Full wwPDB EM Validation Report ⓘ

Apr 16, 2024 – 10:32 am BST

PDB ID	:	8OVA
EMDB ID	:	EMD-17208
Title	:	CRYO-EM STRUCTURE OF TRYPANOSOMA BRUCEI PROCYCLIC FORM 80S RIBOSOME : PARENTAL STRAIN
Authors	:	Rajan, K.S.; Yonath, A.
Deposited on	:	2023-04-25
Resolution	:	2.47 Å(reported)

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

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

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

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

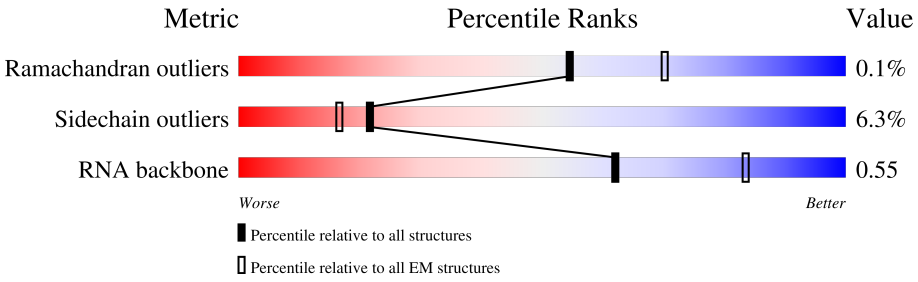
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.47 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	BA	1920	65% 17% • 16%
2	AA	2282	62% 20% • 16%
3	BB	1536	56% 16% • 27%
4	BH	136	67% 20% • 12%
5	BG	183	83% 17% •
6	BF	78	64% 24% 12%
7	BE	216	63% 22% • 13%
8	BD	119	87% 13%
9	BC	209	63% 13% 23%

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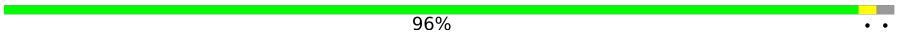
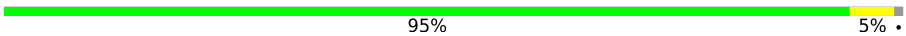
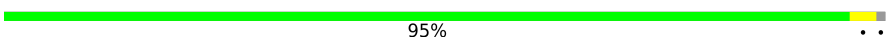
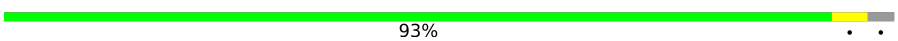
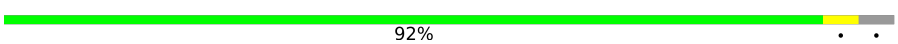
Mol	Chain	Length	Quality of chain
10	AB	19	
11	AQ	117	
12	A8	57	
13	A9	153	
14	Az	279	
15	AH	144	
16	AI	152	
17	AJ	130	
18	AK	149	
19	AM	153	
20	AO	167	
21	AP	266	
22	AR	194	
23	AS	143	
24	AT	137	
25	AU	113	
26	AV	111	
27	AW	86	
28	AX	214	
29	AY	66	
30	AZ	103	
31	AL	142	
32	A0	256	
33	A1	273	
34	A2	190	

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Mol	Chain	Length	Quality of chain
35	A3	250	89% 6% 5%
36	A4	202	88% 10%
37	A5	220	79% 6% 15%
38	A6	190	89% 5% 6%
39	A7	318	90% 8%
40	AC	277	72% 25%
41	AD	172	53% 5% 42%
42	AE	174	83% 5% 12%
43	AG	151	95% 5%
44	Bh	188	77% 6% 17%
45	Ba	133	89% 11%
46	Bb	145	94% 5%
47	Bc	146	95%
48	Bd	71	89% 6% 6%
49	Be	260	95%
50	Bz	34	94% 6%
51	Bg	105	82% 6% 12%
52	Bf	429	89% 8%
53	BI	193	95%
54	Bj	170	66% 32%
55	BK	213	85% 6% 9%
56	Bk	127	91% 6%
57	BL	194	78% 7% 14%
58	Bl	149	94%
59	Bm	109	86% 10%

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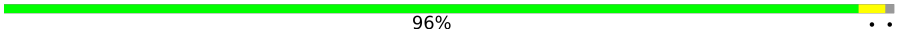
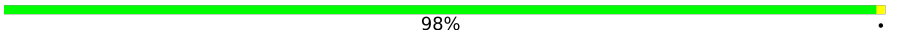
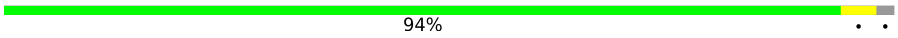
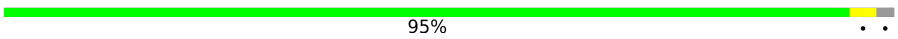
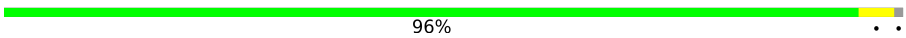
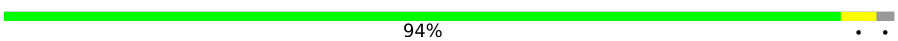
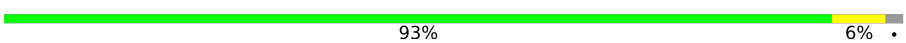
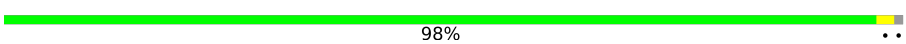
Mol	Chain	Length	Quality of chain
60	BN	218	
61	Bn	84	
62	BO	222	
63	Bo	93	
64	Bp	82	
65	Bq	51	
66	BQ	221	
67	BR	166	
68	Br	374	
69	BS	179	
70	Bs	128	
71	BT	260	
72	Bt	106	
73	BU	159	
74	Bu	308	
75	BV	130	
76	Bv	192	
77	BW	139	
78	BX	164	
79	Bw	257	
80	Bx	276	
81	BY	125	
82	By	189	
83	BZ	143	
84	Bi	132	

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Mol	Chain	Length	Quality of chain
85	BP	189	
86	AF	144	

2 Entry composition (i)

There are 91 unique types of molecules in this entry. The entry contains 209127 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called LSUa rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	BA	1604	34346	15345	6216	11181	1604	0	0

- Molecule 2 is a RNA chain called SSU rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	AA	1919	40964	18316	7328	13401	1919	0	0

- Molecule 3 is a RNA chain called LSUb rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	BB	1119	23918	10699	4282	7818	1119	0	0

- Molecule 4 is a RNA chain called SrRNA-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	BH	119	2538	1131	451	837	119	0	0

- Molecule 5 is a RNA chain called SrRNA-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	BG	183	3919	1746	708	1282	183	0	0

- Molecule 6 is a RNA chain called SrRNA-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	BF	69	1444	646	239	490	69	0	0

- Molecule 7 is a RNA chain called SrRNA-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	BE	188	Total	C	N	O	P	0	0
			3981	1780	692	1321	188		

- Molecule 8 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	BD	119	Total	C	N	O	P	0	0
			2533	1131	449	835	118		

- Molecule 9 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	BC	160	Total	C	N	O	P	0	0
			3411	1529	610	1113	159		

- Molecule 10 is a RNA chain called E-SITE TRNA.

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

- Molecule 11 is a protein called Ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AQ	100	Total	C	N	O	S	0	0
			800	501	152	144	3		

- Molecule 12 is a protein called uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	A8	56	Total	C	N	O	S	0	0
			461	284	97	75	5		

- Molecule 13 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	A9	70	Total	C	N	O	S	0	1
			569	361	109	92	7		

- Molecule 14 is a protein called RNA-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Az	100	Total	C	N	O	S	0	0
			807	504	154	148	1		

- Molecule 15 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AH	134	Total	C	N	O	S	0	0
			992	607	193	183	9		

- Molecule 16 is a protein called 40S ribosomal protein S15, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AI	119	Total	C	N	O	S	0	0
			966	614	188	161	3		

- Molecule 17 is a protein called 40S ribosomal protein S15a, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AJ	129	Total	C	N	O	S	0	0
			1018	645	191	174	8		

- Molecule 18 is a protein called 40S ribosomal protein S16, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AK	142	Total	C	N	O	S	0	0
			1140	728	215	194	3		

- Molecule 19 is a protein called 40S ribosomal protein S18, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AM	141	Total	C	N	O	S	0	0
			1143	713	227	198	5		

- Molecule 20 is a protein called Ribosomal protein S19, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AO	154	Total	C	N	O	S	0	0
			1220	770	242	199	9		

- Molecule 21 is a protein called 40S ribosomal protein S2, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AP	218	Total	C	N	O	S	0	0
			1688	1078	298	303	9		

- Molecule 22 is a protein called 40S ribosomal protein S21, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AR	89	Total	C	N	O	S	0	0
			666	415	119	129	3		

- Molecule 23 is a protein called 40S ribosomal protein S23, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AS	140	Total	C	N	O	S	0	0
			1096	696	213	185	2		

- Molecule 24 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AT	129	Total	C	N	O	S	0	0
			1034	659	202	170	3		

- Molecule 25 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	AU	73	Total	C	N	O	S	0	0
			575	365	105	100	5		

- Molecule 26 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	AV	103	Total	C	N	O	S	0	0
			830	512	175	135	8		

- Molecule 27 is a protein called 40S ribosomal protein S27, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	AW	85	Total	C	N	O	S	0	0
			660	411	124	116	9		

- Molecule 28 is a protein called 40S ribosomal protein S3, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	AX	208	Total	C	N	O	S	0	0
			1652	1036	310	294	12		

- Molecule 29 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	AY	55	Total	C	N	O	S	0	0
			448	283	93	71	1		

- Molecule 30 is a protein called 40S ribosomal protein S33, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	AZ	58	Total	C	N	O	S	0	0
			449	271	94	80	4		

- Molecule 31 is a protein called 40S ribosomal protein S17, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	AL	122	Total	C	N	O	S	0	0
			945	600	184	156	5		

- Molecule 32 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	A0	220	Total	C	N	O	S	0	0
			1789	1129	336	316	8		

- Molecule 33 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	A1	262	Total	C	N	O	S	0	0
			2062	1306	388	359	9		

- Molecule 34 is a protein called 40S ribosomal protein S5, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	A2	183	Total	C	N	O	S	0	0
			1464	915	282	262	5		

- Molecule 35 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	A3	238	Total	C	N	O	S	0	0
			1871	1161	383	323	4		

- Molecule 36 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	A4	198	Total	C	N	O	S	0	0
			1602	1023	308	266	5		

- Molecule 37 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	A5	187	Total	C	N	O	S	0	0
			1471	927	291	251	2		

- Molecule 38 is a protein called Probable 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	A6	179	Total	C	N	O	S	0	0
			1477	929	297	243	8		

- Molecule 39 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	A7	309	Total	C	N	O	S	0	0
			2371	1483	418	458	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	AC	208	Total	C	N	O	S	0	0
			1648	1049	297	291	11		

- Molecule 41 is a protein called 40S ribosomal protein S10, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	AD	99	Total	C	N	O	S	0	0
			814	531	140	139	4		

- Molecule 42 is a protein called 40S ribosomal proteins S11, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	AE	153	Total	C	N	O	S	0	0
			1249	782	253	209	5		

- Molecule 43 is a protein called 40S ribosomal protein S13, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	AG	150	Total	C	N	O	S	0	0
			1203	756	236	203	8		

- Molecule 44 is a protein called 60S ribosomal subunit protein L31, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Bh	156	Total	C	N	O	S	0	0
			1249	785	253	207	4		

- Molecule 45 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Ba	132	Total	C	N	O	S	0	0
			1085	688	219	175	3		

- Molecule 46 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Bb	144	Total	C	N	O	S	0	0
			1137	717	228	186	6		

- Molecule 47 is a protein called 60S ribosomal protein L28, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Bc	144	Total	C	N	O	S	0	0
			1162	723	234	197	8		

- Molecule 48 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Bd	67	Total	C	N	O	S	0	0
			547	335	123	88	1		

- Molecule 49 is a protein called 60S ribosomal protein L2, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Be	254	Total	C	N	O	S	1	0
			1907	1189	394	312	12		

- Molecule 50 is a protein called Ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Bz	32	Total	C	N	O	S	0	0
			284	172	74	36	2		

- Molecule 51 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Bg	92	Total	C	N	O	S	0	0
			708	441	128	134	5		

- Molecule 52 is a protein called Ribosomal protein L3, mitochondrial, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	Bf	396	Total	C	N	O	S	0	0
			3174	2001	626	534	13		

- Molecule 53 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	BI	191	Total	C	N	O	S	0	0
			1517	950	313	246	8		

- Molecule 54 is a protein called 60S ribosomal protein L34, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	Bj	116	Total	C	N	O	S	0	0
			959	593	214	148	4		

- Molecule 55 is a protein called 60S ribosomal protein L10, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	BK	194	Total	C	N	O	S	0	0
			1588	1002	314	260	12		

- Molecule 56 is a protein called 60S ribosomal protein L35, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	Bk	123	Total	C	N	O	S	0	0
			1010	634	217	156	3		

- Molecule 57 is a protein called 60S ribosomal protein L11, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	BL	166	Total	C	N	O	S	0	0
			1325	836	247	235	7		

- Molecule 58 is a protein called 60S ribosomal protein L35A, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	Bl	144	Total	C	N	O	S	0	0
			1163	728	239	193	3		

- Molecule 59 is a protein called Ribosomal protein L36, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	Bm	98	Total	C	N	O	S	0	0
			786	493	164	127	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
60	BN	215	Total	C	N	O	S	0	0
			1762	1097	365	294	6		

- Molecule 61 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	Bn	80	Total	C	N	O	S	0	0
			676	410	157	103	6		

- Molecule 62 is a protein called 60S ribosomal protein L13a, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	BO	221	Total	C	N	O	S	0	0
			1801	1141	364	289	7		

- Molecule 63 is a protein called 60S ribosomal protein L37a, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	Bo	89	Total	C	N	O	S	0	0
			699	434	144	115	6		

- Molecule 64 is a protein called 60S ribosomal protein L38, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	Bp	77	Total	C	N	O	S	0	0
			626	393	125	104	4		

- Molecule 65 is a protein called 60S ribosomal protein L39, putative.

Mol	Chain	Residues	Atoms				AltConf	Trace
65	Bq	50	Total	C	N	O	0	0
			457	297	98	62		

- Molecule 66 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	BQ	203	Total	C	N	O	S	0	0
			1716	1077	370	264	5		

- Molecule 67 is a protein called 60S ribosomal protein L17, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	BR	151	Total	C	N	O	S	0	0
			1219	767	242	202	8		

- Molecule 68 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	Br	367	Total	C	N	O	S	0	0
			2882	1802	575	488	17		

- Molecule 69 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	BS	178	Total	C	N	O	S	0	0
			1465	926	289	243	7		

- Molecule 70 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	Bs	50	Total	C	N	O	S	0	0
			394	247	80	60	7		

- Molecule 71 is a protein called 60S ribosomal protein L19, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	BT	196	Total	C	N	O	S	0	0
			1590	974	349	259	8		

- Molecule 72 is a protein called 60S ribosomal protein L44.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	Bt	97	Total	C	N	O	S	0	0
			801	507	159	130	5		

- Molecule 73 is a protein called 60S ribosomal protein L21E, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	BU	157	Total	C	N	O	S	0	0
			1247	793	245	203	6		

- Molecule 74 is a protein called 60S ribosomal protein L5, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Bu	247	Total	C	N	O	S	0	0
			1964	1234	378	347	5		

- Molecule 75 is a protein called 60S ribosomal protein L22, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	BV	122	Total	C	N	O	S	0	0
			979	629	179	168	3		

- Molecule 76 is a protein called 60S ribosomal protein L6, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	Bv	143	Total	C	N	O	S	0	0
			1101	699	202	197	3		

- Molecule 77 is a protein called 60S ribosomal protein L23, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	BW	136	Total	C	N	O	S	0	0
			1029	651	195	178	5		

- Molecule 78 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	BX	120	Total	C	N	O	S	0	0
			982	624	185	171	2		

- Molecule 79 is a protein called 60S ribosomal protein L7, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Bw	230	Total	C	N	O	S	0	0
			1872	1190	362	312	8		

- Molecule 80 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Bx	235	Total	C	N	O	S	0	0
			1874	1178	369	321	6		

- Molecule 81 is a protein called 60S ribosomal protein L24, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	BY	64	Total	C	N	O	S	0	0
			550	358	108	79	5		

- Molecule 82 is a protein called 60S ribosomal protein L9, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	By	186	Total	C	N	O	S	0	0
			1515	961	281	269	4		

- Molecule 83 is a protein called 60S ribosomal protein L26, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	BZ	122	Total	C	N	O	S	0	0
			993	614	210	164	5		

- Molecule 84 is a protein called 60S ribosomal protein L32, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	Bi	131	Total 1075	C 678	N 217	O 176	S 4	0	0

- Molecule 85 is a protein called 40S ribosomal protein L14, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	BP	152	Total 1237	C 784	N 240	O 209	S 4	0	0

- Molecule 86 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	AF	115	Total 868	C 531	N 156	O 173	S 8	0	0

- Molecule 87 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
87	BA	67	Total 67	Mg 67	0
87	AA	88	Total 88	Mg 88	0
87	BB	61	Total 61	Mg 61	0
87	BG	5	Total 5	Mg 5	0
87	BE	1	Total 1	Mg 1	0
87	BD	1	Total 1	Mg 1	0
87	BC	1	Total 1	Mg 1	0
87	AH	1	Total 1	Mg 1	0
87	AO	2	Total 2	Mg 2	0
87	A0	1	Total 1	Mg 1	0
87	Be	2	Total 2	Mg 2	0
87	Bf	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms	AltConf
87	BN	1	Total Mg 1 1	0
87	BR	1	Total Mg 1 1	0
87	BW	1	Total Mg 1 1	0

- Molecule 88 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
88	BA	8	Total K 8 8	0
88	AA	25	Total K 25 25	0
88	BB	12	Total K 12 12	0
88	AH	1	Total K 1 1	0
88	BZ	1	Total K 1 1	0

- Molecule 89 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	AltConf
89	BA	10	Total Na 10 10	0
89	AA	14	Total Na 14 14	0
89	BB	14	Total Na 14 14	0
89	A3	1	Total Na 1 1	0
89	BK	1	Total Na 1 1	0

- Molecule 90 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
90	A9	1	Total Zn 1 1	0
90	Bn	1	Total Zn 1 1	0

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Mol	Chain	Residues	Atoms	AltConf
90	Bo	1	Total Zn 1 1	0
90	Bs	1	Total Zn 1 1	0

- Molecule 91 is water.

Mol	Chain	Residues	Atoms	AltConf
91	BA	53	Total O 53 53	0
91	AA	40	Total O 40 40	0
91	BB	61	Total O 61 61	0
91	BH	2	Total O 2 2	0
91	BG	4	Total O 4 4	0
91	BE	1	Total O 1 1	0
91	BC	1	Total O 1 1	0
91	A8	1	Total O 1 1	0
91	AH	1	Total O 1 1	0
91	AK	1	Total O 1 1	0
91	AV	3	Total O 3 3	0
91	A2	1	Total O 1 1	0
91	AG	1	Total O 1 1	0
91	Bb	3	Total O 3 3	0
91	Bd	1	Total O 1 1	0
91	Be	7	Total O 7 7	0
91	Bj	1	Total O 1 1	0

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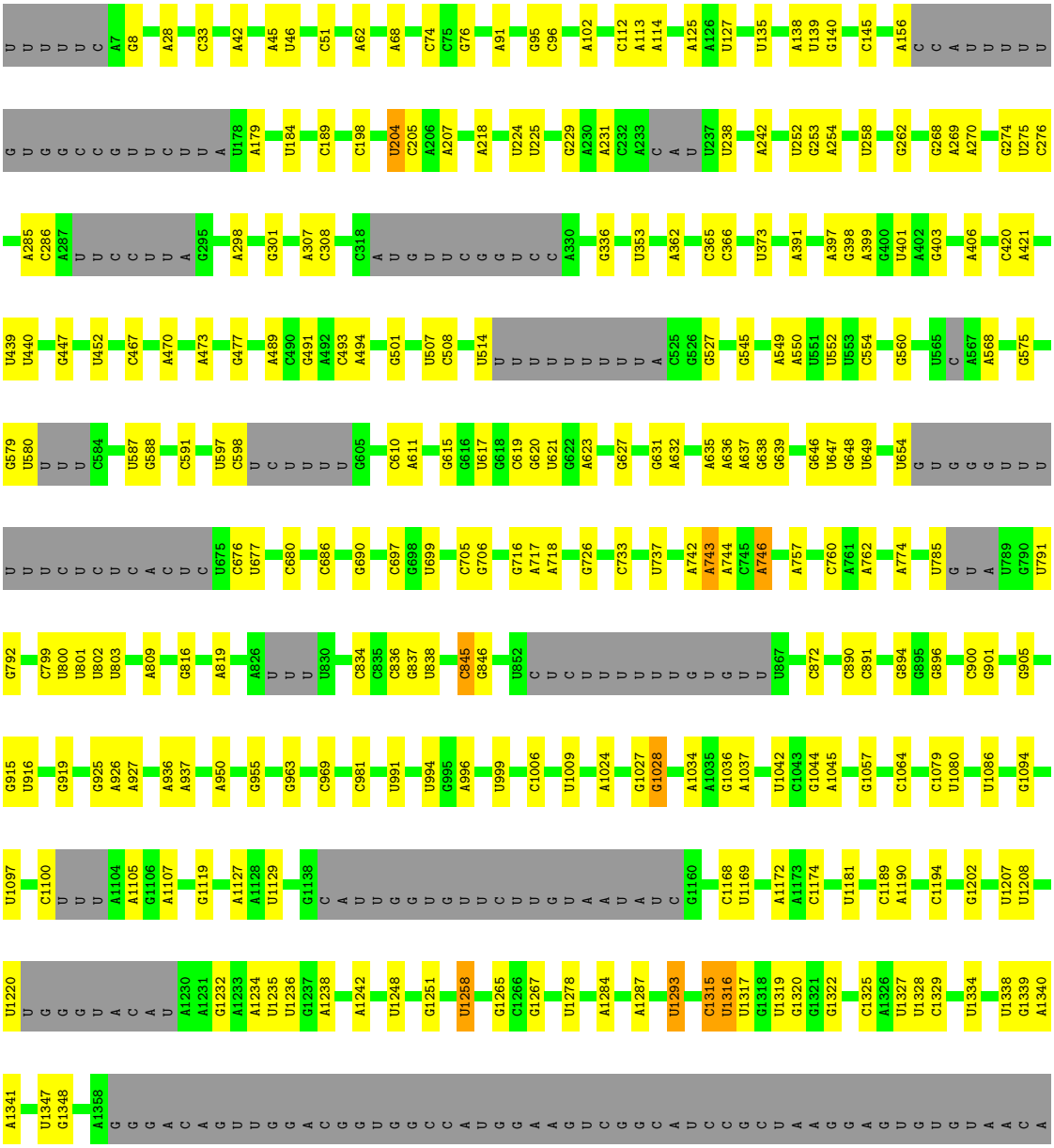
Mol	Chain	Residues	Atoms	AltConf
91	BK	1	Total O 1 1	0
91	BN	1	Total O 1 1	0
91	Bn	1	Total O 1 1	0
91	BQ	2	Total O 2 2	0
91	Br	1	Total O 1 1	0
91	Bi	1	Total O 1 1	0

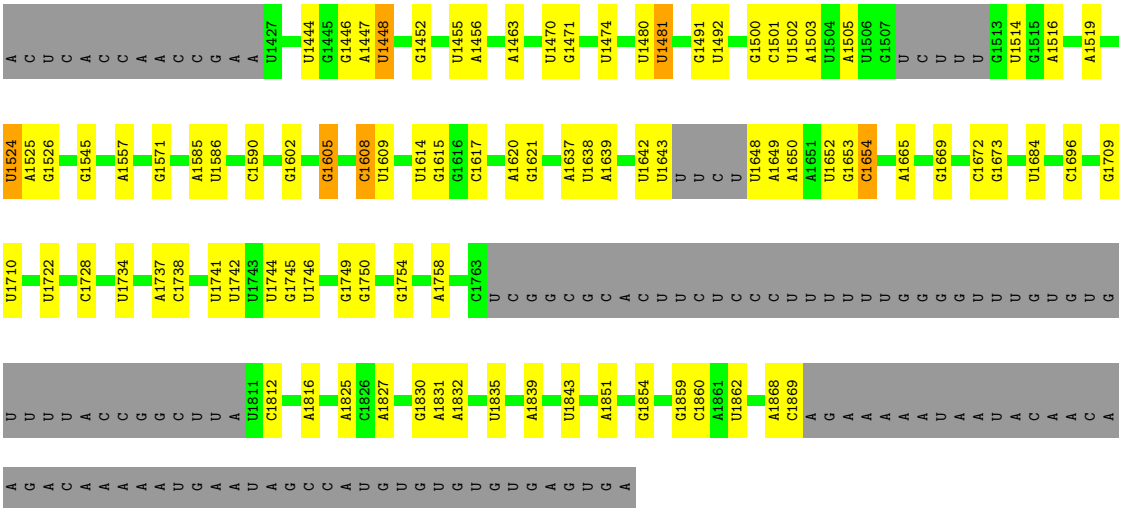
3 Residue-property plots (i)

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

- Molecule 1: LSUa rRNA

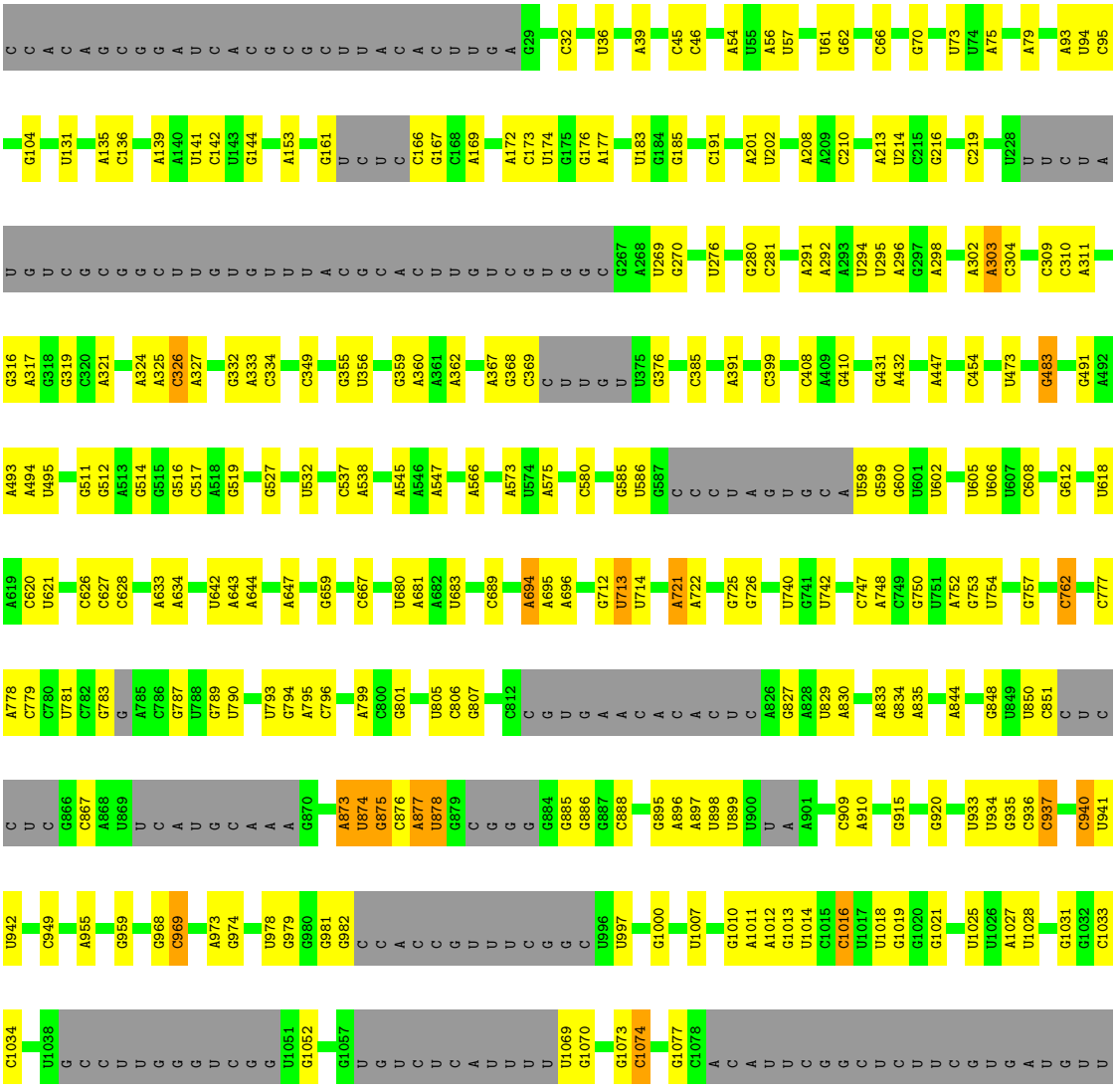
Chain BA:

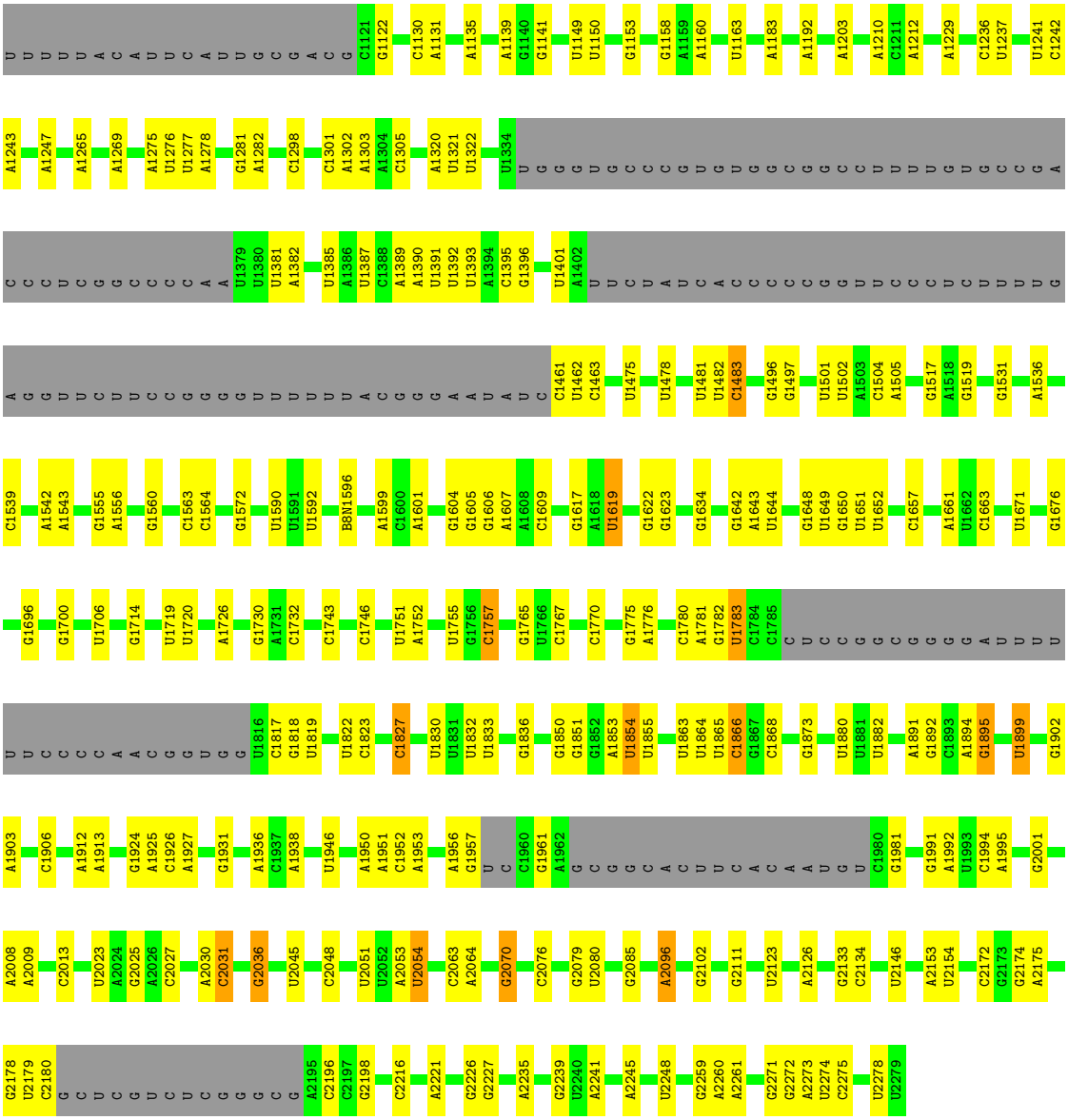




• Molecule 2: SSU rRNA

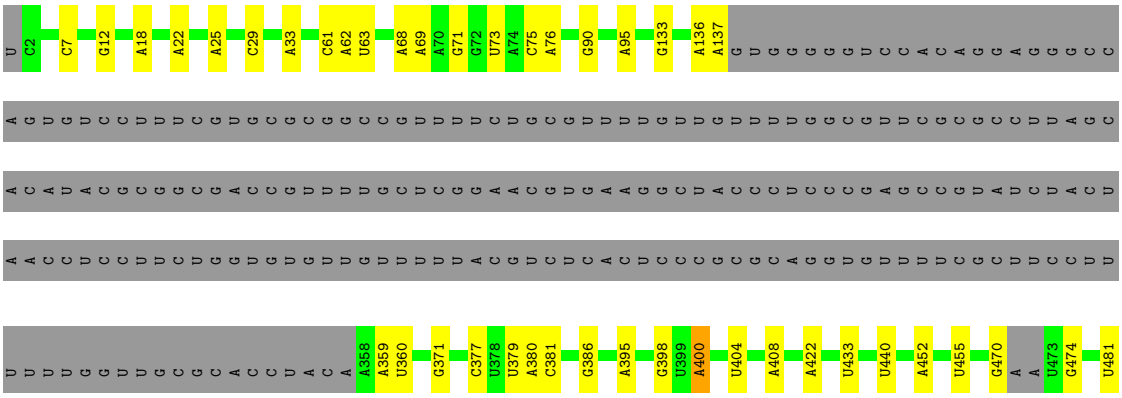
Chain AA:

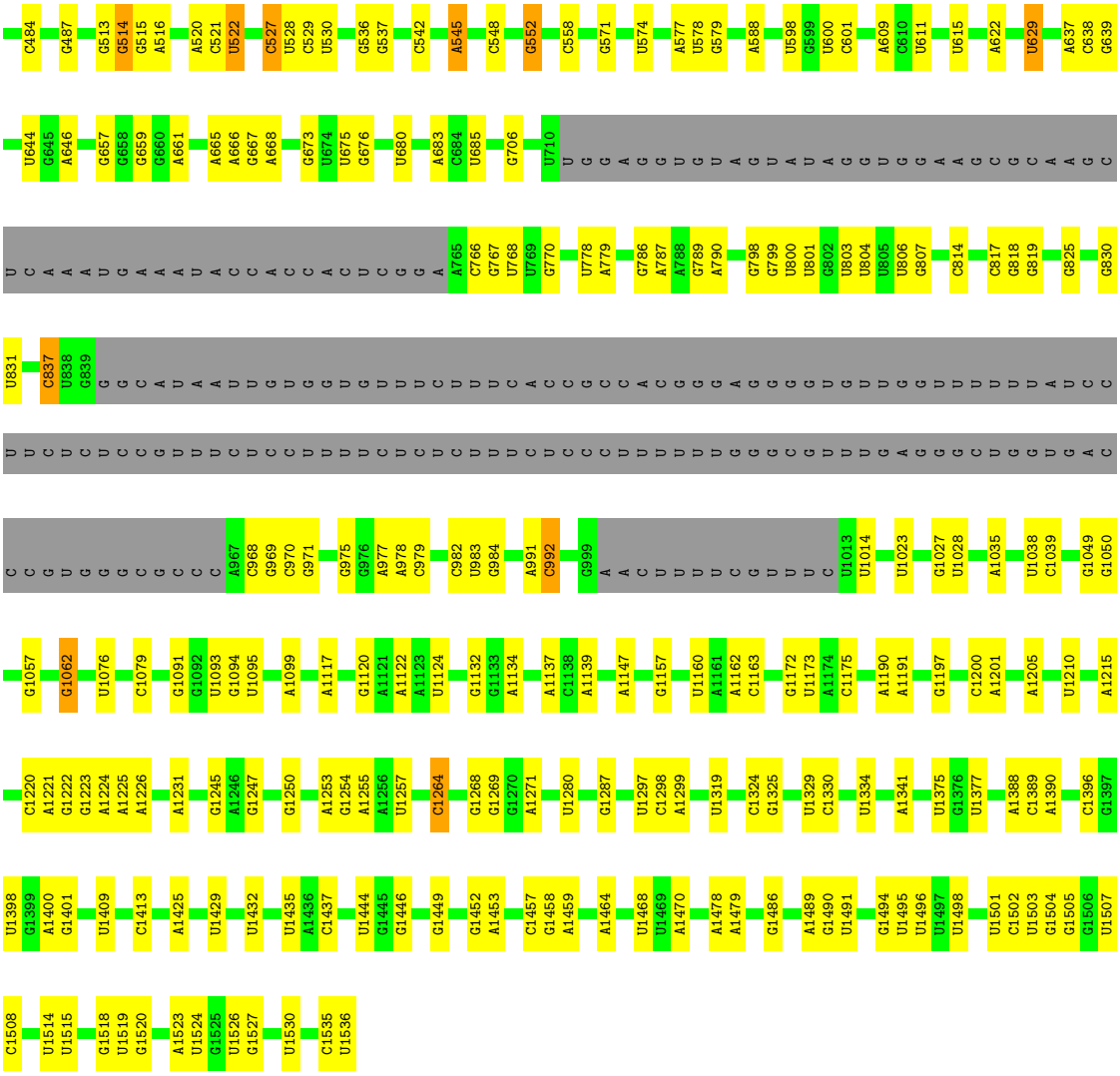




• Molecule 3: LSUb rRNA

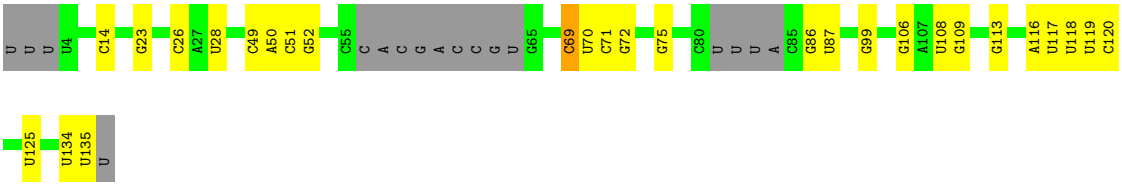
Chain BB:





• Molecule 4: SrRNA-4

Chain BH:

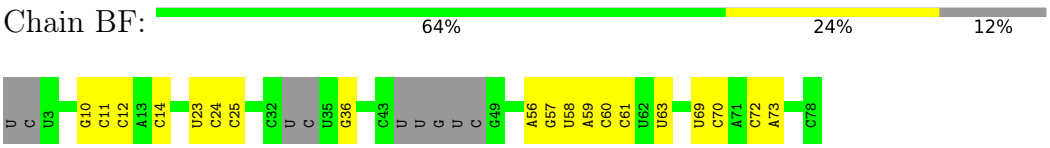


• Molecule 5: SrRNA-2

Chain BG:

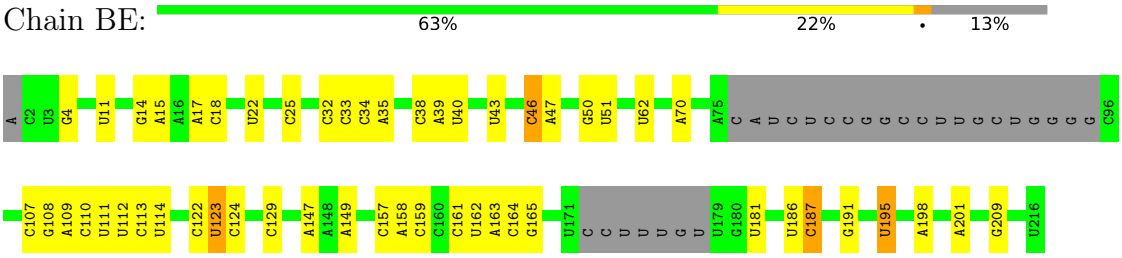
• Molecule 6: SrRNA-6

Chain BF:



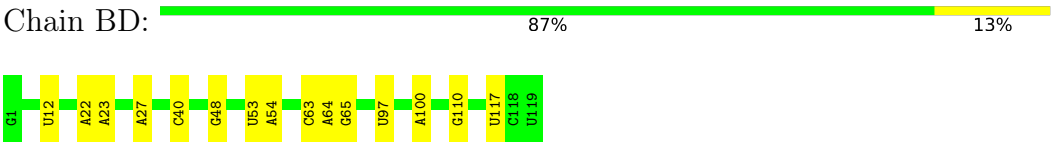
• Molecule 7: SrRNA-1

Chain BE:



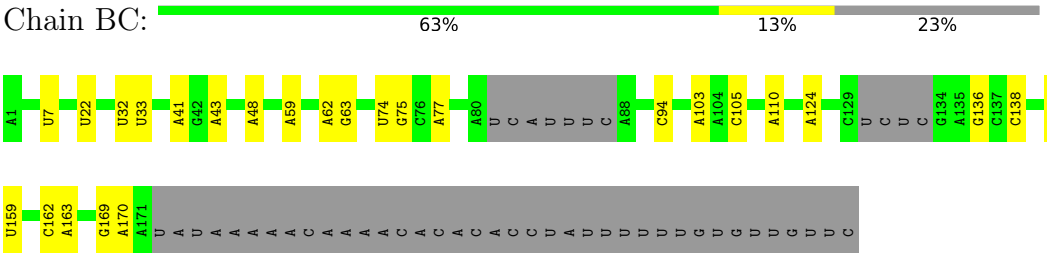
• Molecule 8: 5S rRNA

Chain BD:



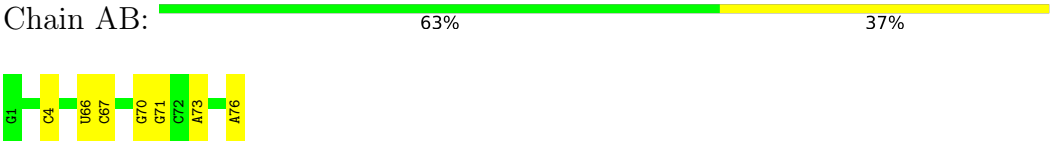
• Molecule 9: 5.8S rRNA

Chain BC:



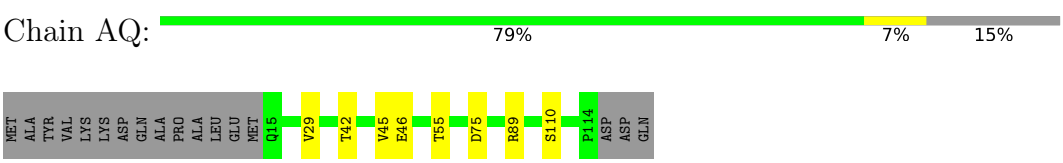
• Molecule 10: E-SITE TRNA

Chain AB:



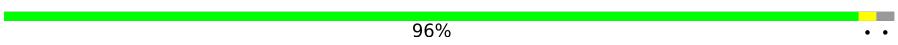
• Molecule 11: Ribosomal protein S10

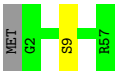
Chain AQ:



• Molecule 12: uS14

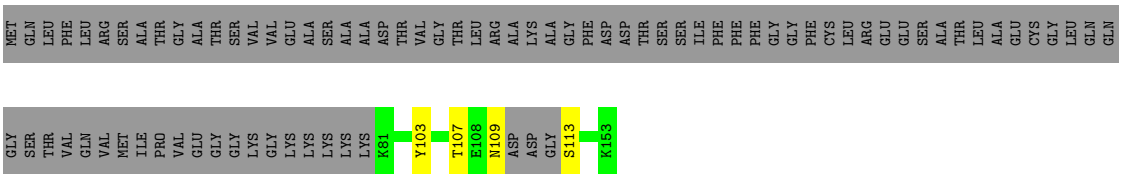
Chain A8:





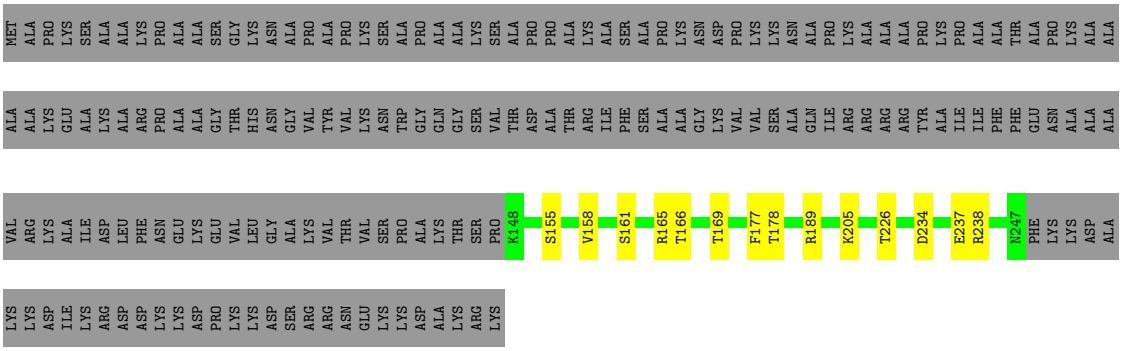
• Molecule 13: Ubiquitin-60S ribosomal protein L40

Chain A9:



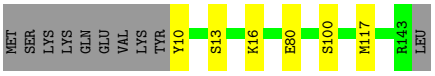
• Molecule 14: RNA-binding protein

Chain Az:



• Molecule 15: 40S ribosomal protein S14

Chain AH:

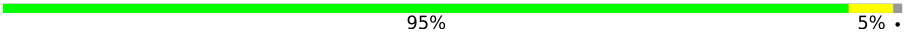


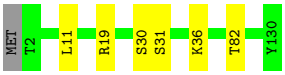
• Molecule 16: 40S ribosomal protein S15, putative

Chain AI:

• Molecule 17: 40S ribosomal protein S15a, putative

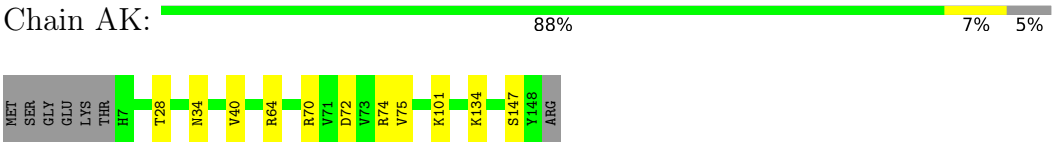
Chain AJ:





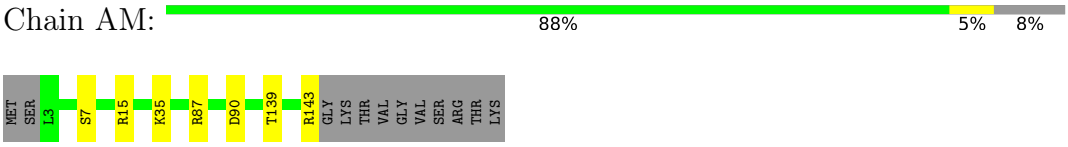
• Molecule 18: 40S ribosomal protein S16, putative

Chain AK:



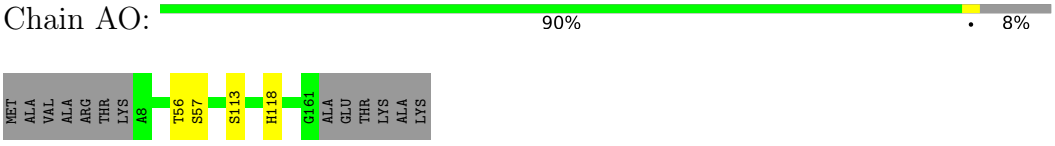
• Molecule 19: 40S ribosomal protein S18, putative

Chain AM:



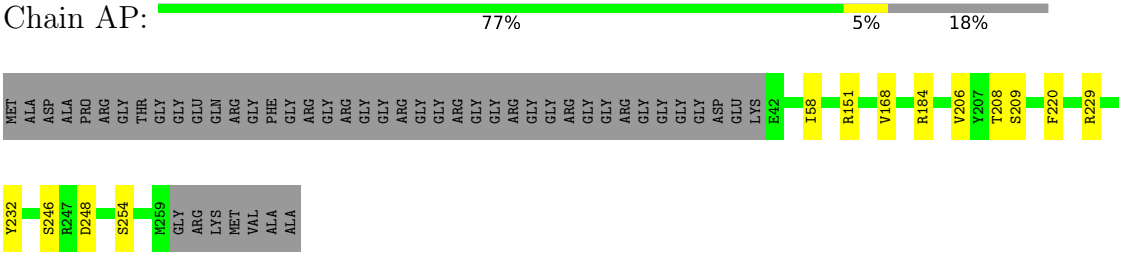
• Molecule 20: Ribosomal protein S19, putative

Chain AO:



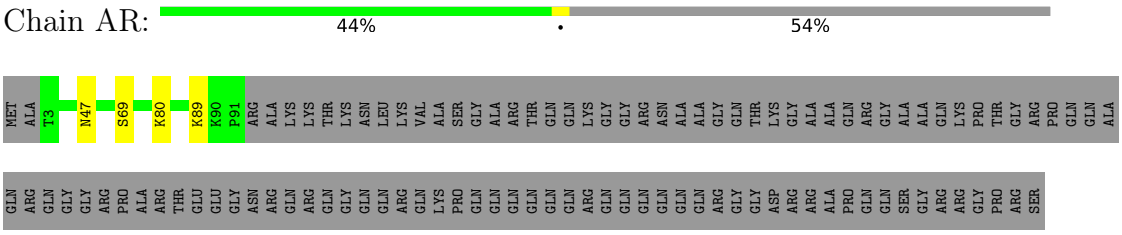
• Molecule 21: 40S ribosomal protein S2, putative

Chain AP:



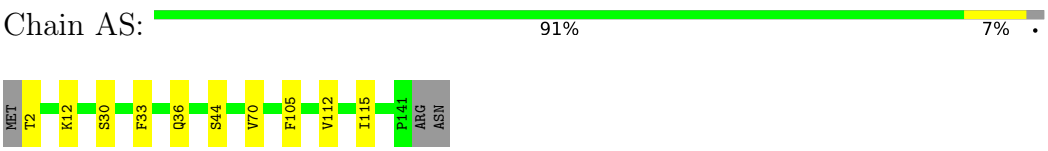
• Molecule 22: 40S ribosomal protein S21, putative

Chain AR:



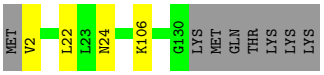
• Molecule 23: 40S ribosomal protein S23, putative

Chain AS:



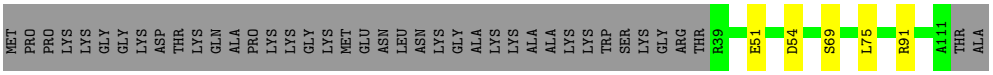
• Molecule 24: 40S ribosomal protein S24

Chain AT:



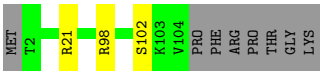
• Molecule 25: 40S ribosomal protein S25

Chain AU:



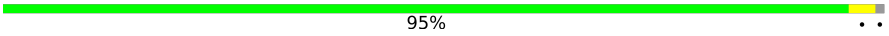
• Molecule 26: 40S ribosomal protein S26

Chain AV:



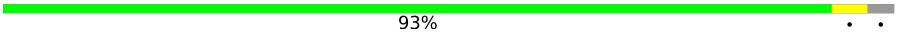
• Molecule 27: 40S ribosomal protein S27, putative

Chain AW:



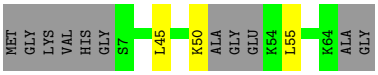
• Molecule 28: 40S ribosomal protein S3, putative

Chain AX:



• Molecule 29: 40S ribosomal protein S30

Chain AY:

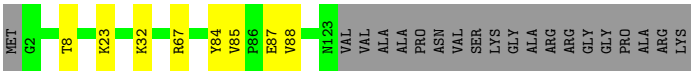


• Molecule 30: 40S ribosomal protein S33, putative

Chain AZ:

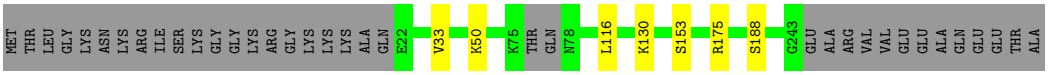
• Molecule 31: 40S ribosomal protein S17, putative

Chain AL:



• Molecule 32: 40S ribosomal protein S3a

Chain A0:

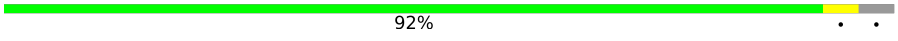


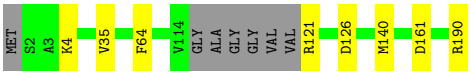
• Molecule 33: 40S ribosomal protein S4

Chain A1:

• Molecule 34: 40S ribosomal protein S5, putative

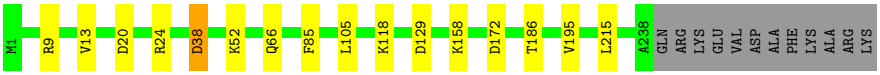
Chain A2:





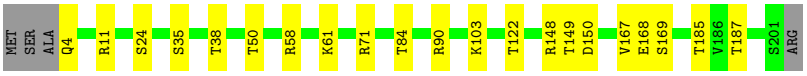
• Molecule 35: 40S ribosomal protein S6

Chain A3:



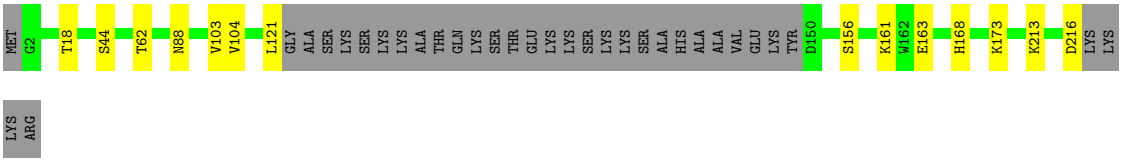
• Molecule 36: 40S ribosomal protein S7

Chain A4:



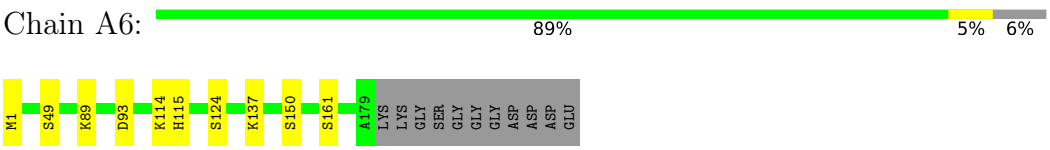
• Molecule 37: 40S ribosomal protein S8

Chain A5:



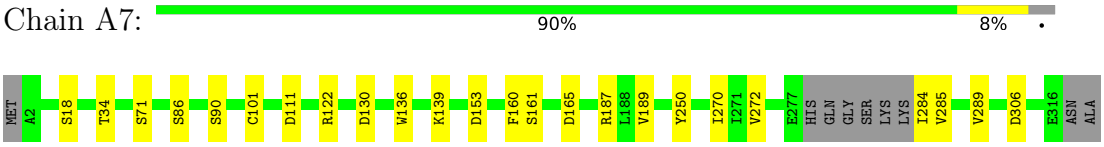
• Molecule 38: Probable 40S ribosomal protein S9

Chain A6:



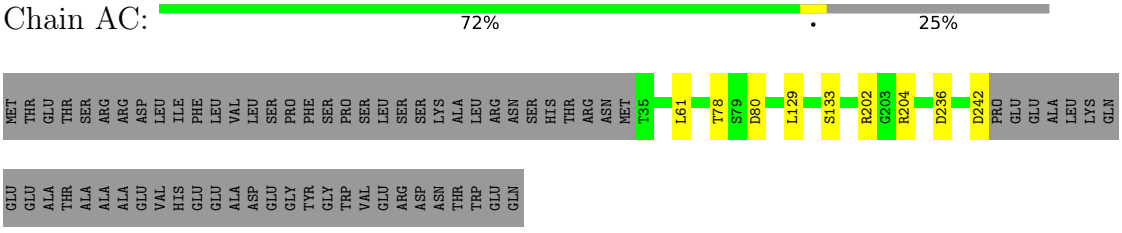
• Molecule 39: Guanine nucleotide-binding protein subunit beta-like protein

Chain A7:



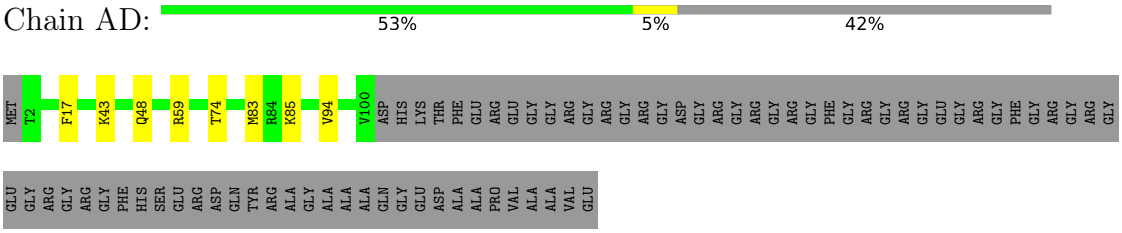
• Molecule 40: 40S ribosomal protein SA

Chain AC:



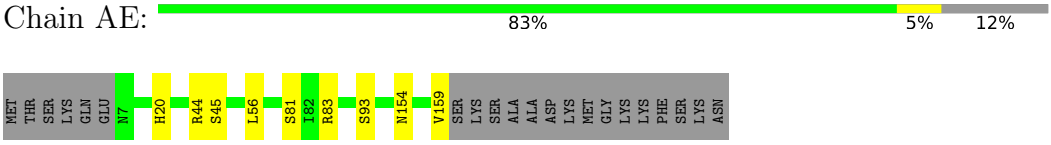
• Molecule 41: 40S ribosomal protein S10, putative

Chain AD:



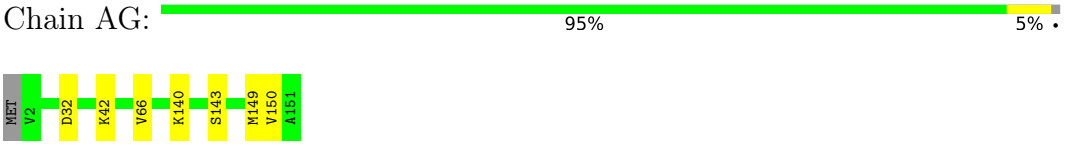
• Molecule 42: 40S ribosomal proteins S11, putative

Chain AE:



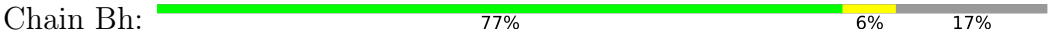
• Molecule 43: 40S ribosomal protein S13, putative

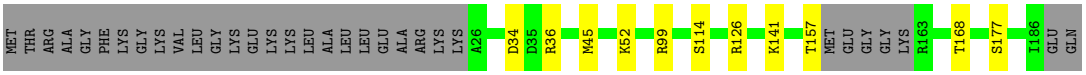
Chain AG:



• Molecule 44: 60S ribosomal subunit protein L31, putative

Chain Bh:



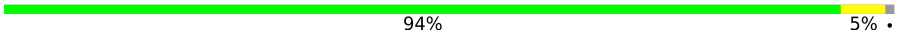


• Molecule 45: 60S ribosomal protein L27

Chain Ba:

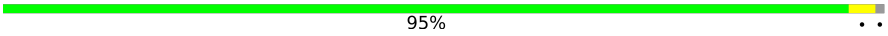
• Molecule 46: 60S ribosomal protein L27a

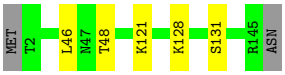
Chain Bb:



• Molecule 47: 60S ribosomal protein L28, putative

Chain Bc:



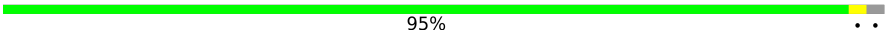


• Molecule 48: 60S ribosomal protein L29

Chain Bd:

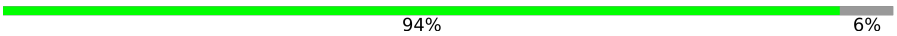
• Molecule 49: 60S ribosomal protein L2, putative

Chain Be:



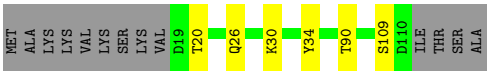
• Molecule 50: Ribosomal protein L41

Chain Bz:



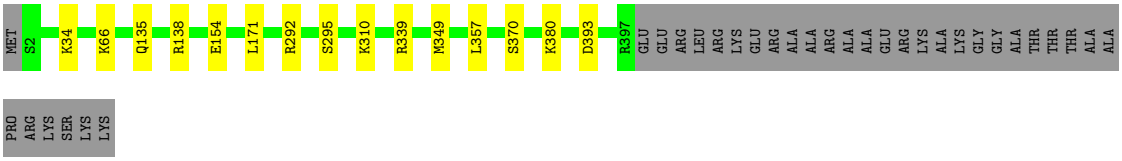
• Molecule 51: 60S ribosomal protein L30

Chain Bg:



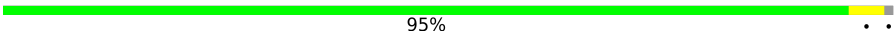
• Molecule 52: Ribosomal protein L3, mitochondrial, putative

Chain Bf:



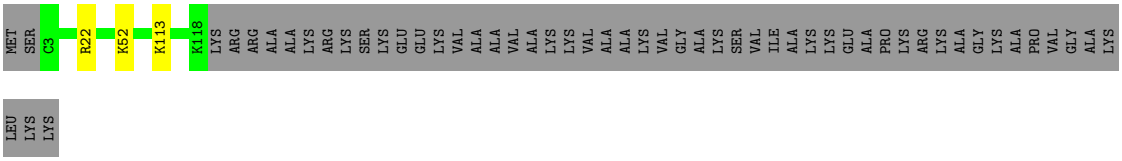
• Molecule 53: 60S ribosomal protein L18

Chain BI:



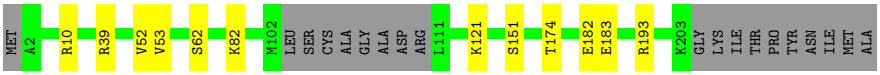
• Molecule 54: 60S ribosomal protein L34, putative

Chain Bj:



• Molecule 55: 60S ribosomal protein L10, putative

Chain BK:



• Molecule 56: 60S ribosomal protein L35, putative

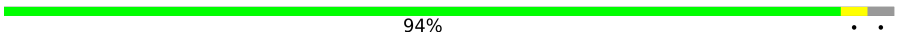
Chain Bk:

• Molecule 57: 60S ribosomal protein L11, putative

Chain BL:

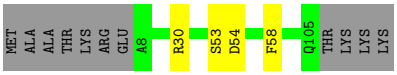
• Molecule 58: 60S ribosomal protein L35A, putative

Chain Bl:



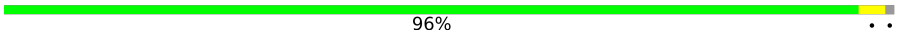
• Molecule 59: Ribosomal protein L36, putative

Chain Bm:



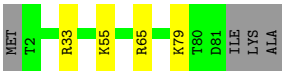
• Molecule 60: 60S ribosomal protein L13

Chain BN:



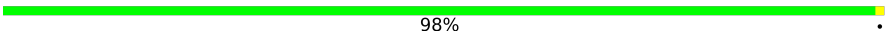
• Molecule 61: Ribosomal protein L37

Chain Bn:



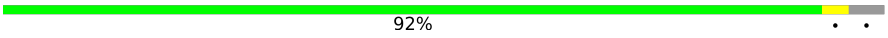
• Molecule 62: 60S ribosomal protein L13a, putative

Chain BO:



• Molecule 63: 60S ribosomal protein L37a, putative

Chain Bo:

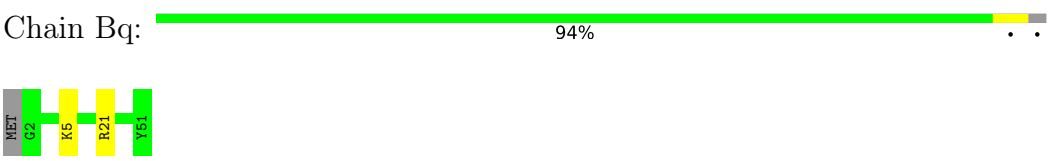


• Molecule 64: 60S ribosomal protein L38, putative

Chain Bp:

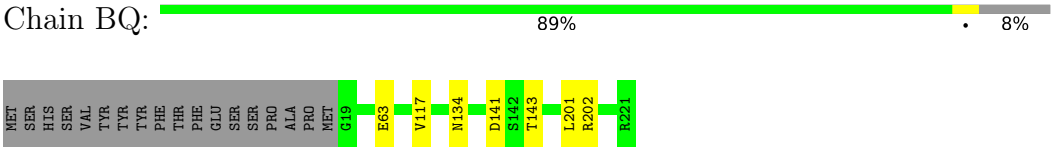
• Molecule 65: 60S ribosomal protein L39, putative

Chain Bq:



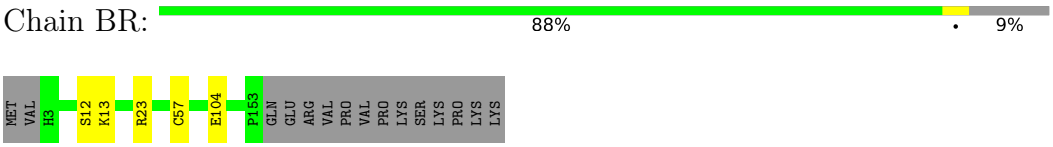
• Molecule 66: Ribosomal protein L15

Chain BQ:



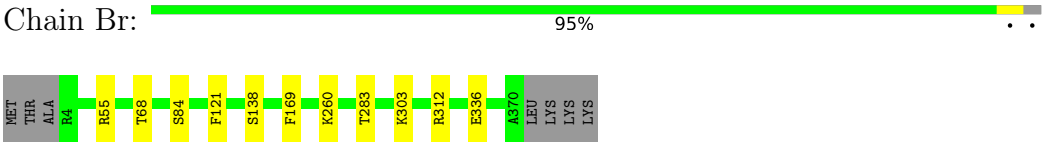
• Molecule 67: 60S ribosomal protein L17, putative

Chain BR:



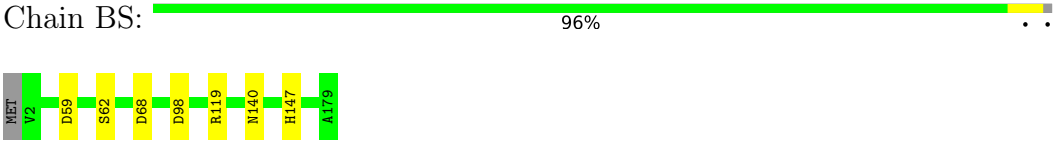
• Molecule 68: 60S ribosomal protein L4

Chain Br:



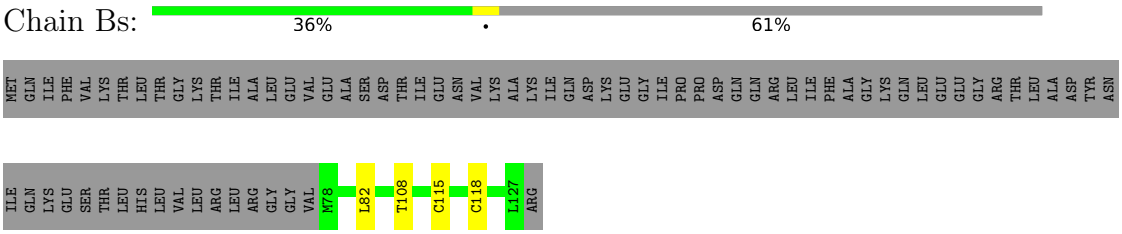
• Molecule 69: 60S ribosomal protein L18a

Chain BS:



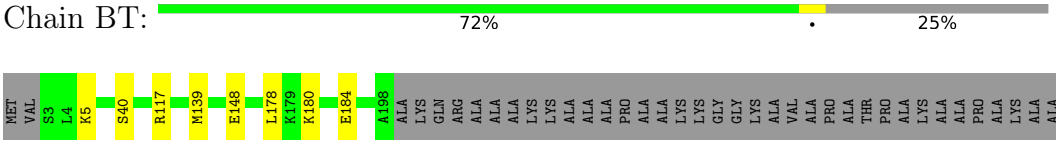
• Molecule 70: Ubiquitin-60S ribosomal protein L40

Chain Bs:



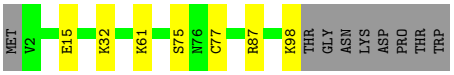
• Molecule 71: 60S ribosomal protein L19, putative

Chain BT:



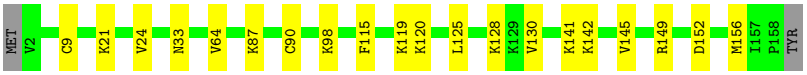
• Molecule 72: 60S ribosomal protein L44

Chain Bt:



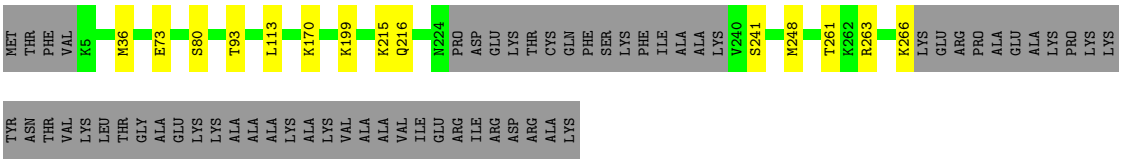
• Molecule 73: 60S ribosomal protein L21E, putative

Chain BU:



• Molecule 74: 60S ribosomal protein L5, putative

Chain Bu:

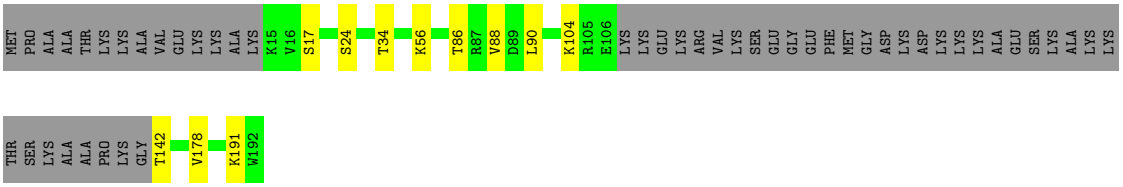


• Molecule 75: 60S ribosomal protein L22, putative

Chain BV:

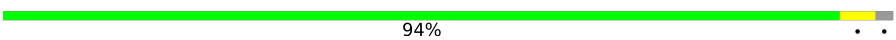
• Molecule 76: 60S ribosomal protein L6, putative

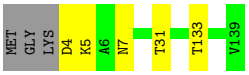
Chain Bv:



• Molecule 77: 60S ribosomal protein L23, putative

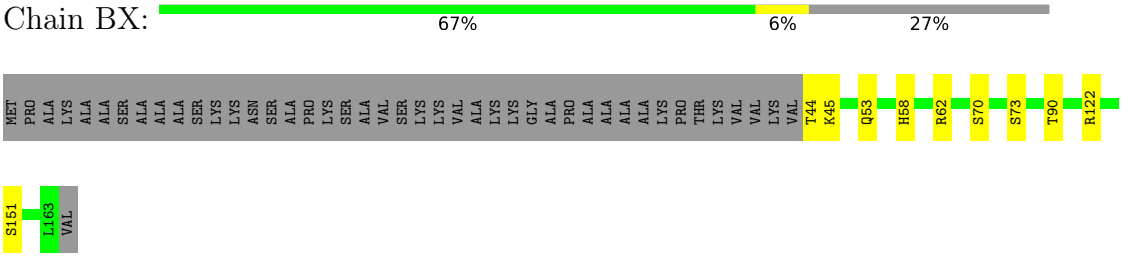
Chain BW:





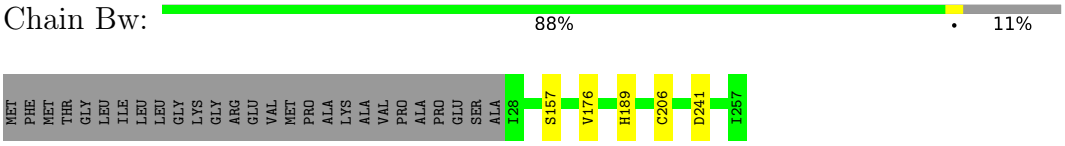
• Molecule 78: 60S ribosomal protein L23a

Chain BX:



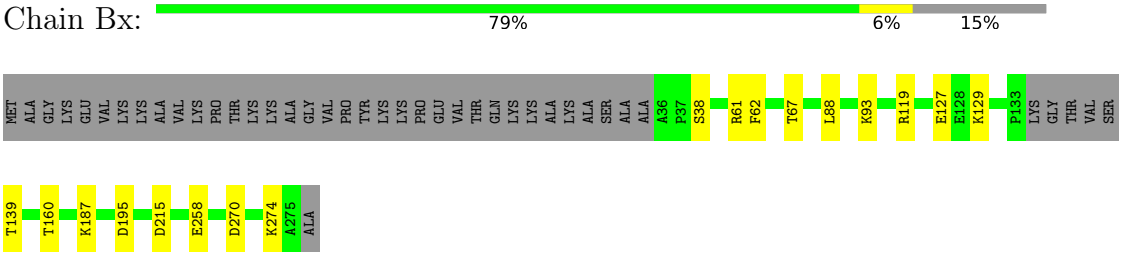
• Molecule 79: 60S ribosomal protein L7, putative

Chain Bw:



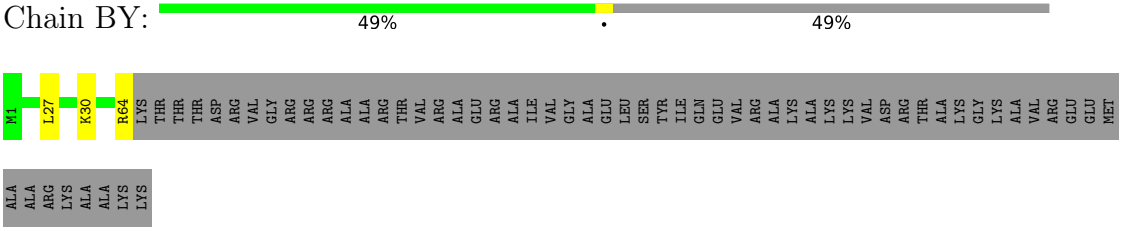
• Molecule 80: 60S ribosomal protein L7a

Chain Bx:



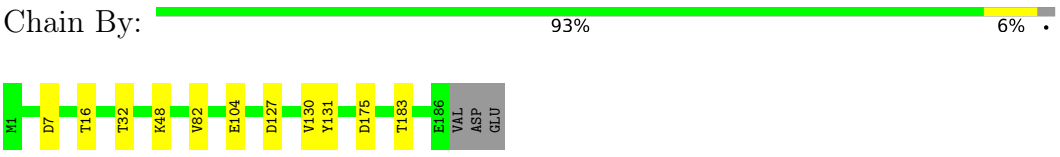
• Molecule 81: 60S ribosomal protein L24, putative

Chain BY:



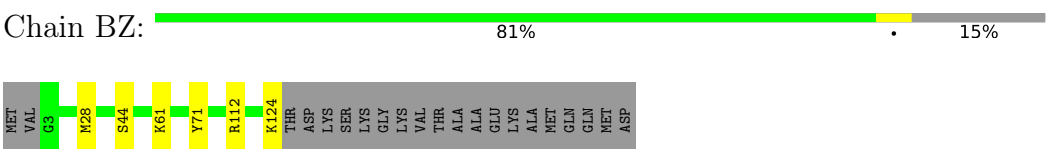
• Molecule 82: 60S ribosomal protein L9, putative

Chain By:



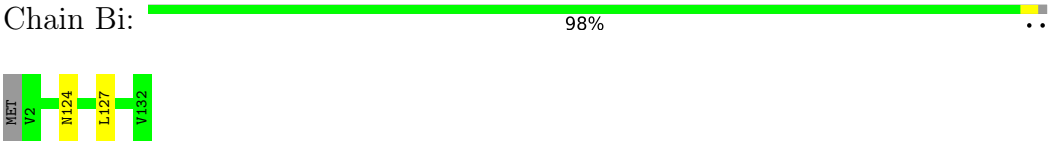
• Molecule 83: 60S ribosomal protein L26, putative

Chain BZ:



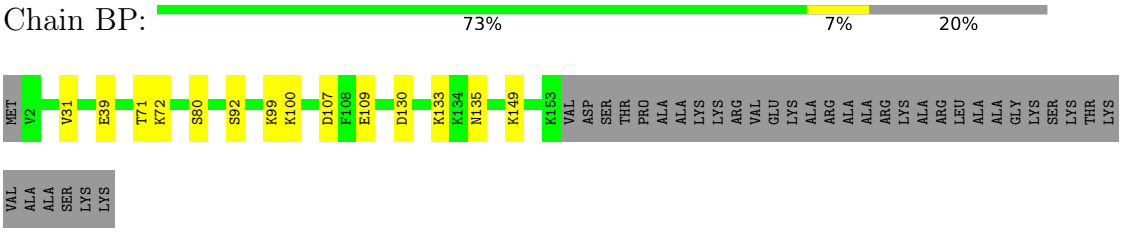
• Molecule 84: 60S ribosomal protein L32, putative

Chain Bi:



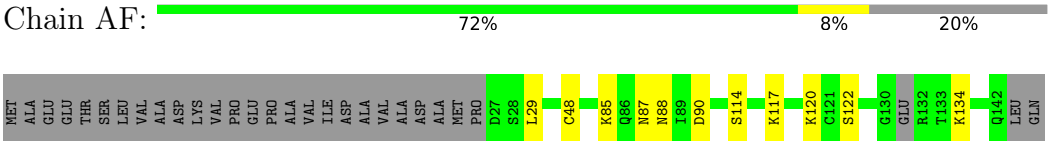
• Molecule 85: 40S ribosomal protein L14, putative

Chain BP:



• Molecule 86: 40S ribosomal protein S12

Chain AF:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	459985	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.17	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (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: 7MG, 5MC, PSU, NA, K, B8N, A2M, OMG, OMU, ZN, OMC, MG, 1MA, MA6

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	BA	0.41	0/37519	0.85	40/58462 (0.1%)
2	AA	0.49	0/44961	0.90	88/70031 (0.1%)
3	BB	0.44	0/25592	0.85	18/39885 (0.0%)
4	BH	0.39	0/2833	0.83	3/4410 (0.1%)
5	BG	0.41	0/4383	0.83	4/6835 (0.1%)
6	BF	0.35	0/1604	0.89	2/2487 (0.1%)
7	BE	0.41	0/4442	0.91	11/6910 (0.2%)
8	BD	0.36	0/2830	0.74	0/4410
9	BC	0.36	0/3662	0.78	0/5700
10	AB	0.41	0/450	0.95	0/698
11	AQ	0.28	0/809	0.60	0/1091
12	A8	0.27	0/468	0.55	0/619
13	A9	0.30	0/582	0.59	0/773
14	Az	0.29	0/820	0.62	0/1100
15	AH	0.29	0/1006	0.61	0/1349
16	AI	0.29	0/986	0.51	0/1321
17	AJ	0.29	0/1035	0.53	0/1386
18	AK	0.29	0/1161	0.55	0/1561
19	AM	0.27	0/1161	0.55	0/1554
20	AO	0.27	0/1245	0.52	0/1665
21	AP	0.30	0/1723	0.52	0/2328
22	AR	0.27	0/676	0.48	0/919
23	AS	0.28	0/1117	0.54	0/1495
24	AT	0.28	0/1050	0.52	0/1395
25	AU	0.27	0/581	0.57	1/776 (0.1%)
26	AV	0.33	0/846	0.64	0/1132
27	AW	0.30	0/674	0.58	0/904
28	AX	0.27	0/1674	0.54	0/2236
29	AY	0.29	0/453	0.52	0/596
30	AZ	0.29	0/448	0.62	0/595
31	AL	0.26	0/957	0.50	0/1282
32	A0	0.28	0/1815	0.54	0/2440

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	A1	0.28	0/2096	0.56	1/2819 (0.0%)
34	A2	0.27	0/1486	0.51	0/1997
35	A3	0.27	0/1893	0.61	1/2533 (0.0%)
36	A4	0.27	0/1634	0.52	0/2208
37	A5	0.28	0/1494	0.57	0/2004
38	A6	0.28	0/1507	0.54	0/2023
39	A7	0.26	0/2428	0.52	0/3311
40	AC	0.30	0/1682	0.50	0/2275
41	AD	0.29	0/837	0.49	0/1129
42	AE	0.30	0/1274	0.56	0/1714
43	AG	0.28	0/1225	0.53	0/1642
44	Bh	0.26	0/1270	0.57	0/1696
45	Ba	0.29	0/1105	0.55	0/1472
46	Bb	0.26	0/1165	0.53	0/1554
47	Bc	0.25	0/1179	0.52	0/1573
48	Bd	0.25	0/558	0.52	0/747
49	Be	0.29	0/1948	0.57	0/2621
50	Bz	0.28	0/288	0.70	0/374
51	Bg	0.28	0/718	0.48	0/969
52	Bf	0.27	0/3244	0.54	0/4360
53	BI	0.25	0/1543	0.55	0/2059
54	Bj	0.26	0/977	0.59	0/1304
55	BK	0.27	0/1620	0.56	0/2171
56	Bk	0.26	0/1018	0.57	0/1346
57	BL	0.28	0/1346	0.53	0/1800
58	Bl	0.28	0/1187	0.57	0/1592
59	Bm	0.26	0/796	0.59	1/1057 (0.1%)
60	BN	0.26	0/1793	0.55	0/2391
61	Bn	0.27	0/690	0.64	0/920
62	BO	0.26	0/1832	0.53	0/2446
63	Bo	0.30	0/711	0.58	0/946
64	Bp	0.27	0/635	0.55	0/844
65	Bq	0.26	0/471	0.53	0/626
66	BQ	0.27	0/1755	0.59	0/2346
67	BR	0.26	0/1244	0.52	0/1669
68	Br	0.25	0/2936	0.54	0/3941
69	BS	0.28	0/1500	0.54	0/2018
70	Bs	0.29	0/400	0.58	0/531
71	BT	0.27	0/1607	0.59	0/2130
72	Bt	0.27	0/815	0.53	0/1077
73	BU	0.28	0/1276	0.55	0/1716
74	Bu	0.28	0/1999	0.56	0/2684
75	BV	0.29	0/995	0.60	0/1329

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
76	Bv	0.27	0/1120	0.51	0/1511
77	BW	0.29	0/1046	0.54	0/1408
78	BX	0.26	0/999	0.55	0/1343
79	Bw	0.27	0/1907	0.51	0/2556
80	Bx	0.25	0/1901	0.54	0/2557
81	BY	0.30	0/570	0.58	0/766
82	By	0.27	0/1536	0.55	0/2065
83	BZ	0.26	0/1006	0.61	0/1340
84	Bi	0.27	0/1097	0.55	0/1468
85	BP	0.27	0/1256	0.50	0/1683
86	AF	0.26	0/870	0.53	0/1169
All	All	0.38	0/221048	0.76	170/324175 (0.1%)

There are no bond length outliers.

All (170) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	BB	515	G	P-O3'-C3'	-9.67	108.09	119.70
3	BB	528	U	P-O3'-C3'	-9.66	108.11	119.70
2	AA	878	U	P-O3'-C3'	-9.57	108.21	119.70
3	BB	514	G	P-O3'-C3'	-8.94	108.98	119.70
1	BA	74	C	C2-N1-C1'	8.83	128.52	118.80
2	AA	874	U	P-O3'-C3'	-8.71	109.25	119.70
3	BB	529	C	P-O3'-C3'	-8.69	109.28	119.70
2	AA	875	G	P-O3'-C3'	-8.48	109.53	119.70
1	BA	74	C	N1-C2-O2	8.36	123.92	118.90
1	BA	1524	U	N3-C2-O2	-8.34	116.36	122.20
3	BB	516	A	P-O3'-C3'	-8.28	109.76	119.70
2	AA	876	C	P-O3'-C3'	-8.23	109.82	119.70
3	BB	527	C	P-O3'-C3'	-8.22	109.84	119.70
1	BA	1843	U	C2-N1-C1'	8.12	127.45	117.70
1	BA	1315	C	C2-N1-C1'	7.92	127.51	118.80
2	AA	1278	A	P-O3'-C3'	-7.80	110.34	119.70
2	AA	873	A	P-O3'-C3'	-7.56	110.63	119.70
1	BA	1524	U	N1-C2-O2	7.23	127.86	122.80
2	AA	1277	U	P-O3'-C3'	-7.19	111.07	119.70
3	BB	1079	C	C2-N1-C1'	7.12	126.63	118.80
1	BA	1315	C	N1-C2-O2	7.06	123.14	118.90
3	BB	530	U	P-O3'-C3'	-7.06	111.23	119.70
1	BA	1524	U	C2-N1-C1'	7.04	126.15	117.70
2	AA	877	A	P-O3'-C3'	-7.01	111.29	119.70
1	BA	1843	U	N1-C2-O2	7.00	127.70	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	AA	2027	C	N3-C2-O2	-6.75	117.17	121.90
1	BA	74	C	N3-C2-O2	-6.72	117.19	121.90
2	AA	142	C	OP1-P-OP2	-6.70	109.56	119.60
1	BA	1843	U	N3-C2-O2	-6.59	117.59	122.20
2	AA	1461	C	C2-N1-C1'	6.58	126.04	118.80
2	AA	1074	C	N1-C2-O2	6.49	122.79	118.90
1	BA	74	C	C6-N1-C1'	-6.44	113.07	120.80
1	BA	1042	U	C2-N1-C1'	6.42	125.41	117.70
1	BA	204	U	C2-N1-C1'	6.32	125.28	117.70
2	AA	2180	C	C2-N1-C1'	6.26	125.69	118.80
2	AA	2031	C	N1-C2-O2	6.15	122.59	118.90
2	AA	2196	C	C2-N1-C1'	6.04	125.45	118.80
2	AA	627	C	C2-N1-C1'	5.97	125.37	118.80
2	AA	1461	C	N1-C2-O2	5.90	122.44	118.90
3	BB	837	C	N1-C2-O2	5.89	122.44	118.90
7	BE	195	U	C2-N1-C1'	5.89	124.77	117.70
2	AA	628	C	C2-N1-C1'	5.88	125.27	118.80
2	AA	1016	C	N1-C2-O2	5.81	122.39	118.90
33	A1	26	PRO	C-N-CA	-5.78	107.24	121.70
2	AA	1827	C	C2-N1-C1'	5.78	125.16	118.80
2	AA	713	U	N3-C2-O2	-5.76	118.17	122.20
1	BA	1315	C	N3-C2-O2	-5.75	117.87	121.90
2	AA	620	C	C2-N1-C1'	5.75	125.12	118.80
2	AA	1663	C	N3-C2-O2	-5.74	117.88	121.90
2	AA	281	C	C2-N1-C1'	5.73	125.10	118.80
2	AA	1757	C	N3-C2-O2	-5.72	117.90	121.90
4	BH	69	C	N1-C2-O2	5.71	122.33	118.90
1	BA	477	G	O4'-C1'-N9	5.71	112.77	108.20
4	BH	69	C	C2-N1-C1'	5.71	125.08	118.80
2	AA	1242	C	C2-N1-C1'	5.71	125.08	118.80
7	BE	129	C	C2-N1-C1'	5.71	125.08	118.80
2	AA	626	C	C2-N1-C1'	5.71	125.08	118.80
1	BA	198	C	C2-N1-C1'	5.70	125.07	118.80
2	AA	683	U	C2-N1-C1'	5.70	124.54	117.70
2	AA	95	C	C2-N1-C1'	5.68	125.04	118.80
2	AA	1823	C	N1-C2-O2	5.65	122.29	118.90
2	AA	385	C	C2-N1-C1'	5.64	125.00	118.80
2	AA	1539	C	N3-C2-O2	-5.63	117.96	121.90
2	AA	937	C	C2-N1-C1'	5.60	124.96	118.80
2	AA	779	C	N1-C2-O2	5.58	122.25	118.90
2	AA	969	C	C2-N1-C1'	5.58	124.94	118.80
3	BB	1079	C	N1-C2-O2	5.57	122.24	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	AA	2036	G	O4'-C1'-N9	5.57	112.65	108.20
2	AA	694	A	O4'-C1'-N9	5.56	112.65	108.20
3	BB	992	C	C2-N1-C1'	5.56	124.92	118.80
2	AA	940	C	C2-N1-C1'	5.54	124.89	118.80
2	AA	2180	C	N1-C2-O2	5.54	122.22	118.90
2	AA	1074	C	C2-N1-C1'	5.54	124.89	118.80
1	BA	1315	C	C6-N1-C1'	-5.53	114.16	120.80
2	AA	1539	C	C2-N1-C1'	5.51	124.86	118.80
2	AA	1609	C	N3-C2-O2	-5.50	118.05	121.90
3	BB	814	C	N1-C2-O2	5.50	122.20	118.90
59	Bm	54	ASP	CB-CG-OD1	5.50	123.25	118.30
1	BA	1843	U	C6-N1-C1'	-5.50	113.51	121.20
5	BG	148	C	N1-C2-O2	5.49	122.19	118.90
6	BF	61	C	C2-N1-C1'	5.48	124.83	118.80
7	BE	18	C	C2-N1-C1'	5.48	124.82	118.80
1	BA	189	C	C2-N1-C1'	5.43	124.78	118.80
2	AA	2031	C	N3-C2-O2	-5.43	118.10	121.90
2	AA	712	G	C4-N9-C1'	5.43	133.56	126.50
2	AA	349	C	C2-N1-C1'	5.42	124.76	118.80
7	BE	187	C	C2-N1-C1'	5.42	124.76	118.80
2	AA	1866	C	N1-C2-O2	5.41	122.14	118.90
2	AA	2048	C	N1-C2-O2	5.40	122.14	118.90
3	BB	814	C	C2-N1-C1'	5.39	124.73	118.80
2	AA	1663	C	C2-N1-C1'	5.38	124.72	118.80
1	BA	204	U	N1-C2-O2	5.38	126.57	122.80
2	AA	1757	C	N1-C2-O2	5.37	122.12	118.90
2	AA	2027	C	N1-C2-O2	5.37	122.12	118.90
1	BA	1293	U	C2-N1-C1'	5.35	124.12	117.70
2	AA	1854	U	C2-N1-C1'	5.35	124.12	117.70
6	BF	61	C	N1-C2-O2	5.34	122.11	118.90
2	AA	1478	U	C2-N1-C1'	5.34	124.11	117.70
7	BE	38	C	C2-N1-C1'	5.34	124.68	118.80
2	AA	620	C	N3-C2-O2	-5.33	118.17	121.90
2	AA	1767	C	C2-N1-C1'	5.33	124.66	118.80
1	BA	467	C	C2-N1-C1'	5.33	124.66	118.80
2	AA	796	C	C2-N1-C1'	5.32	124.65	118.80
2	AA	621	U	N3-C2-O2	-5.32	118.48	122.20
2	AA	1823	C	C2-N1-C1'	5.31	124.64	118.80
5	BG	148	C	C2-N1-C1'	5.31	124.64	118.80
2	AA	969	C	N1-C2-O2	5.30	122.08	118.90
7	BE	25	C	C2-N1-C1'	5.29	124.62	118.80
2	AA	909	C	C2-N1-C1'	5.29	124.62	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	BB	1200	C	N3-C2-O2	-5.29	118.20	121.90
1	BA	1860	C	C2-N1-C1'	5.28	124.60	118.80
2	AA	580	C	C2-N1-C1'	5.28	124.61	118.80
1	BA	1684	U	C2-N1-C1'	5.28	124.03	117.70
3	BB	558	C	C2-N1-C1'	5.28	124.60	118.80
2	AA	2031	C	C2-N1-C1'	5.27	124.59	118.80
1	BA	955	G	O4'-C1'-N9	5.26	112.41	108.20
2	AA	1475	U	C2-N1-C1'	5.26	124.01	117.70
2	AA	2048	C	N3-C2-O2	-5.25	118.22	121.90
3	BB	837	C	N3-C2-O2	-5.25	118.23	121.90
2	AA	1663	C	N1-C2-O2	5.24	122.05	118.90
7	BE	43	U	C2-N1-C1'	5.24	123.99	117.70
7	BE	43	U	N3-C2-O2	-5.24	118.53	122.20
2	AA	1866	C	C2-N1-C1'	5.23	124.55	118.80
2	AA	2048	C	C2-N1-C1'	5.22	124.55	118.80
2	AA	326	C	C2-N1-C1'	5.22	124.54	118.80
1	BA	1741	U	N3-C2-O2	-5.21	118.55	122.20
2	AA	1609	C	C6-N1-C2	-5.21	118.22	120.30
1	BA	1734	U	N3-C2-O2	-5.20	118.56	122.20
1	BA	1481	U	C2-N1-C1'	5.20	123.94	117.70
2	AA	689	C	C2-N1-C1'	5.20	124.52	118.80
2	AA	1952	C	C2-N1-C1'	5.20	124.52	118.80
2	AA	1743	C	C2-N1-C1'	5.19	124.51	118.80
2	AA	326	C	N1-C2-O2	5.19	122.02	118.90
2	AA	762	C	N1-C2-O2	5.19	122.02	118.90
1	BA	845	C	C2-N1-C1'	5.18	124.50	118.80
2	AA	2076	C	C2-N1-C1'	5.18	124.50	118.80
2	AA	1823	C	N3-C2-O2	-5.18	118.28	121.90
2	AA	1868	C	C2-N1-C1'	5.17	124.49	118.80
2	AA	796	C	N1-C2-O2	5.17	122.00	118.90
2	AA	1483	C	N1-C2-O2	5.17	122.00	118.90
4	BH	108	U	C2-N1-C1'	5.17	123.90	117.70
2	AA	747	C	N1-C2-O2	5.14	121.98	118.90
3	BB	970	C	N1-C2-O2	5.14	121.98	118.90
2	AA	747	C	C2-N1-C1'	5.13	124.45	118.80
1	BA	1654	C	C2-N1-C1'	5.13	124.44	118.80
1	BA	1207	U	N1-C2-O2	5.10	126.37	122.80
1	BA	1524	U	C6-N1-C2	-5.10	117.94	121.00
5	BG	85	C	N3-C2-O2	-5.10	118.33	121.90
35	A3	38	ASP	CB-CG-OD2	5.08	122.88	118.30
7	BE	46	C	N1-C2-O2	5.08	121.95	118.90
1	BA	1654	C	N1-C2-O2	5.08	121.95	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	AA	303	A	O4'-C1'-N9	5.08	112.27	108.20
2	AA	1539	C	N1-C2-O2	5.08	121.95	118.90
1	BA	1168	C	C2-N1-C1'	5.08	124.39	118.80
5	BG	148	C	N3-C2-O2	-5.08	118.35	121.90
1	BA	204	U	N3-C2-O2	-5.07	118.65	122.20
1	BA	1316	U	C2-N1-C1'	5.07	123.78	117.70
2	AA	1074	C	N3-C2-O2	-5.07	118.35	121.90
1	BA	1654	C	N3-C2-O2	-5.07	118.35	121.90
7	BE	46	C	N3-C2-O2	-5.07	118.35	121.90
3	BB	1297	U	C2-N1-C1'	5.06	123.78	117.70
1	BA	127	U	C2-N1-C1'	5.05	123.76	117.70
2	AA	1827	C	N1-C2-O2	5.04	121.93	118.90
7	BE	123	U	P-O3'-C3'	5.04	125.75	119.70
2	AA	620	C	C6-N1-C2	-5.04	118.28	120.30
25	AU	54	ASP	CB-CG-OD1	5.03	122.83	118.30
2	AA	483	G	N3-C4-N9	-5.03	122.98	126.00
2	AA	1783	U	C2-N1-C1'	5.01	123.72	117.70
2	AA	1483	C	C2-N1-C1'	5.01	124.31	118.80
1	BA	1860	C	C6-N1-C2	-5.00	118.30	120.30

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	
11	AQ	98/117 (84%)	96 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	A8	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
13	A9	66/153 (43%)	61 (92%)	5 (8%)	0	100	100
14	Az	98/279 (35%)	84 (86%)	13 (13%)	1 (1%)	15	26
15	AH	132/144 (92%)	118 (89%)	14 (11%)	0	100	100
16	AI	115/152 (76%)	112 (97%)	3 (3%)	0	100	100
17	AJ	127/130 (98%)	123 (97%)	4 (3%)	0	100	100
18	AK	140/149 (94%)	134 (96%)	6 (4%)	0	100	100
19	AM	139/153 (91%)	134 (96%)	5 (4%)	0	100	100
20	AO	152/167 (91%)	147 (97%)	5 (3%)	0	100	100
21	AP	216/266 (81%)	203 (94%)	12 (6%)	1 (0%)	29	46
22	AR	87/194 (45%)	85 (98%)	2 (2%)	0	100	100
23	AS	138/143 (96%)	128 (93%)	10 (7%)	0	100	100
24	AT	127/137 (93%)	118 (93%)	9 (7%)	0	100	100
25	AU	71/113 (63%)	67 (94%)	4 (6%)	0	100	100
26	AV	101/111 (91%)	94 (93%)	7 (7%)	0	100	100
27	AW	83/86 (96%)	80 (96%)	3 (4%)	0	100	100
28	AX	206/214 (96%)	196 (95%)	10 (5%)	0	100	100
29	AY	51/66 (77%)	50 (98%)	1 (2%)	0	100	100
30	AZ	54/103 (52%)	52 (96%)	2 (4%)	0	100	100
31	AL	120/142 (84%)	115 (96%)	5 (4%)	0	100	100
32	A0	216/256 (84%)	211 (98%)	5 (2%)	0	100	100
33	A1	260/273 (95%)	245 (94%)	15 (6%)	0	100	100
34	A2	179/190 (94%)	177 (99%)	2 (1%)	0	100	100
35	A3	236/250 (94%)	228 (97%)	8 (3%)	0	100	100
36	A4	196/202 (97%)	187 (95%)	9 (5%)	0	100	100
37	A5	183/220 (83%)	176 (96%)	7 (4%)	0	100	100
38	A6	177/190 (93%)	173 (98%)	4 (2%)	0	100	100
39	A7	305/318 (96%)	294 (96%)	11 (4%)	0	100	100
40	AC	206/277 (74%)	200 (97%)	6 (3%)	0	100	100
41	AD	97/172 (56%)	94 (97%)	3 (3%)	0	100	100
42	AE	151/174 (87%)	143 (95%)	8 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	AG	148/151 (98%)	144 (97%)	4 (3%)	0	100	100
44	Bh	152/188 (81%)	142 (93%)	10 (7%)	0	100	100
45	Ba	130/133 (98%)	129 (99%)	1 (1%)	0	100	100
46	Bb	142/145 (98%)	136 (96%)	6 (4%)	0	100	100
47	Bc	142/146 (97%)	139 (98%)	3 (2%)	0	100	100
48	Bd	65/71 (92%)	63 (97%)	2 (3%)	0	100	100
49	Be	253/260 (97%)	247 (98%)	6 (2%)	0	100	100
50	Bz	30/34 (88%)	30 (100%)	0	0	100	100
51	Bg	90/105 (86%)	90 (100%)	0	0	100	100
52	Bf	394/429 (92%)	388 (98%)	6 (2%)	0	100	100
53	BI	189/193 (98%)	183 (97%)	6 (3%)	0	100	100
54	Bj	114/170 (67%)	111 (97%)	3 (3%)	0	100	100
55	BK	190/213 (89%)	182 (96%)	8 (4%)	0	100	100
56	Bk	121/127 (95%)	115 (95%)	5 (4%)	1 (1%)	19	33
57	BL	164/194 (84%)	155 (94%)	9 (6%)	0	100	100
58	Bl	142/149 (95%)	136 (96%)	6 (4%)	0	100	100
59	Bm	96/109 (88%)	95 (99%)	1 (1%)	0	100	100
60	BN	213/218 (98%)	202 (95%)	11 (5%)	0	100	100
61	Bn	78/84 (93%)	76 (97%)	2 (3%)	0	100	100
62	BO	219/222 (99%)	218 (100%)	1 (0%)	0	100	100
63	Bo	87/93 (94%)	83 (95%)	4 (5%)	0	100	100
64	Bp	75/82 (92%)	71 (95%)	4 (5%)	0	100	100
65	Bq	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
66	BQ	201/221 (91%)	197 (98%)	4 (2%)	0	100	100
67	BR	149/166 (90%)	147 (99%)	2 (1%)	0	100	100
68	Br	365/374 (98%)	352 (96%)	13 (4%)	0	100	100
69	BS	176/179 (98%)	170 (97%)	6 (3%)	0	100	100
70	Bs	48/128 (38%)	46 (96%)	2 (4%)	0	100	100
71	BT	194/260 (75%)	186 (96%)	8 (4%)	0	100	100
72	Bt	95/106 (90%)	91 (96%)	4 (4%)	0	100	100
73	BU	155/159 (98%)	143 (92%)	11 (7%)	1 (1%)	25	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
74	Bu	243/308 (79%)	234 (96%)	9 (4%)	0	100 100
75	BV	120/130 (92%)	111 (92%)	8 (7%)	1 (1%)	19 33
76	Bv	139/192 (72%)	134 (96%)	5 (4%)	0	100 100
77	BW	134/139 (96%)	132 (98%)	2 (2%)	0	100 100
78	BX	118/164 (72%)	114 (97%)	4 (3%)	0	100 100
79	Bw	228/257 (89%)	223 (98%)	5 (2%)	0	100 100
80	Bx	231/276 (84%)	220 (95%)	11 (5%)	0	100 100
81	BY	62/125 (50%)	60 (97%)	2 (3%)	0	100 100
82	By	184/189 (97%)	175 (95%)	9 (5%)	0	100 100
83	BZ	120/143 (84%)	118 (98%)	2 (2%)	0	100 100
84	Bi	129/132 (98%)	125 (97%)	4 (3%)	0	100 100
85	BP	150/189 (79%)	144 (96%)	6 (4%)	0	100 100
86	AF	111/144 (77%)	107 (96%)	3 (3%)	1 (1%)	17 29
All	All	11215/13146 (85%)	10789 (96%)	420 (4%)	6 (0%)	54 71

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	Az	169	THR
56	Bk	6	LYS
73	BU	33	ASN
75	BV	17	ARG
86	AF	122	SER
21	AP	58	ILE

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
11	AQ	90/104 (86%)	82 (91%)	8 (9%)	9 17
12	A8	49/50 (98%)	48 (98%)	1 (2%)	55 77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
13	A9	62/126 (49%)	58 (94%)	4 (6%)	17 31
14	Az	86/216 (40%)	73 (85%)	13 (15%)	3 4
15	AH	101/112 (90%)	95 (94%)	6 (6%)	19 35
16	AI	100/128 (78%)	93 (93%)	7 (7%)	15 27
17	AJ	108/109 (99%)	102 (94%)	6 (6%)	21 38
18	AK	117/124 (94%)	106 (91%)	11 (9%)	8 15
19	AM	123/133 (92%)	116 (94%)	7 (6%)	20 37
20	AO	127/137 (93%)	123 (97%)	4 (3%)	40 64
21	AP	181/204 (89%)	169 (93%)	12 (7%)	16 30
22	AR	73/150 (49%)	69 (94%)	4 (6%)	21 39
23	AS	115/118 (98%)	105 (91%)	10 (9%)	10 18
24	AT	108/116 (93%)	104 (96%)	4 (4%)	34 57
25	AU	64/94 (68%)	60 (94%)	4 (6%)	18 32
26	AV	90/97 (93%)	87 (97%)	3 (3%)	38 61
27	AW	74/75 (99%)	71 (96%)	3 (4%)	30 53
28	AX	176/180 (98%)	167 (95%)	9 (5%)	24 42
29	AY	47/53 (89%)	44 (94%)	3 (6%)	17 31
30	AZ	49/84 (58%)	45 (92%)	4 (8%)	11 20
31	AL	96/122 (79%)	88 (92%)	8 (8%)	11 20
32	A0	190/218 (87%)	183 (96%)	7 (4%)	34 57
33	A1	221/231 (96%)	206 (93%)	15 (7%)	16 28
34	A2	157/160 (98%)	149 (95%)	8 (5%)	24 42
35	A3	191/207 (92%)	175 (92%)	16 (8%)	11 19
36	A4	173/187 (92%)	152 (88%)	21 (12%)	5 8
37	A5	147/180 (82%)	133 (90%)	14 (10%)	8 15
38	A6	159/166 (96%)	149 (94%)	10 (6%)	18 32
39	A7	260/267 (97%)	236 (91%)	24 (9%)	9 16
40	AC	183/243 (75%)	174 (95%)	9 (5%)	25 44
41	AD	87/131 (66%)	79 (91%)	8 (9%)	9 16
42	AE	137/156 (88%)	128 (93%)	9 (7%)	16 30
43	AG	130/131 (99%)	123 (95%)	7 (5%)	22 40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
44	Bh	133/162 (82%)	122 (92%)	11 (8%)	11 20
45	Ba	115/117 (98%)	101 (88%)	14 (12%)	5 8
46	Bb	115/116 (99%)	108 (94%)	7 (6%)	18 34
47	Bc	128/130 (98%)	123 (96%)	5 (4%)	32 55
48	Bd	56/59 (95%)	52 (93%)	4 (7%)	14 26
49	Be	191/204 (94%)	185 (97%)	6 (3%)	40 64
50	Bz	29/31 (94%)	29 (100%)	0	100 100
51	Bg	81/92 (88%)	75 (93%)	6 (7%)	13 25
52	Bf	337/360 (94%)	322 (96%)	15 (4%)	27 48
53	BI	163/165 (99%)	156 (96%)	7 (4%)	29 50
54	Bj	99/137 (72%)	96 (97%)	3 (3%)	41 65
55	BK	169/185 (91%)	157 (93%)	12 (7%)	14 26
56	Bk	104/114 (91%)	97 (93%)	7 (7%)	16 29
57	BL	142/167 (85%)	128 (90%)	14 (10%)	8 13
58	Bl	122/126 (97%)	118 (97%)	4 (3%)	38 61
59	Bm	81/90 (90%)	78 (96%)	3 (4%)	34 57
60	BN	185/188 (98%)	179 (97%)	6 (3%)	39 63
61	Bn	68/71 (96%)	64 (94%)	4 (6%)	19 35
62	BO	194/195 (100%)	191 (98%)	3 (2%)	65 83
63	Bo	72/76 (95%)	69 (96%)	3 (4%)	30 51
64	Bp	72/77 (94%)	64 (89%)	8 (11%)	6 10
65	Bq	46/47 (98%)	44 (96%)	2 (4%)	29 50
66	BQ	176/193 (91%)	169 (96%)	7 (4%)	31 53
67	BR	129/144 (90%)	124 (96%)	5 (4%)	32 55
68	Br	304/310 (98%)	293 (96%)	11 (4%)	35 58
69	BS	159/160 (99%)	152 (96%)	7 (4%)	28 49
70	Bs	41/111 (37%)	37 (90%)	4 (10%)	8 14
71	BT	153/198 (77%)	145 (95%)	8 (5%)	23 41
72	Bt	87/95 (92%)	80 (92%)	7 (8%)	12 21
73	BU	132/134 (98%)	113 (86%)	19 (14%)	3 5
74	Bu	199/247 (81%)	185 (93%)	14 (7%)	15 27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
75	BV	100/116 (86%)	87 (87%)	13 (13%)	4 7
76	Bv	119/160 (74%)	108 (91%)	11 (9%)	9 16
77	BW	106/108 (98%)	101 (95%)	5 (5%)	26 46
78	BX	107/136 (79%)	97 (91%)	10 (9%)	9 15
79	Bw	193/213 (91%)	188 (97%)	5 (3%)	46 70
80	Bx	199/229 (87%)	182 (92%)	17 (8%)	10 19
81	BY	57/102 (56%)	54 (95%)	3 (5%)	22 40
82	By	169/172 (98%)	158 (94%)	11 (6%)	17 31
83	BZ	108/125 (86%)	102 (94%)	6 (6%)	21 38
84	Bi	116/117 (99%)	114 (98%)	2 (2%)	60 81
85	BP	132/158 (84%)	118 (89%)	14 (11%)	6 12
86	AF	93/120 (78%)	83 (89%)	10 (11%)	6 11
All	All	9652/11066 (87%)	9040 (94%)	612 (6%)	21 32

All (612) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	AQ	29	VAL
11	AQ	42	THR
11	AQ	45	VAL
11	AQ	46	GLU
11	AQ	55	THR
11	AQ	75	ASP
11	AQ	89	ARG
11	AQ	110	SER
12	A8	9	SER
13	A9	103	TYR
13	A9	107	THR
13	A9	109	ASN
13	A9	113	SER
14	Az	155	SER
14	Az	158	VAL
14	Az	161	SER
14	Az	165	ARG
14	Az	166	THR
14	Az	177	PHE
14	Az	178	THR
14	Az	189	ARG

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Mol	Chain	Res	Type
14	Az	205	LYS
14	Az	226	THR
14	Az	234	ASP
14	Az	237	GLU
14	Az	238	ARG
15	AH	10	TYR
15	AH	13	SER
15	AH	16	LYS
15	AH	80	GLU
15	AH	100	SER
15	AH	117	MET
16	AI	20	HIS
16	AI	25	ARG
16	AI	30	ASP
16	AI	50	ARG
16	AI	71	LYS
16	AI	75	LYS
16	AI	137	ARG
17	AJ	11	LEU
17	AJ	19	ARG
17	AJ	30	SER
17	AJ	31	SER
17	AJ	36	LYS
17	AJ	82	THR
18	AK	28	THR
18	AK	34	ASN
18	AK	40	VAL
18	AK	64	ARG
18	AK	70	ARG
18	AK	72	ASP
18	AK	74	ARG
18	AK	75	VAL
18	AK	101	LYS
18	AK	134	LYS
18	AK	147	SER
19	AM	7	SER
19	AM	15	ARG
19	AM	35	LYS
19	AM	87	ARG
19	AM	90	ASP
19	AM	139	THR
19	AM	143	ARG

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Mol	Chain	Res	Type
20	AO	56	THR
20	AO	57	SER
20	AO	113	SER
20	AO	118	HIS
21	AP	151	ARG
21	AP	168	VAL
21	AP	184	ARG
21	AP	206	VAL
21	AP	208	THR
21	AP	209	SER
21	AP	220	PHE
21	AP	229	ARG
21	AP	232	TYR
21	AP	246	SER
21	AP	248	ASP
21	AP	254	SER
22	AR	47	ASN
22	AR	69	SER
22	AR	80	LYS
22	AR	89	LYS
23	AS	2	THR
23	AS	12	LYS
23	AS	30	SER
23	AS	33	PHE
23	AS	36	GLN
23	AS	44	SER
23	AS	70	VAL
23	AS	105	PHE
23	AS	112	VAL
23	AS	115	ILE
24	AT	2	VAL
24	AT	22	LEU
24	AT	24	ASN
24	AT	106	LYS
25	AU	51	GLU
25	AU	69	SER
25	AU	75	LEU
25	AU	91	ARG
26	AV	21	ARG
26	AV	98	ARG
26	AV	102	SER
27	AW	45	THR

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Mol	Chain	Res	Type
27	AW	57	CYS
27	AW	66	ARG
28	AX	25	LYS
28	AX	38	HIS
28	AX	43	THR
28	AX	50	ARG
28	AX	89	ARG
28	AX	112	LEU
28	AX	144	GLN
28	AX	169	THR
28	AX	205	THR
29	AY	45	LEU
29	AY	50	LYS
29	AY	55	LEU
30	AZ	45	LYS
30	AZ	61	VAL
30	AZ	64	MET
30	AZ	100	ARG
31	AL	8	THR
31	AL	23	LYS
31	AL	32	LYS
31	AL	67	ARG
31	AL	84	TYR
31	AL	85	VAL
31	AL	87	GLU
31	AL	88	VAL
32	A0	33	VAL
32	A0	50	LYS
32	A0	116	LEU
32	A0	130	LYS
32	A0	153	SER
32	A0	175	ARG
32	A0	188	SER
33	A1	54	ASN
33	A1	91	LYS
33	A1	99	LEU
33	A1	118	ILE
33	A1	135	VAL
33	A1	138	THR
33	A1	150	ARG
33	A1	164	LYS
33	A1	165	LYS

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Mol	Chain	Res	Type
33	A1	167	LEU
33	A1	179	MET
33	A1	208	LYS
33	A1	211	SER
33	A1	228	ASP
33	A1	238	LYS
34	A2	4	LYS
34	A2	35	VAL
34	A2	64	PHE
34	A2	121	ARG
34	A2	126	ASP
34	A2	140	MET
34	A2	161	ASP
34	A2	190	ARG
35	A3	9	ARG
35	A3	13	VAL
35	A3	20	ASP
35	A3	24	ARG
35	A3	38	ASP
35	A3	52	LYS
35	A3	66	GLN
35	A3	85	PHE
35	A3	105	LEU
35	A3	118	LYS
35	A3	129	ASP
35	A3	158	LYS
35	A3	172	ASP
35	A3	186	THR
35	A3	195	VAL
35	A3	215	LEU
36	A4	4	GLN
36	A4	11	ARG
36	A4	24	SER
36	A4	35	SER
36	A4	38	THR
36	A4	50	THR
36	A4	58	ARG
36	A4	61	LYS
36	A4	71	ARG
36	A4	84	THR
36	A4	90	ARG
36	A4	103	LYS

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Mol	Chain	Res	Type
36	A4	122	THR
36	A4	148	ARG
36	A4	149	THR
36	A4	150	ASP
36	A4	167	VAL
36	A4	168	GLU
36	A4	169	SER
36	A4	185	THR
36	A4	187	THR
37	A5	18	THR
37	A5	44	SER
37	A5	62	THR
37	A5	88	ASN
37	A5	103	VAL
37	A5	104	VAL
37	A5	121	LEU
37	A5	156	SER
37	A5	161	LYS
37	A5	163	GLU
37	A5	168	HIS
37	A5	173	LYS
37	A5	213	LYS
37	A5	216	ASP
38	A6	1	MET
38	A6	49	SER
38	A6	89	LYS
38	A6	93	ASP
38	A6	114	LYS
38	A6	115	HIS
38	A6	124	SER
38	A6	137	LYS
38	A6	150	SER
38	A6	161	SER
39	A7	18	SER
39	A7	34	THR
39	A7	71	SER
39	A7	86	SER
39	A7	90	SER
39	A7	101	CYS
39	A7	111	ASP
39	A7	122	ARG
39	A7	130	ASP

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Mol	Chain	Res	Type
39	A7	136	TRP
39	A7	139	LYS
39	A7	153	ASP
39	A7	160	PHE
39	A7	161	SER
39	A7	165	ASP
39	A7	187	ARG
39	A7	189	VAL
39	A7	250	TYR
39	A7	270	ILE
39	A7	272	VAL
39	A7	284	ILE
39	A7	285	VAL
39	A7	289	VAL
39	A7	306	ASP
40	AC	61	LEU
40	AC	78	THR
40	AC	80	ASP
40	AC	129	LEU
40	AC	133	SER
40	AC	202	ARG
40	AC	204	ARG
40	AC	236	ASP
40	AC	242	ASP
41	AD	17	PHE
41	AD	43	LYS
41	AD	48	GLN
41	AD	59	ARG
41	AD	74	THR
41	AD	83	MET
41	AD	85	LYS
41	AD	94	VAL
42	AE	20	HIS
42	AE	44	ARG
42	AE	45	SER
42	AE	56	LEU
42	AE	81	SER
42	AE	83	ARG
42	AE	93	SER
42	AE	154	ASN
42	AE	159	VAL
43	AG	32	ASP

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Mol	Chain	Res	Type
43	AG	42	LYS
43	AG	66	VAL
43	AG	140	LYS
43	AG	143	SER
43	AG	149	MET
43	AG	150	VAL
44	Bh	34	ASP
44	Bh	36	ARG
44	Bh	45	MET
44	Bh	52	LYS
44	Bh	99	ARG
44	Bh	114	SER
44	Bh	126	ARG
44	Bh	141	LYS
44	Bh	157	THR
44	Bh	168	THR
44	Bh	177	SER
45	Ba	29	ASP
45	Ba	30	THR
45	Ba	31	ARG
45	Ba	33	LYS
45	Ba	50	ARG
45	Ba	57	SER
45	Ba	80	LEU
45	Ba	83	ARG
45	Ba	89	SER
45	Ba	90	ARG
45	Ba	93	ARG
45	Ba	97	ASN
45	Ba	107	SER
45	Ba	123	ASN
46	Bb	9	ARG
46	Bb	26	ARG
46	Bb	27	LYS
46	Bb	60	HIS
46	Bb	86	GLU
46	Bb	88	MET
46	Bb	119	CYS
47	Bc	46	LEU
47	Bc	48	THR
47	Bc	121	LYS
47	Bc	128	LYS

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Mol	Chain	Res	Type
47	Bc	131	SER
48	Bd	13	SER
48	Bd	34	ARG
48	Bd	57	LYS
48	Bd	67	GLN
49	Be	18	VAL
49	Be	115	ASN
49	Be	130	SER
49	Be	147	ARG
49	Be	218	HIS
49	Be	242	ARG
51	Bg	20	THR
51	Bg	26	GLN
51	Bg	30	LYS
51	Bg	34	TYR
51	Bg	90	THR
51	Bg	109	SER
52	Bf	34	LYS
52	Bf	66	LYS
52	Bf	135	GLN
52	Bf	138	ARG
52	Bf	154	GLU
52	Bf	171	LEU
52	Bf	292	ARG
52	Bf	295	SER
52	Bf	310	LYS
52	Bf	339	ARG
52	Bf	349	MET
52	Bf	357	LEU
52	Bf	370	SER
52	Bf	380	LYS
52	Bf	393	ASP
53	BI	3	VAL
53	BI	75	THR
53	BI	76	VAL
53	BI	89	ILE
53	BI	101	ARG
53	BI	183	SER
53	BI	187	ARG
54	Bj	22	ARG
54	Bj	52	LYS
54	Bj	113	LYS

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Mol	Chain	Res	Type
55	BK	10	ARG
55	BK	39	ARG
55	BK	52	VAL
55	BK	53	VAL
55	BK	62	SER
55	BK	82	LYS
55	BK	121	LYS
55	BK	151	SER
55	BK	174	THR
55	BK	182	GLU
55	BK	183	GLU
55	BK	193	ARG
56	Bk	21	GLN
56	Bk	25	PHE
56	Bk	68	GLU
56	Bk	78	LYS
56	Bk	80	ARG
56	Bk	86	THR
56	Bk	120	ARG
57	BL	21	VAL
57	BL	25	CYS
57	BL	37	LEU
57	BL	45	GLU
57	BL	47	LEU
57	BL	81	LYS
57	BL	92	LYS
57	BL	141	ARG
57	BL	152	VAL
57	BL	154	ARG
57	BL	163	LYS
57	BL	174	HIS
57	BL	175	ASP
57	BL	177	ILE
58	Bl	15	ARG
58	Bl	23	THR
58	Bl	24	LYS
58	Bl	81	CYS
59	Bm	30	ARG
59	Bm	53	SER
59	Bm	58	PHE
60	BN	71	ASN
60	BN	72	MET

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Mol	Chain	Res	Type
60	BN	135	ARG
60	BN	139	GLN
60	BN	140	LYS
60	BN	171	ARG
61	Bn	33	ARG
61	Bn	55	LYS
61	Bn	65	ARG
61	Bn	79	LYS
62	BO	23	ASP
62	BO	115	ARG
62	BO	218	LYS
63	Bo	25	ARG
63	Bo	47	PHE
63	Bo	78	THR
64	Bp	6	LYS
64	Bp	12	LEU
64	Bp	18	LYS
64	Bp	19	ASP
64	Bp	31	VAL
64	Bp	39	SER
64	Bp	59	SER
64	Bp	63	SER
65	Bq	5	LYS
65	Bq	21	ARG
66	BQ	63	GLU
66	BQ	117	VAL
66	BQ	134	ASN
66	BQ	141	ASP
66	BQ	143	THR
66	BQ	201	LEU
66	BQ	202	ARG
67	BR	12	SER
67	BR	13	LYS
67	BR	23	ARG
67	BR	57	CYS
67	BR	104	GLU
68	Br	55	ARG
68	Br	68	THR
68	Br	84	SER
68	Br	121	PHE
68	Br	138	SER
68	Br	169	PHE

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Mol	Chain	Res	Type
68	Br	260	LYS
68	Br	283	THR
68	Br	303	LYS
68	Br	312	ARG
68	Br	336	GLU
69	BS	59	ASP
69	BS	62	SER
69	BS	68	ASP
69	BS	98	ASP
69	BS	119	ARG
69	BS	140	ASN
69	BS	147	HIS
70	Bs	82	LEU
70	Bs	108	THR
70	Bs	115	CYS
70	Bs	118	CYS
71	BT	5	LYS
71	BT	40	SER
71	BT	117	ARG
71	BT	139	MET
71	BT	148	GLU
71	BT	178	LEU
71	BT	180	LYS
71	BT	184	GLU
72	Bt	15	GLU
72	Bt	32	LYS
72	Bt	61	LYS
72	Bt	75	SER
72	Bt	77	CYS
72	Bt	87	ARG
72	Bt	98	LYS
73	BU	9	CYS
73	BU	21	LYS
73	BU	24	VAL
73	BU	64	VAL
73	BU	87	LYS
73	BU	90	CYS
73	BU	98	LYS
73	BU	115	PHE
73	BU	119	LYS
73	BU	120	LYS
73	BU	125	LEU

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Mol	Chain	Res	Type
73	BU	128	LYS
73	BU	130	VAL
73	BU	141	LYS
73	BU	142	LYS
73	BU	145	VAL
73	BU	149	ARG
73	BU	152	ASP
73	BU	156	MET
74	Bu	36	MET
74	Bu	73	GLU
74	Bu	80	SER
74	Bu	93	THR
74	Bu	113	LEU
74	Bu	170	LYS
74	Bu	199	LYS
74	Bu	215	LYS
74	Bu	216	GLN
74	Bu	241	SER
74	Bu	248	MET
74	Bu	261	THR
74	Bu	263	ARG
74	Bu	266	LYS
75	BV	15	ARG
75	BV	25	VAL
75	BV	30	CYS
75	BV	35	SER
75	BV	66	SER
75	BV	72	MET
75	BV	75	ASN
75	BV	78	SER
75	BV	80	THR
75	BV	81	THR
75	BV	82	THR
75	BV	93	LEU
75	BV	102	ASP
76	Bv	17	SER
76	Bv	24	SER
76	Bv	34	THR
76	Bv	56	LYS
76	Bv	86	THR
76	Bv	88	VAL
76	Bv	90	LEU

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Mol	Chain	Res	Type
76	Bv	104	LYS
76	Bv	142	THR
76	Bv	178	VAL
76	Bv	191	LYS
77	BW	4	ASP
77	BW	5	LYS
77	BW	7	ASN
77	BW	31	THR
77	BW	133	THR
78	BX	44	THR
78	BX	45	LYS
78	BX	53	GLN
78	BX	58	HIS
78	BX	62	ARG
78	BX	70	SER
78	BX	73	SER
78	BX	90	THR
78	BX	122	ARG
78	BX	151	SER
79	Bw	157	SER
79	Bw	176	VAL
79	Bw	189	HIS
79	Bw	206	CYS
79	Bw	241	ASP
80	Bx	38	SER
80	Bx	61	ARG
80	Bx	62	PHE
80	Bx	67	THR
80	Bx	88	LEU
80	Bx	93	LYS
80	Bx	119	ARG
80	Bx	127	GLU
80	Bx	129	LYS
80	Bx	139	THR
80	Bx	160	THR
80	Bx	187	LYS
80	Bx	195	ASP
80	Bx	215	ASP
80	Bx	258	GLU
80	Bx	270	ASP
80	Bx	274	LYS
81	BY	27	LEU

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Mol	Chain	Res	Type
81	BY	30	LYS
81	BY	64	ARG
82	By	7	ASP
82	By	16	THR
82	By	32	THR
82	By	48	LYS
82	By	82	VAL
82	By	104	GLU
82	By	127	ASP
82	By	130	VAL
82	By	131	TYR
82	By	175	ASP
82	By	183	THR
83	BZ	28	MET
83	BZ	44	SER
83	BZ	61	LYS
83	BZ	71	TYR
83	BZ	112	ARG
83	BZ	124	LYS
84	Bi	124	ASN
84	Bi	127	LEU
85	BP	31	VAL
85	BP	39	GLU
85	BP	71	THR
85	BP	72	LYS
85	BP	80	SER
85	BP	92	SER
85	BP	99	LYS
85	BP	100	LYS
85	BP	107	ASP
85	BP	109	GLU
85	BP	130	ASP
85	BP	133	LYS
85	BP	135	ASN
85	BP	149	LYS
86	AF	29	LEU
86	AF	48	CYS
86	AF	85	LYS
86	AF	87	ASN
86	AF	88	ASN
86	AF	90	ASP
86	AF	114	SER

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Mol	Chain	Res	Type
86	AF	117	LYS
86	AF	120	LYS
86	AF	134	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
36	A4	115	GLN
38	A6	64	ASN
39	A7	97	GLN
46	Bb	116	GLN
59	Bm	66	GLN
77	BW	30	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	BA	1585/1920 (82%)	300 (18%)	9 (0%)
10	AB	17/19 (89%)	7 (41%)	1 (5%)
2	AA	1899/2282 (83%)	424 (22%)	13 (0%)
3	BB	1113/1536 (72%)	209 (18%)	5 (0%)
4	BH	116/136 (85%)	27 (23%)	0
5	BG	182/183 (99%)	30 (16%)	1 (0%)
6	BF	66/78 (84%)	17 (25%)	1 (1%)
7	BE	185/216 (85%)	47 (25%)	4 (2%)
8	BD	118/119 (99%)	15 (12%)	0
9	BC	157/209 (75%)	22 (14%)	0
All	All	5438/6698 (81%)	1098 (20%)	34 (0%)

All (1098) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	BA	8	G
1	BA	28	A
1	BA	33	C
1	BA	42	A
1	BA	45	A
1	BA	51	C
1	BA	62	A
1	BA	68	A

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Mol	Chain	Res	Type
1	BA	76	G
1	BA	91	A
1	BA	95	G
1	BA	96	C
1	BA	102	A
1	BA	112	C
1	BA	113	A
1	BA	114	A
1	BA	125	A
1	BA	135	U
1	BA	138	A
1	BA	139	U
1	BA	140	G
1	BA	145	C
1	BA	156	A
1	BA	179	A
1	BA	184	U
1	BA	204	U
1	BA	205	C
1	BA	207	A
1	BA	218	A
1	BA	224	U
1	BA	225	U
1	BA	229	G
1	BA	231	A
1	BA	238	U
1	BA	242	A
1	BA	252	U
1	BA	253	G
1	BA	262	G
1	BA	268	G
1	BA	269	A
1	BA	270	A
1	BA	274	G
1	BA	275	U
1	BA	276	C
1	BA	285	A
1	BA	286	C
1	BA	298	A
1	BA	301	G
1	BA	307	A
1	BA	308	C

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Mol	Chain	Res	Type
1	BA	336	G
1	BA	353	U
1	BA	362	A
1	BA	365	C
1	BA	366	C
1	BA	373	U
1	BA	391	A
1	BA	397	A
1	BA	398	G
1	BA	399	A
1	BA	401	U
1	BA	403	G
1	BA	406	A
1	BA	420	C
1	BA	421	A
1	BA	439	U
1	BA	440	U
1	BA	447	G
1	BA	470	A
1	BA	473	A
1	BA	489	A
1	BA	491	G
1	BA	493	C
1	BA	494	A
1	BA	501	G
1	BA	507	U
1	BA	508	C
1	BA	514	U
1	BA	527	G
1	BA	545	G
1	BA	549	A
1	BA	550	A
1	BA	552	U
1	BA	554	C
1	BA	560	G
1	BA	568	A
1	BA	575	G
1	BA	579	G
1	BA	580	U
1	BA	587	U
1	BA	588	G
1	BA	591	C

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Mol	Chain	Res	Type
1	BA	597	U
1	BA	598	C
1	BA	610	C
1	BA	611	A
1	BA	615	G
1	BA	617	U
1	BA	619	C
1	BA	620	G
1	BA	621	U
1	BA	623	A
1	BA	627	G
1	BA	631	G
1	BA	632	A
1	BA	635	A
1	BA	636	A
1	BA	637	A
1	BA	638	G
1	BA	639	G
1	BA	646	G
1	BA	647	U
1	BA	648	G
1	BA	649	U
1	BA	654	U
1	BA	676	C
1	BA	677	U
1	BA	680	C
1	BA	686	C
1	BA	690	G
1	BA	697	C
1	BA	699	U
1	BA	705	C
1	BA	706	G
1	BA	716	G
1	BA	717	A
1	BA	718	A
1	BA	726	G
1	BA	733	C
1	BA	743	A2M
1	BA	744	A
1	BA	746	A2M
1	BA	757	A
1	BA	774	A

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Mol	Chain	Res	Type
1	BA	785	U
1	BA	791	U
1	BA	792	G
1	BA	799	C
1	BA	800	U
1	BA	801	U
1	BA	802	U
1	BA	803	U
1	BA	809	A
1	BA	816	G
1	BA	819	A
1	BA	834	C
1	BA	836	C
1	BA	837	G
1	BA	838	U
1	BA	845	C
1	BA	846	G
1	BA	872	C
1	BA	890	C
1	BA	891	C
1	BA	894	G
1	BA	896	G
1	BA	900	C
1	BA	901	G
1	BA	905	G
1	BA	919	G
1	BA	926	A
1	BA	936	A
1	BA	937	A
1	BA	950	A
1	BA	963	G
1	BA	969	C
1	BA	981	C
1	BA	991	U
1	BA	994	U
1	BA	999	U
1	BA	1027	G
1	BA	1028	OMG
1	BA	1034	A
1	BA	1036	G
1	BA	1037	A
1	BA	1044	G

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Mol	Chain	Res	Type
1	BA	1045	A
1	BA	1057	G
1	BA	1064	C
1	BA	1079	C
1	BA	1080	U
1	BA	1094	G
1	BA	1097	U
1	BA	1100	C
1	BA	1105	A
1	BA	1107	A
1	BA	1119	G
1	BA	1127	A
1	BA	1172	A
1	BA	1174	C
1	BA	1189	C
1	BA	1190	A
1	BA	1194	C
1	BA	1202	G
1	BA	1208	U
1	BA	1220	U
1	BA	1232	G
1	BA	1234	A
1	BA	1235	U
1	BA	1236	U
1	BA	1238	A
1	BA	1242	A
1	BA	1251	G
1	BA	1258	PSU
1	BA	1265	G
1	BA	1278	U
1	BA	1284	A
1	BA	1287	A
1	BA	1293	U
1	BA	1315	C
1	BA	1316	U
1	BA	1317	U
1	BA	1319	U
1	BA	1320	G
1	BA	1322	G
1	BA	1325	C
1	BA	1327	U
1	BA	1328	U

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Mol	Chain	Res	Type
1	BA	1334	U
1	BA	1338	U
1	BA	1339	G
1	BA	1340	A
1	BA	1341	A
1	BA	1347	U
1	BA	1348	G
1	BA	1444	U
1	BA	1446	G
1	BA	1447	A
1	BA	1448	OMU
1	BA	1452	G
1	BA	1455	U
1	BA	1456	A
1	BA	1463	A
1	BA	1470	U
1	BA	1471	G
1	BA	1474	U
1	BA	1480	U
1	BA	1481	U
1	BA	1491	G
1	BA	1492	U
1	BA	1500	G
1	BA	1501	C
1	BA	1502	U
1	BA	1503	A
1	BA	1505	A
1	BA	1514	U
1	BA	1516	A
1	BA	1519	A
1	BA	1525	A
1	BA	1526	G
1	BA	1545	G
1	BA	1557	A
1	BA	1571	G
1	BA	1585	A
1	BA	1586	U
1	BA	1590	C
1	BA	1602	G
1	BA	1605	OMG
1	BA	1608	OMC
1	BA	1615	G

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Mol	Chain	Res	Type
1	BA	1617	C
1	BA	1637	A
1	BA	1638	U
1	BA	1639	A
1	BA	1642	U
1	BA	1643	U
1	BA	1649	A
1	BA	1650	A
1	BA	1652	U
1	BA	1653	G
1	BA	1654	C
1	BA	1669	G
1	BA	1672	C
1	BA	1673	G
1	BA	1696	C
1	BA	1710	U
1	BA	1722	U
1	BA	1728	C
1	BA	1737	A
1	BA	1738	C
1	BA	1744	U
1	BA	1746	U
1	BA	1749	G
1	BA	1750	G
1	BA	1754	G
1	BA	1758	A
1	BA	1812	C
1	BA	1816	A
1	BA	1825	A
1	BA	1827	A
1	BA	1831	A
1	BA	1832	A
1	BA	1835	U
1	BA	1839	A
1	BA	1851	A
1	BA	1854	G
1	BA	1859	G
1	BA	1862	U
1	BA	1868	A
1	BA	1869	C
2	AA	32	C
2	AA	39	A

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Mol	Chain	Res	Type
2	AA	45	C
2	AA	54	A
2	AA	62	G
2	AA	70	G
2	AA	73	U
2	AA	75	A
2	AA	79	A
2	AA	93	A
2	AA	94	U
2	AA	104	G
2	AA	135	A
2	AA	136	C
2	AA	139	A
2	AA	141	U
2	AA	144	G
2	AA	153	A
2	AA	161	G
2	AA	167	G
2	AA	169	A
2	AA	172	A
2	AA	173	C
2	AA	174	U
2	AA	176	G
2	AA	177	A
2	AA	183	U
2	AA	185	G
2	AA	191	C
2	AA	201	A
2	AA	202	U
2	AA	208	A
2	AA	210	C
2	AA	213	A
2	AA	214	U
2	AA	216	G
2	AA	219	C
2	AA	269	U
2	AA	270	G
2	AA	276	U
2	AA	280	G
2	AA	292	A
2	AA	294	U
2	AA	295	U

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Mol	Chain	Res	Type
2	AA	296	A
2	AA	298	A
2	AA	302	A
2	AA	303	A
2	AA	304	C
2	AA	309	C
2	AA	310	C
2	AA	311	A
2	AA	316	G
2	AA	317	A
2	AA	319	G
2	AA	321	A
2	AA	324	A
2	AA	325	A
2	AA	326	C
2	AA	327	A
2	AA	332	G
2	AA	333	A
2	AA	334	C
2	AA	355	G
2	AA	356	U
2	AA	359	G
2	AA	360	A
2	AA	362	A
2	AA	367	A
2	AA	368	G
2	AA	369	C
2	AA	376	G
2	AA	391	A
2	AA	399	C
2	AA	408	C
2	AA	410	G
2	AA	431	G
2	AA	432	A
2	AA	447	A
2	AA	454	C
2	AA	473	U
2	AA	483	G
2	AA	491	G
2	AA	493	A
2	AA	494	A
2	AA	495	U

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Mol	Chain	Res	Type
2	AA	511	G
2	AA	512	G
2	AA	514	G
2	AA	516	G
2	AA	517	C
2	AA	519	G
2	AA	527	G
2	AA	532	U
2	AA	537	C
2	AA	538	A
2	AA	545	A
2	AA	547	A
2	AA	566	A
2	AA	573	A
2	AA	575	A
2	AA	585	G
2	AA	586	U
2	AA	599	G
2	AA	600	G
2	AA	602	U
2	AA	605	U
2	AA	606	U
2	AA	608	C
2	AA	612	G
2	AA	618	U
2	AA	633	A
2	AA	634	A
2	AA	642	U
2	AA	643	A
2	AA	644	A
2	AA	647	A
2	AA	659	G
2	AA	667	C
2	AA	680	U
2	AA	681	A
2	AA	694	A
2	AA	695	A
2	AA	696	A
2	AA	713	U
2	AA	721	A2M
2	AA	722	A
2	AA	725	G

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Mol	Chain	Res	Type
2	AA	726	G
2	AA	740	U
2	AA	742	U
2	AA	748	A
2	AA	750	G
2	AA	752	A
2	AA	753	G
2	AA	754	U
2	AA	757	G
2	AA	762	C
2	AA	777	C
2	AA	778	A
2	AA	781	U
2	AA	783	G
2	AA	787	G
2	AA	789	G
2	AA	790	U
2	AA	793	U
2	AA	794	G
2	AA	795	A
2	AA	799	A
2	AA	801	G
2	AA	805	U
2	AA	806	C
2	AA	807	G
2	AA	827	G
2	AA	829	U
2	AA	830	A
2	AA	833	A
2	AA	834	G
2	AA	835	A
2	AA	844	A
2	AA	848	G
2	AA	850	U
2	AA	851	C
2	AA	867	C
2	AA	873	A
2	AA	874	U
2	AA	875	G
2	AA	877	A
2	AA	878	U
2	AA	885	G

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Mol	Chain	Res	Type
2	AA	886	G
2	AA	888	C
2	AA	895	G
2	AA	896	A
2	AA	897	A
2	AA	898	U
2	AA	899	U
2	AA	910	A
2	AA	915	G
2	AA	920	G
2	AA	933	U
2	AA	934	U
2	AA	935	G
2	AA	936	C
2	AA	937	C
2	AA	940	C
2	AA	941	U
2	AA	949	C
2	AA	955	A
2	AA	959	G
2	AA	968	G
2	AA	969	C
2	AA	973	A
2	AA	974	G
2	AA	978	U
2	AA	979	G
2	AA	981	G
2	AA	982	G
2	AA	997	U
2	AA	1000	G
2	AA	1007	U
2	AA	1010	G
2	AA	1011	A
2	AA	1012	A
2	AA	1013	G
2	AA	1014	U
2	AA	1016	C
2	AA	1018	U
2	AA	1019	G
2	AA	1021	G
2	AA	1025	U
2	AA	1027	A

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Mol	Chain	Res	Type
2	AA	1028	U
2	AA	1031	G
2	AA	1033	C
2	AA	1034	C
2	AA	1052	G
2	AA	1070	G
2	AA	1073	G
2	AA	1074	C
2	AA	1077	G
2	AA	1122	G
2	AA	1130	C
2	AA	1131	A
2	AA	1135	A
2	AA	1139	A
2	AA	1141	G
2	AA	1149	U
2	AA	1150	U
2	AA	1153	G
2	AA	1158	G
2	AA	1160	A
2	AA	1163	U
2	AA	1183	A
2	AA	1192	A
2	AA	1203	A
2	AA	1210	A
2	AA	1212	A
2	AA	1229	A
2	AA	1236	C
2	AA	1237	U
2	AA	1241	U
2	AA	1243	A
2	AA	1247	A
2	AA	1265	A
2	AA	1269	A
2	AA	1275	A
2	AA	1281	G
2	AA	1282	A
2	AA	1298	C
2	AA	1301	C
2	AA	1302	A
2	AA	1303	A
2	AA	1305	C

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Mol	Chain	Res	Type
2	AA	1320	A
2	AA	1322	U
2	AA	1381	U
2	AA	1382	A
2	AA	1385	U
2	AA	1387	U
2	AA	1389	A
2	AA	1391	U
2	AA	1392	U
2	AA	1393	U
2	AA	1395	C
2	AA	1396	G
2	AA	1401	U
2	AA	1462	U
2	AA	1463	C
2	AA	1481	U
2	AA	1482	U
2	AA	1483	C
2	AA	1496	G
2	AA	1497	G
2	AA	1501	U
2	AA	1502	U
2	AA	1504	C
2	AA	1505	A
2	AA	1519	G
2	AA	1536	A
2	AA	1542	A
2	AA	1543	A
2	AA	1555	G
2	AA	1556	A
2	AA	1560	G
2	AA	1563	C
2	AA	1564	C
2	AA	1572	G
2	AA	1590	U
2	AA	1599	A
2	AA	1601	A
2	AA	1604	G
2	AA	1605	G
2	AA	1606	G
2	AA	1607	A
2	AA	1617	G

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Mol	Chain	Res	Type
2	AA	1619	PSU
2	AA	1622	G
2	AA	1623	G
2	AA	1634	G
2	AA	1642	G
2	AA	1643	A
2	AA	1644	U
2	AA	1648	G
2	AA	1649	U
2	AA	1650	G
2	AA	1651	U
2	AA	1657	C
2	AA	1661	A
2	AA	1671	U
2	AA	1696	G
2	AA	1706	U
2	AA	1714	G
2	AA	1719	U
2	AA	1720	U
2	AA	1726	A
2	AA	1730	G
2	AA	1732	C
2	AA	1746	C
2	AA	1751	U
2	AA	1752	A
2	AA	1755	U
2	AA	1757	C
2	AA	1765	G
2	AA	1770	C
2	AA	1775	G
2	AA	1776	A
2	AA	1780	C
2	AA	1781	A
2	AA	1782	G
2	AA	1783	U
2	AA	1817	C
2	AA	1818	G
2	AA	1819	U
2	AA	1822	U
2	AA	1827	C
2	AA	1830	U
2	AA	1832	U

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Mol	Chain	Res	Type
2	AA	1833	U
2	AA	1836	G
2	AA	1850	G
2	AA	1851	G
2	AA	1853	A
2	AA	1854	U
2	AA	1855	U
2	AA	1863	U
2	AA	1864	U
2	AA	1865	U
2	AA	1866	C
2	AA	1873	G
2	AA	1880	U
2	AA	1882	U
2	AA	1891	A
2	AA	1892	G
2	AA	1894	A
2	AA	1895	OMG
2	AA	1899	OMU
2	AA	1902	G
2	AA	1903	A
2	AA	1906	C
2	AA	1912	A
2	AA	1913	A
2	AA	1924	G
2	AA	1925	A
2	AA	1926	C
2	AA	1927	A
2	AA	1936	A
2	AA	1938	A
2	AA	1946	U
2	AA	1950	A
2	AA	1951	A
2	AA	1953	A
2	AA	1956	A
2	AA	1957	G
2	AA	1961	G
2	AA	1981	G
2	AA	1991	G
2	AA	1992	A
2	AA	1994	C
2	AA	1995	A

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Mol	Chain	Res	Type
2	AA	2001	G
2	AA	2008	A
2	AA	2009	A
2	AA	2013	C
2	AA	2023	U
2	AA	2025	G
2	AA	2030	A
2	AA	2031	C
2	AA	2036	G
2	AA	2051	U
2	AA	2053	A
2	AA	2054	OMU
2	AA	2063	C
2	AA	2064	A
2	AA	2070	7MG
2	AA	2079	G
2	AA	2080	U
2	AA	2085	G
2	AA	2096	A2M
2	AA	2102	G
2	AA	2111	G
2	AA	2126	A
2	AA	2133	G
2	AA	2172	C
2	AA	2174	G
2	AA	2175	A
2	AA	2178	G
2	AA	2179	U
2	AA	2198	G
2	AA	2216	C
2	AA	2221	A
2	AA	2226	G
2	AA	2235	A
2	AA	2239	G
2	AA	2241	A
2	AA	2245	A
2	AA	2248	U
2	AA	2259	G
2	AA	2271	G
2	AA	2272	G
2	AA	2273	A
2	AA	2274	U

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Mol	Chain	Res	Type
2	AA	2275	C
2	AA	2278	U
3	BB	7	C
3	BB	12	G
3	BB	18	A
3	BB	22	A
3	BB	25	A
3	BB	29	C
3	BB	33	A
3	BB	61	C
3	BB	62	A
3	BB	63	U
3	BB	68	A
3	BB	69	A
3	BB	75	C
3	BB	76	A
3	BB	90	G
3	BB	133	G
3	BB	136	A
3	BB	137	A
3	BB	359	A
3	BB	360	U
3	BB	371	G
3	BB	380	A
3	BB	381	C
3	BB	386	G
3	BB	395	A
3	BB	398	G
3	BB	400	A2M
3	BB	404	U
3	BB	408	A
3	BB	422	A
3	BB	433	U
3	BB	440	U
3	BB	452	A
3	BB	470	G
3	BB	474	G
3	BB	481	U
3	BB	484	C
3	BB	487	G
3	BB	513	G
3	BB	514	G

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Mol	Chain	Res	Type
3	BB	520	A
3	BB	521	C
3	BB	522	PSU
3	BB	527	C
3	BB	536	G
3	BB	537	G
3	BB	545	A2M
3	BB	548	C
3	BB	552	OMG
3	BB	571	G
3	BB	574	U
3	BB	577	A
3	BB	579	G
3	BB	598	U
3	BB	600	U
3	BB	629	PSU
3	BB	637	A
3	BB	638	C
3	BB	639	G
3	BB	657	G
3	BB	661	A
3	BB	665	A
3	BB	666	A
3	BB	667	G
3	BB	668	A
3	BB	675	U
3	BB	676	G
3	BB	683	A
3	BB	706	G
3	BB	766	C
3	BB	767	G
3	BB	768	U
3	BB	770	G
3	BB	778	U
3	BB	779	A
3	BB	786	G
3	BB	787	A
3	BB	789	G
3	BB	790	A
3	BB	798	G
3	BB	799	G
3	BB	800	U

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Mol	Chain	Res	Type
3	BB	801	U
3	BB	803	U
3	BB	804	U
3	BB	806	U
3	BB	807	G
3	BB	817	C
3	BB	818	G
3	BB	819	G
3	BB	825	G
3	BB	830	G
3	BB	831	U
3	BB	837	C
3	BB	968	C
3	BB	969	G
3	BB	971	G
3	BB	975	G
3	BB	977	A
3	BB	978	A
3	BB	979	C
3	BB	982	C
3	BB	983	U
3	BB	984	G
3	BB	991	A
3	BB	992	C
3	BB	1014	U
3	BB	1023	U
3	BB	1027	G
3	BB	1028	U
3	BB	1035	A
3	BB	1038	U
3	BB	1039	C
3	BB	1049	G
3	BB	1050	G
3	BB	1057	G
3	BB	1062	OMG
3	BB	1091	G
3	BB	1095	U
3	BB	1099	A
3	BB	1117	A
3	BB	1120	G
3	BB	1122	A
3	BB	1124	U

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Mol	Chain	Res	Type
3	BB	1132	G
3	BB	1134	A
3	BB	1137	A
3	BB	1139	A
3	BB	1147	A
3	BB	1157	G
3	BB	1162	A
3	BB	1163	C
3	BB	1172	G
3	BB	1173	U
3	BB	1190	A
3	BB	1191	A
3	BB	1197	G
3	BB	1205	A
3	BB	1215	A
3	BB	1220	C
3	BB	1221	A
3	BB	1222	G
3	BB	1223	G
3	BB	1225	A
3	BB	1226	A
3	BB	1231	A
3	BB	1250	G
3	BB	1253	A
3	BB	1254	G
3	BB	1255	A
3	BB	1257	U
3	BB	1264	OMC
3	BB	1268	G
3	BB	1271	A
3	BB	1287	G
3	BB	1298	C
3	BB	1299	A
3	BB	1325	G
3	BB	1329	U
3	BB	1330	C
3	BB	1341	A
3	BB	1377	U
3	BB	1389	C
3	BB	1390	A
3	BB	1396	C
3	BB	1401	G

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Mol	Chain	Res	Type
3	BB	1425	A
3	BB	1432	U
3	BB	1437	C
3	BB	1444	U
3	BB	1446	G
3	BB	1449	G
3	BB	1452	G
3	BB	1453	A
3	BB	1457	C
3	BB	1458	G
3	BB	1459	A
3	BB	1464	A
3	BB	1468	U
3	BB	1470	A
3	BB	1478	A
3	BB	1479	A
3	BB	1486	G
3	BB	1489	A
3	BB	1490	G
3	BB	1491	U
3	BB	1494	G
3	BB	1495	U
3	BB	1496	U
3	BB	1498	U
3	BB	1501	U
3	BB	1502	C
3	BB	1503	U
3	BB	1504	G
3	BB	1505	G
3	BB	1507	U
3	BB	1508	C
3	BB	1514	U
3	BB	1515	U
3	BB	1518	G
3	BB	1519	U
3	BB	1520	G
3	BB	1523	A
3	BB	1524	U
3	BB	1526	U
3	BB	1527	G
3	BB	1530	U
3	BB	1535	C

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Mol	Chain	Res	Type
3	BB	1536	U
4	BH	14	C
4	BH	23	G
4	BH	26	C
4	BH	28	U
4	BH	49	C
4	BH	50	A
4	BH	51	C
4	BH	52	G
4	BH	69	C
4	BH	70	U
4	BH	71	C
4	BH	72	G
4	BH	75	G
4	BH	86	G
4	BH	87	U
4	BH	99	G
4	BH	106	G
4	BH	109	G
4	BH	113	G
4	BH	116	A
4	BH	117	U
4	BH	118	U
4	BH	119	U
4	BH	120	C
4	BH	125	U
4	BH	134	U
4	BH	135	U
5	BG	5	G
5	BG	8	U
5	BG	9	G
5	BG	10	U
5	BG	12	A
5	BG	19	C
5	BG	25	G
5	BG	39	A
5	BG	40	G
5	BG	58	G
5	BG	60	A
5	BG	74	G
5	BG	85	C
5	BG	86	U

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Mol	Chain	Res	Type
5	BG	102	G
5	BG	114	A
5	BG	120	U
5	BG	121	C
5	BG	127	G
5	BG	132	U
5	BG	139	U
5	BG	145	C
5	BG	149	U
5	BG	150	A
5	BG	157	A
5	BG	158	A
5	BG	159	A
5	BG	168	A
5	BG	171	A
5	BG	173	C
6	BF	10	G
6	BF	11	C
6	BF	12	C
6	BF	14	C
6	BF	23	U
6	BF	24	C
6	BF	25	C
6	BF	36	G
6	BF	57	G
6	BF	58	U
6	BF	59	A
6	BF	60	C
6	BF	63	U
6	BF	69	U
6	BF	70	C
6	BF	72	C
6	BF	73	A
7	BE	4	G
7	BE	11	U
7	BE	14	G
7	BE	15	A
7	BE	17	A
7	BE	22	U
7	BE	32	C
7	BE	33	C
7	BE	34	C

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Mol	Chain	Res	Type
7	BE	35	A
7	BE	39	A
7	BE	40	U
7	BE	46	C
7	BE	47	A
7	BE	50	G
7	BE	51	U
7	BE	62	U
7	BE	70	A
7	BE	107	C
7	BE	108	G
7	BE	109	A
7	BE	110	C
7	BE	111	U
7	BE	112	U
7	BE	113	C
7	BE	114	U
7	BE	122	C
7	BE	123	U
7	BE	124	C
7	BE	147	A
7	BE	149	A
7	BE	157	C
7	BE	158	A
7	BE	159	C
7	BE	161	C
7	BE	162	U
7	BE	163	A
7	BE	164	C
7	BE	165	G
7	BE	181	U
7	BE	186	U
7	BE	187	C
7	BE	191	G
7	BE	195	U
7	BE	198	A
7	BE	201	A
7	BE	209	G
8	BD	12	U
8	BD	22	A
8	BD	23	A
8	BD	27	A

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Mol	Chain	Res	Type
8	BD	40	C
8	BD	48	G
8	BD	53	U
8	BD	54	A
8	BD	63	C
8	BD	64	A
8	BD	65	G
8	BD	97	U
8	BD	100	A
8	BD	110	G
8	BD	117	U
9	BC	22	U
9	BC	32	U
9	BC	33	U
9	BC	48	A
9	BC	59	A
9	BC	62	A
9	BC	63	G
9	BC	77	A
9	BC	94	C
9	BC	103	A
9	BC	105	C
9	BC	110	A
9	BC	124	A
9	BC	136	G
9	BC	138	C
9	BC	149	A
9	BC	157	U
9	BC	158	U
9	BC	159	U
9	BC	162	C
9	BC	169	G
9	BC	170	A
10	AB	4	C
10	AB	66	U
10	AB	67	C
10	AB	70	G
10	AB	71	G
10	AB	73	A
10	AB	76	A

All (34) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	BA	268	G
1	BA	597	U
1	BA	610	C
1	BA	1036	G
1	BA	1316	U
1	BA	1524	U
1	BA	1648	U
1	BA	1745	G
1	BA	1830	G
2	AA	166	C
2	AA	172	A
2	AA	291	A
2	AA	324	A
2	AA	598	U
2	AA	978	U
2	AA	1069	U
2	AA	1321	U
2	AA	1381	U
2	AA	1390	A
2	AA	1832	U
2	AA	1853	A
2	AA	1924	G
3	BB	379	U
3	BB	817	C
3	BB	1038	U
3	BB	1224	A
3	BB	1507	U
5	BG	18	U
6	BF	56	A
7	BE	123	U
7	BE	158	A
7	BE	162	U
7	BE	186	U
10	AB	66	U

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

125 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	A2M	BB	646	3	18,25,26	3.63	7 (38%)	18,36,39	3.76	4 (22%)
3	OMU	BB	1093	3	19,22,23	3.01	8 (42%)	26,31,34	1.73	5 (19%)
2	OMU	AA	57	2	19,22,23	2.96	8 (42%)	26,31,34	1.72	5 (19%)
1	PSU	BA	1129	1	18,21,22	4.43	7 (38%)	22,30,33	1.82	5 (22%)
1	OMC	BA	1006	1	19,22,23	2.91	8 (42%)	26,31,34	0.74	0
3	OMU	BB	73	3	19,22,23	2.96	8 (42%)	26,31,34	1.69	5 (19%)
3	PSU	BB	1398	87,3	18,21,22	4.41	8 (44%)	22,30,33	1.86	6 (27%)
1	A2M	BA	743	1,3	18,25,26	3.62	8 (44%)	18,36,39	3.92	4 (22%)
3	OMG	BB	1062	3	18,26,27	2.51	8 (44%)	19,38,41	1.56	4 (21%)
1	PSU	BA	1086	1,87,88	18,21,22	4.38	7 (38%)	22,30,33	1.83	5 (22%)
2	PSU	AA	1619	2,13	18,21,22	4.38	8 (44%)	22,30,33	1.64	4 (18%)
2	OMG	AA	1700	2	18,26,27	2.43	8 (44%)	19,38,41	1.65	5 (26%)
3	PSU	BB	680	87,3	18,21,22	4.39	7 (38%)	22,30,33	1.83	5 (22%)
1	PSU	BA	737	1,87	18,21,22	4.39	7 (38%)	22,30,33	1.77	5 (22%)
2	OMU	AA	36	2	19,22,23	2.95	8 (42%)	26,31,34	1.86	5 (19%)
9	OMG	BC	75	9	18,26,27	2.55	8 (44%)	19,38,41	1.56	4 (21%)
2	B8N	AA	1596	2	24,29,30	3.01	6 (25%)	29,42,45	1.72	5 (17%)
2	A2M	AA	2096	2	18,25,26	3.62	7 (38%)	18,36,39	3.87	5 (27%)
3	PSU	BB	1076	3	18,21,22	4.41	7 (38%)	22,30,33	1.94	5 (22%)
1	PSU	BA	1609	1	18,21,22	4.44	7 (38%)	22,30,33	1.84	5 (22%)
2	A2M	AA	56	2,89	18,25,26	3.63	7 (38%)	18,36,39	3.72	4 (22%)
2	PSU	AA	61	2	18,21,22	4.46	7 (38%)	22,30,33	1.87	5 (22%)
2	OMG	AA	1531	2	18,26,27	2.42	8 (44%)	19,38,41	1.60	4 (21%)
3	OMU	BB	685	3	19,22,23	2.98	8 (42%)	26,31,34	1.73	5 (19%)
9	OMU	BC	7	1,9	19,22,23	2.99	8 (42%)	26,31,34	1.72	5 (19%)
9	A2M	BC	43	9	18,25,26	3.59	7 (38%)	18,36,39	3.72	4 (22%)
3	A2M	BB	588	1,3	18,25,26	3.63	8 (44%)	18,36,39	3.78	5 (27%)
2	OMG	AA	1931	2,89	18,26,27	2.51	8 (44%)	19,38,41	1.62	5 (26%)
2	OMU	AA	2054	2	19,22,23	2.97	8 (42%)	26,31,34	1.73	4 (15%)
9	A2M	BC	41	9	18,25,26	3.62	8 (44%)	18,36,39	3.77	4 (22%)
2	MA6	AA	2261	2	18,26,27	1.17	1 (5%)	19,38,41	3.01	2 (10%)
2	OMU	AA	1652	2	19,22,23	2.99	8 (42%)	26,31,34	1.72	5 (19%)
3	A2M	BB	622	1,3	18,25,26	3.59	7 (38%)	18,36,39	3.76	4 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	OMG	AA	1895	2,87	18,26,27	2.49	8 (44%)	19,38,41	1.55	4 (21%)
1	OMG	BA	1267	1	18,26,27	2.49	8 (44%)	19,38,41	1.63	5 (26%)
3	OMU	BB	578	3,89	19,22,23	2.95	8 (42%)	26,31,34	1.73	4 (15%)
1	PSU	BA	1009	1	18,21,22	4.39	7 (38%)	22,30,33	1.85	5 (22%)
1	OMC	BA	1608	1	19,22,23	2.95	8 (42%)	26,31,34	0.96	2 (7%)
1	OMU	BA	1742	1	19,22,23	2.96	8 (42%)	26,31,34	1.71	4 (15%)
1	OMC	BA	760	1	19,22,23	2.91	8 (42%)	26,31,34	0.72	0
3	A2M	BB	609	3	18,25,26	3.62	7 (38%)	18,36,39	3.67	4 (22%)
3	PSU	BB	522	3	18,21,22	4.42	7 (38%)	22,30,33	1.77	5 (22%)
2	OMG	AA	1517	2	18,26,27	2.53	8 (44%)	19,38,41	1.57	4 (21%)
3	PSU	BB	644	3	18,21,22	4.41	7 (38%)	22,30,33	1.82	5 (22%)
3	PSU	BB	1160	3	18,21,22	4.46	7 (38%)	22,30,33	1.83	5 (22%)
3	OMG	BB	1269	3	18,26,27	2.48	8 (44%)	19,38,41	1.54	5 (26%)
2	OMG	AA	1676	2,88	18,26,27	2.51	8 (44%)	19,38,41	1.56	4 (21%)
1	PSU	BA	452	1	18,21,22	4.46	7 (38%)	22,30,33	1.78	5 (22%)
1	A2M	BA	996	1,89	18,25,26	3.62	7 (38%)	18,36,39	3.68	4 (22%)
3	A2M	BB	545	87,3	18,25,26	3.69	8 (44%)	18,36,39	3.89	5 (27%)
3	OMG	BB	1245	3	18,26,27	2.51	8 (44%)	19,38,41	1.54	4 (21%)
1	A2M	BA	254	1	18,25,26	3.61	8 (44%)	18,36,39	3.77	4 (22%)
3	PSU	BB	615	3	18,21,22	4.42	7 (38%)	22,30,33	1.82	5 (22%)
1	1MA	BA	742	1,87	16,25,26	3.96	4 (25%)	18,37,40	1.75	3 (16%)
3	OMG	BB	71	3	18,26,27	2.52	8 (44%)	19,38,41	1.58	4 (21%)
3	OMC	BB	377	3	19,22,23	2.98	8 (42%)	26,31,34	0.71	0
1	PSU	BA	1248	1	18,21,22	4.44	7 (38%)	22,30,33	1.84	6 (27%)
2	OMU	AA	2154	2	19,22,23	2.98	8 (42%)	26,31,34	1.74	5 (19%)
3	PSU	BB	1409	3	18,21,22	4.47	7 (38%)	22,30,33	1.74	5 (22%)
3	5MC	BB	542	87,3	18,22,23	3.41	7 (38%)	26,32,35	1.08	2 (7%)
1	OMC	BA	1329	1	19,22,23	3.03	8 (42%)	26,31,34	0.78	0
1	PSU	BA	258	1	18,21,22	4.49	7 (38%)	22,30,33	1.78	5 (22%)
1	A2M	BA	927	1	18,25,26	3.62	7 (38%)	18,36,39	3.66	4 (22%)
3	OMC	BB	1264	3	19,22,23	2.95	8 (42%)	26,31,34	0.82	0
3	A2M	BB	1400	87,3	18,25,26	3.61	8 (44%)	18,36,39	3.76	4 (22%)
1	A2M	BA	1024	1	18,25,26	3.58	7 (38%)	18,36,39	3.70	4 (22%)
2	OMC	AA	46	2	19,22,23	2.86	8 (42%)	26,31,34	0.77	0
1	OMG	BA	1605	1	18,26,27	2.52	8 (44%)	19,38,41	1.61	4 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	OMU	BB	1375	3	19,22,23	2.96	8 (42%)	26,31,34	1.71	5 (19%)
3	PSU	BB	455	88,87,3	18,21,22	4.41	7 (38%)	22,30,33	1.84	5 (22%)
2	OMG	AA	2227	2	18,26,27	2.49	8 (44%)	19,38,41	1.56	4 (21%)
9	PSU	BC	74	9	18,21,22	4.49	7 (38%)	22,30,33	1.88	5 (22%)
3	A2M	BB	1201	3	18,25,26	3.61	8 (44%)	18,36,39	3.72	4 (22%)
1	OMU	BA	46	1	19,22,23	2.96	8 (42%)	26,31,34	1.78	5 (19%)
2	PSU	AA	131	2	18,21,22	4.41	7 (38%)	22,30,33	1.74	3 (13%)
1	OMU	BA	916	1	19,22,23	2.96	8 (42%)	26,31,34	1.77	5 (19%)
3	PSU	BB	1429	3	18,21,22	4.37	7 (38%)	22,30,33	1.87	5 (22%)
2	A2M	AA	2153	2	18,25,26	3.64	9 (50%)	18,36,39	3.90	4 (22%)
3	OMC	BB	1175	3	19,22,23	2.95	8 (42%)	26,31,34	0.78	0
2	OMU	AA	1899	2	19,22,23	3.00	8 (42%)	26,31,34	1.78	5 (19%)
2	OMU	AA	2123	2	19,22,23	2.87	7 (36%)	26,31,34	1.81	4 (15%)
3	OMC	BB	1413	3	19,22,23	2.92	8 (42%)	26,31,34	0.76	0
9	A2M	BC	163	1,9	18,25,26	3.59	7 (38%)	18,36,39	3.79	4 (22%)
3	OMG	BB	552	3	18,26,27	2.46	8 (44%)	19,38,41	1.50	4 (21%)
1	PSU	BA	1258	1	18,21,22	4.41	7 (38%)	22,30,33	1.84	5 (22%)
2	MA6	AA	2260	2	18,26,27	1.14	1 (5%)	19,38,41	3.21	2 (10%)
1	OMG	BA	925	1	18,26,27	2.50	8 (44%)	19,38,41	1.54	3 (15%)
2	OMC	AA	2134	2	19,22,23	2.84	8 (42%)	26,31,34	0.72	0
3	PSU	BB	1319	3	18,21,22	4.46	8 (44%)	22,30,33	1.83	6 (27%)
2	PSU	AA	942	2	18,21,22	4.41	7 (38%)	22,30,33	1.68	5 (22%)
3	OMG	BB	1247	3	18,26,27	2.52	8 (44%)	19,38,41	1.52	4 (21%)
1	A2M	BA	1620	1,87,3	18,25,26	3.61	8 (44%)	18,36,39	3.75	4 (22%)
2	PSU	AA	2045	2	18,21,22	4.39	7 (38%)	22,30,33	1.81	5 (22%)
1	OMU	BA	1181	1	19,22,23	2.97	8 (42%)	26,31,34	1.80	5 (19%)
3	PSU	BB	629	3	18,21,22	4.40	7 (38%)	22,30,33	1.79	5 (22%)
3	A2M	BB	400	3	18,25,26	3.62	8 (44%)	18,36,39	3.71	4 (22%)
3	A2M	BB	95	3	18,25,26	3.60	8 (44%)	18,36,39	3.72	4 (22%)
3	OMG	BB	1094	3	18,26,27	2.50	8 (44%)	19,38,41	1.64	4 (21%)
1	A2M	BA	762	1	18,25,26	3.60	7 (38%)	18,36,39	3.79	4 (22%)
1	A2M	BA	746	1	18,25,26	3.65	7 (38%)	18,36,39	3.74	4 (22%)
1	OMU	BA	1448	1	19,22,23	2.97	8 (42%)	26,31,34	1.74	4 (15%)
1	PSU	BA	1614	1,3	18,21,22	4.43	7 (38%)	22,30,33	1.79	5 (22%)
3	OMC	BB	601	3	19,22,23	2.91	8 (42%)	26,31,34	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	PSU	BB	1280	3	18,21,22	4.41	7 (38%)	22,30,33	1.86	6 (27%)
2	A2M	AA	721	2,87	18,25,26	3.64	8 (44%)	18,36,39	3.82	4 (22%)
3	PSU	BB	611	3	18,21,22	4.37	8 (44%)	22,30,33	1.65	4 (18%)
2	PSU	AA	2146	2	18,21,22	4.39	7 (38%)	22,30,33	1.70	4 (18%)
2	OMC	AA	66	2	19,22,23	2.93	8 (42%)	26,31,34	0.77	0
3	OMG	BB	673	3	18,26,27	2.52	8 (44%)	19,38,41	1.61	4 (21%)
2	PSU	AA	1592	2	18,21,22	4.39	7 (38%)	22,30,33	1.85	5 (22%)
1	OMG	BA	1028	1	18,26,27	2.50	8 (44%)	19,38,41	1.52	4 (21%)
2	PSU	AA	1276	2	18,21,22	4.37	7 (38%)	22,30,33	1.87	5 (22%)
3	A2M	BB	1388	3	18,25,26	3.64	7 (38%)	18,36,39	3.88	4 (22%)
3	OMU	BB	1435	3	19,22,23	2.98	8 (42%)	26,31,34	1.72	5 (19%)
1	OMG	BA	1709	1	18,26,27	2.53	8 (44%)	19,38,41	1.56	4 (21%)
1	OMG	BA	1621	1,3	18,26,27	2.46	8 (44%)	19,38,41	1.52	5 (26%)
3	PSU	BB	1210	3	18,21,22	4.45	7 (38%)	22,30,33	1.78	5 (22%)
2	7MG	AA	2070	2	22,26,27	4.14	10 (45%)	29,39,42	2.05	9 (31%)
1	OMG	BA	915	1	18,26,27	2.51	8 (44%)	19,38,41	1.59	4 (21%)
3	OMG	BB	659	3	18,26,27	2.50	8 (44%)	19,38,41	1.61	5 (26%)
3	PSU	BB	1334	3	18,21,22	4.38	7 (38%)	22,30,33	1.80	5 (22%)
3	5MC	BB	1324	3	18,22,23	3.51	7 (38%)	26,32,35	1.10	1 (3%)
1	A2M	BA	1665	1,3	18,25,26	3.61	8 (44%)	18,36,39	3.70	4 (22%)
1	PSU	BA	1169	1	18,21,22	4.43	7 (38%)	22,30,33	1.87	5 (22%)
2	OMU	AA	714	2	19,22,23	2.94	8 (42%)	26,31,34	1.71	5 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A2M	BB	646	3	-	0/5/27/28	0/3/3/3
3	OMU	BB	1093	3	-	0/9/27/28	0/2/2/2
2	OMU	AA	57	2	-	1/9/27/28	0/2/2/2
1	PSU	BA	1129	1	-	0/7/25/26	0/2/2/2
1	OMC	BA	1006	1	-	0/9/27/28	0/2/2/2
3	OMU	BB	73	3	-	0/9/27/28	0/2/2/2
3	PSU	BB	1398	87,3	-	1/7/25/26	0/2/2/2
1	A2M	BA	743	1,3	-	2/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMG	BB	1062	3	-	3/5/27/28	0/3/3/3
1	PSU	BA	1086	1,87,88	-	0/7/25/26	0/2/2/2
2	PSU	AA	1619	2,13	-	2/7/25/26	0/2/2/2
2	OMG	AA	1700	2	-	0/5/27/28	0/3/3/3
3	PSU	BB	680	87,3	-	0/7/25/26	0/2/2/2
1	PSU	BA	737	1,87	-	0/7/25/26	0/2/2/2
2	OMU	AA	36	2	-	6/9/27/28	0/2/2/2
9	OMG	BC	75	9	-	1/5/27/28	0/3/3/3
2	B8N	AA	1596	2	-	5/16/34/35	0/2/2/2
2	A2M	AA	2096	2	-	2/5/27/28	0/3/3/3
3	PSU	BB	1076	3	-	0/7/25/26	0/2/2/2
1	PSU	BA	1609	1	-	0/7/25/26	0/2/2/2
2	A2M	AA	56	2,89	-	1/5/27/28	0/3/3/3
2	PSU	AA	61	2	-	0/7/25/26	0/2/2/2
2	OMG	AA	1531	2	-	1/5/27/28	0/3/3/3
3	OMU	BB	685	3	-	1/9/27/28	0/2/2/2
9	OMU	BC	7	1,9	-	1/9/27/28	0/2/2/2
9	A2M	BC	43	9	-	1/5/27/28	0/3/3/3
3	A2M	BB	588	1,3	-	1/5/27/28	0/3/3/3
2	OMG	AA	1931	2,89	-	0/5/27/28	0/3/3/3
2	OMU	AA	2054	2	-	2/9/27/28	0/2/2/2
9	A2M	BC	41	9	-	0/5/27/28	0/3/3/3
2	MA6	AA	2261	2	-	1/7/29/30	0/3/3/3
2	OMU	AA	1652	2	-	0/9/27/28	0/2/2/2
3	A2M	BB	622	1,3	-	1/5/27/28	0/3/3/3
2	OMG	AA	1895	2,87	-	1/5/27/28	0/3/3/3
1	OMG	BA	1267	1	-	0/5/27/28	0/3/3/3
3	OMU	BB	578	3,89	-	5/9/27/28	0/2/2/2
1	PSU	BA	1009	1	-	0/7/25/26	0/2/2/2
1	OMC	BA	1608	1	-	3/9/27/28	0/2/2/2
1	OMU	BA	1742	1	-	1/9/27/28	0/2/2/2
1	OMC	BA	760	1	-	1/9/27/28	0/2/2/2
3	A2M	BB	609	3	-	1/5/27/28	0/3/3/3
3	PSU	BB	522	3	-	2/7/25/26	0/2/2/2
2	OMG	AA	1517	2	-	1/5/27/28	0/3/3/3
3	PSU	BB	644	3	-	0/7/25/26	0/2/2/2
3	PSU	BB	1160	3	-	0/7/25/26	0/2/2/2
3	OMG	BB	1269	3	-	0/5/27/28	0/3/3/3
2	OMG	AA	1676	2,88	-	1/5/27/28	0/3/3/3
1	PSU	BA	452	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	A2M	BA	996	1,89	-	1/5/27/28	0/3/3/3
3	A2M	BB	545	87,3	-	2/5/27/28	0/3/3/3
3	OMG	BB	1245	3	-	0/5/27/28	0/3/3/3
1	A2M	BA	254	1	-	0/5/27/28	0/3/3/3
3	PSU	BB	615	3	-	0/7/25/26	0/2/2/2
1	1MA	BA	742	1,87	-	0/3/25/26	0/3/3/3
3	OMG	BB	71	3	-	0/5/27/28	0/3/3/3
3	OMC	BB	377	3	-	0/9/27/28	0/2/2/2
1	PSU	BA	1248	1	-	0/7/25/26	0/2/2/2
2	OMU	AA	2154	2	-	1/9/27/28	0/2/2/2
3	PSU	BB	1409	3	-	0/7/25/26	0/2/2/2
3	5MC	BB	542	87,3	-	1/7/25/26	0/2/2/2
1	OMC	BA	1329	1	-	1/9/27/28	0/2/2/2
1	PSU	BA	258	1	-	0/7/25/26	0/2/2/2
1	A2M	BA	927	1	-	0/5/27/28	0/3/3/3
3	OMC	BB	1264	3	-	1/9/27/28	0/2/2/2
3	A2M	BB	1400	87,3	-	0/5/27/28	0/3/3/3
1	A2M	BA	1024	1	-	1/5/27/28	0/3/3/3
2	OMC	AA	46	2	-	0/9/27/28	0/2/2/2
1	OMG	BA	1605	1	-	2/5/27/28	0/3/3/3
3	OMU	BB	1375	3	-	1/9/27/28	0/2/2/2
3	PSU	BB	455	88,87,3	-	0/7/25/26	0/2/2/2
2	OMG	AA	2227	2	-	0/5/27/28	0/3/3/3
9	PSU	BC	74	9	-	0/7/25/26	0/2/2/2
3	A2M	BB	1201	3	-	3/5/27/28	0/3/3/3
1	OMU	BA	46	1	-	0/9/27/28	0/2/2/2
2	PSU	AA	131	2	-	2/7/25/26	0/2/2/2
1	OMU	BA	916	1	-	0/9/27/28	0/2/2/2
3	PSU	BB	1429	3	-	0/7/25/26	0/2/2/2
2	A2M	AA	2153	2	-	1/5/27/28	0/3/3/3
3	OMC	BB	1175	3	-	0/9/27/28	0/2/2/2
2	OMU	AA	1899	2	-	4/9/27/28	0/2/2/2
2	OMU	AA	2123	2	-	0/9/27/28	0/2/2/2
3	OMC	BB	1413	3	-	0/9/27/28	0/2/2/2
9	A2M	BC	163	1,9	-	1/5/27/28	0/3/3/3
3	OMG	BB	552	3	-	2/5/27/28	0/3/3/3
1	PSU	BA	1258	1	-	2/7/25/26	0/2/2/2
2	MA6	AA	2260	2	-	0/7/29/30	0/3/3/3
1	OMG	BA	925	1	-	0/5/27/28	0/3/3/3
2	OMC	AA	2134	2	-	1/9/27/28	0/2/2/2
3	PSU	BB	1319	3	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PSU	AA	942	2	-	4/7/25/26	0/2/2/2
3	OMG	BB	1247	3	-	0/5/27/28	0/3/3/3
1	A2M	BA	1620	1,87,3	-	0/5/27/28	0/3/3/3
2	PSU	AA	2045	2	-	0/7/25/26	0/2/2/2
1	OMU	BA	1181	1	-	0/9/27/28	0/2/2/2
3	PSU	BB	629	3	-	2/7/25/26	0/2/2/2
3	A2M	BB	400	3	-	2/5/27/28	0/3/3/3
3	A2M	BB	95	3	-	1/5/27/28	0/3/3/3
3	OMG	BB	1094	3	-	0/5/27/28	0/3/3/3
1	A2M	BA	762	1	-	1/5/27/28	0/3/3/3
1	A2M	BA	746	1	-	0/5/27/28	0/3/3/3
1	OMU	BA	1448	1	-	2/9/27/28	0/2/2/2
1	PSU	BA	1614	1,3	-	2/7/25/26	0/2/2/2
3	OMC	BB	601	3	-	0/9/27/28	0/2/2/2
3	PSU	BB	1280	3	-	0/7/25/26	0/2/2/2
2	A2M	AA	721	2,87	-	3/5/27/28	0/3/3/3
3	PSU	BB	611	3	-	0/7/25/26	0/2/2/2
2	PSU	AA	2146	2	-	0/7/25/26	0/2/2/2
2	OMC	AA	66	2	-	0/9/27/28	0/2/2/2
3	OMG	BB	673	3	-	0/5/27/28	0/3/3/3
2	PSU	AA	1592	2	-	2/7/25/26	0/2/2/2
1	OMG	BA	1028	1	-	2/5/27/28	0/3/3/3
2	PSU	AA	1276	2	-	0/7/25/26	0/2/2/2
3	A2M	BB	1388	3	-	0/5/27/28	0/3/3/3
3	OMU	BB	1435	3	-	0/9/27/28	0/2/2/2
1	OMG	BA	1709	1	-	0/5/27/28	0/3/3/3
1	OMG	BA	1621	1,3	-	0/5/27/28	0/3/3/3
3	PSU	BB	1210	3	-	0/7/25/26	0/2/2/2
2	7MG	AA	2070	2	-	1/7/37/38	0/3/3/3
1	OMG	BA	915	1	-	0/5/27/28	0/3/3/3
3	OMG	BB	659	3	-	0/5/27/28	0/3/3/3
3	PSU	BB	1334	3	-	0/7/25/26	0/2/2/2
3	5MC	BB	1324	3	-	4/7/25/26	0/2/2/2
1	A2M	BA	1665	1,3	-	3/5/27/28	0/3/3/3
1	PSU	BA	1169	1	-	0/7/25/26	0/2/2/2
2	OMU	AA	714	2	-	0/9/27/28	0/2/2/2

All (935) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BA	742	1MA	C2-N3	14.22	1.46	1.29
1	BA	258	PSU	C6-C5	11.65	1.48	1.35
3	BB	1409	PSU	C6-C5	11.60	1.48	1.35
1	BA	452	PSU	C6-C5	11.60	1.48	1.35
9	BC	74	PSU	C6-C5	11.56	1.48	1.35
3	BB	1160	PSU	C6-C5	11.55	1.48	1.35
1	BA	1129	PSU	C6-C5	11.55	1.48	1.35
3	BB	1319	PSU	C6-C5	11.55	1.48	1.35
3	BB	1210	PSU	C6-C5	11.53	1.48	1.35
2	AA	942	PSU	C6-C5	11.52	1.48	1.35
1	BA	1609	PSU	C6-C5	11.48	1.48	1.35
3	BB	644	PSU	C6-C5	11.48	1.48	1.35
2	AA	61	PSU	C6-C5	11.48	1.48	1.35
3	BB	522	PSU	C6-C5	11.47	1.48	1.35
2	AA	2146	PSU	C6-C5	11.46	1.48	1.35
1	BA	1248	PSU	C6-C5	11.44	1.48	1.35
1	BA	1614	PSU	C6-C5	11.42	1.48	1.35
2	AA	131	PSU	C6-C5	11.42	1.48	1.35
1	BA	1086	PSU	C6-C5	11.42	1.48	1.35
3	BB	615	PSU	C6-C5	11.40	1.48	1.35
2	AA	2045	PSU	C6-C5	11.40	1.48	1.35
1	BA	1258	PSU	C6-C5	11.39	1.48	1.35
1	BA	1169	PSU	C6-C5	11.38	1.48	1.35
3	BB	611	PSU	C6-C5	11.37	1.48	1.35
3	BB	680	PSU	C6-C5	11.37	1.48	1.35
3	BB	455	PSU	C6-C5	11.36	1.48	1.35
2	AA	1592	PSU	C6-C5	11.35	1.48	1.35
3	BB	1398	PSU	C6-C5	11.34	1.48	1.35
1	BA	1009	PSU	C6-C5	11.33	1.48	1.35
3	BB	629	PSU	C6-C5	11.33	1.48	1.35
2	AA	1619	PSU	C6-C5	11.32	1.48	1.35
3	BB	1076	PSU	C6-C5	11.30	1.48	1.35
3	BB	1429	PSU	C6-C5	11.30	1.48	1.35
1	BA	737	PSU	C6-C5	11.29	1.48	1.35
3	BB	1334	PSU	C6-C5	11.28	1.48	1.35
3	BB	1280	PSU	C6-C5	11.27	1.48	1.35
2	AA	1276	PSU	C6-C5	11.23	1.48	1.35
2	AA	2070	7MG	C8-N9	10.67	1.51	1.46
2	AA	131	PSU	C2-N1	9.71	1.49	1.36
1	BA	258	PSU	C2-N1	9.66	1.49	1.36
3	BB	1160	PSU	C2-N1	9.62	1.49	1.36
9	BC	74	PSU	C2-N1	9.60	1.49	1.36
2	AA	61	PSU	C2-N1	9.60	1.49	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BA	452	PSU	C2-N1	9.58	1.49	1.36
1	BA	1169	PSU	C2-N1	9.55	1.49	1.36
3	BB	1319	PSU	C2-N1	9.53	1.49	1.36
3	BB	1409	PSU	C2-N1	9.53	1.49	1.36
3	BB	1210	PSU	C2-N1	9.52	1.49	1.36
1	BA	1609	PSU	C2-N1	9.50	1.49	1.36
3	BB	615	PSU	C2-N1	9.49	1.49	1.36
3	BB	629	PSU	C2-N1	9.47	1.49	1.36
1	BA	1248	PSU	C2-N1	9.47	1.49	1.36
3	BB	455	PSU	C2-N1	9.47	1.49	1.36
1	BA	737	PSU	C2-N1	9.47	1.49	1.36
1	BA	1129	PSU	C2-N1	9.45	1.49	1.36
1	BA	1614	PSU	C2-N1	9.45	1.49	1.36
3	BB	1280	PSU	C2-N1	9.44	1.49	1.36
3	BB	1334	PSU	C2-N1	9.44	1.49	1.36
3	BB	1076	PSU	C2-N1	9.44	1.49	1.36
3	BB	644	PSU	C2-N1	9.43	1.49	1.36
1	BA	1009	PSU	C2-N1	9.42	1.49	1.36
2	AA	1276	PSU	C2-N1	9.42	1.49	1.36
3	BB	522	PSU	C2-N1	9.40	1.49	1.36
2	AA	1592	PSU	C2-N1	9.39	1.49	1.36
1	BA	1258	PSU	C2-N1	9.39	1.49	1.36
3	BB	680	PSU	C2-N1	9.38	1.49	1.36
3	BB	1398	PSU	C2-N1	9.37	1.49	1.36
2	AA	1619	PSU	C2-N1	9.36	1.49	1.36
2	AA	2045	PSU	C2-N1	9.34	1.49	1.36
1	BA	1086	PSU	C2-N1	9.33	1.49	1.36
3	BB	1429	PSU	C2-N1	9.30	1.49	1.36
3	BB	611	PSU	C2-N1	9.30	1.49	1.36
2	AA	2146	PSU	C2-N1	9.27	1.49	1.36
2	AA	942	PSU	C2-N1	9.18	1.49	1.36
2	AA	2070	7MG	C5-N7	9.14	1.46	1.35
3	BB	1324	5MC	C6-C5	9.14	1.49	1.34
3	BB	400	A2M	C3'-C4'	-8.96	1.30	1.53
2	AA	2153	A2M	C3'-C4'	-8.92	1.30	1.53
3	BB	1388	A2M	C3'-C4'	-8.83	1.30	1.53
2	AA	2096	A2M	C3'-C4'	-8.83	1.30	1.53
3	BB	1400	A2M	C3'-C4'	-8.82	1.30	1.53
1	BA	927	A2M	C3'-C4'	-8.81	1.30	1.53
3	BB	1201	A2M	C3'-C4'	-8.80	1.30	1.53
1	BA	1665	A2M	C3'-C4'	-8.79	1.30	1.53
3	BB	646	A2M	C3'-C4'	-8.77	1.30	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AA	56	A2M	C3'-C4'	-8.77	1.30	1.53
1	BA	1620	A2M	C3'-C4'	-8.76	1.30	1.53
3	BB	542	5MC	C6-C5	8.74	1.49	1.34
1	BA	996	A2M	C3'-C4'	-8.74	1.30	1.53
2	AA	721	A2M	C3'-C4'	-8.73	1.30	1.53
1	BA	1024	A2M	C3'-C4'	-8.72	1.30	1.53
3	BB	622	A2M	C3'-C4'	-8.68	1.30	1.53
9	BC	41	A2M	C3'-C4'	-8.68	1.30	1.53
9	BC	43	A2M	C3'-C4'	-8.67	1.30	1.53
1	BA	254	A2M	C3'-C4'	-8.67	1.30	1.53
3	BB	609	A2M	C3'-C4'	-8.67	1.30	1.53
9	BC	163	A2M	C3'-C4'	-8.65	1.30	1.53
3	BB	95	A2M	C3'-C4'	-8.65	1.30	1.53
1	BA	762	A2M	C3'-C4'	-8.65	1.30	1.53
3	BB	588	A2M	C3'-C4'	-8.65	1.30	1.53
1	BA	746	A2M	C3'-C4'	-8.65	1.30	1.53
3	BB	545	A2M	C3'-C4'	-8.47	1.31	1.53
1	BA	743	A2M	C3'-C4'	-8.41	1.31	1.53
2	AA	1596	B8N	C6-N1	8.09	1.56	1.36
3	BB	545	A2M	O4'-C1'	-8.03	1.29	1.41
9	BC	41	A2M	O4'-C4'	7.77	1.62	1.45
3	BB	1400	A2M	O4'-C4'	7.76	1.62	1.45
1	BA	746	A2M	O4'-C4'	7.74	1.62	1.45
3	BB	609	A2M	O4'-C4'	7.73	1.62	1.45
1	BA	254	A2M	O4'-C4'	7.73	1.62	1.45
9	BC	43	A2M	O4'-C4'	7.71	1.62	1.45
3	BB	646	A2M	O4'-C4'	7.70	1.62	1.45
3	BB	1388	A2M	O4'-C4'	7.68	1.62	1.45
3	BB	588	A2M	O4'-C4'	7.67	1.62	1.45
1	BA	1665	A2M	O4'-C4'	7.67	1.62	1.45
1	BA	743	A2M	O4'-C1'	-7.66	1.30	1.41
3	BB	622	A2M	O4'-C4'	7.66	1.62	1.45
1	BA	762	A2M	O4'-C4'	7.65	1.62	1.45
3	BB	400	A2M	O4'-C4'	7.65	1.62	1.45
2	AA	56	A2M	O4'-C4'	7.64	1.62	1.45
1	BA	1620	A2M	O4'-C4'	7.64	1.62	1.45
2	AA	2096	A2M	O4'-C4'	7.64	1.62	1.45
1	BA	996	A2M	O4'-C4'	7.64	1.62	1.45
3	BB	545	A2M	O4'-C4'	7.64	1.62	1.45
9	BC	163	A2M	O4'-C4'	7.61	1.62	1.45
3	BB	95	A2M	O4'-C4'	7.59	1.62	1.45
1	BA	743	A2M	O4'-C4'	7.59	1.62	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BA	746	A2M	O4'-C1'	-7.59	1.30	1.41
1	BA	1024	A2M	O4'-C4'	7.58	1.61	1.45
2	AA	2153	A2M	O4'-C4'	7.58	1.61	1.45
3	BB	1201	A2M	O4'-C4'	7.54	1.61	1.45
2	AA	721	A2M	O4'-C1'	-7.54	1.30	1.41
9	BC	74	PSU	C2-N3	7.52	1.50	1.37
3	BB	1409	PSU	C2-N3	7.47	1.50	1.37
3	BB	522	PSU	C2-N3	7.47	1.50	1.37
1	BA	927	A2M	O4'-C1'	-7.46	1.30	1.41
2	AA	942	PSU	C2-N3	7.44	1.50	1.37
2	AA	61	PSU	C2-N3	7.44	1.50	1.37
3	BB	1210	PSU	C2-N3	7.42	1.50	1.37
1	BA	927	A2M	O4'-C4'	7.42	1.61	1.45
1	BA	1609	PSU	C2-N3	7.42	1.50	1.37
3	BB	588	A2M	O4'-C1'	-7.42	1.30	1.41
1	BA	1248	PSU	C2-N3	7.41	1.50	1.37
2	AA	721	A2M	O4'-C4'	7.41	1.61	1.45
1	BA	258	PSU	C2-N3	7.41	1.50	1.37
1	BA	1258	PSU	C2-N3	7.40	1.50	1.37
1	BA	452	PSU	C2-N3	7.40	1.50	1.37
3	BB	1280	PSU	C2-N3	7.38	1.50	1.37
1	BA	1129	PSU	C2-N3	7.38	1.50	1.37
2	AA	1596	B8N	C4-N3	-7.37	1.26	1.40
3	BB	1319	PSU	C2-N3	7.36	1.50	1.37
2	AA	56	A2M	O4'-C1'	-7.36	1.30	1.41
2	AA	2045	PSU	C2-N3	7.36	1.50	1.37
1	BA	1169	PSU	C2-N3	7.36	1.50	1.37
3	BB	1160	PSU	C2-N3	7.35	1.50	1.37
1	BA	1614	PSU	C2-N3	7.35	1.50	1.37
3	BB	629	PSU	C2-N3	7.33	1.50	1.37
3	BB	1398	PSU	C2-N3	7.32	1.50	1.37
1	BA	996	A2M	O4'-C1'	-7.32	1.30	1.41
2	AA	2146	PSU	C2-N3	7.32	1.50	1.37
3	BB	615	PSU	C2-N3	7.32	1.50	1.37
3	BB	609	A2M	O4'-C1'	-7.31	1.30	1.41
3	BB	646	A2M	O4'-C1'	-7.31	1.30	1.41
3	BB	1076	PSU	C2-N3	7.31	1.50	1.37
3	BB	455	PSU	C2-N3	7.30	1.50	1.37
1	BA	1086	PSU	C2-N3	7.29	1.50	1.37
3	BB	1388	A2M	O4'-C1'	-7.29	1.30	1.41
3	BB	1429	PSU	C2-N3	7.29	1.50	1.37
2	AA	2153	A2M	O4'-C1'	-7.28	1.30	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	BB	644	PSU	C2-N3	7.28	1.50	1.37
2	AA	2096	A2M	O4'-C1'	-7.27	1.30	1.41
9	BC	41	A2M	O4'-C1'	-7.27	1.30	1.41
3	BB	1334	PSU	C2-N3	7.27	1.50	1.37
2	AA	1592	PSU	C2-N3	7.26	1.49	1.37
2	AA	2070	7MG	C4-N9	7.26	1.46	1.37
1	BA	1009	PSU	C2-N3	7.24	1.49	1.37
1	BA	762	A2M	O4'-C1'	-7.24	1.31	1.41
1	BA	737	PSU	C2-N3	7.24	1.49	1.37
3	BB	611	PSU	C2-N3	7.23	1.49	1.37
9	BC	163	A2M	O4'-C1'	-7.23	1.31	1.41
3	BB	680	PSU	C2-N3	7.23	1.49	1.37
1	BA	254	A2M	O4'-C1'	-7.22	1.31	1.41
3	BB	1201	A2M	O4'-C1'	-7.22	1.31	1.41
3	BB	95	A2M	O4'-C1'	-7.20	1.31	1.41
1	BA	1620	A2M	O4'-C1'	-7.19	1.31	1.41
2	AA	1619	PSU	C2-N3	7.18	1.49	1.37
1	BA	1665	A2M	O4'-C1'	-7.18	1.31	1.41
2	AA	1276	PSU	C2-N3	7.18	1.49	1.37
1	BA	1024	A2M	O4'-C1'	-7.16	1.31	1.41
3	BB	622	A2M	O4'-C1'	-7.16	1.31	1.41
9	BC	43	A2M	O4'-C1'	-7.13	1.31	1.41
3	BB	1400	A2M	O4'-C1'	-7.03	1.31	1.41
2	AA	131	PSU	C2-N3	7.03	1.49	1.37
2	AA	1899	OMU	C2-N1	7.00	1.49	1.38
3	BB	400	A2M	O4'-C1'	-6.96	1.31	1.41
3	BB	1093	OMU	C2-N1	6.90	1.49	1.38
2	AA	1652	OMU	C2-N1	6.89	1.49	1.38
3	BB	578	OMU	C2-N1	6.89	1.49	1.38
3	BB	1435	OMU	C2-N1	6.88	1.49	1.38
1	BA	1448	OMU	C2-N1	6.88	1.49	1.38
2	AA	2054	OMU	C2-N1	6.88	1.49	1.38
1	BA	46	OMU	C2-N1	6.88	1.49	1.38
1	BA	916	OMU	C2-N1	6.86	1.49	1.38
9	BC	7	OMU	C2-N1	6.85	1.49	1.38
3	BB	685	OMU	C2-N1	6.83	1.49	1.38
2	AA	36	OMU	C2-N1	6.82	1.49	1.38
1	BA	1742	OMU	C2-N1	6.82	1.49	1.38
1	BA	1181	OMU	C2-N1	6.79	1.49	1.38
2	AA	1899	OMU	C2-N3	6.79	1.50	1.38
2	AA	2154	OMU	C2-N1	6.77	1.49	1.38
3	BB	73	OMU	C2-N1	6.76	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AA	2154	OMU	C2-N3	6.75	1.50	1.38
2	AA	57	OMU	C2-N1	6.74	1.49	1.38
3	BB	1375	OMU	C2-N1	6.73	1.49	1.38
3	BB	1093	OMU	C2-N3	6.72	1.49	1.38
2	AA	714	OMU	C2-N1	6.72	1.49	1.38
9	BC	7	OMU	C2-N3	6.69	1.49	1.38
2	AA	2054	OMU	C2-N3	6.63	1.49	1.38
3	BB	73	OMU	C2-N3	6.63	1.49	1.38
2	AA	1652	OMU	C2-N3	6.62	1.49	1.38
1	BA	1181	OMU	C2-N3	6.61	1.49	1.38
3	BB	685	OMU	C2-N3	6.61	1.49	1.38
2	AA	2123	OMU	C2-N1	6.61	1.49	1.38
1	BA	916	OMU	C2-N3	6.59	1.49	1.38
3	BB	1435	OMU	C2-N3	6.58	1.49	1.38
2	AA	57	OMU	C2-N3	6.58	1.49	1.38
1	BA	1742	OMU	C2-N3	6.58	1.49	1.38
1	BA	1448	OMU	C2-N3	6.58	1.49	1.38
3	BB	578	OMU	C2-N3	6.55	1.49	1.38
3	BB	1375	OMU	C2-N3	6.53	1.49	1.38
1	BA	46	OMU	C2-N3	6.52	1.49	1.38
1	BA	1329	OMC	C2-N3	6.47	1.49	1.36
2	AA	36	OMU	C2-N3	6.44	1.49	1.38
2	AA	714	OMU	C2-N3	6.44	1.49	1.38
3	BB	377	OMC	C2-N3	6.30	1.49	1.36
2	AA	2123	OMU	C2-N3	6.22	1.49	1.38
1	BA	760	OMC	C2-N3	6.20	1.48	1.36
2	AA	2070	7MG	C2-N3	6.20	1.48	1.33
3	BB	1175	OMC	C2-N3	6.17	1.48	1.36
3	BB	601	OMC	C2-N3	6.15	1.48	1.36
2	AA	66	OMC	C2-N3	6.15	1.48	1.36
3	BB	1264	OMC	C2-N3	6.13	1.48	1.36
1	BA	1608	OMC	C2-N3	6.12	1.48	1.36
1	BA	1006	OMC	C2-N3	6.10	1.48	1.36
3	BB	542	5MC	C4-N3	6.10	1.44	1.34
3	BB	1324	5MC	C4-N3	6.09	1.44	1.34
3	BB	1413	OMC	C2-N3	6.06	1.48	1.36
1	BA	1329	OMC	C6-C5	6.00	1.49	1.35
2	AA	46	OMC	C2-N3	5.99	1.48	1.36
3	BB	1264	OMC	C6-C5	5.96	1.48	1.35
3	BB	377	OMC	C6-C5	5.95	1.48	1.35
3	BB	542	5MC	C2-N3	5.93	1.48	1.36
3	BB	1413	OMC	C6-C5	5.92	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	BB	1175	OMC	C6-C5	5.89	1.48	1.35
1	BA	1608	OMC	C6-C5	5.88	1.48	1.35
2	AA	66	OMC	C6-C5	5.86	1.48	1.35
2	AA	2134	OMC	C2-N3	5.85	1.48	1.36
1	BA	1006	OMC	C6-C5	5.83	1.48	1.35
1	BA	760	OMC	C6-C5	5.83	1.48	1.35
3	BB	1324	5MC	C2-N3	5.82	1.48	1.36
3	BB	601	OMC	C6-C5	5.78	1.48	1.35
2	AA	46	OMC	C6-C5	5.77	1.48	1.35
2	AA	2134	OMC	C6-C5	5.73	1.48	1.35
3	BB	1093	OMU	C6-C5	5.70	1.48	1.35
9	BC	7	OMU	C6-C5	5.68	1.48	1.35
2	AA	36	OMU	C6-C5	5.65	1.48	1.35
2	AA	1652	OMU	C6-C5	5.65	1.48	1.35
2	AA	1596	B8N	C2-N1	5.65	1.56	1.39
3	BB	1375	OMU	C6-C5	5.63	1.48	1.35
2	AA	2154	OMU	C6-C5	5.63	1.48	1.35
3	BB	685	OMU	C6-C5	5.63	1.48	1.35
1	BA	1448	OMU	C6-C5	5.61	1.48	1.35
1	BA	46	OMU	C6-C5	5.61	1.48	1.35
3	BB	1435	OMU	C6-C5	5.61	1.48	1.35
2	AA	57	OMU	C6-C5	5.58	1.48	1.35
3	BB	73	OMU	C6-C5	5.58	1.48	1.35
2	AA	714	OMU	C6-C5	5.58	1.48	1.35
1	BA	1181	OMU	C6-C5	5.57	1.48	1.35
2	AA	1899	OMU	C6-C5	5.57	1.48	1.35
1	BA	916	OMU	C6-C5	5.57	1.48	1.35
3	BB	578	OMU	C6-C5	5.56	1.48	1.35
1	BA	1742	OMU	C6-C5	5.55	1.48	1.35
2	AA	2054	OMU	C6-C5	5.54	1.47	1.35
2	AA	2123	OMU	C6-C5	5.37	1.47	1.35
9	BC	74	PSU	C6-N1	5.35	1.45	1.36
1	BA	258	PSU	C6-N1	5.34	1.45	1.36
2	AA	2070	7MG	C4-N3	5.33	1.46	1.34
1	BA	1329	OMC	C4-N3	5.32	1.45	1.34
2	AA	942	PSU	C6-N1	5.27	1.45	1.36
1	BA	1169	PSU	C6-N1	5.26	1.45	1.36
3	BB	1160	PSU	C6-N1	5.25	1.45	1.36
2	AA	1619	PSU	C6-N1	5.25	1.44	1.36
1	BA	1248	PSU	C6-N1	5.25	1.44	1.36
3	BB	1210	PSU	C6-N1	5.24	1.44	1.36
1	BA	452	PSU	C6-N1	5.24	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	BB	1409	PSU	C6-N1	5.24	1.44	1.36
1	BA	1609	PSU	C6-N1	5.24	1.44	1.36
2	AA	1676	OMG	C2-N3	5.23	1.45	1.33
1	BA	1028	OMG	C2-N3	5.22	1.45	1.33
3	BB	1319	PSU	C6-N1	5.21	1.44	1.36
9	BC	75	OMG	C2-N3	5.21	1.45	1.33
3	BB	455	PSU	C6-N1	5.21	1.44	1.36
1	BA	1009	PSU	C6-N1	5.21	1.44	1.36
2	AA	1517	OMG	C2-N3	5.21	1.45	1.33
2	AA	61	PSU	C6-N1	5.21	1.44	1.36
1	BA	1709	OMG	C2-N3	5.20	1.45	1.33
1	BA	1605	OMG	C2-N3	5.20	1.45	1.33
3	BB	615	PSU	C6-N1	5.20	1.44	1.36
1	BA	1129	PSU	C6-N1	5.19	1.44	1.36
3	BB	680	PSU	C6-N1	5.19	1.44	1.36
3	BB	1247	OMG	C2-N3	5.19	1.45	1.33
3	BB	1076	PSU	C6-N1	5.18	1.44	1.36
3	BB	1062	OMG	C2-N3	5.17	1.45	1.33
3	BB	1245	OMG	C2-N3	5.16	1.45	1.33
2	AA	131	PSU	C6-N1	5.15	1.44	1.36
1	BA	1614	PSU	C6-N1	5.14	1.44	1.36
3	BB	1398	PSU	C6-N1	5.14	1.44	1.36
3	BB	71	OMG	C2-N3	5.14	1.45	1.33
3	BB	611	PSU	C6-N1	5.14	1.44	1.36
3	BB	522	PSU	C6-N1	5.13	1.44	1.36
2	AA	2227	OMG	C2-N3	5.13	1.45	1.33
3	BB	377	OMC	C4-N3	5.13	1.44	1.34
3	BB	629	PSU	C6-N1	5.13	1.44	1.36
2	AA	2146	PSU	C6-N1	5.13	1.44	1.36
2	AA	1276	PSU	C6-N1	5.13	1.44	1.36
3	BB	1334	PSU	C6-N1	5.12	1.44	1.36
1	BA	737	PSU	C6-N1	5.12	1.44	1.36
1	BA	1258	PSU	C6-N1	5.11	1.44	1.36
2	AA	1596	B8N	C6-C5	5.11	1.42	1.34
3	BB	1280	PSU	C6-N1	5.11	1.44	1.36
2	AA	1592	PSU	C6-N1	5.11	1.44	1.36
2	AA	2045	PSU	C6-N1	5.11	1.44	1.36
3	BB	673	OMG	C2-N3	5.10	1.45	1.33
1	BA	915	OMG	C2-N3	5.09	1.45	1.33
3	BB	644	PSU	C6-N1	5.08	1.44	1.36
1	BA	925	OMG	C2-N3	5.05	1.45	1.33
2	AA	1895	OMG	C2-N3	5.03	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	BB	1269	OMG	C2-N3	5.01	1.45	1.33
3	BB	601	OMC	C4-N3	5.01	1.44	1.34
1	BA	1086	PSU	C6-N1	5.01	1.44	1.36
3	BB	1175	OMC	C4-N3	5.00	1.44	1.34
1	BA	1006	OMC	C4-N3	5.00	1.44	1.34
2	AA	1931	OMG	C2-N3	4.98	1.45	1.33
1	BA	1608	OMC	C4-N3	4.97	1.44	1.34
2	AA	66	OMC	C4-N3	4.97	1.44	1.34
3	BB	1429	PSU	C6-N1	4.97	1.44	1.36
1	BA	760	OMC	C4-N3	4.96	1.44	1.34
3	BB	659	OMG	C2-N3	4.95	1.45	1.33
3	BB	1094	OMG	C2-N3	4.95	1.45	1.33
2	AA	1531	OMG	C2-N3	4.94	1.45	1.33
1	BA	1621	OMG	C2-N3	4.93	1.45	1.33
3	BB	1264	OMC	C4-N3	4.93	1.44	1.34
3	BB	1413	OMC	C4-N3	4.93	1.44	1.34
2	AA	1517	OMG	C4-N3	4.90	1.49	1.37
3	BB	552	OMG	C2-N3	4.89	1.45	1.33
1	BA	1267	OMG	C2-N3	4.86	1.45	1.33
2	AA	1676	OMG	C4-N3	4.85	1.49	1.37
9	BC	75	OMG	C4-N3	4.83	1.49	1.37
1	BA	1329	OMC	C4-N4	4.81	1.45	1.33
1	BA	1709	OMG	C4-N3	4.80	1.49	1.37
3	BB	1247	OMG	C4-N3	4.79	1.49	1.37
1	BA	1605	OMG	C4-N3	4.79	1.49	1.37
2	AA	46	OMC	C4-N3	4.79	1.44	1.34
1	BA	1028	OMG	C4-N3	4.78	1.49	1.37
2	AA	2134	OMC	C4-N3	4.78	1.44	1.34
3	BB	377	OMC	C4-N4	4.78	1.45	1.33
3	BB	673	OMG	C4-N3	4.77	1.48	1.37
2	AA	1700	OMG	C2-N3	4.76	1.44	1.33
3	BB	1175	OMC	C4-N4	4.75	1.45	1.33
3	BB	1245	OMG	C4-N3	4.75	1.48	1.37
3	BB	1062	OMG	C4-N3	4.75	1.48	1.37
2	AA	1931	OMG	C4-N3	4.75	1.48	1.37
3	BB	1264	OMC	C4-N4	4.74	1.45	1.33
3	BB	1413	OMC	C4-N4	4.74	1.45	1.33
2	AA	2227	OMG	C4-N3	4.74	1.48	1.37
2	AA	1895	OMG	C4-N3	4.73	1.48	1.37
3	BB	71	OMG	C4-N3	4.72	1.48	1.37
1	BA	915	OMG	C4-N3	4.72	1.48	1.37
1	BA	925	OMG	C4-N3	4.71	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BA	760	OMC	C4-N4	4.71	1.45	1.33
3	BB	1247	OMG	C2-N2	4.67	1.45	1.34
2	AA	66	OMC	C4-N4	4.67	1.44	1.33
3	BB	552	OMG	C4-N3	4.67	1.48	1.37
3	BB	659	OMG	C4-N3	4.66	1.48	1.37
3	BB	1094	OMG	C4-N3	4.65	1.48	1.37
1	BA	1608	OMC	C4-N4	4.65	1.44	1.33
1	BA	1621	OMG	C4-N3	4.64	1.48	1.37
2	AA	2134	OMC	C4-N4	4.63	1.44	1.33
3	BB	1269	OMG	C4-N3	4.63	1.48	1.37
3	BB	71	OMG	C2-N2	4.62	1.45	1.34
3	BB	1062	OMG	C2-N2	4.62	1.45	1.34
3	BB	601	OMC	C4-N4	4.61	1.44	1.33
9	BC	75	OMG	C2-N2	4.61	1.45	1.34
1	BA	1028	OMG	C2-N2	4.60	1.45	1.34
1	BA	1006	OMC	C4-N4	4.60	1.44	1.33
3	BB	1245	OMG	C2-N2	4.60	1.45	1.34
2	AA	46	OMC	C4-N4	4.59	1.44	1.33
1	BA	1709	OMG	C2-N2	4.59	1.45	1.34
3	BB	673	OMG	C2-N2	4.58	1.45	1.34
1	BA	1605	OMG	C2-N2	4.58	1.45	1.34
2	AA	1517	OMG	C2-N2	4.58	1.45	1.34
3	BB	1324	5MC	C6-N1	4.57	1.45	1.38
1	BA	915	OMG	C2-N2	4.57	1.45	1.34
1	BA	1608	OMC	C2-N1	4.56	1.49	1.40
2	AA	1931	OMG	C2-N2	4.56	1.45	1.34
3	BB	1076	PSU	C1'-C5	-4.56	1.39	1.50
1	BA	925	OMG	C2-N2	4.56	1.45	1.34
2	AA	1895	OMG	C2-N2	4.55	1.45	1.34
2	AA	1676	OMG	C2-N2	4.55	1.45	1.34
1	BA	1267	OMG	C4-N3	4.55	1.48	1.37
3	BB	659	OMG	C2-N2	4.53	1.45	1.34
3	BB	1269	OMG	C2-N2	4.52	1.44	1.34
3	BB	1094	OMG	C2-N2	4.51	1.44	1.34
2	AA	1700	OMG	C4-N3	4.50	1.48	1.37
2	AA	2227	OMG	C2-N2	4.47	1.44	1.34
3	BB	1398	PSU	C1'-C5	-4.46	1.40	1.50
1	BA	742	1MA	C2-N1	4.46	1.44	1.35
3	BB	552	OMG	C2-N2	4.46	1.44	1.34
2	AA	1700	OMG	C2-N2	4.46	1.44	1.34
9	BC	74	PSU	C1'-C5	-4.46	1.40	1.50
1	BA	1267	OMG	C2-N2	4.45	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BA	1621	OMG	C2-N2	4.45	1.44	1.34
2	AA	1531	OMG	C4-N3	4.44	1.48	1.37
3	BB	1429	PSU	C1'-C5	-4.44	1.40	1.50
2	AA	61	PSU	C1'-C5	-4.44	1.40	1.50
1	BA	1329	OMC	C2-N1	4.43	1.49	1.40
3	BB	1264	OMC	C2-N1	4.43	1.49	1.40
1	BA	1009	PSU	C1'-C5	-4.42	1.40	1.50
2	AA	1276	PSU	C1'-C5	-4.41	1.40	1.50
3	BB	1160	PSU	C1'-C5	-4.41	1.40	1.50
2	AA	1596	B8N	C1'-C5	-4.41	1.40	1.50
2	AA	1592	PSU	C1'-C5	-4.40	1.40	1.50
1	BA	1248	PSU	C1'-C5	-4.39	1.40	1.50
3	BB	1280	PSU	C1'-C5	-4.39	1.40	1.50
3	BB	1175	OMC	C2-N1	4.37	1.49	1.40
1	BA	1169	PSU	C1'-C5	-4.37	1.40	1.50
2	AA	1531	OMG	C2-N2	4.36	1.44	1.34
1	BA	1129	PSU	C1'-C5	-4.35	1.40	1.50
3	BB	455	PSU	C1'-C5	-4.35	1.40	1.50
3	BB	615	PSU	C1'-C5	-4.34	1.40	1.50
1	BA	452	PSU	C1'-C5	-4.32	1.40	1.50
2	AA	2045	PSU	C1'-C5	-4.32	1.40	1.50
3	BB	1319	PSU	C1'-C5	-4.32	1.40	1.50
3	BB	377	OMC	C2-N1	4.31	1.49	1.40
1	BA	737	PSU	C1'-C5	-4.31	1.40	1.50
1	BA	1258	PSU	C1'-C5	-4.30	1.40	1.50
1	BA	1614	PSU	C1'-C5	-4.29	1.40	1.50
1	BA	1086	PSU	C1'-C5	-4.28	1.40	1.50
3	BB	1409	PSU	C1'-C5	-4.28	1.40	1.50
3	BB	644	PSU	C1'-C5	-4.27	1.40	1.50
1	BA	1609	PSU	C1'-C5	-4.27	1.40	1.50
3	BB	680	PSU	C1'-C5	-4.27	1.40	1.50
3	BB	1324	5MC	C4-N4	4.26	1.45	1.34
1	BA	258	PSU	C1'-C5	-4.25	1.40	1.50
2	AA	66	OMC	C2-N1	4.24	1.49	1.40
3	BB	1210	PSU	C1'-C5	-4.24	1.40	1.50
3	BB	629	PSU	C1'-C5	-4.23	1.40	1.50
3	BB	1334	PSU	C1'-C5	-4.22	1.40	1.50
1	BA	1006	OMC	C2-N1	4.20	1.49	1.40
2	AA	2146	PSU	C1'-C5	-4.20	1.40	1.50
3	BB	601	OMC	C2-N1	4.19	1.49	1.40
1	BA	760	OMC	C2-N1	4.18	1.49	1.40
3	BB	542	5MC	C4-N4	4.17	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	BB	542	5MC	C6-N1	4.16	1.45	1.38
3	BB	522	PSU	C1'-C5	-4.15	1.40	1.50
3	BB	1413	OMC	C2-N1	4.12	1.48	1.40
3	BB	611	PSU	C1'-C5	-4.10	1.40	1.50
2	AA	46	OMC	C2-N1	4.10	1.48	1.40
1	BA	742	1MA	C4-N3	4.08	1.50	1.37
2	AA	131	PSU	C1'-C5	-4.08	1.40	1.50
3	BB	1324	5MC	C2-N1	4.05	1.48	1.40
3	BB	542	5MC	C2-N1	4.05	1.48	1.40
1	BA	1181	OMU	C4-N3	4.01	1.45	1.38
2	AA	2154	OMU	C4-N3	4.01	1.45	1.38
2	AA	942	PSU	C1'-C5	-4.00	1.41	1.50
2	AA	1619	PSU	C1'-C5	-4.00	1.41	1.50
3	BB	1375	OMU	C4-N3	4.00	1.45	1.38
3	BB	1435	OMU	C4-N3	4.00	1.45	1.38
9	BC	7	OMU	C4-N3	3.99	1.45	1.38
2	AA	1652	OMU	C4-N3	3.99	1.45	1.38
3	BB	73	OMU	C4-N3	3.98	1.45	1.38
3	BB	1093	OMU	C4-N3	3.98	1.45	1.38
2	AA	57	OMU	C4-N3	3.97	1.45	1.38
2	AA	2134	OMC	C2-N1	3.97	1.48	1.40
1	BA	1742	OMU	C4-N3	3.94	1.45	1.38
1	BA	1448	OMU	C4-N3	3.93	1.45	1.38
2	AA	1899	OMU	C4-N3	3.92	1.45	1.38
3	BB	522	PSU	C4-N3	3.91	1.46	1.38
2	AA	942	PSU	C4-N3	3.91	1.46	1.38
3	BB	1409	PSU	C4-N3	3.91	1.46	1.38
2	AA	2054	OMU	C4-N3	3.90	1.45	1.38
3	BB	685	OMU	C4-N3	3.89	1.45	1.38
9	BC	74	PSU	C4-N3	3.84	1.46	1.38
1	BA	258	PSU	C4-N3	3.83	1.46	1.38
1	BA	916	OMU	C4-N3	3.82	1.45	1.38
2	AA	714	OMU	C4-N3	3.81	1.45	1.38
2	AA	1619	PSU	C4-N3	3.80	1.45	1.38
1	BA	452	PSU	C4-N3	3.79	1.45	1.38
2	AA	1592	PSU	C4-N3	3.77	1.45	1.38
1	BA	1614	PSU	C4-N3	3.77	1.45	1.38
1	BA	1129	PSU	C4-N3	3.76	1.45	1.38
2	AA	61	PSU	C4-N3	3.76	1.45	1.38
3	BB	1210	PSU	C4-N3	3.76	1.45	1.38
3	BB	611	PSU	C4-N3	3.75	1.45	1.38
1	BA	1609	PSU	C4-N3	3.75	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BA	46	OMU	C4-N3	3.75	1.45	1.38
1	BA	1258	PSU	C4-N3	3.75	1.45	1.38
3	BB	1280	PSU	C4-N3	3.74	1.45	1.38
2	AA	2045	PSU	C4-N3	3.74	1.45	1.38
3	BB	615	PSU	C4-N3	3.74	1.45	1.38
3	BB	629	PSU	C4-N3	3.74	1.45	1.38
1	BA	737	PSU	C4-N3	3.72	1.45	1.38
2	AA	2146	PSU	C4-N3	3.71	1.45	1.38
3	BB	578	OMU	C4-N3	3.71	1.45	1.38
3	BB	1334	PSU	C4-N3	3.70	1.45	1.38
3	BB	1319	PSU	C4-N3	3.70	1.45	1.38
3	BB	1160	PSU	C4-N3	3.70	1.45	1.38
1	BA	1267	OMG	C6-N1	3.69	1.43	1.37
9	BC	75	OMG	C6-N1	3.69	1.43	1.37
1	BA	1086	PSU	C4-N3	3.69	1.45	1.38
1	BA	1248	PSU	C4-N3	3.69	1.45	1.38
3	BB	1429	PSU	C4-N3	3.69	1.45	1.38
1	BA	1169	PSU	C4-N3	3.67	1.45	1.38
2	AA	36	OMU	C4-N3	3.67	1.45	1.38
3	BB	455	PSU	C4-N3	3.66	1.45	1.38
3	BB	644	PSU	C4-N3	3.66	1.45	1.38
1	BA	1009	PSU	C4-N3	3.64	1.45	1.38
3	BB	680	PSU	C4-N3	3.63	1.45	1.38
3	BB	1398	PSU	C4-N3	3.63	1.45	1.38
2	AA	1276	PSU	C4-N3	3.61	1.45	1.38
2	AA	2123	OMU	C4-N3	3.60	1.45	1.38
3	BB	1076	PSU	C4-N3	3.60	1.45	1.38
1	BA	1605	OMG	C6-N1	3.60	1.43	1.37
3	BB	1094	OMG	C6-N1	3.60	1.43	1.37
2	AA	131	PSU	C4-N3	3.58	1.45	1.38
3	BB	673	OMG	C6-N1	3.56	1.43	1.37
3	BB	1269	OMG	C6-N1	3.55	1.43	1.37
3	BB	1245	OMG	C6-N1	3.54	1.43	1.37
3	BB	659	OMG	C6-N1	3.54	1.43	1.37
2	AA	1517	OMG	C6-N1	3.53	1.43	1.37
2	AA	1931	OMG	C6-N1	3.52	1.43	1.37
1	BA	1709	OMG	C6-N1	3.51	1.43	1.37
3	BB	71	OMG	C6-N1	3.50	1.43	1.37
3	BB	1247	OMG	C6-N1	3.50	1.43	1.37
2	AA	1895	OMG	C6-N1	3.49	1.43	1.37
1	BA	1621	OMG	C6-N1	3.47	1.43	1.37
2	AA	2227	OMG	C6-N1	3.47	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	BB	1062	OMG	C6-N1	3.47	1.43	1.37
2	AA	2070	7MG	C6-N1	3.46	1.45	1.38
1	BA	925	OMG	C6-N1	3.45	1.43	1.37
1	BA	915	OMG	C6-N1	3.45	1.43	1.37
1	BA	1028	OMG	C6-N1	3.43	1.43	1.37
2	AA	2123	OMU	O4-C4	-3.41	1.17	1.24
3	BB	552	OMG	C6-N1	3.41	1.43	1.37
2	AA	1676	OMG	C6-N1	3.37	1.42	1.37
2	AA	2070	7MG	C2-N1	3.36	1.46	1.37
1	BA	1329	OMC	C6-N1	3.33	1.46	1.38
2	AA	2070	7MG	C5-C6	3.31	1.52	1.43
2	AA	36	OMU	O4-C4	-3.28	1.18	1.24
2	AA	1531	OMG	C6-N1	3.27	1.42	1.37
2	AA	1700	OMG	C6-N1	3.24	1.42	1.37
2	AA	2070	7MG	O6-C6	-3.23	1.17	1.23
2	AA	2070	7MG	C2-N2	3.23	1.41	1.34
2	AA	714	OMU	O4-C4	-3.22	1.18	1.24
2	AA	1531	OMG	C5-C4	-3.20	1.34	1.43
1	BA	1608	OMC	C6-N1	3.18	1.45	1.38
1	BA	46	OMU	O4-C4	-3.18	1.18	1.24
3	BB	377	OMC	C6-N1	3.18	1.45	1.38
2	AA	2054	OMU	O4-C4	-3.18	1.18	1.24
2	AA	1700	OMG	C5-C4	-3.17	1.35	1.43
2	AA	2134	OMC	O2-C2	-3.17	1.17	1.23
3	BB	1413	OMC	C6-N1	3.16	1.45	1.38
1	BA	1006	OMC	C6-N1	3.15	1.45	1.38
3	BB	1375	OMU	O4-C4	-3.13	1.18	1.24
2	AA	66	OMC	C6-N1	3.12	1.45	1.38
1	BA	916	OMU	O4-C4	-3.12	1.18	1.24
3	BB	545	A2M	O3'-C3'	3.12	1.50	1.43
2	AA	721	A2M	O3'-C3'	3.12	1.50	1.43
1	BA	1448	OMU	O4-C4	-3.12	1.18	1.24
3	BB	1264	OMC	C6-N1	3.12	1.45	1.38
3	BB	601	OMC	C6-N1	3.11	1.45	1.38
3	BB	685	OMU	O4-C4	-3.11	1.18	1.24
2	AA	1652	OMU	O4-C4	-3.11	1.18	1.24
3	BB	1175	OMC	C6-N1	3.11	1.45	1.38
3	BB	1094	OMG	C5-C6	3.11	1.53	1.47
2	AA	2153	A2M	C6-N6	3.09	1.45	1.34
3	BB	1435	OMU	O4-C4	-3.09	1.18	1.24
1	BA	743	A2M	O3'-C3'	3.08	1.50	1.43
1	BA	1181	OMU	O4-C4	-3.08	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AA	57	OMU	O4-C4	-3.08	1.18	1.24
3	BB	73	OMU	O4-C4	-3.07	1.18	1.24
1	BA	254	A2M	C6-N6	3.07	1.45	1.34
9	BC	75	OMG	C5-C6	3.07	1.53	1.47
1	BA	915	OMG	C5-C6	3.06	1.53	1.47
1	BA	1665	A2M	C6-N6	3.06	1.45	1.34
9	BC	7	OMU	O4-C4	-3.06	1.18	1.24
1	BA	927	A2M	C6-N6	3.06	1.45	1.34
3	BB	1093	OMU	O4-C4	-3.05	1.18	1.24
2	AA	46	OMC	C6-N1	3.05	1.45	1.38
3	BB	673	OMG	C5-C6	3.05	1.53	1.47
2	AA	1899	OMU	O4-C4	-3.05	1.18	1.24
2	AA	2096	A2M	C6-N6	3.05	1.45	1.34
9	BC	43	A2M	C6-N6	3.04	1.45	1.34
1	BA	743	A2M	C6-N6	3.04	1.45	1.34
3	BB	646	A2M	C6-N6	3.04	1.45	1.34
1	BA	1605	OMG	C5-C6	3.04	1.53	1.47
3	BB	1201	A2M	C6-N6	3.04	1.45	1.34
3	BB	71	OMG	C5-C6	3.04	1.53	1.47
3	BB	95	A2M	C6-N6	3.03	1.45	1.34
3	BB	622	A2M	C6-N6	3.03	1.45	1.34
1	BA	746	A2M	C6-N6	3.03	1.45	1.34
3	BB	1388	A2M	C6-N6	3.03	1.45	1.34
1	BA	1742	OMU	O4-C4	-3.03	1.18	1.24
2	AA	1931	OMG	C5-C6	3.03	1.53	1.47
1	BA	762	A2M	C6-N6	3.03	1.45	1.34
2	AA	56	A2M	C6-N6	3.03	1.45	1.34
9	BC	163	A2M	C6-N6	3.02	1.45	1.34
3	BB	588	A2M	C6-N6	3.02	1.45	1.34
1	BA	1024	A2M	C6-N6	3.02	1.45	1.34
1	BA	1267	OMG	C5-C4	-3.02	1.35	1.43
3	BB	588	A2M	O3'-C3'	3.02	1.50	1.43
3	BB	659	OMG	C5-C4	-3.02	1.35	1.43
1	BA	996	A2M	C6-N6	3.02	1.45	1.34
2	AA	721	A2M	C6-N6	3.02	1.45	1.34
1	BA	760	OMC	C6-N1	3.01	1.45	1.38
3	BB	1400	A2M	C6-N6	3.01	1.45	1.34
1	BA	925	OMG	C5-C6	3.01	1.53	1.47
2	AA	131	PSU	O4-C4	-3.01	1.17	1.23
3	BB	578	OMU	O4-C4	-3.01	1.18	1.24
9	BC	41	A2M	C6-N6	3.01	1.45	1.34
1	BA	1620	A2M	C6-N6	3.01	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AA	2096	A2M	O3'-C3'	3.00	1.50	1.43
3	BB	601	OMC	O2-C2	-3.00	1.18	1.23
3	BB	609	A2M	C6-N6	3.00	1.45	1.34
2	AA	46	OMC	O2-C2	-2.99	1.18	1.23
3	BB	400	A2M	C6-N6	2.99	1.44	1.34
2	AA	2154	OMU	O4-C4	-2.98	1.18	1.24
1	BA	1006	OMC	O2-C2	-2.98	1.18	1.23
2	AA	2261	MA6	C5-C4	-2.98	1.33	1.40
3	BB	1269	OMG	C5-C6	2.98	1.53	1.47
2	AA	1676	OMG	C5-C6	2.97	1.53	1.47
3	BB	1413	OMC	O2-C2	-2.97	1.18	1.23
3	BB	1094	OMG	C5-C4	-2.97	1.35	1.43
3	BB	545	A2M	C6-N6	2.96	1.44	1.34
1	BA	1267	OMG	C5-C6	2.96	1.53	1.47
2	AA	66	OMC	O2-C2	-2.96	1.18	1.23
1	BA	1608	OMC	O2-C2	-2.95	1.18	1.23
3	BB	659	OMG	C5-C6	2.95	1.53	1.47
3	BB	1264	OMC	O2-C2	-2.95	1.18	1.23
2	AA	2134	OMC	C6-N1	2.95	1.45	1.38
3	BB	1247	OMG	C5-C6	2.94	1.53	1.47
3	BB	95	A2M	O3'-C3'	2.94	1.49	1.43
1	BA	1709	OMG	C5-C6	2.94	1.53	1.47
1	BA	1621	OMG	C5-C6	2.93	1.53	1.47
3	BB	552	OMG	C5-C6	2.93	1.53	1.47
1	BA	1665	A2M	O3'-C3'	2.93	1.49	1.43
1	BA	746	A2M	O3'-C3'	2.92	1.49	1.43
3	BB	1388	A2M	C5-C4	-2.92	1.33	1.40
1	BA	915	OMG	C5-C4	-2.92	1.35	1.43
2	AA	1931	OMG	C5-C4	-2.91	1.35	1.43
3	BB	1398	PSU	O4-C4	-2.91	1.18	1.23
1	BA	760	OMC	O2-C2	-2.91	1.18	1.23
3	BB	1062	OMG	C5-C6	2.90	1.53	1.47
2	AA	1895	OMG	C5-C4	-2.90	1.35	1.43
3	BB	622	A2M	O3'-C3'	2.90	1.49	1.43
3	BB	1245	OMG	C5-C6	2.90	1.53	1.47
3	BB	646	A2M	O3'-C3'	2.90	1.49	1.43
3	BB	1201	A2M	O3'-C3'	2.90	1.49	1.43
1	BA	1621	OMG	C5-C4	-2.90	1.35	1.43
3	BB	1388	A2M	O3'-C3'	2.89	1.49	1.43
1	BA	927	A2M	O3'-C3'	2.89	1.49	1.43
3	BB	545	A2M	C5-C4	-2.89	1.33	1.40
3	BB	552	OMG	C5-C4	-2.89	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	BC	41	A2M	O3'-C3'	2.88	1.49	1.43
2	AA	56	A2M	C5-C4	-2.88	1.33	1.40
2	AA	721	A2M	C5-C4	-2.88	1.33	1.40
3	BB	1324	5MC	O2-C2	-2.88	1.18	1.23
2	AA	2227	OMG	C5-C4	-2.87	1.35	1.43
1	BA	254	A2M	O3'-C3'	2.87	1.49	1.43
3	BB	1175	OMC	O2-C2	-2.87	1.18	1.23
2	AA	2227	OMG	C5-C6	2.86	1.53	1.47
3	BB	1245	OMG	C5-C4	-2.85	1.35	1.43
1	BA	1620	A2M	O3'-C3'	2.85	1.49	1.43
9	BC	43	A2M	O3'-C3'	2.85	1.49	1.43
3	BB	1400	A2M	O3'-C3'	2.85	1.49	1.43
1	BA	996	A2M	C5-C4	-2.85	1.33	1.40
3	BB	680	PSU	O4-C4	-2.85	1.18	1.23
1	BA	996	A2M	O3'-C3'	2.85	1.49	1.43
1	BA	762	A2M	O3'-C3'	2.85	1.49	1.43
2	AA	1517	OMG	C5-C6	2.84	1.53	1.47
1	BA	1028	OMG	C5-C6	2.84	1.53	1.47
2	AA	2153	A2M	C5-C4	-2.84	1.33	1.40
3	BB	400	A2M	C5-C4	-2.84	1.33	1.40
2	AA	1895	OMG	C5-C6	2.84	1.53	1.47
2	AA	2096	A2M	C5-C4	-2.84	1.33	1.40
1	BA	925	OMG	C5-C4	-2.84	1.35	1.43
3	BB	609	A2M	O3'-C3'	2.83	1.49	1.43
3	BB	1334	PSU	O4-C4	-2.83	1.18	1.23
3	BB	1269	OMG	C5-C4	-2.83	1.35	1.43
1	BA	1709	OMG	C5-C4	-2.83	1.35	1.43
2	AA	2123	OMU	O2-C2	-2.83	1.17	1.23
1	BA	743	A2M	C5-C4	-2.83	1.33	1.40
1	BA	1248	PSU	O4-C4	-2.83	1.18	1.23
2	AA	714	OMU	C6-N1	2.82	1.44	1.38
9	BC	163	A2M	O3'-C3'	2.82	1.49	1.43
9	BC	163	A2M	C5-C4	-2.82	1.33	1.40
3	BB	1400	A2M	C5-C4	-2.82	1.33	1.40
3	BB	71	OMG	C5-C4	-2.82	1.35	1.43
3	BB	588	A2M	C5-C4	-2.82	1.33	1.40
2	AA	1652	OMU	C6-N1	2.82	1.44	1.38
2	AA	1276	PSU	O4-C4	-2.82	1.18	1.23
3	BB	1076	PSU	O4-C4	-2.82	1.18	1.23
3	BB	609	A2M	C5-C4	-2.82	1.33	1.40
3	BB	673	OMG	C5-C4	-2.82	1.35	1.43
1	BA	1665	A2M	C5-C4	-2.81	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BA	1024	A2M	C5-C4	-2.81	1.33	1.40
2	AA	1517	OMG	C5-C4	-2.81	1.35	1.43
1	BA	1009	PSU	O4-C4	-2.81	1.18	1.23
3	BB	1062	OMG	C5-C4	-2.81	1.35	1.43
3	BB	646	A2M	C5-C4	-2.80	1.33	1.40
3	BB	1435	OMU	C6-N1	2.80	1.44	1.38
2	AA	1899	OMU	C6-N1	2.80	1.44	1.38
3	BB	1201	A2M	C5-C4	-2.80	1.33	1.40
3	BB	644	PSU	O4-C4	-2.80	1.18	1.23
3	BB	685	OMU	C6-N1	2.80	1.44	1.38
3	BB	73	OMU	C6-N1	2.80	1.44	1.38
9	BC	43	A2M	C5-C4	-2.80	1.33	1.40
1	BA	1620	A2M	C5-C4	-2.80	1.33	1.40
1	BA	746	A2M	C5-C4	-2.80	1.33	1.40
3	BB	1093	OMU	C6-N1	2.79	1.44	1.38
1	BA	1169	PSU	O4-C4	-2.79	1.18	1.23
2	AA	942	PSU	O4-C4	-2.79	1.18	1.23
3	BB	455	PSU	O4-C4	-2.79	1.18	1.23
1	BA	737	PSU	O4-C4	-2.78	1.18	1.23
9	BC	7	OMU	C6-N1	2.78	1.44	1.38
3	BB	578	OMU	C6-N1	2.78	1.44	1.38
2	AA	1676	OMG	C5-C4	-2.78	1.36	1.43
1	BA	1181	OMU	C6-N1	2.78	1.44	1.38
1	BA	1742	OMU	C6-N1	2.78	1.44	1.38
9	BC	75	OMG	C5-C4	-2.78	1.36	1.43
1	BA	1086	PSU	O4-C4	-2.78	1.18	1.23
3	BB	1247	OMG	C5-C4	-2.77	1.36	1.43
9	BC	41	A2M	C5-C4	-2.77	1.33	1.40
3	BB	622	A2M	C5-C4	-2.77	1.33	1.40
3	BB	377	OMC	O2-C2	-2.77	1.18	1.23
3	BB	1280	PSU	O4-C4	-2.77	1.18	1.23
1	BA	1605	OMG	C5-C4	-2.77	1.36	1.43
1	BA	742	1MA	C5-C4	-2.77	1.36	1.43
1	BA	254	A2M	C5-C4	-2.77	1.33	1.40
1	BA	916	OMU	C6-N1	2.76	1.44	1.38
3	BB	95	A2M	C5-C4	-2.76	1.33	1.40
3	BB	615	PSU	O4-C4	-2.76	1.18	1.23
2	AA	57	OMU	C6-N1	2.76	1.44	1.38
1	BA	927	A2M	C5-C4	-2.76	1.33	1.40
1	BA	1448	OMU	C6-N1	2.76	1.44	1.38
2	AA	1700	OMG	C5-C6	2.75	1.53	1.47
1	BA	1024	A2M	O3'-C3'	2.75	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	BB	1375	OMU	C6-N1	2.75	1.44	1.38
3	BB	1160	PSU	O4-C4	-2.75	1.18	1.23
3	BB	542	5MC	O2-C2	-2.75	1.18	1.23
3	BB	1429	PSU	O4-C4	-2.74	1.18	1.23
2	AA	36	OMU	C6-N1	2.74	1.44	1.38
2	AA	56	A2M	O3'-C3'	2.74	1.49	1.43
1	BA	1620	A2M	O2'-C2'	-2.74	1.35	1.42
1	BA	1028	OMG	C5-C4	-2.74	1.36	1.43
1	BA	762	A2M	C5-C4	-2.73	1.33	1.40
1	BA	46	OMU	C6-N1	2.73	1.44	1.38
2	AA	2054	OMU	C6-N1	2.73	1.44	1.38
2	AA	1619	PSU	O4-C4	-2.73	1.18	1.23
1	BA	1614	PSU	O4-C4	-2.73	1.18	1.23
2	AA	1592	PSU	O4-C4	-2.72	1.18	1.23
9	BC	75	OMG	C2-N1	2.72	1.44	1.37
3	BB	629	PSU	O4-C4	-2.72	1.18	1.23
3	BB	545	A2M	O2'-C2'	-2.72	1.35	1.42
2	AA	2153	A2M	O2'-C2'	-2.71	1.35	1.42
1	BA	1609	PSU	O4-C4	-2.70	1.18	1.23
3	BB	400	A2M	O3'-C3'	2.70	1.49	1.43
3	BB	1400	A2M	O2'-C2'	-2.70	1.35	1.42
2	AA	2154	OMU	C6-N1	2.70	1.44	1.38
1	BA	1258	PSU	O4-C4	-2.69	1.18	1.23
3	BB	1319	PSU	O4-C4	-2.69	1.18	1.23
1	BA	1267	OMG	C2-N1	2.69	1.44	1.37
1	BA	927	A2M	O2'-C2'	-2.69	1.35	1.42
2	AA	2146	PSU	O4-C4	-2.69	1.18	1.23
2	AA	2153	A2M	O3'-C3'	2.69	1.49	1.43
3	BB	400	A2M	O2'-C2'	-2.68	1.35	1.42
2	AA	61	PSU	O4-C4	-2.68	1.18	1.23
1	BA	1329	OMC	O2-C2	-2.68	1.18	1.23
3	BB	1201	A2M	O2'-C2'	-2.68	1.35	1.42
3	BB	1210	PSU	O4-C4	-2.68	1.18	1.23
3	BB	673	OMG	C2-N1	2.67	1.44	1.37
1	BA	1709	OMG	C2-N1	2.67	1.44	1.37
1	BA	452	PSU	O4-C4	-2.67	1.18	1.23
3	BB	1094	OMG	C2-N1	2.66	1.44	1.37
1	BA	258	PSU	O4-C4	-2.65	1.18	1.23
3	BB	1409	PSU	O4-C4	-2.65	1.18	1.23
9	BC	74	PSU	O4-C4	-2.65	1.18	1.23
1	BA	762	A2M	O2'-C2'	-2.65	1.35	1.42
2	AA	56	A2M	O2'-C2'	-2.64	1.35	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AA	2260	MA6	C5-C4	-2.64	1.33	1.40
3	BB	646	A2M	O2'-C2'	-2.64	1.35	1.42
1	BA	254	A2M	O2'-C2'	-2.64	1.35	1.42
3	BB	659	OMG	C2-N1	2.64	1.44	1.37
1	BA	1129	PSU	O4-C4	-2.63	1.18	1.23
1	BA	1621	OMG	C2-N1	2.63	1.44	1.37
3	BB	1247	OMG	C2-N1	2.63	1.44	1.37
1	BA	1605	OMG	C2-N1	2.63	1.44	1.37
1	BA	746	A2M	O2'-C2'	-2.63	1.35	1.42
2	AA	2045	PSU	O4-C4	-2.63	1.18	1.23
3	BB	1062	OMG	C2-N1	2.63	1.44	1.37
9	BC	41	A2M	O2'-C2'	-2.62	1.35	1.42
2	AA	721	A2M	O2'-C2'	-2.62	1.35	1.42
3	BB	71	OMG	C2-N1	2.62	1.44	1.37
3	BB	1388	A2M	O2'-C2'	-2.62	1.35	1.42
3	BB	1245	OMG	C2-N1	2.62	1.44	1.37
2	AA	1931	OMG	C2-N1	2.61	1.44	1.37
2	AA	1895	OMG	C2-N1	2.61	1.44	1.37
2	AA	1531	OMG	O6-C6	-2.61	1.18	1.23
3	BB	1269	OMG	C2-N1	2.61	1.44	1.37
2	AA	1531	OMG	C5-C6	2.60	1.52	1.47
1	BA	996	A2M	O2'-C2'	-2.60	1.36	1.42
1	BA	925	OMG	C2-N1	2.60	1.44	1.37
2	AA	2123	OMU	C6-N1	2.60	1.44	1.38
3	BB	611	PSU	O4-C4	-2.59	1.18	1.23
3	BB	522	PSU	O4-C4	-2.58	1.18	1.23
3	BB	622	A2M	O2'-C2'	-2.58	1.36	1.42
1	BA	1028	OMG	C2-N1	2.58	1.44	1.37
1	BA	915	OMG	C2-N1	2.57	1.44	1.37
3	BB	552	OMG	C2-N1	2.57	1.44	1.37
3	BB	609	A2M	O2'-C2'	-2.56	1.36	1.42
2	AA	36	OMU	O2-C2	-2.56	1.18	1.23
2	AA	714	OMU	O2-C2	-2.56	1.18	1.23
3	BB	1375	OMU	O2-C2	-2.56	1.18	1.23
2	AA	1676	OMG	C2-N1	2.55	1.44	1.37
2	AA	1700	OMG	O6-C6	-2.55	1.18	1.23
2	AA	2227	OMG	C2-N1	2.55	1.44	1.37
1	BA	1742	OMU	O2-C2	-2.55	1.18	1.23
1	BA	46	OMU	O2-C2	-2.55	1.18	1.23
1	BA	743	A2M	O2'-C2'	-2.54	1.36	1.42
1	BA	1665	A2M	O2'-C2'	-2.54	1.36	1.42
3	BB	95	A2M	O2'-C2'	-2.53	1.36	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	BB	1435	OMU	O2-C2	-2.53	1.18	1.23
3	BB	685	OMU	O2-C2	-2.53	1.18	1.23
1	BA	1024	A2M	O2'-C2'	-2.52	1.36	1.42
2	AA	1517	OMG	C2-N1	2.52	1.43	1.37
2	AA	57	OMU	O2-C2	-2.51	1.18	1.23
9	BC	163	A2M	O2'-C2'	-2.51	1.36	1.42
1	BA	1329	OMC	C5-C4	2.51	1.48	1.42
9	BC	43	A2M	O2'-C2'	-2.49	1.36	1.42
2	AA	2054	OMU	O2-C2	-2.49	1.18	1.23
3	BB	578	OMU	O2-C2	-2.49	1.18	1.23
3	BB	659	OMG	O6-C6	-2.48	1.18	1.23
2	AA	1700	OMG	C2-N1	2.48	1.43	1.37
2	AA	1517	OMG	O6-C6	-2.47	1.18	1.23
1	BA	1448	OMU	O2-C2	-2.47	1.18	1.23
2	AA	1895	OMG	O6-C6	-2.47	1.18	1.23
3	BB	1413	OMC	C5-C4	2.47	1.48	1.42
1	BA	916	OMU	O2-C2	-2.47	1.18	1.23
9	BC	7	OMU	O2-C2	-2.45	1.18	1.23
3	BB	377	OMC	C5-C4	2.44	1.48	1.42
2	AA	1652	OMU	O2-C2	-2.44	1.18	1.23
2	AA	1899	OMU	O2-C2	-2.44	1.18	1.23
3	BB	73	OMU	O2-C2	-2.44	1.18	1.23
2	AA	1676	OMG	O6-C6	-2.43	1.18	1.23
1	BA	1267	OMG	O6-C6	-2.43	1.18	1.23
1	BA	925	OMG	O6-C6	-2.43	1.18	1.23
1	BA	1181	OMU	O2-C2	-2.43	1.18	1.23
3	BB	1269	OMG	O6-C6	-2.43	1.18	1.23
3	BB	552	OMG	O6-C6	-2.42	1.18	1.23
3	BB	673	OMG	O6-C6	-2.42	1.18	1.23
3	BB	1062	OMG	O6-C6	-2.42	1.18	1.23
1	BA	1028	OMG	O6-C6	-2.41	1.18	1.23
3	BB	588	A2M	O2'-C2'	-2.41	1.36	1.42
3	BB	1093	OMU	O2-C2	-2.41	1.18	1.23
3	BB	1245	OMG	O6-C6	-2.41	1.18	1.23
1	BA	915	OMG	O6-C6	-2.41	1.18	1.23
1	BA	1709	OMG	O6-C6	-2.40	1.18	1.23
2	AA	2227	OMG	O6-C6	-2.40	1.18	1.23
2	AA	1931	OMG	O6-C6	-2.40	1.18	1.23
3	BB	1247	OMG	O6-C6	-2.40	1.18	1.23
1	BA	1621	OMG	O6-C6	-2.40	1.18	1.23
2	AA	1531	OMG	C2-N1	2.39	1.43	1.37
2	AA	2154	OMU	O2-C2	-2.39	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	BB	1264	OMC	C5-C4	2.39	1.48	1.42
3	BB	1175	OMC	C5-C4	2.39	1.48	1.42
3	BB	1094	OMG	O6-C6	-2.38	1.18	1.23
3	BB	1093	OMU	C5-C4	2.35	1.48	1.43
3	BB	71	OMG	O6-C6	-2.35	1.18	1.23
2	AA	66	OMC	C5-C4	2.33	1.48	1.42
2	AA	2154	OMU	C5-C4	2.32	1.48	1.43
2	AA	1652	OMU	C5-C4	2.32	1.48	1.43
3	BB	601	OMC	C5-C4	2.32	1.48	1.42
3	BB	685	OMU	C5-C4	2.31	1.48	1.43
1	BA	1006	OMC	C5-C4	2.31	1.48	1.42
1	BA	1181	OMU	C5-C4	2.31	1.48	1.43
9	BC	75	OMG	O6-C6	-2.30	1.18	1.23
3	BB	578	OMU	C5-C4	2.30	1.48	1.43
2	AA	2134	OMC	C5-C4	2.30	1.48	1.42
2	AA	2096	A2M	O2'-C2'	-2.27	1.36	1.42
3	BB	1375	OMU	C5-C4	2.27	1.48	1.43
1	BA	760	OMC	C5-C4	2.27	1.48	1.42
9	BC	7	OMU	C5-C4	2.27	1.48	1.43
1	BA	46	OMU	C5-C4	2.26	1.48	1.43
1	BA	1448	OMU	C5-C4	2.24	1.48	1.43
1	BA	1742	OMU	C5-C4	2.24	1.48	1.43
3	BB	1435	OMU	C5-C4	2.23	1.48	1.43
2	AA	57	OMU	C5-C4	2.23	1.48	1.43
2	AA	46	OMC	C5-C4	2.23	1.48	1.42
1	BA	1608	OMC	C5-C4	2.22	1.48	1.42
1	BA	916	OMU	C5-C4	2.22	1.48	1.43
2	AA	1899	OMU	C5-C4	2.22	1.48	1.43
2	AA	714	OMU	C5-C4	2.22	1.48	1.43
2	AA	2054	OMU	C5-C4	2.22	1.48	1.43
2	AA	36	OMU	C5-C4	2.21	1.48	1.43
3	BB	73	OMU	C5-C4	2.19	1.48	1.43
2	AA	1596	B8N	O2-C2	-2.18	1.18	1.22
1	BA	1605	OMG	O6-C6	-2.18	1.18	1.23
2	AA	1619	PSU	C4-C5	2.17	1.50	1.44
3	BB	400	A2M	O5'-C5'	-2.16	1.39	1.44
1	BA	743	A2M	O5'-C5'	-2.11	1.39	1.44
1	BA	1620	A2M	C2-N3	2.11	1.35	1.32
2	AA	721	A2M	O5'-C5'	-2.09	1.39	1.44
3	BB	1201	A2M	C2-N3	2.08	1.35	1.32
1	BA	254	A2M	C2-N3	2.08	1.35	1.32
3	BB	1319	PSU	O4'-C1'	-2.07	1.41	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	BC	41	A2M	C2-N3	2.07	1.35	1.32
3	BB	95	A2M	C2-N3	2.05	1.35	1.32
3	BB	588	A2M	C2-N3	2.05	1.35	1.32
2	AA	2153	A2M	O5'-C5'	-2.05	1.39	1.44
2	AA	2153	A2M	C2-N3	2.04	1.35	1.32
1	BA	1665	A2M	C2-N3	2.04	1.35	1.32
3	BB	611	PSU	C4-C5	2.02	1.49	1.44
3	BB	545	A2M	O5'-C5'	-2.02	1.39	1.44
3	BB	1400	A2M	C2-N3	2.01	1.35	1.32
3	BB	1398	PSU	O4'-C1'	-2.00	1.41	1.43

All (508) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	AA	2260	MA6	N1-C6-N6	-12.60	103.80	117.06
2	AA	2261	MA6	N1-C6-N6	-11.59	104.85	117.06
1	BA	762	A2M	C5-C6-N6	10.89	136.89	120.35
1	BA	743	A2M	C5-C6-N6	10.71	136.62	120.35
2	AA	2096	A2M	C5-C6-N6	10.70	136.61	120.35
3	BB	1388	A2M	C5-C6-N6	10.66	136.55	120.35
3	BB	95	A2M	C5-C6-N6	10.64	136.52	120.35
9	BC	41	A2M	C5-C6-N6	10.59	136.44	120.35
1	BA	1620	A2M	C5-C6-N6	10.56	136.40	120.35
1	BA	1665	A2M	C5-C6-N6	10.52	136.34	120.35
2	AA	721	A2M	C5-C6-N6	10.51	136.33	120.35
3	BB	622	A2M	C5-C6-N6	10.51	136.32	120.35
3	BB	646	A2M	C5-C6-N6	10.50	136.31	120.35
3	BB	545	A2M	C5-C6-N6	10.50	136.31	120.35
1	BA	746	A2M	C5-C6-N6	10.49	136.29	120.35
9	BC	163	A2M	C5-C6-N6	10.48	136.28	120.35
1	BA	927	A2M	C5-C6-N6	10.48	136.27	120.35
1	BA	996	A2M	C5-C6-N6	10.46	136.25	120.35
2	AA	56	A2M	C5-C6-N6	10.42	136.19	120.35
9	BC	43	A2M	C5-C6-N6	10.42	136.19	120.35
3	BB	1400	A2M	C5-C6-N6	10.41	136.17	120.35
2	AA	2153	A2M	C5-C6-N6	10.41	136.16	120.35
1	BA	254	A2M	C5-C6-N6	10.40	136.16	120.35
3	BB	400	A2M	C5-C6-N6	10.37	136.12	120.35
3	BB	609	A2M	C5-C6-N6	10.37	136.10	120.35
1	BA	1024	A2M	C5-C6-N6	10.35	136.09	120.35
3	BB	588	A2M	C5-C6-N6	10.35	136.08	120.35
3	BB	1201	A2M	C5-C6-N6	10.32	136.03	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	AA	2153	A2M	C1'-N9-C4	-8.71	111.34	126.64
3	BB	1388	A2M	C1'-N9-C4	-8.15	112.33	126.64
3	BB	545	A2M	C1'-N9-C4	-7.98	112.61	126.64
1	BA	743	A2M	C1'-N9-C4	-7.92	112.72	126.64
1	BA	254	A2M	C1'-N9-C4	-7.77	112.98	126.64
2	AA	721	A2M	C1'-N9-C4	-7.70	113.12	126.64
9	BC	163	A2M	C1'-N9-C4	-7.70	113.12	126.64
2	AA	2096	A2M	C1'-N9-C4	-7.65	113.20	126.64
3	BB	646	A2M	C1'-N9-C4	-7.63	113.24	126.64
3	BB	1201	A2M	C1'-N9-C4	-7.60	113.29	126.64
9	BC	41	A2M	C1'-N9-C4	-7.55	113.38	126.64
3	BB	588	A2M	C1'-N9-C4	-7.53	113.42	126.64
3	BB	1400	A2M	C1'-N9-C4	-7.51	113.44	126.64
3	BB	622	A2M	C1'-N9-C4	-7.50	113.47	126.64
9	BC	43	A2M	C1'-N9-C4	-7.40	113.64	126.64
1	BA	743	A2M	N6-C6-N1	-7.39	103.23	118.57
1	BA	1024	A2M	C1'-N9-C4	-7.39	113.67	126.64
2	AA	2096	A2M	N6-C6-N1	-7.38	103.25	118.57
1	BA	1620	A2M	N6-C6-N1	-7.34	103.33	118.57
2	AA	721	A2M	N6-C6-N1	-7.31	103.40	118.57
3	BB	1388	A2M	N6-C6-N1	-7.30	103.42	118.57
3	BB	400	A2M	C1'-N9-C4	-7.30	113.82	126.64
1	BA	927	A2M	N6-C6-N1	-7.29	103.44	118.57
3	BB	545	A2M	N6-C6-N1	-7.28	103.46	118.57
2	AA	56	A2M	C1'-N9-C4	-7.27	113.86	126.64
1	BA	1665	A2M	N6-C6-N1	-7.26	103.49	118.57
3	BB	95	A2M	N6-C6-N1	-7.23	103.56	118.57
9	BC	41	A2M	N6-C6-N1	-7.23	103.57	118.57
3	BB	646	A2M	N6-C6-N1	-7.22	103.58	118.57
1	BA	762	A2M	N6-C6-N1	-7.22	103.58	118.57
3	BB	622	A2M	N6-C6-N1	-7.21	103.61	118.57
1	BA	746	A2M	N6-C6-N1	-7.21	103.61	118.57
1	BA	996	A2M	N6-C6-N1	-7.21	103.62	118.57
9	BC	163	A2M	N6-C6-N1	-7.20	103.62	118.57
1	BA	762	A2M	C1'-N9-C4	-7.20	114.00	126.64
9	BC	43	A2M	N6-C6-N1	-7.19	103.64	118.57
3	BB	1400	A2M	N6-C6-N1	-7.19	103.65	118.57
3	BB	609	A2M	C1'-N9-C4	-7.18	114.02	126.64
1	BA	1620	A2M	C1'-N9-C4	-7.18	114.03	126.64
2	AA	56	A2M	N6-C6-N1	-7.17	103.70	118.57
2	AA	2153	A2M	N6-C6-N1	-7.13	103.78	118.57
1	BA	254	A2M	N6-C6-N1	-7.11	103.81	118.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	BA	1024	A2M	N6-C6-N1	-7.11	103.82	118.57
3	BB	400	A2M	N6-C6-N1	-7.11	103.82	118.57
3	BB	588	A2M	N6-C6-N1	-7.10	103.83	118.57
3	BB	1201	A2M	N6-C6-N1	-7.06	103.91	118.57
3	BB	609	A2M	N6-C6-N1	-7.05	103.94	118.57
1	BA	746	A2M	C1'-N9-C4	-6.94	114.44	126.64
3	BB	95	A2M	C1'-N9-C4	-6.92	114.47	126.64
1	BA	1665	A2M	C1'-N9-C4	-6.89	114.54	126.64
1	BA	996	A2M	C1'-N9-C4	-6.78	114.73	126.64
1	BA	927	A2M	C1'-N9-C4	-6.46	115.29	126.64
2	AA	36	OMU	C4-N3-C2	-5.61	119.18	126.58
3	BB	1388	A2M	N3-C2-N1	-5.61	119.92	128.68
1	BA	746	A2M	N3-C2-N1	-5.59	119.94	128.68
3	BB	1400	A2M	N3-C2-N1	-5.58	119.95	128.68
3	BB	545	A2M	N3-C2-N1	-5.58	119.96	128.68
1	BA	743	A2M	N3-C2-N1	-5.57	119.97	128.68
2	AA	2153	A2M	N3-C2-N1	-5.56	119.99	128.68
9	BC	163	A2M	N3-C2-N1	-5.56	119.99	128.68
1	BA	1665	A2M	N3-C2-N1	-5.55	120.01	128.68
2	AA	56	A2M	N3-C2-N1	-5.55	120.01	128.68
2	AA	721	A2M	N3-C2-N1	-5.55	120.01	128.68
1	BA	762	A2M	N3-C2-N1	-5.54	120.02	128.68
2	AA	2123	OMU	C4-N3-C2	-5.54	119.27	126.58
2	AA	2261	MA6	N3-C2-N1	-5.53	120.03	128.68
1	BA	996	A2M	N3-C2-N1	-5.53	120.04	128.68
1	BA	927	A2M	N3-C2-N1	-5.52	120.05	128.68
1	BA	46	OMU	C4-N3-C2	-5.50	119.32	126.58
3	BB	622	A2M	N3-C2-N1	-5.50	120.08	128.68
9	BC	41	A2M	N3-C2-N1	-5.49	120.10	128.68
3	BB	1201	A2M	N3-C2-N1	-5.49	120.10	128.68
3	BB	646	A2M	N3-C2-N1	-5.48	120.12	128.68
1	BA	1181	OMU	C4-N3-C2	-5.48	119.36	126.58
1	BA	916	OMU	C4-N3-C2	-5.47	119.36	126.58
3	BB	588	A2M	N3-C2-N1	-5.45	120.17	128.68
2	AA	2260	MA6	N3-C2-N1	-5.44	120.18	128.68
9	BC	43	A2M	N3-C2-N1	-5.43	120.18	128.68
1	BA	254	A2M	N3-C2-N1	-5.43	120.19	128.68
3	BB	1093	OMU	C4-N3-C2	-5.43	119.42	126.58
1	BA	1024	A2M	N3-C2-N1	-5.42	120.20	128.68
1	BA	1620	A2M	N3-C2-N1	-5.42	120.20	128.68
2	AA	2096	A2M	N3-C2-N1	-5.42	120.21	128.68
2	AA	2154	OMU	C4-N3-C2	-5.41	119.45	126.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	BB	609	A2M	N3-C2-N1	-5.41	120.23	128.68
1	BA	1448	OMU	C4-N3-C2	-5.37	119.50	126.58
3	BB	685	OMU	C4-N3-C2	-5.35	119.52	126.58
3	BB	400	A2M	N3-C2-N1	-5.34	120.33	128.68
2	AA	2054	OMU	C4-N3-C2	-5.34	119.54	126.58
3	BB	1435	OMU	C4-N3-C2	-5.34	119.54	126.58
2	AA	714	OMU	C4-N3-C2	-5.32	119.56	126.58
2	AA	1652	OMU	C4-N3-C2	-5.32	119.56	126.58
3	BB	578	OMU	C4-N3-C2	-5.30	119.59	126.58
9	BC	7	OMU	C4-N3-C2	-5.29	119.60	126.58
3	BB	1375	OMU	C4-N3-C2	-5.29	119.61	126.58
2	AA	1899	OMU	C4-N3-C2	-5.27	119.62	126.58
1	BA	1742	OMU	C4-N3-C2	-5.26	119.64	126.58
2	AA	57	OMU	C4-N3-C2	-5.24	119.67	126.58
3	BB	95	A2M	N3-C2-N1	-5.20	120.55	128.68
3	BB	73	OMU	C4-N3-C2	-5.20	119.72	126.58
1	BA	742	1MA	N1-C2-N3	-5.12	120.06	126.02
2	AA	1596	B8N	C5-C4-N3	5.11	125.64	116.17
2	AA	2070	7MG	C5-C6-N1	4.98	119.77	110.99
1	BA	1169	PSU	C4-N3-C2	-4.76	119.48	126.34
3	BB	1076	PSU	C4-N3-C2	-4.72	119.53	126.34
2	AA	1276	PSU	C4-N3-C2	-4.71	119.56	126.34
3	BB	455	PSU	C4-N3-C2	-4.67	119.61	126.34
9	BC	74	PSU	C4-N3-C2	-4.66	119.62	126.34
2	AA	131	PSU	C4-N3-C2	-4.66	119.63	126.34
3	BB	1398	PSU	C4-N3-C2	-4.65	119.63	126.34
1	BA	1248	PSU	C4-N3-C2	-4.65	119.64	126.34
2	AA	61	PSU	C4-N3-C2	-4.63	119.67	126.34
3	BB	644	PSU	C4-N3-C2	-4.61	119.69	126.34
1	BA	1009	PSU	C4-N3-C2	-4.60	119.72	126.34
1	BA	1258	PSU	C4-N3-C2	-4.59	119.72	126.34
3	BB	615	PSU	C4-N3-C2	-4.59	119.72	126.34
2	AA	1592	PSU	C4-N3-C2	-4.59	119.72	126.34
3	BB	680	PSU	C4-N3-C2	-4.59	119.72	126.34
3	BB	1429	PSU	C4-N3-C2	-4.59	119.73	126.34
3	BB	1334	PSU	C4-N3-C2	-4.58	119.74	126.34
1	BA	1129	PSU	C4-N3-C2	-4.58	119.74	126.34
3	BB	1160	PSU	C4-N3-C2	-4.56	119.77	126.34
3	BB	1280	PSU	C4-N3-C2	-4.55	119.78	126.34
3	BB	1210	PSU	C4-N3-C2	-4.55	119.79	126.34
1	BA	737	PSU	C4-N3-C2	-4.55	119.79	126.34
1	BA	1086	PSU	C4-N3-C2	-4.54	119.79	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	BA	1614	PSU	C4-N3-C2	-4.51	119.84	126.34
1	BA	1609	PSU	C4-N3-C2	-4.51	119.84	126.34
3	BB	629	PSU	C4-N3-C2	-4.50	119.85	126.34
3	BB	1409	PSU	C4-N3-C2	-4.50	119.85	126.34
1	BA	452	PSU	C4-N3-C2	-4.50	119.86	126.34
1	BA	258	PSU	C4-N3-C2	-4.48	119.89	126.34
3	BB	1319	PSU	C4-N3-C2	-4.47	119.89	126.34
3	BB	1076	PSU	N1-C2-N3	4.45	120.17	115.13
2	AA	2045	PSU	C4-N3-C2	-4.42	119.97	126.34
2	AA	1596	B8N	C4-N3-C2	-4.41	119.88	125.46
3	BB	522	PSU	C4-N3-C2	-4.39	120.01	126.34
3	BB	1429	PSU	N1-C2-N3	4.39	120.11	115.13
2	AA	1592	PSU	N1-C2-N3	4.39	120.10	115.13
1	BA	1258	PSU	N1-C2-N3	4.36	120.07	115.13
2	AA	1619	PSU	C4-N3-C2	-4.34	120.08	126.34
2	AA	1276	PSU	N1-C2-N3	4.32	120.03	115.13
1	BA	1086	PSU	N1-C2-N3	4.32	120.02	115.13
2	AA	2070	7MG	C2-N3-C4	4.31	119.97	112.30
1	BA	1169	PSU	N1-C2-N3	4.30	120.00	115.13
2	AA	61	PSU	N1-C2-N3	4.30	120.00	115.13
1	BA	1609	PSU	N1-C2-N3	4.29	120.00	115.13
9	BC	74	PSU	N1-C2-N3	4.29	119.99	115.13
3	BB	455	PSU	N1-C2-N3	4.29	119.99	115.13
1	BA	1009	PSU	N1-C2-N3	4.29	119.99	115.13
3	BB	680	PSU	N1-C2-N3	4.28	119.98	115.13
3	BB	1160	PSU	N1-C2-N3	4.26	119.96	115.13
3	BB	1398	PSU	N1-C2-N3	4.26	119.96	115.13
2	AA	36	OMU	N3-C2-N1	4.25	120.54	114.89
2	AA	2045	PSU	N1-C2-N3	4.25	119.94	115.13
2	AA	2146	PSU	C4-N3-C2	-4.24	120.22	126.34
1	BA	1129	PSU	N1-C2-N3	4.24	119.94	115.13
3	BB	1319	PSU	N1-C2-N3	4.24	119.94	115.13
3	BB	644	PSU	N1-C2-N3	4.24	119.93	115.13
1	BA	1614	PSU	N1-C2-N3	4.23	119.92	115.13
3	BB	615	PSU	N1-C2-N3	4.22	119.92	115.13
3	BB	1280	PSU	N1-C2-N3	4.21	119.90	115.13
3	BB	522	PSU	N1-C2-N3	4.19	119.88	115.13
3	BB	611	PSU	C4-N3-C2	-4.18	120.31	126.34
2	AA	2123	OMU	N3-C2-N1	4.18	120.44	114.89
1	BA	1248	PSU	N1-C2-N3	4.18	119.86	115.13
1	BA	258	PSU	N1-C2-N3	4.17	119.86	115.13
3	BB	629	PSU	N1-C2-N3	4.17	119.85	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	BB	1334	PSU	N1-C2-N3	4.15	119.84	115.13
3	BB	1210	PSU	N1-C2-N3	4.14	119.82	115.13
2	AA	2070	7MG	C5-C4-N3	-4.13	120.25	128.13
1	BA	737	PSU	N1-C2-N3	4.09	119.77	115.13
1	BA	452	PSU	N1-C2-N3	4.09	119.76	115.13
2	AA	942	PSU	C4-N3-C2	-4.07	120.48	126.34
1	BA	742	1MA	C5-C6-N1	4.06	119.95	113.90
2	AA	131	PSU	N1-C2-N3	4.06	119.72	115.13
2	AA	2146	PSU	N1-C2-N3	4.04	119.71	115.13
3	BB	1409	PSU	N1-C2-N3	4.03	119.69	115.13
3	BB	685	OMU	N3-C2-N1	4.01	120.22	114.89
1	BA	916	OMU	N3-C2-N1	4.00	120.20	114.89
9	BC	7	OMU	N3-C2-N1	3.99	120.19	114.89
3	BB	1093	OMU	N3-C2-N1	3.97	120.16	114.89
3	BB	578	OMU	N3-C2-N1	3.93	120.10	114.89
1	BA	46	OMU	N3-C2-N1	3.93	120.10	114.89
2	AA	1899	OMU	N3-C2-N1	3.90	120.06	114.89
3	BB	611	PSU	N1-C2-N3	3.90	119.54	115.13
1	BA	1448	OMU	N3-C2-N1	3.89	120.06	114.89
3	BB	1375	OMU	N3-C2-N1	3.89	120.05	114.89
1	BA	1181	OMU	N3-C2-N1	3.89	120.05	114.89
2	AA	57	OMU	N3-C2-N1	3.89	120.05	114.89
2	AA	714	OMU	N3-C2-N1	3.88	120.04	114.89
2	AA	942	PSU	N1-C2-N3	3.86	119.51	115.13
2	AA	1652	OMU	N3-C2-N1	3.86	120.02	114.89
1	BA	1742	OMU	N3-C2-N1	3.85	120.00	114.89
2	AA	1619	PSU	N1-C2-N3	3.84	119.48	115.13
2	AA	2154	OMU	N3-C2-N1	3.83	119.98	114.89
2	AA	2054	OMU	N3-C2-N1	3.83	119.98	114.89
3	BB	1435	OMU	N3-C2-N1	3.79	119.93	114.89
3	BB	1324	5MC	C5-C6-N1	-3.75	119.48	123.34
3	BB	73	OMU	N3-C2-N1	3.74	119.85	114.89
2	AA	1517	OMG	C5-C6-N1	3.64	120.38	113.95
2	AA	1676	OMG	C5-C6-N1	3.63	120.36	113.95
2	AA	1931	OMG	C5-C6-N1	3.62	120.35	113.95
1	BA	915	OMG	C5-C6-N1	3.60	120.32	113.95
2	AA	1700	OMG	C5-C6-N1	3.59	120.29	113.95
3	BB	1062	OMG	C5-C6-N1	3.58	120.28	113.95
2	AA	1531	OMG	C5-C6-N1	3.57	120.26	113.95
1	BA	1709	OMG	C5-C6-N1	3.56	120.23	113.95
1	BA	46	OMU	C5-C4-N3	3.56	120.16	114.84
2	AA	2123	OMU	C5-C4-N3	3.56	120.16	114.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	AA	2227	OMG	C5-C6-N1	3.54	120.20	113.95
3	BB	1245	OMG	C5-C6-N1	3.54	120.20	113.95
3	BB	673	OMG	C5-C6-N1	3.54	120.19	113.95
3	BB	1094	OMG	C5-C6-N1	3.53	120.18	113.95
2	AA	714	OMU	C5-C4-N3	3.52	120.11	114.84
3	BB	71	OMG	C5-C6-N1	3.52	120.16	113.95
9	BC	75	OMG	C5-C6-N1	3.51	120.15	113.95
3	BB	1269	OMG	C5-C6-N1	3.51	120.14	113.95
2	AA	36	OMU	C5-C4-N3	3.51	120.09	114.84
1	BA	1181	OMU	C5-C4-N3	3.50	120.07	114.84
3	BB	1247	OMG	C5-C6-N1	3.50	120.13	113.95
1	BA	925	OMG	C5-C6-N1	3.49	120.12	113.95
3	BB	659	OMG	C5-C6-N1	3.49	120.11	113.95
3	BB	1435	OMU	C5-C4-N3	3.48	120.05	114.84
2	AA	1895	OMG	C5-C6-N1	3.48	120.09	113.95
1	BA	1028	OMG	C5-C6-N1	3.46	120.06	113.95
1	BA	1605	OMG	C5-C6-N1	3.45	120.05	113.95
2	AA	2054	OMU	C5-C4-N3	3.45	120.00	114.84
1	BA	1621	OMG	C5-C6-N1	3.43	120.01	113.95
1	BA	916	OMU	C5-C4-N3	3.42	119.96	114.84
1	BA	1448	OMU	C5-C4-N3	3.41	119.94	114.84
3	BB	1093	OMU	C5-C4-N3	3.41	119.94	114.84
2	AA	1652	OMU	C5-C4-N3	3.41	119.94	114.84
1	BA	1267	OMG	C5-C6-N1	3.40	119.95	113.95
3	BB	73	OMU	C5-C4-N3	3.39	119.92	114.84
3	BB	552	OMG	C5-C6-N1	3.39	119.94	113.95
3	BB	685	OMU	C5-C4-N3	3.39	119.91	114.84
1	BA	1742	OMU	C5-C4-N3	3.38	119.90	114.84
3	BB	1375	OMU	C5-C4-N3	3.37	119.89	114.84
3	BB	578	OMU	C5-C4-N3	3.37	119.88	114.84
9	BC	7	OMU	C5-C4-N3	3.36	119.87	114.84
2	AA	2154	OMU	C5-C4-N3	3.36	119.86	114.84
2	AA	57	OMU	C5-C4-N3	3.34	119.84	114.84
2	AA	2070	7MG	C4-C5-N7	3.31	110.12	105.53
2	AA	1899	OMU	C5-C4-N3	3.27	119.73	114.84
2	AA	942	PSU	C6-N1-C2	-3.23	119.38	122.68
3	BB	542	5MC	C5-C6-N1	-3.20	120.04	123.34
3	BB	1076	PSU	C6-C5-C4	3.20	120.44	118.20
3	BB	1429	PSU	C6-N1-C2	-3.18	119.43	122.68
2	AA	2045	PSU	C6-N1-C2	-3.17	119.44	122.68
3	BB	522	PSU	C6-N1-C2	-3.17	119.44	122.68
2	AA	2070	7MG	C5-C4-N9	3.13	110.42	106.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	BA	1609	PSU	C6-N1-C2	-3.11	119.50	122.68
2	AA	2146	PSU	C6-N1-C2	-3.10	119.51	122.68
1	BA	1086	PSU	C6-N1-C2	-3.09	119.53	122.68
2	AA	1592	PSU	C6-N1-C2	-3.07	119.54	122.68
2	AA	1596	B8N	N3-C2-N1	3.07	121.09	116.76
3	BB	1160	PSU	C6-N1-C2	-3.06	119.55	122.68
3	BB	1319	PSU	C6-N1-C2	-3.01	119.60	122.68
2	AA	1517	OMG	C2-N1-C6	-3.01	119.56	125.10
3	BB	615	PSU	C6-N1-C2	-3.00	119.61	122.68
1	BA	1709	OMG	C2-N1-C6	-3.00	119.57	125.10
2	AA	2123	OMU	O4-C4-C5	-3.00	119.89	125.16
2	AA	1676	OMG	C2-N1-C6	-3.00	119.58	125.10
2	AA	1531	OMG	C2-N1-C6	-3.00	119.58	125.10
2	AA	2070	7MG	C2-N1-C6	-2.99	119.65	125.10
9	BC	74	PSU	C6-C5-C4	2.99	120.29	118.20
3	BB	1062	OMG	C2-N1-C6	-2.98	119.60	125.10
1	BA	915	OMG	C2-N1-C6	-2.98	119.61	125.10
1	BA	1258	PSU	C6-N1-C2	-2.98	119.63	122.68
3	BB	455	PSU	C6-N1-C2	-2.98	119.64	122.68
2	AA	1700	OMG	C8-N7-C5	2.98	108.66	102.99
3	BB	680	PSU	C6-N1-C2	-2.97	119.64	122.68
3	BB	1076	PSU	C6-N1-C2	-2.97	119.65	122.68
1	BA	1605	OMG	C2-N1-C6	-2.97	119.64	125.10
3	BB	644	PSU	C6-N1-C2	-2.97	119.65	122.68
3	BB	1280	PSU	C6-N1-C2	-2.96	119.65	122.68
2	AA	2227	OMG	C2-N1-C6	-2.96	119.65	125.10
1	BA	1181	OMU	O4-C4-C5	-2.96	119.96	125.16
2	AA	1276	PSU	C6-N1-C2	-2.95	119.66	122.68
3	BB	659	OMG	C8-N7-C5	2.95	108.61	102.99
3	BB	73	OMU	O4-C4-C5	-2.94	119.99	125.16
1	BA	1129	PSU	C6-N1-C2	-2.94	119.68	122.68
2	AA	2054	OMU	O4-C4-C5	-2.94	120.00	125.16
3	BB	673	OMG	C8-N7-C5	2.94	108.58	102.99
3	BB	1210	PSU	C6-N1-C2	-2.94	119.68	122.68
3	BB	1269	OMG	C2-N1-C6	-2.94	119.69	125.10
3	BB	1435	OMU	O4-C4-C5	-2.93	120.01	125.16
3	BB	71	OMG	C2-N1-C6	-2.93	119.71	125.10
3	BB	1245	OMG	C2-N1-C6	-2.92	119.72	125.10
1	BA	915	OMG	C8-N7-C5	2.92	108.55	102.99
2	AA	61	PSU	C6-N1-C2	-2.91	119.70	122.68
2	AA	1531	OMG	C8-N7-C5	2.91	108.54	102.99
3	BB	629	PSU	C6-N1-C2	-2.91	119.71	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	AA	2154	OMU	O4-C4-C5	-2.91	120.05	125.16
1	BA	1267	OMG	C8-N7-C5	2.91	108.53	102.99
2	AA	1899	OMU	O4-C4-C5	-2.91	120.05	125.16
1	BA	1605	OMG	C8-N7-C5	2.91	108.53	102.99
1	BA	1742	OMU	O4-C4-C5	-2.90	120.05	125.16
9	BC	75	OMG	C2-N1-C6	-2.90	119.76	125.10
1	BA	258	PSU	C6-N1-C2	-2.90	119.72	122.68
3	BB	1094	OMG	C8-N7-C5	2.90	108.50	102.99
3	BB	1334	PSU	C6-N1-C2	-2.89	119.72	122.68
3	BB	1375	OMU	O4-C4-C5	-2.89	120.08	125.16
1	BA	1009	PSU	C6-N1-C2	-2.89	119.73	122.68
3	BB	673	OMG	C2-N1-C6	-2.89	119.78	125.10
9	BC	74	PSU	C6-N1-C2	-2.88	119.74	122.68
2	AA	1700	OMG	C2-N1-C6	-2.88	119.80	125.10
1	BA	1028	OMG	C2-N1-C6	-2.88	119.80	125.10
1	BA	1614	PSU	C6-N1-C2	-2.87	119.75	122.68
2	AA	1931	OMG	C2-N1-C6	-2.87	119.82	125.10
3	BB	611	PSU	C6-N1-C2	-2.87	119.75	122.68
2	AA	1895	OMG	C2-N1-C6	-2.87	119.82	125.10
2	AA	57	OMU	O4-C4-C5	-2.86	120.13	125.16
1	BA	916	OMU	O4-C4-C5	-2.85	120.14	125.16
2	AA	1895	OMG	C8-N7-C5	2.85	108.43	102.99
3	BB	1247	OMG	C2-N1-C6	-2.85	119.84	125.10
2	AA	1652	OMU	O4-C4-C5	-2.85	120.14	125.16
3	BB	71	OMG	C8-N7-C5	2.85	108.41	102.99
2	AA	2227	OMG	C8-N7-C5	2.83	108.39	102.99
2	AA	1676	OMG	C8-N7-C5	2.83	108.38	102.99
3	BB	1398	PSU	C6-N1-C2	-2.83	119.79	122.68
3	BB	1062	OMG	C8-N7-C5	2.82	108.37	102.99
9	BC	75	OMG	C8-N7-C5	2.82	108.37	102.99
2	AA	2070	7MG	O6-C6-C5	-2.82	120.62	127.54
1	BA	925	OMG	C8-N7-C5	2.82	108.36	102.99
3	BB	659	OMG	C2-N1-C6	-2.82	119.91	125.10
1	BA	452	PSU	C6-N1-C2	-2.82	119.80	122.68
3	BB	1094	OMG	C2-N1-C6	-2.81	119.92	125.10
9	BC	7	OMU	O4-C4-C5	-2.81	120.22	125.16
2	AA	1931	OMG	C8-N7-C5	2.81	108.34	102.99
1	BA	1267	OMG	C2-N1-C6	-2.81	119.93	125.10
1	BA	742	1MA	C8-N7-C5	2.80	108.33	102.99
3	BB	1429	PSU	O2-C2-N1	-2.80	119.71	122.79
1	BA	1621	OMG	C8-N7-C5	2.80	108.32	102.99
2	AA	131	PSU	C6-N1-C2	-2.80	119.83	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	BB	1245	OMG	C8-N7-C5	2.79	108.31	102.99
1	BA	1448	OMU	O4-C4-C5	-2.79	120.25	125.16
1	BA	1248	PSU	C6-N1-C2	-2.78	119.84	122.68
2	AA	36	OMU	O4-C4-C5	-2.78	120.27	125.16
1	BA	1621	OMG	C2-N1-C6	-2.78	119.98	125.10
3	BB	1093	OMU	O4-C4-C5	-2.77	120.29	125.16
3	BB	1247	OMG	C8-N7-C5	2.77	108.27	102.99
2	AA	61	PSU	C6-C5-C4	2.77	120.13	118.20
1	BA	1258	PSU	O2-C2-N1	-2.77	119.75	122.79
1	BA	925	OMG	C2-N1-C6	-2.77	120.01	125.10
1	BA	1169	PSU	C6-N1-C2	-2.76	119.86	122.68
3	BB	1269	OMG	C8-N7-C5	2.76	108.25	102.99
3	BB	1409	PSU	C6-N1-C2	-2.76	119.86	122.68
1	BA	1169	PSU	C6-C5-C4	2.76	120.13	118.20
3	BB	685	OMU	O4-C4-C5	-2.75	120.32	125.16
1	BA	1709	OMG	C8-N7-C5	2.75	108.23	102.99
3	BB	578	OMU	O4-C4-C5	-2.75	120.33	125.16
2	AA	1276	PSU	C6-C5-C4	2.74	120.11	118.20
1	BA	1086	PSU	O2-C2-N1	-2.73	119.79	122.79
1	BA	737	PSU	C6-N1-C2	-2.72	119.90	122.68
2	AA	714	OMU	O4-C4-C5	-2.72	120.37	125.16
2	AA	1517	OMG	C8-N7-C5	2.72	108.17	102.99
3	BB	552	OMG	C2-N1-C6	-2.71	120.10	125.10
1	BA	1248	PSU	C6-C5-C4	2.71	120.09	118.20
1	BA	1009	PSU	C6-C5-C4	2.71	120.09	118.20
2	AA	2045	PSU	O2-C2-N1	-2.70	119.81	122.79
3	BB	552	OMG	C8-N7-C5	2.70	108.12	102.99
3	BB	1280	PSU	C6-C5-C4	2.68	120.07	118.20
3	BB	1398	PSU	C6-C5-C4	2.68	120.07	118.20
1	BA	1028	OMG	C8-N7-C5	2.67	108.08	102.99
1	BA	1609	PSU	C6-C5-C4	2.65	120.05	118.20
1	BA	46	OMU	O4-C4-C5	-2.64	120.51	125.16
3	BB	615	PSU	O2-C2-N1	-2.64	119.88	122.79
2	AA	1596	B8N	O4-C4-N3	-2.62	115.52	119.98
2	AA	1592	PSU	O2-C2-N1	-2.62	119.91	122.79
3	BB	1076	PSU	O2-C2-N1	-2.62	119.91	122.79
3	BB	455	PSU	O2-C2-N1	-2.61	119.91	122.79
2	AA	61	PSU	O2-C2-N1	-2.61	119.92	122.79
3	BB	629	PSU	O2-C2-N1	-2.60	119.92	122.79
2	AA	1619	PSU	C6-N1-C2	-2.59	120.03	122.68
3	BB	522	PSU	O2-C2-N1	-2.58	119.95	122.79
2	AA	2070	7MG	N9-C4-N3	2.58	129.33	125.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	BB	1280	PSU	O2-C2-N1	-2.58	119.95	122.79
1	BA	1614	PSU	O2-C2-N1	-2.57	119.96	122.79
3	BB	1319	PSU	C6-C5-C4	2.56	119.99	118.20
3	BB	1334	PSU	O2-C2-N1	-2.52	120.01	122.79
2	AA	2070	7MG	N9-C8-N7	2.51	106.96	103.38
3	BB	1398	PSU	O2-C2-N1	-2.50	120.04	122.79
1	BA	1129	PSU	O2-C2-N1	-2.49	120.05	122.79
2	AA	1592	PSU	C6-C5-C4	2.49	119.94	118.20
1	BA	258	PSU	C6-C5-C4	2.48	119.93	118.20
3	BB	1160	PSU	C6-C5-C4	2.48	119.93	118.20
3	BB	1409	PSU	O2-C2-N1	-2.47	120.07	122.79
9	BC	74	PSU	O2-C2-N1	-2.47	120.07	122.79
3	BB	680	PSU	O2-C2-N1	-2.46	120.08	122.79
1	BA	452	PSU	C6-C5-C4	2.46	119.92	118.20
2	AA	2146	PSU	O2-C2-N1	-2.46	120.09	122.79
1	BA	1609	PSU	O2-C2-N1	-2.44	120.11	122.79
3	BB	644	PSU	O2-C2-N1	-2.43	120.11	122.79
3	BB	1429	PSU	C6-C5-C4	2.43	119.90	118.20
1	BA	737	PSU	O2-C2-N1	-2.43	120.12	122.79
2	AA	942	PSU	O2-C2-N1	-2.42	120.12	122.79
1	BA	1169	PSU	O2-C2-N1	-2.40	120.15	122.79
3	BB	1160	PSU	O2-C2-N1	-2.40	120.15	122.79
1	BA	1608	OMC	O2-C2-N3	-2.40	118.43	122.33
1	BA	1248	PSU	O2-C2-N1	-2.39	120.16	122.79
1	BA	1009	PSU	O2-C2-N1	-2.37	120.18	122.79
1	BA	1086	PSU	C6-C5-C4	2.37	119.85	118.20
1	BA	1181	OMU	O2-C2-N1	-2.36	119.65	122.79
1	BA	452	PSU	O2-C2-N1	-2.34	120.22	122.79
1	BA	737	PSU	C6-C5-C4	2.34	119.83	118.20
1	BA	1129	PSU	C6-C5-C4	2.34	119.83	118.20
1	BA	1709	OMG	O6-C6-C5	-2.33	119.82	124.37
2	AA	1517	OMG	O6-C6-C5	-2.32	119.84	124.37
3	BB	1210	PSU	O2-C2-N1	-2.32	120.24	122.79
2	AA	2154	OMU	O2-C2-N1	-2.32	119.71	122.79
2	AA	1276	PSU	O2-C2-N1	-2.31	120.24	122.79
3	BB	1062	OMG	O6-C6-C5	-2.31	119.86	124.37
3	BB	542	5MC	CM5-C5-C6	-2.31	119.76	122.85
2	AA	36	OMU	O2-C2-N1	-2.31	119.72	122.79
2	AA	2045	PSU	C6-C5-C4	2.30	119.81	118.20
1	BA	1267	OMG	N2-C2-N1	2.30	121.61	116.71
2	AA	1899	OMU	C1'-N1-C2	2.30	121.73	117.57
1	BA	1608	OMC	C1'-N1-C2	2.29	123.53	118.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	BA	1258	PSU	C6-C5-C4	2.29	119.80	118.20
3	BB	615	PSU	C6-C5-C4	2.29	119.80	118.20
3	BB	680	PSU	C6-C5-C4	2.29	119.80	118.20
1	BA	1028	OMG	O6-C6-C5	-2.28	119.92	124.37
1	BA	1614	PSU	C6-C5-C4	2.28	119.79	118.20
3	BB	588	A2M	O2'-C2'-C1'	2.27	113.58	109.09
3	BB	1319	PSU	O2-C2-N1	-2.25	120.31	122.79
3	BB	629	PSU	C6-C5-C4	2.25	119.77	118.20
3	BB	1319	PSU	O4'-C1'-C2'	2.24	108.30	105.14
3	BB	644	PSU	C6-C5-C4	2.24	119.76	118.20
3	BB	1280	PSU	O4'-C1'-C2'	2.23	108.29	105.14
9	BC	75	OMG	O6-C6-C5	-2.23	120.02	124.37
3	BB	455	PSU	C6-C5-C4	2.22	119.75	118.20
3	BB	611	PSU	O2-C2-N1	-2.21	120.36	122.79
3	BB	1247	OMG	O6-C6-C5	-2.21	120.06	124.37
1	BA	258	PSU	O2-C2-N1	-2.20	120.37	122.79
2	AA	57	OMU	O2-C2-N1	-2.19	119.88	122.79
3	BB	1210	PSU	C6-C5-C4	2.18	119.72	118.20
3	BB	659	OMG	O6-C6-C5	-2.18	120.11	124.37
2	AA	2227	OMG	O6-C6-C5	-2.17	120.13	124.37
3	BB	1245	OMG	O6-C6-C5	-2.17	120.14	124.37
3	BB	1409	PSU	C6-C5-C4	2.16	119.71	118.20
2	AA	1676	OMG	O6-C6-C5	-2.16	120.15	124.37
2	AA	1895	OMG	O6-C6-C5	-2.16	120.15	124.37
2	AA	1700	OMG	N2-C2-N1	2.16	121.31	116.71
3	BB	1398	PSU	O4'-C1'-C2'	2.15	108.17	105.14
2	AA	1596	B8N	C31-N3-C4	2.14	120.47	117.31
3	BB	1334	PSU	C6-C5-C4	2.14	119.69	118.20
2	AA	1931	OMG	O6-C6-C5	-2.14	120.19	124.37
2	AA	2096	A2M	O2'-C2'-C1'	2.14	113.33	109.09
9	BC	7	OMU	O2-C2-N1	-2.13	119.96	122.79
1	BA	1621	OMG	N2-C2-N1	2.13	121.25	116.71
2	AA	1619	PSU	O2-C2-N1	-2.13	120.45	122.79
3	BB	1094	OMG	N2-C2-N1	2.13	121.24	116.71
1	BA	1248	PSU	O4'-C1'-C2'	2.13	108.14	105.14
3	BB	1269	OMG	O6-C6-C5	-2.11	120.25	124.37
3	BB	1375	OMU	O2-C2-N1	-2.11	119.98	122.79
3	BB	73	OMU	O2-C2-N1	-2.11	119.98	122.79
3	BB	685	OMU	O2-C2-N1	-2.11	119.98	122.79
2	AA	714	OMU	O2-C2-N1	-2.11	119.98	122.79
1	BA	1605	OMG	O6-C6-C5	-2.10	120.26	124.37
2	AA	1531	OMG	O6-C6-C5	-2.10	120.27	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	BA	1621	OMG	O6-C6-C5	-2.10	120.27	124.37
1	BA	916	OMU	O2-C2-N1	-2.10	120.00	122.79
1	BA	46	OMU	O2-C2-N1	-2.10	120.00	122.79
3	BB	1093	OMU	O2-C2-N1	-2.09	120.00	122.79
3	BB	545	A2M	O4'-C1'-C2'	-2.09	102.97	106.59
3	BB	71	OMG	O6-C6-C5	-2.08	120.31	124.37
3	BB	1435	OMU	O2-C2-N1	-2.05	120.06	122.79
2	AA	1700	OMG	O6-C6-C5	-2.05	120.37	124.37
3	BB	552	OMG	O6-C6-C5	-2.05	120.38	124.37
3	BB	673	OMG	O6-C6-C5	-2.04	120.38	124.37
2	AA	1931	OMG	N2-C2-N1	2.04	121.06	116.71
1	BA	1267	OMG	O6-C6-C5	-2.04	120.38	124.37
3	BB	1269	OMG	N2-C2-N1	2.04	121.05	116.71
3	BB	659	OMG	N2-C2-N1	2.04	121.05	116.71
3	BB	522	PSU	C6-C5-C4	2.03	119.62	118.20
1	BA	915	OMG	O6-C6-C5	-2.03	120.40	124.37
2	AA	942	PSU	O4'-C1'-C2'	2.03	108.00	105.14
2	AA	1652	OMU	O2-C2-N1	-2.02	120.10	122.79

There are no chirality outliers.

All (105) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	BC	7	OMU	C1'-C2'-O2'-CM2
9	BC	43	A2M	C1'-C2'-O2'-CM'
9	BC	163	A2M	C1'-C2'-O2'-CM'
1	BA	743	A2M	C1'-C2'-O2'-CM'
1	BA	760	OMC	C1'-C2'-O2'-CM2
1	BA	762	A2M	C1'-C2'-O2'-CM'
1	BA	996	A2M	C1'-C2'-O2'-CM'
1	BA	1024	A2M	C1'-C2'-O2'-CM'
1	BA	1028	OMG	O4'-C4'-C5'-O5'
1	BA	1028	OMG	C3'-C4'-C5'-O5'
1	BA	1258	PSU	C3'-C4'-C5'-O5'
1	BA	1258	PSU	O4'-C4'-C5'-O5'
1	BA	1329	OMC	C1'-C2'-O2'-CM2
1	BA	1665	A2M	C1'-C2'-O2'-CM'
1	BA	1742	OMU	C1'-C2'-O2'-CM2
2	AA	56	A2M	C1'-C2'-O2'-CM'
2	AA	57	OMU	C1'-C2'-O2'-CM2
2	AA	131	PSU	O4'-C1'-C5-C4
2	AA	131	PSU	O4'-C1'-C5-C6

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Mol	Chain	Res	Type	Atoms
2	AA	721	A2M	O4'-C4'-C5'-O5'
2	AA	721	A2M	C3'-C4'-C5'-O5'
2	AA	721	A2M	C1'-C2'-O2'-CM'
2	AA	942	PSU	O4'-C1'-C5-C4
2	AA	942	PSU	C2'-C1'-C5-C6
2	AA	942	PSU	O4'-C1'-C5-C6
2	AA	1596	B8N	O4'-C4'-C5'-O5'
2	AA	1596	B8N	N3-C31-C32-C33
2	AA	1619	PSU	C3'-C4'-C5'-O5'
2	AA	1899	OMU	O4'-C1'-N1-C2
2	AA	2054	OMU	O4'-C4'-C5'-O5'
2	AA	2096	A2M	C1'-C2'-O2'-CM'
2	AA	2153	A2M	C1'-C2'-O2'-CM'
2	AA	2154	OMU	C1'-C2'-O2'-CM2
3	BB	95	A2M	C1'-C2'-O2'-CM'
3	BB	400	A2M	O4'-C4'-C5'-O5'
3	BB	400	A2M	C3'-C4'-C5'-O5'
3	BB	522	PSU	C3'-C4'-C5'-O5'
3	BB	552	OMG	O4'-C4'-C5'-O5'
3	BB	552	OMG	C3'-C4'-C5'-O5'
3	BB	578	OMU	O4'-C1'-N1-C2
3	BB	578	OMU	O4'-C1'-N1-C6
3	BB	578	OMU	O4'-C4'-C5'-O5'
3	BB	588	A2M	C1'-C2'-O2'-CM'
3	BB	609	A2M	C1'-C2'-O2'-CM'
3	BB	622	A2M	C1'-C2'-O2'-CM'
3	BB	629	PSU	C3'-C4'-C5'-O5'
3	BB	629	PSU	O4'-C4'-C5'-O5'
3	BB	685	OMU	C1'-C2'-O2'-CM2
3	BB	1062	OMG	O4'-C4'-C5'-O5'
3	BB	1062	OMG	C3'-C4'-C5'-O5'
1	BA	1448	OMU	C3'-C4'-C5'-O5'
2	AA	1596	B8N	C3'-C4'-C5'-O5'
2	AA	2054	OMU	C3'-C4'-C5'-O5'
3	BB	522	PSU	O4'-C4'-C5'-O5'
2	AA	1899	OMU	O4'-C1'-N1-C6
1	BA	1448	OMU	O4'-C4'-C5'-O5'
1	BA	1665	A2M	O4'-C4'-C5'-O5'
2	AA	1619	PSU	O4'-C4'-C5'-O5'
3	BB	578	OMU	C3'-C4'-C5'-O5'
3	BB	1201	A2M	C3'-C4'-C5'-O5'
1	BA	1665	A2M	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	BA	1614	PSU	C3'-C4'-C5'-O5'
2	AA	36	OMU	O4'-C4'-C5'-O5'
2	AA	36	OMU	C2'-C1'-N1-C6
3	BB	1324	5MC	C2'-C1'-N1-C6
2	AA	1592	PSU	O4'-C4'-C5'-O5'
3	BB	1201	A2M	O4'-C4'-C5'-O5'
2	AA	1676	OMG	C1'-C2'-O2'-CM2
3	BB	1324	5MC	O4'-C1'-N1-C6
2	AA	1596	B8N	C31-C32-C33-C34
2	AA	1517	OMG	C3'-C2'-O2'-CM2
3	BB	545	A2M	C3'-C2'-O2'-CM'
1	BA	1605	OMG	C3'-C4'-C5'-O5'
2	AA	36	OMU	C3'-C4'-C5'-O5'
2	AA	36	OMU	O4'-C1'-N1-C6
1	BA	1614	PSU	O4'-C4'-C5'-O5'
2	AA	942	PSU	O4'-C4'-C5'-O5'
2	AA	2070	7MG	O4'-C4'-C5'-O5'
2	AA	2096	A2M	C3'-C4'-C5'-O5'
3	BB	578	OMU	C4'-C5'-O5'-P
3	BB	542	5MC	O4'-C4'-C5'-O5'
3	BB	1324	5MC	C2'-C1'-N1-C2
1	BA	1605	OMG	C3'-C2'-O2'-CM2
3	BB	545	A2M	O4'-C4'-C5'-O5'
3	BB	1324	5MC	O4'-C1'-N1-C2
2	AA	1899	OMU	C4'-C5'-O5'-P
2	AA	2261	MA6	C4'-C5'-O5'-P
1	BA	1608	OMC	C2'-C1'-N1-C6
3	BB	1398	PSU	O4'-C1'-C5-C4
3	BB	1375	OMU	C3'-C2'-O2'-CM2
3	BB	1264	OMC	C4'-C5'-O5'-P
2	AA	1596	B8N	N34-C33-C34-O35
2	AA	36	OMU	O4'-C1'-N1-C2
2	AA	1531	OMG	C4'-C5'-O5'-P
2	AA	1592	PSU	C3'-C4'-C5'-O5'
2	AA	2134	OMC	O4'-C4'-C5'-O5'
9	BC	75	OMG	C1'-C2'-O2'-CM2
3	BB	1062	OMG	C1'-C2'-O2'-CM2
1	BA	743	A2M	O4'-C4'-C5'-O5'
1	BA	1608	OMC	C2'-C1'-N1-C2
2	AA	36	OMU	C2'-C1'-N1-C2
1	BA	1608	OMC	O4'-C4'-C5'-O5'
2	AA	1895	OMG	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
2	AA	1899	OMU	O4'-C4'-C5'-O5'
3	BB	1201	A2M	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 325 ligands modelled in this entry, 325 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
10	AB	1
2	AA	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	AB	7:A	O3'	65:G	P	16.03

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	AA	1596:B8N	O3'	1597:C	P	4.10

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-17208. 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.