60S ribosomal protein L21

Chain S:  92%




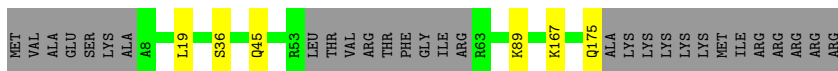
- Molecule 61: Putative 40S ribosomal protein L14

Chain K:  83% 5% 13%



- Molecule 62: 60S ribosomal protein L11

Chain D:  81% 15%



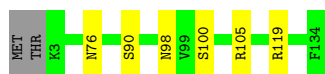
- Molecule 63: Putative 60S ribosomal protein L27A/L29

Chain L:  95%



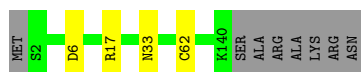
- Molecule 64: 60S ribosomal protein L27

Chain Y:  94%



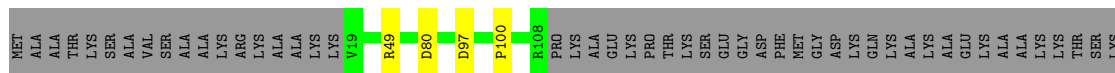
- Molecule 65: Putative 60S ribosomal protein L28

Chain Z:  92%



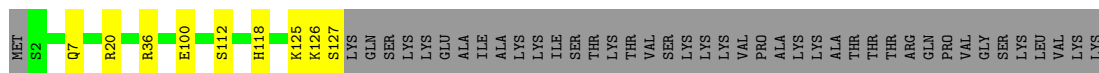
- Molecule 66: Putative 60S ribosomal protein L6

Chain F:  70%



- Molecule 67: Putative 60S ribosomal protein L34

Chain h:  70%




- Molecule 68: Putative ribosomal protein l35a

Chain g:  92%

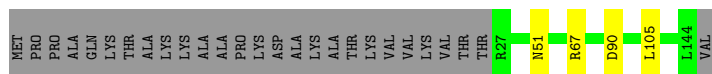
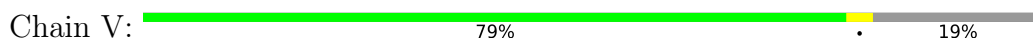


- Molecule 69: Putative 60S ribosomal protein L23

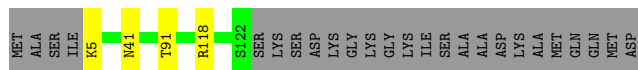
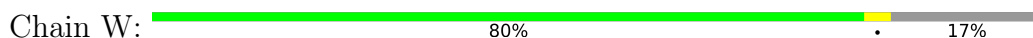
Chain J:  88%



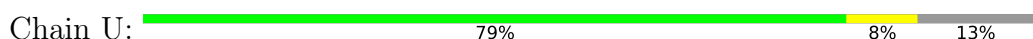
• Molecule 70: Putative 60S ribosomal protein L23a



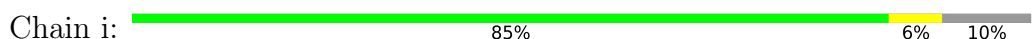
• Molecule 71: Putative 60S ribosomal protein L26



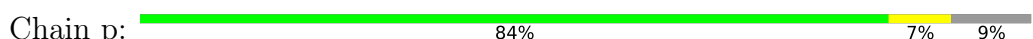
• Molecule 72: Putative 60S ribosomal protein L22



• Molecule 73: Putative 60S Ribosomal protein L36



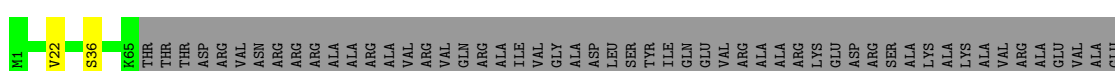
• Molecule 74: Putative 60S ribosomal protein L44



• Molecule 75: 60S ribosomal protein L37a

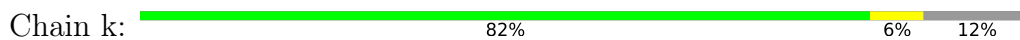


• Molecule 76: Putative ribosomal protein L24



ARG
LYS
LYS
ALA
ALA
LYS
LYS

• Molecule 77: Putative ribosomal protein L38



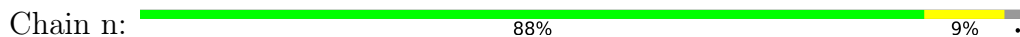
MET
P2
R3
C15
V23
S73
H74
ALA
LYS
THR
ASN
ALA
GLY
SER
LYS
GLN

• Molecule 78: Putative 60S ribosomal protein L39



MET
G2
K5
Y51

• Molecule 79: 60S ribosomal protein L41



MET
G2
T3
V4
M10
R18
K34

• Molecule 80: Putative ribosomal protein L1a



MET
SER
ALA
R4
T68
M64
F107
F121
S134
Q142
D155
S156
F169
R217
R289
K309
K321
V346
R352
K369
SER
ALA
LYS
GLN

• Molecule 81: SR1_chain_3

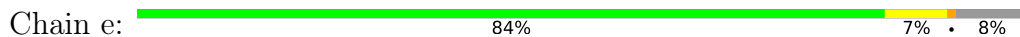


U
A
U
U
U
G
A
U13
G6
U16
A
A
C
C
C
U
U
U
G
G26
C34
U38
A141
G142
A143
U144
A40
A41
U42
C43
C44
U45
C46
U58
U59
U63
A72
C78
A
U
U
C
C
C
C
C
C
C
U
A
C
C
U
U
U
U
U
U
C
G
G
G
G
C

C98
U107
U108
U109
U110
A111
C
U
U
C
U116
G117
G118
C119
U124
G213
U214
G
U


U187
C188
C191
G192
C193
A194
U196
A198
A202
G210
G213
U214
G
U

• Molecule 82: Putative 60S ribosomal subunit protein L31



MET
THR
ARG
ALA
GLY
M1
K11
I14
E23
S24
R25
K31
R32
K46
K47
N57
R74
R61
S88
L114
M115
K116
E151
THR
THR
GLU
GLY
ASN
LYS
LYS
HIS
LYS
H160
S172
Y181
GLU
GLN

- Molecule 83: Ribosomal protein L37

Chain j:  93%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	345376	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 ($e^-/\text{\AA}^2$)	1.0	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: OMG, MA6, 1MA, NA, OMU, MG, 5MC, PSU, C4J, A2M, OMC, K, G7M, ZN

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	SW	0.34	0/804	0.50	0/1090
2	SZ	0.27	0/988	0.51	0/1322
3	SY	0.25	0/610	0.54	0/829
4	SX	0.36	0/1100	0.53	0/1485
5	SV	0.31	0/850	0.50	0/1141
6	SU	0.28	0/1196	0.54	0/1613
7	ST	0.28	0/1168	0.58	0/1567
8	SS	0.37	0/433	0.60	0/578
9	SR	0.35	0/908	0.53	0/1232
10	SB	0.27	0/1679	0.52	0/2273
11	SC	0.31	0/1647	0.53	0/2208
12	SD	0.26	0/1541	0.58	0/2066
13	SE	0.27	0/2100	0.54	0/2830
14	SK	0.27	0/1445	0.59	0/1937
15	S4	0.57	0/450	1.03	0/698
16	Sg	0.33	0/2306	0.56	0/3144
17	Sa	0.34	0/546	0.56	0/738
18	Sc	0.29	0/651	0.57	0/877
19	Se	0.26	0/410	0.59	0/544
20	S1	0.60	0/40111	0.91	99/62469 (0.2%)
21	SQ	0.24	0/178	0.49	0/242
22	SP	0.29	0/1144	0.56	0/1533
23	SO	0.34	0/1027	0.57	0/1382
24	SN	0.34	0/836	0.55	0/1134
25	Sd	0.31	0/468	0.60	0/630
26	SM	0.30	0/821	0.55	0/1112
27	SL	0.35	0/1151	0.50	0/1547
28	SJ	0.28	0/1031	0.52	0/1382
29	SI	0.26	0/1643	0.53	0/2215
30	SH	0.34	0/1459	0.54	0/1958
31	SG	0.27	0/1833	0.58	0/2458
32	SF	0.28	0/1692	0.51	0/2294

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	SA	0.27	0/1862	0.55	0/2505
34	Sb	0.29	0/796	0.57	0/1070
35	Sh	0.27	0/664	0.56	0/904
36	f	0.42	0/1008	0.62	0/1351
37	d	0.39	0/635	0.49	0/871
38	c	0.40	0/1812	0.57	0/2440
39	a	0.36	0/965	0.58	0/1295
40	b	0.34	0/531	0.56	0/712
41	1	0.91	0/37000	1.00	89/57678 (0.2%)
42	2	0.87	0/23546	1.03	78/36681 (0.2%)
43	4	0.82	0/4341	0.95	3/6767 (0.0%)
44	7	0.92	0/3669	0.98	7/5710 (0.1%)
45	B	0.39	0/3283	0.61	0/4421
46	8	0.62	0/2806	0.85	3/4367 (0.1%)
47	5	0.88	0/2650	1.04	10/4123 (0.2%)
48	A	0.39	0/2029	0.65	0/2722
49	O	0.34	0/2007	0.54	0/2696
50	G	0.35	0/1883	0.60	0/2535
51	H	0.39	0/1810	0.60	1/2435 (0.0%)
52	M	0.42	0/1754	0.64	0/2342
53	I	0.36	0/1626	0.56	0/2186
54	P	0.40	0/1564	0.60	0/2092
55	Q	0.37	0/1500	0.61	0/2000
56	R	0.41	0/1481	0.55	0/1997
57	E	0.31	0/1458	0.58	0/1971
58	6	0.70	0/1658	1.04	9/2580 (0.3%)
59	T	0.41	0/1257	0.59	0/1683
60	S	0.38	0/1230	0.58	0/1658
61	K	0.34	0/1212	0.55	0/1634
62	D	0.31	0/1159	0.54	0/1565
63	L	0.41	0/1151	0.59	0/1538
64	Y	0.36	0/1070	0.57	0/1437
65	Z	0.33	0/1066	0.60	0/1431
66	F	0.36	0/1065	0.58	1/1451 (0.1%)
67	h	0.45	2/1035 (0.2%)	0.63	0/1378
68	g	0.45	0/1124	0.64	0/1511
69	J	0.40	0/985	0.60	0/1329
70	V	0.37	0/954	0.56	0/1284
71	W	0.35	0/962	0.62	0/1284
72	U	0.34	0/892	0.51	0/1192
73	i	0.34	0/750	0.55	0/1003
74	p	0.41	0/733	0.61	0/977
75	o	0.44	0/708	0.68	0/944

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	X	0.38	0/574	0.61	0/774
77	k	0.36	0/554	0.58	0/751
78	l	0.40	0/453	0.58	0/606
79	n	0.43	0/263	0.71	0/348
80	C	0.39	0/2847	0.60	0/3836
81	3	0.79	0/3792	1.09	27/5895 (0.5%)
82	e	0.42	0/1314	0.61	0/1761
83	j	0.44	0/676	0.73	0/902
All	All	0.65	2/206390 (0.0%)	0.84	327/303151 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	h	36[A]	ARG	C-O	5.13	1.33	1.23
67	h	36[B]	ARG	C-O	5.13	1.33	1.23

All (327) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	1	214	C	P-O3'-C3'	-12.86	104.27	119.70
42	2	508	A	P-O3'-C3'	-12.19	105.07	119.70
41	1	487	A	P-O3'-C3'	-10.88	106.65	119.70
20	S1	232	C	P-O3'-C3'	-10.87	106.66	119.70
42	2	497	G	P-O3'-C3'	-10.59	107.00	119.70
42	2	507	G	P-O3'-C3'	-10.50	107.10	119.70
41	1	164	U	P-O3'-C3'	-10.23	107.43	119.70
42	2	510	PSU	P-O3'-C3'	-10.00	107.69	119.70
20	S1	780	A	P-O3'-C3'	-9.97	107.73	119.70
41	1	1393	A	P-O3'-C3'	-9.95	107.77	119.70
20	S1	783	A	P-O3'-C3'	-9.78	107.96	119.70
20	S1	234	C	P-O3'-C3'	-9.75	108.00	119.70
41	1	212	U	P-O3'-C3'	-9.72	108.04	119.70
41	1	447	G	O4'-C1'-N9	9.69	115.95	108.20
41	1	1392	G	P-O3'-C3'	-9.59	108.19	119.70
20	S1	2061	5MC	P-O3'-C3'	-9.57	108.22	119.70
81	3	183	G	P-O3'-C3'	-9.52	108.28	119.70
20	S1	1923	A	O4'-C1'-N9	9.47	115.78	108.20
41	1	1382	G	P-O3'-C3'	-9.44	108.37	119.70
20	S1	784	C	P-O3'-C3'	-9.27	108.58	119.70
41	1	159	U	P-O3'-C3'	-9.26	108.59	119.70
41	1	646	C	P-O3'-C3'	-9.23	108.63	119.70
42	2	91	C	C6-N1-C2	-9.19	116.62	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	2	504	PSU	P-O3'-C3'	-9.18	108.69	119.70
42	2	512	U	P-O3'-C3'	-9.13	108.75	119.70
41	1	1761	A	P-O3'-C3'	-9.10	108.78	119.70
20	S1	1510	C	C6-N1-C2	-9.09	116.66	120.30
81	3	58	U	P-O3'-C3'	-9.03	108.86	119.70
81	3	40	A	P-O3'-C3'	-9.02	108.88	119.70
44	7	88	A	P-O3'-C3'	-8.95	108.96	119.70
41	1	160	C	P-O3'-C3'	-8.95	108.97	119.70
42	2	965	C	N1-C2-O2	8.94	124.26	118.90
41	1	1245	G	P-O3'-C3'	-8.87	109.05	119.70
41	1	216	G	P-O3'-C3'	-8.86	109.07	119.70
41	1	211	U	P-O3'-C3'	-8.76	109.19	119.70
20	S1	2065	G	P-O3'-C3'	-8.75	109.20	119.70
44	7	86	C	P-O3'-C3'	-8.73	109.23	119.70
42	2	783	A	P-O3'-C3'	-8.66	109.31	119.70
81	3	34	C	N3-C2-O2	-8.63	115.86	121.90
20	S1	782	C	P-O3'-C3'	-8.62	109.36	119.70
20	S1	1577	U	P-O3'-C3'	-8.61	109.37	119.70
20	S1	1510	C	N3-C2-O2	-8.58	115.89	121.90
41	1	490	C	P-O3'-C3'	-8.56	109.43	119.70
20	S1	231	A	P-O3'-C3'	-8.53	109.47	119.70
42	2	500	PSU	P-O3'-C3'	-8.51	109.49	119.70
44	7	87	U	P-O3'-C3'	-8.51	109.49	119.70
42	2	91	C	N3-C2-O2	-8.50	115.95	121.90
41	1	251	A	P-O3'-C3'	-8.49	109.52	119.70
20	S1	235	C	P-O3'-C3'	-8.47	109.53	119.70
20	S1	1462	G	P-O3'-C3'	-8.47	109.53	119.70
42	2	518	G	P-O3'-C3'	-8.47	109.53	119.70
41	1	1395	U	P-O3'-C3'	-8.46	109.54	119.70
47	5	64	U	P-O3'-C3'	-8.45	109.56	119.70
20	S1	233	G	P-O3'-C3'	-8.36	109.66	119.70
42	2	62	A	P-O3'-C3'	-8.36	109.67	119.70
20	S1	509	G	P-O3'-C3'	-8.34	109.70	119.70
41	1	1762	A	P-O3'-C3'	-8.33	109.71	119.70
20	S1	508	A	P-O3'-C3'	-8.27	109.77	119.70
20	S1	1271	C	C2-N1-C1'	8.21	127.83	118.80
81	3	146	G	P-O3'-C3'	-8.21	109.85	119.70
20	S1	492	U	P-O3'-C3'	-8.20	109.86	119.70
81	3	59	U	P-O3'-C3'	-8.17	109.90	119.70
42	2	965	C	N3-C2-O2	-8.15	116.19	121.90
20	S1	2059	C	P-O3'-C3'	-8.12	109.96	119.70
20	S1	236	C	P-O3'-C3'	-8.11	109.97	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	2	501	A	P-O3'-C3'	-8.11	109.97	119.70
42	2	444	A	P-O3'-C3'	-8.08	110.00	119.70
42	2	786	A	P-O3'-C3'	-8.07	110.01	119.70
42	2	74	A	P-O3'-C3'	-7.99	110.12	119.70
20	S1	510	G	P-O3'-C3'	-7.94	110.17	119.70
42	2	516	A	P-O3'-C3'	-7.94	110.17	119.70
81	3	45	U	P-O3'-C3'	-7.94	110.17	119.70
41	1	1244	G	P-O3'-C3'	-7.93	110.18	119.70
81	3	125	U	O4'-C1'-N1	7.92	114.54	108.20
81	3	34	C	C2-N1-C1'	7.90	127.49	118.80
41	1	213	G	P-O3'-C3'	-7.88	110.24	119.70
42	2	517	A	P-O3'-C3'	-7.86	110.27	119.70
20	S1	117	G	P-O3'-C3'	-7.86	110.27	119.70
20	S1	779	A	P-O3'-C3'	-7.85	110.28	119.70
42	2	965	C	C2-N1-C1'	7.85	127.43	118.80
20	S1	506	U	P-O3'-C3'	-7.84	110.29	119.70
44	7	70	C	P-O3'-C3'	-7.84	110.29	119.70
47	5	92	G	P-O3'-C3'	-7.82	110.32	119.70
81	3	144	U	P-O3'-C3'	-7.82	110.32	119.70
42	2	63	U	P-O3'-C3'	-7.81	110.33	119.70
42	2	1063	C	C2-N1-C1'	7.79	127.37	118.80
41	1	161	A	P-O3'-C3'	-7.76	110.39	119.70
20	S1	1576	A	P-O3'-C3'	-7.74	110.41	119.70
41	1	1255	G	P-O3'-C3'	-7.73	110.42	119.70
20	S1	1922	A	O4'-C1'-N9	7.70	114.36	108.20
42	2	441	C	P-O3'-C3'	-7.66	110.51	119.70
42	2	61	C	P-O3'-C3'	-7.65	110.52	119.70
20	S1	493	C	P-O3'-C3'	-7.58	110.60	119.70
41	1	1588	G	O4'-C1'-N9	7.57	114.25	108.20
20	S1	2058	G	P-O3'-C3'	-7.55	110.64	119.70
42	2	496	G	P-O3'-C3'	-7.54	110.65	119.70
20	S1	113	A	P-O3'-C3'	-7.53	110.66	119.70
47	5	113	A	P-O3'-C3'	-7.52	110.68	119.70
42	2	58	G	P-O3'-C3'	-7.52	110.68	119.70
20	S1	116	U	P-O3'-C3'	-7.49	110.71	119.70
20	S1	496	A	P-O3'-C3'	-7.49	110.71	119.70
41	1	484	A	P-O3'-C3'	-7.44	110.78	119.70
81	3	142	G	P-O3'-C3'	-7.36	110.87	119.70
81	3	145	U	P-O3'-C3'	-7.36	110.87	119.70
42	2	514	U	P-O3'-C3'	-7.33	110.90	119.70
81	3	143	A	P-O3'-C3'	-7.33	110.90	119.70
58	6	67	C	N3-C2-O2	-7.32	116.78	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	S1	1463	G	P-O3'-C3'	-7.31	110.93	119.70
20	S1	2203	U	N1-C2-O2	7.28	127.90	122.80
42	2	1190	U	N3-C2-O2	-7.26	117.11	122.20
20	S1	495	A	P-O3'-C3'	-7.25	111.00	119.70
41	1	1396	G	P-O3'-C3'	-7.25	111.00	119.70
20	S1	2203	U	C2-N1-C1'	7.22	126.36	117.70
20	S1	114	U	P-O3'-C3'	-7.21	111.05	119.70
81	3	46	C	P-O3'-C3'	-7.17	111.09	119.70
41	1	1012	C	O5'-P-OP1	-7.17	99.25	105.70
42	2	495	G	P-O3'-C3'	-7.16	111.10	119.70
58	6	7	A	O4'-C1'-N9	7.14	113.91	108.20
41	1	1381	G	P-O3'-C3'	-7.13	111.14	119.70
20	S1	1461	G	P-O3'-C3'	-7.11	111.16	119.70
20	S1	1987	G	O4'-C1'-N9	7.09	113.88	108.20
20	S1	1983	U	N3-C2-O2	-7.07	117.25	122.20
42	2	479	C	N3-C2-O2	-7.07	116.95	121.90
20	S1	115	C	P-O3'-C3'	-7.03	111.26	119.70
81	3	34	C	C6-N1-C2	-7.03	117.49	120.30
43	4	10	U	N1-C2-O2	7.00	127.70	122.80
41	1	215	U	P-O3'-C3'	-6.96	111.35	119.70
41	1	1760	C	P-O3'-C3'	-6.92	111.40	119.70
20	S1	781	A	P-O3'-C3'	-6.89	111.44	119.70
41	1	247	A	P-O3'-C3'	-6.88	111.45	119.70
20	S1	112	A	P-O3'-C3'	-6.84	111.49	119.70
41	1	1763	A	P-O3'-C3'	-6.83	111.50	119.70
20	S1	1973	C	N3-C2-O2	-6.80	117.14	121.90
42	2	91	C	C2-N1-C1'	6.79	126.26	118.80
42	2	378	C	C6-N1-C2	-6.78	117.59	120.30
66	F	100	PRO	CA-N-CD	-6.76	102.03	111.50
41	1	938	G	P-O3'-C3'	-6.75	111.60	119.70
41	1	250	A	P-O3'-C3'	-6.74	111.61	119.70
81	3	34	C	N1-C2-O2	6.74	122.94	118.90
81	3	141	A	P-O3'-C3'	-6.74	111.62	119.70
81	3	188	C	P-O3'-C3'	-6.73	111.63	119.70
42	2	59	U	P-O3'-C3'	-6.72	111.63	119.70
42	2	1512	G	P-O3'-C3'	-6.70	111.66	119.70
41	1	488	G	P-O3'-C3'	-6.70	111.66	119.70
41	1	481	U	P-O3'-C3'	-6.67	111.69	119.70
20	S1	2056	C	P-O3'-C3'	-6.67	111.70	119.70
42	2	956	C	N1-C2-O2	6.66	122.90	118.90
20	S1	1271	C	C6-N1-C1'	-6.64	112.83	120.80
81	3	43	C	P-O3'-C3'	-6.62	111.75	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	2	800	G	P-O3'-C3'	-6.62	111.76	119.70
20	S1	1956	C	N3-C2-O2	-6.62	117.27	121.90
41	1	645	G	P-O3'-C3'	-6.59	111.79	119.70
81	3	191	C	N3-C2-O2	-6.59	117.29	121.90
20	S1	1510	C	C2-N1-C1'	6.59	126.05	118.80
20	S1	911	A	OP1-P-O3'	6.58	119.67	105.20
43	4	10	U	N3-C2-O2	-6.57	117.60	122.20
20	S1	1956	C	C2-N1-C1'	6.53	125.98	118.80
47	5	84	C	P-O3'-C3'	-6.50	111.90	119.70
81	3	41	A	P-O3'-C3'	-6.50	111.90	119.70
81	3	196	U	P-O3'-C3'	-6.48	111.92	119.70
20	S1	1578	G	P-O3'-C3'	-6.48	111.93	119.70
41	1	1602	C	P-O3'-C3'	-6.45	111.96	119.70
42	2	26	C	C6-N1-C2	-6.44	117.73	120.30
41	1	158	A	P-O3'-C3'	-6.42	112.00	119.70
81	3	38	U	P-O3'-C3'	-6.39	112.03	119.70
20	S1	1464	G	P-O3'-C3'	-6.38	112.04	119.70
41	1	246	A	P-O3'-C3'	-6.37	112.06	119.70
41	1	248	A	P-O3'-C3'	-6.36	112.07	119.70
47	5	63	G	P-O3'-C3'	-6.36	112.07	119.70
41	1	983	U	P-O3'-C3'	6.35	127.32	119.70
20	S1	1212	C	C2-N1-C1'	6.34	125.77	118.80
41	1	1601	U	P-O3'-C3'	-6.34	112.10	119.70
42	2	506	PSU	P-O3'-C3'	-6.33	112.10	119.70
42	2	493	G	P-O3'-C3'	-6.33	112.11	119.70
20	S1	491	G	P-O3'-C3'	-6.31	112.13	119.70
81	3	186	U	P-O3'-C3'	-6.31	112.13	119.70
20	S1	1580	G	P-O3'-C3'	-6.30	112.14	119.70
41	1	191	U	O4'-C1'-N1	6.28	113.22	108.20
81	3	191	C	N1-C2-O2	6.27	122.66	118.90
42	2	515	U	P-O3'-C3'	-6.27	112.18	119.70
41	1	581	G	OP1-P-O3'	6.26	118.97	105.20
41	1	100	G	C4-N9-C1'	6.25	134.63	126.50
20	S1	2203	U	N3-C2-O2	-6.21	117.86	122.20
42	2	965	C	C6-N1-C2	-6.21	117.82	120.30
42	2	782	G	P-O3'-C3'	-6.19	112.27	119.70
20	S1	1956	C	N1-C2-O2	6.19	122.61	118.90
42	2	347	A	P-O3'-C3'	-6.18	112.28	119.70
44	7	6	G	OP1-P-O3'	6.16	118.75	105.20
42	2	1461	C	C2-N1-C1'	6.16	125.58	118.80
42	2	91	C	C4-C5-C6	6.13	120.47	117.40
20	S1	2039	C	N3-C2-O2	-6.12	117.62	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	S1	1973	C	N1-C2-O2	6.12	122.57	118.90
44	7	71	A	P-O3'-C3'	-6.12	112.36	119.70
41	1	234	G	OP1-P-O3'	6.08	118.58	105.20
41	1	1391	U	P-O3'-C3'	-6.08	112.40	119.70
20	S1	1581	G	P-O3'-C3'	-6.08	112.40	119.70
42	2	1156	G	O4'-C1'-N9	6.07	113.06	108.20
42	2	491	C	P-O3'-C3'	-6.07	112.42	119.70
41	1	100	G	C8-N9-C1'	-6.04	119.15	127.00
81	3	157	C	C2-N1-C1'	6.02	125.42	118.80
58	6	67	C	C6-N1-C2	-6.01	117.89	120.30
41	1	1012	C	N3-C2-O2	-5.96	117.72	121.90
20	S1	778	G	P-O3'-C3'	-5.94	112.58	119.70
20	S1	2040	C	N3-C2-O2	-5.91	117.76	121.90
41	1	778	C	N3-C2-O2	-5.89	117.78	121.90
58	6	7	A	C5-N7-C8	-5.89	100.96	103.90
20	S1	1510	C	N1-C2-O2	5.87	122.42	118.90
58	6	7	A	N7-C8-N9	5.87	116.74	113.80
41	1	1012	C	N1-C2-O2	5.85	122.41	118.90
42	2	60	A	P-O3'-C3'	-5.85	112.68	119.70
41	1	68	A	OP1-P-O3'	5.83	118.03	105.20
20	S1	2039	C	C6-N1-C2	-5.83	117.97	120.30
41	1	1724	C	N1-C2-O2	5.83	122.40	118.90
42	2	1063	C	C6-N1-C2	-5.81	117.98	120.30
41	1	926	G	OP1-P-O3'	5.78	117.92	105.20
41	1	869	C	C6-N1-C2	-5.76	118.00	120.30
20	S1	1911	U	N3-C2-O2	-5.75	118.17	122.20
41	1	1598	A	P-O3'-C3'	-5.72	112.83	119.70
20	S1	1909	C	C2-N1-C1'	5.70	125.07	118.80
20	S1	2040	C	C6-N1-C2	-5.69	118.02	120.30
20	S1	1271	C	O4'-C1'-N1	5.69	112.75	108.20
41	1	582	U	C2-N1-C1'	5.68	124.52	117.70
41	1	973	U	C2-N1-C1'	5.67	124.50	117.70
42	2	479	C	C6-N1-C2	-5.62	118.05	120.30
42	2	91	C	N1-C2-N3	5.61	123.13	119.20
42	2	1466	C	N1-C2-O2	5.61	122.27	118.90
41	1	967	G	P-O3'-C3'	5.59	126.41	119.70
42	2	1151	U	OP1-P-O3'	5.58	117.49	105.20
58	6	67	C	N1-C2-O2	5.58	122.25	118.90
20	S1	1980	U	N3-C2-O2	-5.57	118.30	122.20
20	S1	1931	G	N3-C4-C5	-5.57	125.82	128.60
20	S1	507	G	P-O3'-C3'	-5.57	113.02	119.70
42	2	75	A	P-O3'-C3'	-5.54	113.05	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	S1	1575	G	P-O3'-C3'	-5.54	113.05	119.70
20	S1	906	U	N3-C2-O2	-5.53	118.33	122.20
20	S1	775	C	N1-C2-O2	5.53	122.22	118.90
51	H	109	TYR	CB-CA-C	5.50	121.41	110.40
20	S1	2057	C	P-O3'-C3'	-5.49	113.11	119.70
42	2	346	C	P-O3'-C3'	-5.49	113.11	119.70
41	1	100	G	O4'-C1'-N9	5.47	112.57	108.20
20	S1	2040	C	C2-N1-C1'	5.46	124.81	118.80
41	1	728	C	P-O3'-C3'	5.45	126.25	119.70
20	S1	659	G	C4-N9-C1'	5.44	133.58	126.50
20	S1	1909	C	N3-C2-O2	-5.44	118.09	121.90
20	S1	1983	U	C2-N1-C1'	5.43	124.21	117.70
41	1	736	C	C2-N1-C1'	5.43	124.77	118.80
42	2	34	G	N3-C4-N9	5.41	129.24	126.00
20	S1	1788	U	C2-N1-C1'	5.40	124.18	117.70
41	1	1613	C	O5'-P-OP1	-5.40	100.84	105.70
20	S1	78	C	C6-N1-C2	-5.38	118.15	120.30
46	8	109	U	C2-N1-C1'	5.37	124.15	117.70
20	S1	1838	U	N3-C2-O2	-5.37	118.44	122.20
41	1	916	U	N3-C2-O2	-5.37	118.44	122.20
42	2	392	C	C6-N1-C2	-5.35	118.16	120.30
42	2	1022	U	C2-N1-C1'	5.34	124.10	117.70
20	S1	1465	A	P-O3'-C3'	-5.33	113.30	119.70
42	2	1066	G	OP1-P-O3'	5.33	116.92	105.20
42	2	479	C	N1-C2-O2	5.33	122.10	118.90
81	3	198	A	P-O3'-C3'	-5.32	113.31	119.70
20	S1	1961	G	O4'-C1'-N9	5.32	112.45	108.20
46	8	39	C	C2-N1-C1'	5.31	124.64	118.80
42	2	1190	U	N1-C2-N3	5.29	118.08	114.90
20	S1	2039	C	C2-N1-C1'	5.29	124.62	118.80
41	1	994	U	N3-C2-O2	-5.29	118.50	122.20
20	S1	76	U	C2-N1-C1'	5.29	124.05	117.70
44	7	164	U	N3-C2-O2	-5.29	118.50	122.20
42	2	956	C	N3-C2-O2	-5.29	118.20	121.90
41	1	736	C	N3-C2-O2	-5.28	118.20	121.90
41	1	1254	C	C2-N1-C1'	5.27	124.60	118.80
42	2	1388	G	O4'-C1'-N9	5.27	112.42	108.20
42	2	1466	C	C2-N1-C1'	5.27	124.60	118.80
41	1	973	U	N3-C2-O2	-5.27	118.51	122.20
20	S1	2052	C	C6-N1-C2	-5.26	118.19	120.30
47	5	112	G	P-O3'-C3'	-5.26	113.39	119.70
41	1	638	C	C2-N1-C1'	5.26	124.59	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	1	1012	C	C2-N1-C1'	5.26	124.58	118.80
41	1	663	C	C6-N1-C2	-5.25	118.20	120.30
42	2	380	G	N3-C4-C5	-5.25	125.98	128.60
42	2	511	C	P-O3'-C3'	-5.25	113.40	119.70
41	1	1632	C	C6-N1-C2	-5.24	118.20	120.30
20	S1	916	G	OP2-P-O3'	5.24	116.72	105.20
42	2	337	A	P-O3'-C3'	5.24	125.99	119.70
42	2	378	C	N3-C2-O2	-5.24	118.23	121.90
20	S1	1108	A	P-O3'-C3'	5.24	125.98	119.70
42	2	569	G	N3-C4-C5	-5.24	125.98	128.60
41	1	1756	A	O4'-C1'-N9	5.22	112.38	108.20
41	1	957	C	C2-N3-C4	-5.22	117.29	119.90
47	5	99	A	C5-N7-C8	-5.22	101.29	103.90
42	2	956	C	C2-N1-C1'	5.21	124.54	118.80
58	6	65	C	N3-C2-O2	-5.21	118.25	121.90
41	1	778	C	C2-N1-C1'	5.21	124.53	118.80
20	S1	1927	U	N3-C2-O2	-5.20	118.56	122.20
20	S1	775	C	N3-C2-O2	-5.19	118.27	121.90
42	2	1010	U	N3-C2-O2	-5.18	118.58	122.20
41	1	581	G	P-O3'-C3'	5.17	125.90	119.70
20	S1	1956	C	C6-N1-C2	-5.17	118.23	120.30
41	1	916	U	C2-N1-C1'	5.16	123.89	117.70
41	1	582	U	N1-C2-O2	5.15	126.41	122.80
58	6	65	C	N1-C2-O2	5.14	121.99	118.90
41	1	973	U	N1-C2-O2	5.13	126.39	122.80
46	8	92	U	C2-N1-C1'	5.13	123.86	117.70
41	1	83	A	P-O3'-C3'	5.12	125.85	119.70
42	2	1063	C	C6-N1-C1'	-5.12	114.65	120.80
41	1	582	U	N3-C2-O2	-5.12	118.62	122.20
42	2	1063	C	N3-C2-O2	-5.12	118.32	121.90
43	4	15	G	P-O3'-C3'	5.12	125.84	119.70
41	1	736	C	N1-C2-O2	5.11	121.96	118.90
42	2	513	C	P-O3'-C3'	-5.10	113.58	119.70
41	1	626	U	C2-N1-C1'	5.09	123.81	117.70
20	S1	78	C	C2-N1-C1'	5.09	124.40	118.80
41	1	19	G	O4'-C1'-N9	5.08	112.26	108.20
41	1	1012	C	C6-N1-C2	-5.07	118.27	120.30
20	S1	1764	U	N3-C2-O2	-5.07	118.65	122.20
42	2	965	C	C6-N1-C1'	-5.06	114.73	120.80
20	S1	78	C	N1-C2-O2	5.05	121.93	118.90
47	5	62	G	P-O3'-C3'	-5.04	113.65	119.70
58	6	65	C	C2-N1-C1'	5.04	124.34	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	5	91	A	P-O3'-C3'	-5.04	113.66	119.70
41	1	1724	C	N3-C2-O2	-5.03	118.38	121.90
42	2	520	U	P-O3'-C3'	-5.03	113.66	119.70
20	S1	76	U	N1-C2-O2	5.03	126.32	122.80
47	5	111	U	P-O3'-C3'	-5.02	113.67	119.70
20	S1	1612	C	P-O3'-C3'	5.02	125.72	119.70
41	1	1655	U	N3-C2-O2	-5.02	118.69	122.20
20	S1	2203	U	C6-N1-C1'	-5.01	114.19	121.20
42	2	1461	C	C5-C6-N1	5.01	123.50	121.00
41	1	63	A	O4'-C1'-N9	5.00	112.20	108.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	SW	101/152 (66%)	97 (96%)	4 (4%)	0	100	100
2	SZ	121/137 (88%)	116 (96%)	5 (4%)	0	100	100
3	SY	81/164 (49%)	79 (98%)	2 (2%)	0	100	100
4	SX	137/161 (85%)	129 (94%)	8 (6%)	0	100	100
5	SV	109/143 (76%)	105 (96%)	4 (4%)	0	100	100
6	SU	146/173 (84%)	139 (95%)	7 (5%)	0	100	100
7	ST	139/151 (92%)	131 (94%)	8 (6%)	0	100	100
8	SS	53/57 (93%)	49 (92%)	4 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	SR	117/153 (76%)	115 (98%)	2 (2%)	0	100	100
10	SB	207/246 (84%)	199 (96%)	8 (4%)	0	100	100
11	SC	212/219 (97%)	206 (97%)	6 (3%)	0	100	100
12	SD	181/190 (95%)	174 (96%)	7 (4%)	0	100	100
13	SE	260/273 (95%)	256 (98%)	4 (2%)	0	100	100
14	SK	176/220 (80%)	173 (98%)	3 (2%)	0	100	100
16	Sg	294/312 (94%)	269 (92%)	25 (8%)	0	100	100
17	Sa	69/120 (58%)	65 (94%)	4 (6%)	0	100	100
18	Sc	82/86 (95%)	78 (95%)	4 (5%)	0	100	100
19	Se	48/66 (73%)	43 (90%)	5 (10%)	0	100	100
21	SQ	24/141 (17%)	24 (100%)	0	0	100	100
22	SP	143/143 (100%)	141 (99%)	2 (1%)	0	100	100
23	SO	135/144 (94%)	130 (96%)	5 (4%)	0	100	100
24	SN	99/168 (59%)	94 (95%)	5 (5%)	0	100	100
25	Sd	63/87 (72%)	57 (90%)	6 (10%)	0	100	100
26	SM	101/116 (87%)	99 (98%)	2 (2%)	0	100	100
27	SL	141/149 (95%)	137 (97%)	4 (3%)	0	100	100
28	SJ	127/130 (98%)	126 (99%)	1 (1%)	0	100	100
29	SI	198/200 (99%)	195 (98%)	3 (2%)	0	100	100
30	SH	180/190 (95%)	175 (97%)	5 (3%)	0	100	100
31	SG	232/249 (93%)	229 (99%)	3 (1%)	0	100	100
32	SF	218/265 (82%)	214 (98%)	4 (2%)	0	100	100
33	SA	225/264 (85%)	224 (100%)	1 (0%)	0	100	100
34	Sb	98/112 (88%)	94 (96%)	4 (4%)	0	100	100
35	Sh	92/235 (39%)	85 (92%)	7 (8%)	0	100	100
36	f	120/133 (90%)	116 (97%)	4 (3%)	0	100	100
37	d	88/104 (85%)	85 (97%)	3 (3%)	0	100	100
38	c	225/252 (89%)	218 (97%)	7 (3%)	0	100	100
39	a	121/127 (95%)	115 (95%)	6 (5%)	0	100	100
40	b	64/70 (91%)	63 (98%)	1 (2%)	0	100	100
45	B	407/419 (97%)	397 (98%)	10 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	A	258/260 (99%)	252 (98%)	6 (2%)	0	100	100
49	O	249/305 (82%)	235 (94%)	14 (6%)	0	100	100
50	G	233/264 (88%)	225 (97%)	8 (3%)	0	100	100
51	H	220/222 (99%)	219 (100%)	1 (0%)	0	100	100
52	M	201/204 (98%)	195 (97%)	6 (3%)	0	100	100
53	I	203/220 (92%)	192 (95%)	11 (5%)	0	100	100
54	P	195/198 (98%)	188 (96%)	7 (4%)	0	100	100
55	Q	187/254 (74%)	184 (98%)	3 (2%)	0	100	100
56	R	176/179 (98%)	174 (99%)	2 (1%)	0	100	100
57	E	184/190 (97%)	174 (95%)	10 (5%)	0	100	100
59	T	151/166 (91%)	148 (98%)	3 (2%)	0	100	100
60	S	150/159 (94%)	143 (95%)	7 (5%)	0	100	100
61	K	151/175 (86%)	145 (96%)	6 (4%)	0	100	100
62	D	155/188 (82%)	146 (94%)	9 (6%)	0	100	100
63	L	142/145 (98%)	137 (96%)	5 (4%)	0	100	100
64	Y	131/134 (98%)	128 (98%)	3 (2%)	0	100	100
65	Z	137/147 (93%)	134 (98%)	3 (2%)	0	100	100
66	F	138/195 (71%)	135 (98%)	3 (2%)	0	100	100
67	h	125/168 (74%)	119 (95%)	6 (5%)	0	100	100
68	g	136/144 (94%)	131 (96%)	4 (3%)	1 (1%)	22	25
69	J	127/139 (91%)	125 (98%)	2 (2%)	0	100	100
70	V	116/145 (80%)	114 (98%)	2 (2%)	0	100	100
71	W	116/143 (81%)	113 (97%)	3 (3%)	0	100	100
72	U	108/129 (84%)	105 (97%)	3 (3%)	0	100	100
73	i	91/105 (87%)	88 (97%)	3 (3%)	0	100	100
74	p	94/106 (89%)	81 (86%)	13 (14%)	0	100	100
75	o	88/92 (96%)	78 (89%)	10 (11%)	0	100	100
76	X	63/124 (51%)	61 (97%)	2 (3%)	0	100	100
77	k	71/83 (86%)	69 (97%)	2 (3%)	0	100	100
78	l	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
79	n	31/34 (91%)	28 (90%)	3 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
80	C	364/373 (98%)	354 (97%)	10 (3%)	0	100	100
82	e	169/188 (90%)	159 (94%)	9 (5%)	1 (1%)	25	29
83	j	78/83 (94%)	76 (97%)	2 (3%)	0	100	100
All	All	10720/12433 (86%)	10343 (96%)	375 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
82	e	47	LYS
68	g	20	LYS

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	SW	74/130 (57%)	71 (96%)	3 (4%)	30	40
2	SZ	100/118 (85%)	99 (99%)	1 (1%)	76	84
3	SY	63/116 (54%)	59 (94%)	4 (6%)	18	22
4	SX	107/131 (82%)	102 (95%)	5 (5%)	26	34
5	SV	83/126 (66%)	80 (96%)	3 (4%)	35	46
6	SU	121/152 (80%)	116 (96%)	5 (4%)	30	40
7	ST	122/132 (92%)	121 (99%)	1 (1%)	81	88
8	SS	42/49 (86%)	40 (95%)	2 (5%)	25	33
9	SR	86/130 (66%)	79 (92%)	7 (8%)	11	13
10	SB	175/202 (87%)	163 (93%)	12 (7%)	15	18
11	SC	168/184 (91%)	158 (94%)	10 (6%)	19	24
12	SD	160/164 (98%)	159 (99%)	1 (1%)	86	91
13	SE	215/225 (96%)	209 (97%)	6 (3%)	43	56
14	SK	138/176 (78%)	134 (97%)	4 (3%)	42	53
16	Sg	235/265 (89%)	207 (88%)	28 (12%)	5	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	Sa	58/95 (61%)	52 (90%)	6 (10%)	7	7
18	Sc	68/76 (90%)	61 (90%)	7 (10%)	7	7
19	Se	40/54 (74%)	38 (95%)	2 (5%)	24	32
21	SQ	15/120 (12%)	15 (100%)	0	100	100
22	SP	114/117 (97%)	107 (94%)	7 (6%)	18	24
23	SO	101/113 (89%)	95 (94%)	6 (6%)	19	25
24	SN	85/128 (66%)	76 (89%)	9 (11%)	6	6
25	Sd	46/75 (61%)	41 (89%)	5 (11%)	6	6
26	SM	94/104 (90%)	90 (96%)	4 (4%)	29	38
27	SL	114/120 (95%)	112 (98%)	2 (2%)	59	71
28	SJ	108/111 (97%)	104 (96%)	4 (4%)	34	45
29	SI	174/186 (94%)	164 (94%)	10 (6%)	20	26
30	SH	150/159 (94%)	145 (97%)	5 (3%)	38	49
31	SG	180/208 (86%)	174 (97%)	6 (3%)	38	49
32	SF	170/208 (82%)	163 (96%)	7 (4%)	30	40
33	SA	198/222 (89%)	183 (92%)	15 (8%)	13	15
34	Sb	80/93 (86%)	79 (99%)	1 (1%)	69	79
35	Sh	59/177 (33%)	46 (78%)	13 (22%)	1	0
36	f	104/115 (90%)	102 (98%)	2 (2%)	57	69
37	d	60/89 (67%)	56 (93%)	4 (7%)	16	20
38	c	174/209 (83%)	169 (97%)	5 (3%)	42	53
39	a	93/118 (79%)	91 (98%)	2 (2%)	52	64
40	b	52/58 (90%)	50 (96%)	2 (4%)	33	43
45	B	331/351 (94%)	319 (96%)	12 (4%)	35	46
48	A	202/204 (99%)	195 (96%)	7 (4%)	36	47
49	O	191/242 (79%)	182 (95%)	9 (5%)	26	34
50	G	192/221 (87%)	187 (97%)	5 (3%)	46	58
51	H	183/188 (97%)	178 (97%)	5 (3%)	44	57
52	M	179/180 (99%)	172 (96%)	7 (4%)	32	42
53	I	165/183 (90%)	159 (96%)	6 (4%)	35	46
54	P	163/164 (99%)	156 (96%)	7 (4%)	29	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	Q	138/198 (70%)	129 (94%)	9 (6%)	17	21
56	R	155/159 (98%)	146 (94%)	9 (6%)	20	25
57	E	157/172 (91%)	143 (91%)	14 (9%)	9	10
59	T	131/143 (92%)	129 (98%)	2 (2%)	65	76
60	S	125/134 (93%)	120 (96%)	5 (4%)	31	41
61	K	121/145 (83%)	113 (93%)	8 (7%)	16	20
62	D	104/162 (64%)	98 (94%)	6 (6%)	20	25
63	L	113/114 (99%)	107 (95%)	6 (5%)	22	29
64	Y	106/116 (91%)	100 (94%)	6 (6%)	20	26
65	Z	106/118 (90%)	102 (96%)	4 (4%)	33	43
66	F	103/153 (67%)	98 (95%)	5 (5%)	25	32
67	h	105/146 (72%)	97 (92%)	8 (8%)	13	15
68	g	112/121 (93%)	108 (96%)	4 (4%)	35	46
69	J	102/111 (92%)	95 (93%)	7 (7%)	15	18
70	V	100/124 (81%)	96 (96%)	4 (4%)	31	41
71	W	102/122 (84%)	98 (96%)	4 (4%)	32	42
72	U	88/114 (77%)	78 (89%)	10 (11%)	5	5
73	i	75/88 (85%)	69 (92%)	6 (8%)	12	14
74	p	66/92 (72%)	59 (89%)	7 (11%)	6	6
75	o	70/74 (95%)	66 (94%)	4 (6%)	20	26
76	X	58/104 (56%)	56 (97%)	2 (3%)	37	48
77	k	56/74 (76%)	51 (91%)	5 (9%)	9	10
78	l	44/47 (94%)	43 (98%)	1 (2%)	50	63
79	n	24/32 (75%)	21 (88%)	3 (12%)	4	3
80	C	287/301 (95%)	272 (95%)	15 (5%)	23	30
82	e	128/158 (81%)	113 (88%)	15 (12%)	5	4
83	j	67/70 (96%)	64 (96%)	3 (4%)	27	36
All	All	8675/10380 (84%)	8229 (95%)	446 (5%)	27	31

All (446) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	SW	22	PHE

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Mol	Chain	Res	Type
1	SW	107	HIS
1	SW	130	TYR
2	SZ	22	LEU
3	SY	8	ASN
3	SY	10	GLU
3	SY	16	LEU
3	SY	40	SER
4	SX	59	LYS
4	SX	72	SER
4	SX	98	LEU
4	SX	116	ASN
4	SX	133	HIS
5	SV	5	ARG
5	SV	7	LYS
5	SV	18	GLU
6	SU	30	ASN
6	SU	62	LYS
6	SU	82	ARG
6	SU	121	SER
6	SU	127	SER
7	ST	31	ARG
8	SS	26	SER
8	SS	37	LEU
9	SR	5	LEU
9	SR	14	VAL
9	SR	32	ARG
9	SR	44	LEU
9	SR	66	GLU
9	SR	74	ASP
9	SR	101	SER
10	SB	10	VAL
10	SB	14	LYS
10	SB	31	ARG
10	SB	56	MET
10	SB	84	LEU
10	SB	91	TYR
10	SB	101	PHE
10	SB	132	THR
10	SB	144	ASN
10	SB	177	MET
10	SB	201	LYS
10	SB	203	ASP

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Mol	Chain	Res	Type
11	SC	44	ARG
11	SC	46	GLU
11	SC	66[A]	ARG
11	SC	66[B]	ARG
11	SC	84	GLN
11	SC	89	ARG
11	SC	101	VAL
11	SC	108	LEU
11	SC	149	MET
11	SC	173	HIS
12	SD	181	ARG
13	SE	96	PHE
13	SE	197	CYS
13	SE	202	PHE
13	SE	227	LYS
13	SE	239	GLN
13	SE	253	ARG
14	SK	37	ARG
14	SK	77	ARG
14	SK	159	GLN
14	SK	160	ARG
16	Sg	2	ASN
16	Sg	6	HIS
16	Sg	8	LYS
16	Sg	10	HIS
16	Sg	11	ARG
16	Sg	33	SER
16	Sg	34	ARG
16	Sg	105	LYS
16	Sg	115	PHE
16	Sg	124	SER
16	Sg	127	ARG
16	Sg	139	GLU
16	Sg	147	ASP
16	Sg	167	VAL
16	Sg	178	VAL
16	Sg	181	VAL
16	Sg	188	ARG
16	Sg	189	THR
16	Sg	193	HIS
16	Sg	194	SER
16	Sg	199	THR

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Mol	Chain	Res	Type
16	Sg	205	ASP
16	Sg	209	CYS
16	Sg	227	GLU
16	Sg	262	ASP
16	Sg	264	GLU
16	Sg	269	ILE
16	Sg	302	LEU
17	Sa	42	PHE
17	Sa	59	LEU
17	Sa	85	ARG
17	Sa	90	ARG
17	Sa	100	VAL
17	Sa	103	ARG
18	Sc	4	PHE
18	Sc	13	VAL
18	Sc	17	ARG
18	Sc	75	VAL
18	Sc	80	TYR
18	Sc	81	ARG
18	Sc	85	ASP
19	Se	8	LEU
19	Se	26	LYS
22	SP	7	GLN
22	SP	68	LYS
22	SP	105	PHE
22	SP	119	ARG
22	SP	127	ASN
22	SP	135	ARG
22	SP	138	LYS
23	SO	36	HIS
23	SO	84	ASN
23	SO	89	LYS
23	SO	90	MET
23	SO	123	GLU
23	SO	136	LYS
24	SN	7	LYS
24	SN	11	ASP
24	SN	17	PHE
24	SN	30	MET
24	SN	32	THR
24	SN	40	ASN
24	SN	59	ARG

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Mol	Chain	Res	Type
24	SN	75	LEU
24	SN	96	ASN
25	Sd	28	LYS
25	Sd	36	ARG
25	Sd	41	GLN
25	Sd	44	VAL
25	Sd	46	LEU
26	SM	29	VAL
26	SM	76	THR
26	SM	100	SER
26	SM	105	SER
27	SL	28	THR
27	SL	72	ASP
28	SJ	30	SER
28	SJ	98	GLN
28	SJ	107	SER
28	SJ	118	SER
29	SI	1	MET
29	SI	5	LEU
29	SI	9	ARG
29	SI	17	SER
29	SI	22	SER
29	SI	33	SER
29	SI	51	GLU
29	SI	79	ARG
29	SI	118	SER
29	SI	198	SER
30	SH	25	ARG
30	SH	64	PHE
30	SH	67	ARG
30	SH	131	ARG
30	SH	161	ASP
31	SG	9	ARG
31	SG	131	THR
31	SG	145	ARG
31	SG	173	ARG
31	SG	203	ARG
31	SG	209	ARG
32	SF	50	LYS
32	SF	61	THR
32	SF	79	VAL
32	SF	158	ASN

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Mol	Chain	Res	Type
32	SF	168	MET
32	SF	186	ARG
32	SF	234	TYR
33	SA	24	MET
33	SA	31	ASP
33	SA	37	ASN
33	SA	109	THR
33	SA	110	ASP
33	SA	153	SER
33	SA	182	GLN
33	SA	185	GLU
33	SA	188	SER
33	SA	192	ARG
33	SA	196	SER
33	SA	217	VAL
33	SA	232	SER
33	SA	240	SER
33	SA	246	ARG
34	Sb	21	LYS
35	Sh	134	ASN
35	Sh	138	VAL
35	Sh	149	THR
35	Sh	154	MET
35	Sh	166	ARG
35	Sh	172	PHE
35	Sh	178	ASP
35	Sh	184	LYS
35	Sh	191	ASN
35	Sh	194	GLU
35	Sh	196	ARG
35	Sh	208	SER
35	Sh	213	ARG
36	f	5	THR
36	f	56	LYS
37	d	11	THR
37	d	50	CYS
37	d	75	ASN
37	d	96	ASN
38	c	47	LYS
38	c	87	LEU
38	c	109	GLN
38	c	227	LYS

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Mol	Chain	Res	Type
38	c	242	THR
39	a	44	ARG
39	a	104	LYS
40	b	4	SER
40	b	58	LYS
45	B	5	LYS
45	B	40	LYS
45	B	67	VAL
45	B	79	LEU
45	B	199	LEU
45	B	203	LEU
45	B	211	ASP
45	B	217	SER
45	B	249[A]	ARG
45	B	249[B]	ARG
45	B	347	ARG
45	B	392	LYS
48	A	28	LYS
48	A	71	ARG
48	A	92	GLN
48	A	93	LYS
48	A	119	LYS
48	A	147	ARG
48	A	193	ARG
49	O	10	LYS
49	O	81	HIS
49	O	93	THR
49	O	118	LYS
49	O	128	SER
49	O	132	VAL
49	O	215	LYS
49	O	233	SER
49	O	264	LEU
50	G	26	SER
50	G	84	ASP
50	G	201	LEU
50	G	211	THR
50	G	219	VAL
51	H	10	PHE
51	H	86	LYS
51	H	149	ARG
51	H	177	LYS

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Mol	Chain	Res	Type
51	H	184	SER
52	M	29	GLU
52	M	46	GLU
52	M	60	CYS
52	M	73	ARG
52	M	109	ARG
52	M	125	SER
52	M	187	SER
53	I	46	LEU
53	I	74	ARG
53	I	178	SER
53	I	183	SER
53	I	191	LYS
53	I	202	THR
54	P	16	ARG
54	P	17	HIS
54	P	42	SER
54	P	89	VAL
54	P	113	SER
54	P	131	ASP
54	P	144	TYR
55	Q	12	SER
55	Q	33	GLN
55	Q	89	MET
55	Q	126	ARG
55	Q	150	LYS
55	Q	153	ARG
55	Q	154	GLN
55	Q	179	LYS
55	Q	190	ARG
56	R	65	VAL
56	R	75	ASN
56	R	87	CYS
56	R	89	TYR
56	R	97	ARG
56	R	98	ASP
56	R	133	ASP
56	R	158	THR
56	R	173	THR
57	E	6	SER
57	E	9	THR
57	E	17	THR

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Mol	Chain	Res	Type
57	E	20	VAL
57	E	36	LYS
57	E	39	THR
57	E	95	TYR
57	E	125	VAL
57	E	128	THR
57	E	162	GLN
57	E	166	VAL
57	E	167	LYS
57	E	184	THR
57	E	185	ASN
59	T	11	SER
59	T	93	SER
60	S	46	SER
60	S	92	ARG
60	S	111	GLN
60	S	115	TYR
60	S	128	LEU
61	K	59	LYS
61	K	79	SER
61	K	80	SER
61	K	90	ARG
61	K	101	CYS
61	K	136	VAL
61	K	137	SER
61	K	152	LYS
62	D	19	LEU
62	D	36	SER
62	D	45	GLN
62	D	89	LYS
62	D	167	LYS
62	D	175	GLN
63	L	15	THR
63	L	60	HIS
63	L	79	SER
63	L	86	GLU
63	L	117	VAL
63	L	136	LYS
64	Y	76	ASN
64	Y	90	SER
64	Y	98	ASN
64	Y	100	SER

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Mol	Chain	Res	Type
64	Y	105	ARG
64	Y	119	ARG
65	Z	6	ASP
65	Z	17	ARG
65	Z	33	ASN
65	Z	62	CYS
66	F	49	ARG
66	F	80	ASP
66	F	97	ASP
66	F	147	SER
66	F	167	LYS
67	h	7	GLN
67	h	20	ARG
67	h	100	GLU
67	h	112	SER
67	h	118	HIS
67	h	125	LYS
67	h	126	LYS
67	h	127	SER
68	g	14	LEU
68	g	18	SER
68	g	32	ARG
68	g	63	THR
69	J	14	ARG
69	J	47	ARG
69	J	90	LYS
69	J	120	VAL
69	J	130	LYS
69	J	132	SER
69	J	133	THR
70	V	51	ASN
70	V	67	ARG
70	V	90	ASP
70	V	105	LEU
71	W	5	LYS
71	W	41	ASN
71	W	91	THR
71	W	118	ARG
72	U	24	LYS
72	U	29	ASP
72	U	44	LEU
72	U	71	SER

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Mol	Chain	Res	Type
72	U	75	ASN
72	U	76	VAL
72	U	81	THR
72	U	82	THR
72	U	106	TRP
72	U	109	ILE
73	i	31	ASP
73	i	49	ASP
73	i	51	VAL
73	i	59	ARG
73	i	61	GLN
73	i	79	ARG
74	p	7	LYS
74	p	24	LYS
74	p	74	CYS
74	p	77	CYS
74	p	78	LYS
74	p	79	SER
74	p	81	ARG
75	o	5	THR
75	o	10	VAL
75	o	29	LEU
75	o	61	SER
76	X	22	VAL
76	X	36	SER
77	k	3	ARG
77	k	15	CYS
77	k	23	VAL
77	k	73	SER
77	k	74	HIS
78	l	5	LYS
79	n	4	VAL
79	n	10	MET
79	n	18	ARG
80	C	68	THR
80	C	94	MET
80	C	107	PHE
80	C	121	PHE
80	C	134	SER
80	C	142	GLN
80	C	155	ASP
80	C	156	SER

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Mol	Chain	Res	Type
80	C	169	PHE
80	C	217	ARG
80	C	289	ARG
80	C	309	LYS
80	C	321	LYS
80	C	346	VAL
80	C	352	ARG
82	e	11	LYS
82	e	14	ILE
82	e	23	GLU
82	e	25	ARG
82	e	31	LYS
82	e	32	ARG
82	e	46	LYS
82	e	47	LYS
82	e	57	ASN
82	e	74	ARG
82	e	81	MET
82	e	88	SER
82	e	114	LEU
82	e	116	LYS
82	e	172	SER
83	j	33	ARG
83	j	68	LYS
83	j	80	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (176) such sidechains are listed below:

Mol	Chain	Res	Type
1	SW	108	GLN
1	SW	110	ASN
2	SZ	34	HIS
2	SZ	95	ASN
4	SX	116	ASN
4	SX	153	GLN
5	SV	31	ASN
6	SU	11	HIS
6	SU	26	GLN
6	SU	30	ASN
6	SU	46	HIS
6	SU	116	GLN
6	SU	134	GLN

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Mol	Chain	Res	Type
7	ST	49	GLN
7	ST	65	ASN
7	ST	123	HIS
8	SS	27	ASN
9	SR	98	HIS
10	SB	33	GLN
10	SB	95	GLN
10	SB	102	HIS
10	SB	167	ASN
11	SC	144	GLN
12	SD	65	HIS
12	SD	122	HIS
13	SE	71	ASN
13	SE	185	ASN
13	SE	203	ASN
13	SE	231	ASN
13	SE	239	GLN
13	SE	240	GLN
14	SK	169	HIS
16	Sg	10	HIS
16	Sg	44	ASN
16	Sg	58	ASN
16	Sg	64	HIS
16	Sg	106	HIS
16	Sg	129	ASN
16	Sg	298	HIS
16	Sg	301	ASN
19	Se	60	GLN
22	SP	20	ASN
22	SP	39	ASN
23	SO	36	HIS
24	SN	12	ASN
24	SN	40	ASN
24	SN	48	GLN
24	SN	51	GLN
27	SL	32	GLN
27	SL	89	GLN
28	SJ	42	GLN
28	SJ	98	GLN
28	SJ	120	ASN
29	SI	99	GLN
29	SI	101	GLN

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Mol	Chain	Res	Type
30	SH	134	ASN
30	SH	172	ASN
30	SH	189	ASN
31	SG	35	ASN
31	SG	86	ASN
31	SG	113	ASN
32	SF	158	ASN
33	SA	193	ASN
33	SA	228	GLN
33	SA	245	GLN
35	Sh	198	HIS
35	Sh	220	ASN
37	d	13	ASN
37	d	38	GLN
37	d	75	ASN
37	d	96	ASN
38	c	123	ASN
38	c	177	GLN
38	c	184	ASN
39	a	69	ASN
39	a	102	ASN
39	a	105	ASN
40	b	31	ASN
45	B	94	GLN
45	B	135	GLN
45	B	151	ASN
45	B	174	HIS
48	A	17	GLN
48	A	139	HIS
48	A	140	ASN
48	A	194	ASN
48	A	205	ASN
48	A	216	HIS
48	A	218	HIS
49	O	63	GLN
49	O	81	HIS
49	O	184	ASN
50	G	169	ASN
50	G	174	ASN
50	G	205	ASN
51	H	74	GLN
51	H	90	HIS

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Mol	Chain	Res	Type
51	H	118	ASN
51	H	159	ASN
51	H	186	HIS
51	H	212	ASN
52	M	99	GLN
52	M	171	HIS
53	I	18	ASN
53	I	93	GLN
54	P	17	HIS
54	P	132	GLN
55	Q	33	GLN
55	Q	75	HIS
55	Q	137	ASN
56	R	85	GLN
56	R	143	GLN
56	R	145	HIS
56	R	148	ASN
57	E	42	GLN
57	E	133	GLN
57	E	152	GLN
59	T	97	ASN
59	T	110	ASN
59	T	147	GLN
60	S	33	ASN
60	S	110	HIS
60	S	111	GLN
62	D	45	GLN
62	D	64	ASN
63	L	11	GLN
63	L	25	HIS
63	L	39	HIS
63	L	62	HIS
63	L	77	ASN
63	L	116	GLN
64	Y	21	HIS
64	Y	28	ASN
64	Y	67	GLN
64	Y	76	ASN
64	Y	77	HIS
65	Z	33	ASN
65	Z	71	ASN
65	Z	76	GLN

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Mol	Chain	Res	Type
66	F	154	GLN
66	F	191	HIS
67	h	7	GLN
67	h	13	HIS
67	h	19	ASN
67	h	51	HIS
67	h	87	GLN
67	h	101	GLN
68	g	16	GLN
68	g	25	ASN
68	g	111	HIS
68	g	122	ASN
70	V	34	GLN
70	V	39	HIS
70	V	82	ASN
70	V	140	ASN
72	U	16	GLN
72	U	54	ASN
72	U	58	ASN
72	U	118	GLN
73	i	39	HIS
74	p	3	ASN
75	o	21	ASN
75	o	33	GLN
75	o	75	ASN
76	X	63	HIS
78	l	18	ASN
78	l	19	GLN
78	l	33	ASN
78	l	43	HIS
80	C	292	GLN
82	e	39	ASN
82	e	127	ASN
82	e	147	GLN
83	j	10	GLN
83	j	28	HIS
83	j	30	GLN

5.3.3 RNA

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	S4	17/19 (89%)	6 (35%)	0
20	S1	1699/2204 (77%)	353 (20%)	15 (0%)
41	1	1564/1782 (87%)	316 (20%)	24 (1%)
42	2	1035/1526 (67%)	215 (20%)	17 (1%)
43	4	182/183 (99%)	35 (19%)	2 (1%)
44	7	157/171 (91%)	24 (15%)	0
46	8	116/123 (94%)	13 (11%)	1 (0%)
47	5	107/135 (79%)	26 (24%)	3 (2%)
58	6	70/73 (95%)	29 (41%)	5 (7%)
81	3	156/216 (72%)	33 (21%)	3 (1%)
All	All	5103/6432 (79%)	1050 (20%)	70 (1%)

All (1050) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	S4	2	C
15	S4	5	G
15	S4	7	A
15	S4	69	G
15	S4	70	C
15	S4	76	A
20	S1	2	A
20	S1	3	U
20	S1	17	C
20	S1	26	A
20	S1	32	U
20	S1	33	PSU
20	S1	34	G
20	S1	42	G
20	S1	45	U
20	S1	47	A
20	S1	59	C
20	S1	78	C
20	S1	80	G
20	S1	81	G
20	S1	98	A2M
20	S1	101	A
20	S1	102	C
20	S1	112	A
20	S1	117	G
20	S1	128	C

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Mol	Chain	Res	Type
20	S1	145	A
20	S1	146	U
20	S1	152	A
20	S1	158	G
20	S1	165	G
20	S1	171	C
20	S1	173	A
20	S1	174	A
20	S1	176	A
20	S1	181	A
20	S1	193	G
20	S1	197	U
20	S1	198	C
20	S1	232	C
20	S1	234	C
20	S1	235	C
20	S1	236	C
20	S1	238	G
20	S1	249	A
20	S1	252	G
20	S1	253	U
20	S1	254	A
20	S1	275	A
20	S1	276	G
20	S1	278	A
20	S1	281	A
20	S1	284	C
20	S1	285	A
20	S1	286	G
20	S1	287	C
20	S1	288	A
20	S1	308	C
20	S1	315	A
20	S1	316	A
20	S1	317	G
20	S1	339	U
20	S1	343	G
20	S1	356	A
20	S1	358	C
20	S1	360	G
20	S1	364	G
20	S1	365	U

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Mol	Chain	Res	Type
20	S1	381	G
20	S1	382	A
20	S1	404	C
20	S1	423	U
20	S1	443	A
20	S1	444	A
20	S1	445	U
20	S1	447	G
20	S1	459	A
20	S1	462	G
20	S1	464	G
20	S1	467	C
20	S1	469	G
20	S1	471	A
20	S1	477	G
20	S1	481	A
20	S1	482	U
20	S1	483	U
20	S1	487	C
20	S1	488	A
20	S1	495	A
20	S1	496	A
20	S1	497	A
20	S1	501	A
20	S1	503	C
20	S1	507	G
20	S1	512	A2M
20	S1	516	A
20	S1	523	A
20	S1	553	U
20	S1	555	C
20	S1	565	U
20	S1	566	A
20	S1	586	G
20	S1	588	G
20	S1	589	U
20	S1	591	A
20	S1	600	OMG
20	S1	606	G
20	S1	607	PSU
20	S1	608	C
20	S1	614	C

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Mol	Chain	Res	Type
20	S1	626	G
20	S1	628	A
20	S1	631	U
20	S1	643	A
20	S1	660	U
20	S1	664	U
20	S1	668	A2M
20	S1	669	A
20	S1	671	G
20	S1	672	G
20	S1	673	G
20	S1	688	G
20	S1	689	U
20	S1	690	G
20	S1	693	C
20	S1	746	C
20	S1	750	U
20	S1	752	C
20	S1	753	A
20	S1	757	C
20	S1	758	G
20	S1	778	G
20	S1	779	A
20	S1	782	C
20	S1	783	A
20	S1	785	G
20	S1	787	G
20	S1	788	A
20	S1	789	G
20	S1	790	U
20	S1	791	G
20	S1	792	G
20	S1	811	C
20	S1	815	U
20	S1	816	C
20	S1	819	G
20	S1	820	C
20	S1	821	A
20	S1	834	U
20	S1	839	G
20	S1	842	U
20	S1	843	U

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Mol	Chain	Res	Type
20	S1	856	A
20	S1	863	C
20	S1	866	G
20	S1	867	A
20	S1	875	A
20	S1	876	G
20	S1	883	G
20	S1	884	A
20	S1	886	U
20	S1	887	U
20	S1	894	G
20	S1	895	A
20	S1	897	A2M
20	S1	903	G
20	S1	905	A
20	S1	914	G
20	S1	916	G
20	S1	917	C
20	S1	955	A
20	S1	957	G
20	S1	965	G
20	S1	970	U
20	S1	972	A
20	S1	973	U
20	S1	974	G
20	S1	977	G
20	S1	978	C
20	S1	990	U
20	S1	991	G
20	S1	992	C
20	S1	993	U
20	S1	994	U
20	S1	1101	A
20	S1	1102	G
20	S1	1105	A
20	S1	1109	A
20	S1	1119	U
20	S1	1123	G
20	S1	1129	A
20	S1	1133	U
20	S1	1139	G
20	S1	1142	G

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Mol	Chain	Res	Type
20	S1	1146	G
20	S1	1155	U
20	S1	1168	C
20	S1	1180	A
20	S1	1189	G
20	S1	1191	A
20	S1	1192	PSU
20	S1	1199	A
20	S1	1207	U
20	S1	1213	A
20	S1	1235	A
20	S1	1239	A
20	S1	1245	A
20	S1	1246	PSU
20	S1	1252	A
20	S1	1273	A
20	S1	1275	C
20	S1	1279	G
20	S1	1287	U
20	S1	1289	A
20	S1	1427	U
20	S1	1431	A
20	S1	1432	C
20	S1	1442	U
20	S1	1443	U
20	S1	1444	G
20	S1	1449	U
20	S1	1452	A
20	S1	1466	G
20	S1	1490	A
20	S1	1498	G
20	S1	1502	G
20	S1	1503	A
20	S1	1510	C
20	S1	1511	C
20	S1	1519	G
20	S1	1537	U
20	S1	1546	A
20	S1	1548	A
20	S1	1551	G
20	S1	1552	G
20	S1	1554	A

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Mol	Chain	Res	Type
20	S1	1565	A
20	S1	1567	C
20	S1	1568	C
20	S1	1569	G
20	S1	1570	G
20	S1	1573	A
20	S1	1574	G
20	S1	1578	G
20	S1	1579	A
20	S1	1580	G
20	S1	1589	G
20	S1	1595	G
20	S1	1597	G
20	S1	1598	U
20	S1	1606	C
20	S1	1607	G
20	S1	1608	A
20	S1	1611	C
20	S1	1612	C
20	S1	1613	C
20	S1	1616	A
20	S1	1622	G
20	S1	1636	U
20	S1	1637	U
20	S1	1643	G
20	S1	1653	U
20	S1	1657	PSU
20	S1	1658	U
20	S1	1666	U
20	S1	1667	U
20	S1	1670	G
20	S1	1673	A
20	S1	1677	G
20	S1	1700	G
20	S1	1705	C
20	S1	1706	A
20	S1	1767	G
20	S1	1771	A
20	S1	1775	C
20	S1	1782	G
20	S1	1789	U
20	S1	1795	G

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Mol	Chain	Res	Type
20	S1	1796	U
20	S1	1797	A
20	S1	1801	G
20	S1	1807	G
20	S1	1816	U
20	S1	1822	A
20	S1	1825	A
20	S1	1828	A
20	S1	1829	OMG
20	S1	1833	OMU
20	S1	1834	G
20	S1	1836	G
20	S1	1837	A
20	S1	1847	A
20	S1	1848	U
20	S1	1872	A
20	S1	1875	G
20	S1	1890	A
20	S1	1891	A
20	S1	1907	A
20	S1	1909	C
20	S1	1915	U
20	S1	1919	C
20	S1	1920	A
20	S1	1921	A
20	S1	1922	A
20	S1	1923	A
20	S1	1924	G
20	S1	1928	G
20	S1	1931	G
20	S1	1932	A
20	S1	1933	A
20	S1	1938	C
20	S1	1944	C
20	S1	1948	U
20	S1	1950	G
20	S1	1955	A
20	S1	1956	C
20	S1	1976	U
20	S1	1977	U
20	S1	1978	A
20	S1	1979	OMU

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Mol	Chain	Res	Type
20	S1	1984	C
20	S1	1988	C
20	S1	1995	G7M
20	S1	2004	G
20	S1	2010	G
20	S1	2012	A
20	S1	2021	A2M
20	S1	2027	G
20	S1	2053	A
20	S1	2054	C
20	S1	2055	A
20	S1	2057	C
20	S1	2058	G
20	S1	2065	G
20	S1	2069	U
20	S1	2086	A
20	S1	2097	C
20	S1	2099	G
20	S1	2100	A
20	S1	2102	A
20	S1	2104	G
20	S1	2105	C
20	S1	2157	A
20	S1	2160	G
20	S1	2163	G
20	S1	2165	A
20	S1	2169	A
20	S1	2170	G
20	S1	2172	U
20	S1	2173	A
20	S1	2183	G
20	S1	2186	C
20	S1	2195	G
20	S1	2196	G
20	S1	2197	A
20	S1	2198	U
20	S1	2199	C
20	S1	2202	PSU
20	S1	2203	U
41	1	24	A
41	1	38	A
41	1	41	A

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Mol	Chain	Res	Type
41	1	47	C
41	1	58	A
41	1	64	A
41	1	84	G
41	1	86	G
41	1	87	A
41	1	91	G
41	1	92	C
41	1	98	A
41	1	110	A
41	1	131	U
41	1	134	A
41	1	135	A
41	1	136	G
41	1	141	U
41	1	142	A
41	1	154	A
41	1	155	A
41	1	156	A
41	1	158	A
41	1	159	U
41	1	161	A
41	1	162	U
41	1	163	U
41	1	164	U
41	1	165	C
41	1	171	U
41	1	175	G
41	1	189	A
41	1	191	U
41	1	192	C
41	1	205	A
41	1	206	A
41	1	210	G
41	1	212	U
41	1	214	C
41	1	216	G
41	1	217	A
41	1	218	A
41	1	219	U
41	1	223	A
41	1	230	A

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Mol	Chain	Res	Type
41	1	231	U
41	1	233	U
41	1	234	G
41	1	239	PSU
41	1	249	G
41	1	250	A
41	1	251	A
41	1	255	G
41	1	256	U
41	1	258	A
41	1	266	G
41	1	273	A
41	1	279	G
41	1	280	A
41	1	281	G
41	1	283	G
41	1	290	G
41	1	291	A
41	1	292	A
41	1	301	A
41	1	305	A
41	1	306	G
41	1	307	U
41	1	323	U
41	1	332	A
41	1	335	U
41	1	336	U
41	1	337	G
41	1	341	G
41	1	343	U
41	1	361	A
41	1	367	A
41	1	368	G
41	1	369	A
41	1	374	G
41	1	383	U
41	1	390	C
41	1	391	A
41	1	392	A
41	1	409	U
41	1	410	U
41	1	417	G

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Mol	Chain	Res	Type
41	1	440	A
41	1	443	A
41	1	444	C
41	1	461	G
41	1	462	A
41	1	463	C
41	1	464	A
41	1	477	C
41	1	482	U
41	1	483	C
41	1	485	A
41	1	486	G
41	1	487	A
41	1	488	G
41	1	501	C
41	1	503	A
41	1	506	G
41	1	521	G
41	1	523	G
41	1	526	A
41	1	528	A
41	1	536	G
41	1	538	G
41	1	542	C
41	1	543	G
41	1	544	A
41	1	545	A
41	1	546	G
41	1	547	U
41	1	548	G
41	1	551	A
41	1	563	C
41	1	564	U
41	1	567	G
41	1	569	G
41	1	570	A
41	1	571	A
41	1	572	A
41	1	575	A
41	1	582	U
41	1	583	A
41	1	586	U

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Mol	Chain	Res	Type
41	1	591	U
41	1	592	G
41	1	599	G
41	1	610	A
41	1	611	C
41	1	612	G
41	1	624	U
41	1	625	C
41	1	631	G
41	1	632	A
41	1	633	U
41	1	634	G
41	1	641	G
41	1	651	G
41	1	652	A
41	1	668	C
41	1	681	A2M
41	1	692	A
41	1	709	A
41	1	713	A
41	1	728	C
41	1	729	A
41	1	735	U
41	1	736	C
41	1	737	U
41	1	750	G
41	1	753	A
41	1	754	G
41	1	761	A
41	1	763	U
41	1	767	U
41	1	769	U
41	1	771	U
41	1	788	A
41	1	789	U
41	1	790	C
41	1	791	C
41	1	792	G
41	1	793	U
41	1	803	C
41	1	818	C
41	1	821	C

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Mol	Chain	Res	Type
41	1	822	C
41	1	823	G
41	1	824	U
41	1	832	G
41	1	836	G
41	1	838	G
41	1	850	G
41	1	868	A
41	1	880	C
41	1	886	G
41	1	912	C
41	1	925	U
41	1	930	U
41	1	959	OMG
41	1	965	A
41	1	967	G
41	1	968	A
41	1	972	A
41	1	975	G
41	1	976	A
41	1	983	U
41	1	984	A
41	1	988	G
41	1	995	C
41	1	1010	C
41	1	1012	C
41	1	1029	G
41	1	1031	A
41	1	1045	G
41	1	1102	U
41	1	1105	A
41	1	1108	G
41	1	1114	A
41	1	1116	A
41	1	1118	A
41	1	1128	A
41	1	1134	C
41	1	1135	U
41	1	1148	A
41	1	1150	A
41	1	1156	A
41	1	1159	A

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Mol	Chain	Res	Type
41	1	1165	A
41	1	1174	G
41	1	1181	PSU
41	1	1188	G
41	1	1210	A
41	1	1216	U
41	1	1235	A
41	1	1239	U
41	1	1242	U
41	1	1243	G
41	1	1249	A
41	1	1250	U
41	1	1251	U
41	1	1252	C
41	1	1253	U
41	1	1254	C
41	1	1257	U
41	1	1261	U
41	1	1265	A
41	1	1269	G
41	1	1270	U
41	1	1271	G
41	1	1275	G
41	1	1278	G
41	1	1352	C
41	1	1353	A
41	1	1354	C
41	1	1364	A
41	1	1369	G
41	1	1370	A
41	1	1371	OMU
41	1	1375	G
41	1	1378	U
41	1	1379	A
41	1	1380	A
41	1	1389	A
41	1	1390	G
41	1	1392	G
41	1	1393	A
41	1	1394	A
41	1	1395	U
41	1	1401	U

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Mol	Chain	Res	Type
41	1	1412	G
41	1	1413	U
41	1	1414	A
41	1	1420	G
41	1	1421	G
41	1	1422	A
41	1	1435	A
41	1	1438	A
41	1	1445	G
41	1	1453	G
41	1	1464	G
41	1	1490	G
41	1	1504	A
41	1	1509	C
41	1	1524	OMG
41	1	1527	OMC
41	1	1536	C
41	1	1540	OMG
41	1	1543	A
41	1	1545	G
41	1	1557	A
41	1	1559	A
41	1	1560	U
41	1	1561	A
41	1	1564	C
41	1	1586	G
41	1	1590	G
41	1	1605	G
41	1	1613	C
41	1	1625	A
41	1	1654	A
41	1	1655	U
41	1	1661	U
41	1	1662	G
41	1	1663	U
41	1	1666	G
41	1	1667	G
41	1	1669	A
41	1	1671	G
41	1	1672	U
41	1	1673	G
41	1	1675	A

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Mol	Chain	Res	Type
41	1	1723	A
41	1	1726	G
41	1	1727	A
41	1	1728	A
41	1	1730	A
41	1	1738	C
41	1	1739	A
41	1	1744	A
41	1	1747	U
41	1	1753	U
41	1	1761	A
41	1	1762	A
41	1	1763	A
41	1	1764	A
41	1	1766	G
41	1	1774	A
41	1	1775	U
41	1	1779	G
41	1	1780	G
42	2	7	C
42	2	22	A
42	2	25	A
42	2	33	A
42	2	61	C
42	2	63	U
42	2	68	A
42	2	69	A
42	2	75	A
42	2	78	PSU
42	2	90	G
42	2	91	C
42	2	118	G
42	2	135	A
42	2	136	A
42	2	338	C
42	2	339	A
42	2	340	A
42	2	342	U
42	2	343	U
42	2	349	C
42	2	368	G
42	2	377	A

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Mol	Chain	Res	Type
42	2	380	G
42	2	386	U
42	2	388	A
42	2	390	A
42	2	404	A
42	2	443	OMC
42	2	444	A
42	2	453	A
42	2	454	A
42	2	455	U
42	2	456	G
42	2	485	G
42	2	490	A
42	2	492	G
42	2	495	G
42	2	496	G
42	2	497	G
42	2	498	A
42	2	499	G
42	2	501	A
42	2	502	A
42	2	505	A
42	2	506	PSU
42	2	507	G
42	2	508	A
42	2	509	C
42	2	513	C
42	2	518	G
42	2	519	G
42	2	520	U
42	2	526	A
42	2	527	A2M
42	2	529	G
42	2	530	C
42	2	534	OMG
42	2	544	U
42	2	552	C
42	2	553	G
42	2	554	C
42	2	556	U
42	2	559	A
42	2	561	G

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Mol	Chain	Res	Type
42	2	571	G
42	2	580	U
42	2	582	U
42	2	602	A
42	2	618	A
42	2	620	C
42	2	621	G
42	2	639	G
42	2	643	A
42	2	647	A
42	2	648	A
42	2	649	G
42	2	650	A
42	2	657	U
42	2	658	G
42	2	665	A2M
42	2	685	G
42	2	688	G
42	2	690	C
42	2	750	U
42	2	760	U
42	2	761	A
42	2	769	A
42	2	774	A
42	2	777	A
42	2	780	G
42	2	781	G
42	2	784	U
42	2	785	U
42	2	786	A
42	2	797	C
42	2	798	G
42	2	810	G
42	2	811	U
42	2	814	A
42	2	960	C
42	2	964	G
42	2	968	U
42	2	969	A
42	2	970	A
42	2	972	C
42	2	979	A

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Mol	Chain	Res	Type
42	2	982	G
42	2	983	G
42	2	985	A
42	2	986	U
42	2	1011	G
42	2	1012	U
42	2	1019	A
42	2	1022	U
42	2	1030	A
42	2	1033	G
42	2	1034	G
42	2	1041	G
42	2	1046	OMG
42	2	1055	A
42	2	1064	A
42	2	1075	G
42	2	1079	U
42	2	1083	A
42	2	1101	A
42	2	1116	A
42	2	1118	A
42	2	1121	A
42	2	1123	A
42	2	1126	C
42	2	1131	A
42	2	1132	A
42	2	1146	A
42	2	1147	C
42	2	1156	G
42	2	1157	U
42	2	1165	G
42	2	1180	A
42	2	1181	G
42	2	1189	A
42	2	1215	A
42	2	1234	G
42	2	1237	A
42	2	1238	G
42	2	1239	A
42	2	1241	U
42	2	1248	OMC
42	2	1252	G

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Mol	Chain	Res	Type
42	2	1255	A
42	2	1265	PSU
42	2	1270	C
42	2	1271	G
42	2	1272	G
42	2	1273	C
42	2	1274	C
42	2	1275	A
42	2	1301	G
42	2	1303	PSU
42	2	1305	C
42	2	1308	5MC
42	2	1309	G
42	2	1314	C
42	2	1325	A
42	2	1327	C
42	2	1332	C
42	2	1373	C
42	2	1374	A
42	2	1380	C
42	2	1385	G
42	2	1389	G
42	2	1403	PSU
42	2	1409	A
42	2	1416	U
42	2	1421	C
42	2	1428	U
42	2	1433	G
42	2	1436	A
42	2	1438	U
42	2	1441	C
42	2	1443	A
42	2	1444	G
42	2	1445	A
42	2	1447	A
42	2	1448	A
42	2	1450	G
42	2	1451	A
42	2	1452	U
42	2	1453	U
42	2	1454	A
42	2	1455	U

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Mol	Chain	Res	Type
42	2	1458	G
42	2	1461	C
42	2	1462	A
42	2	1464	A
42	2	1465	G
42	2	1466	C
42	2	1468	G
42	2	1496	G
42	2	1497	C
42	2	1498	G
42	2	1501	G
42	2	1502	G
42	2	1503	G
42	2	1510	U
42	2	1511	U
42	2	1512	G
42	2	1513	G
42	2	1514	U
42	2	1517	G
42	2	1520	C
42	2	1521	A
42	2	1522	U
42	2	1524	A
42	2	1525	C
43	4	8	U
43	4	9	G
43	4	14	G
43	4	16	G
43	4	22	G
43	4	24	A
43	4	25	G
43	4	40	G
43	4	48	U
43	4	50	G
43	4	55	A
43	4	58	G
43	4	85	C
43	4	86	U
43	4	87	G
43	4	102	G
43	4	107	U
43	4	114	A

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Mol	Chain	Res	Type
43	4	120	U
43	4	121	C
43	4	127	G
43	4	128	U
43	4	129	G
43	4	131	U
43	4	139	U
43	4	142	A
43	4	145	C
43	4	150	A
43	4	151	A
43	4	155	A
43	4	157	A
43	4	159	G
43	4	168	A
43	4	173	C
43	4	174	A
44	7	22	U
44	7	33	U
44	7	48	A
44	7	52	A
44	7	59	A
44	7	62	A
44	7	63	G
44	7	85	U
44	7	86	C
44	7	87	U
44	7	88	A
44	7	94	G
44	7	103	A
44	7	104	A
44	7	105	C
44	7	110	A
44	7	120	G
44	7	124	A
44	7	125	A
44	7	126	G
44	7	136	G
44	7	149	A
44	7	157	U
44	7	158	U
46	8	11	G

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Mol	Chain	Res	Type
46	8	32	C
46	8	46	A
46	8	54	A
46	8	57	U
46	8	58	A
46	8	91	G
46	8	94	A
46	8	95	U
46	8	104	A
46	8	113	U
46	8	114	G
46	8	123	U
47	5	5	G
47	5	14	C
47	5	17	A
47	5	23	G
47	5	28	U
47	5	36	C
47	5	38	G
47	5	46	C
47	5	47	G
47	5	48	G
47	5	49	C
47	5	50	A
47	5	51	U
47	5	61	C
47	5	62	G
47	5	64	U
47	5	67	G
47	5	71	C
47	5	98	G
47	5	105	G
47	5	108	G
47	5	111	U
47	5	112	G
47	5	113	A
47	5	119	C
47	5	124	U
58	6	7	A
58	6	11	G
58	6	12	C
58	6	14	A

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Mol	Chain	Res	Type
58	6	15	C
58	6	24	C
58	6	25	U
58	6	26	G
58	6	29	G
58	6	31	U
58	6	32	U
58	6	37	C
58	6	38	C
58	6	39	U
58	6	40	C
58	6	41	G
58	6	42	A
58	6	43	A
58	6	52	G
58	6	53	U
58	6	55	U
58	6	56	A
58	6	58	U
58	6	59	C
58	6	64	U
58	6	67	C
58	6	68	A
58	6	72	C
58	6	73	A
81	3	16	G
81	3	34	C
81	3	41	A
81	3	42	U
81	3	59	U
81	3	63	U
81	3	72	A
81	3	107	U
81	3	109	U
81	3	110	U
81	3	118	G
81	3	119	C
81	3	124	U
81	3	125	U
81	3	126	C
81	3	138	U
81	3	145	U

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Mol	Chain	Res	Type
81	3	146	G
81	3	149	A
81	3	150	A
81	3	151	A
81	3	179	U
81	3	181	G
81	3	183	G
81	3	184	A
81	3	188	C
81	3	191	C
81	3	192	G
81	3	194	A
81	3	202	A
81	3	210	G
81	3	213	G
81	3	214	U

All (70) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
20	S1	1	G
20	S1	277	U
20	S1	494	A
20	S1	607	PSU
20	S1	757	C
20	S1	916	G
20	S1	1108	A
20	S1	1145	A
20	S1	1579	A
20	S1	1612	C
20	S1	1636	U
20	S1	1931	G
20	S1	1983	U
20	S1	2065	G
20	S1	2159	A
41	1	83	A
41	1	141	U
41	1	154	A
41	1	162	U
41	1	163	U
41	1	191	U
41	1	249	G

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Mol	Chain	Res	Type
41	1	443	A
41	1	485	A
41	1	581	G
41	1	728	C
41	1	790	C
41	1	837	A
41	1	947	A
41	1	959	OMG
41	1	967	G
41	1	983	U
41	1	1011	PSU
41	1	1264	A
41	1	1269	G
41	1	1352	C
41	1	1394	A
41	1	1443	U
41	1	1524	OMG
42	2	25	A
42	2	68	A
42	2	134	C
42	2	337	A
42	2	443	OMC
42	2	452	G
42	2	500	PSU
42	2	504	PSU
42	2	646	G
42	2	648	A
42	2	959	A
42	2	985	A
42	2	1156	G
42	2	1403	PSU
42	2	1452	U
42	2	1467	G
42	2	1497	C
43	4	15	G
43	4	149	U
46	8	45	G
47	5	48	G
47	5	105	G
47	5	111	U
58	6	10	C
58	6	38	C

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Mol	Chain	Res	Type
58	6	40	C
58	6	51	A
58	6	72	C
81	3	41	A
81	3	183	G
81	3	187	U

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

152 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$
20	PSU	S1	104	20	18,21,22	4.41	7 (38%)	22,30,33	1.78	5 (22%)
20	5MC	S1	2061	20	18,22,23	0.98	2 (11%)	26,32,35	1.21	2 (7%)
20	PSU	S1	12	20	18,21,22	4.33	7 (38%)	22,30,33	1.98	5 (22%)
44	A2M	7	43	44	18,25,26	3.70	7 (38%)	18,36,39	3.69	4 (22%)
20	PSU	S1	607	20	18,21,22	4.52	7 (38%)	22,30,33	1.75	5 (22%)
20	OMC	S1	2140	20	19,22,23	2.96	8 (42%)	26,31,34	0.81	0
20	OMU	S1	2048	20	19,22,23	2.90	7 (36%)	26,31,34	1.79	5 (19%)
42	PSU	2	1144	42	18,21,22	4.27	8 (44%)	22,30,33	1.93	4 (18%)
42	OMG	2	1078	42	18,26,27	2.36	8 (44%)	19,38,41	1.78	5 (26%)
41	OMG	1	959	41	18,26,27	2.47	8 (44%)	19,38,41	1.71	4 (21%)
41	OMU	1	845	41	19,22,23	2.82	7 (36%)	26,31,34	1.77	4 (15%)
42	OMG	2	1231	42	18,26,27	2.37	8 (44%)	19,38,41	1.59	5 (26%)
20	OMC	S1	38	20	19,22,23	2.92	8 (42%)	26,31,34	0.75	0
20	OMG	S1	1623	20	18,26,27	2.43	8 (44%)	19,38,41	1.56	4 (21%)
41	PSU	1	1402	41	18,21,22	4.13	9 (50%)	22,30,33	1.87	4 (18%)
41	PSU	1	940	41	18,21,22	4.25	8 (44%)	22,30,33	1.81	5 (22%)
20	PSU	S1	1566	20	18,21,22	1.37	2 (11%)	22,30,33	2.00	5 (22%)
42	A2M	2	665	42	18,25,26	3.64	7 (38%)	18,36,39	3.42	4 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
41	PSU	1	1181	41	18,21,22	4.28	7 (38%)	22,30,33	1.78	5 (22%)
42	PSU	2	593	42	18,21,22	4.18	9 (50%)	22,30,33	1.96	5 (22%)
42	OMU	2	1359	42	19,22,23	2.88	8 (42%)	26,31,34	1.79	5 (19%)
20	OMG	S1	600	20	18,26,27	2.52	8 (44%)	19,38,41	1.54	3 (15%)
42	OMG	2	655	42	18,26,27	2.38	8 (44%)	19,38,41	1.63	4 (21%)
42	OMG	2	71	42	18,26,27	2.36	8 (44%)	19,38,41	1.61	5 (26%)
42	OMU	2	1419	42	19,22,23	2.87	8 (42%)	26,31,34	1.69	4 (15%)
20	PSU	S1	455	20	18,21,22	4.46	7 (38%)	22,30,33	1.90	5 (22%)
20	PSU	S1	1192	20	18,21,22	4.37	7 (38%)	22,30,33	1.63	4 (18%)
20	A2M	S1	897	20	18,25,26	3.66	9 (50%)	18,36,39	3.63	5 (27%)
41	OMU	1	1371	41	19,22,23	2.92	8 (42%)	26,31,34	2.09	6 (23%)
41	OMC	1	1552	41	19,22,23	2.80	8 (42%)	26,31,34	0.78	0
42	A2M	2	1384	42	18,25,26	3.63	7 (38%)	18,36,39	3.57	4 (22%)
81	OMU	3	13	81	19,22,23	2.87	7 (36%)	26,31,34	1.82	5 (19%)
42	PSU	2	1060	42	18,21,22	4.32	8 (44%)	22,30,33	1.78	4 (18%)
42	OMC	2	1159	42	19,22,23	2.80	8 (42%)	26,31,34	0.81	0
20	MA6	S1	2184	20	18,26,27	1.16	2 (11%)	19,38,41	2.99	2 (10%)
41	PSU	1	1011	42,41	18,21,22	4.42	7 (38%)	22,30,33	1.91	5 (22%)
42	A2M	2	382	42	18,25,26	3.63	7 (38%)	18,36,39	3.58	4 (22%)
42	PSU	2	1354	42	18,21,22	4.28	8 (44%)	22,30,33	1.90	5 (22%)
20	OMC	S1	1866	20	19,22,23	2.80	8 (42%)	26,31,34	0.71	0
41	PSU	1	239	41	18,21,22	4.34	7 (38%)	22,30,33	1.73	5 (22%)
41	A2M	1	1539	42,87,84,41	18,25,26	3.63	7 (38%)	18,36,39	3.76	5 (27%)
42	5MC	2	1308	42	18,22,23	3.48	7 (38%)	26,32,35	1.25	3 (11%)
20	OMU	S1	1777	20	19,22,23	2.95	8 (42%)	26,31,34	1.74	5 (19%)
20	G7M	S1	1995	20	20,26,27	4.02	10 (50%)	17,39,42	1.00	1 (5%)
41	OMG	1	1524	41	18,26,27	2.40	8 (44%)	19,38,41	1.74	4 (21%)
44	PSU	7	69	44	18,21,22	4.28	8 (44%)	22,30,33	1.78	4 (18%)
42	OMG	2	1253	42	18,26,27	2.35	8 (44%)	19,38,41	1.61	6 (31%)
42	PSU	2	626	42	18,21,22	4.18	8 (44%)	22,30,33	1.75	3 (13%)
20	C4J	S1	1543	20	24,29,30	2.99	9 (37%)	29,42,45	1.46	5 (17%)
42	PSU	2	1265	42	18,21,22	4.46	7 (38%)	22,30,33	1.71	5 (22%)
44	OMG	7	75	44	18,26,27	2.43	8 (44%)	19,38,41	1.62	5 (26%)
41	OMU	1	1107	41	19,22,23	2.80	8 (42%)	26,31,34	1.80	6 (23%)
20	OMG	S1	1550	20	18,26,27	2.49	8 (44%)	19,38,41	1.60	5 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	A2M	S1	98	20	18,25,26	3.60	8 (44%)	18,36,39	3.57	4 (22%)
20	MA6	S1	2185	20	18,26,27	1.17	1 (5%)	19,38,41	3.11	2 (10%)
42	PSU	2	1318	42	18,21,22	4.22	8 (44%)	22,30,33	1.73	4 (18%)
41	A2M	1	437	41	18,25,26	3.66	8 (44%)	18,36,39	3.83	4 (22%)
42	OMC	2	359	42	19,22,23	2.87	8 (42%)	26,31,34	0.66	0
42	PSU	2	1361	42	18,21,22	4.38	7 (38%)	22,30,33	1.93	5 (22%)
42	A2M	2	591	42	18,25,26	3.64	8 (44%)	18,36,39	3.67	4 (22%)
41	OMC	1	695	41	19,22,23	2.72	8 (42%)	26,31,34	0.72	0
20	OMU	S1	1979	20	19,22,23	2.86	8 (42%)	26,31,34	1.79	4 (15%)
42	PSU	2	437	42	18,21,22	4.16	8 (44%)	22,30,33	1.88	5 (22%)
42	A2M	2	628	42	18,25,26	3.68	9 (50%)	18,36,39	3.84	5 (27%)
42	A2M	2	95	42	18,25,26	3.64	7 (38%)	18,36,39	3.47	4 (22%)
20	A2M	S1	512	20	18,25,26	0.97	1 (5%)	18,36,39	1.30	2 (11%)
20	OMG	S1	1647	20	18,26,27	2.40	8 (44%)	19,38,41	1.71	5 (26%)
42	A2M	2	572	42	18,25,26	3.69	7 (38%)	18,36,39	3.81	5 (27%)
41	A2M	1	697	41	18,25,26	3.68	7 (38%)	18,36,39	3.91	4 (22%)
20	OMU	S1	1833	20	19,22,23	3.02	8 (42%)	26,31,34	1.76	5 (19%)
20	5MC	S1	1544	20	18,22,23	3.46	7 (38%)	26,32,35	1.05	1 (3%)
42	PSU	2	1382	42	18,21,22	4.22	9 (50%)	22,30,33	1.79	5 (22%)
41	A2M	1	858	41	18,25,26	3.61	8 (44%)	18,36,39	3.89	4 (22%)
20	OMG	S1	1865	20	18,26,27	2.41	8 (44%)	19,38,41	1.69	5 (26%)
41	PSU	1	1017	41	18,21,22	4.13	8 (44%)	22,30,33	1.74	5 (22%)
20	PSU	S1	1533	20	18,21,22	4.30	7 (38%)	22,30,33	1.84	5 (22%)
20	OMG	S1	1829	20	18,26,27	2.42	8 (44%)	19,38,41	1.52	4 (21%)
41	PSU	1	672	84,41	18,21,22	4.21	8 (44%)	22,30,33	1.91	5 (22%)
20	PSU	S1	1657	20	18,21,22	4.29	7 (38%)	22,30,33	1.64	4 (18%)
42	OMU	2	560	42	19,22,23	2.88	7 (36%)	26,31,34	1.73	4 (15%)
20	A2M	S1	28	20	18,25,26	3.58	7 (38%)	18,36,39	3.74	4 (22%)
41	PSU	1	1528	41	18,21,22	4.25	8 (44%)	22,30,33	1.75	4 (18%)
42	PSU	2	1194	42	18,21,22	4.21	8 (44%)	22,30,33	1.99	5 (22%)
42	PSU	2	1403	42	18,21,22	4.23	9 (50%)	22,30,33	1.74	4 (18%)
20	A2M	S1	479	20	18,25,26	3.64	8 (44%)	18,36,39	3.75	4 (22%)
41	OMG	1	1626	41	18,26,27	2.35	8 (44%)	19,38,41	1.62	5 (26%)
42	A2M	2	604	42,41	18,25,26	3.62	7 (38%)	18,36,39	3.80	4 (22%)
44	A2M	7	162	41,44	18,25,26	3.64	8 (44%)	18,36,39	3.89	4 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
42	OMC	2	443	42	19,22,23	0.86	0	26,31,34	1.02	0
42	OMG	2	1046	42	18,26,27	2.50	8 (44%)	19,38,41	1.55	4 (21%)
20	OMU	S1	1621	20	19,22,23	2.94	8 (42%)	26,31,34	1.76	5 (19%)
20	OMG	S1	2151	20	18,26,27	2.54	8 (44%)	19,38,41	1.62	4 (21%)
42	PSU	2	597	42	18,21,22	4.16	8 (44%)	22,30,33	1.92	4 (18%)
41	PSU	1	1664	41	18,21,22	4.20	8 (44%)	22,30,33	1.70	4 (18%)
44	PSU	7	74	44	18,21,22	4.31	8 (44%)	22,30,33	1.85	5 (22%)
41	A2M	1	681	41	18,25,26	3.65	7 (38%)	18,36,39	3.53	4 (22%)
42	OMU	2	73	42	19,22,23	2.82	7 (36%)	26,31,34	1.70	5 (19%)
41	PSU	1	1171	41	18,21,22	4.13	9 (50%)	22,30,33	1.77	5 (22%)
42	PSU	2	500	42	18,21,22	1.40	2 (11%)	22,30,33	2.08	4 (18%)
42	PSU	2	1413	42	18,21,22	4.19	8 (44%)	22,30,33	1.77	4 (18%)
42	PSU	2	1058	42	18,21,22	4.32	8 (44%)	22,30,33	1.75	4 (18%)
20	PSU	S1	1841	20	18,21,22	4.37	7 (38%)	22,30,33	1.85	5 (22%)
41	OMC	1	1527	41	19,22,23	2.69	7 (36%)	26,31,34	0.72	0
43	OMG	4	74	43	18,26,27	2.29	8 (44%)	19,38,41	1.64	6 (31%)
42	PSU	2	1303	42	18,21,22	4.47	8 (44%)	22,30,33	1.92	6 (27%)
20	PSU	S1	1156	20	18,21,22	4.48	7 (38%)	22,30,33	1.76	5 (22%)
42	A2M	2	527	42	18,25,26	3.78	8 (44%)	18,36,39	3.73	5 (27%)
42	OMG	2	641	42	18,26,27	2.39	8 (44%)	19,38,41	1.74	5 (26%)
20	OMU	S1	661	20	19,22,23	2.94	8 (42%)	26,31,34	1.71	4 (15%)
42	PSU	2	1264	42	18,21,22	4.46	7 (38%)	22,30,33	1.84	5 (22%)
42	OMC	2	1248	42	19,22,23	2.79	8 (42%)	26,31,34	0.91	1 (3%)
42	PSU	2	506	42	18,21,22	1.39	2 (11%)	22,30,33	2.11	5 (22%)
42	OMU	2	667	42	19,22,23	2.86	8 (42%)	26,31,34	1.81	5 (19%)
41	OMG	1	856	41	18,26,27	2.38	8 (44%)	19,38,41	1.63	5 (26%)
42	A2M	2	1372	42	18,25,26	3.70	7 (38%)	18,36,39	3.74	4 (22%)
20	OMU	S1	8	20	19,22,23	2.97	8 (42%)	26,31,34	1.75	5 (19%)
41	1MA	1	677	84,41	16,25,26	1.10	2 (12%)	18,37,40	1.06	1 (5%)
41	PSU	1	870	84,41	18,21,22	4.24	8 (44%)	22,30,33	1.85	4 (18%)
42	OMC	2	583	42	19,22,23	2.70	7 (36%)	26,31,34	0.78	0
42	PSU	2	472	42	18,21,22	4.33	7 (38%)	22,30,33	1.79	5 (22%)
42	OMC	2	1317	42	19,22,23	2.75	8 (42%)	26,31,34	0.87	1 (3%)
20	PSU	S1	33	20	18,21,22	4.48	7 (38%)	22,30,33	1.81	5 (22%)
42	A2M	2	1185	42	18,25,26	3.62	7 (38%)	18,36,39	3.71	4 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	PSU	S1	1539	20	18,21,22	4.29	7 (38%)	22,30,33	1.75	4 (18%)
20	PSU	S1	2046	20	18,21,22	4.34	7 (38%)	22,30,33	1.93	5 (22%)
20	PSU	S1	609	20	18,21,22	4.43	7 (38%)	22,30,33	1.82	5 (22%)
41	PSU	1	1533	42,41	18,21,22	4.16	8 (44%)	22,30,33	2.06	5 (22%)
41	A2M	1	678	42,41	18,25,26	3.66	7 (38%)	18,36,39	3.53	4 (22%)
42	PSU	2	78	42	18,21,22	4.25	9 (50%)	22,30,33	1.77	5 (22%)
42	PSU	2	662	42,84	18,21,22	4.22	8 (44%)	22,30,33	1.80	5 (22%)
42	OMG	2	534	42	18,26,27	2.38	8 (44%)	19,38,41	1.54	4 (21%)
42	PSU	2	510	42	18,21,22	1.41	3 (16%)	22,30,33	1.93	5 (22%)
20	OMG	S1	1478	20	18,26,27	2.43	8 (44%)	19,38,41	1.69	5 (26%)
20	PSU	S1	1246	20	18,21,22	4.42	8 (44%)	22,30,33	1.71	4 (18%)
42	PSU	2	504	42	18,21,22	1.34	2 (11%)	22,30,33	2.14	4 (18%)
42	OMG	2	1360	42	18,26,27	2.40	8 (44%)	19,38,41	1.61	5 (26%)
42	A2M	2	570	42,41	18,25,26	3.67	7 (38%)	18,36,39	3.45	5 (27%)
20	A2M	S1	2021	20	18,25,26	3.65	7 (38%)	18,36,39	3.70	4 (22%)
41	OMG	1	1190	41	18,26,27	2.46	8 (44%)	19,38,41	1.73	5 (26%)
41	A2M	1	955	41	18,25,26	3.61	7 (38%)	18,36,39	3.49	4 (22%)
20	PSU	S1	2202	20	18,21,22	4.43	7 (38%)	22,30,33	1.74	5 (22%)
42	5MC	2	524	42,84	18,22,23	3.24	7 (38%)	26,32,35	1.10	2 (7%)
20	OMC	S1	18	20	19,22,23	2.89	8 (42%)	26,31,34	0.72	0
42	OMU	2	1077	42	19,22,23	2.90	8 (42%)	26,31,34	1.78	4 (15%)
41	OMU	1	847	41	19,22,23	2.78	7 (36%)	26,31,34	1.88	5 (19%)
20	OMU	S1	29	20	19,22,23	3.00	8 (42%)	26,31,34	1.75	5 (19%)
20	A2M	S1	668	20	18,25,26	3.63	7 (38%)	18,36,39	3.75	4 (22%)
41	OMG	1	1540	42,41	18,26,27	2.35	8 (44%)	19,38,41	1.69	5 (26%)
42	OMG	2	1229	42	18,26,27	2.39	8 (44%)	19,38,41	1.71	6 (31%)
41	PSU	1	422	41	18,21,22	4.31	8 (44%)	22,30,33	1.90	5 (22%)
41	OMU	1	1659	41	19,22,23	2.80	7 (36%)	26,31,34	1.82	5 (19%)
42	OMC	2	1397	42	19,22,23	2.72	8 (42%)	26,31,34	0.82	0

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
20	PSU	S1	104	20	-	0/7/25/26	0/2/2/2
20	5MC	S1	2061	20	-	0/7/25/26	0/2/2/2
20	PSU	S1	12	20	-	0/7/25/26	0/2/2/2
44	A2M	7	43	44	-	0/5/27/28	0/3/3/3
20	PSU	S1	607	20	-	6/7/25/26	0/2/2/2
20	OMC	S1	2140	20	-	2/9/27/28	0/2/2/2
20	OMU	S1	2048	20	-	0/9/27/28	0/2/2/2
42	PSU	2	1144	42	-	0/7/25/26	0/2/2/2
42	OMG	2	1078	42	-	0/5/27/28	0/3/3/3
41	OMG	1	959	41	-	2/5/27/28	0/3/3/3
41	OMU	1	845	41	-	0/9/27/28	0/2/2/2
42	OMG	2	1231	42	-	0/5/27/28	0/3/3/3
20	OMC	S1	38	20	-	0/9/27/28	0/2/2/2
20	OMG	S1	1623	20	-	0/5/27/28	0/3/3/3
41	PSU	1	1402	41	-	2/7/25/26	0/2/2/2
41	PSU	1	940	41	-	0/7/25/26	0/2/2/2
20	PSU	S1	1566	20	-	0/7/25/26	0/2/2/2
42	A2M	2	665	42	-	3/5/27/28	0/3/3/3
41	PSU	1	1181	41	-	3/7/25/26	0/2/2/2
42	PSU	2	593	42	-	0/7/25/26	0/2/2/2
42	OMU	2	1359	42	-	1/9/27/28	0/2/2/2
20	OMG	S1	600	20	-	2/5/27/28	0/3/3/3
42	OMG	2	655	42	-	1/5/27/28	0/3/3/3
42	OMG	2	71	42	-	0/5/27/28	0/3/3/3
42	OMU	2	1419	42	-	1/9/27/28	0/2/2/2
20	PSU	S1	455	20	-	0/7/25/26	0/2/2/2
20	PSU	S1	1192	20	-	2/7/25/26	0/2/2/2
20	A2M	S1	897	20	-	2/5/27/28	0/3/3/3
41	OMU	1	1371	41	-	4/9/27/28	0/2/2/2
41	OMC	1	1552	41	-	0/9/27/28	0/2/2/2
42	A2M	2	1384	42	-	1/5/27/28	0/3/3/3
81	OMU	3	13	81	-	0/9/27/28	0/2/2/2
42	PSU	2	1060	42	-	1/7/25/26	0/2/2/2
42	OMC	2	1159	42	-	0/9/27/28	0/2/2/2
20	MA6	S1	2184	20	-	0/7/29/30	0/3/3/3
41	PSU	1	1011	42,41	-	1/7/25/26	0/2/2/2
42	A2M	2	382	42	-	1/5/27/28	0/3/3/3
42	PSU	2	1354	42	-	0/7/25/26	0/2/2/2
20	OMC	S1	1866	20	-	0/9/27/28	0/2/2/2
41	PSU	1	239	41	-	2/7/25/26	0/2/2/2
41	A2M	1	1539	42,87,84,41	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
42	5MC	2	1308	42	-	6/7/25/26	0/2/2/2
20	OMU	S1	1777	20	-	0/9/27/28	0/2/2/2
20	G7M	S1	1995	20	-	0/3/25/26	0/3/3/3
41	OMG	1	1524	41	-	1/5/27/28	0/3/3/3
44	PSU	7	69	44	-	2/7/25/26	0/2/2/2
42	OMG	2	1253	42	-	0/5/27/28	0/3/3/3
42	PSU	2	626	42	-	0/7/25/26	0/2/2/2
20	C4J	S1	1543	20	-	2/16/34/35	0/2/2/2
42	PSU	2	1265	42	-	2/7/25/26	0/2/2/2
44	OMG	7	75	44	-	0/5/27/28	0/3/3/3
41	OMU	1	1107	41	-	0/9/27/28	0/2/2/2
20	OMG	S1	1550	20	-	2/5/27/28	0/3/3/3
20	A2M	S1	98	20	-	1/5/27/28	0/3/3/3
20	MA6	S1	2185	20	-	1/7/29/30	0/3/3/3
42	PSU	2	1318	42	-	0/7/25/26	0/2/2/2
41	A2M	1	437	41	-	1/5/27/28	0/3/3/3
42	OMC	2	359	42	-	0/9/27/28	0/2/2/2
42	PSU	2	1361	42	-	2/7/25/26	0/2/2/2
42	A2M	2	591	42	-	0/5/27/28	0/3/3/3
41	OMC	1	695	41	-	0/9/27/28	0/2/2/2
20	OMU	S1	1979	20	-	3/9/27/28	0/2/2/2
42	PSU	2	437	42	-	0/7/25/26	0/2/2/2
42	A2M	2	628	42	-	0/5/27/28	0/3/3/3
42	A2M	2	95	42	-	1/5/27/28	0/3/3/3
20	A2M	S1	512	20	-	3/5/27/28	0/3/3/3
20	OMG	S1	1647	20	-	0/5/27/28	0/3/3/3
42	A2M	2	572	42	-	0/5/27/28	0/3/3/3
41	A2M	1	697	41	-	1/5/27/28	0/3/3/3
20	OMU	S1	1833	20	-	4/9/27/28	0/2/2/2
20	5MC	S1	1544	20	-	0/7/25/26	0/2/2/2
42	PSU	2	1382	42	-	0/7/25/26	0/2/2/2
41	A2M	1	858	41	-	0/5/27/28	0/3/3/3
20	OMG	S1	1865	20	-	0/5/27/28	0/3/3/3
41	PSU	1	1017	41	-	0/7/25/26	0/2/2/2
20	PSU	S1	1533	20	-	2/7/25/26	0/2/2/2
20	OMG	S1	1829	20	-	2/5/27/28	0/3/3/3
41	PSU	1	672	84,41	-	0/7/25/26	0/2/2/2
20	PSU	S1	1657	20	-	1/7/25/26	0/2/2/2
42	OMU	2	560	42	-	1/9/27/28	0/2/2/2
20	A2M	S1	28	20	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	PSU	1	1528	41	-	0/7/25/26	0/2/2/2
42	PSU	2	1194	42	-	0/7/25/26	0/2/2/2
42	PSU	2	1403	42	-	1/7/25/26	0/2/2/2
20	A2M	S1	479	20	-	1/5/27/28	0/3/3/3
41	OMG	1	1626	41	-	0/5/27/28	0/3/3/3
42	A2M	2	604	42,41	-	1/5/27/28	0/3/3/3
44	A2M	7	162	41,44	-	1/5/27/28	0/3/3/3
42	OMC	2	443	42	-	4/9/27/28	0/2/2/2
42	OMG	2	1046	42	-	2/5/27/28	0/3/3/3
20	OMU	S1	1621	20	-	0/9/27/28	0/2/2/2
20	OMG	S1	2151	20	-	0/5/27/28	0/3/3/3
42	PSU	2	597	42	-	0/7/25/26	0/2/2/2
41	PSU	1	1664	41	-	0/7/25/26	0/2/2/2
44	PSU	7	74	44	-	0/7/25/26	0/2/2/2
41	A2M	1	681	41	-	3/5/27/28	0/3/3/3
42	OMU	2	73	42	-	0/9/27/28	0/2/2/2
41	PSU	1	1171	41	-	2/7/25/26	0/2/2/2
42	PSU	2	500	42	-	3/7/25/26	0/2/2/2
42	PSU	2	1413	42	-	0/7/25/26	0/2/2/2
42	PSU	2	1058	42	-	0/7/25/26	0/2/2/2
20	PSU	S1	1841	20	-	0/7/25/26	0/2/2/2
41	OMC	1	1527	41	-	1/9/27/28	0/2/2/2
43	OMG	4	74	43	-	0/5/27/28	0/3/3/3
42	PSU	2	1303	42	-	2/7/25/26	0/2/2/2
20	PSU	S1	1156	20	-	0/7/25/26	0/2/2/2
42	A2M	2	527	42	-	2/5/27/28	0/3/3/3
42	OMG	2	641	42	-	0/5/27/28	0/3/3/3
20	OMU	S1	661	20	-	0/9/27/28	0/2/2/2
42	PSU	2	1264	42	-	0/7/25/26	0/2/2/2
42	OMC	2	1248	42	-	1/9/27/28	0/2/2/2
42	PSU	2	506	42	-	1/7/25/26	0/2/2/2
42	OMU	2	667	42	-	0/9/27/28	0/2/2/2
41	OMG	1	856	41	-	0/5/27/28	0/3/3/3
42	A2M	2	1372	42	-	0/5/27/28	0/3/3/3
20	OMU	S1	8	20	-	6/9/27/28	0/2/2/2
41	1MA	1	677	84,41	-	0/3/25/26	0/3/3/3
41	PSU	1	870	84,41	-	0/7/25/26	0/2/2/2
42	OMC	2	583	42	-	0/9/27/28	0/2/2/2
42	PSU	2	472	42	-	0/7/25/26	0/2/2/2
42	OMC	2	1317	42	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	PSU	S1	33	20	-	2/7/25/26	0/2/2/2
42	A2M	2	1185	42	-	3/5/27/28	0/3/3/3
20	PSU	S1	1539	20	-	1/7/25/26	0/2/2/2
20	PSU	S1	2046	20	-	0/7/25/26	0/2/2/2
20	PSU	S1	609	20	-	0/7/25/26	0/2/2/2
41	PSU	1	1533	42,41	-	0/7/25/26	0/2/2/2
41	A2M	1	678	42,41	-	0/5/27/28	0/3/3/3
42	PSU	2	78	42	-	2/7/25/26	0/2/2/2
42	PSU	2	662	42,84	-	0/7/25/26	0/2/2/2
42	OMG	2	534	42	-	2/5/27/28	0/3/3/3
42	PSU	2	510	42	-	0/7/25/26	0/2/2/2
20	OMG	S1	1478	20	-	1/5/27/28	0/3/3/3
20	PSU	S1	1246	20	-	2/7/25/26	0/2/2/2
42	PSU	2	504	42	-	3/7/25/26	0/2/2/2
42	OMG	2	1360	42	-	0/5/27/28	0/3/3/3
42	A2M	2	570	42,41	-	1/5/27/28	0/3/3/3
20	A2M	S1	2021	20	-	3/5/27/28	0/3/3/3
41	OMG	1	1190	41	-	0/5/27/28	0/3/3/3
41	A2M	1	955	41	-	0/5/27/28	0/3/3/3
20	PSU	S1	2202	20	-	1/7/25/26	0/2/2/2
42	5MC	2	524	42,84	-	0/7/25/26	0/2/2/2
20	OMC	S1	18	20	-	0/9/27/28	0/2/2/2
42	OMU	2	1077	42	-	0/9/27/28	0/2/2/2
41	OMU	1	847	41	-	0/9/27/28	0/2/2/2
20	OMU	S1	29	20	-	0/9/27/28	0/2/2/2
20	A2M	S1	668	20	-	3/5/27/28	0/3/3/3
41	OMG	1	1540	42,41	-	2/5/27/28	0/3/3/3
42	OMG	2	1229	42	-	0/5/27/28	0/3/3/3
41	PSU	1	422	41	-	0/7/25/26	0/2/2/2
41	OMU	1	1659	41	-	0/9/27/28	0/2/2/2
42	OMC	2	1397	42	-	0/9/27/28	0/2/2/2

All (1107) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	S1	607	PSU	C6-C5	12.03	1.49	1.35
20	S1	33	PSU	C6-C5	11.67	1.48	1.35
20	S1	1156	PSU	C6-C5	11.66	1.48	1.35
20	S1	1246	PSU	C6-C5	11.62	1.48	1.35
41	1	1011	PSU	C6-C5	11.62	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	2	1303	PSU	C6-C5	11.61	1.48	1.35
42	2	1264	PSU	C6-C5	11.59	1.48	1.35
42	2	1265	PSU	C6-C5	11.56	1.48	1.35
20	S1	455	PSU	C6-C5	11.53	1.48	1.35
20	S1	2202	PSU	C6-C5	11.49	1.48	1.35
42	2	1058	PSU	C6-C5	11.40	1.48	1.35
20	S1	1192	PSU	C6-C5	11.40	1.48	1.35
20	S1	609	PSU	C6-C5	11.37	1.48	1.35
20	S1	104	PSU	C6-C5	11.33	1.48	1.35
42	2	1361	PSU	C6-C5	11.31	1.48	1.35
44	7	74	PSU	C6-C5	11.30	1.48	1.35
42	2	1060	PSU	C6-C5	11.30	1.48	1.35
20	S1	1841	PSU	C6-C5	11.27	1.48	1.35
42	2	472	PSU	C6-C5	11.22	1.48	1.35
20	S1	2046	PSU	C6-C5	11.22	1.48	1.35
42	2	1144	PSU	C6-C5	11.21	1.48	1.35
44	7	69	PSU	C6-C5	11.20	1.48	1.35
41	1	1528	PSU	C6-C5	11.19	1.48	1.35
42	2	626	PSU	C6-C5	11.19	1.48	1.35
41	1	239	PSU	C6-C5	11.19	1.48	1.35
20	S1	1539	PSU	C6-C5	11.16	1.48	1.35
42	2	78	PSU	C6-C5	11.15	1.48	1.35
41	1	870	PSU	C6-C5	11.15	1.48	1.35
42	2	1318	PSU	C6-C5	11.14	1.48	1.35
41	1	422	PSU	C6-C5	11.12	1.48	1.35
20	S1	12	PSU	C6-C5	11.10	1.48	1.35
42	2	1354	PSU	C6-C5	11.09	1.48	1.35
41	1	1181	PSU	C6-C5	11.05	1.48	1.35
20	S1	1533	PSU	C6-C5	11.03	1.48	1.35
42	2	662	PSU	C6-C5	11.02	1.48	1.35
42	2	1413	PSU	C6-C5	11.01	1.48	1.35
41	1	672	PSU	C6-C5	10.95	1.48	1.35
41	1	1017	PSU	C6-C5	10.95	1.48	1.35
41	1	1664	PSU	C6-C5	10.94	1.48	1.35
42	2	1403	PSU	C6-C5	10.91	1.48	1.35
41	1	940	PSU	C6-C5	10.91	1.48	1.35
42	2	1194	PSU	C6-C5	10.89	1.48	1.35
20	S1	1657	PSU	C6-C5	10.87	1.48	1.35
42	2	593	PSU	C6-C5	10.86	1.48	1.35
42	2	1382	PSU	C6-C5	10.78	1.47	1.35
41	1	1402	PSU	C6-C5	10.78	1.47	1.35
42	2	597	PSU	C6-C5	10.75	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	2	437	PSU	C6-C5	10.66	1.47	1.35
41	1	1171	PSU	C6-C5	10.61	1.47	1.35
41	1	1533	PSU	C6-C5	10.46	1.47	1.35
20	S1	1995	G7M	C8-N9	10.15	1.51	1.33
20	S1	1995	G7M	C8-N7	10.04	1.51	1.33
20	S1	1543	C4J	C6-C5	9.81	1.48	1.34
20	S1	1156	PSU	C2-N1	9.61	1.49	1.36
42	2	1264	PSU	C2-N1	9.60	1.49	1.36
42	2	1265	PSU	C2-N1	9.60	1.49	1.36
20	S1	33	PSU	C2-N1	9.58	1.49	1.36
20	S1	455	PSU	C2-N1	9.56	1.49	1.36
20	S1	609	PSU	C2-N1	9.53	1.49	1.36
20	S1	104	PSU	C2-N1	9.52	1.49	1.36
20	S1	607	PSU	C2-N1	9.51	1.49	1.36
42	2	1303	PSU	C2-N1	9.50	1.49	1.36
42	2	1308	5MC	C6-C5	9.42	1.50	1.34
20	S1	12	PSU	C2-N1	9.41	1.49	1.36
20	S1	2202	PSU	C2-N1	9.39	1.49	1.36
42	2	1361	PSU	C2-N1	9.32	1.49	1.36
20	S1	1841	PSU	C2-N1	9.32	1.49	1.36
42	2	472	PSU	C2-N1	9.32	1.49	1.36
20	S1	1192	PSU	C2-N1	9.31	1.49	1.36
42	2	1144	PSU	C2-N1	9.31	1.49	1.36
41	1	1011	PSU	C2-N1	9.29	1.49	1.36
41	1	239	PSU	C2-N1	9.26	1.49	1.36
20	S1	2046	PSU	C2-N1	9.19	1.49	1.36
20	S1	1246	PSU	C2-N1	9.18	1.49	1.36
20	S1	897	A2M	C3'-C4'	-9.16	1.29	1.53
42	2	1060	PSU	C2-N1	9.15	1.49	1.36
42	2	1058	PSU	C2-N1	9.14	1.49	1.36
44	7	69	PSU	C2-N1	9.13	1.49	1.36
20	S1	1533	PSU	C2-N1	9.09	1.49	1.36
41	1	422	PSU	C2-N1	9.09	1.49	1.36
41	1	1181	PSU	C2-N1	9.08	1.49	1.36
42	2	1354	PSU	C2-N1	9.07	1.49	1.36
20	S1	1657	PSU	C2-N1	9.05	1.49	1.36
41	1	940	PSU	C2-N1	9.04	1.49	1.36
44	7	74	PSU	C2-N1	9.01	1.48	1.36
20	S1	1544	5MC	C6-C5	8.94	1.49	1.34
20	S1	1539	PSU	C2-N1	8.93	1.48	1.36
42	2	665	A2M	C3'-C4'	-8.92	1.30	1.53
42	2	1372	A2M	C3'-C4'	-8.91	1.30	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	1	1533	PSU	C2-N1	8.91	1.48	1.36
44	7	162	A2M	C3'-C4'	-8.89	1.30	1.53
42	2	1194	PSU	C2-N1	8.89	1.48	1.36
42	2	597	PSU	C2-N1	8.87	1.48	1.36
41	1	1664	PSU	C2-N1	8.87	1.48	1.36
41	1	870	PSU	C2-N1	8.86	1.48	1.36
42	2	628	A2M	C3'-C4'	-8.85	1.30	1.53
42	2	593	PSU	C2-N1	8.82	1.48	1.36
42	2	1403	PSU	C2-N1	8.81	1.48	1.36
42	2	662	PSU	C2-N1	8.81	1.48	1.36
42	2	1382	PSU	C2-N1	8.80	1.48	1.36
42	2	437	PSU	C2-N1	8.80	1.48	1.36
41	1	678	A2M	C3'-C4'	-8.78	1.30	1.53
42	2	95	A2M	C3'-C4'	-8.77	1.30	1.53
42	2	1384	A2M	C3'-C4'	-8.76	1.30	1.53
41	1	672	PSU	C2-N1	8.76	1.48	1.36
41	1	1528	PSU	C2-N1	8.75	1.48	1.36
20	S1	2021	A2M	C3'-C4'	-8.74	1.30	1.53
42	2	570	A2M	C3'-C4'	-8.73	1.30	1.53
44	7	43	A2M	C3'-C4'	-8.71	1.30	1.53
42	2	591	A2M	C3'-C4'	-8.70	1.30	1.53
20	S1	28	A2M	C3'-C4'	-8.69	1.30	1.53
20	S1	668	A2M	C3'-C4'	-8.68	1.30	1.53
41	1	858	A2M	C3'-C4'	-8.68	1.30	1.53
42	2	78	PSU	C2-N1	8.68	1.48	1.36
42	2	626	PSU	C2-N1	8.66	1.48	1.36
42	2	1318	PSU	C2-N1	8.63	1.48	1.36
41	1	955	A2M	C3'-C4'	-8.63	1.30	1.53
42	2	524	5MC	C6-C5	8.63	1.48	1.34
41	1	1171	PSU	C2-N1	8.62	1.48	1.36
41	1	1017	PSU	C2-N1	8.62	1.48	1.36
42	2	604	A2M	C3'-C4'	-8.59	1.31	1.53
42	2	382	A2M	C3'-C4'	-8.55	1.31	1.53
20	S1	98	A2M	C3'-C4'	-8.55	1.31	1.53
20	S1	479	A2M	C3'-C4'	-8.53	1.31	1.53
42	2	1413	PSU	C2-N1	8.53	1.48	1.36
41	1	437	A2M	C3'-C4'	-8.53	1.31	1.53
41	1	697	A2M	C3'-C4'	-8.52	1.31	1.53
42	2	1185	A2M	C3'-C4'	-8.52	1.31	1.53
41	1	681	A2M	C3'-C4'	-8.52	1.31	1.53
42	2	527	A2M	O4'-C1'	-8.49	1.29	1.41
41	1	1539	A2M	C3'-C4'	-8.44	1.31	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	2	527	A2M	C3'-C4'	-8.44	1.31	1.53
42	2	572	A2M	C3'-C4'	-8.41	1.31	1.53
41	1	1402	PSU	C2-N1	8.31	1.48	1.36
42	2	572	A2M	O4'-C4'	7.90	1.62	1.45
42	2	591	A2M	O4'-C4'	7.84	1.62	1.45
41	1	858	A2M	O4'-C1'	-7.83	1.30	1.41
41	1	697	A2M	O4'-C1'	-7.83	1.30	1.41
42	2	382	A2M	O4'-C4'	7.78	1.62	1.45
20	S1	98	A2M	O4'-C4'	7.75	1.62	1.45
44	7	43	A2M	O4'-C1'	-7.75	1.30	1.41
42	2	527	A2M	O4'-C4'	7.73	1.62	1.45
20	S1	897	A2M	O4'-C4'	7.72	1.62	1.45
41	1	681	A2M	O4'-C4'	7.71	1.62	1.45
44	7	43	A2M	O4'-C4'	7.71	1.62	1.45
41	1	678	A2M	O4'-C4'	7.71	1.62	1.45
20	S1	479	A2M	O4'-C4'	7.67	1.62	1.45
42	2	570	A2M	O4'-C4'	7.67	1.62	1.45
42	2	628	A2M	O4'-C4'	7.67	1.62	1.45
41	1	1539	A2M	O4'-C1'	-7.65	1.30	1.41
42	2	604	A2M	O4'-C4'	7.65	1.62	1.45
42	2	1372	A2M	O4'-C1'	-7.63	1.30	1.41
41	1	955	A2M	O4'-C4'	7.63	1.62	1.45
41	1	697	A2M	O4'-C4'	7.63	1.62	1.45
42	2	1185	A2M	O4'-C1'	-7.62	1.30	1.41
20	S1	28	A2M	O4'-C4'	7.62	1.62	1.45
42	2	570	A2M	O4'-C1'	-7.61	1.30	1.41
42	2	572	A2M	O4'-C1'	-7.59	1.30	1.41
41	1	437	A2M	O4'-C4'	7.59	1.62	1.45
20	S1	2021	A2M	O4'-C4'	7.58	1.61	1.45
41	1	437	A2M	O4'-C1'	-7.58	1.30	1.41
20	S1	668	A2M	O4'-C1'	-7.54	1.30	1.41
20	S1	2021	A2M	O4'-C1'	-7.54	1.30	1.41
42	2	1384	A2M	O4'-C4'	7.51	1.61	1.45
41	1	1539	A2M	O4'-C4'	7.50	1.61	1.45
42	2	665	A2M	O4'-C4'	7.50	1.61	1.45
20	S1	479	A2M	O4'-C1'	-7.50	1.30	1.41
20	S1	607	PSU	C2-N3	7.50	1.50	1.37
42	2	95	A2M	O4'-C4'	7.47	1.61	1.45
44	7	162	A2M	O4'-C1'	-7.47	1.30	1.41
42	2	1372	A2M	O4'-C4'	7.46	1.61	1.45
42	2	1384	A2M	O4'-C1'	-7.44	1.30	1.41
41	1	681	A2M	O4'-C1'	-7.44	1.30	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	S1	1246	PSU	C2-N3	7.43	1.50	1.37
44	7	162	A2M	O4'-C4'	7.42	1.61	1.45
20	S1	2046	PSU	C2-N3	7.42	1.50	1.37
20	S1	668	A2M	O4'-C4'	7.41	1.61	1.45
20	S1	455	PSU	C2-N3	7.41	1.50	1.37
20	S1	33	PSU	C2-N3	7.41	1.50	1.37
20	S1	609	PSU	C2-N3	7.40	1.50	1.37
20	S1	2202	PSU	C2-N3	7.40	1.50	1.37
42	2	604	A2M	O4'-C1'	-7.38	1.30	1.41
42	2	1185	A2M	O4'-C4'	7.37	1.61	1.45
20	S1	1156	PSU	C2-N3	7.36	1.50	1.37
42	2	1265	PSU	C2-N3	7.36	1.50	1.37
42	2	1303	PSU	C2-N3	7.35	1.50	1.37
41	1	678	A2M	O4'-C1'	-7.34	1.30	1.41
20	S1	104	PSU	C2-N3	7.33	1.50	1.37
42	2	1361	PSU	C2-N3	7.32	1.50	1.37
42	2	628	A2M	O4'-C1'	-7.30	1.30	1.41
42	2	382	A2M	O4'-C1'	-7.30	1.30	1.41
20	S1	1841	PSU	C2-N3	7.29	1.50	1.37
42	2	95	A2M	O4'-C1'	-7.27	1.30	1.41
20	S1	1657	PSU	C2-N3	7.27	1.50	1.37
42	2	1264	PSU	C2-N3	7.24	1.49	1.37
41	1	1011	PSU	C2-N3	7.23	1.49	1.37
41	1	955	A2M	O4'-C1'	-7.19	1.31	1.41
20	S1	1192	PSU	C2-N3	7.19	1.49	1.37
42	2	591	A2M	O4'-C1'	-7.19	1.31	1.41
41	1	1181	PSU	C2-N3	7.17	1.49	1.37
41	1	858	A2M	O4'-C4'	7.15	1.61	1.45
20	S1	98	A2M	O4'-C1'	-7.15	1.31	1.41
20	S1	1539	PSU	C2-N3	7.14	1.49	1.37
42	2	665	A2M	O4'-C1'	-7.14	1.31	1.41
20	S1	1833	OMU	C2-N1	7.14	1.49	1.38
41	1	239	PSU	C2-N3	7.14	1.49	1.37
41	1	422	PSU	C2-N3	7.13	1.49	1.37
20	S1	28	A2M	O4'-C1'	-7.12	1.31	1.41
41	1	1371	OMU	C2-N1	7.10	1.49	1.38
20	S1	1533	PSU	C2-N3	7.05	1.49	1.37
42	2	472	PSU	C2-N3	7.04	1.49	1.37
44	7	74	PSU	C2-N3	7.03	1.49	1.37
41	1	1533	PSU	C2-N3	7.01	1.49	1.37
20	S1	29	OMU	C2-N1	6.99	1.49	1.38
41	1	1402	PSU	C2-N3	6.98	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	S1	897	A2M	O4'-C1'	-6.96	1.31	1.41
20	S1	12	PSU	C2-N3	6.95	1.49	1.37
41	1	1528	PSU	C2-N3	6.95	1.49	1.37
42	2	1382	PSU	C2-N3	6.94	1.49	1.37
42	2	1354	PSU	C2-N3	6.94	1.49	1.37
42	2	1403	PSU	C2-N3	6.93	1.49	1.37
42	2	1060	PSU	C2-N3	6.91	1.49	1.37
42	2	1194	PSU	C2-N3	6.88	1.49	1.37
41	1	940	PSU	C2-N3	6.85	1.49	1.37
42	2	1318	PSU	C2-N3	6.83	1.49	1.37
41	1	1171	PSU	C2-N3	6.82	1.49	1.37
42	2	1413	PSU	C2-N3	6.82	1.49	1.37
20	S1	8	OMU	C2-N1	6.82	1.49	1.38
41	1	672	PSU	C2-N3	6.81	1.49	1.37
42	2	560	OMU	C2-N1	6.78	1.49	1.38
20	S1	661	OMU	C2-N1	6.78	1.49	1.38
20	S1	1777	OMU	C2-N1	6.77	1.49	1.38
42	2	437	PSU	C2-N3	6.75	1.49	1.37
42	2	1058	PSU	C2-N3	6.73	1.49	1.37
20	S1	1833	OMU	C2-N3	6.72	1.49	1.38
42	2	1077	OMU	C2-N1	6.66	1.49	1.38
44	7	69	PSU	C2-N3	6.65	1.48	1.37
20	S1	2048	OMU	C2-N1	6.65	1.49	1.38
20	S1	29	OMU	C2-N3	6.64	1.49	1.38
42	2	1144	PSU	C2-N3	6.63	1.48	1.37
41	1	870	PSU	C2-N3	6.61	1.48	1.37
20	S1	1979	OMU	C2-N1	6.59	1.49	1.38
41	1	1017	PSU	C2-N3	6.59	1.48	1.37
42	2	78	PSU	C2-N3	6.58	1.48	1.37
42	2	662	PSU	C2-N3	6.57	1.48	1.37
20	S1	1621	OMU	C2-N3	6.56	1.49	1.38
20	S1	8	OMU	C2-N3	6.54	1.49	1.38
41	1	1664	PSU	C2-N3	6.53	1.48	1.37
20	S1	1777	OMU	C2-N3	6.52	1.49	1.38
81	3	13	OMU	C2-N1	6.49	1.48	1.38
42	2	1419	OMU	C2-N1	6.49	1.48	1.38
20	S1	1621	OMU	C2-N1	6.49	1.48	1.38
20	S1	661	OMU	C2-N3	6.48	1.49	1.38
20	S1	2048	OMU	C2-N3	6.45	1.49	1.38
42	2	593	PSU	C2-N3	6.44	1.48	1.37
42	2	597	PSU	C2-N3	6.43	1.48	1.37
41	1	845	OMU	C2-N1	6.35	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	2	626	PSU	C2-N3	6.33	1.48	1.37
42	2	667	OMU	C2-N1	6.30	1.48	1.38
42	2	1077	OMU	C2-N3	6.30	1.49	1.38
42	2	1359	OMU	C2-N1	6.28	1.48	1.38
41	1	1107	OMU	C2-N3	6.28	1.49	1.38
20	S1	1979	OMU	C2-N3	6.27	1.49	1.38
42	2	560	OMU	C2-N3	6.26	1.49	1.38
42	2	667	OMU	C2-N3	6.24	1.49	1.38
41	1	1659	OMU	C2-N1	6.24	1.48	1.38
42	2	1359	OMU	C2-N3	6.22	1.49	1.38
20	S1	2140	OMC	C2-N3	6.21	1.48	1.36
41	1	1371	OMU	C2-N3	6.17	1.49	1.38
42	2	73	OMU	C2-N1	6.17	1.48	1.38
42	2	1419	OMU	C2-N3	6.17	1.49	1.38
81	3	13	OMU	C2-N3	6.16	1.48	1.38
42	2	359	OMC	C2-N3	6.13	1.48	1.36
41	1	847	OMU	C2-N1	6.12	1.48	1.38
42	2	73	OMU	C2-N3	6.12	1.48	1.38
20	S1	1995	G7M	C2-N3	6.11	1.48	1.33
20	S1	38	OMC	C2-N3	6.08	1.48	1.36
41	1	845	OMU	C2-N3	6.08	1.48	1.38
20	S1	18	OMC	C2-N3	6.05	1.48	1.36
41	1	1107	OMU	C2-N1	6.04	1.48	1.38
20	S1	1544	5MC	C4-N3	6.02	1.44	1.34
41	1	847	OMU	C2-N3	5.99	1.48	1.38
42	2	1248	OMC	C6-C5	5.94	1.48	1.35
41	1	1659	OMU	C2-N3	5.88	1.48	1.38
41	1	1552	OMC	C6-C5	5.86	1.48	1.35
42	2	1159	OMC	C2-N3	5.83	1.48	1.36
20	S1	1544	5MC	C2-N3	5.81	1.48	1.36
20	S1	1866	OMC	C2-N3	5.81	1.48	1.36
20	S1	38	OMC	C6-C5	5.81	1.48	1.35
20	S1	1543	C4J	C2-N3	5.80	1.49	1.38
20	S1	18	OMC	C6-C5	5.78	1.48	1.35
20	S1	2140	OMC	C6-C5	5.78	1.48	1.35
41	1	1552	OMC	C2-N3	5.77	1.48	1.36
20	S1	1866	OMC	C6-C5	5.74	1.48	1.35
42	2	359	OMC	C6-C5	5.73	1.48	1.35
42	2	1248	OMC	C2-N3	5.69	1.47	1.36
42	2	1317	OMC	C2-N3	5.69	1.47	1.36
42	2	1159	OMC	C6-C5	5.68	1.48	1.35
42	2	1317	OMC	C6-C5	5.65	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	S1	1833	OMU	C6-C5	5.60	1.48	1.35
20	S1	8	OMU	C6-C5	5.59	1.48	1.35
20	S1	29	OMU	C6-C5	5.58	1.48	1.35
20	S1	1621	OMU	C6-C5	5.56	1.48	1.35
42	2	1397	OMC	C2-N3	5.55	1.47	1.36
42	2	1077	OMU	C6-C5	5.54	1.47	1.35
42	2	583	OMC	C6-C5	5.54	1.47	1.35
41	1	695	OMC	C6-C5	5.53	1.47	1.35
42	2	1359	OMU	C6-C5	5.53	1.47	1.35
20	S1	1777	OMU	C6-C5	5.52	1.47	1.35
41	1	695	OMC	C2-N3	5.51	1.47	1.36
42	2	1308	5MC	C2-N3	5.51	1.47	1.36
20	S1	661	OMU	C6-C5	5.48	1.47	1.35
42	2	524	5MC	C2-N3	5.47	1.47	1.36
41	1	1527	OMC	C6-C5	5.47	1.47	1.35
42	2	1397	OMC	C6-C5	5.47	1.47	1.35
81	3	13	OMU	C6-C5	5.46	1.47	1.35
42	2	524	5MC	C4-N3	5.43	1.43	1.34
42	2	1308	5MC	C4-N3	5.41	1.43	1.34
42	2	1419	OMU	C6-C5	5.39	1.47	1.35
41	1	847	OMU	C6-C5	5.39	1.47	1.35
41	1	1527	OMC	C2-N3	5.36	1.47	1.36
20	S1	607	PSU	C6-N1	5.34	1.45	1.36
20	S1	1156	PSU	C6-N1	5.34	1.45	1.36
42	2	667	OMU	C6-C5	5.34	1.47	1.35
20	S1	2048	OMU	C6-C5	5.34	1.47	1.35
42	2	560	OMU	C6-C5	5.33	1.47	1.35
42	2	73	OMU	C6-C5	5.33	1.47	1.35
41	1	1107	OMU	C6-C5	5.31	1.47	1.35
20	S1	609	PSU	C6-N1	5.30	1.45	1.36
20	S1	1979	OMU	C6-C5	5.30	1.47	1.35
42	2	1264	PSU	C6-N1	5.30	1.45	1.36
42	2	583	OMC	C2-N3	5.30	1.47	1.36
42	2	1265	PSU	C6-N1	5.29	1.45	1.36
20	S1	1657	PSU	C6-N1	5.28	1.45	1.36
20	S1	104	PSU	C6-N1	5.25	1.44	1.36
20	S1	455	PSU	C6-N1	5.23	1.44	1.36
41	1	1371	OMU	C6-C5	5.23	1.47	1.35
20	S1	2151	OMG	C2-N3	5.23	1.45	1.33
20	S1	33	PSU	C6-N1	5.22	1.44	1.36
41	1	1659	OMU	C6-C5	5.19	1.47	1.35
20	S1	2202	PSU	C6-N1	5.18	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	1	959	OMG	C2-N3	5.17	1.45	1.33
20	S1	2140	OMC	C4-N3	5.16	1.44	1.34
42	2	1303	PSU	C6-N1	5.14	1.44	1.36
41	1	239	PSU	C6-N1	5.14	1.44	1.36
20	S1	1246	PSU	C6-N1	5.14	1.44	1.36
44	7	69	PSU	C6-N1	5.13	1.44	1.36
20	S1	600	OMG	C2-N3	5.13	1.45	1.33
41	1	845	OMU	C6-C5	5.13	1.47	1.35
41	1	422	PSU	C6-N1	5.08	1.44	1.36
41	1	1181	PSU	C6-N1	5.07	1.44	1.36
42	2	1058	PSU	C6-N1	5.05	1.44	1.36
20	S1	1550	OMG	C2-N3	5.04	1.45	1.33
42	2	1060	PSU	C6-N1	5.03	1.44	1.36
20	S1	1533	PSU	C6-N1	5.00	1.44	1.36
42	2	472	PSU	C6-N1	5.00	1.44	1.36
20	S1	38	OMC	C4-N3	4.99	1.44	1.34
20	S1	12	PSU	C6-N1	4.99	1.44	1.36
42	2	1361	PSU	C6-N1	4.98	1.44	1.36
20	S1	1192	PSU	C6-N1	4.98	1.44	1.36
20	S1	1539	PSU	C6-N1	4.98	1.44	1.36
20	S1	2046	PSU	C6-N1	4.98	1.44	1.36
20	S1	1841	PSU	C6-N1	4.96	1.44	1.36
42	2	1046	OMG	C2-N3	4.96	1.45	1.33
20	S1	1623	OMG	C2-N3	4.94	1.45	1.33
20	S1	2151	OMG	C4-N3	4.92	1.49	1.37
42	2	1354	PSU	C6-N1	4.88	1.44	1.36
42	2	1308	5MC	C6-N1	4.87	1.46	1.38
20	S1	1995	G7M	C6-N1	4.86	1.45	1.37
42	2	1382	PSU	C6-N1	4.85	1.44	1.36
41	1	1011	PSU	C6-N1	4.85	1.44	1.36
41	1	1524	OMG	C2-N3	4.84	1.45	1.33
44	7	74	PSU	C6-N1	4.84	1.44	1.36
20	S1	600	OMG	C4-N3	4.82	1.49	1.37
20	S1	18	OMC	C4-N3	4.80	1.44	1.34
41	1	672	PSU	C6-N1	4.80	1.44	1.36
20	S1	1478	OMG	C2-N3	4.80	1.44	1.33
41	1	1190	OMG	C2-N3	4.80	1.44	1.33
20	S1	1829	OMG	C2-N3	4.79	1.44	1.33
42	2	662	PSU	C6-N1	4.78	1.44	1.36
41	1	1528	PSU	C6-N1	4.78	1.44	1.36
41	1	940	PSU	C6-N1	4.78	1.44	1.36
42	2	437	PSU	C6-N1	4.77	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	2	78	PSU	C6-N1	4.76	1.44	1.36
20	S1	1866	OMC	C4-N3	4.76	1.44	1.34
42	2	1403	PSU	C6-N1	4.76	1.44	1.36
42	2	359	OMC	C4-N3	4.76	1.44	1.34
41	1	1552	OMC	C4-N3	4.75	1.44	1.34
42	2	1144	PSU	C6-N1	4.73	1.44	1.36
42	2	359	OMC	C4-N4	4.73	1.45	1.33
42	2	1318	PSU	C6-N1	4.72	1.44	1.36
42	2	1229	OMG	C2-N3	4.72	1.44	1.33
20	S1	2140	OMC	C4-N4	4.72	1.45	1.33
20	S1	18	OMC	C4-N4	4.71	1.45	1.33
41	1	870	PSU	C6-N1	4.70	1.44	1.36
42	2	655	OMG	C2-N3	4.69	1.44	1.33
42	2	626	PSU	C6-N1	4.69	1.44	1.36
20	S1	1623	OMG	C4-N3	4.68	1.48	1.37
42	2	534	OMG	C2-N3	4.67	1.44	1.33
20	S1	38	OMC	C4-N4	4.67	1.44	1.33
41	1	1664	PSU	C6-N1	4.66	1.44	1.36
42	2	1413	PSU	C6-N1	4.66	1.44	1.36
42	2	1360	OMG	C2-N3	4.65	1.44	1.33
42	2	597	PSU	C6-N1	4.65	1.43	1.36
41	1	940	PSU	C1'-C5	-4.64	1.39	1.50
42	2	593	PSU	C6-N1	4.62	1.43	1.36
44	7	75	OMG	C2-N3	4.62	1.44	1.33
42	2	1159	OMC	C4-N3	4.61	1.43	1.34
20	S1	12	PSU	C1'-C5	-4.60	1.39	1.50
41	1	1011	PSU	C1'-C5	-4.60	1.39	1.50
20	S1	1550	OMG	C4-N3	4.60	1.48	1.37
42	2	1231	OMG	C2-N3	4.60	1.44	1.33
42	2	1046	OMG	C2-N2	4.59	1.45	1.34
20	S1	1544	5MC	C6-N1	4.57	1.45	1.38
42	2	1046	OMG	C4-N3	4.57	1.48	1.37
20	S1	1865	OMG	C2-N3	4.56	1.44	1.33
41	1	856	OMG	C2-N3	4.56	1.44	1.33
20	S1	1478	OMG	C4-N3	4.56	1.48	1.37
20	S1	600	OMG	C2-N2	4.55	1.45	1.34
41	1	1171	PSU	C6-N1	4.54	1.43	1.36
42	2	1354	PSU	C1'-C5	-4.54	1.39	1.50
20	S1	1533	PSU	C1'-C5	-4.54	1.39	1.50
41	1	1533	PSU	C1'-C5	-4.54	1.39	1.50
20	S1	1550	OMG	C2-N2	4.54	1.45	1.34
20	S1	1623	OMG	C2-N2	4.54	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	2	593	PSU	C1'-C5	-4.54	1.39	1.50
20	S1	1829	OMG	C4-N3	4.54	1.48	1.37
42	2	1159	OMC	C4-N4	4.53	1.44	1.33
20	S1	2151	OMG	C2-N2	4.52	1.44	1.34
42	2	1194	PSU	C6-N1	4.52	1.43	1.36
41	1	959	OMG	C2-N2	4.51	1.44	1.34
41	1	959	OMG	C4-N3	4.50	1.48	1.37
42	2	1231	OMG	C4-N3	4.49	1.48	1.37
42	2	662	PSU	C1'-C5	-4.49	1.39	1.50
41	1	1402	PSU	C6-N1	4.49	1.43	1.36
20	S1	1865	OMG	C4-N3	4.48	1.48	1.37
42	2	1317	OMC	C4-N4	4.48	1.44	1.33
20	S1	1865	OMG	C2-N2	4.48	1.44	1.34
42	2	1382	PSU	C1'-C5	-4.48	1.40	1.50
42	2	655	OMG	C4-N3	4.47	1.48	1.37
42	2	641	OMG	C2-N3	4.47	1.44	1.33
42	2	1397	OMC	C4-N3	4.46	1.43	1.34
20	S1	1647	OMG	C2-N3	4.46	1.44	1.33
41	1	672	PSU	C1'-C5	-4.46	1.40	1.50
41	1	1552	OMC	C4-N4	4.46	1.44	1.33
20	S1	1647	OMG	C4-N3	4.45	1.48	1.37
20	S1	2140	OMC	C2-N1	4.44	1.49	1.40
42	2	1058	PSU	C1'-C5	-4.44	1.40	1.50
20	S1	1841	PSU	C1'-C5	-4.44	1.40	1.50
20	S1	1829	OMG	C2-N2	4.43	1.44	1.34
20	S1	2046	PSU	C1'-C5	-4.42	1.40	1.50
42	2	1078	OMG	C2-N3	4.42	1.43	1.33
41	1	1626	OMG	C2-N3	4.42	1.43	1.33
42	2	1253	OMG	C2-N3	4.41	1.43	1.33
42	2	1194	PSU	C1'-C5	-4.41	1.40	1.50
41	1	1190	OMG	C4-N3	4.39	1.48	1.37
20	S1	1478	OMG	C2-N2	4.39	1.44	1.34
20	S1	455	PSU	C1'-C5	-4.39	1.40	1.50
44	7	75	OMG	C4-N3	4.39	1.48	1.37
20	S1	33	PSU	C1'-C5	-4.38	1.40	1.50
41	1	1190	OMG	C2-N2	4.38	1.44	1.34
42	2	1360	OMG	C4-N3	4.38	1.48	1.37
41	1	1527	OMC	C4-N3	4.38	1.43	1.34
41	1	1524	OMG	C4-N3	4.38	1.48	1.37
41	1	1533	PSU	C6-N1	4.38	1.43	1.36
42	2	472	PSU	C1'-C5	-4.37	1.40	1.50
42	2	71	OMG	C2-N3	4.37	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	S1	1866	OMC	C4-N4	4.37	1.44	1.33
42	2	1144	PSU	C1'-C5	-4.37	1.40	1.50
44	7	74	PSU	C1'-C5	-4.37	1.40	1.50
42	2	1264	PSU	C1'-C5	-4.37	1.40	1.50
41	1	695	OMC	C4-N3	4.36	1.43	1.34
42	2	534	OMG	C4-N3	4.36	1.47	1.37
42	2	1229	OMG	C2-N2	4.36	1.44	1.34
42	2	583	OMC	C4-N3	4.36	1.43	1.34
41	1	239	PSU	C1'-C5	-4.35	1.40	1.50
41	1	870	PSU	C1'-C5	-4.34	1.40	1.50
42	2	1303	PSU	C1'-C5	-4.34	1.40	1.50
20	S1	609	PSU	C1'-C5	-4.33	1.40	1.50
42	2	1253	OMG	C4-N3	4.33	1.47	1.37
41	1	422	PSU	C1'-C5	-4.32	1.40	1.50
42	2	1229	OMG	C4-N3	4.32	1.47	1.37
42	2	1248	OMC	C4-N4	4.32	1.44	1.33
41	1	1017	PSU	C1'-C5	-4.32	1.40	1.50
42	2	641	OMG	C4-N3	4.32	1.47	1.37
41	1	1402	PSU	C1'-C5	-4.31	1.40	1.50
42	2	1361	PSU	C1'-C5	-4.31	1.40	1.50
42	2	1397	OMC	C4-N4	4.31	1.44	1.33
20	S1	104	PSU	C1'-C5	-4.31	1.40	1.50
42	2	1360	OMG	C2-N2	4.30	1.44	1.34
41	1	1664	PSU	C1'-C5	-4.30	1.40	1.50
44	7	75	OMG	C2-N2	4.30	1.44	1.34
42	2	1413	PSU	C1'-C5	-4.29	1.40	1.50
42	2	583	OMC	C4-N4	4.29	1.44	1.33
42	2	1248	OMC	C4-N3	4.29	1.43	1.34
41	1	1017	PSU	C6-N1	4.29	1.43	1.36
42	2	1078	OMG	C2-N2	4.28	1.44	1.34
20	S1	1647	OMG	C2-N2	4.28	1.44	1.34
20	S1	607	PSU	C1'-C5	-4.27	1.40	1.50
20	S1	38	OMC	C2-N1	4.27	1.49	1.40
42	2	1253	OMG	C2-N2	4.26	1.44	1.34
41	1	1540	OMG	C2-N3	4.25	1.43	1.33
42	2	626	PSU	C1'-C5	-4.24	1.40	1.50
20	S1	1544	5MC	C4-N4	4.24	1.45	1.34
41	1	1528	PSU	C1'-C5	-4.23	1.40	1.50
41	1	1626	OMG	C2-N2	4.23	1.44	1.34
43	4	74	OMG	C2-N3	4.22	1.43	1.33
41	1	1626	OMG	C4-N3	4.22	1.47	1.37
41	1	1540	OMG	C4-N3	4.21	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	S1	1156	PSU	C1'-C5	-4.21	1.40	1.50
42	2	437	PSU	C1'-C5	-4.21	1.40	1.50
42	2	1078	OMG	C4-N3	4.21	1.47	1.37
42	2	1060	PSU	C1'-C5	-4.20	1.40	1.50
41	1	1540	OMG	C2-N2	4.20	1.44	1.34
41	1	856	OMG	C4-N3	4.20	1.47	1.37
42	2	534	OMG	C2-N2	4.19	1.44	1.34
42	2	71	OMG	C2-N2	4.18	1.44	1.34
41	1	856	OMG	C2-N2	4.18	1.44	1.34
41	1	1524	OMG	C2-N2	4.17	1.44	1.34
42	2	71	OMG	C4-N3	4.17	1.47	1.37
41	1	1171	PSU	C1'-C5	-4.17	1.40	1.50
42	2	1265	PSU	C1'-C5	-4.17	1.40	1.50
44	7	69	PSU	C1'-C5	-4.16	1.40	1.50
42	2	1317	OMC	C4-N3	4.16	1.42	1.34
20	S1	2202	PSU	C1'-C5	-4.14	1.40	1.50
42	2	1248	OMC	C2-N1	4.14	1.49	1.40
41	1	1181	PSU	C1'-C5	-4.14	1.40	1.50
20	S1	1539	PSU	C1'-C5	-4.13	1.40	1.50
42	2	1231	OMG	C2-N2	4.12	1.44	1.34
42	2	597	PSU	C1'-C5	-4.12	1.40	1.50
43	4	74	OMG	C4-N3	4.12	1.47	1.37
20	S1	1192	PSU	C1'-C5	-4.11	1.40	1.50
20	S1	1657	PSU	C1'-C5	-4.11	1.40	1.50
42	2	1318	PSU	C1'-C5	-4.10	1.40	1.50
42	2	1308	5MC	C4-N4	4.09	1.44	1.34
20	S1	18	OMC	C2-N1	4.08	1.48	1.40
42	2	1308	5MC	C2-N1	4.06	1.48	1.40
42	2	524	5MC	C6-N1	4.06	1.45	1.38
41	1	1527	OMC	C4-N4	4.05	1.43	1.33
20	S1	1621	OMU	C4-N3	4.03	1.45	1.38
41	1	695	OMC	C4-N4	4.02	1.43	1.33
20	S1	1544	5MC	C2-N1	4.01	1.48	1.40
42	2	641	OMG	C2-N2	4.00	1.43	1.34
42	2	655	OMG	C2-N2	3.99	1.43	1.34
20	S1	29	OMU	C4-N3	3.98	1.45	1.38
42	2	78	PSU	C1'-C5	-3.97	1.41	1.50
43	4	74	OMG	C2-N2	3.96	1.43	1.34
41	1	695	OMC	C2-N1	3.93	1.48	1.40
20	S1	1833	OMU	C4-N3	3.92	1.45	1.38
42	2	1265	PSU	C4-N3	3.91	1.46	1.38
42	2	1159	OMC	C2-N1	3.89	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	1	845	OMU	O4-C4	-3.89	1.16	1.24
42	2	78	PSU	O4-C4	-3.88	1.16	1.23
20	S1	1543	C4J	C6-N1	3.87	1.46	1.36
20	S1	1777	OMU	C4-N3	3.86	1.45	1.38
20	S1	1995	G7M	C4-N3	3.86	1.46	1.37
41	1	1527	OMC	C2-N1	3.86	1.48	1.40
20	S1	1246	PSU	C4-N3	3.85	1.46	1.38
20	S1	1866	OMC	C2-N1	3.83	1.48	1.40
41	1	1552	OMC	C2-N1	3.83	1.48	1.40
20	S1	1246	PSU	C1'-C5	-3.83	1.41	1.50
42	2	1403	PSU	C1'-C5	-3.82	1.41	1.50
20	S1	607	PSU	C4-N3	3.82	1.45	1.38
20	S1	609	PSU	C4-N3	3.81	1.45	1.38
42	2	1317	OMC	C2-N1	3.81	1.48	1.40
20	S1	33	PSU	C4-N3	3.81	1.45	1.38
20	S1	1156	PSU	C4-N3	3.80	1.45	1.38
20	S1	2048	OMU	C4-N3	3.80	1.45	1.38
42	2	1397	OMC	C2-N1	3.80	1.48	1.40
42	2	524	5MC	C4-N4	3.78	1.43	1.34
20	S1	661	OMU	C4-N3	3.78	1.45	1.38
20	S1	104	PSU	C4-N3	3.77	1.45	1.38
42	2	560	OMU	O4-C4	-3.77	1.17	1.24
42	2	583	OMC	C2-N1	3.76	1.48	1.40
20	S1	2202	PSU	C4-N3	3.75	1.45	1.38
42	2	359	OMC	C2-N1	3.75	1.48	1.40
20	S1	1657	PSU	C4-N3	3.75	1.45	1.38
42	2	1359	OMU	O4-C4	-3.74	1.17	1.24
41	1	847	OMU	O4-C4	-3.73	1.17	1.24
20	S1	455	PSU	C4-N3	3.72	1.45	1.38
20	S1	8	OMU	C4-N3	3.71	1.45	1.38
20	S1	1192	PSU	C4-N3	3.71	1.45	1.38
81	3	13	OMU	C4-N3	3.70	1.45	1.38
41	1	695	OMC	O2-C2	-3.70	1.16	1.23
42	2	1419	OMU	O4-C4	-3.68	1.17	1.24
42	2	1264	PSU	C4-N3	3.68	1.45	1.38
42	2	583	OMC	O2-C2	-3.67	1.16	1.23
42	2	1303	PSU	C4-N3	3.67	1.45	1.38
42	2	1046	OMG	C6-N1	3.66	1.43	1.37
42	2	667	OMU	O4-C4	-3.65	1.17	1.24
42	2	73	OMU	O4-C4	-3.65	1.17	1.24
41	1	870	PSU	O4-C4	-3.64	1.16	1.23
20	S1	1539	PSU	C4-N3	3.63	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	1	239	PSU	C4-N3	3.62	1.45	1.38
41	1	1107	OMU	O4-C4	-3.62	1.17	1.24
41	1	1659	OMU	O4-C4	-3.61	1.17	1.24
42	2	641	OMG	C5-C4	-3.61	1.33	1.43
20	S1	2046	PSU	C4-N3	3.60	1.45	1.38
20	S1	1979	OMU	C4-N3	3.59	1.45	1.38
42	2	524	5MC	C2-N1	3.59	1.47	1.40
20	S1	1841	PSU	C4-N3	3.59	1.45	1.38
42	2	1361	PSU	C4-N3	3.58	1.45	1.38
41	1	1527	OMC	O2-C2	-3.58	1.17	1.23
42	2	1382	PSU	O4-C4	-3.57	1.16	1.23
41	1	1371	OMU	O4-C4	-3.56	1.17	1.24
42	2	71	OMG	C5-C4	-3.56	1.34	1.43
42	2	1359	OMU	C4-N3	3.56	1.44	1.38
41	1	1664	PSU	O4-C4	-3.56	1.16	1.23
44	7	75	OMG	C6-N1	3.54	1.43	1.37
41	1	1011	PSU	C4-N3	3.54	1.45	1.38
42	2	597	PSU	O4-C4	-3.53	1.16	1.23
20	S1	2151	OMG	C6-N1	3.52	1.43	1.37
42	2	472	PSU	C4-N3	3.51	1.45	1.38
20	S1	600	OMG	C6-N1	3.51	1.43	1.37
42	2	1397	OMC	O2-C2	-3.51	1.17	1.23
81	3	13	OMU	O4-C4	-3.50	1.17	1.24
42	2	1318	PSU	C4-N3	3.49	1.45	1.38
42	2	1403	PSU	C4-N3	3.49	1.45	1.38
41	1	1190	OMG	C6-N1	3.46	1.43	1.37
42	2	662	PSU	O4-C4	-3.46	1.17	1.23
42	2	1317	OMC	O2-C2	-3.45	1.17	1.23
42	2	1077	OMU	C4-N3	3.43	1.44	1.38
42	2	1419	OMU	C4-N3	3.43	1.44	1.38
20	S1	1533	PSU	C4-N3	3.43	1.45	1.38
20	S1	1550	OMG	C6-N1	3.42	1.43	1.37
41	1	1181	PSU	C4-N3	3.42	1.45	1.38
42	2	1413	PSU	C4-N3	3.41	1.45	1.38
20	S1	1979	OMU	O4-C4	-3.40	1.17	1.24
41	1	1659	OMU	C4-N3	3.40	1.44	1.38
41	1	1171	PSU	O4-C4	-3.40	1.17	1.23
41	1	1533	PSU	C4-N3	3.39	1.45	1.38
42	2	437	PSU	C4-N3	3.39	1.45	1.38
20	S1	1543	C4J	C4-N3	3.39	1.46	1.40
20	S1	1647	OMG	C5-C4	-3.39	1.34	1.43
42	2	1159	OMC	O2-C2	-3.38	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	7	74	PSU	C4-N3	3.38	1.45	1.38
20	S1	1543	C4J	C31-C3	3.38	1.59	1.52
41	1	1402	PSU	O4-C4	-3.37	1.17	1.23
20	S1	2048	OMU	O4-C4	-3.36	1.18	1.24
41	1	422	PSU	C4-N3	3.36	1.45	1.38
41	1	959	OMG	C6-N1	3.35	1.42	1.37
42	2	593	PSU	O4-C4	-3.34	1.17	1.23
20	S1	8	OMU	O4-C4	-3.33	1.18	1.24
20	S1	12	PSU	C4-N3	3.33	1.45	1.38
42	2	1318	PSU	O4-C4	-3.32	1.17	1.23
42	2	1248	OMC	O2-C2	-3.32	1.17	1.23
41	1	1107	OMU	C4-N3	3.31	1.44	1.38
41	1	845	OMU	C4-N3	3.31	1.44	1.38
41	1	1528	PSU	O4-C4	-3.31	1.17	1.23
41	1	1402	PSU	C4-N3	3.29	1.44	1.38
20	S1	1647	OMG	C6-N1	3.29	1.42	1.37
20	S1	1478	OMG	C5-C4	-3.28	1.34	1.43
42	2	1058	PSU	C4-N3	3.27	1.44	1.38
42	2	1077	OMU	O4-C4	-3.27	1.18	1.24
44	7	69	PSU	C4-N3	3.27	1.44	1.38
42	2	1360	OMG	C5-C4	-3.27	1.34	1.43
41	1	856	OMG	C6-N1	3.27	1.42	1.37
43	4	74	OMG	C5-C4	-3.26	1.34	1.43
42	2	1078	OMG	C5-C4	-3.26	1.34	1.43
41	1	1540	OMG	C5-C4	-3.26	1.34	1.43
42	2	626	PSU	O4-C4	-3.26	1.17	1.23
42	2	1194	PSU	C4-N3	3.26	1.44	1.38
42	2	1231	OMG	C5-C4	-3.25	1.34	1.43
44	7	75	OMG	C5-C4	-3.25	1.34	1.43
41	1	940	PSU	O4-C4	-3.25	1.17	1.23
41	1	1626	OMG	C5-C4	-3.25	1.34	1.43
20	S1	1829	OMG	C6-N1	3.25	1.42	1.37
42	2	527	A2M	O3'-C3'	3.25	1.50	1.43
20	S1	1995	G7M	C2-N1	3.24	1.45	1.37
42	2	1354	PSU	C4-N3	3.24	1.44	1.38
20	S1	661	OMU	O4-C4	-3.24	1.18	1.24
42	2	560	OMU	C4-N3	3.24	1.44	1.38
42	2	73	OMU	C4-N3	3.24	1.44	1.38
42	2	95	A2M	C5-C4	-3.24	1.32	1.40
20	S1	1621	OMU	O4-C4	-3.23	1.18	1.24
42	2	534	OMG	C5-C4	-3.23	1.34	1.43
41	1	847	OMU	O2-C2	-3.22	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	2	667	OMU	C4-N3	3.22	1.44	1.38
42	2	73	OMU	O2-C2	-3.22	1.17	1.23
41	1	856	OMG	C5-C4	-3.21	1.34	1.43
42	2	572	A2M	O3'-C3'	3.21	1.50	1.43
42	2	1413	PSU	O4-C4	-3.21	1.17	1.23
41	1	672	PSU	O4-C4	-3.21	1.17	1.23
20	S1	1777	OMU	O4-C4	-3.21	1.18	1.24
42	2	1360	OMG	C6-N1	3.21	1.42	1.37
41	1	940	PSU	C4-N3	3.21	1.44	1.38
42	2	437	PSU	O4-C4	-3.21	1.17	1.23
42	2	1194	PSU	O4-C4	-3.20	1.17	1.23
42	2	1060	PSU	C4-N3	3.20	1.44	1.38
20	S1	668	A2M	O3'-C3'	3.20	1.50	1.43
41	1	1540	OMG	C6-N1	3.20	1.42	1.37
42	2	524	5MC	O2-C2	-3.20	1.17	1.23
42	2	572	A2M	C5-C4	-3.19	1.32	1.40
20	S1	1866	OMC	O2-C2	-3.19	1.17	1.23
20	S1	479	A2M	O3'-C3'	3.18	1.50	1.43
42	2	641	OMG	C6-N1	3.18	1.42	1.37
41	1	1371	OMU	C4-N3	3.18	1.44	1.38
41	1	1659	OMU	O2-C2	-3.18	1.17	1.23
42	2	1046	OMG	C5-C6	3.18	1.53	1.47
20	S1	1865	OMG	C6-N1	3.18	1.42	1.37
20	S1	2140	OMC	C6-N1	3.18	1.45	1.38
41	1	1524	OMG	C5-C4	-3.18	1.35	1.43
41	1	1017	PSU	O4-C4	-3.18	1.17	1.23
42	2	1229	OMG	C6-N1	3.17	1.42	1.37
42	2	1372	A2M	C5-C4	-3.17	1.32	1.40
42	2	1253	OMG	C5-C4	-3.17	1.35	1.43
41	1	672	PSU	C4-N3	3.17	1.44	1.38
41	1	955	A2M	C5-C4	-3.16	1.32	1.40
41	1	845	OMU	O2-C2	-3.15	1.17	1.23
42	2	359	OMC	C6-N1	3.15	1.45	1.38
41	1	1171	PSU	C4-N3	3.15	1.44	1.38
42	2	597	PSU	C4-N3	3.14	1.44	1.38
41	1	1528	PSU	C4-N3	3.14	1.44	1.38
20	S1	1865	OMG	C5-C4	-3.14	1.35	1.43
41	1	1190	OMG	C5-C4	-3.14	1.35	1.43
20	S1	1995	G7M	C2-N2	3.14	1.41	1.34
43	4	74	OMG	C6-N1	3.14	1.42	1.37
20	S1	29	OMU	O4-C4	-3.14	1.18	1.24
44	7	43	A2M	C5-C4	-3.14	1.32	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	2	655	OMG	C5-C4	-3.13	1.35	1.43
20	S1	1566	PSU	C6-C5	3.13	1.39	1.35
41	1	697	A2M	C5-C4	-3.13	1.32	1.40
20	S1	18	OMC	O2-C2	-3.13	1.17	1.23
42	2	1078	OMG	C6-N1	3.13	1.42	1.37
41	1	437	A2M	C5-C4	-3.12	1.32	1.40
42	2	1354	PSU	O4-C4	-3.12	1.17	1.23
41	1	681	A2M	C5-C4	-3.12	1.32	1.40
42	2	1361	PSU	O4-C4	-3.12	1.17	1.23
42	2	570	A2M	C5-C4	-3.11	1.32	1.40
42	2	359	OMC	O2-C2	-3.11	1.17	1.23
42	2	527	A2M	C5-C4	-3.11	1.32	1.40
41	1	1524	OMG	C5-C6	3.11	1.53	1.47
20	S1	38	OMC	C6-N1	3.10	1.45	1.38
42	2	1229	OMG	C5-C4	-3.10	1.35	1.43
20	S1	1833	OMU	O4-C4	-3.10	1.18	1.24
42	2	1403	PSU	O4-C4	-3.10	1.17	1.23
42	2	1253	OMG	C5-C6	3.10	1.53	1.47
20	S1	1623	OMG	C6-N1	3.09	1.42	1.37
44	7	69	PSU	O4-C4	-3.09	1.17	1.23
42	2	1382	PSU	C4-N3	3.09	1.44	1.38
41	1	870	PSU	C4-N3	3.09	1.44	1.38
41	1	1664	PSU	C4-N3	3.09	1.44	1.38
42	2	1144	PSU	O4-C4	-3.09	1.17	1.23
42	2	667	OMU	O2-C2	-3.08	1.17	1.23
41	1	678	A2M	C5-C4	-3.08	1.32	1.40
42	2	655	OMG	C5-C6	3.08	1.53	1.47
20	S1	1543	C4J	O4'-C1'	-3.08	1.39	1.43
20	S1	1543	C4J	O4-C4	-3.07	1.16	1.23
42	2	1078	OMG	C5-C6	3.07	1.53	1.47
44	7	162	A2M	C5-C4	-3.07	1.32	1.40
42	2	1308	5MC	O2-C2	-3.07	1.18	1.23
41	1	1552	OMC	O2-C2	-3.06	1.18	1.23
42	2	1231	OMG	C6-N1	3.06	1.42	1.37
20	S1	18	OMC	C6-N1	3.06	1.45	1.38
41	1	677	1MA	C8-N7	-3.06	1.29	1.35
43	4	74	OMG	O6-C6	-3.06	1.17	1.23
42	2	665	A2M	C5-C4	-3.06	1.32	1.40
41	1	1371	OMU	O2-C2	-3.06	1.17	1.23
41	1	1533	PSU	O4-C4	-3.06	1.17	1.23
20	S1	479	A2M	C6-N6	3.06	1.45	1.34
42	2	1144	PSU	C4-N3	3.05	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	1	422	PSU	O4-C4	-3.05	1.17	1.23
20	S1	897	A2M	C6-N6	3.04	1.45	1.34
42	2	1317	OMC	C6-N1	3.04	1.45	1.38
42	2	534	OMG	C6-N1	3.04	1.42	1.37
42	2	1372	A2M	O3'-C3'	3.04	1.50	1.43
44	7	74	PSU	O4-C4	-3.03	1.17	1.23
42	2	78	PSU	C4-N3	3.03	1.44	1.38
42	2	628	A2M	O2'-C2'	-3.03	1.34	1.42
20	S1	28	A2M	C6-N6	3.03	1.45	1.34
41	1	1626	OMG	C6-N1	3.02	1.42	1.37
42	2	655	OMG	C6-N1	3.02	1.42	1.37
42	2	1060	PSU	O4-C4	-3.02	1.17	1.23
20	S1	2021	A2M	C5-C4	-3.02	1.32	1.40
42	2	641	OMG	C5-C6	3.02	1.53	1.47
41	1	1190	OMG	C5-C6	3.02	1.53	1.47
42	2	95	A2M	C6-N6	3.02	1.45	1.34
42	2	504	PSU	C6-C5	3.02	1.38	1.35
20	S1	1995	G7M	O6-C6	-3.02	1.17	1.23
20	S1	2151	OMG	C5-C6	3.02	1.53	1.47
41	1	1524	OMG	C6-N1	3.02	1.42	1.37
42	2	71	OMG	C6-N1	3.01	1.42	1.37
20	S1	600	OMG	C5-C6	3.01	1.53	1.47
42	2	382	A2M	C5-C4	-3.01	1.33	1.40
41	1	858	A2M	O3'-C3'	3.01	1.50	1.43
20	S1	668	A2M	C6-N6	3.01	1.45	1.34
42	2	1185	A2M	C5-C4	-3.01	1.33	1.40
41	1	1017	PSU	C4-N3	3.01	1.44	1.38
20	S1	1533	PSU	O4-C4	-3.00	1.17	1.23
41	1	437	A2M	O3'-C3'	3.00	1.50	1.43
42	2	1185	A2M	O3'-C3'	3.00	1.50	1.43
42	2	510	PSU	C6-C5	3.00	1.38	1.35
41	1	1011	PSU	O4-C4	-3.00	1.17	1.23
41	1	695	OMC	C6-N1	3.00	1.45	1.38
20	S1	1478	OMG	C6-N1	2.99	1.42	1.37
44	7	75	OMG	C5-C6	2.99	1.53	1.47
42	2	626	PSU	C4-N3	2.98	1.44	1.38
42	2	71	OMG	O6-C6	-2.98	1.17	1.23
20	S1	98	A2M	C6-N6	2.98	1.44	1.34
41	1	856	OMG	C5-C6	2.98	1.53	1.47
20	S1	1543	C4J	C2-N1	2.97	1.47	1.39
20	S1	1539	PSU	O4-C4	-2.97	1.17	1.23
42	2	604	A2M	C5-C4	-2.97	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	1	1626	OMG	C5-C6	2.97	1.53	1.47
41	1	239	PSU	O4-C4	-2.96	1.18	1.23
41	1	1539	A2M	O3'-C3'	2.96	1.49	1.43
41	1	1539	A2M	C5-C4	-2.96	1.33	1.40
20	S1	38	OMC	O2-C2	-2.96	1.18	1.23
41	1	1527	OMC	C6-N1	2.95	1.45	1.38
20	S1	1829	OMG	C5-C4	-2.95	1.35	1.43
42	2	1372	A2M	C6-N6	2.94	1.44	1.34
41	1	681	A2M	C6-N6	2.94	1.44	1.34
42	2	1248	OMC	C6-N1	2.94	1.45	1.38
42	2	591	A2M	C5-C4	-2.94	1.33	1.40
42	2	570	A2M	O3'-C3'	2.93	1.49	1.43
41	1	1552	OMC	C6-N1	2.93	1.45	1.38
41	1	437	A2M	O2'-C2'	-2.93	1.35	1.42
42	2	1384	A2M	C5-C4	-2.93	1.33	1.40
42	2	506	PSU	C4-N3	-2.93	1.33	1.38
20	S1	1657	PSU	O4-C4	-2.93	1.18	1.23
42	2	662	PSU	C4-N3	2.92	1.44	1.38
20	S1	1866	OMC	C6-N1	2.92	1.45	1.38
41	1	858	A2M	C6-N6	2.92	1.44	1.34
20	S1	2021	A2M	C6-N6	2.92	1.44	1.34
42	2	1185	A2M	C6-N6	2.91	1.44	1.34
20	S1	1550	OMG	C5-C4	-2.91	1.35	1.43
20	S1	1478	OMG	O6-C6	-2.91	1.17	1.23
20	S1	1829	OMG	C5-C6	2.91	1.53	1.47
42	2	665	A2M	O2'-C2'	-2.91	1.35	1.42
41	1	697	A2M	O3'-C3'	2.90	1.49	1.43
42	2	583	OMC	C6-N1	2.90	1.45	1.38
42	2	593	PSU	C4-N3	2.90	1.44	1.38
41	1	1540	OMG	C5-C6	2.89	1.53	1.47
42	2	506	PSU	C6-C5	2.89	1.38	1.35
20	S1	1544	5MC	O2-C2	-2.89	1.18	1.23
20	S1	1841	PSU	O4-C4	-2.89	1.18	1.23
41	1	1540	OMG	O6-C6	-2.89	1.17	1.23
42	2	604	A2M	C6-N6	2.89	1.44	1.34
41	1	856	OMG	O6-C6	-2.89	1.17	1.23
42	2	500	PSU	C6-C5	2.89	1.38	1.35
42	2	1419	OMU	O2-C2	-2.89	1.17	1.23
42	2	1046	OMG	C5-C4	-2.88	1.35	1.43
42	2	382	A2M	O3'-C3'	2.88	1.49	1.43
44	7	43	A2M	C6-N6	2.88	1.44	1.34
41	1	681	A2M	O3'-C3'	2.88	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	2	1360	OMG	C5-C6	2.88	1.53	1.47
42	2	1359	OMU	C6-N1	2.88	1.44	1.38
41	1	1539	A2M	O2'-C2'	-2.87	1.35	1.42
42	2	1253	OMG	O6-C6	-2.87	1.17	1.23
42	2	628	A2M	O3'-C3'	2.87	1.49	1.43
20	S1	98	A2M	C5-C4	-2.87	1.33	1.40
20	S1	668	A2M	C5-C4	-2.87	1.33	1.40
42	2	510	PSU	C4-N3	-2.87	1.33	1.38
81	3	13	OMU	O2-C2	-2.86	1.17	1.23
20	S1	98	A2M	O3'-C3'	2.86	1.49	1.43
20	S1	2184	MA6	C5-C4	-2.86	1.33	1.40
20	S1	1550	OMG	C5-C6	2.85	1.53	1.47
42	2	641	OMG	O6-C6	-2.85	1.17	1.23
20	S1	1623	OMG	C5-C4	-2.85	1.35	1.43
41	1	1626	OMG	O6-C6	-2.85	1.17	1.23
20	S1	28	A2M	C5-C4	-2.85	1.33	1.40
41	1	437	A2M	C6-N6	2.85	1.44	1.34
20	S1	2021	A2M	O3'-C3'	2.85	1.49	1.43
42	2	1159	OMC	C6-N1	2.85	1.44	1.38
42	2	570	A2M	C6-N6	2.85	1.44	1.34
42	2	1078	OMG	O6-C6	-2.84	1.17	1.23
41	1	678	A2M	O3'-C3'	2.84	1.49	1.43
42	2	604	A2M	O3'-C3'	2.84	1.49	1.43
42	2	1253	OMG	C6-N1	2.84	1.42	1.37
42	2	1229	OMG	O6-C6	-2.83	1.17	1.23
20	S1	12	PSU	O4-C4	-2.83	1.18	1.23
42	2	534	OMG	O6-C6	-2.83	1.17	1.23
41	1	847	OMU	C4-N3	2.83	1.43	1.38
42	2	1264	PSU	O4-C4	-2.83	1.18	1.23
42	2	591	A2M	C6-N6	2.83	1.44	1.34
42	2	527	A2M	C6-N6	2.83	1.44	1.34
41	1	697	A2M	O2'-C2'	-2.83	1.35	1.42
20	S1	600	OMG	C5-C4	-2.83	1.35	1.43
20	S1	661	OMU	C6-N1	2.83	1.44	1.38
42	2	500	PSU	C4-N3	-2.82	1.33	1.38
41	1	678	A2M	O2'-C2'	-2.82	1.35	1.42
42	2	472	PSU	O4-C4	-2.82	1.18	1.23
20	S1	2048	OMU	O2-C2	-2.82	1.17	1.23
20	S1	1543	C4J	O2-C2	-2.82	1.17	1.22
42	2	628	A2M	C6-N6	2.81	1.44	1.34
20	S1	29	OMU	C6-N1	2.81	1.44	1.38
42	2	1303	PSU	O4-C4	-2.81	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	7	162	A2M	C6-N6	2.81	1.44	1.34
42	2	534	OMG	C5-C6	2.81	1.53	1.47
42	2	1229	OMG	C5-C6	2.81	1.53	1.47
41	1	955	A2M	C6-N6	2.81	1.44	1.34
20	S1	1833	OMU	C6-N1	2.81	1.44	1.38
20	S1	1647	OMG	O6-C6	-2.81	1.17	1.23
44	7	162	A2M	O2'-C2'	-2.81	1.35	1.42
20	S1	1623	OMG	C5-C6	2.81	1.53	1.47
41	1	678	A2M	C6-N6	2.81	1.44	1.34
42	2	1384	A2M	C6-N6	2.81	1.44	1.34
42	2	572	A2M	O2'-C2'	-2.81	1.35	1.42
20	S1	1621	OMU	O2-C2	-2.80	1.17	1.23
20	S1	2185	MA6	C5-C4	-2.80	1.33	1.40
42	2	1231	OMG	O6-C6	-2.80	1.17	1.23
42	2	665	A2M	C6-N6	2.80	1.44	1.34
20	S1	1192	PSU	O4-C4	-2.79	1.18	1.23
41	1	1181	PSU	O4-C4	-2.79	1.18	1.23
20	S1	479	A2M	C5-C4	-2.79	1.33	1.40
41	1	697	A2M	C6-N6	2.79	1.44	1.34
20	S1	28	A2M	O3'-C3'	2.79	1.49	1.43
42	2	655	OMG	O6-C6	-2.79	1.17	1.23
42	2	382	A2M	C6-N6	2.79	1.44	1.34
41	1	955	A2M	O2'-C2'	-2.79	1.35	1.42
42	2	1397	OMC	C6-N1	2.79	1.44	1.38
42	2	560	OMU	O2-C2	-2.78	1.18	1.23
42	2	1185	A2M	O2'-C2'	-2.78	1.35	1.42
41	1	1539	A2M	C6-N6	2.78	1.44	1.34
20	S1	8	OMU	C6-N1	2.78	1.44	1.38
20	S1	2140	OMC	O2-C2	-2.78	1.18	1.23
42	2	1359	OMU	O2-C2	-2.77	1.18	1.23
20	S1	1246	PSU	O4-C4	-2.77	1.18	1.23
42	2	604	A2M	O2'-C2'	-2.77	1.35	1.42
20	S1	1777	OMU	C6-N1	2.77	1.44	1.38
42	2	665	A2M	O3'-C3'	2.76	1.49	1.43
42	2	1384	A2M	O2'-C2'	-2.76	1.35	1.42
20	S1	1478	OMG	C5-C6	2.76	1.53	1.47
20	S1	897	A2M	C5-C4	-2.76	1.33	1.40
44	7	43	A2M	O2'-C2'	-2.75	1.35	1.42
41	1	858	A2M	C5-C4	-2.75	1.33	1.40
41	1	959	OMG	C5-C4	-2.74	1.36	1.43
42	2	71	OMG	C5-C6	2.73	1.53	1.47
20	S1	455	PSU	O4-C4	-2.73	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	S1	1566	PSU	C4-N3	-2.73	1.33	1.38
42	2	591	A2M	O3'-C3'	2.73	1.49	1.43
42	2	1419	OMU	C6-N1	2.73	1.44	1.38
20	S1	2151	OMG	C5-C4	-2.72	1.36	1.43
42	2	591	A2M	O2'-C2'	-2.72	1.35	1.42
42	2	667	OMU	C6-N1	2.72	1.44	1.38
42	2	1058	PSU	O4-C4	-2.72	1.18	1.23
42	2	504	PSU	C4-N3	-2.72	1.33	1.38
20	S1	1979	OMU	O2-C2	-2.71	1.18	1.23
20	S1	1156	PSU	O4-C4	-2.71	1.18	1.23
20	S1	897	A2M	O2'-C2'	-2.71	1.35	1.42
20	S1	1621	OMU	C6-N1	2.71	1.44	1.38
42	2	1372	A2M	O2'-C2'	-2.70	1.35	1.42
42	2	1077	OMU	C6-N1	2.70	1.44	1.38
20	S1	609	PSU	O4-C4	-2.70	1.18	1.23
20	S1	2046	PSU	O4-C4	-2.69	1.18	1.23
42	2	572	A2M	C6-N6	2.69	1.43	1.34
20	S1	897	A2M	O3'-C3'	2.69	1.49	1.43
20	S1	2202	PSU	O4-C4	-2.69	1.18	1.23
42	2	95	A2M	O3'-C3'	2.68	1.49	1.43
42	2	1360	OMG	O6-C6	-2.68	1.17	1.23
20	S1	98	A2M	O2'-C2'	-2.68	1.35	1.42
41	1	1371	OMU	C6-N1	2.68	1.44	1.38
42	2	1231	OMG	C5-C6	2.67	1.52	1.47
42	2	1046	OMG	C2-N1	2.67	1.44	1.37
20	S1	1865	OMG	O6-C6	-2.67	1.17	1.23
42	2	1077	OMU	O2-C2	-2.67	1.18	1.23
41	1	858	A2M	O2'-C2'	-2.67	1.35	1.42
20	S1	2021	A2M	O2'-C2'	-2.67	1.35	1.42
42	2	95	A2M	O2'-C2'	-2.67	1.35	1.42
44	7	43	A2M	O3'-C3'	2.66	1.49	1.43
20	S1	661	OMU	O2-C2	-2.66	1.18	1.23
41	1	959	OMG	C5-C6	2.66	1.52	1.47
42	2	597	PSU	O2-C2	-2.66	1.17	1.23
20	S1	1865	OMG	C5-C6	2.65	1.52	1.47
20	S1	28	A2M	O2'-C2'	-2.63	1.35	1.42
20	S1	33	PSU	O4-C4	-2.63	1.18	1.23
41	1	1190	OMG	C2-N1	2.62	1.44	1.37
20	S1	607	PSU	O4-C4	-2.62	1.18	1.23
20	S1	2151	OMG	C2-N1	2.62	1.44	1.37
41	1	1107	OMU	O2-C2	-2.61	1.18	1.23
20	S1	1865	OMG	C2-N1	2.61	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	S1	104	PSU	O4-C4	-2.61	1.18	1.23
41	1	681	A2M	O2'-C2'	-2.61	1.35	1.42
41	1	959	OMG	C2-N1	2.61	1.44	1.37
41	1	1190	OMG	O6-C6	-2.60	1.18	1.23
20	S1	1550	OMG	C2-N1	2.60	1.44	1.37
41	1	1659	OMU	C6-N1	2.59	1.44	1.38
42	2	527	A2M	O2'-C2'	-2.59	1.36	1.42
20	S1	1777	OMU	O2-C2	-2.59	1.18	1.23
20	S1	600	OMG	C2-N1	2.59	1.44	1.37
20	S1	8	OMU	O2-C2	-2.59	1.18	1.23
42	2	1384	A2M	O3'-C3'	2.58	1.49	1.43
41	1	1107	OMU	C6-N1	2.58	1.44	1.38
41	1	959	OMG	O6-C6	-2.58	1.18	1.23
81	3	13	OMU	C6-N1	2.57	1.44	1.38
42	2	1265	PSU	O4-C4	-2.57	1.18	1.23
20	S1	1829	OMG	C2-N1	2.57	1.44	1.37
42	2	382	A2M	O2'-C2'	-2.57	1.36	1.42
20	S1	2048	OMU	C6-N1	2.57	1.44	1.38
42	2	628	A2M	C5-C4	-2.56	1.34	1.40
20	S1	1550	OMG	O6-C6	-2.56	1.18	1.23
20	S1	1647	OMG	C5-C6	2.55	1.52	1.47
20	S1	1979	OMU	C6-N1	2.55	1.44	1.38
20	S1	1623	OMG	O6-C6	-2.54	1.18	1.23
20	S1	479	A2M	O2'-C2'	-2.54	1.36	1.42
42	2	73	OMU	C6-N1	2.54	1.44	1.38
41	1	845	OMU	C6-N1	2.53	1.44	1.38
43	4	74	OMG	C5-C6	2.52	1.52	1.47
20	S1	1647	OMG	C2-N1	2.52	1.43	1.37
20	S1	29	OMU	O2-C2	-2.52	1.18	1.23
44	7	75	OMG	O6-C6	-2.52	1.18	1.23
41	1	1171	PSU	O2-C2	-2.51	1.18	1.23
41	1	677	1MA	C5-C4	-2.51	1.36	1.43
42	2	78	PSU	O4'-C1'	-2.50	1.40	1.43
20	S1	668	A2M	O2'-C2'	-2.50	1.36	1.42
20	S1	2061	5MC	C6-N1	-2.50	1.33	1.38
42	2	626	PSU	O2-C2	-2.49	1.18	1.23
20	S1	1995	G7M	C5-C6	2.48	1.51	1.45
41	1	847	OMU	C6-N1	2.48	1.44	1.38
41	1	1540	OMG	C2-N1	2.48	1.43	1.37
41	1	1017	PSU	O2-C2	-2.47	1.18	1.23
44	7	162	A2M	O3'-C3'	2.47	1.48	1.43
41	1	1524	OMG	O6-C6	-2.47	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	S1	600	OMG	O6-C6	-2.46	1.18	1.23
20	S1	1829	OMG	O6-C6	-2.46	1.18	1.23
20	S1	1833	OMU	O2-C2	-2.46	1.18	1.23
42	2	1194	PSU	O2-C2	-2.46	1.18	1.23
42	2	1360	OMG	C2-N1	2.45	1.43	1.37
20	S1	1623	OMG	C2-N1	2.45	1.43	1.37
42	2	78	PSU	O2-C2	-2.44	1.18	1.23
42	2	560	OMU	C6-N1	2.44	1.43	1.38
42	2	662	PSU	O2-C2	-2.43	1.18	1.23
42	2	1403	PSU	O4'-C1'	-2.42	1.40	1.43
42	2	593	PSU	O2-C2	-2.42	1.18	1.23
44	7	75	OMG	C2-N1	2.42	1.43	1.37
41	1	955	A2M	O3'-C3'	2.40	1.48	1.43
41	1	870	PSU	O2-C2	-2.39	1.18	1.23
20	S1	38	OMC	C5-C4	2.39	1.48	1.42
20	S1	2140	OMC	C5-C4	2.38	1.48	1.42
42	2	1231	OMG	C2-N1	2.38	1.43	1.37
41	1	1664	PSU	O2-C2	-2.37	1.18	1.23
42	2	534	OMG	C2-N1	2.36	1.43	1.37
42	2	1046	OMG	O6-C6	-2.35	1.18	1.23
42	2	1382	PSU	O2-C2	-2.35	1.18	1.23
41	1	1524	OMG	C2-N1	2.35	1.43	1.37
20	S1	2061	5MC	C6-C5	2.34	1.38	1.34
42	2	1413	PSU	O2-C2	-2.34	1.18	1.23
42	2	655	OMG	C2-N1	2.33	1.43	1.37
41	1	856	OMG	C2-N1	2.33	1.43	1.37
42	2	1077	OMU	C5-C4	2.33	1.48	1.43
20	S1	512	A2M	C5-C4	2.32	1.47	1.40
20	S1	2151	OMG	O6-C6	-2.31	1.18	1.23
41	1	1626	OMG	C2-N1	2.30	1.43	1.37
42	2	1078	OMG	C2-N1	2.30	1.43	1.37
42	2	641	OMG	C2-N1	2.29	1.43	1.37
20	S1	897	A2M	O5'-C5'	-2.29	1.39	1.44
20	S1	29	OMU	C5-C4	2.28	1.48	1.43
42	2	359	OMC	C5-C4	2.28	1.48	1.42
42	2	570	A2M	O2'-C2'	-2.28	1.36	1.42
20	S1	8	OMU	C5-C4	2.27	1.48	1.43
42	2	1058	PSU	O2-C2	-2.27	1.18	1.23
42	2	437	PSU	O2-C2	-2.27	1.18	1.23
20	S1	1478	OMG	C2-N1	2.27	1.43	1.37
41	1	1528	PSU	O2-C2	-2.26	1.18	1.23
20	S1	18	OMC	C5-C4	2.26	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	S1	1833	OMU	C5-C4	2.25	1.48	1.43
42	2	1144	PSU	O2-C2	-2.24	1.18	1.23
42	2	527	A2M	O5'-C5'	-2.24	1.39	1.44
42	2	1318	PSU	O2-C2	-2.24	1.18	1.23
41	1	672	PSU	O2-C2	-2.23	1.18	1.23
41	1	1371	OMU	C5-C4	2.23	1.48	1.43
41	1	1533	PSU	O2-C2	-2.21	1.18	1.23
20	S1	1777	OMU	C5-C4	2.21	1.48	1.43
43	4	74	OMG	C2-N1	2.21	1.43	1.37
42	2	71	OMG	C2-N1	2.21	1.43	1.37
42	2	1229	OMG	C2-N1	2.20	1.43	1.37
20	S1	1246	PSU	O4'-C1'	-2.19	1.40	1.43
42	2	1248	OMC	C5-C4	2.19	1.47	1.42
42	2	1253	OMG	C2-N1	2.18	1.43	1.37
41	1	1552	OMC	C5-C4	2.17	1.47	1.42
20	S1	1621	OMU	C5-C4	2.17	1.48	1.43
41	1	1171	PSU	O4'-C1'	-2.17	1.40	1.43
42	2	1403	PSU	O2-C2	-2.16	1.18	1.23
42	2	1060	PSU	O2-C2	-2.14	1.18	1.23
20	S1	661	OMU	C5-C4	2.14	1.48	1.43
42	2	1359	OMU	C5-C4	2.14	1.48	1.43
41	1	422	PSU	O2-C2	-2.13	1.18	1.23
20	S1	1866	OMC	C5-C4	2.13	1.47	1.42
42	2	628	A2M	C6-C5	-2.13	1.35	1.43
42	2	667	OMU	C5-C4	2.12	1.48	1.43
41	1	940	PSU	O2-C2	-2.12	1.18	1.23
41	1	1402	PSU	O2-C2	-2.12	1.18	1.23
41	1	1107	OMU	C5-C4	2.12	1.48	1.43
42	2	1382	PSU	O4'-C1'	-2.12	1.40	1.43
42	2	628	A2M	C4-N3	-2.11	1.32	1.35
42	2	593	PSU	O4'-C1'	-2.10	1.40	1.43
20	S1	98	A2M	C2-N3	2.10	1.35	1.32
42	2	1317	OMC	C5-C4	2.10	1.47	1.42
20	S1	897	A2M	C2-N3	2.09	1.35	1.32
41	1	1402	PSU	O4'-C1'	-2.09	1.40	1.43
42	2	1419	OMU	C5-C4	2.09	1.48	1.43
44	7	162	A2M	O5'-C5'	-2.08	1.39	1.44
44	7	74	PSU	O2-C2	-2.08	1.19	1.23
20	S1	2184	MA6	C2-N3	2.08	1.35	1.32
41	1	695	OMC	C5-C4	2.08	1.47	1.42
20	S1	479	A2M	C2-N3	2.07	1.35	1.32
44	7	69	PSU	O4'-C1'	-2.06	1.41	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	1	437	A2M	O5'-C5'	-2.06	1.39	1.44
42	2	591	A2M	O5'-C5'	-2.05	1.39	1.44
20	S1	1979	OMU	C5-C4	2.04	1.48	1.43
42	2	1397	OMC	C5-C4	2.04	1.47	1.42
42	2	1159	OMC	C5-C4	2.01	1.47	1.42
42	2	510	PSU	C2-N3	-2.01	1.34	1.37
42	2	1303	PSU	C4-C5	2.01	1.49	1.44
41	1	858	A2M	O5'-C5'	-2.01	1.39	1.44
42	2	1354	PSU	O2-C2	-2.00	1.19	1.23
20	S1	1995	G7M	C5-C4	2.00	1.43	1.39

All (612) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	S1	2185	MA6	N1-C6-N6	-12.06	104.36	117.06
20	S1	2184	MA6	N1-C6-N6	-11.54	104.91	117.06
41	1	858	A2M	C5-C6-N6	11.39	137.67	120.35
42	2	628	A2M	C5-C6-N6	11.38	137.65	120.35
41	1	697	A2M	C5-C6-N6	11.23	137.42	120.35
42	2	604	A2M	C5-C6-N6	10.76	136.70	120.35
42	2	591	A2M	C5-C6-N6	10.64	136.52	120.35
41	1	437	A2M	C5-C6-N6	10.60	136.46	120.35
42	2	572	A2M	C5-C6-N6	10.58	136.43	120.35
42	2	1185	A2M	C5-C6-N6	10.46	136.25	120.35
44	7	43	A2M	C5-C6-N6	10.46	136.25	120.35
20	S1	479	A2M	C5-C6-N6	10.45	136.24	120.35
44	7	162	A2M	C5-C6-N6	10.44	136.22	120.35
20	S1	28	A2M	C5-C6-N6	10.39	136.13	120.35
20	S1	2021	A2M	C5-C6-N6	10.37	136.11	120.35
41	1	1539	A2M	C5-C6-N6	10.36	136.10	120.35
20	S1	668	A2M	C5-C6-N6	10.35	136.08	120.35
42	2	1372	A2M	C5-C6-N6	10.35	136.08	120.35
20	S1	897	A2M	C5-C6-N6	10.14	135.76	120.35
42	2	1384	A2M	C5-C6-N6	10.11	135.72	120.35
42	2	382	A2M	C5-C6-N6	10.11	135.71	120.35
41	1	955	A2M	C5-C6-N6	10.10	135.69	120.35
20	S1	98	A2M	C5-C6-N6	10.06	135.64	120.35
41	1	678	A2M	C5-C6-N6	10.01	135.57	120.35
42	2	527	A2M	C5-C6-N6	9.94	135.45	120.35
42	2	95	A2M	C5-C6-N6	9.93	135.45	120.35
42	2	665	A2M	C5-C6-N6	9.79	135.24	120.35
41	1	681	A2M	C5-C6-N6	9.77	135.20	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	2	570	A2M	C5-C6-N6	9.43	134.68	120.35
44	7	162	A2M	C1'-N9-C4	-8.29	112.08	126.64
41	1	858	A2M	N6-C6-N1	-8.05	101.86	118.57
41	1	697	A2M	N6-C6-N1	-7.70	102.60	118.57
42	2	1372	A2M	C1'-N9-C4	-7.53	113.42	126.64
20	S1	28	A2M	C1'-N9-C4	-7.51	113.45	126.64
42	2	572	A2M	N6-C6-N1	-7.49	103.02	118.57
20	S1	479	A2M	C1'-N9-C4	-7.47	113.52	126.64
20	S1	668	A2M	C1'-N9-C4	-7.47	113.52	126.64
41	1	437	A2M	C1'-N9-C4	-7.45	113.55	126.64
42	2	604	A2M	C1'-N9-C4	-7.39	113.65	126.64
41	1	437	A2M	N6-C6-N1	-7.37	103.27	118.57
42	2	604	A2M	N6-C6-N1	-7.34	103.33	118.57
41	1	697	A2M	C1'-N9-C4	-7.31	113.80	126.64
42	2	1372	A2M	N6-C6-N1	-7.22	103.58	118.57
20	S1	2021	A2M	N6-C6-N1	-7.22	103.58	118.57
42	2	591	A2M	N6-C6-N1	-7.20	103.63	118.57
20	S1	28	A2M	N6-C6-N1	-7.17	103.69	118.57
44	7	162	A2M	N6-C6-N1	-7.16	103.70	118.57
42	2	1185	A2M	N6-C6-N1	-7.16	103.72	118.57
42	2	1185	A2M	C1'-N9-C4	-7.14	114.10	126.64
44	7	43	A2M	N6-C6-N1	-7.14	103.76	118.57
20	S1	479	A2M	N6-C6-N1	-7.12	103.79	118.57
41	1	1539	A2M	C1'-N9-C4	-7.12	114.13	126.64
20	S1	668	A2M	N6-C6-N1	-7.10	103.83	118.57
41	1	678	A2M	N6-C6-N1	-7.06	103.92	118.57
42	2	527	A2M	C1'-N9-C4	-7.04	114.27	126.64
20	S1	98	A2M	C1'-N9-C4	-6.96	114.42	126.64
20	S1	897	A2M	N6-C6-N1	-6.94	104.18	118.57
20	S1	897	A2M	C1'-N9-C4	-6.93	114.47	126.64
42	2	527	A2M	N6-C6-N1	-6.93	104.20	118.57
42	2	382	A2M	N6-C6-N1	-6.92	104.21	118.57
41	1	955	A2M	N6-C6-N1	-6.87	104.30	118.57
42	2	572	A2M	C1'-N9-C4	-6.85	114.61	126.64
42	2	628	A2M	N6-C6-N1	-6.83	104.40	118.57
41	1	1539	A2M	N6-C6-N1	-6.80	104.45	118.57
20	S1	98	A2M	N6-C6-N1	-6.77	104.52	118.57
42	2	95	A2M	N6-C6-N1	-6.72	104.62	118.57
42	2	1384	A2M	C1'-N9-C4	-6.72	114.84	126.64
42	2	1384	A2M	N6-C6-N1	-6.71	104.65	118.57
44	7	43	A2M	C1'-N9-C4	-6.66	114.94	126.64
41	1	681	A2M	N6-C6-N1	-6.64	104.78	118.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	2	665	A2M	N6-C6-N1	-6.59	104.90	118.57
20	S1	2021	A2M	C1'-N9-C4	-6.53	115.17	126.64
41	1	681	A2M	C1'-N9-C4	-6.48	115.26	126.64
42	2	570	A2M	N6-C6-N1	-6.47	105.14	118.57
42	2	382	A2M	C1'-N9-C4	-6.44	115.32	126.64
42	2	95	A2M	C1'-N9-C4	-6.35	115.48	126.64
42	2	506	PSU	N1-C2-N3	6.35	122.33	115.13
42	2	628	A2M	C1'-N9-C4	-6.34	115.50	126.64
42	2	591	A2M	C1'-N9-C4	-6.33	115.52	126.64
42	2	500	PSU	N1-C2-N3	6.21	122.16	115.13
41	1	1371	OMU	C4-N3-C2	-6.18	118.43	126.58
41	1	858	A2M	C1'-N9-C4	-6.12	115.88	126.64
42	2	510	PSU	N1-C2-N3	6.04	121.97	115.13
41	1	678	A2M	C1'-N9-C4	-6.03	116.05	126.64
42	2	504	PSU	N1-C2-N3	5.95	121.87	115.13
41	1	955	A2M	C1'-N9-C4	-5.94	116.21	126.64
20	S1	1566	PSU	N1-C2-N3	5.92	121.83	115.13
42	2	527	A2M	N3-C2-N1	-5.91	119.44	128.68
44	7	162	A2M	N3-C2-N1	-5.90	119.45	128.68
42	2	572	A2M	N3-C2-N1	-5.86	119.52	128.68
44	7	43	A2M	N3-C2-N1	-5.72	119.74	128.68
41	1	1659	OMU	C4-N3-C2	-5.70	119.06	126.58
41	1	858	A2M	N3-C2-N1	-5.69	119.78	128.68
41	1	1539	A2M	N3-C2-N1	-5.67	119.82	128.68
81	3	13	OMU	C4-N3-C2	-5.67	119.10	126.58
42	2	665	A2M	C1'-N9-C4	-5.67	116.68	126.64
41	1	678	A2M	N3-C2-N1	-5.66	119.83	128.68
42	2	1077	OMU	C4-N3-C2	-5.65	119.13	126.58
42	2	570	A2M	N3-C2-N1	-5.64	119.86	128.68
42	2	1359	OMU	C4-N3-C2	-5.63	119.15	126.58
20	S1	2184	MA6	N3-C2-N1	-5.63	119.88	128.68
42	2	382	A2M	N3-C2-N1	-5.63	119.89	128.68
20	S1	28	A2M	N3-C2-N1	-5.62	119.90	128.68
20	S1	1979	OMU	C4-N3-C2	-5.59	119.20	126.58
20	S1	2021	A2M	N3-C2-N1	-5.56	119.98	128.68
42	2	1372	A2M	N3-C2-N1	-5.56	119.98	128.68
41	1	847	OMU	C4-N3-C2	-5.55	119.26	126.58
42	2	665	A2M	N3-C2-N1	-5.55	120.00	128.68
20	S1	668	A2M	N3-C2-N1	-5.54	120.03	128.68
42	2	604	A2M	N3-C2-N1	-5.53	120.03	128.68
20	S1	2185	MA6	N3-C2-N1	-5.53	120.04	128.68
20	S1	1621	OMU	C4-N3-C2	-5.50	119.32	126.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	1	437	A2M	N3-C2-N1	-5.49	120.09	128.68
42	2	1185	A2M	N3-C2-N1	-5.47	120.12	128.68
42	2	667	OMU	C4-N3-C2	-5.47	119.37	126.58
41	1	1107	OMU	C4-N3-C2	-5.46	119.38	126.58
42	2	591	A2M	N3-C2-N1	-5.46	120.15	128.68
41	1	697	A2M	N3-C2-N1	-5.45	120.15	128.68
20	S1	479	A2M	N3-C2-N1	-5.44	120.18	128.68
41	1	955	A2M	N3-C2-N1	-5.43	120.20	128.68
20	S1	2048	OMU	C4-N3-C2	-5.42	119.43	126.58
41	1	681	A2M	N3-C2-N1	-5.39	120.25	128.68
42	2	560	OMU	C4-N3-C2	-5.39	119.47	126.58
42	2	570	A2M	C1'-N9-C4	-5.39	117.17	126.64
20	S1	897	A2M	N3-C2-N1	-5.39	120.25	128.68
20	S1	1777	OMU	C4-N3-C2	-5.38	119.49	126.58
42	2	1384	A2M	N3-C2-N1	-5.33	120.34	128.68
20	S1	8	OMU	C4-N3-C2	-5.33	119.55	126.58
42	2	1419	OMU	C4-N3-C2	-5.32	119.56	126.58
20	S1	98	A2M	N3-C2-N1	-5.29	120.40	128.68
41	1	845	OMU	C4-N3-C2	-5.28	119.62	126.58
20	S1	661	OMU	C4-N3-C2	-5.28	119.62	126.58
20	S1	29	OMU	C4-N3-C2	-5.24	119.67	126.58
42	2	597	PSU	C4-N3-C2	-5.09	119.00	126.34
42	2	628	A2M	N3-C2-N1	-5.09	120.72	128.68
42	2	73	OMU	C4-N3-C2	-5.08	119.87	126.58
20	S1	1833	OMU	C4-N3-C2	-5.06	119.90	126.58
42	2	95	A2M	N3-C2-N1	-5.02	120.83	128.68
41	1	870	PSU	C4-N3-C2	-4.99	119.15	126.34
42	2	593	PSU	N1-C2-N3	4.98	120.78	115.13
42	2	437	PSU	C4-N3-C2	-4.92	119.24	126.34
42	2	78	PSU	C4-N3-C2	-4.91	119.27	126.34
42	2	1144	PSU	C4-N3-C2	-4.90	119.28	126.34
42	2	1194	PSU	C4-N3-C2	-4.90	119.29	126.34
42	2	1382	PSU	C4-N3-C2	-4.89	119.29	126.34
41	1	1533	PSU	C4-N3-C2	-4.89	119.29	126.34
41	1	1533	PSU	N1-C2-N3	4.88	120.66	115.13
41	1	672	PSU	C4-N3-C2	-4.84	119.36	126.34
42	2	593	PSU	C4-N3-C2	-4.83	119.39	126.34
41	1	422	PSU	C4-N3-C2	-4.80	119.42	126.34
42	2	1194	PSU	N1-C2-N3	4.78	120.55	115.13
42	2	1354	PSU	C4-N3-C2	-4.77	119.46	126.34
41	1	847	OMU	N3-C2-N1	4.77	121.22	114.89
42	2	1318	PSU	C4-N3-C2	-4.77	119.47	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	7	74	PSU	C4-N3-C2	-4.76	119.48	126.34
42	2	597	PSU	N1-C2-N3	4.76	120.52	115.13
42	2	1361	PSU	C4-N3-C2	-4.75	119.50	126.34
20	S1	1533	PSU	C4-N3-C2	-4.74	119.50	126.34
42	2	1144	PSU	N1-C2-N3	4.74	120.50	115.13
20	S1	2046	PSU	C4-N3-C2	-4.73	119.52	126.34
20	S1	12	PSU	C4-N3-C2	-4.72	119.54	126.34
42	2	1303	PSU	C4-N3-C2	-4.72	119.54	126.34
41	1	1011	PSU	C4-N3-C2	-4.71	119.56	126.34
42	2	1264	PSU	C4-N3-C2	-4.69	119.58	126.34
41	1	672	PSU	N1-C2-N3	4.68	120.43	115.13
41	1	1528	PSU	C4-N3-C2	-4.67	119.61	126.34
44	7	69	PSU	C4-N3-C2	-4.66	119.63	126.34
20	S1	455	PSU	C4-N3-C2	-4.66	119.63	126.34
20	S1	1841	PSU	C4-N3-C2	-4.63	119.67	126.34
20	S1	12	PSU	N1-C2-N3	4.62	120.37	115.13
41	1	1371	OMU	N3-C2-N1	4.60	121.00	114.89
42	2	1303	PSU	N1-C2-N3	4.59	120.33	115.13
42	2	1354	PSU	N1-C2-N3	4.59	120.33	115.13
20	S1	33	PSU	C4-N3-C2	-4.59	119.73	126.34
20	S1	609	PSU	C4-N3-C2	-4.59	119.73	126.34
20	S1	104	PSU	C4-N3-C2	-4.59	119.73	126.34
41	1	940	PSU	C4-N3-C2	-4.57	119.75	126.34
42	2	1413	PSU	C4-N3-C2	-4.57	119.75	126.34
42	2	1361	PSU	N1-C2-N3	4.54	120.28	115.13
42	2	472	PSU	C4-N3-C2	-4.54	119.80	126.34
20	S1	1657	PSU	C4-N3-C2	-4.53	119.81	126.34
20	S1	2046	PSU	N1-C2-N3	4.53	120.26	115.13
42	2	626	PSU	C4-N3-C2	-4.53	119.82	126.34
41	1	239	PSU	C4-N3-C2	-4.52	119.82	126.34
41	1	422	PSU	N1-C2-N3	4.52	120.25	115.13
20	S1	455	PSU	N1-C2-N3	4.51	120.24	115.13
20	S1	1156	PSU	C4-N3-C2	-4.50	119.86	126.34
41	1	1181	PSU	C4-N3-C2	-4.48	119.89	126.34
42	2	437	PSU	N1-C2-N3	4.47	120.19	115.13
42	2	662	PSU	C4-N3-C2	-4.45	119.92	126.34
20	S1	2202	PSU	C4-N3-C2	-4.42	119.97	126.34
41	1	1402	PSU	C4-N3-C2	-4.41	119.98	126.34
42	2	1060	PSU	C4-N3-C2	-4.41	119.99	126.34
41	1	1402	PSU	N1-C2-N3	4.40	120.11	115.13
42	2	626	PSU	N1-C2-N3	4.39	120.11	115.13
41	1	1171	PSU	C4-N3-C2	-4.39	120.01	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	7	74	PSU	N1-C2-N3	4.39	120.10	115.13
41	1	1664	PSU	C4-N3-C2	-4.37	120.04	126.34
41	1	1011	PSU	N1-C2-N3	4.37	120.08	115.13
42	2	1403	PSU	C4-N3-C2	-4.36	120.05	126.34
42	2	662	PSU	N1-C2-N3	4.35	120.06	115.13
20	S1	1539	PSU	C4-N3-C2	-4.35	120.07	126.34
41	1	870	PSU	N1-C2-N3	4.34	120.05	115.13
42	2	1264	PSU	N1-C2-N3	4.34	120.05	115.13
20	S1	1841	PSU	N1-C2-N3	4.32	120.02	115.13
42	2	1060	PSU	N1-C2-N3	4.31	120.02	115.13
20	S1	1533	PSU	N1-C2-N3	4.29	119.99	115.13
41	1	1017	PSU	C4-N3-C2	-4.29	120.16	126.34
42	2	1265	PSU	C4-N3-C2	-4.28	120.17	126.34
41	1	1181	PSU	N1-C2-N3	4.28	119.98	115.13
20	S1	2202	PSU	N1-C2-N3	4.27	119.97	115.13
20	S1	1246	PSU	C4-N3-C2	-4.25	120.22	126.34
42	2	1058	PSU	C4-N3-C2	-4.24	120.23	126.34
20	S1	33	PSU	N1-C2-N3	4.23	119.93	115.13
20	S1	1539	PSU	N1-C2-N3	4.22	119.91	115.13
20	S1	609	PSU	N1-C2-N3	4.22	119.91	115.13
42	2	667	OMU	N3-C2-N1	4.21	120.48	114.89
44	7	69	PSU	N1-C2-N3	4.21	119.90	115.13
20	S1	607	PSU	C4-N3-C2	-4.21	120.28	126.34
42	2	1058	PSU	N1-C2-N3	4.20	119.89	115.13
42	2	1413	PSU	N1-C2-N3	4.20	119.88	115.13
41	1	1017	PSU	N1-C2-N3	4.19	119.88	115.13
42	2	472	PSU	N1-C2-N3	4.18	119.86	115.13
42	2	1359	OMU	N3-C2-N1	4.17	120.42	114.89
41	1	940	PSU	N1-C2-N3	4.17	119.85	115.13
20	S1	607	PSU	N1-C2-N3	4.15	119.83	115.13
42	2	504	PSU	C3'-C2'-C1'	4.13	106.45	101.64
42	2	1077	OMU	N3-C2-N1	4.11	120.35	114.89
20	S1	104	PSU	N1-C2-N3	4.11	119.79	115.13
42	2	1382	PSU	N1-C2-N3	4.11	119.78	115.13
20	S1	1156	PSU	N1-C2-N3	4.08	119.76	115.13
42	2	73	OMU	N3-C2-N1	4.08	120.30	114.89
41	1	1171	PSU	N1-C2-N3	4.07	119.75	115.13
42	2	1318	PSU	N1-C2-N3	4.07	119.74	115.13
20	S1	1566	PSU	C4-N3-C2	-4.07	120.48	126.34
20	S1	1192	PSU	C4-N3-C2	-4.06	120.48	126.34
20	S1	1543	C4J	C4-N3-C2	-4.05	120.33	125.46
42	2	78	PSU	N1-C2-N3	4.04	119.71	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	S1	29	OMU	N3-C2-N1	4.03	120.23	114.89
42	2	506	PSU	C4-N3-C2	-4.02	120.55	126.34
41	1	1528	PSU	N1-C2-N3	4.01	119.68	115.13
42	2	1403	PSU	N1-C2-N3	4.00	119.66	115.13
20	S1	1246	PSU	N1-C2-N3	3.98	119.64	115.13
42	2	560	OMU	N3-C2-N1	3.97	120.16	114.89
42	2	1265	PSU	N1-C2-N3	3.97	119.62	115.13
41	1	1664	PSU	N1-C2-N3	3.95	119.61	115.13
20	S1	1777	OMU	N3-C2-N1	3.94	120.12	114.89
41	1	239	PSU	N1-C2-N3	3.94	119.60	115.13
20	S1	1478	OMG	C5-C6-N1	3.94	120.91	113.95
42	2	524	5MC	C5-C6-N1	-3.93	119.30	123.34
41	1	1659	OMU	N3-C2-N1	3.93	120.11	114.89
42	2	1229	OMG	C5-C6-N1	3.91	120.86	113.95
20	S1	1979	OMU	N3-C2-N1	3.91	120.08	114.89
81	3	13	OMU	C5-C4-N3	3.90	120.67	114.84
41	1	1659	OMU	C5-C4-N3	3.88	120.64	114.84
42	2	1419	OMU	N3-C2-N1	3.87	120.03	114.89
42	2	504	PSU	C4-N3-C2	-3.87	120.77	126.34
41	1	845	OMU	N3-C2-N1	3.86	120.02	114.89
41	1	1371	OMU	C5-C4-N3	3.86	120.62	114.84
20	S1	1621	OMU	N3-C2-N1	3.86	120.01	114.89
20	S1	8	OMU	N3-C2-N1	3.85	120.00	114.89
42	2	510	PSU	C4-N3-C2	-3.85	120.79	126.34
81	3	13	OMU	N3-C2-N1	3.84	119.99	114.89
20	S1	1833	OMU	N3-C2-N1	3.83	119.97	114.89
20	S1	1657	PSU	N1-C2-N3	3.82	119.46	115.13
20	S1	1192	PSU	N1-C2-N3	3.82	119.46	115.13
20	S1	661	OMU	N3-C2-N1	3.81	119.95	114.89
42	2	1078	OMG	C5-C6-N1	3.80	120.66	113.95
42	2	500	PSU	C4-N3-C2	-3.80	120.86	126.34
20	S1	2048	OMU	N3-C2-N1	3.79	119.92	114.89
41	1	1107	OMU	C5-C4-N3	3.78	120.49	114.84
42	2	1359	OMU	C5-C4-N3	3.76	120.47	114.84
20	S1	2061	5MC	C5-C6-N1	-3.73	119.50	123.34
20	S1	1544	5MC	C5-C6-N1	-3.73	119.51	123.34
43	4	74	OMG	C5-C6-N1	3.72	120.53	113.95
42	2	504	PSU	O2-C2-N1	-3.71	118.71	122.79
42	2	1231	OMG	C5-C6-N1	3.68	120.45	113.95
20	S1	1550	OMG	C5-C6-N1	3.67	120.43	113.95
41	1	1190	OMG	C5-C6-N1	3.67	120.43	113.95
42	2	1419	OMU	C5-C4-N3	3.67	120.33	114.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	S1	1979	OMU	C5-C4-N3	3.66	120.31	114.84
42	2	1253	OMG	C5-C6-N1	3.65	120.41	113.95
42	2	667	OMU	C5-C4-N3	3.63	120.27	114.84
41	1	845	OMU	C5-C4-N3	3.62	120.25	114.84
42	2	641	OMG	C5-C6-N1	3.62	120.34	113.95
42	2	534	OMG	C5-C6-N1	3.60	120.31	113.95
41	1	1107	OMU	N3-C2-N1	3.60	119.67	114.89
20	S1	2151	OMG	C5-C6-N1	3.59	120.30	113.95
20	S1	1865	OMG	C5-C6-N1	3.59	120.29	113.95
42	2	500	PSU	C3'-C2'-C1'	3.59	105.82	101.64
20	S1	1623	OMG	C5-C6-N1	3.59	120.28	113.95
42	2	1360	OMG	C5-C6-N1	3.59	120.28	113.95
20	S1	1647	OMG	C5-C6-N1	3.59	120.28	113.95
20	S1	2048	OMU	C5-C4-N3	3.58	120.20	114.84
42	2	1077	OMU	C5-C4-N3	3.58	120.19	114.84
20	S1	12	PSU	C6-C5-C4	3.57	120.69	118.20
20	S1	1621	OMU	C5-C4-N3	3.57	120.18	114.84
42	2	506	PSU	C3'-C2'-C1'	3.56	105.79	101.64
41	1	1402	PSU	C6-N1-C2	-3.55	119.06	122.68
41	1	959	OMG	C5-C6-N1	3.55	120.21	113.95
41	1	1626	OMG	C5-C6-N1	3.54	120.21	113.95
20	S1	600	OMG	C5-C6-N1	3.53	120.19	113.95
41	1	1533	PSU	O2-C2-N1	-3.52	118.91	122.79
41	1	1524	OMG	C5-C6-N1	3.52	120.17	113.95
41	1	1402	PSU	O2-C2-N1	-3.51	118.93	122.79
41	1	1533	PSU	C6-N1-C2	-3.51	119.10	122.68
20	S1	1777	OMU	C5-C4-N3	3.49	120.06	114.84
41	1	856	OMG	C5-C6-N1	3.49	120.12	113.95
44	7	75	OMG	C5-C6-N1	3.49	120.11	113.95
41	1	1540	OMG	C5-C6-N1	3.49	120.11	113.95
42	2	655	OMG	C5-C6-N1	3.48	120.09	113.95
20	S1	8	OMU	C5-C4-N3	3.47	120.03	114.84
20	S1	661	OMU	C5-C4-N3	3.46	120.02	114.84
42	2	506	PSU	O2-C2-N1	-3.45	118.99	122.79
42	2	1361	PSU	C6-N1-C2	-3.45	119.16	122.68
20	S1	1566	PSU	C3'-C2'-C1'	3.43	105.63	101.64
42	2	71	OMG	C5-C6-N1	3.41	119.98	113.95
42	2	1060	PSU	C6-N1-C2	-3.40	119.20	122.68
42	2	1046	OMG	C5-C6-N1	3.40	119.95	113.95
42	2	641	OMG	C8-N7-C5	3.39	109.46	102.99
41	1	1171	PSU	C6-N1-C2	-3.35	119.26	122.68
20	S1	512	A2M	N3-C2-N1	-3.34	123.45	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	S1	1829	OMG	C5-C6-N1	3.34	119.85	113.95
42	2	593	PSU	C6-N1-C2	-3.32	119.28	122.68
20	S1	1246	PSU	C6-N1-C2	-3.31	119.30	122.68
42	2	500	PSU	O2-C2-N1	-3.30	119.15	122.79
20	S1	29	OMU	C5-C4-N3	3.28	119.75	114.84
20	S1	607	PSU	C6-N1-C2	-3.28	119.33	122.68
42	2	560	OMU	C5-C4-N3	3.27	119.73	114.84
42	2	510	PSU	O2-C2-N1	-3.24	119.22	122.79
41	1	1524	OMG	C2-N1-C6	-3.23	119.16	125.10
42	2	570	A2M	O2'-C2'-C1'	3.22	115.48	109.09
20	S1	2046	PSU	C6-N1-C2	-3.22	119.39	122.68
20	S1	2048	OMU	O4-C4-C5	-3.21	119.51	125.16
41	1	1371	OMU	C1'-N1-C2	3.21	123.38	117.57
42	2	1308	5MC	C5-C6-N1	-3.21	120.04	123.34
20	S1	1833	OMU	C5-C4-N3	3.20	119.62	114.84
20	S1	1566	PSU	O2-C2-N1	-3.20	119.27	122.79
20	S1	1539	PSU	C6-N1-C2	-3.19	119.42	122.68
42	2	662	PSU	C6-N1-C2	-3.19	119.42	122.68
41	1	422	PSU	C6-N1-C2	-3.17	119.44	122.68
42	2	1078	OMG	C8-N7-C5	3.16	109.01	102.99
42	2	1058	PSU	C6-N1-C2	-3.16	119.46	122.68
41	1	847	OMU	C5-C4-N3	3.15	119.56	114.84
42	2	1194	PSU	C6-N1-C2	-3.14	119.48	122.68
42	2	1354	PSU	C6-N1-C2	-3.14	119.48	122.68
20	S1	455	PSU	C6-N1-C2	-3.12	119.49	122.68
42	2	73	OMU	C5-C4-N3	3.12	119.50	114.84
41	1	856	OMG	C8-N7-C5	3.11	108.91	102.99
42	2	655	OMG	C8-N7-C5	3.10	108.90	102.99
42	2	1403	PSU	C6-N1-C2	-3.10	119.51	122.68
42	2	1361	PSU	O2-C2-N1	-3.09	119.39	122.79
41	1	1011	PSU	C6-C5-C4	3.09	120.36	118.20
20	S1	2202	PSU	C6-N1-C2	-3.08	119.53	122.68
20	S1	1192	PSU	C6-N1-C2	-3.08	119.54	122.68
20	S1	1841	PSU	C6-N1-C2	-3.07	119.54	122.68
41	1	1524	OMG	C8-N7-C5	3.06	108.82	102.99
41	1	1540	OMG	C8-N7-C5	3.06	108.82	102.99
20	S1	1995	G7M	C2-N1-C6	-3.04	119.51	125.10
81	3	13	OMU	O4-C4-C5	-3.03	119.83	125.16
41	1	959	OMG	C2-N1-C6	-3.03	119.52	125.10
41	1	1190	OMG	C2-N1-C6	-3.03	119.53	125.10
41	1	1659	OMU	O4-C4-C5	-3.03	119.84	125.16
42	2	1265	PSU	C6-N1-C2	-3.02	119.59	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	1	845	OMU	O4-C4-C5	-3.02	119.86	125.16
42	2	1194	PSU	O2-C2-N1	-3.01	119.48	122.79
20	S1	12	PSU	C6-N1-C2	-3.00	119.61	122.68
44	7	75	OMG	C8-N7-C5	2.99	108.69	102.99
41	1	1181	PSU	C6-N1-C2	-2.99	119.62	122.68
20	S1	609	PSU	C6-N1-C2	-2.99	119.62	122.68
41	1	1017	PSU	C6-N1-C2	-2.98	119.63	122.68
41	1	1190	OMG	C8-N7-C5	2.98	108.67	102.99
42	2	1144	PSU	C6-N1-C2	-2.98	119.64	122.68
20	S1	1550	OMG	C2-N1-C6	-2.97	119.62	125.10
42	2	1303	PSU	C6-N1-C2	-2.96	119.66	122.68
42	2	628	A2M	O4'-C4'-C3'	-2.95	99.27	105.11
20	S1	1979	OMU	O4-C4-C5	-2.95	119.96	125.16
41	1	1664	PSU	C6-N1-C2	-2.95	119.67	122.68
42	2	1078	OMG	C2-N1-C6	-2.95	119.67	125.10
42	2	1360	OMG	C2-N1-C6	-2.95	119.67	125.10
20	S1	1647	OMG	C8-N7-C5	2.95	108.60	102.99
20	S1	2151	OMG	C8-N7-C5	2.95	108.60	102.99
41	1	1533	PSU	C6-C5-C4	2.94	120.26	118.20
42	2	597	PSU	C6-N1-C2	-2.94	119.68	122.68
20	S1	1777	OMU	O4-C4-C5	-2.93	120.00	125.16
20	S1	1657	PSU	C6-N1-C2	-2.93	119.68	122.68
42	2	472	PSU	C6-N1-C2	-2.93	119.69	122.68
42	2	1229	OMG	C8-N7-C5	2.93	108.57	102.99
42	2	1264	PSU	C6-N1-C2	-2.93	119.69	122.68
20	S1	33	PSU	C6-N1-C2	-2.92	119.69	122.68
41	1	1540	OMG	N2-C2-N1	2.92	122.93	116.71
41	1	847	OMU	O2-C2-N1	-2.92	118.90	122.79
20	S1	1623	OMG	C2-N1-C6	-2.92	119.72	125.10
41	1	672	PSU	C6-N1-C2	-2.92	119.70	122.68
42	2	1046	OMG	C8-N7-C5	2.91	108.54	102.99
41	1	1011	PSU	C6-N1-C2	-2.90	119.72	122.68
42	2	534	OMG	C2-N1-C6	-2.90	119.76	125.10
20	S1	600	OMG	C8-N7-C5	2.90	108.51	102.99
20	S1	1647	OMG	C2-N1-C6	-2.89	119.77	125.10
20	S1	29	OMU	O4-C4-C5	-2.89	120.07	125.16
20	S1	1865	OMG	C2-N1-C6	-2.89	119.78	125.10
20	S1	1478	OMG	C8-N7-C5	2.88	108.48	102.99
20	S1	1621	OMU	O4-C4-C5	-2.87	120.11	125.16
42	2	626	PSU	C6-N1-C2	-2.86	119.75	122.68
41	1	1371	OMU	O4-C4-C5	-2.85	120.15	125.16
42	2	71	OMG	C8-N7-C5	2.85	108.42	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	S1	600	OMG	C2-N1-C6	-2.85	119.85	125.10
41	1	1626	OMG	C8-N7-C5	2.85	108.41	102.99
20	S1	1623	OMG	C8-N7-C5	2.84	108.40	102.99
20	S1	1829	OMG	C8-N7-C5	2.84	108.39	102.99
42	2	437	PSU	C6-N1-C2	-2.83	119.79	122.68
42	2	1360	OMG	C8-N7-C5	2.82	108.37	102.99
20	S1	455	PSU	C6-C5-C4	2.82	120.17	118.20
41	1	940	PSU	C6-N1-C2	-2.80	119.82	122.68
20	S1	8	OMU	O4-C4-C5	-2.80	120.23	125.16
43	4	74	OMG	C2-N1-C6	-2.80	119.95	125.10
20	S1	1833	OMU	O4-C4-C5	-2.79	120.25	125.16
20	S1	2151	OMG	C2-N1-C6	-2.79	119.96	125.10
20	S1	1865	OMG	C8-N7-C5	2.79	108.30	102.99
42	2	1413	PSU	C6-N1-C2	-2.79	119.83	122.68
42	2	1046	OMG	C2-N1-C6	-2.78	119.97	125.10
20	S1	1156	PSU	C6-N1-C2	-2.78	119.84	122.68
42	2	1194	PSU	C6-C5-C4	2.78	120.14	118.20
20	S1	661	OMU	O4-C4-C5	-2.78	120.28	125.16
44	7	74	PSU	C6-N1-C2	-2.77	119.85	122.68
41	1	1540	OMG	C2-N1-C6	-2.77	120.00	125.10
20	S1	1478	OMG	C2-N1-C6	-2.77	120.00	125.10
41	1	856	OMG	C2-N1-C6	-2.76	120.02	125.10
44	7	75	OMG	C2-N1-C6	-2.75	120.03	125.10
20	S1	1829	OMG	C2-N1-C6	-2.75	120.03	125.10
20	S1	512	A2M	C4-C5-N7	-2.73	106.55	109.40
42	2	1413	PSU	O2-C2-N1	-2.73	119.79	122.79
42	2	73	OMU	O4-C4-C5	-2.73	120.37	125.16
20	S1	2046	PSU	C6-C5-C4	2.72	120.10	118.20
41	1	1626	OMG	C2-N1-C6	-2.72	120.08	125.10
20	S1	1533	PSU	C6-N1-C2	-2.72	119.90	122.68
42	2	641	OMG	C2-N1-C6	-2.72	120.09	125.10
42	2	1253	OMG	C8-N7-C5	2.71	108.15	102.99
41	1	1528	PSU	O2-C2-N1	-2.71	119.81	122.79
41	1	1107	OMU	O4-C4-C5	-2.70	120.41	125.16
42	2	1303	PSU	O2-C2-N1	-2.70	119.82	122.79
20	S1	1550	OMG	C8-N7-C5	2.70	108.13	102.99
43	4	74	OMG	C8-N7-C5	2.69	108.12	102.99
42	2	1231	OMG	C8-N7-C5	2.69	108.12	102.99
42	2	655	OMG	C2-N1-C6	-2.69	120.14	125.10
42	2	527	A2M	O4'-C1'-C2'	-2.69	101.92	106.59
42	2	71	OMG	N2-C2-N1	2.69	122.44	116.71
20	S1	104	PSU	C6-N1-C2	-2.68	119.94	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	S1	1246	PSU	O2-C2-N1	-2.68	119.84	122.79
42	2	1144	PSU	C6-C5-C4	2.68	120.07	118.20
42	2	1303	PSU	C6-C5-C4	2.68	120.07	118.20
20	S1	2202	PSU	O2-C2-N1	-2.67	119.86	122.79
20	S1	1647	OMG	N2-C2-N1	2.66	122.38	116.71
20	S1	1833	OMU	C1'-N1-C2	2.66	122.39	117.57
42	2	534	OMG	C8-N7-C5	2.66	108.05	102.99
42	2	572	A2M	O4'-C1'-C2'	-2.66	101.98	106.59
42	2	641	OMG	N2-C2-N1	2.65	122.35	116.71
20	S1	1841	PSU	O2-C2-N1	-2.64	119.88	122.79
42	2	1229	OMG	C2-N1-C6	-2.64	120.24	125.10
41	1	847	OMU	O4-C4-C5	-2.64	120.52	125.16
42	2	1359	OMU	O4-C4-C5	-2.64	120.52	125.16
20	S1	2046	PSU	O2-C2-N1	-2.63	119.90	122.79
41	1	1107	OMU	O2-C2-N1	-2.62	119.30	122.79
42	2	1253	OMG	N2-C2-N1	2.62	122.30	116.71
41	1	1626	OMG	N2-C2-N1	2.61	122.28	116.71
42	2	667	OMU	O4-C4-C5	-2.61	120.57	125.16
41	1	239	PSU	C6-N1-C2	-2.60	120.02	122.68
44	7	69	PSU	C6-N1-C2	-2.60	120.02	122.68
44	7	74	PSU	O2-C2-N1	-2.60	119.93	122.79
20	S1	609	PSU	C6-C5-C4	2.60	120.02	118.20
41	1	672	PSU	O2-C2-N1	-2.59	119.94	122.79
42	2	1253	OMG	C2-N1-C6	-2.59	120.33	125.10
42	2	1382	PSU	C6-N1-C2	-2.59	120.04	122.68
20	S1	1539	PSU	O2-C2-N1	-2.58	119.95	122.79
20	S1	1865	OMG	N2-C2-N1	2.57	122.19	116.71
41	1	1171	PSU	O2-C2-N1	-2.56	119.97	122.79
20	S1	1533	PSU	O2-C2-N1	-2.55	119.98	122.79
42	2	78	PSU	C6-N1-C2	-2.55	120.08	122.68
42	2	1078	OMG	N2-C2-N1	2.54	122.12	116.71
42	2	1419	OMU	O4-C4-C5	-2.54	120.70	125.16
20	S1	607	PSU	O2-C2-N1	-2.53	120.00	122.79
42	2	437	PSU	O2-C2-N1	-2.52	120.01	122.79
42	2	71	OMG	C2-N1-C6	-2.52	120.45	125.10
41	1	422	PSU	O2-C2-N1	-2.51	120.03	122.79
42	2	73	OMU	O2-C2-N1	-2.51	119.45	122.79
20	S1	1543	C4J	N3-C2-N1	2.50	120.28	116.76
42	2	1077	OMU	O4-C4-C5	-2.49	120.77	125.16
42	2	1231	OMG	N1-C2-N3	-2.49	118.67	123.32
43	4	74	OMG	N2-C2-N1	2.49	122.02	116.71
20	S1	1533	PSU	C6-C5-C4	2.49	119.94	118.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	2	1229	OMG	O6-C6-N1	-2.48	117.72	120.65
20	S1	1841	PSU	C6-C5-C4	2.46	119.92	118.20
20	S1	1865	OMG	O6-C6-C5	-2.45	119.58	124.37
41	1	1190	OMG	N2-C2-N1	2.45	121.92	116.71
20	S1	1621	OMU	O2-C2-N1	-2.45	119.53	122.79
44	7	75	OMG	N2-C2-N1	2.45	121.92	116.71
41	1	1528	PSU	C6-N1-C2	-2.45	120.18	122.68
42	2	1231	OMG	C2-N1-C6	-2.45	120.59	125.10
42	2	593	PSU	C6-C5-C4	2.44	119.91	118.20
41	1	940	PSU	C6-C5-C4	2.44	119.91	118.20
41	1	940	PSU	O2-C2-N1	-2.44	120.10	122.79
20	S1	1543	C4J	C31-C3-N3	-2.44	107.43	112.00
20	S1	455	PSU	O2-C2-N1	-2.44	120.11	122.79
42	2	1229	OMG	N1-C2-N3	-2.43	118.77	123.32
20	S1	609	PSU	O2-C2-N1	-2.42	120.12	122.79
42	2	597	PSU	O2-C2-N1	-2.42	120.12	122.79
41	1	959	OMG	C8-N7-C5	2.42	107.61	102.99
41	1	959	OMG	O6-C6-C5	-2.42	119.64	124.37
42	2	1360	OMG	N2-C2-N1	2.42	121.86	116.71
20	S1	1543	C4J	C3-N3-C4	2.41	120.86	117.31
41	1	1524	OMG	N2-C2-N1	2.39	121.81	116.71
20	S1	33	PSU	C6-C5-C4	2.39	119.87	118.20
20	S1	104	PSU	C6-C5-C4	2.39	119.87	118.20
41	1	856	OMG	N2-C2-N1	2.39	121.80	116.71
42	2	510	PSU	C3'-C2'-C1'	2.38	104.41	101.64
42	2	1354	PSU	O2-C2-N1	-2.38	120.17	122.79
42	2	667	OMU	O2-C2-N1	-2.38	119.62	122.79
42	2	593	PSU	O2-C2-N1	-2.38	120.17	122.79
42	2	655	OMG	N2-C2-N1	2.38	121.78	116.71
42	2	1264	PSU	C6-C5-C4	2.38	119.86	118.20
42	2	1248	OMC	O2-C2-N3	-2.37	118.47	122.33
41	1	1107	OMU	C2'-C1'-N1	-2.37	109.62	114.22
41	1	1664	PSU	O2-C2-N1	-2.37	120.18	122.79
42	2	472	PSU	O2-C2-N1	-2.37	120.19	122.79
41	1	672	PSU	C6-C5-C4	2.37	119.85	118.20
20	S1	33	PSU	O2-C2-N1	-2.36	120.19	122.79
20	S1	1657	PSU	O2-C2-N1	-2.35	120.21	122.79
42	2	1265	PSU	O2-C2-N1	-2.34	120.22	122.79
20	S1	1478	OMG	N1-C2-N3	-2.33	118.96	123.32
20	S1	1550	OMG	O6-C6-C5	-2.33	119.82	124.37
42	2	1403	PSU	O2-C2-N1	-2.33	120.23	122.79
42	2	1308	5MC	O2-C2-N3	-2.33	118.55	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	S1	1156	PSU	C6-C5-C4	2.32	119.82	118.20
41	1	1017	PSU	O2-C2-N1	-2.32	120.24	122.79
42	2	1359	OMU	O2-C2-N1	-2.31	119.71	122.79
42	2	1317	OMC	O2-C2-N3	-2.30	118.59	122.33
20	S1	1192	PSU	O2-C2-N1	-2.29	120.27	122.79
41	1	1371	OMU	O2-C2-N3	-2.28	117.25	121.50
20	S1	1478	OMG	N2-C2-N1	2.28	121.56	116.71
42	2	78	PSU	C5-C4-N3	2.27	121.71	116.58
20	S1	1550	OMG	N2-C2-N1	2.26	121.52	116.71
42	2	560	OMU	O4-C4-C5	-2.26	121.19	125.16
20	S1	104	PSU	O2-C2-N1	-2.26	120.31	122.79
20	S1	607	PSU	C6-C5-C4	2.26	119.78	118.20
41	1	422	PSU	C6-C5-C4	2.26	119.78	118.20
20	S1	12	PSU	O2-C2-N1	-2.25	120.31	122.79
20	S1	2061	5MC	C5-C4-N3	-2.23	119.26	121.67
20	S1	8	OMU	O2-C2-N1	-2.22	119.83	122.79
42	2	1058	PSU	C6-C5-C4	2.22	119.75	118.20
41	1	1539	A2M	O4'-C1'-C2'	-2.20	102.77	106.59
42	2	1229	OMG	N2-C2-N1	2.20	121.39	116.71
44	7	74	PSU	C6-C5-C4	2.20	119.73	118.20
42	2	472	PSU	C6-C5-C4	2.19	119.73	118.20
42	2	1253	OMG	N1-C2-N3	-2.19	119.22	123.32
42	2	1046	OMG	N2-C2-N1	2.19	121.38	116.71
42	2	641	OMG	N1-C2-N3	-2.19	119.22	123.32
42	2	1318	PSU	C6-N1-C2	-2.19	120.44	122.68
42	2	1361	PSU	C6-C5-C4	2.18	119.72	118.20
20	S1	1647	OMG	O6-C6-C5	-2.16	120.16	124.37
44	7	69	PSU	O4'-C1'-C2'	2.16	108.19	105.14
41	1	1011	PSU	O2-C2-N1	-2.16	120.42	122.79
20	S1	2202	PSU	C6-C5-C4	2.15	119.70	118.20
81	3	13	OMU	O2-C2-N1	-2.15	119.92	122.79
42	2	1308	5MC	C5-C4-N3	-2.15	119.36	121.67
42	2	534	OMG	O6-C6-C5	-2.15	120.18	124.37
42	2	1303	PSU	O4'-C1'-C2'	2.14	108.16	105.14
20	S1	1156	PSU	O2-C2-N1	-2.14	120.44	122.79
41	1	239	PSU	O2-C2-N1	-2.14	120.44	122.79
20	S1	1566	PSU	C5-C6-N1	-2.13	118.91	122.11
42	2	1264	PSU	O2-C2-N1	-2.13	120.44	122.79
42	2	1318	PSU	O2-C2-N1	-2.13	120.44	122.79
20	S1	1777	OMU	O2-C2-N1	-2.13	119.95	122.79
42	2	524	5MC	CM5-C5-C6	-2.12	120.01	122.85
20	S1	1543	C4J	C5-C4-N3	2.12	120.10	116.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	S1	1829	OMG	N2-C2-N1	2.12	121.22	116.71
42	2	1360	OMG	O6-C6-C5	-2.11	120.24	124.37
42	2	78	PSU	O2-C2-N1	-2.11	120.47	122.79
42	2	1354	PSU	C6-C5-C4	2.11	119.67	118.20
42	2	1253	OMG	O6-C6-N1	-2.11	118.16	120.65
42	2	1382	PSU	O2-C2-N1	-2.11	120.47	122.79
41	1	870	PSU	C6-C5-C4	2.11	119.67	118.20
42	2	71	OMG	N1-C2-N3	-2.10	119.39	123.32
43	4	74	OMG	O6-C6-C5	-2.10	120.27	124.37
41	1	1190	OMG	O6-C6-C5	-2.10	120.27	124.37
42	2	1060	PSU	O2-C2-N1	-2.09	120.48	122.79
20	S1	2151	OMG	O6-C6-C5	-2.09	120.29	124.37
41	1	1181	PSU	O2-C2-N1	-2.09	120.49	122.79
44	7	75	OMG	N1-C2-N3	-2.09	119.42	123.32
43	4	74	OMG	N1-C2-N3	-2.09	119.42	123.32
42	2	1265	PSU	C6-C5-C4	2.08	119.65	118.20
41	1	1171	PSU	O4'-C1'-C2'	2.08	108.07	105.14
42	2	510	PSU	C5-C6-N1	-2.07	119.00	122.11
20	S1	1623	OMG	O6-C6-C5	-2.07	120.32	124.37
42	2	1078	OMG	O6-C6-N1	-2.07	118.20	120.65
41	1	1017	PSU	C6-C5-C4	2.07	119.65	118.20
20	S1	29	OMU	O2-C2-N1	-2.07	120.03	122.79
42	2	437	PSU	C6-C5-C4	2.07	119.64	118.20
41	1	856	OMG	N1-C2-N3	-2.07	119.46	123.32
42	2	1382	PSU	O4'-C1'-C2'	2.07	108.06	105.14
20	S1	2048	OMU	C1'-N1-C2	2.06	121.30	117.57
41	1	1540	OMG	N1-C2-N3	-2.06	119.48	123.32
42	2	1231	OMG	N2-C2-N1	2.05	121.08	116.71
41	1	1659	OMU	O2-C2-N1	-2.05	120.06	122.79
42	2	662	PSU	O4'-C1'-C2'	2.05	108.03	105.14
42	2	662	PSU	O2-C2-N1	-2.04	120.55	122.79
41	1	677	1MA	C5-C6-N1	-2.03	110.87	113.90
41	1	239	PSU	C6-C5-C4	2.02	119.61	118.20
41	1	1626	OMG	N1-C2-N3	-2.02	119.54	123.32
41	1	870	PSU	C6-N1-C2	-2.02	120.62	122.68
20	S1	897	A2M	C5'-C4'-C3'	-2.02	107.62	115.18
42	2	506	PSU	C5-C6-N1	-2.02	119.08	122.11
41	1	1181	PSU	C6-C5-C4	2.02	119.61	118.20

There are no chirality outliers.

All (132) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
44	7	69	PSU	O4'-C1'-C5-C4
44	7	69	PSU	O4'-C1'-C5-C6
44	7	162	A2M	C1'-C2'-O2'-CM'
20	S1	33	PSU	C3'-C4'-C5'-O5'
20	S1	33	PSU	O4'-C4'-C5'-O5'
20	S1	479	A2M	C1'-C2'-O2'-CM'
20	S1	512	A2M	C1'-C2'-O2'-CM'
20	S1	607	PSU	C2'-C1'-C5-C4
20	S1	607	PSU	O4'-C1'-C5-C4
20	S1	607	PSU	C2'-C1'-C5-C6
20	S1	607	PSU	O4'-C1'-C5-C6
20	S1	607	PSU	C3'-C4'-C5'-O5'
20	S1	668	A2M	O4'-C4'-C5'-O5'
20	S1	668	A2M	C3'-C4'-C5'-O5'
20	S1	668	A2M	C1'-C2'-O2'-CM'
20	S1	897	A2M	O4'-C4'-C5'-O5'
20	S1	897	A2M	C3'-C4'-C5'-O5'
20	S1	1192	PSU	C3'-C4'-C5'-O5'
20	S1	1192	PSU	O4'-C4'-C5'-O5'
20	S1	1246	PSU	C3'-C4'-C5'-O5'
20	S1	1833	OMU	O4'-C1'-N1-C2
20	S1	1833	OMU	O4'-C1'-N1-C6
20	S1	1979	OMU	C3'-C4'-C5'-O5'
20	S1	1979	OMU	O4'-C4'-C5'-O5'
41	1	239	PSU	C3'-C4'-C5'-O5'
41	1	239	PSU	O4'-C4'-C5'-O5'
41	1	437	A2M	C1'-C2'-O2'-CM'
41	1	959	OMG	O4'-C4'-C5'-O5'
41	1	959	OMG	C1'-C2'-O2'-CM2
41	1	1371	OMU	O4'-C1'-N1-C2
41	1	1371	OMU	O4'-C1'-N1-C6
41	1	1371	OMU	C3'-C4'-C5'-O5'
41	1	1540	OMG	O4'-C4'-C5'-O5'
42	2	78	PSU	C3'-C4'-C5'-O5'
42	2	95	A2M	C1'-C2'-O2'-CM'
42	2	382	A2M	C1'-C2'-O2'-CM'
42	2	500	PSU	C2'-C1'-C5-C4
42	2	500	PSU	O4'-C1'-C5-C4
42	2	500	PSU	O4'-C1'-C5-C6
42	2	504	PSU	C4'-C5'-O5'-P
42	2	534	OMG	O4'-C4'-C5'-O5'
42	2	534	OMG	C3'-C4'-C5'-O5'
42	2	570	A2M	C1'-C2'-O2'-CM'

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Mol	Chain	Res	Type	Atoms
42	2	1046	OMG	O4'-C4'-C5'-O5'
42	2	1265	PSU	C3'-C4'-C5'-O5'
42	2	1265	PSU	O4'-C4'-C5'-O5'
42	2	1303	PSU	C3'-C4'-C5'-O5'
42	2	1303	PSU	O4'-C4'-C5'-O5'
42	2	1308	5MC	C3'-C4'-C5'-O5'
42	2	1384	A2M	C1'-C2'-O2'-CM'
42	2	1419	OMU	C1'-C2'-O2'-CM2
20	S1	512	A2M	O4'-C4'-C5'-O5'
20	S1	600	OMG	O4'-C4'-C5'-O5'
20	S1	2140	OMC	C3'-C4'-C5'-O5'
41	1	681	A2M	O4'-C4'-C5'-O5'
41	1	681	A2M	C3'-C4'-C5'-O5'
41	1	1540	OMG	C3'-C4'-C5'-O5'
42	2	527	A2M	O4'-C4'-C5'-O5'
42	2	527	A2M	C3'-C4'-C5'-O5'
42	2	1046	OMG	C3'-C4'-C5'-O5'
20	S1	512	A2M	C3'-C4'-C5'-O5'
20	S1	600	OMG	C3'-C4'-C5'-O5'
20	S1	1550	OMG	C3'-C4'-C5'-O5'
20	S1	2140	OMC	O4'-C4'-C5'-O5'
41	1	1371	OMU	O4'-C4'-C5'-O5'
42	2	78	PSU	O4'-C4'-C5'-O5'
42	2	665	A2M	O4'-C4'-C5'-O5'
42	2	1308	5MC	O4'-C4'-C5'-O5'
42	2	443	OMC	C2'-C1'-N1-C6
20	S1	8	OMU	C2'-C1'-N1-C6
42	2	443	OMC	C2'-C1'-N1-C2
20	S1	1246	PSU	O4'-C4'-C5'-O5'
42	2	504	PSU	O4'-C4'-C5'-O5'
42	2	665	A2M	C3'-C4'-C5'-O5'
20	S1	1543	C4J	C4'-C5'-O5'-P
20	S1	607	PSU	O4'-C4'-C5'-O5'
20	S1	1533	PSU	C3'-C4'-C5'-O5'
20	S1	1550	OMG	O4'-C4'-C5'-O5'
41	1	1181	PSU	C3'-C4'-C5'-O5'
42	2	1308	5MC	C2'-C1'-N1-C6
20	S1	2021	A2M	C3'-C4'-C5'-O5'
42	2	1185	A2M	C3'-C4'-C5'-O5'
42	2	443	OMC	O4'-C1'-N1-C6
20	S1	2021	A2M	O4'-C4'-C5'-O5'
42	2	604	A2M	C1'-C2'-O2'-CM'

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Mol	Chain	Res	Type	Atoms
42	2	1308	5MC	O4'-C1'-N1-C6
41	1	681	A2M	C4'-C5'-O5'-P
42	2	1361	PSU	C4'-C5'-O5'-P
20	S1	1829	OMG	O4'-C4'-C5'-O5'
42	2	655	OMG	C3'-C2'-O2'-CM2
20	S1	8	OMU	O4'-C1'-N1-C6
42	2	443	OMC	O4'-C1'-N1-C2
42	2	1308	5MC	O4'-C1'-N1-C2
42	2	506	PSU	C4'-C5'-O5'-P
42	2	560	OMU	C4'-C5'-O5'-P
20	S1	1533	PSU	O4'-C4'-C5'-O5'
41	1	1181	PSU	O4'-C4'-C5'-O5'
42	2	1185	A2M	O4'-C4'-C5'-O5'
20	S1	1478	OMG	C4'-C5'-O5'-P
41	1	1181	PSU	C4'-C5'-O5'-P
42	2	1248	OMC	C4'-C5'-O5'-P
20	S1	8	OMU	O4'-C4'-C5'-O5'
20	S1	1833	OMU	C4'-C5'-O5'-P
20	S1	8	OMU	C2'-C1'-N1-C2
20	S1	8	OMU	O4'-C1'-N1-C2
41	1	1171	PSU	O4'-C1'-C5-C4
42	2	1361	PSU	O4'-C1'-C5-C4
42	2	1359	OMU	C3'-C2'-O2'-CM2
42	2	504	PSU	C3'-C4'-C5'-O5'
42	2	1060	PSU	C3'-C4'-C5'-O5'
20	S1	1543	C4J	N33-C32-C34-O36
20	S1	1829	OMG	C4'-C5'-O5'-P
42	2	1308	5MC	C2'-C1'-N1-C2
41	1	1402	PSU	O4'-C4'-C5'-O5'
42	2	1403	PSU	C3'-C4'-C5'-O5'
20	S1	1979	OMU	C2'-C1'-N1-C2
20	S1	98	A2M	O4'-C4'-C5'-O5'
20	S1	2021	A2M	C1'-C2'-O2'-CM'
41	1	697	A2M	C1'-C2'-O2'-CM'
42	2	665	A2M	C1'-C2'-O2'-CM'
20	S1	8	OMU	C3'-C2'-O2'-CM2
20	S1	2202	PSU	O4'-C1'-C5-C6
41	1	1011	PSU	O4'-C1'-C5-C6
41	1	1171	PSU	O4'-C1'-C5-C6
20	S1	2185	MA6	C4'-C5'-O5'-P
20	S1	1833	OMU	O4'-C4'-C5'-O5'
41	1	1402	PSU	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
41	1	1524	OMG	C3'-C2'-O2'-CM2
41	1	1527	OMC	O4'-C4'-C5'-O5'
20	S1	1657	PSU	C4'-C5'-O5'-P
42	2	1185	A2M	C4'-C5'-O5'-P
20	S1	1539	PSU	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 144 ligands modelled in this entry, 144 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
41	1	2
15	S4	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S4	7:A	O3'	65:G	P	19.26
1	1	1097:A	O3'	1100:C	P	10.20
1	1	552:G	O3'	554:A	P	4.04

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-15272. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

7 Map analysis

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

7.1 Map-value distribution

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

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

9 Map-model fit

This section was not generated.