



Full wwPDB EM Validation Report ⓘ

Nov 8, 2022 – 01:24 AM EST

PDB ID : 6MTB
EMDB ID : EMD-9237
Title : Rabbit 80S ribosome with P- and Z-site tRNAs (unrotated state)
Authors : Brown, A.; Baird, M.R.; Yip, M.C.J.; Murray, J.; Shao, S.
Deposited on : 2018-10-19
Resolution : 3.60 Å (reported)
Based on initial model : 5LZV

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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

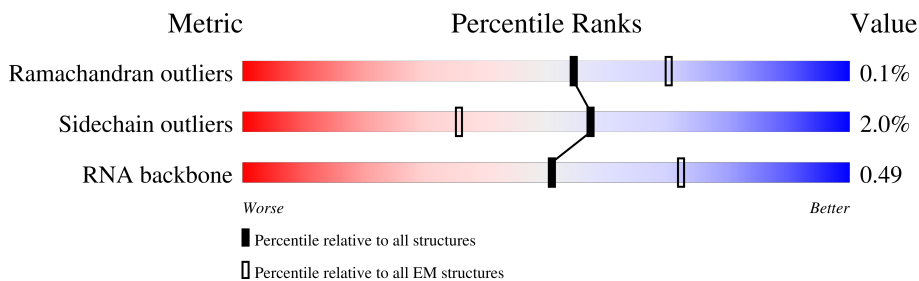
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	7	
2	2	76	
3	4	75	
4	5	3597	
5	7	120	
6	8	151	
7	A	248	
8	B	394	

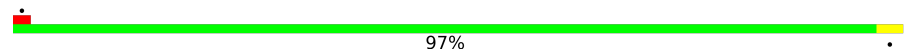
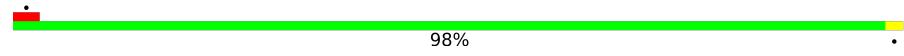
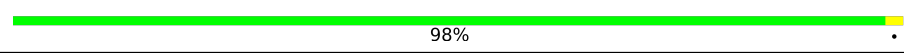
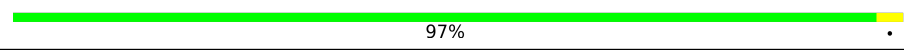
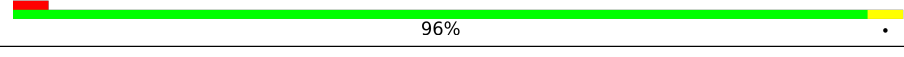
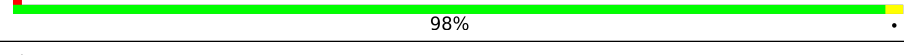
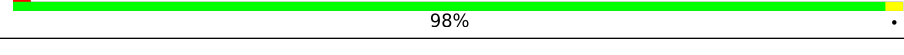
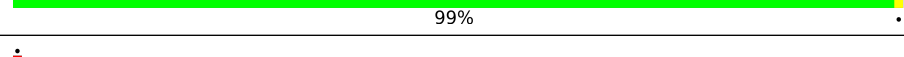
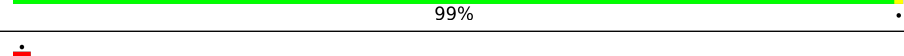
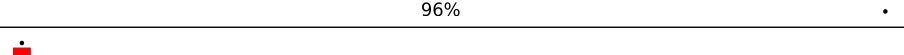
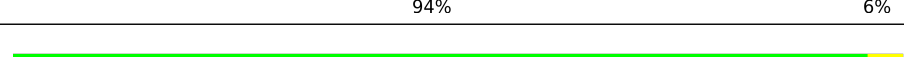
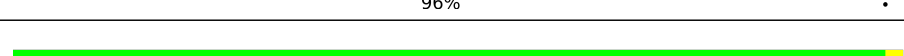
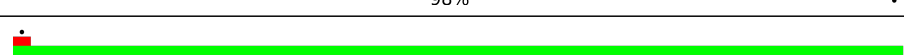
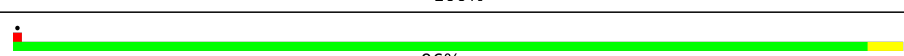
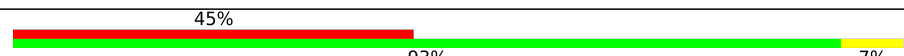
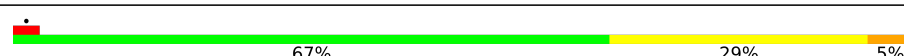
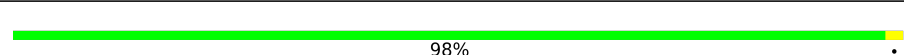
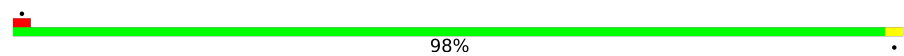
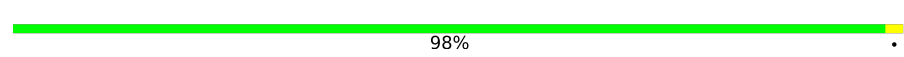
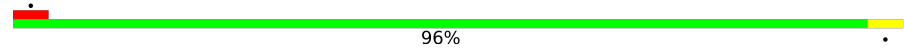
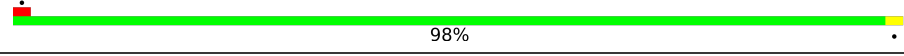
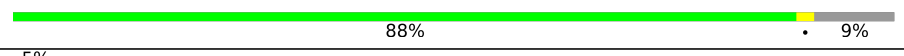
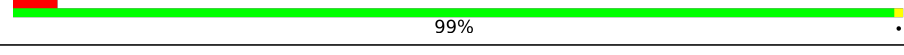
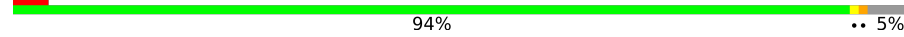

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Mol	Chain	Length	Quality of chain
9	C	362	98%
10	D	293	97%
11	E	291	72% 26%
12	F	247	90% 9%
13	G	319	70% 27%
14	H	190	97%
15	I	214	95%
16	J	178	94%
17	L	210	99%
18	M	138	97%
19	N	203	97%
20	O	199	97%
21	P	153	99%
22	Q	187	98%
23	R	180	98%
24	S	176	98%
25	T	159	97%
26	U	99	97%
27	V	131	98%
28	W	157	5% 66% 32%
29	X	118	100%
30	Y	134	97%
31	Z	135	99%
32	a	147	99%
33	b	245	40% 58%

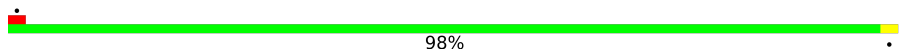
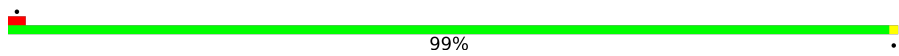
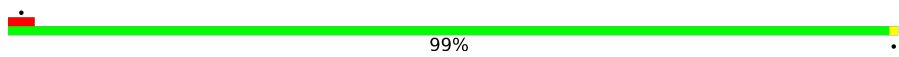

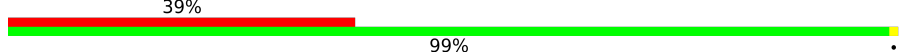
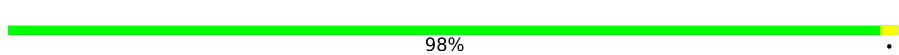
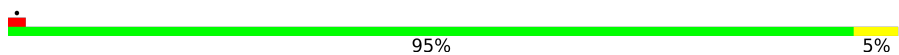
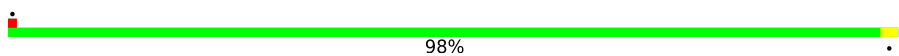
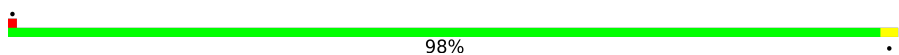
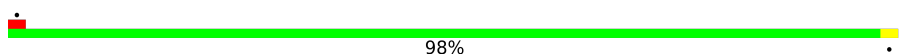
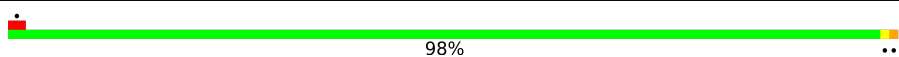
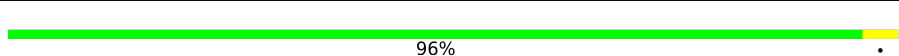
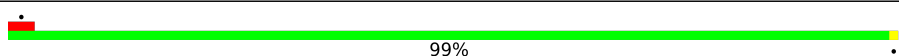
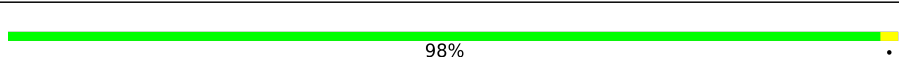
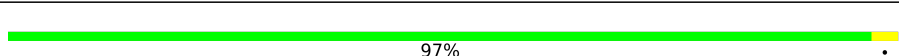
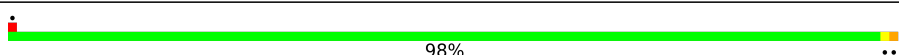
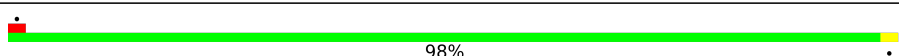
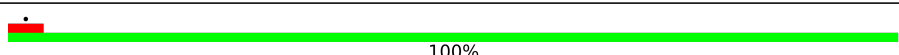
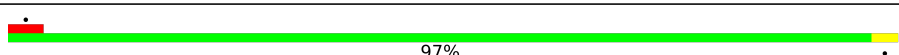
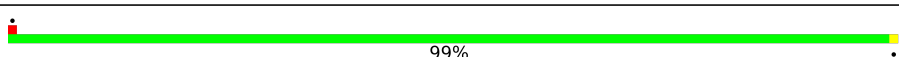
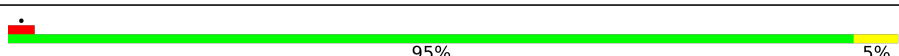
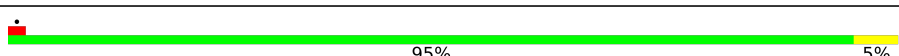
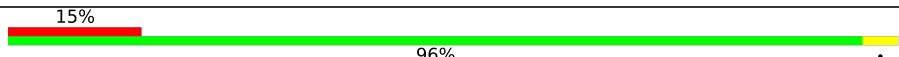

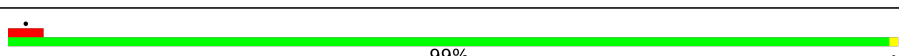
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Mol	Chain	Length	Quality of chain
34	c	98	 97%
35	d	107	 98%
36	e	128	 98%
37	f	109	 97%
38	g	114	 96%
39	h	122	 98%
40	i	102	 98%
41	j	86	 99%
42	k	69	 99%
43	l	50	 96%
44	m	52	 94% 6%
45	n	25	 96%
46	o	103	 98%
47	p	91	 100%
48	r	124	 96%
49	u	206	 45% 93% 7%
50	9	1698	 67% 29% 5%
51	AA	217	 98%
52	BB	213	 98%
53	CC	221	 98%
54	DD	228	 96%
55	EE	262	 98%
56	FF	204	 88% 9%
57	GG	237	 99%
58	HH	194	 94% 5%

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Mol	Chain	Length	Quality of chain
59	II	206	 98%
60	JJ	185	 99%
61	KK	96	 99%
62	LL	158	 89% 9%
63	MM	117	 39% 99%
64	NN	149	 98%
65	OO	136	 95% 5%
66	PP	120	 98%
67	QQ	142	 98%
68	RR	132	 98%
69	SS	144	 98%
70	TT	141	 96%
71	UU	100	 99%
72	VV	83	 98%
73	WW	129	 97%
74	XX	141	 98%
75	YY	124	 98%
76	ZZ	75	 100%
77	aa	101	 97%
78	bb	83	 99%
79	cc	62	 95% 5%
80	dd	55	 95% 5%
81	ee	55	 15% 96%
82	ff	68	 38% 79% 18%
83	gg	313	 99%

2 Entry composition [i](#)

There are 85 unique types of molecules in this entry. The entry contains 216003 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 mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	1	7	149	67	27	48	7	0	0

- Molecule 2 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	2	76	1616	723	291	527	75	0	0

- Molecule 3 is a RNA chain called Z-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	4	75	1593	712	281	526	74	0	0

- Molecule 4 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	5	3597	77254	34469	14127	25061	3597	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	7	120	2558	1141	456	842	119	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	8	151	3209	1433	564	1062	150	0	0

- Molecule 7 is a protein called 60S ribosomal protein L8.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	B	394	3172	2020	597	542	13	0	0

- Molecule 9 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	C	362	2884	1813	577	480	14	0	0

- Molecule 10 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	D	293	2391	1512	438	427	14	0	0

- Molecule 11 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	E	216	1729	1115	329	282	3	0	0

- Molecule 12 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	F	225	1875	1205	358	303	9	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	G	233	1879	1199	361	315	4	0	0

- Molecule 14 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	H	190	1516	954	284	272	6	0	0

- Molecule 15 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	I	205	1664	1056	321	274	13	0	0

- Molecule 16 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	J	170	1362	861	254	241	6	0	0

- Molecule 17 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	L	210	1702	1065	354	279	4	0	0

- Molecule 18 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	M	138	1137	727	221	182	7	0	0

- Molecule 19 is a protein called 60S ribosomal protein L15.

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

- Molecule 20 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	O	199	1630	1051	319	255	5	0	0

- Molecule 21 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	P	153	1242	777	241	215	9	0	0

- Molecule 22 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	Q	187	1515	946	315	250	4	0	0

- Molecule 23 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	R	180	1508	933	328	238	9	0	0

- Molecule 24 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	S	176	1462	930	285	236	11	0	0

- Molecule 25 is a protein called 60S ribosomal protein L21.

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

- Molecule 26 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	U	99	809	519	141	147	2	0	0

- Molecule 27 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	V	131	979	618	184	172	5	0	0

- Molecule 28 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	W	106	860	538	174	144	4	0	0

- Molecule 29 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	X	118	967	618	181	167	1	0	0

- Molecule 30 is a protein called 60S ribosomal protein L26.

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

- Molecule 31 is a protein called 60S ribosomal protein L27.

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

- Molecule 32 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	a	147	1162	734	239	185	4	0	0

- Molecule 33 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	b	104	848	527	189	129	3	0	0

- Molecule 34 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	c	98	761	481	134	140	6	0	0

- Molecule 35 is a protein called 60S ribosomal protein L31.

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

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

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

- Molecule 37 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	f	109	Total	C	N	O	S	0	0
			876	555	174	143	4		

- Molecule 38 is a protein called 60S ribosomal protein L34.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	h	122	Total	C	N	O	S	0	0
			1013	640	204	168	1		

- Molecule 40 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	i	102	Total	C	N	O	S	0	0
			830	520	176	129	5		

- Molecule 41 is a protein called 60S ribosomal protein L37.

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

- Molecule 42 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	k	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

- Molecule 43 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	l	50	Total	C	N	O	S	0	0
			447	286	96	64	1		

- Molecule 44 is a protein called 60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	m	52	Total	C	N	O	S	0	0
			430	267	90	67	6		

- Molecule 45 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	n	25	Total	C	N	O	S	0	0
			239	145	64	27	3		

- Molecule 46 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	o	103	Total	C	N	O	S	0	0
			842	528	172	136	6		

- Molecule 47 is a protein called 60S ribosomal protein L37a.

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

- Molecule 48 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	r	124	Total	C	N	O	S	0	0
			994	616	205	167	6		

- Molecule 49 is a protein called 60S ribosomal protein L10a.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	u	206	Total	C	N	O	S	0	0
			1654	1058	297	291	8		

- Molecule 50 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	9	1698	Total	C	N	O	P	0	0
			36291	16217	6509	11868	1697		

- Molecule 51 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	AA	217	Total	C	N	O	S	0	0
			1710	1086	300	316	8		

- Molecule 52 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	BB	213	Total	C	N	O	S	0	0
			1729	1098	309	308	14		

- Molecule 53 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	CC	221	Total	C	N	O	S	0	0
			1716	1111	295	301	9		

- Molecule 54 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	DD	228	Total	C	N	O	S	0	0
			1768	1126	318	316	8		

- Molecule 55 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	EE	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

- Molecule 56 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	FF	185	Total	C	N	O	S	0	0
			1471	921	277	266	7		

- Molecule 57 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	GG	237	Total	C	N	O	S	0	0
			1923	1200	387	329	7		

- Molecule 58 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	HH	185	Total	C	N	O	S	0	0
			1488	952	271	264	1		

- Molecule 59 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	II	206	Total	C	N	O	S	0	0
			1686	1058	332	291	5		

- Molecule 60 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	JJ	185	Total	C	N	O	S	0	0
			1525	969	306	248	2		

- Molecule 61 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	KK	96	Total	C	N	O	S	0	0
			810	530	143	131	6		

- Molecule 62 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	LL	143	Total	C	N	O	S	0	0
			1175	749	222	198	6		

- Molecule 63 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
63	MM	117	908	570	161	169	8	0	0

- Molecule 64 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
64	NN	149	1202	770	228	203	1	0	0

- Molecule 65 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
65	OO	136	1016	621	199	190	6	0	0

- Molecule 66 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
66	PP	120	997	635	187	168	7	0	0

- Molecule 67 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
67	QQ	142	1128	717	213	195	3	0	0

- Molecule 68 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
68	RR	132	1068	670	199	195	4	0	0

- Molecule 69 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
69	SS	144	1190	746	241	202	1	0	0

- Molecule 70 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
70	TT	141	1097	688	211	195	3	0	0

- Molecule 71 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
71	UU	100	795	498	152	141	4	0	0

- Molecule 72 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
72	VV	83	636	393	117	121	5	0	0

- Molecule 73 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
73	WW	129	1034	659	193	176	6	0	0

- Molecule 74 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
74	XX	141	1098	693	219	183	3	0	0

- Molecule 75 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
75	YY	124	1011	640	198	168	5	0	0

- Molecule 76 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
76	ZZ	75	598	382	111	104	1	0	0

- Molecule 77 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	aa	101	Total	C	N	O	S	0	0
			814	507	170	132	5		

- Molecule 78 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	bb	83	Total	C	N	O	S	0	0
			651	408	121	115	7		

- Molecule 79 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	cc	62	Total	C	N	O	S	0	0
			488	297	97	92	2		

- Molecule 80 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	dd	55	Total	C	N	O	S	0	0
			459	286	94	74	5		

- Molecule 81 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	ee	55	Total	C	N	O	S	0	0
			443	274	97	71	1		

- Molecule 82 is a protein called 40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	ff	68	Total	C	N	O	S	0	0
			555	351	103	94	7		

- Molecule 83 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	gg	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

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

Mol	Chain	Residues	Atoms	AltConf
84	5	199	Total Mg 199 199	0
84	7	7	Total Mg 7 7	0
84	8	7	Total Mg 7 7	0
84	A	1	Total Mg 1 1	0
84	P	1	Total Mg 1 1	0
84	Q	1	Total Mg 1 1	0
84	V	1	Total Mg 1 1	0
84	a	1	Total Mg 1 1	0
84	9	78	Total Mg 78 78	0
84	aa	1	Total Mg 1 1	0

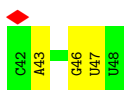
- Molecule 85 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
85	g	1	Total Zn 1 1	0
85	j	1	Total Zn 1 1	0
85	m	1	Total Zn 1 1	0
85	o	1	Total Zn 1 1	0
85	p	1	Total Zn 1 1	0
85	aa	1	Total Zn 1 1	0
85	dd	1	Total Zn 1 1	0
85	ff	1	Total Zn 1 1	0

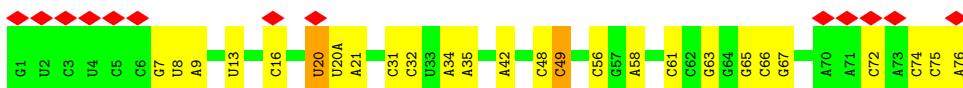
3 Residue-property plots

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

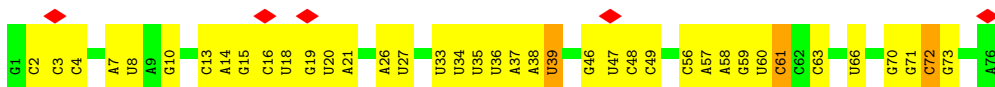
- Molecule 1: mRNA



- Molecule 2: P-site tRNA

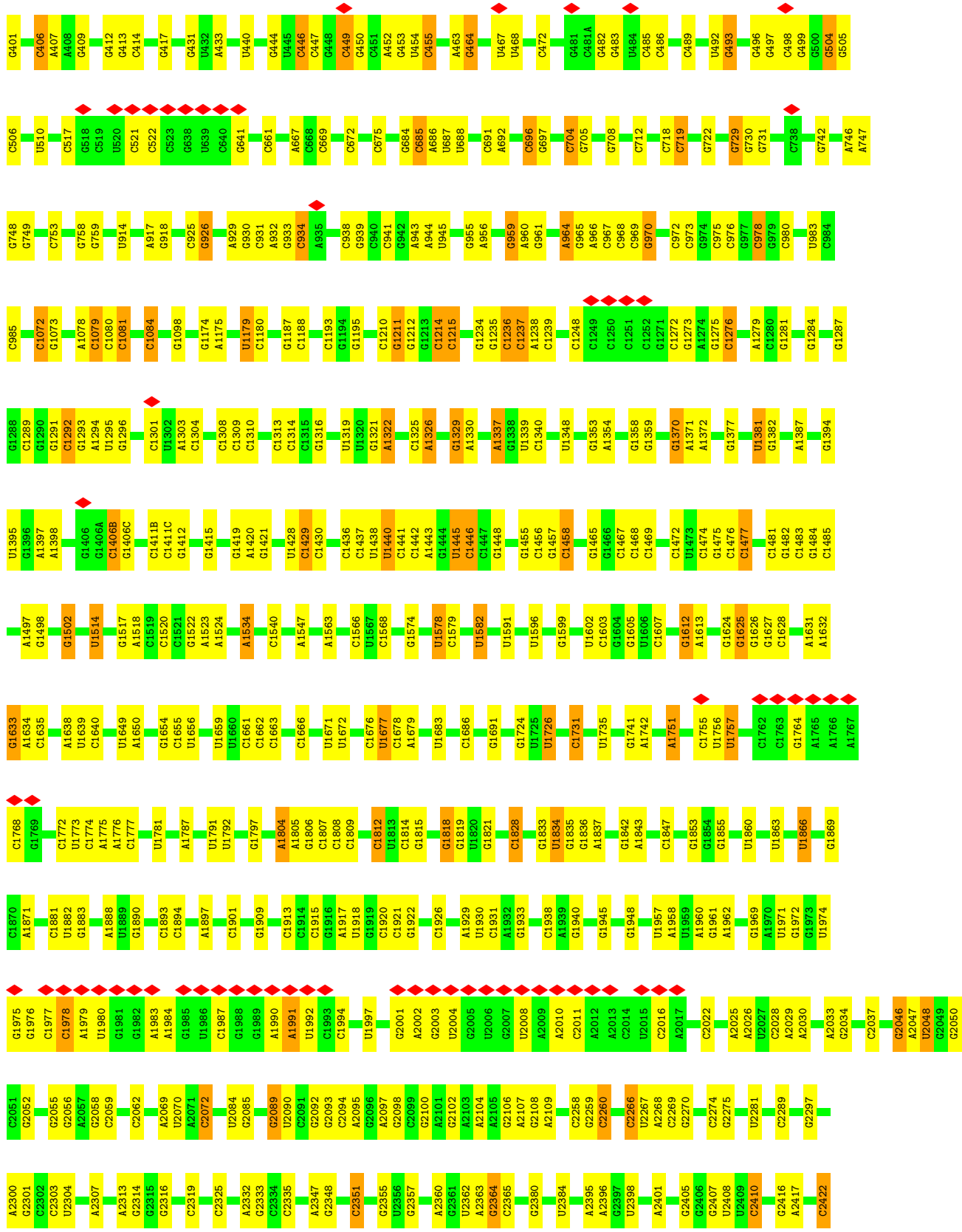


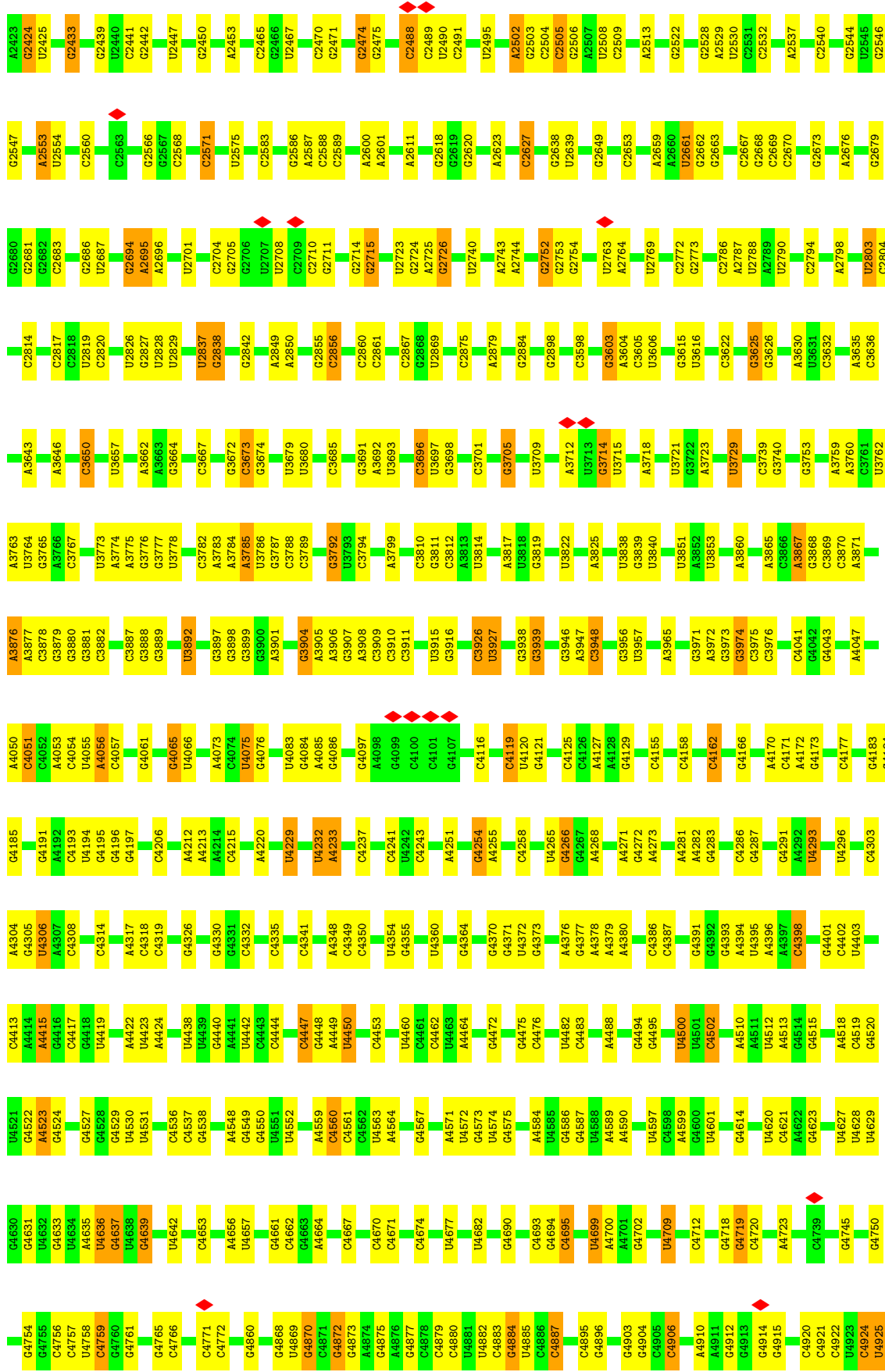
- Molecule 3: Z-site tRNA

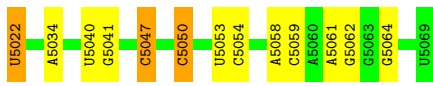
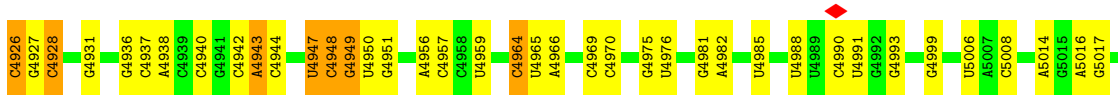


- Molecule 4: 28S rRNA

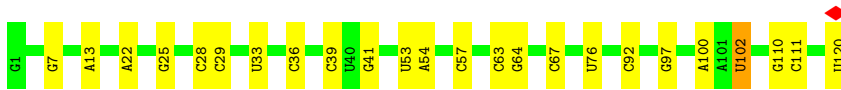
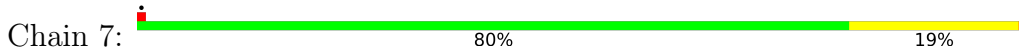




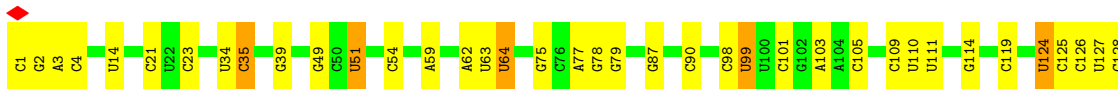




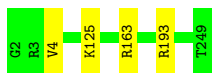
• Molecule 5: 5S rRNA



• Molecule 6: 5.8S rRNA



• Molecule 7: 60S ribosomal protein L8



• Molecule 8: 60S ribosomal protein L3

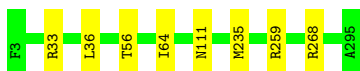


• Molecule 9: 60S ribosomal protein L4



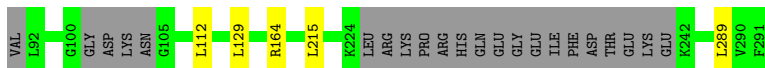
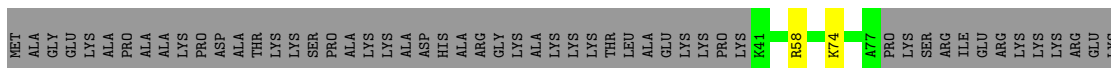
• Molecule 10: 60S ribosomal protein L5





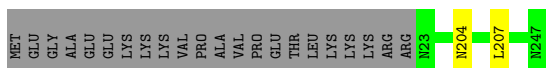
- Molecule 11: 60S ribosomal protein L6

Chain E: 72% 26%



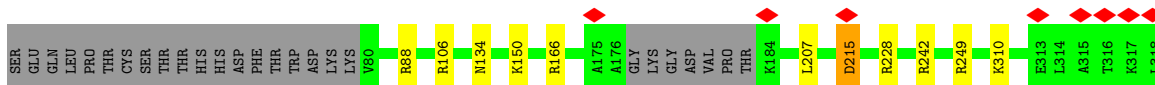
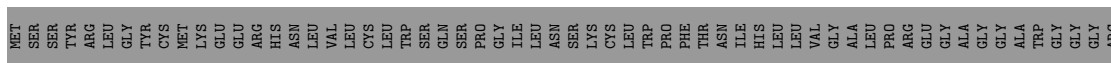
- Molecule 12: 60S ribosomal protein L7

Chain F: 90% 9%



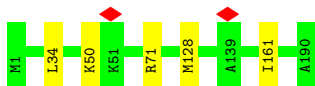
- Molecule 13: 60S ribosomal protein L7a

Chain G: 70% 27%



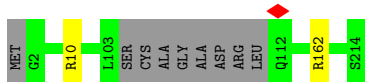
- Molecule 14: 60S ribosomal protein L9

Chain H: 97%



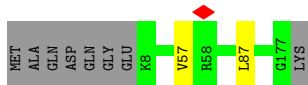
- Molecule 15: 60S ribosomal protein L10

Chain I: 95%



- Molecule 16: 60S ribosomal protein L11

Chain J:  94%



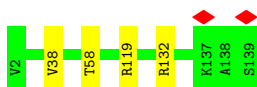
- Molecule 17: 60S ribosomal protein L13

Chain L:  99%



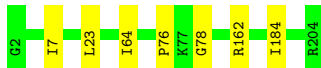
- Molecule 18: 60S ribosomal protein L14

Chain M:  97%



- Molecule 19: 60S ribosomal protein L15

Chain N:  97%



- Molecule 20: 60S ribosomal protein L13a

Chain O:  97%



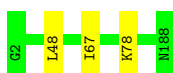
- Molecule 21: 60S ribosomal protein L17

Chain P:  99%

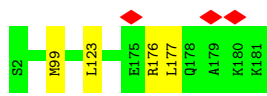


- Molecule 22: 60S ribosomal protein L18

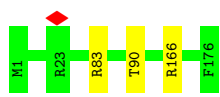
Chain Q:  98%



- Molecule 23: 60S ribosomal protein L19



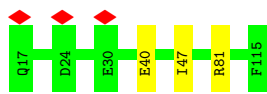
• Molecule 24: 60S ribosomal protein L18a



• Molecule 25: 60S ribosomal protein L21



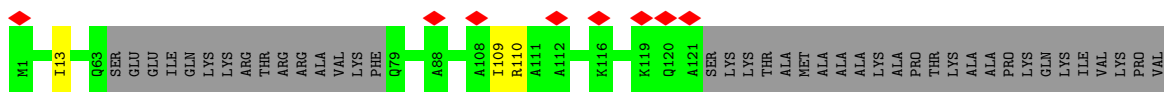
• Molecule 26: 60S ribosomal protein L22



• Molecule 27: 60S ribosomal protein L23



• Molecule 28: 60S ribosomal protein L24



LYS
VAL
SER
ALA
PRO
ARG
VAL
GLY
GLY
LYS
ARG

• Molecule 29: 60S ribosomal protein L23a





- Molecule 36: 60S ribosomal protein L32

Chain e: 98%



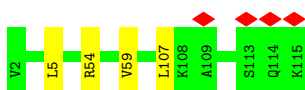
- Molecule 37: 60S ribosomal protein L35a

Chain f: 97%



- Molecule 38: 60S ribosomal protein L34

Chain g: 96%



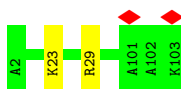
- Molecule 39: 60S ribosomal protein L35

Chain h: 98%



- Molecule 40: 60S ribosomal protein L36

Chain i: 98%



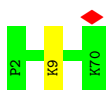
- Molecule 41: 60S ribosomal protein L37

Chain j: 99%



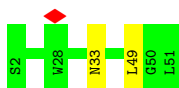
- Molecule 42: 60S ribosomal protein L38

Chain k:  99%



- Molecule 43: 60S ribosomal protein L39

Chain l:  96%



- Molecule 44: 60S ribosomal protein L40

Chain m:  94% 6%



- Molecule 45: 60S ribosomal protein L41

Chain n:  96%



- Molecule 46: 60S ribosomal protein L36a

Chain o:  98%



- Molecule 47: 60S ribosomal protein L37a

Chain p:  100%

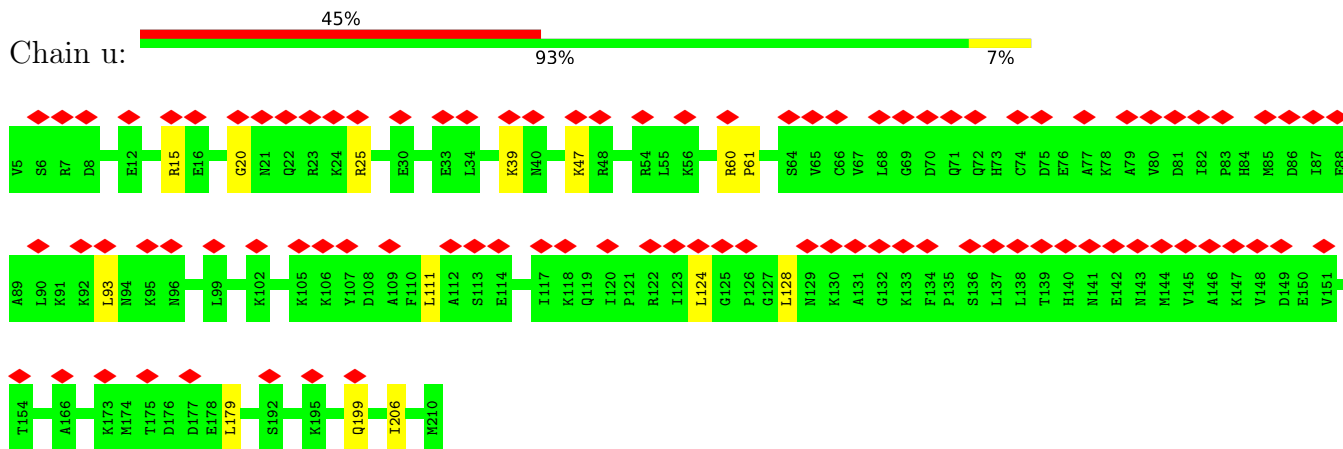


- Molecule 48: 60S ribosomal protein L28

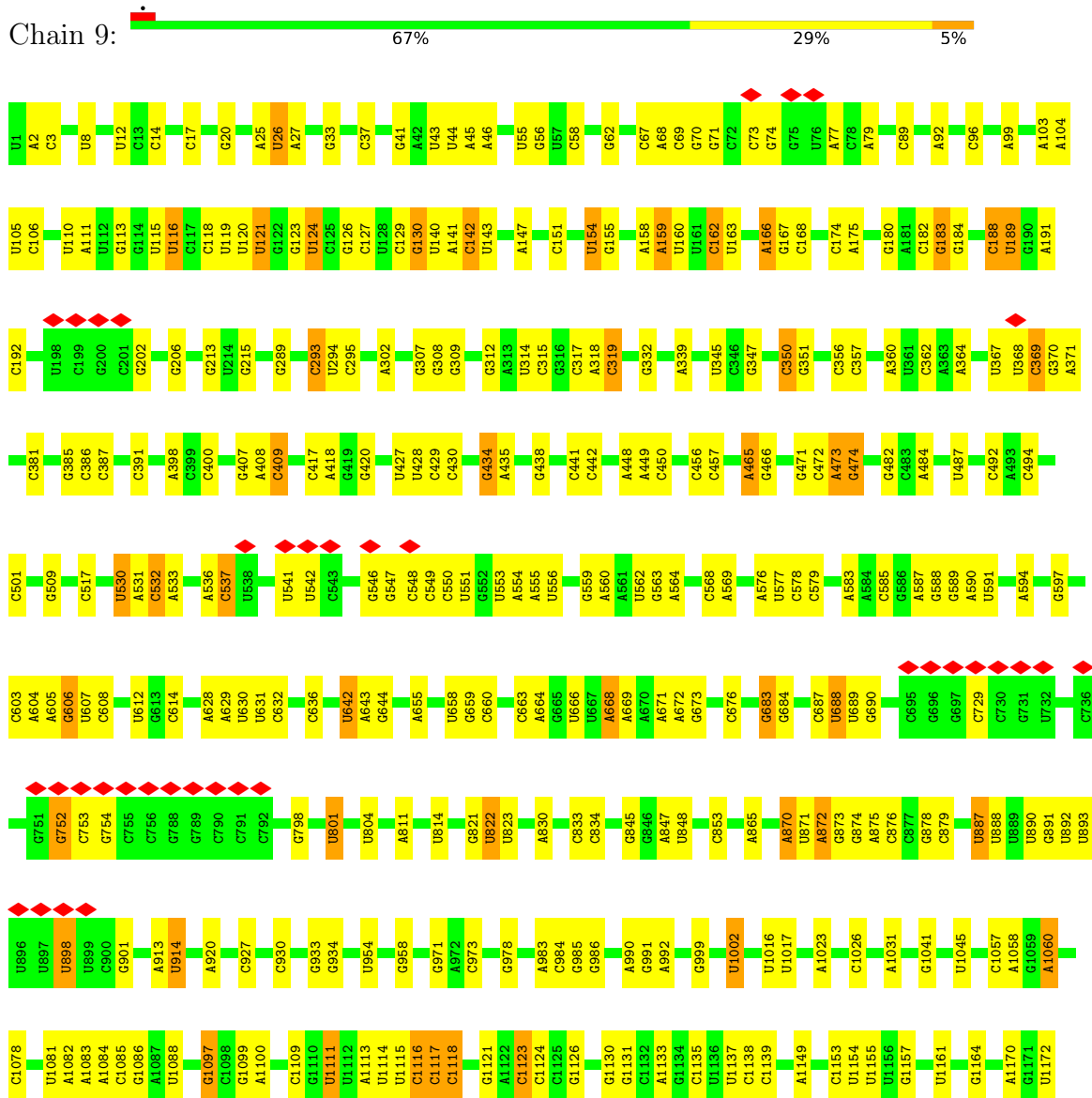
Chain r:  96%

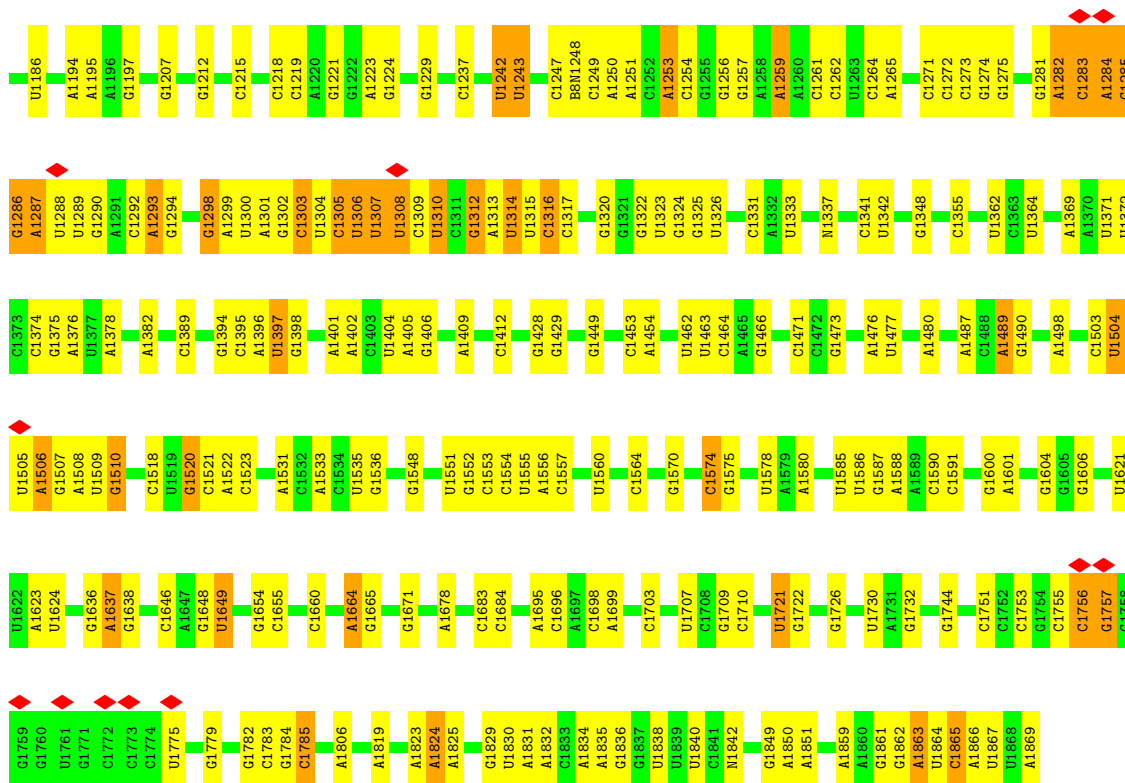


• Molecule 49: 60S ribosomal protein L10a



• Molecule 50: 18S rRNA

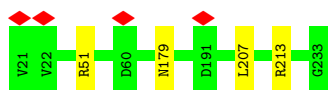




• Molecule 51: 40S ribosomal protein SA



• Molecule 52: 40S ribosomal protein S3a

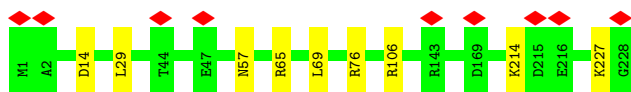


• Molecule 53: 40S ribosomal protein S2



• Molecule 54: 40S ribosomal protein S3

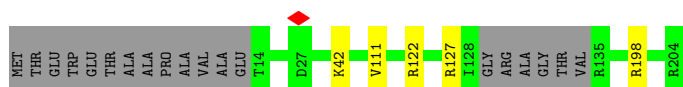




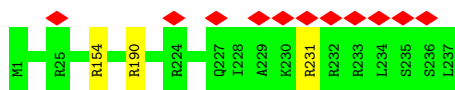
- Molecule 55: 40S ribosomal protein S4, X isoform



- Molecule 56: 40S ribosomal protein S5



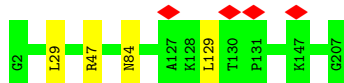
- Molecule 57: 40S ribosomal protein S6



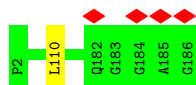
- Molecule 58: 40S ribosomal protein S7



- Molecule 59: 40S ribosomal protein S8

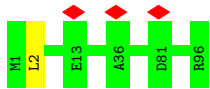


- Molecule 60: 40S ribosomal protein S9




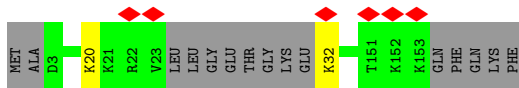
- Molecule 61: 40S ribosomal protein S10

Chain KK:  99%

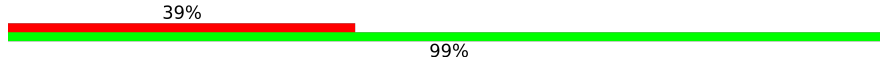


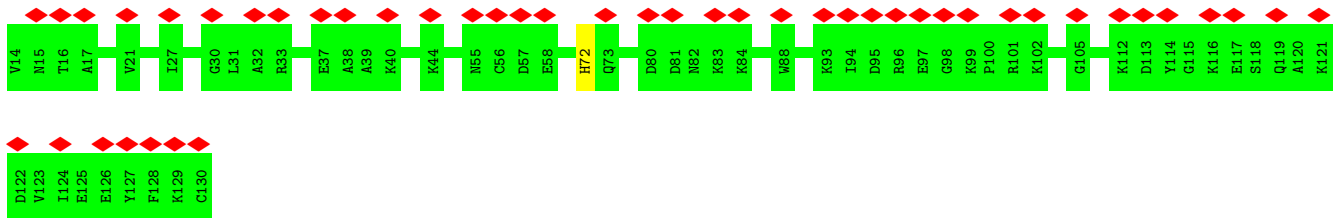
- Molecule 62: 40S ribosomal protein S11

Chain LL:  89%



- Molecule 63: 40S ribosomal protein S12

Chain MM:  39%



- Molecule 64: 40S ribosomal protein S13

Chain NN:  98%



- Molecule 65: 40S ribosomal protein S14

Chain OO:  95%



- Molecule 66: 40S ribosomal protein S15

Chain PP:  98%

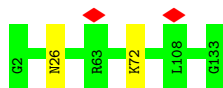


- Molecule 67: 40S ribosomal protein S16

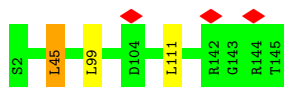
Chain QQ:  98%



- Molecule 68: 40S ribosomal protein S17



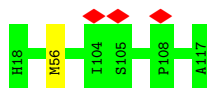
- Molecule 69: 40S ribosomal protein S18



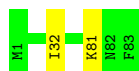
- Molecule 70: 40S ribosomal protein S19



- Molecule 71: 40S ribosomal protein S20



- Molecule 72: 40S ribosomal protein S21



- Molecule 73: 40S ribosomal protein S15a



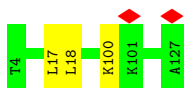
- Molecule 74: 40S ribosomal protein S23

Chain XX:  98%



- Molecule 75: 40S ribosomal protein S24

Chain YY:  98%



- Molecule 76: 40S ribosomal protein S25

Chain ZZ:  100%



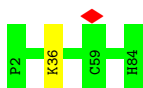
- Molecule 77: 40S ribosomal protein S26

Chain aa:  97%



- Molecule 78: 40S ribosomal protein S27

Chain bb:  99%



- Molecule 79: 40S ribosomal protein S28

Chain cc:  95%

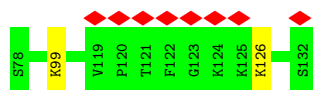


- Molecule 80: 40S ribosomal protein S29

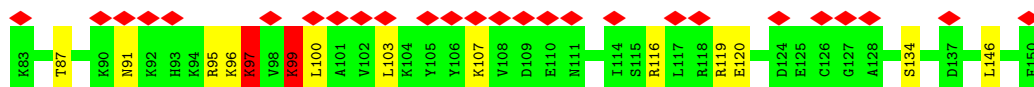
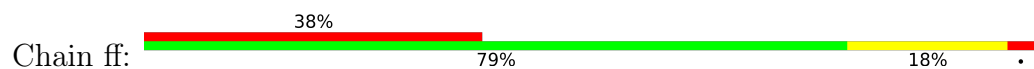
Chain dd:  95%



- Molecule 81: 40S ribosomal protein S30



- Molecule 82: 40S ribosomal protein S27a



- Molecule 83: Receptor of activated protein C kinase 1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	62560	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.797	Depositor
Minimum map value	-0.567	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	536.0, 536.0, 536.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	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: B8W, 5MC, 1MA, I4U, B9B, A2M, P4U, E6G, B9H, OMG, P7G, B8N, PSU, MHG, 5MU, B8H, B8Q, 2MG, MLZ, M7A, MA6, ZN, OMC, BGH, UR3, 7MG, E3C, B8K, MG, B8T, 4AC, E7G, OMU, 6MZ

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	1	0.66	0/166	1.02	0/256
2	2	0.58	0/1805	1.19	19/2809 (0.7%)
3	4	0.42	0/1779	1.11	11/2771 (0.4%)
4	5	1.03	6/83825 (0.0%)	1.23	727/130614 (0.6%)
5	7	1.03	0/2858	1.19	17/4455 (0.4%)
6	8	1.01	0/3559	1.22	27/5543 (0.5%)
7	A	0.62	0/1936	0.69	0/2596
8	B	0.65	0/3240	0.70	0/4339
9	C	0.56	0/2927	0.67	1/3932 (0.0%)
10	D	0.55	0/2437	0.61	0/3264
11	E	0.51	0/1762	0.71	3/2362 (0.1%)
12	F	0.61	0/1911	0.68	1/2549 (0.0%)
13	G	0.49	0/1910	0.66	1/2569 (0.0%)
14	H	0.56	0/1535	0.69	1/2063 (0.0%)
15	I	0.55	0/1702	0.61	0/2272
16	J	0.52	0/1385	0.71	1/1852 (0.1%)
17	L	0.47	0/1733	0.64	0/2316
18	M	0.58	0/1158	0.68	0/1547
19	N	0.61	0/1746	0.68	0/2338
20	O	0.63	1/1662 (0.1%)	0.73	2/2222 (0.1%)
21	P	0.64	0/1268	0.69	0/1700
22	Q	0.56	0/1539	0.72	2/2054 (0.1%)
23	R	0.47	0/1524	0.70	2/2013 (0.1%)
24	S	0.60	0/1501	0.65	0/2012
25	T	0.58	0/1326	0.62	0/1770
26	U	0.45	0/823	0.67	0/1104
27	V	0.62	0/993	0.70	1/1332 (0.1%)
28	W	0.59	1/873 (0.1%)	0.64	0/1158
29	X	0.51	0/984	0.62	0/1323
30	Y	0.59	0/1132	0.66	0/1504

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	Z	0.57	0/1130	0.61	0/1507
32	a	0.61	0/1191	0.65	1/1590 (0.1%)
33	b	0.39	0/861	0.60	0/1138
34	c	0.56	0/771	0.65	0/1034
35	d	0.54	0/903	0.69	0/1216
36	e	0.60	0/1071	0.62	0/1429
37	f	0.69	0/895	0.71	0/1198
38	g	0.54	0/916	0.67	0/1220
39	h	0.48	0/1021	0.66	0/1348
40	i	0.44	0/841	0.59	0/1112
41	j	0.59	0/720	0.67	0/952
42	k	0.44	0/575	0.63	0/761
43	l	0.55	0/459	0.69	1/608 (0.2%)
44	m	0.55	0/425	0.77	0/561
45	n	0.48	0/240	0.77	0/305
46	o	0.50	0/855	0.59	0/1128
47	p	0.59	0/718	0.65	0/953
48	r	0.60	0/1010	0.72	0/1354
49	u	0.35	0/1680	0.76	3/2255 (0.1%)
50	9	0.96	32/39723 (0.1%)	1.33	508/61870 (0.8%)
51	AA	0.55	1/1747 (0.1%)	0.68	0/2374
52	BB	0.47	0/1756	0.66	0/2350
53	CC	0.59	0/1753	0.73	1/2369 (0.0%)
54	DD	0.46	0/1796	0.73	3/2417 (0.1%)
55	EE	0.50	0/2118	0.69	1/2849 (0.0%)
56	FF	0.47	0/1492	0.66	0/2005
57	GG	0.42	0/1946	0.63	0/2590
58	HH	0.44	0/1510	0.69	1/2022 (0.0%)
59	II	0.51	0/1715	0.68	2/2287 (0.1%)
60	JJ	0.47	0/1550	0.67	1/2069 (0.0%)
61	KK	0.46	0/834	0.70	1/1125 (0.1%)
62	LL	0.56	0/1195	0.65	0/1597
63	MM	0.35	0/918	0.71	0/1233
64	NN	0.49	0/1226	0.70	2/1649 (0.1%)
65	OO	0.48	0/1029	0.69	0/1380
66	PP	0.43	0/1017	0.63	0/1358
67	QQ	0.48	0/1146	0.68	0/1534
68	RR	0.44	0/1082	0.64	0/1452
69	SS	0.43	0/1208	0.71	2/1618 (0.1%)
70	TT	0.42	0/1115	0.66	1/1493 (0.1%)
71	UU	0.39	0/805	0.64	0/1081
72	VV	0.55	0/643	0.64	0/860
73	WW	0.57	0/1051	0.69	0/1406

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
74	XX	0.54	0/1116	0.64	0/1490
75	YY	0.42	0/1028	0.64	0/1366
76	ZZ	0.42	0/604	0.69	0/810
77	aa	0.53	0/828	0.63	0/1109
78	bb	0.43	0/665	0.67	0/891
79	cc	0.46	0/490	0.68	0/656
80	dd	0.53	0/470	0.68	1/623 (0.2%)
81	ee	0.43	0/447	0.59	0/587
82	ff	0.88	3/567 (0.5%)	1.35	8/753 (1.1%)
83	gg	0.38	0/2493	0.68	1/3394 (0.0%)
All	All	0.84	44/228364 (0.0%)	1.08	1354/334975 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
8	B	0	1
9	C	0	2
10	D	0	1
13	G	0	1
14	H	0	1
19	N	0	3
25	T	0	1
30	Y	0	1
33	b	0	1
35	d	0	1
46	o	0	1
49	u	0	3
51	AA	0	2
63	MM	0	1
65	OO	0	1
69	SS	0	1
70	TT	0	1
71	UU	0	1
72	VV	0	1
73	WW	0	1
74	XX	0	1
82	ff	0	6
All	All	0	33

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	9	1287	A	N9-C4	12.29	1.45	1.37
50	9	1287	A	N7-C5	-10.18	1.33	1.39
50	9	1286	G	C5'-C4'	9.64	1.62	1.51
50	9	1287	A	P-O5'	8.68	1.68	1.59
50	9	1286	G	C3'-O3'	8.59	1.54	1.42
50	9	1287	A	C5'-C4'	8.49	1.61	1.51
50	9	1286	G	C4'-C3'	8.39	1.62	1.53
50	9	1287	A	N9-C8	-8.29	1.31	1.37
50	9	1286	G	O3'-P	8.25	1.71	1.61
50	9	1504	U	C5-C6	-7.66	1.27	1.34
50	9	1287	A	C5-C4	7.65	1.44	1.38
50	9	1307	U	C2-N3	7.61	1.43	1.37
82	ff	97	LYS	CD-CE	-7.41	1.32	1.51
82	ff	97	LYS	CB-CG	-7.22	1.33	1.52
50	9	1286	G	P-O5'	6.96	1.66	1.59
28	W	13	ILE	C-N	-6.61	1.18	1.34
50	9	1285	G	O3'-P	6.50	1.69	1.61
50	9	1314	U	C4-O4	-6.15	1.18	1.23
50	9	1307	U	N1-C6	-5.95	1.32	1.38
50	9	1504	U	N1-C2	5.84	1.43	1.38
50	9	1324	G	C6-O6	-5.84	1.18	1.24
50	9	1504	U	N1-C6	-5.75	1.32	1.38
82	ff	99	LYS	CB-CG	5.71	1.68	1.52
50	9	1287	A	C8-N7	-5.64	1.27	1.31
50	9	1306	U	C2-O2	-5.57	1.17	1.22
50	9	1285	G	P-O5'	5.42	1.65	1.59
50	9	1283	C	O3'-P	5.38	1.67	1.61
4	5	4488	A	N9-C4	-5.37	1.34	1.37
50	9	1284	A	C3'-O3'	5.33	1.49	1.42
50	9	1324	G	C5-C4	-5.29	1.34	1.38
50	9	1506	A	C6-N6	-5.26	1.29	1.33
50	9	1824	A	N9-C4	5.24	1.41	1.37
4	5	3871	A	N7-C5	-5.22	1.36	1.39
50	9	1285	G	C3'-O3'	5.20	1.49	1.42
4	5	1337	A	N9-C4	-5.20	1.34	1.37
4	5	1890	G	N9-C4	-5.19	1.33	1.38
4	5	1502	G	N9-C4	-5.17	1.33	1.38
4	5	4538	G	N7-C5	-5.16	1.36	1.39
50	9	1504	U	C4-C5	-5.16	1.39	1.43
51	AA	76	VAL	CB-CG1	-5.14	1.42	1.52
50	9	1506	A	N1-C2	-5.14	1.29	1.34
50	9	1285	G	C5'-C4'	5.13	1.57	1.51
50	9	1834	A	N7-C5	-5.10	1.36	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	O	27	VAL	CB-CG1	-5.00	1.42	1.52

All (1354) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	9	1287	A	N7-C8-N9	38.37	132.99	113.80
50	9	1287	A	C8-N9-C4	-37.37	90.85	105.80
50	9	1307	U	C5-C6-N1	32.51	138.95	122.70
50	9	1307	U	C6-N1-C2	-22.81	107.32	121.00
50	9	1504	U	C5-C4-O4	-20.00	113.90	125.90
50	9	1287	A	C5-N7-C8	-17.08	95.36	103.90
50	9	1287	A	C4-C5-C6	16.31	125.16	117.00
50	9	1324	G	C5-C6-N1	15.20	119.10	111.50
50	9	1287	A	C4-N9-C1'	15.01	153.32	126.30
50	9	1308	U	O4'-C1'-N1	14.39	119.72	108.20
50	9	1287	A	N3-C4-C5	-14.09	116.94	126.80
50	9	501	C	C2-N1-C1'	13.95	134.15	118.80
50	9	1504	U	N3-C2-O2	-13.30	112.89	122.20
50	9	1307	U	C2-N1-C1'	12.83	133.10	117.70
50	9	1306	U	C6-N1-C2	-12.51	113.49	121.00
50	9	501	C	N1-C2-O2	12.39	126.33	118.90
50	9	1324	G	C6-N1-C2	-12.32	117.71	125.10
4	5	2505	C	C6-N1-C2	-12.29	115.39	120.30
50	9	1504	U	N3-C4-O4	12.17	127.92	119.40
50	9	1287	A	C6-C5-N7	-11.99	123.90	132.30
50	9	1453	C	C2-N1-C1'	11.94	131.93	118.80
50	9	1324	G	C5-C6-O6	-11.90	121.46	128.60
50	9	1503	C	N1-C2-O2	11.84	126.00	118.90
50	9	1504	U	N1-C2-O2	11.80	131.06	122.80
50	9	1309	C	C5-C6-N1	11.74	126.87	121.00
4	5	2505	C	N3-C2-O2	-11.73	113.69	121.90
4	5	4056	A	OP1-P-O3'	-11.63	79.61	105.20
50	9	1535	U	C2-N1-C1'	11.60	131.62	117.70
4	5	1079	C	N1-C2-O2	11.54	125.82	118.90
4	5	2505	C	N1-C2-O2	11.40	125.74	118.90
50	9	1504	U	C2-N1-C1'	11.40	131.38	117.70
50	9	1307	U	N3-C4-O4	11.15	127.20	119.40
50	9	1506	A	N1-C6-N6	-11.09	111.94	118.60
50	9	1307	U	O4'-C1'-N1	10.92	116.93	108.20
50	9	1314	U	N3-C4-C5	10.91	121.14	114.60
2	2	20	U	C2-N1-C1'	10.83	130.70	117.70
50	9	1306	U	N3-C2-O2	-10.80	114.64	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	9	1453	C	N1-C2-O2	10.64	125.28	118.90
50	9	1303	C	N1-C2-O2	10.45	125.17	118.90
2	2	20	U	N1-C2-O2	10.39	130.07	122.80
4	5	100	C	C2-N1-C1'	10.32	130.16	118.80
50	9	1139	C	N1-C2-O2	10.27	125.06	118.90
50	9	1506	A	C5-C6-N1	10.27	122.83	117.70
4	5	3788	C	N1-C2-O2	10.17	125.00	118.90
50	9	1261	C	N3-C2-O2	-10.15	114.80	121.90
50	9	1286	G	P-O3'-C3'	10.04	131.75	119.70
50	9	1314	U	N3-C4-O4	-10.00	112.40	119.40
4	5	1978	C	N1-C2-O2	9.94	124.86	118.90
50	9	1116	C	N1-C2-O2	9.93	124.86	118.90
50	9	853	C	N1-C2-O2	9.91	124.85	118.90
50	9	1116	C	C2-N1-C1'	9.88	129.67	118.80
50	9	501	C	C6-N1-C1'	-9.86	108.97	120.80
50	9	1261	C	N1-C2-O2	9.84	124.80	118.90
4	5	1639	U	C2-N1-C1'	9.82	129.49	117.70
50	9	1271	C	N1-C2-O2	9.71	124.72	118.90
4	5	4119	C	C2-N1-C1'	9.68	129.45	118.80
50	9	1307	U	N3-C4-C5	-9.68	108.79	114.60
50	9	1317	C	O5'-P-OP1	-9.68	96.99	105.70
50	9	1520	G	N3-C4-C5	-9.64	123.78	128.60
50	9	1306	U	C2-N1-C1'	9.61	129.23	117.70
2	2	20	U	N3-C2-O2	-9.55	115.51	122.20
50	9	1316	C	N1-C2-O2	9.53	124.62	118.90
50	9	1060	A	O4'-C1'-N9	9.51	115.81	108.20
4	5	4942	C	N1-C2-O2	9.49	124.59	118.90
4	5	1079	C	N3-C2-O2	-9.48	115.26	121.90
50	9	1139	C	N3-C2-O2	-9.44	115.29	121.90
50	9	1287	A	N3-C4-N9	9.41	134.93	127.40
50	9	914	U	C2-N1-C1'	9.39	128.97	117.70
50	9	1506	A	C2-N3-C4	9.38	115.29	110.60
50	9	853	C	N3-C2-O2	-9.37	115.34	121.90
50	9	501	C	N3-C2-O2	-9.36	115.35	121.90
4	5	4942	C	N3-C2-O2	-9.34	115.36	121.90
50	9	1287	A	N1-C2-N3	9.31	133.95	129.30
4	5	521	C	N3-C2-O2	-9.30	115.39	121.90
4	5	1612	G	N3-C4-N9	9.29	131.57	126.00
4	5	4303	C	C2-N1-C1'	9.29	129.02	118.80
50	9	1323	U	C5-C4-O4	-9.21	120.38	125.90
50	9	1314	U	C2-N3-C4	-9.20	121.48	127.00
50	9	1287	A	P-O5'-C5'	9.16	135.56	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	9	1300	U	C2-N1-C1'	9.15	128.68	117.70
50	9	183	G	C2-N3-C4	9.13	116.46	111.90
50	9	1535	U	N1-C2-O2	9.10	129.17	122.80
50	9	1520	G	C2-N3-C4	9.07	116.43	111.90
50	9	853	C	C2-N1-C1'	9.05	128.75	118.80
50	9	1289	U	C5-C4-O4	-9.01	120.49	125.90
50	9	1303	C	N3-C2-O2	-8.99	115.60	121.90
4	5	2022	C	N1-C2-O2	8.97	124.28	118.90
6	8	128	C	N1-C2-O2	8.96	124.28	118.90
82	ff	100	LEU	CA-CB-CG	8.90	135.78	115.30
53	CC	175	GLY	C-N-CA	8.87	143.88	121.70
50	9	356	C	N1-C2-O2	8.87	124.22	118.90
50	9	350	C	N1-C2-O2	8.83	124.20	118.90
50	9	1284	A	O4'-C1'-N9	-8.81	101.15	108.20
4	5	4303	C	N1-C2-O2	8.81	124.19	118.90
4	5	1485	C	N1-C2-O2	8.80	124.18	118.90
50	9	1453	C	N3-C2-O2	-8.78	115.75	121.90
4	5	1882	U	C5-C4-O4	-8.76	120.64	125.90
4	5	1079	C	C6-N1-C2	-8.74	116.80	120.30
4	5	1079	C	C2-N1-C1'	8.74	128.41	118.80
4	5	691	C	C2-N1-C1'	8.73	128.41	118.80
50	9	1453	C	C6-N1-C1'	-8.72	110.33	120.80
50	9	1139	C	C2-N1-C1'	8.71	128.38	118.80
50	9	1504	U	C2-N3-C4	-8.70	121.78	127.00
50	9	1286	G	C5'-C4'-C3'	8.68	129.89	116.00
50	9	501	C	C5-C6-N1	8.68	125.34	121.00
50	9	1503	C	N3-C2-O2	-8.68	115.83	121.90
50	9	1300	U	N1-C2-O2	8.66	128.86	122.80
50	9	1504	U	C6-N1-C1'	-8.64	109.10	121.20
4	5	4653	C	C6-N1-C2	-8.64	116.84	120.30
50	9	1306	U	C5-C6-N1	8.62	127.01	122.70
50	9	501	C	C6-N1-C2	-8.62	116.85	120.30
5	7	67	C	C6-N1-C2	-8.61	116.86	120.30
4	5	4119	C	N1-C2-O2	8.60	124.06	118.90
4	5	100	C	N1-C2-O2	8.59	124.05	118.90
50	9	293	C	N1-C2-O2	8.52	124.01	118.90
4	5	100	C	N3-C2-O2	-8.49	115.96	121.90
50	9	1535	U	N3-C2-O2	-8.46	116.28	122.20
50	9	1283	C	C6-N1-C2	-8.46	116.92	120.30
50	9	1624	U	C2-N1-C1'	8.46	127.85	117.70
50	9	1865	C	C6-N1-C2	-8.46	116.92	120.30
4	5	112	C	C2-N1-C1'	8.45	128.10	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	9	356	C	C2-N1-C1'	8.44	128.08	118.80
50	9	1364	U	N1-C2-O2	8.32	128.62	122.80
4	5	2819	U	N3-C2-O2	-8.30	116.39	122.20
4	5	2627	C	N1-C2-O2	8.29	123.87	118.90
5	7	67	C	C5-C6-N1	8.26	125.13	121.00
4	5	4162	C	N1-C2-O2	8.22	123.83	118.90
50	9	1306	U	N1-C2-N3	8.18	119.81	114.90
50	9	1397	U	N3-C2-O2	-8.17	116.48	122.20
4	5	1084	C	C2-N1-C1'	8.17	127.79	118.80
4	5	1612	G	C4-N9-C1'	8.16	137.11	126.50
50	9	1520	G	C8-N9-C4	-8.16	103.13	106.40
4	5	1612	G	C8-N9-C1'	-8.16	116.39	127.00
50	9	632	C	C6-N1-C2	-8.16	117.04	120.30
2	2	31	C	C2-N1-C1'	8.15	127.76	118.80
50	9	124	U	N1-C2-O2	8.15	128.50	122.80
4	5	220	C	N1-C2-O2	8.14	123.78	118.90
4	5	1309	C	C5-C6-N1	8.14	125.07	121.00
50	9	124	U	C2-N1-C1'	8.13	127.46	117.70
4	5	1429	C	N1-C2-O2	8.12	123.77	118.90
4	5	685	C	O5'-P-OP2	-8.11	98.40	105.70
4	5	49	U	N1-C2-O2	8.09	128.47	122.80
4	5	4759	C	N1-C2-O2	8.07	123.74	118.90
4	5	1309	C	C6-N1-C2	-8.05	117.08	120.30
50	9	1535	U	C6-N1-C1'	-8.06	109.92	121.20
4	5	1686	C	C6-N1-C2	-8.04	117.08	120.30
4	5	1978	C	N3-C2-O2	-8.04	116.27	121.90
50	9	1364	U	N3-C2-O2	-8.04	116.57	122.20
4	5	2351	C	C6-N1-C2	-8.04	117.09	120.30
50	9	1261	C	C6-N1-C2	-8.03	117.09	120.30
50	9	1303	C	C2-N1-C1'	8.03	127.63	118.80
4	5	1429	C	C2-N1-C1'	8.00	127.60	118.80
4	5	2410	C	C2-N1-C1'	7.98	127.58	118.80
4	5	1236	C	C6-N1-C2	-7.96	117.11	120.30
4	5	2028	C	C2-N1-C1'	7.88	127.47	118.80
4	5	3788	C	N3-C2-O2	-7.88	116.38	121.90
82	ff	99	LYS	CA-CB-CG	7.87	130.72	113.40
4	5	2022	C	N3-C2-O2	-7.86	116.40	121.90
6	8	4	C	C5-C6-N1	7.79	124.90	121.00
4	5	2627	C	C6-N1-C2	-7.79	117.18	120.30
50	9	1364	U	C2-N1-C1'	7.77	127.02	117.70
4	5	1485	C	C2-N1-C1'	7.74	127.31	118.80
50	9	1292	C	C6-N1-C2	-7.72	117.21	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5	4695	C	N1-C2-O2	7.72	123.53	118.90
50	9	183	G	N3-C4-C5	-7.72	124.74	128.60
4	5	2683	C	C6-N1-C2	-7.72	117.21	120.30
50	9	1289	U	N3-C4-O4	7.72	124.80	119.40
4	5	4880	C	C2-N1-C1'	7.71	127.28	118.80
4	5	4041	C	N1-C2-O2	7.71	123.52	118.90
6	8	21	C	C5-C6-N1	7.71	124.85	121.00
50	9	319	C	O5'-P-OP1	7.70	119.94	110.70
4	5	934	C	C6-N1-C2	-7.68	117.23	120.30
4	5	1084	C	C5-C6-N1	7.68	124.84	121.00
4	5	1429	C	C5-C6-N1	7.67	124.84	121.00
4	5	2667	C	N1-C2-O2	7.67	123.50	118.90
4	5	2837	U	N3-C2-O2	-7.67	116.83	122.20
50	9	293	C	C2-N1-C1'	7.66	127.23	118.80
4	5	220	C	C2-N1-C1'	7.66	127.22	118.80
50	9	1287	A	C6-N1-C2	-7.66	114.01	118.60
50	9	1116	C	N3-C2-O2	-7.64	116.55	121.90
50	9	1016	U	N3-C2-O2	-7.63	116.86	122.20
50	9	1265	A	O4'-C1'-N9	7.62	114.30	108.20
4	5	2505	C	C5-C6-N1	7.62	124.81	121.00
50	9	124	U	N3-C2-O2	-7.59	116.89	122.20
4	5	4162	C	C2-N1-C1'	7.57	127.13	118.80
4	5	4266	G	N3-C4-C5	-7.56	124.82	128.60
50	9	1287	A	OP1-P-OP2	-7.56	108.26	119.60
4	5	1777	C	C2-N1-C1'	7.55	127.11	118.80
6	8	21	C	C6-N1-C2	-7.53	117.29	120.30
4	5	1792	U	C2-N1-C1'	7.53	126.73	117.70
50	9	183	G	C8-N9-C4	-7.53	103.39	106.40
6	8	4	C	C6-N1-C2	-7.52	117.29	120.30
50	9	1325	G	C5-C6-N1	7.52	115.26	111.50
50	9	1300	U	N3-C2-O2	-7.51	116.94	122.20
50	9	1314	U	N3-C2-O2	-7.51	116.95	122.20
4	5	4653	C	C5-C6-N1	7.50	124.75	121.00
4	5	2704	C	C2-N1-C1'	7.50	127.05	118.80
4	5	2046	G	P-O3'-C3'	7.49	128.69	119.70
50	9	1315	U	N3-C2-O2	-7.49	116.96	122.20
6	8	128	C	N3-C2-O2	-7.47	116.67	121.90
4	5	100	C	C6-N1-C1'	-7.46	111.84	120.80
4	5	323	C	C6-N1-C2	-7.45	117.32	120.30
4	5	4423	U	C2-N1-C1'	7.45	126.64	117.70
50	9	1389	C	C2-N1-C1'	7.45	126.99	118.80
50	9	1310	U	C5-C6-N1	7.44	126.42	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5	4667	C	C6-N1-C2	-7.43	117.33	120.30
4	5	1686	C	C5-C6-N1	7.43	124.72	121.00
50	9	1624	U	N3-C2-O2	-7.43	117.00	122.20
4	5	2819	U	N1-C2-O2	7.42	128.00	122.80
5	7	29	C	C2-N1-C1'	7.42	126.97	118.80
50	9	1305	C	C2-N1-C1'	7.42	126.97	118.80
50	9	1397	U	N1-C2-O2	7.42	128.00	122.80
4	5	1484	G	C4-N9-C1'	7.42	136.14	126.50
50	9	1824	A	C2-N3-C4	7.42	114.31	110.60
4	5	1484	G	N3-C4-C5	-7.41	124.90	128.60
50	9	1261	C	C2-N1-C1'	7.39	126.93	118.80
4	5	4928	C	C2-N1-C1'	7.37	126.91	118.80
4	5	1084	C	C6-N1-C2	-7.37	117.35	120.30
4	5	1847	C	C2-N1-C1'	7.36	126.89	118.80
4	5	4303	C	N3-C2-O2	-7.35	116.75	121.90
2	2	61	C	C2-N1-C1'	7.35	126.89	118.80
50	9	494	C	N1-C2-O2	7.35	123.31	118.90
50	9	914	U	C6-N1-C1'	-7.35	110.91	121.20
50	9	1118	C	C2-N1-C1'	7.34	126.88	118.80
4	5	2281	U	N1-C2-O2	7.34	127.94	122.80
4	5	2405	G	N3-C4-N9	7.33	130.40	126.00
50	9	1290	G	N7-C8-N9	7.33	116.77	113.10
3	4	63	C	C2-N1-C1'	7.33	126.86	118.80
82	ff	97	LYS	CB-CG-CD	-7.33	92.55	111.60
4	5	1612	G	C6-C5-N7	-7.32	126.01	130.40
4	5	1514	U	N3-C2-O2	-7.32	117.08	122.20
50	9	853	C	C6-N1-C2	-7.31	117.38	120.30
50	9	914	U	C5-C4-O4	-7.31	121.52	125.90
50	9	1305	C	N1-C2-O2	7.30	123.28	118.90
4	5	4266	G	N3-C4-N9	7.30	130.38	126.00
4	5	4423	U	N3-C2-O2	-7.29	117.10	122.20
4	5	2627	C	N3-C2-O2	-7.29	116.80	121.90
4	5	4162	C	N3-C2-O2	-7.29	116.80	121.90
4	5	1484	G	N3-C4-N9	7.28	130.37	126.00
50	9	1289	U	C2-N1-C1'	7.28	126.44	117.70
4	5	3876	A	P-O3'-C3'	7.27	128.43	119.70
4	5	4413	C	C2-N1-C1'	7.27	126.80	118.80
50	9	1624	U	N1-C2-O2	7.27	127.89	122.80
4	5	1325	C	N3-C2-O2	-7.26	116.82	121.90
4	5	1446	C	C5-C6-N1	7.26	124.63	121.00
4	5	2772	C	C6-N1-C2	-7.25	117.40	120.30
4	5	4258	C	C5-C6-N1	7.24	124.62	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5	704	C	N1-C2-O2	7.24	123.24	118.90
6	8	141	C	C5-C6-N1	7.24	124.62	121.00
4	5	4682	U	N3-C2-O2	-7.23	117.14	122.20
50	9	1161	U	N3-C2-O2	-7.23	117.14	122.20
4	5	4266	G	C4-N9-C1'	7.22	135.89	126.50
4	5	49	U	N3-C2-O2	-7.22	117.15	122.20
4	5	2072	C	C6-N1-C2	-7.21	117.42	120.30
4	5	521	C	N1-C2-O2	7.21	123.23	118.90
50	9	1315	U	C2-N1-C1'	7.20	126.34	117.70
4	5	1381	U	N3-C2-O2	-7.19	117.17	122.20
50	9	350	C	N3-C2-O2	-7.19	116.87	121.90
4	5	4759	C	N3-C2-O2	-7.18	116.87	121.90
50	9	1116	C	C6-N1-C1'	-7.18	112.18	120.80
4	5	4964	C	N3-C2-O2	-7.18	116.87	121.90
4	5	691	C	C6-N1-C2	-7.17	117.43	120.30
3	4	66	U	N1-C2-O2	7.17	127.82	122.80
50	9	188	C	C2-N1-C1'	7.16	126.67	118.80
4	5	4056	A	OP2-P-O3'	-7.14	89.48	105.20
50	9	350	C	C6-N1-C2	-7.14	117.44	120.30
4	5	2838	G	C4-N9-C1'	7.14	135.78	126.50
4	5	1468	C	C6-N1-C2	-7.13	117.45	120.30
4	5	2820	C	N1-C2-O2	7.13	123.18	118.90
50	9	632	C	C2-N1-C1'	7.13	126.64	118.80
4	5	1445	U	C5-C6-N1	7.12	126.26	122.70
4	5	2505	C	C2-N1-C1'	7.11	126.62	118.80
4	5	1481	C	N1-C2-O2	7.10	123.16	118.90
50	9	1290	G	C6-C5-N7	-7.09	126.14	130.40
4	5	2407	G	C4-N9-C1'	7.09	135.72	126.50
50	9	356	C	N3-C2-O2	-7.08	116.94	121.90
50	9	1520	G	C4-N9-C1'	7.07	135.69	126.50
4	5	1663	C	C5-C6-N1	7.05	124.53	121.00
4	5	3926	C	C6-N1-C2	-7.05	117.48	120.30
4	5	4879	C	C6-N1-C2	-7.05	117.48	120.30
4	5	4502	C	N1-C2-O2	7.05	123.13	118.90
4	5	2281	U	N3-C2-O2	-7.04	117.28	122.20
4	5	3911	C	C5-C6-N1	7.04	124.52	121.00
2	2	20	U	C6-N1-C1'	-7.03	111.36	121.20
4	5	4759	C	C2-N1-C1'	7.02	126.52	118.80
50	9	55	U	C2-N1-C1'	7.02	126.12	117.70
50	9	1139	C	C6-N1-C2	-7.02	117.49	120.30
4	5	1893	C	C2-N1-C1'	7.00	126.50	118.80
50	9	1308	U	C2-N1-C1'	-7.00	109.30	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5	472	C	N1-C2-O2	7.00	123.10	118.90
50	9	1751	C	N1-C2-O2	7.00	123.10	118.90
4	5	4560	C	N3-C2-O2	-6.99	117.01	121.90
50	9	1755	C	C6-N1-C2	-6.99	117.51	120.30
50	9	1315	U	N1-C2-O2	6.98	127.69	122.80
4	5	2695	A	P-O3'-C3'	6.98	128.07	119.70
4	5	2362	U	C2-N1-C1'	6.96	126.06	117.70
4	5	4925	U	P-O3'-C3'	6.95	128.04	119.70
4	5	3767	C	C5-C6-N1	6.95	124.47	121.00
4	5	3778	U	N1-C2-O2	6.95	127.66	122.80
50	9	1057	C	N3-C2-O2	-6.95	117.04	121.90
4	5	2856	C	N1-C2-O2	6.93	123.06	118.90
4	5	1978	C	C2-N1-C1'	6.92	126.41	118.80
4	5	7	C	C5-C6-N1	6.91	124.46	121.00
4	5	4119	C	C6-N1-C1'	-6.90	112.52	120.80
50	9	1309	C	C4-C5-C6	-6.90	113.95	117.40
50	9	1286	G	P-O5'-C5'	6.90	131.94	120.90
4	5	1882	U	N3-C4-O4	6.89	124.22	119.40
4	5	4303	C	C6-N1-C1'	-6.89	112.54	120.80
4	5	4155	C	N1-C2-O2	6.88	123.03	118.90
50	9	105	U	N3-C2-O2	-6.88	117.38	122.20
4	5	4869	U	C2-N1-C1'	6.88	125.96	117.70
4	5	4233	A	O5'-P-OP1	-6.87	99.51	105.70
4	5	1828	C	C6-N1-C2	-6.87	117.55	120.30
4	5	2325	C	N3-C2-O2	-6.86	117.10	121.90
50	9	55	U	N1-C2-O2	6.86	127.60	122.80
4	5	2072	C	C5-C6-N1	6.86	124.43	121.00
50	9	1590	C	N1-C2-O2	6.85	123.01	118.90
50	9	26	U	C5-C6-N1	6.84	126.12	122.70
4	5	2627	C	C2-N1-C1'	6.83	126.32	118.80
4	5	1632	A	C2-N3-C4	6.83	114.01	110.60
50	9	494	C	N3-C2-O2	-6.83	117.12	121.90
2	2	31	C	N1-C2-O2	6.82	122.99	118.90
4	5	1079	C	C5-C6-N1	6.81	124.41	121.00
4	5	4964	C	N1-C2-O2	6.81	122.99	118.90
6	8	64	U	N3-C2-O2	-6.81	117.43	122.20
50	9	632	C	C5-C6-N1	6.80	124.40	121.00
4	5	1485	C	N3-C2-O2	-6.80	117.14	121.90
50	9	1111	U	N3-C2-O2	-6.79	117.44	122.20
50	9	1503	C	C2-N1-C1'	6.77	126.25	118.80
4	5	1607	C	N3-C2-O2	-6.77	117.16	121.90
4	5	1847	C	C6-N1-C2	-6.77	117.59	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	9	1287	A	C8-N9-C1'	-6.77	115.52	127.70
50	9	1314	U	C6-N1-C1'	-6.76	111.73	121.20
4	5	4695	C	C2-N1-C1'	6.76	126.24	118.80
50	9	1316	C	N3-C2-O2	-6.75	117.17	121.90
4	5	112	C	N1-C2-O2	6.75	122.95	118.90
4	5	2683	C	C5-C6-N1	6.74	124.37	121.00
50	9	293	C	N3-C2-O2	-6.74	117.18	121.90
50	9	1130	G	C2-N3-C4	6.74	115.27	111.90
4	5	1639	U	N3-C2-O2	-6.73	117.49	122.20
50	9	1314	U	N1-C2-O2	6.73	127.51	122.80
50	9	1271	C	C5-C6-N1	6.72	124.36	121.00
4	5	4949	G	O4'-C1'-N9	6.72	113.58	108.20
50	9	350	C	C5-C6-N1	6.71	124.36	121.00
4	5	1469	C	C6-N1-C2	-6.71	117.62	120.30
4	5	1481	C	C2-N1-C1'	6.71	126.18	118.80
4	5	1329	G	C8-N9-C4	-6.71	103.72	106.40
50	9	1057	C	C2-N1-C1'	6.70	126.17	118.80
50	9	1551	U	C2-N1-C1'	6.70	125.74	117.70
4	5	4229	U	N3-C2-O2	-6.69	117.52	122.20
50	9	1309	C	C6-N1-C2	-6.69	117.62	120.30
4	5	1847	C	C5-C6-N1	6.69	124.34	121.00
4	5	2274	C	N1-C2-O2	6.68	122.91	118.90
4	5	672	C	N1-C2-O2	6.67	122.91	118.90
70	TT	118	ASP	CB-CG-OD1	6.67	124.30	118.30
4	5	4206	C	C6-N1-C2	-6.67	117.63	120.30
50	9	1218	C	C5-C6-N1	6.67	124.33	121.00
4	5	2837	U	N1-C2-O2	6.66	127.46	122.80
50	9	1281	G	C4-N9-C1'	6.66	135.15	126.50
4	5	2704	C	N1-C2-O2	6.65	122.89	118.90
4	5	1072	C	P-O3'-C3'	6.64	127.67	119.70
4	5	2667	C	N3-C2-O2	-6.64	117.25	121.90
4	5	1429	C	C6-N1-C2	-6.64	117.64	120.30
50	9	130	G	C4-N9-C1'	6.64	135.13	126.50
4	5	282	C	N1-C2-O2	6.63	122.88	118.90
4	5	4723	A	C2-N3-C4	6.63	113.92	110.60
4	5	1607	C	N1-C2-O2	6.63	122.88	118.90
6	8	135	C	C2-N1-C1'	6.63	126.09	118.80
4	5	2351	C	C5-C6-N1	6.63	124.31	121.00
4	5	4880	C	N3-C2-O2	-6.63	117.26	121.90
4	5	1340	C	C5-C6-N1	6.62	124.31	121.00
4	5	1445	U	C2-N1-C1'	6.62	125.64	117.70
4	5	4119	C	N3-C2-O2	-6.62	117.27	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5	4682	U	N1-C2-O2	6.62	127.43	122.80
50	9	1298	G	N3-C4-N9	6.61	129.97	126.00
4	5	4075	U	OP1-P-O3'	6.61	119.74	105.20
50	9	189	U	C2-N1-C1'	6.61	125.63	117.70
4	5	4942	C	C2-N1-C1'	6.61	126.07	118.80
4	5	2528	G	N3-C4-N9	6.60	129.96	126.00
50	9	1130	G	N3-C4-C5	-6.60	125.30	128.60
69	SS	45	LEU	CA-CB-CG	6.59	130.47	115.30
50	9	1325	G	N3-C4-N9	6.59	129.96	126.00
4	5	4051	C	N1-C2-O2	6.59	122.85	118.90
3	4	66	U	N3-C2-O2	-6.57	117.60	122.20
4	5	112	C	C6-N1-C2	-6.57	117.67	120.30
50	9	494	C	C6-N1-C2	-6.57	117.67	120.30
6	8	141	C	C6-N1-C2	-6.57	117.67	120.30
4	5	1828	C	C5-C6-N1	6.56	124.28	121.00
6	8	21	C	C2-N1-C1'	6.55	126.01	118.80
4	5	2407	G	C8-N9-C1'	-6.55	118.49	127.00
4	5	4924	C	N3-C2-O2	-6.55	117.31	121.90
50	9	1293	A	C8-N9-C4	6.55	108.42	105.80
50	9	1520	G	N3-C4-N9	6.54	129.92	126.00
50	9	1660	C	N3-C2-O2	-6.54	117.32	121.90
4	5	2528	G	C4-N9-C1'	6.53	135.00	126.50
50	9	43	U	N3-C2-O2	-6.53	117.63	122.20
50	9	457	C	C6-N1-C2	-6.53	117.69	120.30
50	9	898	U	C2-N1-C1'	6.53	125.53	117.70
50	9	752	G	P-O3'-C3'	6.53	127.53	119.70
4	5	2532	C	C2-N1-C1'	6.52	125.98	118.80
4	5	4041	C	N3-C2-O2	-6.52	117.33	121.90
50	9	1506	A	N7-C8-N9	6.51	117.06	113.80
4	5	4695	C	N3-C2-O2	-6.51	117.34	121.90
4	5	1411(B)	C	N3-C2-O2	-6.51	117.34	121.90
50	9	1306	U	C5-C4-O4	6.50	129.80	125.90
50	9	1111	U	N1-C2-O2	6.49	127.34	122.80
50	9	1453	C	C6-N1-C2	-6.49	117.70	120.30
50	9	688	U	P-O3'-C3'	6.48	127.48	119.70
4	5	118	C	C2-N1-C1'	6.48	125.93	118.80
50	9	1289	U	C5-C6-N1	6.48	125.94	122.70
4	5	1656	U	N1-C2-O2	6.47	127.33	122.80
4	5	472	C	C2-N1-C1'	6.47	125.92	118.80
50	9	1591	C	N1-C2-O2	6.47	122.78	118.90
4	5	2407	G	N3-C4-N9	6.47	129.88	126.00
4	5	2362	U	N3-C2-O2	-6.46	117.68	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5	4254	G	N3-C4-C5	-6.46	125.37	128.60
50	9	1389	C	N1-C2-O2	6.46	122.78	118.90
2	2	31	C	C6-N1-C2	-6.46	117.72	120.30
50	9	314	U	N3-C2-O2	-6.45	117.68	122.20
50	9	1262	C	N1-C2-O2	6.45	122.77	118.90
3	4	66	U	C2-N1-C1'	6.45	125.44	117.70
4	5	2008	U	C2-N1-C1'	6.45	125.44	117.70
50	9	369	C	N1-C2-O2	6.45	122.77	118.90
50	9	958	G	C4-N9-C1'	6.45	134.89	126.50
4	5	1994	C	N3-C2-O2	-6.45	117.39	121.90
50	9	1303	C	C6-N1-C2	-6.45	117.72	120.30
4	5	4065	G	P-O3'-C3'	6.44	127.42	119.70
4	5	115	C	C2-N1-C1'	6.44	125.88	118.80
4	5	126	C	C2-N1-C1'	6.43	125.88	118.80
4	5	1612	G	N3-C4-C5	-6.43	125.39	128.60
4	5	4057	C	OP1-P-OP2	6.43	129.24	119.60
50	9	579	C	N1-C2-O2	6.43	122.76	118.90
4	5	1568	C	C2-N1-C1'	6.42	125.86	118.80
4	5	1395	U	C6-N1-C2	-6.42	117.15	121.00
4	5	3775	A	N7-C8-N9	6.41	117.01	113.80
4	5	4206	C	C2-N1-C1'	6.41	125.86	118.80
82	ff	99	LYS	CD-CE-NZ	6.41	126.45	111.70
50	9	183	G	N3-C2-N2	-6.41	115.42	119.90
2	2	31	C	C5-C6-N1	6.40	124.20	121.00
4	5	417	G	O4'-C1'-N9	6.40	113.32	108.20
50	9	1506	A	N3-C4-N9	6.40	132.52	127.40
4	5	2772	C	C5-C6-N1	6.40	124.20	121.00
50	9	1362	U	N1-C2-O2	6.40	127.28	122.80
4	5	3636	C	N3-C2-O2	-6.39	117.43	121.90
5	7	28	C	C6-N1-C2	-6.39	117.74	120.30
50	9	1057	C	N1-C2-O2	6.39	122.74	118.90
4	5	1639	U	N1-C2-O2	6.39	127.27	122.80
4	5	4402	C	C6-N1-C2	-6.39	117.74	120.30
4	5	4258	C	C6-N1-C2	-6.38	117.75	120.30
4	5	250	C	C6-N1-C2	-6.38	117.75	120.30
4	5	4193	C	C2-N1-C1'	6.37	125.81	118.80
50	9	1834	A	N7-C8-N9	6.37	116.99	113.80
4	5	2532	C	C5-C6-N1	6.37	124.18	121.00
4	5	2059	C	C6-N1-C2	-6.37	117.75	120.30
50	9	1308	U	P-O3'-C3'	6.37	127.34	119.70
5	7	92	C	C6-N1-C2	-6.36	117.75	120.30
4	5	4401	G	C4-N9-C1'	6.36	134.77	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	9	1282	A	C8-N9-C4	-6.36	103.26	105.80
4	5	220	C	C6-N1-C2	-6.35	117.76	120.30
4	5	1893	C	C5-C6-N1	6.35	124.17	121.00
4	5	2362	U	N1-C2-O2	6.34	127.24	122.80
4	5	4360	U	N3-C2-O2	-6.34	117.76	122.20
50	9	130	G	N3-C4-C5	-6.34	125.43	128.60
4	5	1468	C	C5-C6-N1	6.34	124.17	121.00
50	9	636	C	C5-C6-N1	6.34	124.17	121.00
4	5	4402	C	N1-C2-O2	6.33	122.70	118.90
4	5	4537	C	C6-N1-C2	-6.33	117.77	120.30
4	5	77	U	N3-C2-O2	-6.33	117.77	122.20
4	5	1635	C	C6-N1-C2	-6.33	117.77	120.30
4	5	1791	U	N1-C2-O2	6.33	127.23	122.80
50	9	1300	U	C6-N1-C1'	-6.33	112.34	121.20
50	9	105	U	N1-C2-O2	6.32	127.22	122.80
50	9	118	C	N1-C2-O2	6.31	122.69	118.90
50	9	1325	G	N3-C2-N2	6.31	124.32	119.90
4	5	2008	U	N1-C2-O2	6.31	127.22	122.80
50	9	1259	A	C2-N3-C4	6.31	113.75	110.60
4	5	2037	C	C6-N1-C2	-6.30	117.78	120.30
4	5	2661	U	P-O3'-C3'	6.30	127.26	119.70
4	5	195	C	C6-N1-C2	-6.30	117.78	120.30
4	5	1325	C	N1-C2-O2	6.29	122.68	118.90
4	5	1994	C	N1-C2-O2	6.29	122.67	118.90
50	9	1293	A	C5-N7-C8	6.29	107.04	103.90
4	5	4075	U	P-O3'-C3'	6.29	127.24	119.70
50	9	1293	A	N7-C8-N9	-6.28	110.66	113.80
54	DD	29	LEU	CB-CG-CD2	-6.28	100.32	111.00
4	5	220	C	N3-C2-O2	-6.28	117.50	121.90
4	5	3910	C	C6-N1-C2	-6.28	117.79	120.30
50	9	887	U	C2-N1-C1'	6.28	125.23	117.70
4	5	1514	U	N1-C2-O2	6.27	127.19	122.80
4	5	2008	U	N3-C2-O2	-6.27	117.81	122.20
50	9	1218	C	C6-N1-C2	-6.27	117.79	120.30
50	9	1287	A	C5'-C4'-O4'	6.26	116.62	109.10
50	9	1284	A	N7-C8-N9	6.26	116.93	113.80
4	5	1381	U	N1-C2-O2	6.26	127.18	122.80
50	9	1506	A	N3-C4-C5	-6.25	122.42	126.80
50	9	1564	C	C2-N1-C1'	6.25	125.68	118.80
4	5	661	C	C2-N1-C1'	6.25	125.67	118.80
4	5	719	C	C5-C6-N1	6.25	124.12	121.00
50	9	130	G	N3-C4-N9	6.25	129.75	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5	13	U	N3-C2-O2	-6.24	117.83	122.20
55	EE	189	LEU	CA-CB-CG	6.24	129.66	115.30
4	5	220	C	C5-C6-N1	6.23	124.12	121.00
50	9	1281	G	C8-N9-C1'	-6.23	118.90	127.00
50	9	473	A	OP2-P-O3'	6.23	118.90	105.20
4	5	4286	C	C6-N1-C2	-6.23	117.81	120.30
4	5	4177	C	C6-N1-C2	-6.22	117.81	120.30
50	9	1271	C	N3-C2-O2	-6.22	117.54	121.90
4	5	719	C	C2-N1-C1'	6.22	125.64	118.80
6	8	101	C	C2-N1-C1'	6.22	125.65	118.80
4	5	323	C	C5-C6-N1	6.22	124.11	121.00
50	9	1574	C	C5-C6-N1	6.22	124.11	121.00
4	5	691	C	C5-C6-N1	6.21	124.10	121.00
4	5	4719	G	OP1-P-O3'	6.21	118.85	105.20
4	5	1340	C	C6-N1-C2	-6.21	117.82	120.30
4	5	1990	A	OP1-P-O3'	6.20	118.84	105.20
4	5	323	C	C2-N1-C1'	6.20	125.62	118.80
4	5	1639	U	C6-N1-C1'	-6.20	112.52	121.20
4	5	2571	C	N1-C2-O2	6.19	122.62	118.90
4	5	4398	C	N1-C2-O2	6.19	122.62	118.90
50	9	356	C	C6-N1-C1'	-6.19	113.37	120.80
50	9	729	C	N1-C2-O2	6.18	122.61	118.90
50	9	1730	U	N3-C2-O2	-6.18	117.87	122.20
4	5	1926	C	C5-C6-N1	6.17	124.09	121.00
4	5	3622	C	C6-N1-C2	-6.17	117.83	120.30
50	9	1453	C	C5-C6-N1	6.17	124.08	121.00
50	9	1503	C	C6-N1-C1'	-6.17	113.39	120.80
50	9	1286	G	OP1-P-OP2	-6.16	110.35	119.60
50	9	1157	G	N3-C4-N9	6.15	129.69	126.00
50	9	1324	G	N3-C4-N9	6.15	129.69	126.00
4	5	4766	C	C5-C6-N1	6.15	124.07	121.00
50	9	1326	U	N3-C2-O2	-6.15	117.90	122.20
4	5	4215	C	C6-N1-C2	-6.15	117.84	120.30
50	9	142	C	N1-C2-O2	6.15	122.59	118.90
4	5	406	C	P-O3'-C3'	6.14	127.07	119.70
4	5	4709	U	N1-C2-O2	6.14	127.10	122.80
50	9	1518	C	C2-N1-C1'	6.14	125.55	118.80
50	9	1660	C	N1-C2-O2	6.13	122.58	118.90
4	5	4970	C	C6-N1-C2	-6.13	117.85	120.30
50	9	1172	U	N1-C2-O2	6.13	127.09	122.80
4	5	976	C	C6-N1-C2	-6.13	117.85	120.30
4	5	1210	C	N1-C2-O2	6.13	122.58	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5	1210	C	C2-N1-C1'	6.12	125.54	118.80
4	5	3788	C	C2-N1-C1'	6.12	125.54	118.80
4	5	1484	G	C8-N9-C1'	-6.12	119.04	127.00
2	2	20	U	C5-C6-N1	6.12	125.76	122.70
23	R	99	MET	CA-CB-CG	-6.12	102.90	113.30
50	9	188	C	C6-N1-C2	-6.12	117.85	120.30
4	5	2528	G	N3-C4-C5	-6.11	125.55	128.60
50	9	1307	U	C5'-C4'-O4'	6.11	116.43	109.10
50	9	1161	U	N1-C2-O2	6.11	127.07	122.80
50	9	494	C	C2-N1-C1'	6.10	125.51	118.80
50	9	958	G	O4'-C1'-N9	6.10	113.08	108.20
49	u	179	LEU	CA-CB-CG	6.09	129.31	115.30
4	5	4926	C	C2-N1-C1'	6.09	125.50	118.80
4	5	5016	A	C5-N7-C8	-6.09	100.86	103.90
4	5	1612	G	C4-C5-N7	6.09	113.23	110.80
4	5	4766	C	C6-N1-C2	-6.09	117.86	120.30
50	9	1229	G	C6-C5-N7	-6.09	126.75	130.40
50	9	1309	C	C2-N1-C1'	6.08	125.49	118.80
4	5	4041	C	C2-N1-C1'	6.08	125.49	118.80
4	5	112	C	C5-C6-N1	6.08	124.04	121.00
4	5	1081	C	C2-N1-C1'	6.08	125.48	118.80
4	5	1612	G	C5-C6-O6	-6.08	124.95	128.60
4	5	1639	U	C5-C6-N1	6.07	125.74	122.70
4	5	4709	U	N3-C2-O2	-6.07	117.95	122.20
4	5	2325	C	N1-C2-O2	6.07	122.54	118.90
4	5	1248	C	N1-C2-O2	6.06	122.54	118.90
22	Q	48	LEU	CA-CB-CG	6.06	129.24	115.30
6	8	90	C	C2-N1-C1'	6.06	125.47	118.80
6	8	119	C	C2-N1-C1'	6.06	125.47	118.80
4	5	1514	U	C2-N1-C1'	6.06	124.97	117.70
4	5	2627	C	C5-C6-N1	6.06	124.03	121.00
4	5	4928	C	C6-N1-C2	-6.06	117.88	120.30
50	9	1285	G	N3-C4-C5	-6.05	125.57	128.60
4	5	1656	U	N3-C2-O2	-6.05	117.97	122.20
50	9	1637	A	P-O3'-C3'	6.05	126.96	119.70
4	5	4948	C	C2-N1-C1'	6.05	125.45	118.80
4	5	4948	C	N3-C2-O2	-6.05	117.67	121.90
50	9	898	U	N1-C2-O2	6.05	127.03	122.80
50	9	1285	G	N3-C4-N9	6.05	129.63	126.00
4	5	5047	C	C6-N1-C2	-6.05	117.88	120.30
5	7	57	C	C6-N1-C2	-6.05	117.88	120.30
50	9	1834	A	C5-N7-C8	-6.05	100.88	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5	115	C	N1-C2-O2	6.04	122.53	118.90
4	5	1458	C	N1-C2-O2	6.04	122.53	118.90
4	5	1807	C	C2-N1-C1'	6.04	125.45	118.80
50	9	1290	G	C4-C5-N7	6.04	113.22	110.80
50	9	1755	C	C5-C6-N1	6.04	124.02	121.00
50	9	191	A	OP1-P-O3'	6.04	118.49	105.20
4	5	4266	G	C8-N9-C1'	-6.04	119.15	127.00
50	9	1286	G	C6-C5-N7	-6.04	126.78	130.40
4	5	48	G	P-O3'-C3'	6.03	126.94	119.70
4	5	4922	C	C6-N1-C2	-6.03	117.89	120.30
50	9	120	U	N3-C2-O2	-6.03	117.98	122.20
4	5	4155	C	N3-C2-O2	-6.03	117.68	121.90
4	5	696	C	P-O3'-C3'	6.03	126.94	119.70
4	5	1469	C	C5-C6-N1	6.03	124.02	121.00
4	5	2752	G	N3-C4-N9	6.03	129.62	126.00
4	5	3778	U	N3-C2-O2	-6.01	117.99	122.20
50	9	930	C	N1-C2-O2	6.01	122.51	118.90
50	9	1283	C	C5-C6-N1	6.01	124.01	121.00
4	5	4232	U	P-O3'-C3'	6.01	126.91	119.70
4	5	691	C	N1-C2-O2	6.01	122.50	118.90
4	5	4502	C	C6-N1-C2	-6.00	117.90	120.30
4	5	2553	A	O4'-C1'-N9	6.00	113.00	108.20
50	9	1362	U	N3-C2-O2	-5.99	118.01	122.20
4	5	1579	C	C6-N1-C2	-5.98	117.91	120.30
4	5	1440	U	N3-C2-O2	-5.98	118.01	122.20
50	9	1284	A	C8-N9-C4	-5.98	103.41	105.80
4	5	1428	U	N1-C2-O2	5.98	126.98	122.80
4	5	934	C	N3-C2-O2	-5.98	117.72	121.90
4	5	1828	C	C2-N1-C1'	5.97	125.37	118.80
58	HH	28	LEU	CA-CB-CG	5.97	129.04	115.30
50	9	1281	G	N3-C4-N9	5.97	129.58	126.00
4	5	449	C	P-O3'-C3'	5.97	126.86	119.70
50	9	879	C	N1-C2-O2	5.97	122.48	118.90
4	5	1276	C	N1-C2-O2	5.96	122.48	118.90
4	5	1612	G	N9-C4-C5	-5.96	103.02	105.40
50	9	1016	U	N1-C2-O2	5.96	126.97	122.80
50	9	1636	G	C4-N9-C1'	5.96	134.25	126.50
4	5	1929	A	C2-N3-C4	5.96	113.58	110.60
50	9	1282	A	O4'-C1'-N9	5.96	112.97	108.20
50	9	578	C	N1-C2-O2	5.95	122.47	118.90
50	9	1272	C	N1-C2-O2	5.95	122.47	118.90
4	5	2405	G	N9-C4-C5	-5.95	103.02	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5	1289	C	C6-N1-C2	-5.95	117.92	120.30
4	5	1890	G	C4-C5-N7	5.94	113.18	110.80
4	5	4926	C	N1-C2-O2	5.94	122.47	118.90
50	9	1506	A	C4-N9-C1'	5.94	136.99	126.30
50	9	1756	C	C2-N1-C1'	5.94	125.33	118.80
4	5	275	C	C6-N1-C2	-5.93	117.93	120.30
50	9	1304	U	N3-C2-O2	-5.93	118.05	122.20
4	5	3657	U	C2-N1-C1'	5.93	124.82	117.70
50	9	151	C	C6-N1-C2	-5.92	117.93	120.30
50	9	1324	G	C2-N3-C4	5.92	114.86	111.90
50	9	1471	C	N1-C2-O2	5.92	122.45	118.90
50	9	1118	C	C6-N1-C2	-5.92	117.93	120.30
50	9	1117	C	N1-C2-O2	5.91	122.45	118.90
4	5	493	G	O5'-P-OP2	-5.91	100.38	105.70
4	5	1633	G	N1-C6-O6	-5.90	116.36	119.90
9	C	100	ARG	NE-CZ-NH1	-5.90	117.35	120.30
4	5	2410	C	C6-N1-C2	-5.90	117.94	120.30
4	5	4947	U	P-O3'-C3'	5.90	126.78	119.70
4	5	2474	G	P-O3'-C3'	5.90	126.78	119.70
50	9	1520	G	N7-C8-N9	5.89	116.05	113.10
4	5	1915	C	N3-C2-O2	-5.89	117.78	121.90
50	9	1123	C	N1-C2-O2	5.89	122.43	118.90
4	5	1929	A	C4-N9-C1'	5.89	136.90	126.30
4	5	2059	C	C5-C6-N1	5.89	123.94	121.00
50	9	69	C	C2-N1-C1'	5.88	125.27	118.80
4	5	4766	C	C2-N1-C1'	5.88	125.27	118.80
50	9	1636	G	N3-C4-N9	5.88	129.53	126.00
4	5	704	C	C2-N1-C1'	5.88	125.26	118.80
50	9	1308	U	C6-N1-C1'	5.88	129.43	121.20
4	5	115	C	N3-C2-O2	-5.87	117.79	121.90
4	5	964	A	N7-C8-N9	5.87	116.74	113.80
50	9	1253	A	P-O3'-C3'	5.87	126.75	119.70
4	5	26	C	C6-N1-C2	-5.87	117.95	120.30
4	5	4423	U	N1-C2-O2	5.87	126.91	122.80
4	5	4254	G	P-O3'-C3'	5.87	126.74	119.70
50	9	1298	G	C8-N9-C1'	-5.87	119.38	127.00
50	9	1753	C	C6-N1-C2	-5.86	117.95	120.30
4	5	2089	G	P-O3'-C3'	5.86	126.73	119.70
4	5	322	C	C5-C6-N1	5.86	123.93	121.00
4	5	3870	C	C6-N1-C2	-5.86	117.96	120.30
50	9	189	U	N1-C2-O2	5.85	126.90	122.80
4	5	2820	C	N3-C2-O2	-5.85	117.80	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5	1276	C	C5-C6-N1	5.85	123.93	121.00
64	NN	149	LEU	CA-CB-CG	5.85	128.76	115.30
4	5	2705	G	C4-N9-C1'	5.85	134.10	126.50
4	5	2838	G	C8-N9-C1'	-5.85	119.40	127.00
50	9	1397	U	N3-C4-O4	-5.85	115.31	119.40
50	9	1660	C	C2-N1-C1'	5.85	125.23	118.80
4	5	2560	C	N1-C2-O2	5.85	122.41	118.90
4	5	3636	C	C6-N1-C2	-5.85	117.96	120.30
11	E	289	LEU	CA-CB-CG	5.85	128.75	115.30
4	5	2258	C	OP1-P-O3'	5.85	118.06	105.20
4	5	1807	C	C6-N1-C2	-5.84	117.96	120.30
4	5	4970	C	C2-N1-C1'	5.84	125.23	118.80
5	7	76	U	N3-C2-O2	-5.84	118.11	122.20
4	5	4229	U	N1-C2-O2	5.84	126.89	122.80
4	5	517	C	C5-C6-N1	5.84	123.92	121.00
4	5	1179	U	C2-N1-C1'	5.84	124.70	117.70
4	5	2532	C	C6-N1-C2	-5.84	117.97	120.30
4	5	1502	G	N3-C4-C5	5.83	131.51	128.60
4	5	2752	G	C8-N9-C1'	-5.83	119.43	127.00
4	5	2772	C	C2-N1-C1'	5.83	125.21	118.80
6	8	51	U	N3-C2-O2	-5.82	118.13	122.20
50	9	427	U	C2-N1-C1'	5.82	124.69	117.70
50	9	1574	C	N1-C2-O2	5.82	122.39	118.90
50	9	1281	G	C5-C6-O6	-5.82	125.11	128.60
4	5	4662	C	C6-N1-C2	-5.81	117.97	120.30
4	5	41	C	C5-C6-N1	5.81	123.91	121.00
4	5	3860	A	C5-C6-N6	-5.81	119.05	123.70
50	9	876	C	C2-N1-C1'	5.81	125.19	118.80
50	9	1002	U	C5-C6-N1	5.81	125.60	122.70
4	5	4695	C	C6-N1-C2	-5.80	117.98	120.30
50	9	350	C	C2-N1-C1'	5.80	125.18	118.80
4	5	1474	C	C6-N1-C2	-5.80	117.98	120.30
50	9	442	C	C5-C6-N1	5.80	123.90	121.00
3	4	72	C	P-O3'-C3'	5.80	126.66	119.70
4	5	2752	G	C6-C5-N7	-5.80	126.92	130.40
4	5	1472	C	C5-C6-N1	5.79	123.90	121.00
50	9	162	C	C6-N1-C2	-5.79	117.98	120.30
4	5	4527	G	N3-C4-N9	5.79	129.48	126.00
50	9	853	C	C6-N1-C1'	-5.79	113.85	120.80
4	5	266	C	O5'-P-OP2	-5.79	100.49	105.70
4	5	3870	C	C5-C6-N1	5.79	123.89	121.00
4	5	1440	U	N1-C2-O2	5.78	126.85	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5	1915	C	C6-N1-C2	-5.78	117.99	120.30
50	9	1664	A	P-O3'-C3'	5.78	126.64	119.70
4	5	3974	G	C4-N9-C1'	5.78	134.01	126.50
50	9	579	C	N3-C2-O2	-5.78	117.86	121.90
4	5	2860	C	C6-N1-C2	-5.78	117.99	120.30
50	9	317	C	C2-N1-C1'	5.78	125.15	118.80
50	9	530	U	C2-N1-C1'	5.78	124.63	117.70
50	9	1314	U	C2-N1-C1'	5.77	124.63	117.70
4	5	2704	C	C5-C6-N1	5.77	123.89	121.00
4	5	4286	C	C5-C6-N1	5.77	123.89	121.00
4	5	1890	G	C5-N7-C8	-5.77	101.42	104.30
4	5	1792	U	C5-C6-N1	5.77	125.58	122.70
4	5	2274	C	N3-C2-O2	-5.77	117.86	121.90
4	5	4561	C	C5-C6-N1	5.77	123.88	121.00
4	5	100	C	O4'-C1'-N1	5.76	112.81	108.20
4	5	712	C	C6-N1-C2	-5.76	118.00	120.30
3	4	61	C	N1-C2-O2	5.76	122.36	118.90
4	5	4928	C	N3-C2-O2	-5.76	117.87	121.90
4	5	1731	C	C2-N1-C1'	5.75	125.13	118.80
4	5	2838	G	C6-C5-N7	-5.75	126.95	130.40
50	9	1265	A	C6-C5-N7	-5.75	128.27	132.30
50	9	1298	G	C4-N9-C1'	5.75	133.98	126.50
4	5	1276	C	C6-N1-C2	-5.75	118.00	120.30
4	5	100	C	C6-N1-C2	-5.75	118.00	120.30
50	9	1753	C	C5-C6-N1	5.75	123.87	121.00
50	9	14	C	C6-N1-C2	-5.75	118.00	120.30
4	5	1663	C	C6-N1-C2	-5.73	118.01	120.30
4	5	250	C	C2-N1-C1'	5.73	125.10	118.80
4	5	5059	C	N1-C2-O2	5.73	122.34	118.90
4	5	661	C	C6-N1-C2	-5.72	118.01	120.30
50	9	96	C	C6-N1-C2	-5.72	118.01	120.30
4	5	3685	C	C6-N1-C2	-5.72	118.01	120.30
4	5	4887	C	C5-C6-N1	5.72	123.86	121.00
50	9	532	C	C6-N1-C2	-5.72	118.01	120.30
82	ff	103	LEU	CA-CB-CG	5.72	128.45	115.30
4	5	1481	C	N3-C2-O2	-5.71	117.90	121.90
4	5	4869	U	N3-C2-O2	-5.71	118.20	122.20
4	5	1804	A	P-O3'-C3'	5.71	126.55	119.70
50	9	958	G	C8-N9-C1'	-5.71	119.58	127.00
4	5	1370	G	P-O3'-C3'	5.71	126.55	119.70
4	5	1791	U	N3-C2-O2	-5.71	118.20	122.20
4	5	4254	G	N3-C4-N9	5.71	129.43	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	9	465	A	P-O3'-C3'	5.71	126.55	119.70
4	5	4402	C	N3-C2-O2	-5.71	117.91	121.90
50	9	1097	G	C4-C5-N7	5.70	113.08	110.80
50	9	1287	A	N9-C4-C5	5.70	108.08	105.80
50	9	1135	C	C5-C6-N1	5.70	123.85	121.00
4	5	1520	C	C6-N1-C2	-5.70	118.02	120.30
4	5	2351	C	N3-C2-O2	-5.70	117.91	121.90
4	5	1735	U	N1-C2-O2	5.70	126.79	122.80
50	9	898	U	N3-C2-O2	-5.70	118.21	122.20
4	5	521	C	C6-N1-C2	-5.69	118.02	120.30
4	5	4699	U	OP1-P-O3'	5.69	117.73	105.20
50	9	1865	C	C5-C6-N1	5.69	123.85	121.00
50	9	870	A	P-O3'-C3'	5.69	126.53	119.70
4	5	985	C	C6-N1-C2	-5.69	118.03	120.30
4	5	1339	U	C5-C6-N1	5.68	125.54	122.70
4	5	1502	G	N3-C4-N9	-5.68	122.59	126.00
4	5	3904	G	OP1-P-O3'	5.68	117.71	105.20
4	5	4341	C	N1-C2-O2	5.68	122.31	118.90
4	5	691	C	C6-N1-C1'	-5.68	113.98	120.80
4	5	4413	C	N1-C2-O2	5.68	122.31	118.90
4	5	4502	C	N3-C2-O2	-5.68	117.93	121.90
4	5	4906	C	N1-C2-O2	5.67	122.31	118.90
14	H	34	LEU	CA-CB-CG	5.67	128.35	115.30
4	5	125	C	C6-N1-C2	-5.67	118.03	120.30
50	9	1730	U	N1-C2-O2	5.67	126.77	122.80
4	5	294	G	N3-C4-N9	5.67	129.40	126.00
4	5	4119	C	C6-N1-C2	-5.67	118.03	120.30
4	5	2474	G	OP1-P-O3'	5.67	117.66	105.20
4	5	2405	G	C6-C5-N7	-5.66	127.00	130.40
4	5	2405	G	C4-C5-N7	5.66	113.06	110.80
6	8	124	U	P-O3'-C3'	5.66	126.49	119.70
50	9	154	U	N3-C2-O2	-5.66	118.24	122.20
4	5	1990	A	P-O3'-C3'	5.66	126.49	119.70
50	9	531	A	OP1-P-O3'	5.65	117.63	105.20
4	5	245	C	P-O3'-C3'	5.65	126.48	119.70
4	5	975	C	C6-N1-C2	-5.65	118.04	120.30
4	5	4538	G	C4-N9-C1'	5.65	133.84	126.50
4	5	2470	C	N1-C2-O2	5.65	122.29	118.90
4	5	1215	C	N1-C2-O2	5.65	122.29	118.90
4	5	3882	C	C6-N1-C2	-5.64	118.04	120.30
50	9	1286	G	N3-C4-N9	5.64	129.39	126.00
50	9	427	U	N3-C2-O2	-5.64	118.25	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	9	1707	U	N3-C2-O2	-5.64	118.25	122.20
5	7	76	U	N1-C2-O2	5.63	126.75	122.80
50	9	872	A	C6-N1-C2	-5.63	115.22	118.60
4	5	2037	C	C5-C6-N1	5.63	123.81	121.00
50	9	537	C	N1-C2-O2	5.63	122.28	118.90
4	5	1901	C	C6-N1-C2	-5.63	118.05	120.30
4	5	4206	C	C5-C6-N1	5.63	123.81	121.00
4	5	4601	U	N1-C2-O2	5.63	126.74	122.80
4	5	4906	C	C2-N1-C1'	5.63	124.99	118.80
4	5	1310	C	C5-C6-N1	5.62	123.81	121.00
50	9	1172	U	N3-C2-O2	-5.62	118.26	122.20
50	9	1751	C	N3-C2-O2	-5.62	117.97	121.90
4	5	1628	C	C5-C6-N1	5.62	123.81	121.00
4	5	5059	C	N3-C2-O2	-5.62	117.97	121.90
4	5	1978	C	C6-N1-C2	-5.61	118.06	120.30
4	5	4041	C	C6-N1-C2	-5.61	118.06	120.30
4	5	4237	C	C6-N1-C2	-5.61	118.06	120.30
50	9	106	C	C5-C6-N1	5.61	123.81	121.00
50	9	876	C	N1-C2-O2	5.61	122.27	118.90
4	5	217	C	P-O3'-C3'	5.61	126.43	119.70
4	5	2528	G	C8-N9-C1'	-5.61	119.71	127.00
4	5	3860	A	C4-C5-N7	5.61	113.51	110.70
50	9	1536	G	C8-N9-C4	-5.61	104.16	106.40
4	5	1467	C	C6-N1-C2	-5.61	118.06	120.30
4	5	3693	U	N1-C2-O2	5.61	126.72	122.80
4	5	112	C	C6-N1-C1'	-5.60	114.08	120.80
4	5	2701	U	N1-C2-O2	5.60	126.72	122.80
50	9	1130	G	N3-C4-N9	5.60	129.36	126.00
5	7	28	C	C5-C6-N1	5.60	123.80	121.00
50	9	879	C	C2-N1-C1'	5.60	124.96	118.80
50	9	1057	C	C6-N1-C2	-5.59	118.06	120.30
4	5	3911	C	C6-N1-C2	-5.59	118.06	120.30
50	9	55	U	N3-C2-O2	-5.59	118.29	122.20
4	5	2752	G	C4-N9-C1'	5.59	133.77	126.50
50	9	1097	G	C6-C5-N7	-5.59	127.05	130.40
50	9	1139	C	C6-N1-C1'	-5.59	114.10	120.80
4	5	3693	U	N3-C2-O2	-5.58	118.29	122.20
50	9	930	C	C2-N1-C1'	5.58	124.94	118.80
50	9	1123	C	C6-N1-C2	-5.58	118.07	120.30
4	5	4386	C	N1-C2-O2	5.58	122.25	118.90
4	5	1237	C	C6-N1-C2	-5.57	118.07	120.30
4	5	1485	C	C6-N1-C1'	-5.57	114.11	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	8	99	U	C2-N1-C1'	5.57	124.39	117.70
4	5	4243	C	C6-N1-C2	-5.57	118.07	120.30
4	5	4880	C	C6-N1-C1'	-5.57	114.12	120.80
4	5	1777	C	N1-C2-O2	5.57	122.24	118.90
4	5	2867	C	C2-N1-C1'	5.56	124.92	118.80
4	5	3794	C	C6-N1-C2	-5.56	118.07	120.30
4	5	1440	U	P-O3'-C3'	5.56	126.37	119.70
50	9	151	C	C5-C6-N1	5.56	123.78	121.00
4	5	4177	C	C5-C6-N1	5.56	123.78	121.00
50	9	1124	C	C6-N1-C2	-5.56	118.08	120.30
5	7	39	C	C6-N1-C2	-5.55	118.08	120.30
50	9	983	A	N3-C4-N9	5.55	131.84	127.40
4	5	1929	A	N7-C8-N9	5.55	116.58	113.80
4	5	1540	C	C6-N1-C2	-5.55	118.08	120.30
4	5	1915	C	C2-N1-C1'	5.55	124.90	118.80
4	5	4943	A	O5'-P-OP1	-5.54	100.71	105.70
6	8	119	C	C5-C6-N1	5.54	123.77	121.00
6	8	119	C	C6-N1-C2	-5.54	118.08	120.30
4	5	1792	U	N1-C2-O2	5.54	126.68	122.80
50	9	55	U	C6-N1-C1'	-5.54	113.45	121.20
4	5	1428	U	C5-C6-N1	5.54	125.47	122.70
4	5	3632	C	C6-N1-C2	-5.54	118.09	120.30
50	9	1520	G	N1-C6-O6	-5.53	116.58	119.90
50	9	1721	U	N1-C2-O2	5.53	126.67	122.80
4	5	1666	C	C6-N1-C2	-5.53	118.09	120.30
4	5	2325	C	C6-N1-C2	-5.53	118.09	120.30
4	5	4254	G	C2-N3-C4	5.53	114.67	111.90
4	5	134	G	P-O3'-C3'	5.53	126.33	119.70
4	5	3721	U	N3-C2-O2	-5.53	118.33	122.20
50	9	371	A	O5'-P-OP2	-5.53	100.72	105.70
4	5	2803	U	C5-C6-N1	5.52	125.46	122.70
4	5	455	C	C5-C6-N1	5.52	123.76	121.00
4	5	2817	C	C5-C6-N1	5.52	123.76	121.00
4	5	4051	C	N3-C2-O2	-5.52	118.03	121.90
50	9	1506	A	C6-N1-C2	-5.52	115.29	118.60
4	5	3696	C	C2-N1-C1'	5.52	124.87	118.80
50	9	1518	C	N3-C2-O2	-5.52	118.04	121.90
50	9	1591	C	N3-C2-O2	-5.52	118.04	121.90
4	5	1893	C	C6-N1-C2	-5.52	118.09	120.30
4	5	2726	G	C4-N9-C1'	5.52	133.67	126.50
4	5	7	C	C6-N1-C2	-5.51	118.09	120.30
4	5	2266	C	P-O3'-C3'	5.51	126.31	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5	4639	G	C4-N9-C1'	5.51	133.66	126.50
4	5	4880	C	N1-C2-O2	5.51	122.21	118.90
50	9	457	C	C5-C6-N1	5.51	123.75	121.00
50	9	1172	U	C2-N1-C1'	5.51	124.31	117.70
50	9	1118	C	N3-C2-O2	-5.51	118.04	121.90
4	5	1672	U	N3-C2-O2	-5.51	118.35	122.20
50	9	1684	C	C6-N1-C2	-5.50	118.10	120.30
4	5	1777	C	C6-N1-C1'	-5.50	114.20	120.80
4	5	1248	C	C6-N1-C2	-5.50	118.10	120.30
4	5	3673	C	N1-C2-O2	5.50	122.20	118.90
50	9	1684	C	C2-N1-C1'	5.50	124.85	118.80
4	5	4527	G	N3-C4-C5	-5.49	125.85	128.60
50	9	130	G	C8-N9-C1'	-5.49	119.86	127.00
50	9	1753	C	C2-N1-C1'	5.49	124.84	118.80
20	O	141	LEU	CB-CG-CD1	-5.49	101.67	111.00
50	9	1506	A	C8-N9-C4	-5.49	103.61	105.80
83	gg	281	ALA	C-N-CA	5.48	135.41	121.70
4	5	4561	C	C6-N1-C2	-5.48	118.11	120.30
50	9	1535	U	C5-C6-N1	5.48	125.44	122.70
32	a	81	LEU	CB-CG-CD2	-5.48	101.69	111.00
4	5	2028	C	C6-N1-C2	-5.48	118.11	120.30
50	9	183	G	N1-C6-O6	-5.48	116.61	119.90
4	5	1248	C	N3-C2-O2	-5.48	118.07	121.90
4	5	1081	C	N1-C2-O2	5.47	122.19	118.90
4	5	1214	C	N1-C2-O2	5.47	122.18	118.90
4	5	1308	C	C6-N1-C2	-5.47	118.11	120.30
4	5	2028	C	C6-N1-C1'	-5.47	114.23	120.80
50	9	118	C	N3-C2-O2	-5.47	118.07	121.90
50	9	183	G	O4'-C1'-N9	5.47	112.58	108.20
3	4	63	C	C6-N1-C2	-5.47	118.11	120.30
4	5	1757	U	N3-C2-O2	-5.46	118.38	122.20
4	5	3876	A	OP2-P-O3'	5.46	117.22	105.20
4	5	4444	C	N1-C2-O2	5.46	122.18	118.90
4	5	4563	U	C5-C6-N1	5.46	125.43	122.70
50	9	1290	G	C8-N9-C4	-5.46	104.22	106.40
4	5	959	G	P-O3'-C3'	5.46	126.25	119.70
4	5	2072	C	C2-N1-C1'	5.46	124.80	118.80
4	5	3904	G	P-O3'-C3'	5.46	126.25	119.70
4	5	2410	C	C5-C6-N1	5.46	123.73	121.00
4	5	1628	C	C6-N1-C2	-5.45	118.12	120.30
4	5	4674	C	C6-N1-C2	-5.45	118.12	120.30
6	8	35	C	C6-N1-C2	-5.45	118.12	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	9	1649	U	N1-C2-O2	5.45	126.62	122.80
50	9	1785	C	N1-C2-O2	5.45	122.17	118.90
4	5	1292	C	C6-N1-C2	-5.45	118.12	120.30
4	5	3778	U	C2-N1-C1'	5.45	124.23	117.70
50	9	183	G	N1-C2-N2	5.45	121.10	116.20
50	9	642	U	P-O3'-C3'	5.45	126.23	119.70
4	5	5008	C	N1-C2-O2	5.44	122.17	118.90
50	9	1186	U	N3-C2-O2	-5.44	118.39	122.20
4	5	294	G	C4-N9-C1'	5.44	133.57	126.50
4	5	2281	U	C2-N1-C1'	5.44	124.23	117.70
4	5	2410	C	N1-C2-O2	5.44	122.16	118.90
4	5	4906	C	C5-C6-N1	5.44	123.72	121.00
50	9	1229	G	N7-C8-N9	5.44	115.82	113.10
4	5	2667	C	C2-N1-C1'	5.43	124.78	118.80
4	5	2705	G	C8-N9-C1'	-5.43	119.94	127.00
59	II	129	LEU	CA-CB-CG	5.43	127.80	115.30
4	5	1894	C	C6-N1-C2	-5.43	118.13	120.30
4	5	2260	C	C2-N1-C1'	5.43	124.78	118.80
4	5	3622	C	C5-C6-N1	5.43	123.72	121.00
4	5	2303	C	C6-N1-C2	-5.43	118.13	120.30
4	5	3705	G	C4-N9-C1'	5.43	133.56	126.50
4	5	4949	G	C4-N9-C1'	5.43	133.56	126.50
50	9	1157	G	C4-N9-C1'	5.43	133.56	126.50
50	9	1624	U	C6-N1-C1'	-5.43	113.60	121.20
50	9	1655	C	C6-N1-C2	-5.43	118.13	120.30
4	5	672	C	C2-N1-C1'	5.42	124.76	118.80
4	5	3657	U	C5-C6-N1	5.42	125.41	122.70
4	5	4969	C	C5-C6-N1	5.42	123.71	121.00
4	5	719	C	C6-N1-C2	-5.42	118.13	120.30
50	9	1281	G	C6-C5-N7	-5.42	127.15	130.40
4	5	13	U	N1-C2-O2	5.42	126.59	122.80
4	5	1853	G	C4-N9-C1'	5.41	133.54	126.50
4	5	1863	U	C5-C6-N1	5.41	125.41	122.70
4	5	978	C	C6-N1-C2	-5.41	118.14	120.30
4	5	1578	U	N3-C2-O2	-5.41	118.41	122.20
4	5	4051	C	C6-N1-C2	-5.41	118.14	120.30
4	5	1915	C	N1-C2-O2	5.41	122.14	118.90
50	9	1306	U	N3-C4-C5	-5.41	111.36	114.60
4	5	4631	G	N3-C4-N9	5.41	129.24	126.00
4	5	4981	G	N3-C4-N9	5.40	129.24	126.00
50	9	1262	C	N3-C2-O2	-5.40	118.12	121.90
4	5	4162	C	C6-N1-C1'	-5.40	114.32	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5	4969	C	C6-N1-C2	-5.40	118.14	120.30
4	5	2715	G	C4-N9-C1'	5.40	133.52	126.50
4	5	1599	G	C6-C5-N7	-5.40	127.16	130.40
61	KK	2	LEU	C-N-CA	5.40	135.19	121.70
50	9	1307	U	N1-C2-N3	5.39	118.14	114.90
4	5	1933	G	C8-N9-C4	-5.39	104.24	106.40
11	E	215	LEU	CA-CB-CG	5.39	127.70	115.30
50	9	973	C	N1-C2-O2	5.39	122.14	118.90
50	9	1117	C	N3-C2-O2	-5.39	118.13	121.90
82	ff	97	LYS	C-N-CA	5.39	135.18	121.70
4	5	386	A	OP1-P-O3'	5.39	117.05	105.20
4	5	1809	C	C6-N1-C2	-5.39	118.14	120.30
4	5	4560	C	N1-C2-O2	5.39	122.13	118.90
50	9	532	C	P-O3'-C3'	5.39	126.16	119.70
50	9	687	C	N1-C2-O2	5.39	122.13	118.90
50	9	1292	C	N3-C2-O2	-5.39	118.13	121.90
4	5	322	C	C6-N1-C2	-5.38	118.15	120.30
4	5	1890	G	N3-C4-C5	5.38	131.29	128.60
4	5	5047	C	N3-C2-O2	-5.38	118.13	121.90
4	5	2488	C	N1-C2-O2	5.38	122.13	118.90
50	9	1111	U	C2-N1-C1'	5.38	124.16	117.70
50	9	1262	C	C2-N1-C1'	5.38	124.72	118.80
50	9	1116	C	C6-N1-C2	-5.38	118.15	120.30
4	5	2571	C	C6-N1-C2	-5.38	118.15	120.30
4	5	4193	C	C6-N1-C2	-5.38	118.15	120.30
4	5	1084	C	N1-C2-O2	5.38	122.12	118.90
4	5	4621	C	C6-N1-C2	-5.37	118.15	120.30
4	5	1632	A	C4-N9-C1'	5.37	135.97	126.30
4	5	2867	C	N1-C2-O2	5.37	122.12	118.90
4	5	49	U	C2-N1-C1'	5.37	124.14	117.70
50	9	879	C	C6-N1-C2	-5.37	118.15	120.30
4	5	1607	C	C6-N1-C2	-5.37	118.15	120.30
4	5	2726	G	N3-C4-N9	5.37	129.22	126.00
50	9	96	C	C2-N1-C1'	5.37	124.70	118.80
50	9	1286	G	N3-C2-N2	5.37	123.66	119.90
4	5	47	A	OP1-P-O3'	5.36	117.00	105.20
4	5	2028	C	C5-C6-N1	5.36	123.68	121.00
4	5	455	C	C6-N1-C2	-5.36	118.16	120.30
4	5	1812	C	C2-N1-C1'	5.36	124.69	118.80
4	5	1429	C	N3-C2-O2	-5.35	118.15	121.90
4	5	2410	C	C6-N1-C1'	-5.35	114.38	120.80
50	9	474	G	C4-N9-C1'	5.35	133.46	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	9	1757	G	N3-C4-C5	-5.35	125.92	128.60
4	5	1406(B)	C	OP1-P-O3'	5.35	116.97	105.20
4	5	1455	G	C6-C5-N7	-5.35	127.19	130.40
4	5	126	C	N1-C2-O2	5.35	122.11	118.90
4	5	4401	G	C8-N9-C1'	-5.34	120.05	127.00
50	9	183	G	C4-N9-C1'	5.34	133.45	126.50
2	2	66	C	N1-C2-O2	5.34	122.11	118.90
4	5	2661	U	OP1-P-O3'	5.34	116.95	105.20
4	5	4758	U	C2-N1-C1'	5.34	124.11	117.70
50	9	434	G	P-O3'-C3'	5.34	126.11	119.70
50	9	1412	C	C2-N1-C1'	5.34	124.68	118.80
4	5	3974	G	C8-N9-C1'	-5.34	120.06	127.00
4	5	4552	U	N3-C2-O2	-5.34	118.46	122.20
4	5	4453	C	C5-C6-N1	5.34	123.67	121.00
4	5	1395	U	C5-C6-N1	5.34	125.37	122.70
50	9	1315	U	O4'-C1'-N1	5.34	112.47	108.20
50	9	887	U	N1-C2-O2	5.33	126.53	122.80
4	5	4350	C	C2-N1-C1'	5.33	124.66	118.80
4	5	4502	C	C5-C6-N1	5.33	123.66	121.00
50	9	20	G	C4-N9-C1'	5.32	133.42	126.50
50	9	606	G	C4-C5-N7	5.32	112.93	110.80
50	9	1649	U	C2-N1-C1'	5.32	124.09	117.70
4	5	1472	C	C6-N1-C2	-5.32	118.17	120.30
50	9	474	G	O5'-P-OP1	-5.32	100.91	105.70
50	9	1281	G	C4-C5-N7	5.32	112.93	110.80
50	9	1305	C	C6-N1-C2	-5.32	118.17	120.30
50	9	1309	C	C2-N3-C4	5.32	122.56	119.90
5	7	29	C	C6-N1-C2	-5.32	118.17	120.30
50	9	676	C	C5-C6-N1	5.32	123.66	121.00
50	9	124	U	C5-C6-N1	5.32	125.36	122.70
50	9	1536	G	N9-C4-C5	5.32	107.53	105.40
4	5	1430	C	C6-N1-C2	-5.31	118.17	120.30
4	5	1440	U	C5-C6-N1	5.31	125.36	122.70
4	5	4360	U	N1-C2-O2	5.31	126.52	122.80
23	R	99	MET	CG-SD-CE	-5.31	91.70	100.20
50	9	1116	C	C5-C6-N1	5.31	123.66	121.00
2	2	31	C	C6-N1-C1'	-5.31	114.43	120.80
4	5	975	C	C5-C6-N1	5.31	123.65	121.00
50	9	891	G	N3-C4-N9	5.31	129.18	126.00
50	9	1412	C	N1-C2-O2	5.31	122.08	118.90
50	9	577	U	N1-C2-O2	5.30	126.51	122.80
4	5	3739	C	N1-C2-O2	5.30	122.08	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5	1568	C	C6-N1-C2	-5.30	118.18	120.30
4	5	3650	C	C6-N1-C2	-5.30	118.18	120.30
50	9	1078	C	C2-N1-C1'	5.30	124.63	118.80
3	4	39	U	C2-N1-C1'	5.30	124.06	117.70
4	5	4709	U	C2-N1-C1'	5.30	124.06	117.70
50	9	663	C	C5-C6-N1	5.30	123.65	121.00
50	9	1290	G	C5-N7-C8	-5.30	101.65	104.30
50	9	1721	U	N3-C2-O2	-5.30	118.49	122.20
4	5	4928	C	N1-C2-O2	5.29	122.08	118.90
50	9	465	A	OP2-P-O3'	5.29	116.85	105.20
50	9	1290	G	N1-C6-O6	5.29	123.08	119.90
50	9	8	U	C5-C4-O4	-5.29	122.72	125.90
4	5	672	C	N3-C2-O2	-5.29	118.20	121.90
4	5	2803	U	N3-C2-O2	-5.29	118.50	122.20
50	9	1316	C	C2-N1-C1'	5.29	124.62	118.80
4	5	2351	C	N1-C2-O2	5.29	122.07	118.90
50	9	1412	C	C6-N1-C2	-5.29	118.18	120.30
4	5	1933	G	N7-C8-N9	5.29	115.74	113.10
50	9	1237	C	C6-N1-C2	-5.28	118.19	120.30
4	5	4119	C	C5-C6-N1	5.28	123.64	121.00
4	5	4887	C	C6-N1-C2	-5.28	118.19	120.30
50	9	37	C	C6-N1-C2	-5.28	118.19	120.30
4	5	1929	A	C8-N9-C4	-5.28	103.69	105.80
80	dd	6	LEU	CA-CB-CG	5.27	127.43	115.30
4	5	3622	C	C2-N1-C1'	5.27	124.60	118.80
4	5	3927	U	N3-C2-O2	-5.27	118.51	122.20
4	5	4462	C	C6-N1-C2	-5.27	118.19	120.30
50	9	1397	U	C5-C4-O4	5.27	129.06	125.90
50	9	386	C	C6-N1-C2	-5.27	118.19	120.30
4	5	1	C	N1-C2-O2	5.27	122.06	118.90
4	5	2509	C	C2-N1-C1'	5.27	124.60	118.80
50	9	659	G	N3-C4-N9	5.27	129.16	126.00
4	5	2837	U	C6-N1-C2	-5.27	117.84	121.00
50	9	1574	C	C6-N1-C2	-5.27	118.19	120.30
50	9	293	C	C6-N1-C1'	-5.27	114.48	120.80
4	5	4417	C	C6-N1-C2	-5.26	118.19	120.30
50	9	1504	U	N3-C4-C5	5.26	117.76	114.60
11	E	129	LEU	CA-CB-CG	5.26	127.40	115.30
4	5	4413	C	N3-C2-O2	-5.26	118.22	121.90
4	5	446	C	C6-N1-C2	-5.26	118.20	120.30
50	9	630	U	C2-N1-C1'	5.25	124.01	117.70
4	5	343	C	C5-C6-N1	5.25	123.63	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5	1807	C	N1-C2-O2	5.25	122.05	118.90
50	9	1325	G	N9-C4-C5	-5.25	103.30	105.40
4	5	955	G	P-O3'-C3'	5.25	126.00	119.70
4	5	3926	C	C5-C6-N1	5.25	123.62	121.00
6	8	51	U	N1-C2-O2	5.25	126.47	122.80
13	G	207	LEU	CA-CB-CG	5.25	127.37	115.30
50	9	1518	C	N1-C2-O2	5.25	122.05	118.90
4	5	1853	G	C8-N9-C1'	-5.25	120.18	127.00
4	5	3603	G	P-O3'-C3'	5.25	125.99	119.70
22	Q	48	LEU	CB-CG-CD2	-5.24	102.09	111.00
4	5	2701	U	N3-C2-O2	-5.24	118.53	122.20
50	9	1757	G	N3-C4-N9	5.24	129.15	126.00
50	9	1389	C	C6-N1-C1'	-5.24	114.51	120.80
4	5	118	C	C5-C6-N1	5.24	123.62	121.00
4	5	3672	G	N3-C4-C5	5.24	131.22	128.60
4	5	2850	A	C2-N3-C4	5.24	113.22	110.60
4	5	1751	A	N9-C4-C5	-5.24	103.70	105.80
50	9	409	C	C6-N1-C2	-5.24	118.21	120.30
50	9	1696	C	N1-C2-O2	5.23	122.04	118.90
4	5	1599	G	C4-N9-C1'	5.23	133.30	126.50
27	V	49	LEU	CA-CB-CG	5.23	127.33	115.30
4	5	77	U	N1-C2-O2	5.23	126.46	122.80
50	9	958	G	C6-C5-N7	-5.23	127.26	130.40
4	5	4413	C	C6-N1-C1'	-5.23	114.53	120.80
50	9	663	C	C6-N1-C2	-5.23	118.21	120.30
50	9	1331	C	C2-N1-C1'	5.23	124.55	118.80
50	9	1229	G	C4-N9-C1'	5.22	133.29	126.50
4	5	447	C	C6-N1-C2	-5.22	118.21	120.30
4	5	1474	C	C5-C6-N1	5.22	123.61	121.00
4	5	5050	C	C2-N1-C1'	5.22	124.54	118.80
4	5	2571	C	C5-C6-N1	5.22	123.61	121.00
50	9	578	C	N3-C2-O2	-5.22	118.25	121.90
4	5	1289	C	C5-C6-N1	5.21	123.61	121.00
50	9	387	C	C6-N1-C2	-5.21	118.21	120.30
50	9	1118	C	N1-C2-O2	5.21	122.03	118.90
4	5	3871	A	N7-C8-N9	5.21	116.41	113.80
4	5	4758	U	N3-C2-O2	-5.21	118.55	122.20
4	5	2838	G	N7-C8-N9	5.21	115.70	113.10
4	5	2704	C	C6-N1-C2	-5.21	118.22	120.30
50	9	1283	C	N3-C4-C5	-5.20	119.82	121.90
4	5	1484	G	C6-C5-N7	-5.20	127.28	130.40
49	u	124	LEU	CA-CB-CG	5.20	127.26	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	9	142	C	N3-C2-O2	-5.20	118.26	121.90
4	5	1446	C	C6-N1-C2	-5.20	118.22	120.30
50	9	606	G	C4-N9-C1'	5.20	133.25	126.50
50	9	1164	G	C4-N9-C1'	5.20	133.25	126.50
4	5	973	C	N3-C2-O2	-5.19	118.27	121.90
6	8	98	C	C6-N1-C2	-5.19	118.22	120.30
43	1	49	LEU	CA-CB-CG	5.19	127.24	115.30
50	9	391	C	C6-N1-C2	-5.19	118.22	120.30
50	9	1510	G	C6-C5-N7	-5.19	127.29	130.40
50	9	1161	U	C2-N1-C1'	5.19	123.93	117.70
4	5	3767	C	C6-N1-C2	-5.19	118.22	120.30
50	9	914	U	O4'-C1'-N1	5.19	112.35	108.20
4	5	4869	U	N1-C2-O2	5.18	126.43	122.80
4	5	1406(B)	C	P-O3'-C3'	5.18	125.92	119.70
50	9	585	C	C2-N1-C1'	5.18	124.50	118.80
50	9	541	U	N1-C2-O2	5.18	126.42	122.80
6	8	153	C	C2-N1-C1'	5.18	124.49	118.80
4	5	294	G	C8-N9-C1'	-5.17	120.27	127.00
6	8	54	C	N1-C2-O2	5.17	122.00	118.90
4	5	1458	C	N3-C2-O2	-5.17	118.28	121.90
4	5	4386	C	N3-C2-O2	-5.17	118.28	121.90
50	9	531	A	P-O3'-C3'	5.17	125.90	119.70
50	9	1308	U	C5'-C4'-O4'	5.17	115.30	109.10
4	5	5022	U	N1-C2-O2	5.17	126.42	122.80
59	II	29	LEU	CA-CB-CG	5.17	127.18	115.30
50	9	1863	A	N7-C8-N9	5.16	116.38	113.80
4	5	2704	C	C6-N1-C1'	-5.16	114.61	120.80
4	5	4949	G	C8-N9-C1'	-5.16	120.29	127.00
50	9	151	C	C2-N1-C1'	5.16	124.48	118.80
4	5	1211	G	P-O3'-C3'	5.16	125.89	119.70
3	4	61	C	C2-N1-C1'	5.16	124.47	118.80
4	5	1726	U	N3-C2-O2	-5.15	118.59	122.20
50	9	1303	C	C6-N1-C1'	-5.15	114.62	120.80
4	5	4057	C	N1-C2-O2	5.15	121.99	118.90
50	9	430	C	C6-N1-C2	-5.15	118.24	120.30
4	5	472	C	N3-C2-O2	-5.15	118.30	121.90
4	5	2465	C	C6-N1-C2	-5.15	118.24	120.30
4	5	3853	U	C2-N1-C1'	5.15	123.88	117.70
4	5	1289	C	N3-C2-O2	-5.15	118.30	121.90
4	5	3775	A	C5-N7-C8	-5.15	101.33	103.90
50	9	1315	U	C6-N1-C2	-5.15	117.91	121.00
50	9	848	U	N3-C2-O2	-5.15	118.60	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5	1442	C	C5-C6-N1	5.14	123.57	121.00
4	5	2089	G	OP2-P-O3'	5.14	116.51	105.20
50	9	345	U	C5-C6-N1	5.14	125.27	122.70
50	9	659	G	C4-N9-C1'	5.14	133.18	126.50
4	5	517	C	C6-N1-C2	-5.14	118.25	120.30
50	9	1315	U	C5-C6-N1	5.14	125.27	122.70
50	9	124	U	C6-N1-C1'	-5.14	114.01	121.20
82	ff	120	GLU	C-N-CA	5.14	134.55	121.70
50	9	537	C	C2-N1-C1'	5.14	124.45	118.80
2	2	32	C	N1-C2-O2	5.13	121.98	118.90
4	5	4639	G	C8-N9-C1'	-5.13	120.33	127.00
50	9	12	U	N3-C2-O2	-5.13	118.61	122.20
4	5	1603	C	C6-N1-C2	-5.13	118.25	120.30
4	5	444	G	C4-N9-C1'	5.13	133.17	126.50
4	5	2384	U	C2-N1-C1'	5.13	123.86	117.70
4	5	718	C	C6-N1-C2	-5.13	118.25	120.30
50	9	1684	C	C5-C6-N1	5.13	123.56	121.00
4	5	282	C	N3-C2-O2	-5.13	118.31	121.90
4	5	1834	U	C2-N1-C1'	5.13	123.85	117.70
4	5	2016	C	N1-C2-O2	5.13	121.98	118.90
82	ff	97	LYS	CA-CB-CG	5.13	124.68	113.40
4	5	3709	U	C2-N1-C1'	5.12	123.85	117.70
4	5	118	C	C6-N1-C2	-5.12	118.25	120.30
4	5	4887	C	N1-C2-O2	5.12	121.97	118.90
50	9	1124	C	C5-C6-N1	5.12	123.56	121.00
3	4	63	C	C5-C6-N1	5.12	123.56	121.00
4	5	1289	C	N1-C2-O2	5.12	121.97	118.90
4	5	3667	C	C6-N1-C2	-5.12	118.25	120.30
50	9	1305	C	C6-N1-C1'	-5.12	114.66	120.80
4	5	941	C	C6-N1-C2	-5.12	118.25	120.30
4	5	4283	G	C4-N9-C1'	5.12	133.15	126.50
50	9	927	C	C6-N1-C2	-5.12	118.25	120.30
50	9	1304	U	N1-C2-O2	5.12	126.38	122.80
4	5	464	G	N3-C4-N9	5.11	129.07	126.00
4	5	1188	C	N3-C2-O2	-5.11	118.32	121.90
4	5	1313	C	O4'-C1'-N1	-5.11	104.11	108.20
4	5	1329	G	C6-C5-N7	-5.11	127.33	130.40
4	5	1329	G	N7-C8-N9	5.11	115.66	113.10
50	9	891	G	N3-C4-C5	-5.11	126.04	128.60
4	5	4662	C	C5-C6-N1	5.11	123.56	121.00
4	5	1455	G	C4-C5-N7	5.11	112.84	110.80
4	5	4460	U	C5-C6-N1	5.11	125.25	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	9	1271	C	C2-N1-C1'	5.11	124.42	118.80
5	7	102	U	N3-C2-O2	-5.11	118.63	122.20
50	9	1164	G	C8-N9-C1'	-5.11	120.36	127.00
4	5	4601	U	N3-C2-O2	-5.10	118.63	122.20
50	9	1271	C	C6-N1-C2	-5.10	118.26	120.30
4	5	1792	U	N3-C2-O2	-5.10	118.63	122.20
4	5	1814	C	C5-C6-N1	5.10	123.55	121.00
4	5	2502	A	OP1-P-O3'	5.10	116.42	105.20
2	2	20	U	C6-N1-C2	-5.10	117.94	121.00
12	F	207	LEU	CB-CG-CD1	-5.10	102.33	111.00
4	5	43	U	N1-C2-O2	5.10	126.37	122.80
4	5	455	C	C2-N1-C1'	5.10	124.41	118.80
4	5	1818	G	C4-N9-C1'	5.10	133.12	126.50
4	5	2694	G	C4-C5-N7	5.10	112.84	110.80
4	5	2502	A	P-O3'-C3'	5.09	125.81	119.70
50	9	1398	G	N3-C4-N9	5.09	129.06	126.00
50	9	1590	C	N3-C2-O2	-5.09	118.33	121.90
4	5	1672	U	N1-C2-O2	5.09	126.36	122.80
4	5	3948	C	C2-N1-C1'	5.09	124.40	118.80
50	9	983	A	C4-N9-C1'	5.09	135.47	126.30
4	5	5016	A	N7-C8-N9	5.09	116.34	113.80
50	9	1564	C	N1-C2-O2	5.09	121.95	118.90
4	5	2072	C	N1-C2-O2	5.09	121.95	118.90
4	5	1477	C	C6-N1-C2	-5.08	118.27	120.30
4	5	5022	U	N3-C2-O2	-5.08	118.64	122.20
4	5	302	C	C6-N1-C2	-5.08	118.27	120.30
4	5	1655	C	C6-N1-C2	-5.08	118.27	120.30
4	5	1735	U	N3-C2-O2	-5.08	118.64	122.20
4	5	3882	C	C2-N1-C1'	5.08	124.39	118.80
50	9	1242	U	N1-C2-O2	5.08	126.36	122.80
4	5	1276	C	C2-N1-C1'	5.08	124.39	118.80
4	5	1339	U	C2-N1-C1'	5.08	123.79	117.70
4	5	2571	C	C2-N1-C1'	5.08	124.39	118.80
4	5	3625	G	P-O3'-C3'	5.08	125.80	119.70
2	2	61	C	C6-N1-C1'	-5.08	114.71	120.80
4	5	1662	C	C5-C6-N1	5.07	123.54	121.00
4	5	4561	C	C2-N1-C1'	5.07	124.38	118.80
50	9	1118	C	O4'-C1'-N1	5.07	112.26	108.20
49	u	111	LEU	CA-CB-CG	5.07	126.97	115.30
50	9	1757	G	C4-N9-C1'	5.07	133.09	126.50
50	9	1834	A	C4-N9-C1'	5.07	135.42	126.30
60	JJ	110	LEU	CB-CG-CD2	-5.07	102.38	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5	3714	G	C4-N9-C1'	5.07	133.09	126.50
50	9	1308	U	C1'-O4'-C4'	-5.07	105.85	109.90
4	5	1632	A	N7-C8-N9	5.07	116.33	113.80
4	5	3871	A	C8-N9-C4	-5.07	103.77	105.80
4	5	4884	G	P-O3'-C3'	5.07	125.78	119.70
4	5	3775	A	O4'-C1'-N9	5.06	112.25	108.20
50	9	1591	C	C2-N1-C1'	5.06	124.37	118.80
4	5	753	C	C6-N1-C2	-5.06	118.28	120.30
4	5	2048	U	N3-C2-O2	-5.06	118.66	122.20
4	5	4538	G	C6-C5-N7	-5.06	127.36	130.40
4	5	2433	G	C4-C5-N7	5.06	112.82	110.80
50	9	1591	C	C6-N1-C2	-5.06	118.28	120.30
50	9	984	C	C6-N1-C2	-5.06	118.28	120.30
50	9	1824	A	N3-C4-C5	-5.06	123.26	126.80
4	5	1429	C	C6-N1-C1'	-5.06	114.73	120.80
50	9	189	U	N3-C2-O2	-5.06	118.66	122.20
4	5	675	C	C5-C6-N1	5.06	123.53	121.00
4	5	2683	C	C2-N1-C1'	5.06	124.36	118.80
4	5	3892	U	N3-C2-O2	-5.05	118.66	122.20
20	O	29	LEU	CB-CG-CD2	-5.05	102.41	111.00
4	5	250	C	C5-C6-N1	5.05	123.53	121.00
4	5	2705	G	N3-C4-N9	5.05	129.03	126.00
4	5	2803	U	C6-N1-C2	-5.05	117.97	121.00
4	5	2837	U	C5-C6-N1	5.05	125.22	122.70
6	8	21	C	N1-C2-O2	5.05	121.93	118.90
50	9	1300	U	C5-C6-N1	5.05	125.22	122.70
50	9	1624	U	O4'-C1'-N1	5.05	112.24	108.20
50	9	1636	G	C8-N9-C1'	-5.05	120.44	127.00
2	2	74	C	C6-N1-C2	-5.05	118.28	120.30
4	5	390	C	C5-C6-N1	5.05	123.52	121.00
4	5	4667	C	C5-C6-N1	5.05	123.52	121.00
50	9	1308	U	C2-N3-C4	-5.05	123.97	127.00
69	SS	111	LEU	CB-CG-CD1	-5.05	102.42	111.00
2	2	49	C	C2-N1-C1'	5.04	124.35	118.80
54	DD	69	LEU	CA-CB-CG	5.04	126.90	115.30
2	2	74	C	C5-C6-N1	5.04	123.52	121.00
4	5	504	G	P-O3'-C3'	5.04	125.75	119.70
4	5	1084	C	C6-N1-C1'	-5.04	114.75	120.80
16	J	87	LEU	CA-CB-CG	-5.04	103.70	115.30
54	DD	14	ASP	CB-CG-OD1	5.04	122.84	118.30
3	4	63	C	N1-C2-O2	5.04	121.92	118.90
50	9	1097	G	C4-N9-C1'	5.04	133.05	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5	4283	G	C6-C5-N7	-5.04	127.38	130.40
50	9	1157	G	C8-N9-C1'	-5.04	120.45	127.00
50	9	1510	G	N3-C4-N9	5.04	129.02	126.00
4	5	4614	G	C6-C5-N7	-5.04	127.38	130.40
4	5	5016	A	C4-C5-N7	5.04	113.22	110.70
5	7	29	C	C6-N1-C1'	-5.04	114.76	120.80
5	7	57	C	C5-C6-N1	5.04	123.52	121.00
50	9	1312	G	N1-C2-N3	5.04	126.92	123.90
4	5	4266	G	C2-N3-C4	5.03	114.42	111.90
4	5	1639	U	C6-N1-C2	-5.03	117.98	121.00
6	8	119	C	N1-C2-O2	5.03	121.92	118.90
50	9	1298	G	N3-C4-C5	-5.03	126.08	128.60
4	5	1633	G	P-O3'-C3'	5.03	125.73	119.70
4	5	2803	U	C2-N1-C1'	5.03	123.73	117.70
64	NN	45	LEU	CA-CB-CG	5.03	126.87	115.30
4	5	975	C	N1-C2-O2	5.03	121.92	118.90
4	5	1079	C	C6-N1-C1'	-5.03	114.77	120.80
4	5	3739	C	C2-N1-C1'	5.03	124.33	118.80
50	9	659	G	C8-N9-C1'	-5.03	120.47	127.00
50	9	1307	U	O5'-C5'-C4'	5.03	121.25	111.70
4	5	3927	U	C2-N1-C1'	5.02	123.73	117.70
50	9	1286	G	O5'-C5'-C4'	5.02	121.25	111.70
50	9	293	C	C6-N1-C2	-5.02	118.29	120.30
50	9	1824	A	N3-C4-N9	5.02	131.42	127.40
4	5	4642	U	N3-C2-O2	-5.02	118.69	122.20
5	7	102	U	N1-C2-O2	5.02	126.31	122.80
4	5	2439	G	C4-N9-C1'	5.02	133.02	126.50
5	7	36	C	C6-N1-C2	-5.02	118.29	120.30
50	9	729	C	N3-C2-O2	-5.02	118.39	121.90
50	9	1324	G	C8-N9-C4	5.02	108.41	106.40
50	9	345	U	N3-C2-O2	-5.01	118.69	122.20
50	9	1834	A	C4-C5-N7	5.01	113.21	110.70
50	9	295	C	C5-C6-N1	5.01	123.51	121.00
4	5	2540	C	C6-N1-C2	-5.01	118.30	120.30
4	5	4712	C	C6-N1-C2	-5.01	118.30	120.30
5	7	39	C	N1-C2-O2	5.01	121.91	118.90
50	9	801	U	C2-N1-C1'	5.01	123.71	117.70
2	2	61	C	C6-N1-C2	-5.01	118.30	120.30
4	5	970	G	C4-N9-C1'	5.01	133.01	126.50
4	5	985	C	C5-C6-N1	5.01	123.50	121.00
4	5	1991	A	OP1-P-OP2	-5.01	112.09	119.60
4	5	3939	G	N3-C4-N9	5.01	129.01	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5	4272	G	C4-N9-C1'	5.01	133.01	126.50
4	5	4444	C	N3-C2-O2	-5.01	118.39	121.90
50	9	1078	C	N1-C2-O2	5.01	121.91	118.90
4	5	1913	C	C6-N1-C2	-5.01	118.30	120.30
4	5	4667	C	N3-C2-O2	-5.01	118.39	121.90
6	8	1	C	N1-C2-O2	5.01	121.90	118.90
50	9	89	C	C6-N1-C2	-5.01	118.30	120.30
50	9	1123	C	N3-C2-O2	-5.01	118.40	121.90
50	9	1574	C	C2-N1-C1'	5.01	124.31	118.80
4	5	926	G	N3-C4-N9	5.00	129.00	126.00
50	9	456	C	C6-N1-C2	-5.00	118.30	120.30
50	9	1840	U	C5-C6-N1	5.00	125.20	122.70
4	5	2820	C	C2-N1-C1'	5.00	124.30	118.80
50	9	407	G	N3-C4-N9	5.00	129.00	126.00
50	9	1489	A	P-O3'-C3'	5.00	125.70	119.70

There are no chirality outliers.

All (33) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
51	AA	42	LYS	Peptide
51	AA	43	SER	Peptide
8	B	16	PHE	Peptide
9	C	69	THR	Peptide
9	C	73	VAL	Peptide
10	D	235	MET	Peptide
13	G	215	ASP	Peptide
14	H	50	LYS	Peptide
63	MM	72	HIS	Peptide
19	N	184	ILE	Peptide
19	N	76	PRO	Peptide
19	N	78	GLY	Peptide
65	OO	38	ASN	Peptide
69	SS	99	LEU	Peptide
25	T	80	VAL	Peptide
70	TT	117	GLN	Peptide
71	UU	56	MET	Peptide
72	VV	32	ILE	Peptide
73	WW	54	ASP	Peptide
74	XX	61	GLN	Peptide
30	Y	82	ILE	Peptide
33	b	101	HIS	Peptide

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Mol	Chain	Res	Type	Group
35	d	95	ASP	Peptide
82	ff	134	SER	Mainchain
82	ff	146	LEU	Peptide
82	ff	91	ASN	Peptide
82	ff	95	ARG	Peptide
82	ff	97	LYS	Peptide
82	ff	99	LYS	Peptide
46	o	74	GLU	Peptide
49	u	128	LEU	Peptide
49	u	20	GLY	Peptide
49	u	60	ARG	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	A	246/248 (99%)	225 (92%)	21 (8%)	0	100	100
8	B	392/394 (100%)	366 (93%)	26 (7%)	0	100	100
9	C	359/362 (99%)	340 (95%)	19 (5%)	0	100	100
10	D	291/293 (99%)	275 (94%)	16 (6%)	0	100	100
11	E	208/291 (72%)	198 (95%)	10 (5%)	0	100	100
12	F	223/247 (90%)	212 (95%)	11 (5%)	0	100	100
13	G	229/319 (72%)	221 (96%)	8 (4%)	0	100	100
14	H	188/190 (99%)	175 (93%)	13 (7%)	0	100	100
15	I	201/214 (94%)	186 (92%)	15 (8%)	0	100	100
16	J	168/178 (94%)	160 (95%)	8 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	L	208/210 (99%)	198 (95%)	9 (4%)	1 (0%)	29	68
18	M	136/138 (99%)	122 (90%)	14 (10%)	0	100	100
19	N	201/203 (99%)	187 (93%)	14 (7%)	0	100	100
20	O	197/199 (99%)	191 (97%)	6 (3%)	0	100	100
21	P	151/153 (99%)	145 (96%)	6 (4%)	0	100	100
22	Q	185/187 (99%)	173 (94%)	12 (6%)	0	100	100
23	R	178/180 (99%)	172 (97%)	6 (3%)	0	100	100
24	S	174/176 (99%)	159 (91%)	14 (8%)	1 (1%)	25	64
25	T	157/159 (99%)	150 (96%)	7 (4%)	0	100	100
26	U	97/99 (98%)	92 (95%)	5 (5%)	0	100	100
27	V	129/131 (98%)	121 (94%)	8 (6%)	0	100	100
28	W	102/157 (65%)	97 (95%)	5 (5%)	0	100	100
29	X	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
30	Y	132/134 (98%)	128 (97%)	4 (3%)	0	100	100
31	Z	133/135 (98%)	125 (94%)	7 (5%)	1 (1%)	19	59
32	a	145/147 (99%)	137 (94%)	8 (6%)	0	100	100
33	b	100/245 (41%)	93 (93%)	7 (7%)	0	100	100
34	c	96/98 (98%)	89 (93%)	7 (7%)	0	100	100
35	d	105/107 (98%)	95 (90%)	10 (10%)	0	100	100
36	e	126/128 (98%)	114 (90%)	12 (10%)	0	100	100
37	f	107/109 (98%)	100 (94%)	7 (6%)	0	100	100
38	g	112/114 (98%)	107 (96%)	5 (4%)	0	100	100
39	h	120/122 (98%)	117 (98%)	3 (2%)	0	100	100
40	i	100/102 (98%)	96 (96%)	4 (4%)	0	100	100
41	j	84/86 (98%)	77 (92%)	7 (8%)	0	100	100
42	k	67/69 (97%)	66 (98%)	1 (2%)	0	100	100
43	l	48/50 (96%)	43 (90%)	5 (10%)	0	100	100
44	m	49/52 (94%)	44 (90%)	4 (8%)	1 (2%)	7	41
45	n	23/25 (92%)	23 (100%)	0	0	100	100
46	o	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
47	p	89/91 (98%)	84 (94%)	5 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	r	122/124 (98%)	116 (95%)	6 (5%)	0	100	100
49	u	204/206 (99%)	171 (84%)	32 (16%)	1 (0%)	29	68
51	AA	215/217 (99%)	203 (94%)	12 (6%)	0	100	100
52	BB	211/213 (99%)	198 (94%)	13 (6%)	0	100	100
53	CC	219/221 (99%)	212 (97%)	7 (3%)	0	100	100
54	DD	226/228 (99%)	219 (97%)	7 (3%)	0	100	100
55	EE	260/262 (99%)	241 (93%)	19 (7%)	0	100	100
56	FF	181/204 (89%)	169 (93%)	12 (7%)	0	100	100
57	GG	235/237 (99%)	227 (97%)	8 (3%)	0	100	100
58	HH	181/194 (93%)	169 (93%)	12 (7%)	0	100	100
59	II	204/206 (99%)	191 (94%)	13 (6%)	0	100	100
60	JJ	183/185 (99%)	180 (98%)	3 (2%)	0	100	100
61	KK	94/96 (98%)	86 (92%)	8 (8%)	0	100	100
62	LL	139/158 (88%)	128 (92%)	11 (8%)	0	100	100
63	MM	115/117 (98%)	105 (91%)	10 (9%)	0	100	100
64	NN	147/149 (99%)	140 (95%)	7 (5%)	0	100	100
65	OO	134/136 (98%)	124 (92%)	10 (8%)	0	100	100
66	PP	118/120 (98%)	114 (97%)	4 (3%)	0	100	100
67	QQ	140/142 (99%)	130 (93%)	10 (7%)	0	100	100
68	RR	130/132 (98%)	125 (96%)	5 (4%)	0	100	100
69	SS	142/144 (99%)	134 (94%)	8 (6%)	0	100	100
70	TT	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
71	UU	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
72	VV	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
73	WW	127/129 (98%)	119 (94%)	8 (6%)	0	100	100
74	XX	139/141 (99%)	128 (92%)	8 (6%)	3 (2%)	6	39
75	YY	122/124 (98%)	118 (97%)	4 (3%)	0	100	100
76	ZZ	73/75 (97%)	71 (97%)	2 (3%)	0	100	100
77	aa	99/101 (98%)	92 (93%)	7 (7%)	0	100	100
78	bb	81/83 (98%)	76 (94%)	5 (6%)	0	100	100
79	cc	60/62 (97%)	57 (95%)	3 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
80	dd	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
81	ee	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
82	ff	66/68 (97%)	49 (74%)	17 (26%)	0	100	100
83	gg	311/313 (99%)	279 (90%)	32 (10%)	0	100	100
All	All	11375/11984 (95%)	10695 (94%)	672 (6%)	8 (0%)	54	83

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
44	m	73	CYS
24	S	166	ARG
49	u	61	PRO
74	XX	62	PRO
31	Z	90	PRO
74	XX	86	PRO
74	XX	61	GLN
17	L	62	PRO

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	
7	A	190/190 (100%)	186 (98%)	4 (2%)	53	78
8	B	342/342 (100%)	336 (98%)	6 (2%)	59	81
9	C	301/301 (100%)	295 (98%)	6 (2%)	55	79
10	D	247/247 (100%)	240 (97%)	7 (3%)	43	72
11	E	190/251 (76%)	186 (98%)	4 (2%)	53	78
12	F	196/215 (91%)	195 (100%)	1 (0%)	88	95
13	G	200/272 (74%)	190 (95%)	10 (5%)	24	59
14	H	169/169 (100%)	166 (98%)	3 (2%)	59	81
15	I	175/181 (97%)	173 (99%)	2 (1%)	73	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	J	143/149 (96%)	142 (99%)	1 (1%)	84	93
17	L	175/175 (100%)	174 (99%)	1 (1%)	86	94
18	M	117/117 (100%)	113 (97%)	4 (3%)	37	69
19	N	171/171 (100%)	167 (98%)	4 (2%)	50	76
20	O	171/171 (100%)	168 (98%)	3 (2%)	59	81
21	P	134/134 (100%)	133 (99%)	1 (1%)	84	93
22	Q	164/164 (100%)	162 (99%)	2 (1%)	71	87
23	R	159/159 (100%)	156 (98%)	3 (2%)	57	80
24	S	157/157 (100%)	155 (99%)	2 (1%)	69	86
25	T	139/139 (100%)	136 (98%)	3 (2%)	52	77
26	U	89/89 (100%)	86 (97%)	3 (3%)	37	69
27	V	101/101 (100%)	99 (98%)	2 (2%)	55	79
28	W	86/126 (68%)	84 (98%)	2 (2%)	50	76
29	X	106/106 (100%)	106 (100%)	0	100	100
30	Y	124/124 (100%)	121 (98%)	3 (2%)	49	75
31	Z	117/117 (100%)	116 (99%)	1 (1%)	78	90
32	a	119/119 (100%)	118 (99%)	1 (1%)	81	91
33	b	84/184 (46%)	80 (95%)	4 (5%)	25	60
34	c	84/84 (100%)	81 (96%)	3 (4%)	35	67
35	d	98/98 (100%)	97 (99%)	1 (1%)	76	88
36	e	114/114 (100%)	111 (97%)	3 (3%)	46	74
37	f	88/88 (100%)	85 (97%)	3 (3%)	37	69
38	g	98/98 (100%)	94 (96%)	4 (4%)	30	64
39	h	109/109 (100%)	107 (98%)	2 (2%)	59	81
40	i	86/86 (100%)	84 (98%)	2 (2%)	50	76
41	j	73/73 (100%)	72 (99%)	1 (1%)	67	85
42	k	64/64 (100%)	63 (98%)	1 (2%)	62	83
43	l	47/47 (100%)	46 (98%)	1 (2%)	53	78
44	m	47/47 (100%)	45 (96%)	2 (4%)	29	63
45	n	24/24 (100%)	23 (96%)	1 (4%)	30	63
46	o	91/91 (100%)	90 (99%)	1 (1%)	73	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	p	74/74 (100%)	74 (100%)	0	100	100
48	r	108/108 (100%)	103 (95%)	5 (5%)	27	61
49	u	186/186 (100%)	179 (96%)	7 (4%)	33	66
51	AA	180/181 (99%)	178 (99%)	2 (1%)	73	88
52	BB	194/194 (100%)	190 (98%)	4 (2%)	53	78
53	CC	187/187 (100%)	184 (98%)	3 (2%)	62	83
54	DD	190/190 (100%)	184 (97%)	6 (3%)	39	70
55	EE	224/224 (100%)	220 (98%)	4 (2%)	59	81
56	FF	158/170 (93%)	153 (97%)	5 (3%)	39	70
57	GG	207/207 (100%)	204 (99%)	3 (1%)	67	85
58	HH	165/174 (95%)	162 (98%)	3 (2%)	59	81
59	II	178/178 (100%)	176 (99%)	2 (1%)	73	88
60	JJ	161/161 (100%)	161 (100%)	0	100	100
61	KK	87/87 (100%)	87 (100%)	0	100	100
62	LL	130/142 (92%)	128 (98%)	2 (2%)	65	84
63	MM	99/99 (100%)	99 (100%)	0	100	100
64	NN	130/130 (100%)	129 (99%)	1 (1%)	81	91
65	OO	106/106 (100%)	100 (94%)	6 (6%)	20	55
66	PP	109/109 (100%)	107 (98%)	2 (2%)	59	81
67	QQ	117/117 (100%)	114 (97%)	3 (3%)	46	74
68	RR	119/119 (100%)	117 (98%)	2 (2%)	60	82
69	SS	125/125 (100%)	124 (99%)	1 (1%)	81	91
70	TT	111/111 (100%)	108 (97%)	3 (3%)	44	73
71	UU	92/92 (100%)	92 (100%)	0	100	100
72	VV	67/67 (100%)	66 (98%)	1 (2%)	65	84
73	WW	112/112 (100%)	109 (97%)	3 (3%)	44	73
74	XX	113/113 (100%)	113 (100%)	0	100	100
75	YY	107/107 (100%)	104 (97%)	3 (3%)	43	72
76	ZZ	66/66 (100%)	66 (100%)	0	100	100
77	aa	88/88 (100%)	85 (97%)	3 (3%)	37	69
78	bb	75/75 (100%)	74 (99%)	1 (1%)	69	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
79	cc	55/55 (100%)	52 (94%)	3 (6%)	21	57
80	dd	48/48 (100%)	46 (96%)	2 (4%)	30	63
81	ee	46/46 (100%)	44 (96%)	2 (4%)	29	63
82	ff	61/61 (100%)	54 (88%)	7 (12%)	5	29
83	gg	272/272 (100%)	271 (100%)	1 (0%)	91	97
All	All	9936/10274 (97%)	9738 (98%)	198 (2%)	57	79

All (198) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	A	4	VAL
7	A	125	LYS
7	A	163	ARG
7	A	193	ARG
8	B	10	ARG
8	B	24	ARG
8	B	81	THR
8	B	261	ARG
8	B	278	THR
8	B	297	LYS
9	C	38	ASN
9	C	57	LEU
9	C	188	ARG
9	C	204	ARG
9	C	274	LYS
9	C	312	ARG
10	D	33	ARG
10	D	36	LEU
10	D	56	THR
10	D	64	ILE
10	D	111	ASN
10	D	259	ARG
10	D	268	ARG
11	E	58	ARG
11	E	74	LYS
11	E	112	LEU
11	E	164	ARG
12	F	204	ASN
13	G	88	ARG
13	G	106	ARG

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Mol	Chain	Res	Type
13	G	134	ASN
13	G	150	LYS
13	G	166	ARG
13	G	215	ASP
13	G	228	ARG
13	G	242	ARG
13	G	249	ARG
13	G	310	LYS
14	H	71	ARG
14	H	128	MET
14	H	161	ILE
15	I	10	ARG
15	I	162	ARG
16	J	57	VAL
17	L	45	ARG
18	M	38	VAL
18	M	58	THR
18	M	119	ARG
18	M	132	ARG
19	N	7	ILE
19	N	23	LEU
19	N	64	ILE
19	N	162	ARG
20	O	117	ARG
20	O	140	ARG
20	O	180	GLN
21	P	140	MET
22	Q	67	ILE
22	Q	78	LYS
23	R	123	LEU
23	R	176	ARG
23	R	177	LEU
24	S	83	ARG
24	S	90	THR
25	T	68	THR
25	T	81	LYS
25	T	159	MET
26	U	40	GLU
26	U	47	ILE
26	U	81	ARG
27	V	18	LEU
27	V	48	ARG

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Mol	Chain	Res	Type
28	W	109	ILE
28	W	110	ARG
30	Y	2	LYS
30	Y	84	ARG
30	Y	103	LYS
31	Z	98	LYS
32	a	94	LYS
33	b	60	ASN
33	b	68	ARG
33	b	91	ARG
33	b	117	ARG
34	c	17	ARG
34	c	20	LEU
34	c	90	ARG
35	d	57	MET
36	e	33	ARG
36	e	92	ASN
36	e	121	ARG
37	f	16	ARG
37	f	63	LYS
37	f	76	ARG
38	g	5	LEU
38	g	54	ARG
38	g	59	VAL
38	g	107	LEU
39	h	56	ARG
39	h	109	ARG
40	i	23	LYS
40	i	29	ARG
41	j	67	LEU
42	k	9	LYS
43	l	33	ASN
44	m	93	ASN
44	m	102	LYS
45	n	6	ARG
46	o	82	MET
48	r	11	ARG
48	r	67	ARG
48	r	106	LEU
48	r	107	ARG
48	r	119	ARG
49	u	15	ARG

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Mol	Chain	Res	Type
49	u	25	ARG
49	u	39	LYS
49	u	47	LYS
49	u	93	LEU
49	u	199	GLN
49	u	206	ILE
51	AA	184	ARG
51	AA	212	LYS
52	BB	51	ARG
52	BB	179	ASN
52	BB	207	LEU
52	BB	213	ARG
53	CC	121	ARG
53	CC	137	VAL
53	CC	209	VAL
54	DD	57	ASN
54	DD	65	ARG
54	DD	76	ARG
54	DD	106	ARG
54	DD	214	LYS
54	DD	227	LYS
55	EE	16	LYS
55	EE	45	ILE
55	EE	148	ARG
55	EE	256	LEU
56	FF	42	LYS
56	FF	111	VAL
56	FF	122	ARG
56	FF	127	ARG
56	FF	198	ARG
57	GG	154	ARG
57	GG	190	ARG
57	GG	231	ARG
58	HH	28	LEU
58	HH	36	LEU
58	HH	144	ILE
59	II	47	ARG
59	II	84	ASN
62	LL	20	LYS
62	LL	32	LYS
64	NN	28	LEU
65	OO	20	GLN

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Mol	Chain	Res	Type
65	OO	84	ARG
65	OO	88	LEU
65	OO	117	ARG
65	OO	142	ARG
65	OO	149	ARG
66	PP	35	GLN
66	PP	104	GLN
67	QQ	41	MET
67	QQ	53	GLU
67	QQ	60	LYS
68	RR	26	ASN
68	RR	72	LYS
69	SS	45	LEU
70	TT	24	LYS
70	TT	28	LEU
70	TT	75	MET
72	VV	81	LYS
73	WW	28	ARG
73	WW	52	ILE
73	WW	104	LEU
75	YY	17	LEU
75	YY	18	LEU
75	YY	100	LYS
77	aa	5	ARG
77	aa	28	ARG
77	aa	51	ARG
78	bb	36	LYS
79	cc	17	VAL
79	cc	31	ARG
79	cc	66	ARG
80	dd	19	ARG
80	dd	44	ARG
81	ee	99	LYS
81	ee	126	LYS
82	ff	87	THR
82	ff	96	LYS
82	ff	97	LYS
82	ff	99	LYS
82	ff	107	LYS
82	ff	116	ARG
82	ff	119	ARG
83	gg	38	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
8	B	175	GLN
18	M	20	HIS
18	M	48	GLN
33	b	60	ASN
49	u	44	GLN
52	BB	179	ASN
53	CC	267	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	6/7 (85%)	3 (50%)	0
2	2	74/76 (97%)	21 (28%)	0
3	4	74/75 (98%)	37 (50%)	1 (1%)
4	5	3526/3597 (98%)	859 (24%)	67 (1%)
5	7	119/120 (99%)	16 (13%)	0
50	9	1671/1698 (98%)	413 (24%)	26 (1%)
6	8	149/151 (98%)	30 (20%)	1 (0%)
All	All	5619/5724 (98%)	1379 (24%)	95 (1%)

All (1379) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	43	A
1	1	46	G
1	1	47	U
2	2	7	G
2	2	8	U
2	2	9	A
2	2	13	U
2	2	16	C
2	2	20	U
2	2	20(A)	U
2	2	21	A
2	2	34	A
2	2	35	A
2	2	42	A
2	2	48	C
2	2	49	C
2	2	56	C

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Mol	Chain	Res	Type
2	2	58	A
2	2	63	G
2	2	65	G
2	2	67	G
2	2	72	C
2	2	75	C
2	2	76	A
3	4	2	C
3	4	3	C
3	4	4	C
3	4	7	A
3	4	8	U
3	4	10	G
3	4	13	C
3	4	14	A
3	4	15	G
3	4	16	C
3	4	18	U
3	4	19	G
3	4	20	U
3	4	21	A
3	4	26	A
3	4	27	U
3	4	33	U
3	4	34	U
3	4	35	U
3	4	36	U
3	4	37	A
3	4	38	A
3	4	39	U
3	4	46	G
3	4	47	U
3	4	48	C
3	4	49	C
3	4	56	C
3	4	57	A
3	4	58	A
3	4	59	G
3	4	60	U
3	4	61	C
3	4	70	G
3	4	71	G

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Mol	Chain	Res	Type
3	4	72	C
3	4	73	G
4	5	5	A
4	5	12	A
4	5	13	U
4	5	17	A
4	5	21	G
4	5	25	A
4	5	39	A
4	5	42	A
4	5	43	U
4	5	47	A
4	5	48	G
4	5	49	U
4	5	56	A
4	5	58	G
4	5	59	A
4	5	64	A
4	5	65	A
4	5	71	C
4	5	72	C
4	5	73	A
4	5	76	A
4	5	84	A
4	5	91	G
4	5	93	G
4	5	104	G
4	5	108	A
4	5	109	G
4	5	110	C
4	5	116	G
4	5	119	G
4	5	120	A
4	5	122	U
4	5	126	C
4	5	134	G
4	5	135	G
4	5	136	C
4	5	137	G
4	5	142	G
4	5	146	G
4	5	151	G

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Mol	Chain	Res	Type
4	5	157	U
4	5	159	C
4	5	167	C
4	5	170	C
4	5	172	C
4	5	173	C
4	5	182	G
4	5	195	C
4	5	200	U
4	5	201	C
4	5	203	U
4	5	205	C
4	5	209	U
4	5	216	C
4	5	218	A
4	5	220	C
4	5	224	U
4	5	225	G
4	5	233	U
4	5	234	G
4	5	245	C
4	5	246	G
4	5	256	G
4	5	265	C
4	5	266	C
4	5	275	C
4	5	276	C
4	5	280	G
4	5	297	U
4	5	306	A
4	5	309	C
4	5	310	G
4	5	315	G
4	5	316	U
4	5	334	A
4	5	340	C
4	5	345	C
4	5	349	A
4	5	350	C
4	5	357	U
4	5	362	A
4	5	363	A

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Mol	Chain	Res	Type
4	5	379	G
4	5	386	A
4	5	387	G
4	5	398	A2M
4	5	401	G
4	5	407	A
4	5	409	G
4	5	412	G
4	5	413	G
4	5	414	C
4	5	431	G
4	5	433	A
4	5	440	U
4	5	446	C
4	5	449	C
4	5	450	G
4	5	452	A
4	5	453	G
4	5	454	U
4	5	455	C
4	5	463	A
4	5	464	G
4	5	467	U
4	5	468	U
4	5	482	G
4	5	483	G
4	5	486	C
4	5	489	C
4	5	492	U
4	5	493	G
4	5	496	G
4	5	497	G
4	5	498	C
4	5	499	G
4	5	505	G
4	5	506	C
4	5	510	U
4	5	522	C
4	5	641	G
4	5	667	A
4	5	669	C
4	5	684	G

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Mol	Chain	Res	Type
4	5	685	C
4	5	686	A
4	5	687	U
4	5	688	U
4	5	692	A
4	5	696	C
4	5	697	G
4	5	704	C
4	5	705	G
4	5	708	G
4	5	719	C
4	5	722	G
4	5	729	2MG
4	5	730	G
4	5	731	G
4	5	742	G
4	5	746	A
4	5	747	A
4	5	748	G
4	5	749	G
4	5	758	G
4	5	759	G
4	5	914	U
4	5	917	A
4	5	918	G
4	5	925	C
4	5	926	G
4	5	929	A
4	5	931	C
4	5	932	A
4	5	933	G
4	5	934	C
4	5	938	C
4	5	939	G
4	5	943	A
4	5	944	A
4	5	945	U
4	5	956	A
4	5	959	G
4	5	960	A
4	5	961	G
4	5	964	A

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Mol	Chain	Res	Type
4	5	965	G
4	5	966	A
4	5	967	C
4	5	968	C
4	5	969	C
4	5	970	G
4	5	972	C
4	5	978	C
4	5	980	C
4	5	983	U
4	5	1072	C
4	5	1073	G
4	5	1078	A
4	5	1079	C
4	5	1080	C
4	5	1081	C
4	5	1084	C
4	5	1098	G
4	5	1175	A
4	5	1179	U
4	5	1180	C
4	5	1187	G
4	5	1193	C
4	5	1195	G
4	5	1211	G
4	5	1212	G
4	5	1214	C
4	5	1215	C
4	5	1234	G
4	5	1235	G
4	5	1236	C
4	5	1237	C
4	5	1238	A
4	5	1239	C
4	5	1272	C
4	5	1273	G
4	5	1275	G
4	5	1276	C
4	5	1279	A
4	5	1281	G
4	5	1284	G
4	5	1287	G

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Mol	Chain	Res	Type
4	5	1292	C
4	5	1293	G
4	5	1294	A
4	5	1295	U
4	5	1296	G
4	5	1301	C
4	5	1303	A
4	5	1304	C
4	5	1314	C
4	5	1319	U
4	5	1321	G
4	5	1322	1MA
4	5	1326	A2M
4	5	1330	A
4	5	1337	A
4	5	1353	G
4	5	1354	A
4	5	1358	G
4	5	1359	G
4	5	1371	A
4	5	1372	A
4	5	1377	G
4	5	1381	U
4	5	1382	G
4	5	1387	A
4	5	1394	G
4	5	1397	A
4	5	1398	A
4	5	1406(C)	G
4	5	1411(C)	C
4	5	1412	G
4	5	1415	G
4	5	1419	G
4	5	1420	A
4	5	1421	G
4	5	1429	C
4	5	1436	C
4	5	1437	C
4	5	1438	U
4	5	1441	C
4	5	1443	A
4	5	1445	U

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Mol	Chain	Res	Type
4	5	1446	C
4	5	1448	G
4	5	1457	G
4	5	1458	C
4	5	1465	G
4	5	1475	G
4	5	1476	C
4	5	1477	C
4	5	1482	G
4	5	1483	C
4	5	1497	A
4	5	1498	G
4	5	1502	G
4	5	1514	U
4	5	1518	A
4	5	1523	A
4	5	1534	A2M
4	5	1547	A
4	5	1563	A
4	5	1566	C
4	5	1578	U
4	5	1582	PSU
4	5	1591	U
4	5	1596	U
4	5	1602	U
4	5	1612	G
4	5	1613	A
4	5	1624	G
4	5	1625	OMG
4	5	1626	G
4	5	1627	G
4	5	1631	A
4	5	1633	G
4	5	1634	A
4	5	1638	A
4	5	1640	C
4	5	1649	U
4	5	1650	A
4	5	1654	G
4	5	1661	C
4	5	1671	U
4	5	1676	C

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Mol	Chain	Res	Type
4	5	1677	PSU
4	5	1678	C
4	5	1679	A
4	5	1691	G
4	5	1724	G
4	5	1726	U
4	5	1731	C
4	5	1741	G
4	5	1742	A
4	5	1751	A
4	5	1755	C
4	5	1756	U
4	5	1757	U
4	5	1764	G
4	5	1768	C
4	5	1772	C
4	5	1773	U
4	5	1774	C
4	5	1775	A
4	5	1776	A
4	5	1781	U
4	5	1787	A
4	5	1804	A
4	5	1805	A
4	5	1806	G
4	5	1808	C
4	5	1812	C
4	5	1815	G
4	5	1819	G
4	5	1821	G
4	5	1828	C
4	5	1833	G
4	5	1834	U
4	5	1835	G
4	5	1836	G
4	5	1837	A
4	5	1842	G
4	5	1843	A
4	5	1855	G
4	5	1866	UR3
4	5	1869	G
4	5	1881	C

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Mol	Chain	Res	Type
4	5	1888	A
4	5	1897	A
4	5	1917	A
4	5	1918	U
4	5	1920	C
4	5	1921	C
4	5	1922	G
4	5	1930	U
4	5	1931	C
4	5	1938	C
4	5	1940	G
4	5	1945	G
4	5	1948	G
4	5	1957	U
4	5	1958	A
4	5	1960	A
4	5	1961	G
4	5	1962	A
4	5	1969	G
4	5	1971	U
4	5	1972	G
4	5	1974	U
4	5	1975	G
4	5	1976	G
4	5	1977	C
4	5	1978	C
4	5	1980	U
4	5	1983	A
4	5	1984	A
4	5	1987	C
4	5	1991	A
4	5	1992	U
4	5	1997	U
4	5	2001	G
4	5	2002	A
4	5	2003	G
4	5	2004	U
4	5	2010	A
4	5	2011	C
4	5	2025	A
4	5	2026	A
4	5	2029	A

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Mol	Chain	Res	Type
4	5	2030	A
4	5	2033	A
4	5	2034	G
4	5	2046	G
4	5	2047	A
4	5	2048	U
4	5	2052	G
4	5	2055	G
4	5	2056	G
4	5	2058	G
4	5	2062	C
4	5	2069	A
4	5	2070	U
4	5	2072	C
4	5	2084	U
4	5	2085	G
4	5	2089	G
4	5	2090	U
4	5	2092	G
4	5	2093	G
4	5	2094	C
4	5	2095	A
4	5	2097	A
4	5	2098	G
4	5	2100	G
4	5	2102	G
4	5	2104	A
4	5	2106	G
4	5	2107	A
4	5	2108	G
4	5	2109	A
4	5	2259	G
4	5	2260	C
4	5	2267	U
4	5	2268	A
4	5	2269	C
4	5	2270	G
4	5	2275	G
4	5	2289	C
4	5	2300	A
4	5	2301	G
4	5	2304	U

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Mol	Chain	Res	Type
4	5	2307	A
4	5	2313	A
4	5	2314	G
4	5	2316	G
4	5	2319	C
4	5	2332	A
4	5	2333	G
4	5	2335	C
4	5	2347	A
4	5	2348	G
4	5	2351	C
4	5	2355	G
4	5	2357	G
4	5	2360	A
4	5	2364	OMG
4	5	2395	A
4	5	2396	A
4	5	2398	U
4	5	2408	U
4	5	2410	C
4	5	2416	G
4	5	2417	A
4	5	2422	OMC
4	5	2424	OMG
4	5	2425	U
4	5	2433	G
4	5	2441	C
4	5	2442	G
4	5	2447	U
4	5	2450	G
4	5	2453	A
4	5	2467	U
4	5	2471	G
4	5	2474	G
4	5	2475	G
4	5	2488	C
4	5	2489	C
4	5	2490	U
4	5	2491	C
4	5	2495	U
4	5	2503	G
4	5	2504	C

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Mol	Chain	Res	Type
4	5	2505	C
4	5	2506	G
4	5	2513	A
4	5	2529	A
4	5	2530	U
4	5	2537	A
4	5	2544	G
4	5	2546	G
4	5	2547	G
4	5	2553	A
4	5	2554	U
4	5	2566	G
4	5	2568	C
4	5	2571	C
4	5	2575	U
4	5	2583	C
4	5	2586	G
4	5	2587	A
4	5	2588	C
4	5	2589	C
4	5	2600	A
4	5	2601	A
4	5	2611	A
4	5	2618	G
4	5	2620	G
4	5	2623	A
4	5	2627	C
4	5	2638	G
4	5	2639	U
4	5	2649	G
4	5	2653	C
4	5	2659	A
4	5	2661	U
4	5	2662	G
4	5	2663	G
4	5	2668	G
4	5	2669	C
4	5	2670	C
4	5	2673	G
4	5	2676	A
4	5	2679	G
4	5	2681	G

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Mol	Chain	Res	Type
4	5	2686	G
4	5	2687	U
4	5	2694	G
4	5	2695	A
4	5	2696	A
4	5	2708	U
4	5	2710	C
4	5	2711	G
4	5	2714	G
4	5	2715	G
4	5	2723	U
4	5	2724	G
4	5	2725	A
4	5	2726	G
4	5	2740	U
4	5	2743	A
4	5	2744	A
4	5	2752	G
4	5	2753	G
4	5	2763	U
4	5	2764	A
4	5	2769	U
4	5	2787	A
4	5	2788	U
4	5	2790	U
4	5	2794	C
4	5	2798	A
4	5	2803	U
4	5	2814	C
4	5	2826	U
4	5	2827	G
4	5	2828	U
4	5	2829	U
4	5	2837	U
4	5	2838	G
4	5	2842	G
4	5	2849	A
4	5	2855	G
4	5	2856	C
4	5	2869	U
4	5	2875	C
4	5	2879	A

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Mol	Chain	Res	Type
4	5	2884	G
4	5	2898	G
4	5	3598	C
4	5	3604	A
4	5	3605	C
4	5	3606	U
4	5	3615	G
4	5	3616	U
4	5	3625	G
4	5	3626	G
4	5	3630	A
4	5	3635	A
4	5	3643	A
4	5	3646	A
4	5	3650	C
4	5	3662	A
4	5	3664	G
4	5	3673	C
4	5	3674	G
4	5	3679	U
4	5	3680	U
4	5	3691	G
4	5	3692	A
4	5	3696	C
4	5	3698	G
4	5	3705	G
4	5	3712	A
4	5	3714	G
4	5	3729	PSU
4	5	3740	G
4	5	3753	G
4	5	3759	A
4	5	3760	A
4	5	3763	A
4	5	3765	G
4	5	3773	U
4	5	3774	A
4	5	3776	G
4	5	3777	G
4	5	3783	A
4	5	3784	A
4	5	3785	A2M

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Mol	Chain	Res	Type
4	5	3786	U
4	5	3787	G
4	5	3789	C
4	5	3792	OMG
4	5	3799	A
4	5	3810	C
4	5	3811	G
4	5	3812	C
4	5	3814	U
4	5	3817	A
4	5	3819	G
4	5	3822	U
4	5	3838	U
4	5	3839	G
4	5	3840	U
4	5	3851	U
4	5	3865	A
4	5	3867	A2M
4	5	3868	G
4	5	3876	A
4	5	3877	A
4	5	3878	C
4	5	3879	G
4	5	3881	G
4	5	3889	G
4	5	3892	U
4	5	3898	G
4	5	3901	A
4	5	3904	G
4	5	3905	A
4	5	3906	A
4	5	3907	G
4	5	3908	A
4	5	3915	U
4	5	3916	G
4	5	3926	C
4	5	3927	U
4	5	3938	G
4	5	3939	G
4	5	3946	G
4	5	3947	A
4	5	3948	C

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Mol	Chain	Res	Type
4	5	3956	G
4	5	3957	U
4	5	3965	A
4	5	3971	G
4	5	3972	A
4	5	3973	G
4	5	3974	G
4	5	3975	C
4	5	3976	C
4	5	4043	G
4	5	4047	A
4	5	4050	A
4	5	4051	C
4	5	4053	A
4	5	4054	C
4	5	4055	U
4	5	4056	A
4	5	4061	G
4	5	4066	U
4	5	4073	A
4	5	4076	G
4	5	4084	G
4	5	4085	A
4	5	4086	G
4	5	4097	G
4	5	4116	C
4	5	4119	C
4	5	4120	U
4	5	4121	G
4	5	4125	C
4	5	4127	A
4	5	4158	C
4	5	4162	C
4	5	4166	G
4	5	4170	A
4	5	4171	C
4	5	4172	A
4	5	4173	G
4	5	4183	G
4	5	4184	G
4	5	4191	G
4	5	4195	G

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Mol	Chain	Res	Type
4	5	4197	G
4	5	4212	A
4	5	4213	A
4	5	4229	U
4	5	4232	U
4	5	4233	A
4	5	4241	C
4	5	4251	A
4	5	4254	G
4	5	4255	A
4	5	4265	U
4	5	4266	G
4	5	4268	A
4	5	4271	A
4	5	4273	A
4	5	4281	A
4	5	4282	A
4	5	4287	G
4	5	4291	G
4	5	4293	PSU
4	5	4304	A
4	5	4305	G
4	5	4306	OMU
4	5	4308	C
4	5	4314	C
4	5	4317	A
4	5	4318	C
4	5	4319	C
4	5	4326	G
4	5	4330	G
4	5	4332	C
4	5	4348	A
4	5	4349	C
4	5	4354	U
4	5	4364	G
4	5	4372	U
4	5	4373	G
4	5	4376	A
4	5	4377	G
4	5	4378	A
4	5	4379	A
4	5	4380	A

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Mol	Chain	Res	Type
4	5	4387	C
4	5	4391	G
4	5	4393	G
4	5	4394	A
4	5	4395	U
4	5	4396	A
4	5	4398	C
4	5	4415	1MA
4	5	4419	U
4	5	4422	A
4	5	4424	A
4	5	4438	U
4	5	4440	G
4	5	4448	G
4	5	4449	A
4	5	4450	PSU
4	5	4464	A
4	5	4475	G
4	5	4476	C
4	5	4482	U
4	5	4495	G
4	5	4500	PSU
4	5	4502	C
4	5	4510	A
4	5	4512	U
4	5	4513	A
4	5	4515	G
4	5	4518	A
4	5	4519	C
4	5	4520	G
4	5	4522	G
4	5	4523	A2M
4	5	4524	G
4	5	4548	A
4	5	4549	G
4	5	4560	C
4	5	4567	G
4	5	4572	U
4	5	4573	G
4	5	4574	U
4	5	4575	G
4	5	4584	A

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Mol	Chain	Res	Type
4	5	4586	G
4	5	4587	G
4	5	4589	A
4	5	4590	A
4	5	4599	A
4	5	4627	U
4	5	4629	U
4	5	4633	G
4	5	4635	A
4	5	4636	PSU
4	5	4637	OMG
4	5	4639	G
4	5	4656	A
4	5	4657	U
4	5	4661	G
4	5	4664	A
4	5	4670	C
4	5	4677	U
4	5	4693	C
4	5	4694	G
4	5	4695	C
4	5	4700	A
4	5	4702	G
4	5	4709	U
4	5	4718	G
4	5	4719	G
4	5	4720	C
4	5	4745	G
4	5	4750	G
4	5	4754	G
4	5	4756	C
4	5	4757	C
4	5	4759	C
4	5	4761	G
4	5	4765	G
4	5	4771	C
4	5	4772	C
4	5	4860	G
4	5	4868	G
4	5	4870	OMG
4	5	4872	2MG
4	5	4873	G

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Mol	Chain	Res	Type
4	5	4875	G
4	5	4877	G
4	5	4882	U
4	5	4883	C
4	5	4885	U
4	5	4887	C
4	5	4895	C
4	5	4896	G
4	5	4903	G
4	5	4904	G
4	5	4906	C
4	5	4910	A
4	5	4912	G
4	5	4914	G
4	5	4915	G
4	5	4920	C
4	5	4921	C
4	5	4924	C
4	5	4925	U
4	5	4926	C
4	5	4927	G
4	5	4928	C
4	5	4931	G
4	5	4937	C
4	5	4938	A
4	5	4940	C
4	5	4943	A
4	5	4944	C
4	5	4947	U
4	5	4948	C
4	5	4949	G
4	5	4950	U
4	5	4951	G
4	5	4956	A
4	5	4957	C
4	5	4959	U
4	5	4964	C
4	5	4965	U
4	5	4966	A
4	5	4975	G
4	5	4976	U
4	5	4982	A

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Mol	Chain	Res	Type
4	5	4985	U
4	5	4988	U
4	5	4990	C
4	5	4991	U
4	5	4993	G
4	5	4999	G
4	5	5006	U
4	5	5014	A
4	5	5017	G
4	5	5022	U
4	5	5034	A
4	5	5040	U
4	5	5041	G
4	5	5047	C
4	5	5050	C
4	5	5053	U
4	5	5054	C
4	5	5058	A
4	5	5061	A
4	5	5062	G
4	5	5064	G
5	7	7	G
5	7	13	A
5	7	22	A
5	7	25	G
5	7	33	U
5	7	41	G
5	7	53	U
5	7	54	A
5	7	63	C
5	7	64	G
5	7	97	G
5	7	100	A
5	7	102	U
5	7	110	G
5	7	111	C
5	7	120	U
6	8	2	G
6	8	3	A
6	8	23	C
6	8	34	U
6	8	35	C

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Mol	Chain	Res	Type
6	8	39	G
6	8	49	G
6	8	51	U
6	8	59	A
6	8	62	A
6	8	63	U
6	8	64	U
6	8	75	G
6	8	77	A
6	8	78	G
6	8	79	G
6	8	87	G
6	8	99	U
6	8	103	A
6	8	105	C
6	8	109	C
6	8	110	U
6	8	111	U
6	8	114	G
6	8	124	U
6	8	125	C
6	8	126	C
6	8	127	U
6	8	137	A
6	8	147	G
50	9	2	A
50	9	3	C
50	9	17	C
50	9	25	A
50	9	26	U
50	9	33	G
50	9	41	G
50	9	44	U
50	9	45	A
50	9	46	A
50	9	56	G
50	9	58	C
50	9	62	G
50	9	67	C
50	9	68	A
50	9	70	G
50	9	71	G

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Mol	Chain	Res	Type
50	9	73	C
50	9	74	G
50	9	77	A
50	9	79	A
50	9	92	A
50	9	99	A
50	9	103	A
50	9	104	A
50	9	110	U
50	9	111	A
50	9	113	G
50	9	115	U
50	9	116	OMU
50	9	121	OMU
50	9	123	G
50	9	124	U
50	9	126	G
50	9	127	C
50	9	129	C
50	9	130	G
50	9	141	A
50	9	142	C
50	9	143	U
50	9	147	A
50	9	154	U
50	9	155	G
50	9	158	A
50	9	159	A2M
50	9	160	U
50	9	162	C
50	9	163	U
50	9	166	A2M
50	9	167	G
50	9	168	C
50	9	175	A
50	9	180	G
50	9	182	C
50	9	183	G
50	9	184	G
50	9	188	C
50	9	189	U
50	9	192	C

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Mol	Chain	Res	Type
50	9	202	G
50	9	206	G
50	9	213	G
50	9	215	G
50	9	289	G
50	9	293	C
50	9	294	U
50	9	302	A
50	9	307	G
50	9	308	G
50	9	309	G
50	9	312	G
50	9	315	C
50	9	318	A
50	9	319	C
50	9	332	G
50	9	339	A
50	9	347	G
50	9	350	C
50	9	351	G
50	9	357	C
50	9	360	A
50	9	362	C
50	9	364	A
50	9	367	U
50	9	368	U
50	9	369	C
50	9	370	G
50	9	381	C
50	9	385	G
50	9	398	A
50	9	400	C
50	9	408	A
50	9	409	C
50	9	417	C
50	9	418	A
50	9	420	G
50	9	428	U
50	9	429	C
50	9	435	A
50	9	438	G
50	9	441	C

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Mol	Chain	Res	Type
50	9	448	A
50	9	449	A
50	9	450	C
50	9	465	A
50	9	466	G
50	9	471	G
50	9	472	C
50	9	473	A
50	9	474	G
50	9	482	G
50	9	487	U
50	9	492	C
50	9	530	U
50	9	532	C
50	9	533	A
50	9	536	A
50	9	537	C
50	9	542	U
50	9	546	G
50	9	547	G
50	9	548	C
50	9	549	C
50	9	550	C
50	9	551	U
50	9	554	A
50	9	555	A
50	9	556	U
50	9	559	G
50	9	560	A
50	9	562	U
50	9	563	G
50	9	564	A
50	9	569	A
50	9	576	A
50	9	583	A
50	9	587	A
50	9	588	G
50	9	589	G
50	9	590	A
50	9	591	U
50	9	594	A
50	9	597	G

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Mol	Chain	Res	Type
50	9	603	C
50	9	604	A
50	9	605	A
50	9	606	G
50	9	607	U
50	9	608	C
50	9	614	C
50	9	628	A
50	9	629	A
50	9	631	U
50	9	643	A
50	9	655	A
50	9	658	U
50	9	660	C
50	9	664	A
50	9	666	U
50	9	668	A2M
50	9	669	A
50	9	671	A
50	9	672	A
50	9	673	G
50	9	683	OMG
50	9	684	G
50	9	688	U
50	9	689	U
50	9	690	G
50	9	752	G
50	9	753	C
50	9	754	G
50	9	798	G
50	9	801	U
50	9	804	U
50	9	811	A
50	9	821	G
50	9	822	PSU
50	9	830	A
50	9	833	C
50	9	834	C
50	9	845	G
50	9	847	A
50	9	865	A
50	9	870	A

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Mol	Chain	Res	Type
50	9	871	U
50	9	872	A
50	9	873	G
50	9	875	A
50	9	878	G
50	9	887	U
50	9	888	U
50	9	890	U
50	9	892	U
50	9	893	U
50	9	898	U
50	9	901	G
50	9	913	A
50	9	914	U
50	9	920	A
50	9	933	G
50	9	934	G
50	9	954	U
50	9	971	G
50	9	978	G
50	9	985	G
50	9	986	G
50	9	990	A
50	9	991	G
50	9	992	A
50	9	999	G
50	9	1002	U
50	9	1017	U
50	9	1023	A
50	9	1026	C
50	9	1041	G
50	9	1045	U
50	9	1058	A
50	9	1060	A
50	9	1082	A
50	9	1083	A
50	9	1084	A
50	9	1085	C
50	9	1086	G
50	9	1088	U
50	9	1097	G
50	9	1099	G

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Mol	Chain	Res	Type
50	9	1100	A
50	9	1109	C
50	9	1111	U
50	9	1113	A
50	9	1114	U
50	9	1115	U
50	9	1116	C
50	9	1117	C
50	9	1118	C
50	9	1121	G
50	9	1123	C
50	9	1126	G
50	9	1131	G
50	9	1133	A
50	9	1138	C
50	9	1149	A
50	9	1153	C
50	9	1154	U
50	9	1155	U
50	9	1170	A
50	9	1194	A
50	9	1195	A
50	9	1197	G
50	9	1207	G
50	9	1212	G
50	9	1215	C
50	9	1221	G
50	9	1223	A
50	9	1224	G
50	9	1242	U
50	9	1243	PSU
50	9	1247	C
50	9	1249	C
50	9	1250	A
50	9	1251	A
50	9	1253	A
50	9	1254	C
50	9	1256	G
50	9	1257	G
50	9	1259	A
50	9	1264	C
50	9	1273	C

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Mol	Chain	Res	Type
50	9	1274	G
50	9	1275	G
50	9	1282	A
50	9	1283	C
50	9	1284	A
50	9	1285	G
50	9	1286	G
50	9	1287	A
50	9	1288	U
50	9	1293	A
50	9	1294	G
50	9	1298	G
50	9	1299	A
50	9	1301	A
50	9	1302	G
50	9	1303	C
50	9	1305	C
50	9	1306	U
50	9	1307	U
50	9	1308	U
50	9	1310	U
50	9	1312	G
50	9	1313	A
50	9	1314	U
50	9	1316	C
50	9	1320	G
50	9	1322	G
50	9	1333	U
50	9	1341	C
50	9	1342	U
50	9	1348	G
50	9	1355	C
50	9	1369	A
50	9	1371	U
50	9	1372	U
50	9	1375	G
50	9	1376	A
50	9	1378	A
50	9	1382	A
50	9	1395	C
50	9	1396	A
50	9	1397	U

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Mol	Chain	Res	Type
50	9	1401	A
50	9	1402	A
50	9	1404	U
50	9	1405	A
50	9	1406	G
50	9	1409	A
50	9	1428	G
50	9	1429	G
50	9	1449	G
50	9	1454	A
50	9	1462	U
50	9	1463	U
50	9	1464	C
50	9	1466	G
50	9	1473	G
50	9	1476	A
50	9	1477	U
50	9	1480	A
50	9	1487	A
50	9	1489	A
50	9	1490	G
50	9	1498	A
50	9	1504	U
50	9	1506	A
50	9	1507	G
50	9	1508	A
50	9	1509	U
50	9	1510	G
50	9	1521	C
50	9	1522	A
50	9	1523	C
50	9	1531	A
50	9	1533	A
50	9	1548	G
50	9	1552	G
50	9	1553	C
50	9	1554	C
50	9	1555	U
50	9	1556	A
50	9	1557	C
50	9	1560	U
50	9	1570	G

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Mol	Chain	Res	Type
50	9	1574	C
50	9	1575	G
50	9	1578	U
50	9	1580	A
50	9	1585	U
50	9	1586	U
50	9	1587	G
50	9	1588	A
50	9	1600	G
50	9	1601	A
50	9	1604	G
50	9	1606	G
50	9	1621	U
50	9	1623	A
50	9	1637	A
50	9	1638	G
50	9	1646	C
50	9	1648	G
50	9	1649	U
50	9	1654	G
50	9	1664	A
50	9	1665	G
50	9	1671	G
50	9	1683	C
50	9	1695	A
50	9	1698	C
50	9	1699	A
50	9	1709	G
50	9	1721	U
50	9	1722	G
50	9	1726	G
50	9	1732	G
50	9	1744	G
50	9	1756	C
50	9	1757	G
50	9	1775	U
50	9	1779	G
50	9	1782	G
50	9	1783	C
50	9	1784	G
50	9	1785	C
50	9	1819	A

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Mol	Chain	Res	Type
50	9	1823	A
50	9	1824	A
50	9	1825	A
50	9	1829	G
50	9	1831	A
50	9	1835	A
50	9	1836	G
50	9	1838	U
50	9	1849	G
50	9	1859	A
50	9	1861	G
50	9	1862	G
50	9	1863	A
50	9	1864	U
50	9	1865	C
50	9	1866	A
50	9	1867	U
50	9	1869	A

All (95) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	4	72	C
4	5	12	A
4	5	47	A
4	5	48	G
4	5	125	C
4	5	134	G
4	5	217	C
4	5	245	C
4	5	265	C
4	5	266	C
4	5	275	C
4	5	385	A
4	5	406	C
4	5	449	C
4	5	485	C
4	5	492	U
4	5	504	G
4	5	684	G
4	5	696	C
4	5	930	G

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Mol	Chain	Res	Type
4	5	959	G
4	5	1072	C
4	5	1174	G
4	5	1211	G
4	5	1236	C
4	5	1238	A
4	5	1291	G
4	5	1329	G
4	5	1370	G
4	5	1406(B)	C
4	5	1440	U
4	5	1445	U
4	5	1633	G
4	5	1804	A
4	5	1818	G
4	5	1979	A
4	5	1983	A
4	5	2046	G
4	5	2089	G
4	5	2266	C
4	5	2474	G
4	5	2502	A
4	5	2546	G
4	5	2587	A
4	5	2661	U
4	5	2695	A
4	5	3603	G
4	5	3625	G
4	5	3697	U
4	5	3876	A
4	5	3888	G
4	5	3904	G
4	5	3973	G
4	5	4053	A
4	5	4065	G
4	5	4075	U
4	5	4119	C
4	5	4232	U
4	5	4254	G
4	5	4447	5MC
4	5	4448	G
4	5	4559	A

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Mol	Chain	Res	Type
4	5	4699	U
4	5	4719	G
4	5	4884	G
4	5	4925	U
4	5	4936	G
4	5	4947	U
6	8	124	U
50	9	110	U
50	9	140	U
50	9	369	C
50	9	434	G
50	9	465	A
50	9	532	C
50	9	553	U
50	9	642	U
50	9	688	U
50	9	752	G
50	9	870	A
50	9	874	G
50	9	1137	U
50	9	1253	A
50	9	1285	G
50	9	1286	G
50	9	1394	G
50	9	1395	C
50	9	1489	A
50	9	1505	U
50	9	1508	A
50	9	1520	G
50	9	1637	A
50	9	1664	A
50	9	1665	G
50	9	1824	A

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

137 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$
50	OMG	9	509	84,50	18,26,27	2.39	8 (44%)	19,38,41	1.58	4 (21%)
4	PSU	5	4450	4,84	18,21,22	1.14	2 (11%)	22,30,33	2.00	5 (22%)
4	2MG	5	4872	4,18	18,26,27	2.61	7 (38%)	16,38,41	1.63	4 (25%)
4	A2M	5	2363	4,84	18,25,26	4.72	10 (55%)	18,36,39	2.76	4 (22%)
4	7MG	5	2522	4	22,26,27	3.38	10 (45%)	29,39,42	2.08	8 (27%)
4	PSU	5	4531	4	18,21,22	1.10	2 (11%)	22,30,33	1.69	4 (18%)
4	OMG	5	2050	4	18,26,27	2.34	8 (44%)	19,38,41	1.56	4 (21%)
4	7MG	5	1605	4	22,26,27	3.32	10 (45%)	29,39,42	2.09	8 (27%)
4	A2M	5	1871	4,84	18,25,26	4.64	10 (55%)	18,36,39	2.72	4 (22%)
4	OMU	5	4306	4	19,22,23	2.71	8 (42%)	26,31,34	1.74	5 (19%)
4	P4U	5	1348	4,84	21,24,25	3.44	8 (38%)	27,33,36	1.59	3 (11%)
4	OMC	5	2861	4	19,22,23	2.84	7 (36%)	26,31,34	1.05	2 (7%)
4	OMG	5	4623	4	18,26,27	2.39	8 (44%)	19,38,41	1.62	4 (21%)
50	A2M	9	668	84,50	18,25,26	4.58	9 (50%)	18,36,39	2.59	5 (27%)
4	5MC	5	3782	4	18,22,23	3.46	7 (38%)	26,32,35	1.42	5 (19%)
50	A2M	9	166	50	18,25,26	4.88	9 (50%)	18,36,39	2.89	5 (27%)
4	B8Q	5	1456	4	17,22,23	2.64	5 (29%)	22,32,35	2.02	5 (22%)
50	6MZ	9	1832	84,50	18,25,26	2.26	4 (22%)	16,36,39	1.70	2 (12%)
4	OMG	5	1522	4	18,26,27	2.40	8 (44%)	19,38,41	1.65	4 (21%)
50	4AC	9	1337	50	21,24,25	3.14	9 (42%)	29,34,37	1.16	4 (13%)
4	OMG	5	1883	4	18,26,27	2.49	8 (44%)	19,38,41	1.77	4 (21%)
50	OMC	9	1703	50	19,22,23	2.86	7 (36%)	26,31,34	0.70	0
4	OMU	5	4620	4	19,22,23	2.61	6 (31%)	26,31,34	1.76	5 (19%)
4	A2M	5	398	4	18,25,26	4.70	8 (44%)	18,36,39	2.57	3 (16%)
4	P7G	5	1909	4	24,28,29	3.90	10 (41%)	27,41,44	1.91	3 (11%)
50	OMG	9	683	50	18,26,27	2.49	8 (44%)	19,38,41	1.59	5 (26%)
4	UR3	5	4597	4	19,22,23	2.58	6 (31%)	26,32,35	1.25	4 (15%)
50	5MU	9	814	50	19,22,23	4.77	7 (36%)	28,32,35	3.39	13 (46%)
4	B9B	5	2754	4,84	21,28,29	6.32	8 (38%)	23,40,43	2.02	6 (26%)
50	A2M	9	1031	50	18,25,26	4.82	9 (50%)	18,36,39	2.42	3 (16%)
50	A2M	9	1678	50	18,25,26	4.71	9 (50%)	18,36,39	2.92	3 (16%)
4	A2M	5	3723	4	18,25,26	4.77	9 (50%)	18,36,39	2.57	3 (16%)
4	PSU	5	3729	4	18,21,22	1.09	1 (5%)	22,30,33	1.84	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PSU	5	2508	4	18,21,22	0.98	1 (5%)	22,30,33	1.64	4 (18%)
4	7MG	5	4550	4	22,26,27	3.28	10 (45%)	29,39,42	1.92	9 (31%)
50	PSU	9	1243	50	18,21,22	1.28	1 (5%)	22,30,33	1.47	4 (18%)
9	MLZ	C	333	9	8,9,10	0.96	0	4,9,11	0.99	0
4	B8T	5	4483	4	19,22,23	3.00	8 (42%)	26,31,34	1.09	1 (3%)
50	MA6	9	1851	50	19,26,27	1.09	1 (5%)	18,38,41	2.77	2 (11%)
50	M7A	9	1806	50	20,25,26	2.02	3 (15%)	28,37,40	3.72	8 (28%)
4	B8W	5	4529	4,84	18,26,27	5.33	8 (44%)	21,38,41	6.53	9 (42%)
50	OMU	9	121	50	19,22,23	2.83	7 (36%)	26,31,34	1.83	5 (19%)
50	OMC	9	1710	50	19,22,23	2.88	7 (36%)	26,31,34	1.03	1 (3%)
50	A2M	9	484	50	18,25,26	4.65	8 (44%)	18,36,39	2.70	4 (22%)
4	E7G	5	1797	4	24,27,28	3.43	11 (45%)	30,40,43	2.18	9 (30%)
4	PSU	5	4403	4	18,21,22	1.06	2 (11%)	22,30,33	1.82	5 (22%)
4	OMG	5	4494	4	18,26,27	2.45	8 (44%)	19,38,41	1.73	5 (26%)
4	B8W	5	4129	4	18,26,27	5.31	8 (44%)	21,38,41	6.22	12 (57%)
4	I4U	5	4194	4	21,24,25	4.92	16 (76%)	27,34,37	1.34	4 (14%)
4	PSU	5	4636	4	18,21,22	1.08	2 (11%)	22,30,33	2.05	5 (22%)
4	2MG	5	1517	4	18,26,27	2.48	7 (38%)	16,38,41	1.69	4 (25%)
50	A2M	9	27	84,50	18,25,26	4.71	9 (50%)	18,36,39	2.70	3 (16%)
4	OMC	5	2422	4,84	19,22,23	2.83	7 (36%)	26,31,34	0.82	1 (3%)
4	PSU	5	3764	4	18,21,22	1.01	1 (5%)	22,30,33	1.62	4 (18%)
4	PSU	5	4293	4	18,21,22	1.09	3 (16%)	22,30,33	1.80	4 (18%)
4	A2M	5	4523	4,84	18,25,26	4.73	9 (50%)	18,36,39	2.89	5 (27%)
4	B8W	5	4472	4	18,26,27	5.25	9 (50%)	21,38,41	5.81	9 (42%)
4	MHG	5	4371	4	29,32,33	3.92	11 (37%)	34,46,49	2.26	8 (23%)
4	UR3	5	4530	4	19,22,23	2.51	6 (31%)	26,32,35	1.41	3 (11%)
4	A2M	5	3718	4	18,25,26	4.77	12 (66%)	18,36,39	2.44	3 (16%)
4	E7G	5	2297	4	24,27,28	3.32	11 (45%)	30,40,43	2.14	9 (30%)
4	B8H	5	4296	4	19,22,23	6.89	7 (36%)	22,32,35	2.59	5 (22%)
50	5MC	9	1374	50	18,22,23	3.66	7 (38%)	26,32,35	1.10	1 (3%)
50	OMU	9	116	50	19,22,23	2.74	7 (36%)	26,31,34	1.84	5 (19%)
4	UR3	5	1866	4	19,22,23	2.37	6 (31%)	26,32,35	1.17	2 (7%)
4	B8K	5	4690	4,14	24,28,29	4.94	16 (66%)	30,42,45	2.80	12 (40%)
50	4AC	9	1842	50	21,24,25	3.06	10 (47%)	29,34,37	1.49	7 (24%)
4	OMG	5	2364	4	18,26,27	2.35	7 (38%)	19,38,41	1.56	4 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	A2M	5	2401	4,84	18,25,26	4.70	8 (44%)	18,36,39	2.61	3 (16%)
6	OMU	8	14	4,6	19,22,23	2.64	6 (31%)	26,31,34	1.85	5 (19%)
50	PSU	9	823	50	18,21,22	1.09	3 (16%)	22,30,33	1.67	4 (18%)
4	OMG	5	3792	4	18,26,27	2.45	8 (44%)	19,38,41	1.66	4 (21%)
4	OMG	5	1316	4	18,26,27	2.42	7 (38%)	19,38,41	1.61	5 (26%)
50	B8Q	9	1219	84,50	17,22,23	2.89	5 (29%)	22,32,35	2.62	7 (31%)
50	MA6	9	1850	50	19,26,27	1.09	1 (5%)	18,38,41	2.84	2 (11%)
4	OMG	5	4637	4	18,26,27	2.32	8 (44%)	19,38,41	1.63	4 (21%)
4	OMG	5	373	4	18,26,27	2.42	8 (44%)	19,38,41	1.56	5 (26%)
4	OMC	5	3869	4	19,22,23	2.69	7 (36%)	26,31,34	0.90	0
4	6MZ	5	4220	4	18,25,26	2.16	4 (22%)	16,36,39	1.96	4 (25%)
4	OMC	5	3887	4	19,22,23	2.84	7 (36%)	26,31,34	0.88	0
4	OMG	5	2424	4	18,26,27	2.52	8 (44%)	19,38,41	1.60	4 (21%)
4	A2M	5	1534	4,84	18,25,26	4.73	9 (50%)	18,36,39	2.66	3 (16%)
4	PSU	5	1582	4	18,21,22	1.13	2 (11%)	22,30,33	1.77	4 (18%)
4	A2M	5	3825	4	18,25,26	4.71	8 (44%)	18,36,39	2.66	3 (16%)
4	OMC	5	3909	4	19,22,23	2.68	7 (36%)	26,31,34	0.94	1 (3%)
50	PSU	9	822	50	18,21,22	1.08	2 (11%)	22,30,33	2.02	6 (27%)
4	B8H	5	1860	4	19,22,23	6.81	6 (31%)	22,32,35	2.36	5 (22%)
4	OMG	5	4870	4	18,26,27	2.47	8 (44%)	19,38,41	1.60	4 (21%)
4	B9H	5	2786	4	20,25,26	2.95	3 (15%)	22,35,38	1.94	3 (13%)
4	P7G	5	3880	4	24,28,29	3.74	10 (41%)	27,41,44	1.69	4 (14%)
4	I4U	5	1659	4	21,24,25	4.86	15 (71%)	27,34,37	1.53	2 (7%)
50	PSU	9	119	50	18,21,22	0.87	1 (5%)	22,30,33	1.66	3 (13%)
4	OMG	5	4196	4,2	18,26,27	2.41	8 (44%)	19,38,41	1.50	4 (21%)
50	PSU	9	612	50	18,21,22	1.03	3 (16%)	22,30,33	1.59	3 (13%)
4	PSU	5	3715	4	18,21,22	0.95	1 (5%)	22,30,33	1.68	4 (18%)
50	UR3	9	1830	50	19,22,23	2.52	6 (31%)	26,32,35	1.76	4 (15%)
4	1MA	5	1322	4,84	16,25,26	3.74	5 (31%)	18,37,40	1.93	3 (16%)
4	A2M	5	1326	4	18,25,26	4.72	9 (50%)	18,36,39	2.78	3 (16%)
4	PSU	5	1683	4	18,21,22	1.18	2 (11%)	22,30,33	1.85	4 (18%)
4	OMG	5	2773	4	18,26,27	2.41	8 (44%)	19,38,41	1.49	4 (21%)
4	B8H	5	3762	4	19,22,23	6.82	6 (31%)	22,32,35	2.45	5 (22%)
4	A2M	5	4571	4	18,25,26	4.63	8 (44%)	18,36,39	2.69	3 (16%)
4	5MC	5	4447	4	18,22,23	3.60	7 (38%)	26,32,35	1.08	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	A2M	5	3867	4	18,25,26	4.67	8 (44%)	18,36,39	2.81	6 (33%)
4	OMG	5	4370	4	18,26,27	2.40	8 (44%)	19,38,41	1.52	4 (21%)
4	OMC	5	3701	4,84	19,22,23	2.72	7 (36%)	26,31,34	0.82	0
4	2MG	5	729	4	18,26,27	2.43	5 (27%)	16,38,41	1.37	3 (18%)
4	PSU	5	1677	4	18,21,22	1.14	3 (16%)	22,30,33	1.87	3 (13%)
50	OMG	9	644	50	18,26,27	2.42	8 (44%)	19,38,41	1.56	4 (21%)
50	A2M	9	159	50	18,25,26	4.79	8 (44%)	18,36,39	2.80	4 (22%)
4	M7A	5	4564	4	20,25,26	1.99	4 (20%)	28,37,40	3.78	7 (25%)
4	B8W	5	2380	4	18,26,27	5.24	8 (44%)	21,38,41	6.18	8 (38%)
50	E3C	9	568	50	18,23,24	3.38	6 (33%)	21,33,36	2.40	6 (28%)
4	B8K	5	3897	4	24,28,29	4.78	16 (66%)	30,42,45	2.57	12 (40%)
44	MLZ	m	72	44	8,9,10	0.82	0	4,9,11	1.09	0
4	PSU	5	4500	4	18,21,22	1.05	3 (16%)	22,30,33	2.05	4 (18%)
4	E6G	5	4355	4	20,27,28	5.75	9 (45%)	22,39,42	2.17	7 (31%)
4	PSU	5	4628	4	18,21,22	1.10	2 (11%)	22,30,33	1.96	4 (18%)
50	B8N	9	1248	50	24,29,30	2.78	7 (29%)	29,42,45	1.84	6 (20%)
4	OMC	5	4536	4	19,22,23	2.69	7 (36%)	26,31,34	1.08	2 (7%)
4	A2M	5	1524	4	18,25,26	4.70	9 (50%)	18,36,39	2.74	3 (16%)
4	B9B	5	1574	4	21,28,29	6.27	9 (42%)	23,40,43	2.16	6 (26%)
4	B8T	5	4671	4	19,22,23	2.91	8 (42%)	26,31,34	0.94	1 (3%)
50	OMC	9	517	50	19,22,23	2.82	7 (36%)	26,31,34	1.01	1 (3%)
4	OMC	5	2365	4	19,22,23	2.78	7 (36%)	26,31,34	0.75	0
4	B8W	5	4185	4	18,26,27	5.17	8 (44%)	21,38,41	5.98	12 (57%)
4	1MA	5	4415	4	16,25,26	4.01	4 (25%)	18,37,40	1.72	3 (16%)
50	PSU	9	1081	50	18,21,22	1.13	3 (16%)	22,30,33	1.78	4 (18%)
4	5MU	5	4083	4	19,22,23	4.65	7 (36%)	28,32,35	3.61	11 (39%)
4	A2M	5	3785	4	18,25,26	4.48	10 (55%)	18,36,39	2.62	4 (22%)
4	OMC	5	2804	4	19,22,23	2.82	7 (36%)	26,31,34	0.88	0
4	B9B	5	237	4	21,28,29	6.30	9 (42%)	23,40,43	2.29	7 (30%)
4	BGH	5	3899	4,84	25,29,30	4.11	16 (64%)	31,43,46	2.66	14 (45%)
4	PSU	5	4442	4	18,21,22	1.08	3 (16%)	22,30,33	2.07	4 (18%)
4	5MC	5	4335	4	18,22,23	3.51	7 (38%)	26,32,35	1.35	3 (11%)
4	OMG	5	1625	4,84	18,26,27	2.39	8 (44%)	19,38,41	1.55	4 (21%)
50	OMC	9	174	50	19,22,23	2.87	7 (36%)	26,31,34	0.84	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	OMG	9	509	84,50	-	0/5/27/28	0/3/3/3
4	PSU	5	4450	4,84	-	4/7/25/26	0/2/2/2
4	2MG	5	4872	4,18	-	2/5/27/28	0/3/3/3
4	A2M	5	2363	4,84	-	1/5/27/28	0/3/3/3
4	7MG	5	2522	4	-	0/7/37/38	0/3/3/3
4	PSU	5	4531	4	-	0/7/25/26	0/2/2/2
4	OMG	5	2050	4	-	0/5/27/28	0/3/3/3
4	7MG	5	1605	4	-	0/7/37/38	0/3/3/3
4	A2M	5	1871	4,84	-	0/5/27/28	0/3/3/3
4	OMU	5	4306	4	-	1/9/27/28	0/2/2/2
4	P4U	5	1348	4,84	-	5/10/29/30	0/2/2/2
4	OMC	5	2861	4	-	1/9/27/28	0/2/2/2
4	OMG	5	4623	4	-	0/5/27/28	0/3/3/3
50	A2M	9	668	84,50	-	3/5/27/28	0/3/3/3
4	5MC	5	3782	4	-	0/7/25/26	0/2/2/2
50	A2M	9	166	50	-	2/5/27/28	0/3/3/3
4	B8Q	5	1456	4	-	0/7/42/43	0/2/2/2
50	6MZ	9	1832	84,50	-	2/5/27/28	0/3/3/3
4	OMG	5	1522	4	-	0/5/27/28	0/3/3/3
50	4AC	9	1337	50	-	2/11/29/30	0/2/2/2
4	OMG	5	1883	4	-	2/5/27/28	0/3/3/3
50	OMC	9	1703	50	-	2/9/27/28	0/2/2/2
4	OMU	5	4620	4	-	1/9/27/28	0/2/2/2
4	A2M	5	398	4	-	2/5/27/28	0/3/3/3
4	P7G	5	1909	4	-	2/10/40/41	0/3/3/3
50	OMG	9	683	50	-	2/5/27/28	0/3/3/3
4	UR3	5	4597	4	-	0/7/25/26	0/2/2/2
50	5MU	9	814	50	-	1/7/25/26	0/2/2/2
4	B9B	5	2754	4,84	-	3/7/29/30	0/3/3/3
50	A2M	9	1031	50	-	0/5/27/28	0/3/3/3
50	A2M	9	1678	50	-	0/5/27/28	0/3/3/3
4	A2M	5	3723	4	-	0/5/27/28	0/3/3/3
4	PSU	5	3729	4	-	2/7/25/26	0/2/2/2
4	PSU	5	2508	4	-	0/7/25/26	0/2/2/2
4	7MG	5	4550	4	-	0/7/37/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	PSU	9	1243	50	-	2/7/25/26	0/2/2/2
9	MLZ	C	333	9	-	3/7/8/10	-
4	B8T	5	4483	4	-	0/7/27/28	0/2/2/2
50	MA6	9	1851	50	-	4/7/29/30	0/3/3/3
50	M7A	9	1806	50	-	0/7/37/38	0/3/3/3
4	B8W	5	4529	4,84	-	4/5/27/28	0/3/3/3
50	OMU	9	121	50	-	2/9/27/28	0/2/2/2
50	OMC	9	1710	50	-	1/9/27/28	0/2/2/2
50	A2M	9	484	50	-	0/5/27/28	0/3/3/3
4	E7G	5	1797	4	-	2/9/39/40	0/3/3/3
4	PSU	5	4403	4	-	3/7/25/26	0/2/2/2
4	OMG	5	4494	4	-	0/5/27/28	0/3/3/3
4	B8W	5	4129	4	-	3/5/27/28	0/3/3/3
4	I4U	5	4194	4	-	4/9/29/30	0/2/2/2
4	PSU	5	4636	4	-	3/7/25/26	0/2/2/2
4	2MG	5	1517	4	-	0/5/27/28	0/3/3/3
50	A2M	9	27	84,50	-	0/5/27/28	0/3/3/3
4	OMC	5	2422	4,84	-	1/9/27/28	0/2/2/2
4	PSU	5	3764	4	-	0/7/25/26	0/2/2/2
4	PSU	5	4293	4	-	2/7/25/26	0/2/2/2
4	A2M	5	4523	4,84	-	3/5/27/28	0/3/3/3
4	B8W	5	4472	4	-	3/5/27/28	0/3/3/3
4	MHG	5	4371	4	-	6/16/46/47	0/3/3/3
4	UR3	5	4530	4	-	1/7/25/26	0/2/2/2
4	A2M	5	3718	4	-	0/5/27/28	0/3/3/3
4	E7G	5	2297	4	-	1/9/39/40	0/3/3/3
4	B8H	5	4296	4	-	0/7/25/26	0/2/2/2
50	5MC	9	1374	50	-	0/7/25/26	0/2/2/2
50	OMU	9	116	50	-	3/9/27/28	0/2/2/2
4	UR3	5	1866	4	-	2/7/25/26	0/2/2/2
4	B8K	5	4690	4,14	-	0/11/41/42	0/3/3/3
50	4AC	9	1842	50	-	0/11/29/30	0/2/2/2
4	OMG	5	2364	4	-	2/5/27/28	0/3/3/3
4	A2M	5	2401	4,84	-	1/5/27/28	0/3/3/3
6	OMU	8	14	4,6	-	1/9/27/28	0/2/2/2
50	PSU	9	823	50	-	0/7/25/26	0/2/2/2
4	OMG	5	3792	4	-	2/5/27/28	0/3/3/3
4	OMG	5	1316	4	-	1/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	B8Q	9	1219	84,50	-	1/7/42/43	0/2/2/2
50	MA6	9	1850	50	-	1/7/29/30	0/3/3/3
4	OMG	5	4637	4	-	2/5/27/28	0/3/3/3
4	OMG	5	373	4	-	0/5/27/28	0/3/3/3
4	OMC	5	3869	4	-	0/9/27/28	0/2/2/2
4	6MZ	5	4220	4	-	1/5/27/28	0/3/3/3
4	OMC	5	3887	4	-	1/9/27/28	0/2/2/2
4	OMG	5	2424	4	-	2/5/27/28	0/3/3/3
4	A2M	5	1534	4,84	-	2/5/27/28	0/3/3/3
4	PSU	5	1582	4	-	2/7/25/26	0/2/2/2
4	A2M	5	3825	4	-	0/5/27/28	0/3/3/3
4	OMC	5	3909	4	-	0/9/27/28	0/2/2/2
50	PSU	9	822	50	-	0/7/25/26	0/2/2/2
4	B8H	5	1860	4	-	0/7/25/26	0/2/2/2
4	OMG	5	4870	4	-	4/5/27/28	0/3/3/3
4	B9H	5	2786	4	-	2/12/47/48	0/2/2/2
4	P7G	5	3880	4	-	2/10/40/41	0/3/3/3
4	I4U	5	1659	4	-	1/9/29/30	0/2/2/2
50	PSU	9	119	50	-	0/7/25/26	0/2/2/2
4	OMG	5	4196	4,2	-	0/5/27/28	0/3/3/3
50	PSU	9	612	50	-	0/7/25/26	0/2/2/2
4	PSU	5	3715	4	-	0/7/25/26	0/2/2/2
50	UR3	9	1830	50	-	2/7/25/26	0/2/2/2
4	1MA	5	1322	4,84	-	0/3/25/26	0/3/3/3
4	A2M	5	1326	4	-	1/5/27/28	0/3/3/3
4	PSU	5	1683	4	-	0/7/25/26	0/2/2/2
4	OMG	5	2773	4	-	0/5/27/28	0/3/3/3
4	B8H	5	3762	4	-	2/7/25/26	0/2/2/2
4	A2M	5	4571	4	-	0/5/27/28	0/3/3/3
4	5MC	5	4447	4	-	4/7/25/26	0/2/2/2
4	A2M	5	3867	4	-	2/5/27/28	0/3/3/3
4	OMG	5	4370	4	-	0/5/27/28	0/3/3/3
4	OMC	5	3701	4,84	-	6/9/27/28	0/2/2/2
4	2MG	5	729	4	-	2/5/27/28	0/3/3/3
4	PSU	5	1677	4	-	1/7/25/26	0/2/2/2
50	OMG	9	644	50	-	2/5/27/28	0/3/3/3
50	A2M	9	159	50	-	3/5/27/28	0/3/3/3
4	M7A	5	4564	4	-	0/7/37/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	B8W	5	2380	4	-	4/5/27/28	0/3/3/3
50	E3C	9	568	50	-	4/9/44/45	0/2/2/2
4	B8K	5	3897	4	-	3/11/41/42	0/3/3/3
44	MLZ	m	72	44	-	1/7/8/10	-
4	PSU	5	4500	4	-	3/7/25/26	0/2/2/2
4	E6G	5	4355	4	-	5/6/28/29	0/3/3/3
4	PSU	5	4628	4	-	0/7/25/26	0/2/2/2
50	B8N	9	1248	50	-	2/16/34/35	0/2/2/2
4	OMC	5	4536	4	-	0/9/27/28	0/2/2/2
4	A2M	5	1524	4	-	0/5/27/28	0/3/3/3
4	B9B	5	1574	4	-	3/7/29/30	0/3/3/3
4	B8T	5	4671	4	-	0/7/27/28	0/2/2/2
50	OMC	9	517	50	-	0/9/27/28	0/2/2/2
4	OMC	5	2365	4	-	0/9/27/28	0/2/2/2
4	B8W	5	4185	4	-	3/5/27/28	0/3/3/3
4	1MA	5	4415	4	-	2/3/25/26	0/3/3/3
50	PSU	9	1081	50	-	1/7/25/26	0/2/2/2
4	5MU	5	4083	4	-	0/7/25/26	0/2/2/2
4	A2M	5	3785	4	-	4/5/27/28	0/3/3/3
4	OMC	5	2804	4	-	0/9/27/28	0/2/2/2
4	B9B	5	237	4	-	4/7/29/30	0/3/3/3
4	BGH	5	3899	4,84	-	3/13/43/44	0/3/3/3
4	PSU	5	4442	4	-	0/7/25/26	0/2/2/2
4	5MC	5	4335	4	-	0/7/25/26	0/2/2/2
4	OMG	5	1625	4,84	-	1/5/27/28	0/3/3/3
50	OMC	9	174	50	-	0/9/27/28	0/2/2/2

All (943) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	5	2754	B9B	C2'-C1'	-18.26	1.26	1.53
4	5	1574	B9B	C2'-C1'	-17.78	1.26	1.53
4	5	237	B9B	C2'-C1'	-17.62	1.27	1.53
4	5	237	B9B	O4'-C1'	17.17	1.65	1.41
50	9	166	A2M	O4'-C1'	16.78	1.64	1.41
4	5	1574	B9B	O4'-C1'	16.48	1.64	1.41
4	5	4296	B8H	C6-C5	-16.42	1.11	1.34
4	5	2754	B9B	O4'-C1'	16.33	1.63	1.41
50	9	1031	A2M	O4'-C1'	16.24	1.63	1.41
4	5	3718	A2M	O4'-C1'	16.09	1.63	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	5	3723	A2M	O4'-C1'	16.04	1.63	1.41
4	5	4355	E6G	C2'-C1'	-15.95	1.29	1.53
50	9	159	A2M	O4'-C1'	15.90	1.63	1.41
4	5	4523	A2M	O4'-C1'	15.89	1.63	1.41
4	5	1860	B8H	C6-C5	-15.87	1.12	1.34
4	5	398	A2M	O4'-C1'	15.86	1.63	1.41
4	5	1534	A2M	O4'-C1'	15.79	1.63	1.41
4	5	2401	A2M	O4'-C1'	15.78	1.63	1.41
4	5	3762	B8H	C6-C5	-15.77	1.12	1.34
4	5	2363	A2M	O4'-C1'	15.75	1.63	1.41
4	5	3825	A2M	O4'-C1'	15.71	1.63	1.41
50	9	27	A2M	O4'-C1'	15.65	1.62	1.41
4	5	1524	A2M	O4'-C1'	15.63	1.62	1.41
50	9	1678	A2M	O4'-C1'	15.63	1.62	1.41
4	5	1326	A2M	O4'-C1'	15.57	1.62	1.41
4	5	1871	A2M	O4'-C1'	15.41	1.62	1.41
4	5	3867	A2M	O4'-C1'	15.41	1.62	1.41
50	9	484	A2M	O4'-C1'	15.36	1.62	1.41
4	5	4296	B8H	C4-N3	-15.31	1.10	1.38
4	5	4355	E6G	O4'-C1'	15.18	1.62	1.41
4	5	4571	A2M	O4'-C1'	15.14	1.62	1.41
4	5	1860	B8H	C4-N3	-15.09	1.10	1.38
4	5	3762	B8H	C4-N3	-15.02	1.11	1.38
4	5	4529	B8W	C2'-C1'	-14.97	1.31	1.53
50	9	668	A2M	O4'-C1'	14.66	1.61	1.41
4	5	3785	A2M	O4'-C1'	14.64	1.61	1.41
4	5	4415	1MA	C2-N3	14.55	1.46	1.29
4	5	4129	B8W	C2'-C1'	-14.51	1.31	1.53
4	5	4472	B8W	C2'-C1'	-14.15	1.32	1.53
4	5	4185	B8W	C2'-C1'	-14.06	1.32	1.53
4	5	2380	B8W	C2'-C1'	-13.99	1.32	1.53
4	5	1322	1MA	C2-N3	13.62	1.45	1.29
4	5	3762	B8H	C4-C5	13.51	1.82	1.44
4	5	4129	B8W	O4'-C1'	13.44	1.59	1.41
4	5	4296	B8H	C4-C5	13.39	1.82	1.44
4	5	1860	B8H	C4-C5	13.34	1.82	1.44
4	5	2380	B8W	O4'-C1'	13.31	1.59	1.41
4	5	3762	B8H	C6-N1	13.23	1.69	1.36
4	5	4472	B8W	O4'-C1'	13.21	1.59	1.41
4	5	1860	B8H	C6-N1	13.19	1.69	1.36
4	5	4529	B8W	O4'-C1'	12.99	1.59	1.41
4	5	4296	B8H	C6-N1	12.92	1.68	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	5	4185	B8W	O4'-C1'	12.89	1.59	1.41
4	5	4690	B8K	C3'-C4'	-11.69	1.23	1.53
4	5	3897	B8K	C3'-C4'	-11.54	1.23	1.53
4	5	4194	I4U	C3'-C2'	-11.45	1.22	1.53
4	5	1659	I4U	C3'-C2'	-11.37	1.22	1.53
4	5	1909	P7G	C8-N9	11.30	1.52	1.46
50	9	814	5MU	C2-N1	11.18	1.56	1.38
4	5	4083	5MU	C6-N1	10.47	1.55	1.38
4	5	3899	BGH	C3'-C4'	-10.38	1.26	1.53
4	5	1348	P4U	C4-N3	10.11	1.44	1.31
4	5	3880	P7G	C8-N9	10.08	1.51	1.46
4	5	1659	I4U	C4-N3	10.07	1.44	1.31
50	9	814	5MU	C6-N1	10.00	1.55	1.38
4	5	4371	MHG	C8-N9	9.88	1.51	1.46
4	5	4194	I4U	C4-N3	9.87	1.44	1.31
4	5	1574	B9B	O6-C6	9.85	1.43	1.35
4	5	4083	5MU	C2-N1	9.82	1.54	1.38
4	5	4690	B8K	C8-N9	9.75	1.51	1.46
4	5	2754	B9B	O6-C6	9.68	1.43	1.35
4	5	4447	5MC	C6-C5	9.37	1.50	1.34
4	5	237	B9B	O6-C6	9.33	1.43	1.35
50	9	1374	5MC	C6-C5	9.14	1.49	1.34
4	5	4083	5MU	C4-C5	9.11	1.59	1.44
50	9	814	5MU	C4-C5	9.10	1.59	1.44
4	5	3899	BGH	O4'-C4'	9.06	1.65	1.45
4	5	2786	B9H	C2-N3	9.02	1.48	1.37
4	5	1909	P7G	C5-N7	8.75	1.45	1.35
4	5	4371	MHG	C5-N7	8.75	1.45	1.35
4	5	3880	P7G	C5-N7	8.72	1.45	1.35
4	5	4335	5MC	C6-C5	8.63	1.48	1.34
4	5	3897	B8K	C2'-C1'	-8.57	1.26	1.53
4	5	4194	I4U	O4'-C4'	-8.53	1.25	1.45
50	9	668	A2M	O4'-C4'	-8.49	1.26	1.45
50	9	814	5MU	C4-N3	-8.43	1.23	1.38
4	5	4083	5MU	C4-N3	-8.38	1.23	1.38
50	9	568	E3C	C2-N3	8.27	1.47	1.37
50	9	1248	B8N	C4-N3	-8.26	1.25	1.40
4	5	4371	MHG	C2-N3	8.25	1.47	1.31
50	9	568	E3C	C2-N1	8.20	1.50	1.38
4	5	3782	5MC	C6-C5	8.11	1.47	1.34
4	5	4690	B8K	C2'-C1'	-8.04	1.27	1.53
4	5	1456	B8Q	C6-C5	8.04	1.51	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	9	1219	B8Q	C6-C5	8.03	1.51	1.33
50	9	1832	6MZ	C6-N6	7.98	1.48	1.35
50	9	159	A2M	O4'-C4'	-7.86	1.27	1.45
4	5	1659	I4U	O4'-C4'	-7.86	1.27	1.45
4	5	1326	A2M	O4'-C4'	-7.86	1.27	1.45
4	5	1797	E7G	C5-N7	7.86	1.44	1.35
4	5	2363	A2M	O4'-C4'	-7.84	1.27	1.45
4	5	4355	E6G	O4'-C4'	-7.79	1.27	1.45
50	9	484	A2M	O4'-C4'	-7.79	1.27	1.45
4	5	4571	A2M	O4'-C4'	-7.77	1.27	1.45
4	5	3867	A2M	O4'-C4'	-7.77	1.27	1.45
50	9	1678	A2M	O4'-C4'	-7.72	1.27	1.45
4	5	1534	A2M	O4'-C4'	-7.70	1.27	1.45
4	5	1524	A2M	O4'-C4'	-7.66	1.27	1.45
4	5	4550	7MG	C8-N9	7.64	1.50	1.46
4	5	4523	A2M	O4'-C4'	-7.61	1.28	1.45
4	5	3825	A2M	O4'-C4'	-7.58	1.28	1.45
4	5	2297	E7G	C5-N7	7.55	1.44	1.35
50	9	1031	A2M	O4'-C4'	-7.53	1.28	1.45
4	5	2522	7MG	C8-N9	7.51	1.50	1.46
4	5	1871	A2M	O4'-C4'	-7.51	1.28	1.45
4	5	3723	A2M	O4'-C4'	-7.49	1.28	1.45
50	9	27	A2M	O4'-C4'	-7.46	1.28	1.45
4	5	3785	A2M	O4'-C4'	-7.46	1.28	1.45
4	5	2401	A2M	O4'-C4'	-7.42	1.28	1.45
4	5	3897	B8K	C8-N9	7.39	1.50	1.46
4	5	2754	B9B	O4'-C4'	-7.37	1.28	1.45
4	5	2522	7MG	C5-N7	7.33	1.44	1.35
4	5	3718	A2M	O4'-C4'	-7.32	1.28	1.45
4	5	398	A2M	O4'-C4'	-7.31	1.28	1.45
4	5	4220	6MZ	C6-N6	7.30	1.47	1.35
4	5	1605	7MG	C5-N7	7.25	1.44	1.35
50	9	166	A2M	O4'-C4'	-7.25	1.28	1.45
4	5	2754	B9B	C2-N2	7.23	1.48	1.33
4	5	1574	B9B	O4'-C4'	-7.22	1.28	1.45
4	5	3897	B8K	O4'-C4'	7.18	1.61	1.45
4	5	4550	7MG	C5-N7	7.16	1.43	1.35
4	5	237	B9B	O4'-C4'	-7.13	1.29	1.45
4	5	1574	B9B	C2-N2	7.11	1.48	1.33
4	5	4529	B8W	C3'-C4'	-7.08	1.34	1.53
50	9	1248	B8N	C6-N1	7.04	1.54	1.36
4	5	237	B9B	C2-N2	7.01	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	5	4185	B8W	C3'-C4'	-6.99	1.35	1.53
4	5	1797	E7G	C8-N9	6.96	1.49	1.46
4	5	4690	B8K	O4'-C4'	6.95	1.60	1.45
50	9	1337	4AC	C4-N3	6.88	1.44	1.32
50	9	1374	5MC	C4-N3	6.86	1.45	1.34
4	5	2786	B9H	C6-C5	6.85	1.48	1.33
4	5	3782	5MC	C4-N3	6.80	1.45	1.34
4	5	4129	B8W	C3'-C4'	-6.77	1.35	1.53
4	5	1605	7MG	C8-N9	6.77	1.49	1.46
4	5	2380	B8W	C3'-C4'	-6.72	1.35	1.53
4	5	4472	B8W	C3'-C4'	-6.67	1.35	1.53
4	5	4335	5MC	C4-N3	6.62	1.45	1.34
50	9	568	E3C	C6-C5	6.51	1.47	1.33
50	9	1219	B8Q	C2-N3	6.47	1.46	1.35
50	9	121	OMU	C2-N3	6.46	1.49	1.38
4	5	4371	MHG	C8-N7	6.42	1.51	1.45
50	9	116	OMU	C2-N3	6.40	1.49	1.38
50	9	1374	5MC	C2-N3	6.35	1.49	1.36
4	5	4872	2MG	C2-N2	6.32	1.47	1.33
4	5	4447	5MC	C4-N3	6.32	1.44	1.34
4	5	4597	UR3	C2-N1	6.30	1.47	1.38
6	8	14	OMU	C2-N3	6.24	1.49	1.38
4	5	2422	OMC	C6-C5	6.23	1.49	1.35
4	5	4371	MHG	C2-N2	6.22	1.47	1.33
50	9	174	OMC	C2-N3	6.22	1.49	1.36
4	5	4483	B8T	C4-N3	6.21	1.43	1.32
4	5	4371	MHG	C2-N1	6.20	1.46	1.36
4	5	1797	E7G	C8-N7	6.19	1.51	1.45
4	5	4671	B8T	C4-N3	6.19	1.43	1.32
4	5	4620	OMU	C2-N3	6.18	1.49	1.38
50	9	1830	UR3	C2-N1	6.18	1.47	1.38
50	9	1703	OMC	C6-C5	6.17	1.49	1.35
4	5	2297	E7G	C8-N9	6.17	1.49	1.46
50	9	1842	4AC	C4-N3	6.16	1.43	1.32
4	5	4530	UR3	C2-N1	6.13	1.47	1.38
50	9	1710	OMC	C6-C5	6.12	1.49	1.35
4	5	4355	E6G	O6-C6	6.10	1.40	1.35
4	5	4306	OMU	C2-N3	6.10	1.48	1.38
4	5	2297	E7G	C8-N7	6.08	1.51	1.45
50	9	174	OMC	C6-C5	6.08	1.49	1.35
50	9	517	OMC	C6-C5	6.08	1.49	1.35
4	5	2804	OMC	C6-C5	6.07	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	5	2365	OMC	C6-C5	6.06	1.49	1.35
4	5	3782	5MC	C2-N3	6.06	1.48	1.36
50	9	1710	OMC	C2-N3	6.05	1.48	1.36
4	5	2861	OMC	C6-C5	6.04	1.49	1.35
4	5	3869	OMC	C6-C5	6.02	1.49	1.35
4	5	3887	OMC	C6-C5	6.02	1.49	1.35
4	5	4483	B8T	C2-N3	6.01	1.48	1.36
4	5	1517	2MG	C2-N2	6.01	1.46	1.33
4	5	2786	B9H	C2-N1	6.01	1.47	1.38
4	5	1659	I4U	C2-N3	6.00	1.48	1.36
4	5	2861	OMC	C2-N3	6.00	1.48	1.36
4	5	1348	P4U	C6-C5	5.99	1.49	1.35
50	9	1842	4AC	C6-C5	5.99	1.49	1.35
4	5	4194	I4U	C1'-N1	-5.98	1.30	1.47
4	5	4335	5MC	C2-N3	5.94	1.48	1.36
4	5	729	2MG	C2-N2	5.94	1.46	1.33
50	9	1337	4AC	C6-C5	5.92	1.48	1.35
50	9	116	OMU	C2-N1	5.92	1.47	1.38
50	9	1830	UR3	C6-C5	5.91	1.48	1.35
50	9	814	5MU	C6-C5	5.91	1.44	1.34
4	5	2804	OMC	C2-N3	5.91	1.48	1.36
4	5	3909	OMC	C6-C5	5.90	1.48	1.35
4	5	1348	P4U	C2-N3	5.89	1.48	1.36
50	9	1337	4AC	C2-N3	5.88	1.48	1.36
4	5	3701	OMC	C6-C5	5.87	1.48	1.35
4	5	3887	OMC	C2-N3	5.87	1.48	1.36
50	9	1806	M7A	C4-N9	5.87	1.49	1.38
4	5	4671	B8T	C2-N3	5.86	1.48	1.36
50	9	1703	OMC	C2-N3	5.84	1.48	1.36
4	5	4530	UR3	C6-C5	5.84	1.48	1.35
4	5	4536	OMC	C2-N3	5.83	1.48	1.36
4	5	4597	UR3	C6-C5	5.83	1.48	1.35
4	5	2422	OMC	C2-N3	5.81	1.48	1.36
4	5	4536	OMC	C6-C5	5.81	1.48	1.35
4	5	4447	5MC	C2-N3	5.80	1.48	1.36
4	5	4483	B8T	C6-C5	5.80	1.48	1.35
4	5	2365	OMC	C2-N3	5.79	1.48	1.36
50	9	1842	4AC	C2-N3	5.76	1.48	1.36
4	5	4306	OMU	C2-N1	5.74	1.47	1.38
50	9	517	OMC	C2-N3	5.73	1.48	1.36
4	5	3701	OMC	C2-N3	5.70	1.47	1.36
4	5	1866	UR3	C6-C5	5.70	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	9	121	OMU	C2-N1	5.69	1.47	1.38
4	5	4564	M7A	C4-N9	5.68	1.48	1.38
4	5	2522	7MG	C2-N3	5.67	1.46	1.33
50	9	174	OMC	C4-N3	5.67	1.45	1.34
4	5	2297	E7G	C2-N3	5.66	1.46	1.33
4	5	2380	B8W	C2-N2	5.64	1.45	1.33
4	5	3899	BGH	C8-N9	5.64	1.49	1.46
4	5	1909	P7G	C2-N1	5.62	1.46	1.33
4	5	4194	I4U	C2-N3	5.60	1.47	1.36
4	5	1797	E7G	C2-N3	5.59	1.46	1.33
4	5	4671	B8T	C6-C5	5.58	1.48	1.35
4	5	4194	I4U	C6-C5	5.58	1.48	1.35
4	5	1605	7MG	C2-N3	5.56	1.46	1.33
4	5	1659	I4U	C6-C5	5.55	1.48	1.35
4	5	4083	5MU	C6-C5	5.55	1.43	1.34
4	5	2861	OMC	C4-N3	5.55	1.45	1.34
50	9	1703	OMC	C4-N3	5.53	1.45	1.34
4	5	3887	OMC	C4-N3	5.53	1.45	1.34
4	5	3880	P7G	C2-N1	5.52	1.46	1.33
4	5	2804	OMC	C4-N3	5.51	1.45	1.34
6	8	14	OMU	C2-N1	5.51	1.47	1.38
4	5	3869	OMC	C2-N3	5.50	1.47	1.36
50	9	1710	OMC	C4-N3	5.50	1.45	1.34
4	5	3701	OMC	C4-N3	5.50	1.45	1.34
4	5	2422	OMC	C4-N3	5.49	1.45	1.34
50	9	121	OMU	C6-C5	5.47	1.47	1.35
4	5	1797	E7G	C4-N9	5.45	1.44	1.37
4	5	4550	7MG	C2-N3	5.43	1.46	1.33
4	5	3762	B8H	C2-N3	5.41	1.47	1.38
4	5	4371	MHG	C4-N3	5.40	1.47	1.34
4	5	4355	E6G	C2-N2	5.39	1.44	1.33
4	5	3897	B8K	C4-N9	5.39	1.44	1.37
4	5	2424	OMG	C2-N3	5.38	1.46	1.33
50	9	517	OMC	C4-N3	5.36	1.45	1.34
4	5	2365	OMC	C4-N3	5.36	1.45	1.34
4	5	4306	OMU	C6-C5	5.34	1.47	1.35
4	5	4870	OMG	C2-N3	5.31	1.46	1.33
4	5	3897	B8K	C3'-C2'	5.29	1.67	1.53
4	5	4690	B8K	C2-N3	5.27	1.45	1.33
4	5	4129	B8W	C2-N2	5.27	1.44	1.33
50	9	644	OMG	C2-N3	5.26	1.46	1.33
4	5	1456	B8Q	C2-N3	5.24	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	5	3909	OMC	C2-N3	5.24	1.47	1.36
4	5	1883	OMG	C2-N3	5.22	1.45	1.33
4	5	2522	7MG	C4-N3	5.22	1.46	1.34
4	5	2297	E7G	C4-N9	5.21	1.43	1.37
4	5	3899	BGH	C2-N3	5.21	1.45	1.33
4	5	1605	7MG	C4-N3	5.21	1.46	1.34
50	9	116	OMU	C6-C5	5.20	1.47	1.35
4	5	1866	UR3	C2-N1	5.19	1.46	1.38
4	5	3880	P7G	C4-N3	5.18	1.46	1.37
4	5	3792	OMG	C2-N3	5.14	1.45	1.33
4	5	1625	OMG	C2-N3	5.14	1.45	1.33
50	9	27	A2M	O3'-C3'	-5.12	1.30	1.43
4	5	4690	B8K	C4-N3	5.10	1.46	1.34
4	5	4620	OMU	C6-C5	5.10	1.46	1.35
50	9	509	OMG	C2-N3	5.10	1.45	1.33
4	5	1659	I4U	C1'-N1	-5.09	1.32	1.47
4	5	3899	BGH	O4'-C1'	-5.08	1.30	1.42
4	5	729	2MG	C4-N3	5.07	1.49	1.37
4	5	4185	B8W	C2-N2	5.05	1.44	1.33
4	5	1909	P7G	C4-N3	5.05	1.46	1.37
4	5	4597	UR3	C2-N3	5.04	1.48	1.39
4	5	4529	B8W	C2-N2	5.04	1.44	1.33
4	5	4690	B8K	C3'-C2'	5.04	1.67	1.53
50	9	1248	B8N	C2-N1	5.04	1.54	1.39
50	9	159	A2M	O3'-C3'	-5.04	1.31	1.43
4	5	3869	OMC	C4-N3	5.04	1.44	1.34
4	5	4620	OMU	C2-N1	5.04	1.46	1.38
4	5	4550	7MG	C4-N3	5.03	1.46	1.34
4	5	3897	B8K	C2-N3	5.03	1.45	1.33
50	9	683	OMG	C2-N3	5.02	1.45	1.33
4	5	4690	B8K	C4-N9	5.02	1.43	1.37
4	5	4623	OMG	C2-N3	5.00	1.45	1.33
4	5	1522	OMG	C2-N3	4.99	1.45	1.33
4	5	1860	B8H	C2-N3	4.97	1.46	1.38
4	5	4370	OMG	C2-N3	4.97	1.45	1.33
4	5	4472	B8W	C2-N2	4.96	1.43	1.33
4	5	2773	OMG	C2-N3	4.96	1.45	1.33
4	5	4196	OMG	C2-N3	4.95	1.45	1.33
4	5	373	OMG	C2-N3	4.93	1.45	1.33
4	5	2050	OMG	C2-N3	4.93	1.45	1.33
4	5	1909	P7G	C4-N9	4.92	1.42	1.35
4	5	4194	I4U	C3'-C4'	4.90	1.65	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	5	3897	B8K	C4-N3	4.89	1.45	1.34
4	5	4371	MHG	C4-N9	4.89	1.43	1.37
4	5	4536	OMC	C4-N3	4.89	1.44	1.34
4	5	4571	A2M	O3'-C3'	-4.89	1.31	1.43
4	5	3897	B8K	C5-N7	4.88	1.48	1.39
4	5	3825	A2M	O3'-C3'	-4.88	1.31	1.43
4	5	3909	OMC	C4-N3	4.86	1.44	1.34
50	9	1337	4AC	C7-N4	4.86	1.46	1.37
4	5	4296	B8H	C2-N3	4.85	1.46	1.38
4	5	3880	P7G	C4-N9	4.84	1.42	1.35
50	9	1374	5MC	C4-N4	4.84	1.46	1.34
4	5	1517	2MG	C4-N3	4.83	1.49	1.37
4	5	4870	OMG	C4-N3	4.82	1.49	1.37
4	5	4637	OMG	C2-N3	4.80	1.44	1.33
50	9	1031	A2M	O3'-C3'	-4.79	1.31	1.43
4	5	3899	BGH	C4-N3	4.78	1.45	1.34
4	5	2364	OMG	C2-N3	4.78	1.44	1.33
4	5	2424	OMG	C4-N3	4.77	1.48	1.37
4	5	4690	B8K	C5-N7	4.77	1.47	1.39
4	5	1524	A2M	O3'-C3'	-4.77	1.31	1.43
4	5	1326	A2M	O3'-C3'	-4.76	1.31	1.43
4	5	1605	7MG	C4-N9	4.76	1.43	1.37
4	5	1316	OMG	C2-N3	4.76	1.44	1.33
4	5	4494	OMG	C2-N3	4.76	1.44	1.33
4	5	2401	A2M	O3'-C3'	-4.74	1.31	1.43
4	5	3723	A2M	O3'-C3'	-4.73	1.31	1.43
4	5	398	A2M	O3'-C3'	-4.71	1.31	1.43
50	9	683	OMG	C4-N3	4.71	1.48	1.37
4	5	4335	5MC	C4-N4	4.70	1.46	1.34
4	5	1883	OMG	C4-N3	4.70	1.48	1.37
4	5	4415	1MA	C2-N1	4.69	1.44	1.35
6	8	14	OMU	C6-C5	4.69	1.45	1.35
4	5	3792	OMG	C4-N3	4.67	1.48	1.37
4	5	3782	5MC	C4-N4	4.67	1.46	1.34
4	5	1625	OMG	C4-N3	4.66	1.48	1.37
50	9	166	A2M	O3'-C3'	-4.65	1.32	1.43
4	5	2522	7MG	C2-N2	4.65	1.45	1.34
4	5	3792	OMG	C2-N2	4.64	1.45	1.34
50	9	668	A2M	O3'-C3'	-4.64	1.32	1.43
4	5	1909	P7G	C2-N2	4.63	1.45	1.34
50	9	1678	A2M	O3'-C3'	-4.63	1.32	1.43
50	9	1842	4AC	C7-N4	4.62	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	9	166	A2M	C6-N6	4.61	1.50	1.34
4	5	1605	7MG	C2-N2	4.61	1.45	1.34
4	5	4447	5MC	C6-N1	4.59	1.45	1.38
4	5	4870	OMG	C2-N2	4.59	1.45	1.34
50	9	683	OMG	C2-N2	4.58	1.45	1.34
4	5	3880	P7G	C2-N2	4.57	1.45	1.34
4	5	3718	A2M	C6-N6	4.57	1.50	1.34
50	9	484	A2M	O3'-C3'	-4.56	1.32	1.43
4	5	4550	7MG	C2-N2	4.55	1.45	1.34
4	5	4690	B8K	C71-N7	4.54	1.49	1.39
4	5	4690	B8K	C2-N2	4.54	1.45	1.34
4	5	1316	OMG	C2-N2	4.54	1.45	1.34
4	5	2424	OMG	C2-N2	4.54	1.45	1.34
4	5	1326	A2M	C6-N6	4.53	1.50	1.34
4	5	4196	OMG	C2-N2	4.53	1.45	1.34
4	5	3867	A2M	C6-N6	4.52	1.50	1.34
4	5	3718	A2M	O3'-C3'	-4.52	1.32	1.43
4	5	4571	A2M	C6-N6	4.52	1.50	1.34
4	5	2364	OMG	C2-N2	4.51	1.44	1.34
4	5	1871	A2M	O3'-C3'	-4.50	1.32	1.43
4	5	398	A2M	C6-N6	4.50	1.50	1.34
50	9	1031	A2M	C6-N6	4.49	1.50	1.34
4	5	1534	A2M	O3'-C3'	-4.49	1.32	1.43
4	5	373	OMG	C2-N2	4.49	1.44	1.34
50	9	159	A2M	C6-N6	4.49	1.50	1.34
4	5	4523	A2M	C6-N6	4.48	1.50	1.34
50	9	644	OMG	C2-N2	4.48	1.44	1.34
4	5	4370	OMG	C2-N2	4.48	1.44	1.34
4	5	4447	5MC	C4-N4	4.48	1.45	1.34
50	9	27	A2M	C6-N6	4.48	1.50	1.34
50	9	644	OMG	C4-N3	4.48	1.48	1.37
4	5	2363	A2M	O3'-C3'	-4.48	1.32	1.43
4	5	2773	OMG	C2-N2	4.47	1.44	1.34
4	5	1871	A2M	C6-N6	4.47	1.50	1.34
4	5	1797	E7G	C4-N3	4.47	1.44	1.34
50	9	1219	B8Q	C2-N1	4.47	1.45	1.38
4	5	1625	OMG	C2-N2	4.47	1.44	1.34
4	5	4494	OMG	C2-N2	4.47	1.44	1.34
4	5	3723	A2M	C6-N6	4.46	1.50	1.34
4	5	373	OMG	C4-N3	4.46	1.48	1.37
4	5	4494	OMG	C4-N3	4.46	1.48	1.37
4	5	4196	OMG	C4-N3	4.45	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	9	1678	A2M	C6-N6	4.45	1.50	1.34
50	9	668	A2M	C6-N6	4.45	1.50	1.34
4	5	3825	A2M	C6-N6	4.45	1.50	1.34
4	5	3899	BGH	C2-N2	4.45	1.44	1.34
4	5	3867	A2M	O3'-C3'	-4.43	1.32	1.43
4	5	4370	OMG	C4-N3	4.43	1.48	1.37
4	5	2050	OMG	C4-N3	4.42	1.48	1.37
4	5	1659	I4U	C3'-C4'	4.42	1.64	1.53
4	5	1348	P4U	O4-C4	4.42	1.40	1.35
50	9	1830	UR3	C2-N3	4.41	1.47	1.39
4	5	1883	OMG	C2-N2	4.41	1.44	1.34
4	5	2773	OMG	C4-N3	4.41	1.48	1.37
4	5	4623	OMG	C2-N2	4.40	1.44	1.34
4	5	2297	E7G	C4-N3	4.39	1.44	1.34
50	9	484	A2M	C6-N6	4.39	1.50	1.34
50	9	1806	M7A	C6-N6	4.38	1.45	1.34
4	5	4872	2MG	C2-N1	4.37	1.43	1.36
4	5	2363	A2M	C6-N6	4.36	1.50	1.34
4	5	2401	A2M	C6-N6	4.36	1.50	1.34
4	5	4483	B8T	C4-N4	4.36	1.44	1.35
4	5	1522	OMG	C2-N2	4.35	1.44	1.34
4	5	1524	A2M	C6-N6	4.35	1.49	1.34
4	5	1534	A2M	C6-N6	4.34	1.49	1.34
4	5	4690	B8K	O4'-C1'	4.34	1.52	1.42
4	5	237	B9B	O3'-C3'	-4.32	1.32	1.43
50	9	1842	4AC	C4-N4	4.32	1.46	1.39
4	5	4623	OMG	C4-N3	4.31	1.47	1.37
4	5	3899	BGH	O2'-C2'	-4.31	1.31	1.42
50	9	509	OMG	C4-N3	4.30	1.47	1.37
50	9	509	OMG	C2-N2	4.30	1.44	1.34
4	5	4671	B8T	C4-N4	4.29	1.44	1.35
4	5	1522	OMG	C4-N3	4.29	1.47	1.37
4	5	4637	OMG	C4-N3	4.28	1.47	1.37
4	5	4564	M7A	C6-N6	4.28	1.44	1.34
4	5	3897	B8K	C2-N2	4.28	1.44	1.34
4	5	2522	7MG	C4-N9	4.26	1.42	1.37
4	5	1316	OMG	C4-N3	4.25	1.47	1.37
4	5	3909	OMC	O2-C2	-4.22	1.15	1.23
4	5	3880	P7G	C8-N7	4.22	1.49	1.45
50	9	1337	4AC	C4-N4	4.20	1.45	1.39
4	5	4637	OMG	C2-N2	4.20	1.44	1.34
50	9	1248	B8N	C6-C5	4.18	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	5	4523	A2M	O3'-C3'	-4.17	1.33	1.43
4	5	3897	B8K	C71-N7	4.17	1.48	1.39
50	9	1374	5MC	C2-N1	4.16	1.49	1.40
4	5	2364	OMG	C4-N3	4.15	1.47	1.37
4	5	1659	I4U	O4'-C1'	4.14	1.51	1.42
4	5	3782	5MC	C2-N1	4.09	1.48	1.40
4	5	3785	A2M	C6-N6	4.09	1.49	1.34
4	5	4872	2MG	C4-N3	4.06	1.47	1.37
50	9	1374	5MC	C6-N1	4.05	1.45	1.38
4	5	4530	UR3	C2-N3	4.04	1.46	1.39
4	5	1909	P7G	C8-N7	4.04	1.49	1.45
4	5	1866	UR3	C2-N3	4.02	1.46	1.39
4	5	2050	OMG	C2-N2	4.01	1.43	1.34
4	5	2297	E7G	C2-N2	4.00	1.43	1.34
4	5	3897	B8K	O4'-C1'	4.00	1.51	1.42
4	5	1348	P4U	C2-N1	3.99	1.48	1.40
4	5	3887	OMC	C4-N4	3.99	1.43	1.33
4	5	1517	2MG	C2-N1	3.97	1.43	1.36
4	5	3899	BGH	C4-N9	3.95	1.42	1.37
4	5	3782	5MC	C6-N1	3.95	1.44	1.38
4	5	2422	OMC	C4-N4	3.90	1.43	1.33
50	9	517	OMC	C4-N4	3.88	1.43	1.33
50	9	1703	OMC	C4-N4	3.88	1.43	1.33
50	9	1710	OMC	C4-N4	3.88	1.43	1.33
4	5	2804	OMC	C4-N4	3.87	1.43	1.33
4	5	1574	B9B	O3'-C3'	-3.83	1.34	1.43
50	9	1710	OMC	C2-N1	3.81	1.48	1.40
4	5	3869	OMC	C4-N4	3.80	1.42	1.33
4	5	4550	7MG	C4-N9	3.80	1.42	1.37
4	5	4335	5MC	C6-N1	3.79	1.44	1.38
4	5	4690	B8K	O6-C6	-3.79	1.16	1.23
50	9	174	OMC	C4-N4	3.77	1.42	1.33
4	5	1348	P4U	C5-C4	3.77	1.48	1.43
4	5	2365	OMC	C4-N4	3.77	1.42	1.33
4	5	1797	E7G	C2-N2	3.77	1.43	1.34
4	5	2861	OMC	C4-N4	3.75	1.42	1.33
50	9	121	OMU	C4-N3	3.75	1.45	1.38
4	5	4447	5MC	C2-N1	3.74	1.48	1.40
4	5	4335	5MC	C2-N1	3.73	1.48	1.40
50	9	517	OMC	C2-N1	3.72	1.48	1.40
4	5	2754	B9B	O3'-C3'	-3.72	1.34	1.43
4	5	3701	OMC	C4-N4	3.71	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	5	4194	I4U	C5-C4	3.69	1.47	1.43
4	5	4494	OMG	C5-C4	-3.67	1.33	1.43
4	5	4472	B8W	O4'-C4'	3.65	1.53	1.45
50	9	174	OMC	C2-N1	3.64	1.47	1.40
4	5	729	2MG	C2-N1	3.63	1.42	1.36
50	9	1806	M7A	C5-N7	3.63	1.48	1.39
4	5	4872	2MG	C5-C4	-3.62	1.33	1.43
50	9	1337	4AC	C5-C4	3.62	1.48	1.40
50	9	1243	PSU	C6-C5	3.60	1.39	1.35
4	5	4536	OMC	C4-N4	3.60	1.42	1.33
4	5	3880	P7G	C2-N3	3.59	1.46	1.37
4	5	2380	B8W	O4'-C4'	3.57	1.53	1.45
50	9	116	OMU	C4-N3	3.57	1.45	1.38
4	5	1316	OMG	C5-C4	-3.56	1.34	1.43
4	5	3785	A2M	O3'-C3'	-3.56	1.34	1.43
6	8	14	OMU	O4-C4	-3.56	1.17	1.24
4	5	1909	P7G	C5-C4	3.55	1.44	1.37
4	5	4671	B8T	C2-N1	3.53	1.47	1.40
4	5	3899	BGH	C5-N7	3.53	1.45	1.39
4	5	4335	5MC	O2-C2	-3.50	1.17	1.23
50	9	1842	4AC	C2-N1	3.50	1.47	1.40
4	5	3723	A2M	O2'-C2'	3.48	1.51	1.42
50	9	1678	A2M	O2'-C2'	3.47	1.51	1.42
4	5	4355	E6G	O2'-C2'	3.46	1.51	1.43
4	5	4872	2MG	O6-C6	-3.46	1.16	1.23
50	9	1703	OMC	O2-C2	-3.45	1.17	1.23
4	5	1322	1MA	C2-N1	3.45	1.42	1.35
4	5	3785	A2M	C5-C4	-3.44	1.31	1.40
4	5	3887	OMC	O2-C2	-3.44	1.17	1.23
4	5	2861	OMC	C2-N1	3.44	1.47	1.40
4	5	4129	B8W	O4'-C4'	3.44	1.52	1.45
4	5	1659	I4U	C5-C4	3.41	1.47	1.43
4	5	4355	E6G	O3'-C3'	-3.41	1.34	1.43
6	8	14	OMU	C4-N3	3.41	1.44	1.38
4	5	3897	B8K	C2-N1	3.39	1.46	1.37
4	5	4637	OMG	C5-C4	-3.39	1.34	1.43
4	5	4196	OMG	C6-N1	3.39	1.42	1.37
4	5	729	2MG	O6-C6	-3.38	1.16	1.23
50	9	159	A2M	O2'-C2'	3.37	1.51	1.42
4	5	3867	A2M	O2'-C2'	3.37	1.51	1.42
4	5	4620	OMU	C4-N3	3.37	1.44	1.38
4	5	4194	I4U	C2-N1	3.37	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	5	1797	E7G	C5-C6	3.37	1.52	1.43
50	9	1703	OMC	C6-N1	3.37	1.46	1.38
50	9	1842	4AC	C5-C4	3.37	1.48	1.40
4	5	4447	5MC	O2-C2	-3.36	1.17	1.23
4	5	2050	OMG	C5-C4	-3.36	1.34	1.43
4	5	2422	OMC	O2-C2	-3.35	1.17	1.23
4	5	1605	7MG	C2-N1	3.35	1.45	1.37
4	5	4483	B8T	C2-N1	3.35	1.47	1.40
4	5	3899	BGH	C5-C6	3.35	1.52	1.43
4	5	4220	6MZ	C5-C4	-3.34	1.32	1.40
4	5	4129	B8W	C3'-C2'	3.34	1.62	1.53
4	5	1659	I4U	O2-C2	-3.34	1.17	1.23
4	5	3909	OMC	C4-N4	3.34	1.41	1.33
4	5	4536	OMC	O2-C2	-3.33	1.17	1.23
4	5	2365	OMC	C6-N1	3.33	1.46	1.38
4	5	4472	B8W	C3'-C2'	3.33	1.62	1.53
4	5	4185	B8W	O4'-C4'	3.32	1.52	1.45
4	5	4415	1MA	C4-N3	3.32	1.47	1.37
4	5	4194	I4U	O4'-C1'	3.32	1.49	1.42
4	5	2773	OMG	C6-N1	3.32	1.42	1.37
50	9	1337	4AC	C2-N1	3.32	1.47	1.40
4	5	1517	2MG	O6-C6	-3.31	1.16	1.23
50	9	568	E3C	C4-N3	3.31	1.53	1.48
4	5	1522	OMG	C5-C4	-3.31	1.34	1.43
4	5	2424	OMG	C6-N1	3.31	1.42	1.37
4	5	2380	B8W	C3'-C2'	3.31	1.62	1.53
4	5	3718	A2M	O2'-C2'	3.31	1.51	1.42
4	5	373	OMG	C5-C4	-3.29	1.34	1.43
4	5	4472	B8W	C5-C4	-3.29	1.32	1.40
4	5	2522	7MG	C2-N1	3.29	1.45	1.37
4	5	2297	E7G	C5-C6	3.28	1.52	1.43
4	5	3867	A2M	C2-N3	3.28	1.37	1.32
4	5	373	OMG	C6-N1	3.28	1.42	1.37
4	5	3880	P7G	C5-C4	3.28	1.43	1.37
50	9	683	OMG	C6-N1	3.27	1.42	1.37
50	9	517	OMC	C6-N1	3.27	1.45	1.38
4	5	2522	7MG	C5-C6	3.27	1.52	1.43
4	5	4620	OMU	O4-C4	-3.27	1.18	1.24
4	5	4194	I4U	O4-C41	-3.25	1.39	1.47
4	5	1534	A2M	C2-N3	3.25	1.37	1.32
4	5	4296	B8H	O4-C4	-3.24	1.17	1.23
4	5	3897	B8K	O6-C6	-3.24	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	5	4872	2MG	C6-N1	3.24	1.42	1.37
4	5	2297	E7G	C2-N1	3.23	1.45	1.37
4	5	4483	B8T	C5-C4	3.23	1.47	1.40
4	5	4483	B8T	O2-C2	-3.23	1.17	1.23
50	9	121	OMU	O4-C4	-3.22	1.18	1.24
4	5	4623	OMG	C5-C4	-3.22	1.34	1.43
4	5	4523	A2M	C5-C4	-3.22	1.32	1.40
4	5	1909	P7G	C2-N3	3.22	1.45	1.37
4	5	1909	P7G	O6-C6	-3.21	1.18	1.23
50	9	116	OMU	O4-C4	-3.21	1.18	1.24
4	5	1316	OMG	C6-N1	3.21	1.42	1.37
4	5	4529	B8W	C3'-C2'	3.21	1.62	1.53
4	5	2804	OMC	O2-C2	-3.21	1.17	1.23
4	5	3899	BGH	O6-C6	-3.20	1.17	1.23
4	5	4306	OMU	C4-N3	3.20	1.44	1.38
4	5	1883	OMG	C5-C4	-3.20	1.34	1.43
4	5	4690	B8K	C2-N1	3.19	1.45	1.37
4	5	2861	OMC	C6-N1	3.19	1.45	1.38
50	9	484	A2M	O2'-C2'	3.19	1.50	1.42
50	9	668	A2M	C5-C4	-3.19	1.32	1.40
4	5	4370	OMG	C5-C4	-3.18	1.35	1.43
4	5	1860	B8H	O4-C4	-3.17	1.17	1.23
4	5	2365	OMC	O2-C2	-3.17	1.17	1.23
4	5	4536	OMC	C2-N1	3.17	1.46	1.40
4	5	4306	OMU	O4-C4	-3.16	1.18	1.24
4	5	4194	I4U	O2'-C2'	3.16	1.50	1.43
4	5	4494	OMG	C6-N1	3.16	1.42	1.37
50	9	1703	OMC	C2-N1	3.16	1.46	1.40
4	5	3825	A2M	C2-N3	3.16	1.37	1.32
50	9	174	OMC	C6-N1	3.16	1.45	1.38
4	5	1797	E7G	C2-N1	3.15	1.45	1.37
50	9	1031	A2M	C5-C4	-3.15	1.32	1.40
4	5	2422	OMC	C6-N1	3.15	1.45	1.38
50	9	1710	OMC	C6-N1	3.15	1.45	1.38
4	5	3869	OMC	O2-C2	-3.14	1.17	1.23
4	5	1326	A2M	O2'-C2'	3.14	1.50	1.42
4	5	4185	B8W	C3'-C2'	3.14	1.61	1.53
4	5	4564	M7A	C5-N7	3.14	1.46	1.39
4	5	4355	E6G	C5-C4	-3.14	1.32	1.40
4	5	1348	P4U	O2-C2	-3.14	1.17	1.23
4	5	3887	OMC	C2-N1	3.13	1.46	1.40
4	5	2364	OMG	C5-C4	-3.13	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	5	3785	A2M	C3'-C4'	3.13	1.61	1.53
4	5	2380	B8W	C5-C4	-3.13	1.32	1.40
4	5	4571	A2M	C2-N3	3.13	1.37	1.32
4	5	398	A2M	O2'-C2'	3.13	1.50	1.42
4	5	3785	A2M	C2-N3	3.13	1.37	1.32
4	5	4870	OMG	C5-C4	-3.13	1.35	1.43
4	5	3792	OMG	C5-C4	-3.13	1.35	1.43
4	5	4370	OMG	C6-N1	3.12	1.42	1.37
4	5	2804	OMC	C2-N1	3.12	1.46	1.40
4	5	1524	A2M	C5-C4	-3.12	1.32	1.40
50	9	644	OMG	C5-C4	-3.12	1.35	1.43
4	5	3762	B8H	O4-C4	-3.12	1.17	1.23
4	5	3701	OMC	C2-N1	3.11	1.46	1.40
50	9	509	OMG	C6-N1	3.11	1.42	1.37
4	5	2861	OMC	O2-C2	-3.11	1.17	1.23
4	5	4571	A2M	C5-C4	-3.10	1.32	1.40
50	9	27	A2M	C5-C4	-3.10	1.32	1.40
50	9	166	A2M	O2'-C2'	3.10	1.50	1.42
4	5	4529	B8W	O4'-C4'	3.09	1.51	1.45
4	5	2422	OMC	C2-N1	3.09	1.46	1.40
4	5	1534	A2M	C5-C4	-3.09	1.32	1.40
50	9	1031	A2M	O2'-C2'	3.09	1.50	1.42
50	9	166	A2M	C2-N3	3.09	1.37	1.32
4	5	2363	A2M	C5-C4	-3.09	1.32	1.40
4	5	1605	7MG	C5-C6	3.08	1.51	1.43
4	5	2364	OMG	C6-N1	3.08	1.42	1.37
4	5	2401	A2M	O2'-C2'	3.07	1.50	1.42
4	5	4083	5MU	O4-C4	-3.07	1.17	1.23
4	5	1659	I4U	O2'-C2'	3.07	1.50	1.43
4	5	729	2MG	C5-C4	-3.07	1.35	1.43
4	5	2804	OMC	C6-N1	3.07	1.45	1.38
4	5	4571	A2M	O2'-C2'	3.06	1.50	1.42
4	5	2401	A2M	C5-C4	-3.06	1.32	1.40
4	5	4550	7MG	C5-C6	3.06	1.51	1.43
50	9	1374	5MC	O2-C2	-3.06	1.18	1.23
4	5	1326	A2M	C5-C4	-3.06	1.32	1.40
4	5	3701	OMC	C6-N1	3.05	1.45	1.38
4	5	4371	MHG	C5-C6	3.05	1.51	1.43
4	5	1524	A2M	O2'-C2'	3.04	1.50	1.42
4	5	1871	A2M	C5-C4	-3.04	1.32	1.40
50	9	121	OMU	O2-C2	-3.04	1.17	1.23
4	5	1522	OMG	C6-N1	3.04	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	5	1322	1MA	C5-C4	-3.03	1.35	1.43
4	5	3785	A2M	O2'-C2'	3.03	1.50	1.42
4	5	1883	OMG	C6-N1	3.03	1.42	1.37
4	5	3825	A2M	O2'-C2'	3.03	1.50	1.42
4	5	3909	OMC	C6-N1	3.03	1.45	1.38
4	5	3869	OMC	C6-N1	3.03	1.45	1.38
4	5	398	A2M	C2-N3	3.03	1.37	1.32
4	5	1524	A2M	C2-N3	3.03	1.37	1.32
4	5	2363	A2M	C2-N3	3.02	1.37	1.32
4	5	4690	B8K	C5-C6	3.02	1.51	1.43
50	9	159	A2M	C2-N3	3.02	1.37	1.32
4	5	4671	B8T	C5-C4	3.02	1.47	1.40
50	9	1710	OMC	O2-C2	-3.01	1.18	1.23
4	5	4371	MHG	C6-N1	3.01	1.44	1.38
4	5	3897	B8K	C5-C6	3.01	1.51	1.43
4	5	1871	A2M	O2'-C2'	3.00	1.50	1.42
4	5	4185	B8W	C5-C4	-3.00	1.33	1.40
50	9	166	A2M	C5-C4	-3.00	1.33	1.40
4	5	4623	OMG	C6-N1	3.00	1.42	1.37
4	5	2773	OMG	C5-C4	-3.00	1.35	1.43
4	5	3782	5MC	O2-C2	-2.99	1.18	1.23
4	5	4550	7MG	C2-N1	2.99	1.45	1.37
50	9	1678	A2M	C2-N3	2.99	1.36	1.32
50	9	1842	4AC	O2-C2	-2.99	1.18	1.23
50	9	484	A2M	C5-C4	-2.98	1.33	1.40
50	9	644	OMG	C6-N1	2.98	1.42	1.37
50	9	1031	A2M	C2-N3	2.98	1.36	1.32
50	9	517	OMC	O2-C2	-2.98	1.18	1.23
4	5	3880	P7G	O6-C6	-2.98	1.19	1.23
50	9	1678	A2M	C5-C4	-2.97	1.33	1.40
4	5	3887	OMC	C6-N1	2.97	1.45	1.38
4	5	1659	I4U	O4-C41	-2.97	1.40	1.47
4	5	3723	A2M	C2-N3	2.97	1.36	1.32
4	5	4671	B8T	O2-C2	-2.96	1.18	1.23
4	5	1517	2MG	C5-C4	-2.96	1.35	1.43
4	5	2401	A2M	C2-N3	2.96	1.36	1.32
4	5	1456	B8Q	C2-N1	2.95	1.42	1.38
4	5	4523	A2M	O2'-C2'	2.95	1.50	1.42
50	9	1832	6MZ	C5-C4	-2.95	1.33	1.40
50	9	484	A2M	C2-N3	2.95	1.36	1.32
4	5	3899	BGH	C2-N1	2.95	1.45	1.37
50	9	683	OMG	C5-C4	-2.94	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	9	1337	4AC	O2-C2	-2.94	1.18	1.23
4	5	1605	7MG	O6-C6	-2.94	1.18	1.23
50	9	509	OMG	C5-C4	-2.94	1.35	1.43
4	5	3825	A2M	C5-C4	-2.94	1.33	1.40
50	9	668	A2M	O2'-C2'	2.93	1.50	1.42
4	5	398	A2M	C5-C4	-2.93	1.33	1.40
4	5	1683	PSU	C6-C5	2.93	1.38	1.35
4	5	2424	OMG	C5-C4	-2.93	1.35	1.43
50	9	159	A2M	C5-C4	-2.92	1.33	1.40
4	5	4523	A2M	C2-N3	2.92	1.36	1.32
4	5	4870	OMG	C6-N1	2.92	1.42	1.37
4	5	1659	I4U	C2-N1	2.92	1.46	1.40
4	5	2365	OMC	C2-N1	2.91	1.46	1.40
4	5	1625	OMG	C5-C4	-2.91	1.35	1.43
4	5	4194	I4U	O2-C2	-2.91	1.18	1.23
4	5	2363	A2M	O2'-C2'	2.91	1.50	1.42
4	5	1625	OMG	C6-N1	2.90	1.42	1.37
4	5	3867	A2M	C5-C4	-2.90	1.33	1.40
4	5	1322	1MA	C4-N3	2.89	1.46	1.37
4	5	2424	OMG	C5-C6	2.89	1.53	1.47
50	9	174	OMC	O2-C2	-2.89	1.18	1.23
4	5	1534	A2M	O2'-C2'	2.89	1.50	1.42
50	9	27	A2M	O2'-C2'	2.87	1.50	1.42
4	5	1326	A2M	C2-N3	2.87	1.36	1.32
50	9	1337	4AC	C6-N1	2.85	1.44	1.38
4	5	4483	B8T	C6-N1	2.84	1.44	1.38
4	5	3723	A2M	C5-C4	-2.84	1.33	1.40
50	9	568	E3C	C6-N1	2.84	1.44	1.38
4	5	1456	B8Q	O2-C2	-2.84	1.17	1.22
50	9	1219	B8Q	O2-C2	-2.84	1.17	1.22
4	5	3701	OMC	O2-C2	-2.83	1.18	1.23
4	5	3764	PSU	C6-C5	2.83	1.38	1.35
4	5	3718	A2M	C2-N3	2.83	1.36	1.32
4	5	1871	A2M	C2-N3	2.82	1.36	1.32
4	5	1582	PSU	C6-C5	2.82	1.38	1.35
50	9	814	5MU	O4-C4	-2.82	1.18	1.23
4	5	4531	PSU	C6-C5	2.82	1.38	1.35
4	5	1883	OMG	C5-C6	2.81	1.53	1.47
4	5	3729	PSU	C6-C5	2.81	1.38	1.35
4	5	4196	OMG	C5-C4	-2.81	1.35	1.43
4	5	4536	OMC	C6-N1	2.80	1.44	1.38
50	9	822	PSU	C6-C5	2.80	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	5	3718	A2M	C5-C4	-2.80	1.33	1.40
4	5	4306	OMU	O2-C2	-2.79	1.17	1.23
4	5	4529	B8W	C5-C4	-2.79	1.33	1.40
50	9	1851	MA6	C5-C4	-2.79	1.33	1.40
50	9	27	A2M	C2-N3	2.78	1.36	1.32
4	5	1517	2MG	C6-N1	2.78	1.42	1.37
4	5	3897	B8K	C6-N1	2.77	1.44	1.38
4	5	2050	OMG	C6-N1	2.76	1.42	1.37
4	5	4220	6MZ	C2-N3	2.76	1.36	1.32
4	5	3909	OMC	C2-N1	2.76	1.46	1.40
4	5	3899	BGH	C71-N7	2.75	1.45	1.39
4	5	1659	I4U	O4-C4	2.74	1.40	1.35
4	5	1605	7MG	C6-N1	2.74	1.43	1.38
4	5	4129	B8W	C5-C4	-2.74	1.33	1.40
4	5	3869	OMC	C2-N1	2.74	1.45	1.40
4	5	2754	B9B	O2'-C2'	2.73	1.49	1.43
50	9	1850	MA6	C5-C4	-2.73	1.33	1.40
4	5	1866	UR3	O4-C4	-2.73	1.17	1.23
50	9	1830	UR3	O2-C2	-2.72	1.17	1.22
4	5	4872	2MG	C5-C6	2.72	1.52	1.47
4	5	3792	OMG	O6-C6	-2.71	1.17	1.23
4	5	4620	OMU	O2-C2	-2.71	1.18	1.23
4	5	2522	7MG	O6-C6	-2.70	1.18	1.23
4	5	3792	OMG	C6-N1	2.70	1.41	1.37
4	5	4637	OMG	C6-N1	2.68	1.41	1.37
4	5	4494	OMG	O6-C6	-2.67	1.17	1.23
4	5	4083	5MU	O2-C2	-2.66	1.18	1.23
4	5	1316	OMG	O6-C6	-2.65	1.17	1.23
4	5	1659	I4U	C6-N1	2.64	1.44	1.38
4	5	2522	7MG	C6-N1	2.64	1.43	1.38
4	5	4293	PSU	C6-C5	2.63	1.38	1.35
4	5	4415	1MA	C5-C4	-2.63	1.36	1.43
50	9	116	OMU	O2-C2	-2.63	1.18	1.23
50	9	823	PSU	C6-C5	2.63	1.38	1.35
4	5	1677	PSU	C6-C5	2.62	1.38	1.35
4	5	4530	UR3	C6-N1	2.62	1.44	1.38
4	5	1522	OMG	O6-C6	-2.61	1.18	1.23
4	5	4442	PSU	C6-C5	2.61	1.38	1.35
4	5	2773	OMG	C2-N1	2.61	1.44	1.37
4	5	237	B9B	O2'-C2'	2.61	1.49	1.43
4	5	4597	UR3	C6-N1	2.60	1.44	1.38
4	5	1866	UR3	O2-C2	-2.60	1.17	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	5	2754	B9B	C5-C4	-2.59	1.34	1.40
4	5	4550	7MG	O6-C6	-2.59	1.18	1.23
4	5	1883	OMG	O6-C6	-2.58	1.18	1.23
4	5	4628	PSU	C6-C5	2.58	1.38	1.35
4	5	237	B9B	C5-C4	-2.58	1.34	1.40
4	5	4550	7MG	C6-N1	2.57	1.43	1.38
50	9	683	OMG	C5-C6	2.57	1.52	1.47
50	9	1081	PSU	O4'-C1'	-2.56	1.40	1.43
4	5	3715	PSU	C6-C5	2.56	1.38	1.35
4	5	2508	PSU	C6-C5	2.55	1.38	1.35
4	5	4371	MHG	O6-C6	-2.55	1.18	1.23
4	5	2364	OMG	O6-C6	-2.55	1.18	1.23
4	5	4637	OMG	O6-C6	-2.55	1.18	1.23
4	5	4623	OMG	O6-C6	-2.55	1.18	1.23
4	5	4530	UR3	O2-C2	-2.55	1.17	1.22
4	5	1574	B9B	O2'-C2'	2.55	1.49	1.43
50	9	668	A2M	C2-N3	2.54	1.36	1.32
50	9	683	OMG	O6-C6	-2.54	1.18	1.23
4	5	2050	OMG	O6-C6	-2.54	1.18	1.23
50	9	1830	UR3	C6-N1	2.52	1.44	1.38
6	8	14	OMU	O2-C2	-2.52	1.18	1.23
50	9	814	5MU	O2-C2	-2.52	1.18	1.23
4	5	1625	OMG	O6-C6	-2.52	1.18	1.23
50	9	1832	6MZ	C2-N3	2.52	1.36	1.32
50	9	1081	PSU	C6-C5	2.52	1.38	1.35
4	5	1677	PSU	O4'-C1'	-2.51	1.40	1.43
50	9	1842	4AC	C6-N1	2.51	1.44	1.38
4	5	4530	UR3	O4-C4	-2.51	1.18	1.23
4	5	1866	UR3	C6-N1	2.51	1.44	1.38
4	5	4870	OMG	O6-C6	-2.50	1.18	1.23
50	9	644	OMG	O6-C6	-2.50	1.18	1.23
4	5	1574	B9B	C5-C4	-2.50	1.34	1.40
4	5	4690	B8K	C6-N1	2.49	1.43	1.38
4	5	2424	OMG	O6-C6	-2.49	1.18	1.23
4	5	1797	E7G	O6-C6	-2.48	1.18	1.23
50	9	1248	B8N	O4-C4	-2.47	1.17	1.23
4	5	4370	OMG	O6-C6	-2.46	1.18	1.23
4	5	1534	A2M	O5'-C5'	-2.46	1.38	1.44
50	9	683	OMG	C2-N1	2.46	1.43	1.37
4	5	3899	BGH	C6-N1	2.45	1.43	1.38
4	5	2297	E7G	C6-N1	2.44	1.43	1.38
4	5	3899	BGH	O5'-C5'	-2.43	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	9	166	A2M	O5'-C5'	-2.43	1.38	1.44
50	9	509	OMG	C2-N1	2.43	1.43	1.37
4	5	1683	PSU	C4-C5	-2.42	1.37	1.44
4	5	4220	6MZ	C6-N1	-2.42	1.30	1.34
4	5	2364	OMG	C2-N1	2.41	1.43	1.37
50	9	509	OMG	O6-C6	-2.41	1.18	1.23
50	9	1248	B8N	O2-C2	-2.41	1.18	1.22
4	5	4636	PSU	C4-C5	-2.41	1.37	1.44
4	5	2773	OMG	O6-C6	-2.41	1.18	1.23
4	5	4403	PSU	C6-C5	2.41	1.38	1.35
50	9	121	OMU	C6-N1	2.40	1.43	1.38
4	5	1522	OMG	C5-C6	2.40	1.52	1.47
4	5	373	OMG	C2-N1	2.38	1.43	1.37
4	5	4306	OMU	C6-N1	2.38	1.43	1.38
4	5	4450	PSU	C4-C5	-2.38	1.37	1.44
50	9	509	OMG	C5-C6	2.38	1.52	1.47
4	5	1797	E7G	C6-N1	2.37	1.43	1.38
50	9	612	PSU	C6-C5	2.37	1.38	1.35
4	5	1348	P4U	C6-N1	2.37	1.43	1.38
50	9	568	E3C	O2-C2	-2.37	1.18	1.22
50	9	668	A2M	C4-N3	-2.36	1.32	1.35
4	5	4370	OMG	C2-N1	2.36	1.43	1.37
4	5	1517	2MG	C5-C6	2.36	1.52	1.47
4	5	4529	B8W	O5'-C5'	-2.36	1.39	1.44
4	5	4194	I4U	C6-N1	2.35	1.43	1.38
4	5	4597	UR3	O2-C2	-2.34	1.18	1.22
4	5	4597	UR3	O4-C4	-2.34	1.18	1.23
4	5	4671	B8T	C6-N1	2.32	1.43	1.38
50	9	644	OMG	C2-N1	2.32	1.43	1.37
50	9	159	A2M	C5'-C4'	2.31	1.58	1.51
4	5	4196	OMG	C2-N1	2.31	1.43	1.37
4	5	373	OMG	O6-C6	-2.30	1.18	1.23
4	5	4196	OMG	C5-C6	2.30	1.52	1.47
50	9	1830	UR3	O4-C4	-2.30	1.18	1.23
4	5	4194	I4U	O5'-C5'	-2.29	1.39	1.44
50	9	822	PSU	O4'-C1'	-2.29	1.40	1.43
4	5	4370	OMG	C5-C6	2.28	1.52	1.47
4	5	4293	PSU	C4-C5	-2.28	1.37	1.44
50	9	1842	4AC	O7-C7	-2.28	1.18	1.23
4	5	3792	OMG	C5-C6	2.28	1.52	1.47
4	5	4870	OMG	C5-C6	2.28	1.52	1.47
4	5	4571	A2M	C5'-C4'	2.27	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	5	4494	OMG	C2-N1	2.27	1.43	1.37
4	5	1326	A2M	C5-N7	-2.26	1.31	1.39
50	9	27	A2M	C5'-C4'	2.25	1.58	1.51
4	5	2424	OMG	C2-N1	2.25	1.43	1.37
4	5	2297	E7G	O6-C6	-2.25	1.19	1.23
4	5	2773	OMG	C5-C6	2.25	1.52	1.47
50	9	823	PSU	C4-C5	-2.25	1.37	1.44
4	5	4450	PSU	O4'-C1'	-2.24	1.40	1.43
4	5	4196	OMG	O6-C6	-2.24	1.18	1.23
4	5	4500	PSU	C4-C5	-2.24	1.37	1.44
4	5	4194	I4U	O4-C4	2.23	1.39	1.35
4	5	4623	OMG	C2-N1	2.22	1.43	1.37
4	5	3825	A2M	O5'-C5'	-2.22	1.39	1.44
4	5	3718	A2M	C3'-C4'	2.22	1.58	1.53
4	5	4523	A2M	O5'-C5'	-2.21	1.39	1.44
50	9	668	A2M	O5'-C5'	-2.20	1.39	1.44
4	5	4628	PSU	O4'-C1'	-2.20	1.40	1.43
4	5	4472	B8W	C4-N3	-2.20	1.32	1.35
4	5	1677	PSU	C4-C5	-2.19	1.37	1.44
50	9	612	PSU	O4'-C1'	-2.19	1.40	1.43
4	5	2380	B8W	O5'-C5'	-2.19	1.39	1.44
4	5	4623	OMG	C5-C6	2.19	1.51	1.47
50	9	1031	A2M	C5'-C4'	2.19	1.58	1.51
4	5	2363	A2M	C5-N7	-2.19	1.31	1.39
4	5	4500	PSU	O4'-C1'	-2.19	1.40	1.43
4	5	4129	B8W	O5'-C5'	-2.19	1.39	1.44
4	5	4531	PSU	O4'-C1'	-2.18	1.40	1.43
4	5	373	OMG	C5-C6	2.18	1.51	1.47
4	5	1582	PSU	O4'-C1'	-2.18	1.40	1.43
4	5	1316	OMG	C2-N1	2.18	1.43	1.37
4	5	2401	A2M	O5'-C5'	-2.17	1.39	1.44
4	5	2363	A2M	O5'-C5'	-2.17	1.39	1.44
4	5	3867	A2M	C5'-C4'	2.17	1.58	1.51
4	5	1625	OMG	C2-N1	2.17	1.43	1.37
4	5	4870	OMG	C2-N1	2.17	1.43	1.37
4	5	4637	OMG	C5-C6	2.16	1.51	1.47
50	9	1219	B8Q	C4-N3	-2.15	1.45	1.48
4	5	1522	OMG	C2-N1	2.15	1.43	1.37
4	5	1574	B9B	C5'-C4'	2.15	1.58	1.51
4	5	1871	A2M	O5'-C5'	-2.15	1.39	1.44
4	5	4472	B8W	O5'-C5'	-2.15	1.39	1.44
4	5	3723	A2M	C5'-C4'	2.15	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	5	3718	A2M	C5'-C4'	2.14	1.58	1.51
4	5	3718	A2M	C4-N3	-2.14	1.32	1.35
4	5	3718	A2M	C5-N7	-2.13	1.32	1.39
50	9	1678	A2M	O5'-C5'	-2.13	1.39	1.44
4	5	2050	OMG	C5-C6	2.12	1.51	1.47
4	5	2050	OMG	C2-N1	2.12	1.42	1.37
4	5	4637	OMG	C2-N1	2.12	1.42	1.37
50	9	1832	6MZ	C6-N1	-2.12	1.31	1.34
4	5	4293	PSU	O4'-C1'	-2.12	1.40	1.43
4	5	4185	B8W	O5'-C5'	-2.11	1.39	1.44
4	5	3785	A2M	C5'-C4'	2.11	1.58	1.51
50	9	484	A2M	C5-N7	-2.11	1.32	1.39
4	5	2363	A2M	C5'-C4'	2.10	1.58	1.51
4	5	3723	A2M	C3'-C4'	2.10	1.58	1.53
50	9	1081	PSU	C4-C5	-2.09	1.38	1.44
4	5	1871	A2M	C5-N7	-2.09	1.32	1.39
4	5	1871	A2M	C5'-C4'	2.09	1.58	1.51
4	5	3792	OMG	C2-N1	2.09	1.42	1.37
4	5	4442	PSU	C4-C5	-2.08	1.38	1.44
4	5	1883	OMG	C2-N1	2.08	1.42	1.37
4	5	4636	PSU	O4'-C1'	-2.08	1.41	1.43
50	9	116	OMU	C6-N1	2.08	1.43	1.38
4	5	3718	A2M	O5'-C5'	-2.07	1.39	1.44
4	5	4306	OMU	C5-C4	2.07	1.48	1.43
4	5	1456	B8Q	C4-N3	-2.07	1.45	1.48
4	5	1524	A2M	C5-N7	-2.07	1.32	1.39
4	5	1625	OMG	C5-C6	2.07	1.51	1.47
4	5	4403	PSU	O4'-C1'	-2.07	1.41	1.43
50	9	1031	A2M	C3'-C4'	2.06	1.58	1.53
50	9	27	A2M	C5-N7	-2.06	1.32	1.39
4	5	4523	A2M	C3'-C4'	2.06	1.58	1.53
50	9	823	PSU	O4'-C1'	-2.05	1.41	1.43
50	9	1678	A2M	C3'-C4'	2.05	1.58	1.53
50	9	119	PSU	C6-C5	2.05	1.37	1.35
4	5	4442	PSU	O4'-C1'	-2.04	1.41	1.43
4	5	4355	E6G	O5'-C5'	-2.04	1.39	1.44
50	9	644	OMG	C5-C6	2.03	1.51	1.47
4	5	4494	OMG	C5-C6	2.03	1.51	1.47
4	5	237	B9B	C5'-C4'	2.03	1.57	1.51
50	9	1248	B8N	O4'-C1'	-2.03	1.41	1.43
4	5	4296	B8H	O4'-C1'	-2.02	1.41	1.43
4	5	4500	PSU	C6-C5	2.02	1.37	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	5	1326	A2M	C4-N3	-2.02	1.32	1.35
4	5	3785	A2M	C5-N7	-2.02	1.32	1.39
4	5	1534	A2M	C5-N7	-2.02	1.32	1.39
50	9	612	PSU	C4-C5	-2.01	1.38	1.44
4	5	398	A2M	C5-N7	-2.01	1.32	1.39
4	5	4564	M7A	C5-C6	-2.01	1.35	1.40
50	9	166	A2M	C5-N7	-2.01	1.32	1.39
4	5	1524	A2M	O5'-C5'	-2.01	1.39	1.44
4	5	1322	1MA	CM1-N1	-2.00	1.42	1.46

All (601) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5	4529	B8W	N2-C2-N3	17.65	146.56	117.79
4	5	2380	B8W	N2-C2-N3	17.41	146.16	117.79
4	5	4185	B8W	N2-C2-N3	16.41	144.54	117.79
4	5	4129	B8W	N2-C2-N3	16.31	144.38	117.79
4	5	4472	B8W	N2-C2-N3	16.08	143.99	117.79
4	5	4529	B8W	N2-C2-N1	-15.93	92.48	117.25
4	5	2380	B8W	N2-C2-N1	-14.94	94.02	117.25
4	5	4472	B8W	N2-C2-N1	-14.40	94.86	117.25
4	5	4185	B8W	N2-C2-N1	-14.12	95.29	117.25
4	5	4529	B8W	C1'-N9-C4	14.10	151.41	126.64
4	5	4129	B8W	N2-C2-N1	-14.07	95.37	117.25
4	5	2380	B8W	C1'-N9-C4	13.23	149.89	126.64
4	5	4564	M7A	C5-C6-N6	13.02	145.97	123.74
4	5	4472	B8W	C1'-N9-C4	12.52	148.65	126.64
4	5	4129	B8W	C1'-N9-C4	12.45	148.51	126.64
50	9	1806	M7A	C5-C6-N6	12.22	144.62	123.74
4	5	4083	5MU	C5-C4-N3	11.54	125.16	115.31
4	5	4185	B8W	C1'-N9-C4	11.25	146.40	126.64
4	5	4564	M7A	N6-C6-N1	-11.08	94.09	118.35
50	9	814	5MU	C5-C4-N3	10.70	124.44	115.31
50	9	1806	M7A	N6-C6-N1	-10.35	95.67	118.35
50	9	1850	MA6	N1-C6-N6	-10.28	106.24	117.06
50	9	1851	MA6	N1-C6-N6	-10.00	106.54	117.06
4	5	4129	B8W	O6-C6-C5	9.13	129.06	116.01
50	9	814	5MU	C5-C6-N1	-9.04	114.04	123.34
4	5	4083	5MU	C5-C6-N1	-8.96	114.12	123.34
50	9	1678	A2M	C5-C6-N6	8.14	132.73	120.35
4	5	1326	A2M	C5-C6-N6	8.13	132.71	120.35
50	9	159	A2M	C5-C6-N6	8.01	132.53	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5	2363	A2M	C5-C6-N6	8.01	132.52	120.35
4	5	1871	A2M	C5-C6-N6	7.83	132.26	120.35
50	9	484	A2M	C5-C6-N6	7.77	132.17	120.35
4	5	3867	A2M	C5-C6-N6	7.77	132.16	120.35
4	5	4523	A2M	C5-C6-N6	7.74	132.11	120.35
4	5	1524	A2M	C5-C6-N6	7.69	132.04	120.35
4	5	4185	B8W	O6-C6-C5	7.68	126.99	116.01
50	9	166	A2M	C5-C6-N6	7.67	132.01	120.35
4	5	2786	B9H	C31-N3-C2	7.59	126.69	117.21
50	9	27	A2M	C5-C6-N6	7.57	131.85	120.35
4	5	3718	A2M	C5-C6-N6	7.52	131.78	120.35
4	5	4296	B8H	C4-N3-C2	-7.51	117.62	127.35
4	5	4571	A2M	C5-C6-N6	7.48	131.71	120.35
4	5	1534	A2M	C5-C6-N6	7.37	131.55	120.35
4	5	3723	A2M	C5-C6-N6	7.33	131.50	120.35
4	5	398	A2M	C5-C6-N6	7.31	131.47	120.35
50	9	668	A2M	C5-C6-N6	7.26	131.39	120.35
4	5	3825	A2M	C5-C6-N6	7.23	131.34	120.35
4	5	2401	A2M	C5-C6-N6	7.13	131.18	120.35
4	5	3785	A2M	C5-C6-N6	7.07	131.10	120.35
4	5	3762	B8H	C4-N3-C2	-7.06	118.21	127.35
4	5	1909	P7G	C4-C5-N7	6.96	110.34	106.67
50	9	1219	B8Q	C1'-N1-C2	6.76	128.40	116.99
4	5	1860	B8H	C4-N3-C2	-6.72	118.65	127.35
4	5	4296	B8H	N3-C2-N1	6.69	122.37	115.14
4	5	4690	B8K	C5-C6-N1	6.61	122.63	110.99
50	9	1031	A2M	C5-C6-N6	6.59	130.36	120.35
4	5	4529	B8W	O6-C6-C5	6.53	125.35	116.01
50	9	568	E3C	C1'-N1-C2	6.51	127.98	116.99
50	9	1806	M7A	N3-C4-N9	6.46	135.02	126.87
4	5	4690	B8K	C72-C71-N7	6.42	128.52	118.86
4	5	3762	B8H	N3-C2-N1	6.36	122.01	115.14
4	5	3880	P7G	C4-C5-N7	6.31	110.00	106.67
4	5	4371	MHG	C2-N3-C4	6.27	119.81	112.04
50	9	1678	A2M	N3-C2-N1	-6.00	119.29	128.68
4	5	1322	1MA	N1-C2-N3	-5.98	119.05	126.02
4	5	3825	A2M	N3-C2-N1	-5.97	119.35	128.68
4	5	3899	BGH	C5-C6-N1	5.95	121.47	110.99
4	5	4523	A2M	N3-C2-N1	-5.93	119.40	128.68
4	5	1860	B8H	N3-C2-N1	5.93	121.55	115.14
50	9	27	A2M	N3-C2-N1	-5.92	119.43	128.68
4	5	2401	A2M	N3-C2-N1	-5.90	119.45	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5	1456	B8Q	C31-N3-C4	5.90	123.14	114.25
4	5	1326	A2M	N3-C2-N1	-5.88	119.48	128.68
50	9	1031	A2M	N3-C2-N1	-5.88	119.49	128.68
50	9	1806	M7A	N3-C2-N1	-5.80	119.54	128.60
50	9	1850	MA6	N3-C2-N1	-5.79	119.63	128.68
4	5	3723	A2M	N3-C2-N1	-5.78	119.64	128.68
4	5	4220	6MZ	N3-C2-N1	-5.78	119.64	128.68
4	5	1797	E7G	C4-C5-N7	5.78	110.05	104.91
50	9	166	A2M	N3-C2-N1	-5.77	119.65	128.68
4	5	4564	M7A	N3-C2-N1	-5.75	119.61	128.60
4	5	1871	A2M	N3-C2-N1	-5.74	119.71	128.68
50	9	1678	A2M	N6-C6-N1	-5.72	106.69	118.57
4	5	3897	B8K	C5-C6-N1	5.71	121.06	110.99
4	5	398	A2M	N3-C2-N1	-5.70	119.77	128.68
4	5	3897	B8K	C72-C71-N7	5.63	127.32	118.86
6	8	14	OMU	C4-N3-C2	-5.62	119.16	126.58
4	5	1524	A2M	N3-C2-N1	-5.60	119.92	128.68
4	5	4564	M7A	N3-C4-N9	5.58	133.92	126.87
4	5	3785	A2M	N3-C2-N1	-5.58	119.96	128.68
4	5	4571	A2M	N3-C2-N1	-5.57	119.97	128.68
4	5	4690	B8K	C4-C5-N7	5.56	109.86	104.91
4	5	2380	B8W	N3-C2-N1	-5.55	119.82	127.22
4	5	1534	A2M	N3-C2-N1	-5.54	120.02	128.68
4	5	3867	A2M	N6-C6-N1	-5.54	107.08	118.57
50	9	1851	MA6	N3-C2-N1	-5.53	120.03	128.68
4	5	3899	BGH	C72-C71-N7	5.53	127.17	118.86
50	9	116	OMU	C4-N3-C2	-5.52	119.30	126.58
4	5	4636	PSU	C4-N3-C2	-5.51	118.40	126.34
50	9	484	A2M	N3-C2-N1	-5.51	120.07	128.68
4	5	2363	A2M	N6-C6-N1	-5.50	107.15	118.57
50	9	159	A2M	N6-C6-N1	-5.50	107.16	118.57
50	9	166	A2M	N6-C6-N1	-5.49	107.18	118.57
4	5	4371	MHG	C4-C5-N7	5.48	109.79	104.91
4	5	3897	B8K	C4-C5-N7	5.48	109.79	104.91
4	5	4306	OMU	C4-N3-C2	-5.48	119.35	126.58
4	5	4500	PSU	C4-N3-C2	-5.47	118.45	126.34
4	5	4083	5MU	N3-C2-N1	5.46	122.14	114.89
4	5	2297	E7G	C4-C5-N7	5.45	109.76	104.91
4	5	1524	A2M	N6-C6-N1	-5.44	107.28	118.57
50	9	159	A2M	N3-C2-N1	-5.41	120.22	128.68
50	9	668	A2M	N3-C2-N1	-5.41	120.22	128.68
4	5	4442	PSU	N1-C2-N3	5.37	121.21	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5	1534	A2M	N6-C6-N1	-5.36	107.45	118.57
4	5	4371	MHG	C5-C6-N1	5.36	120.43	110.99
50	9	121	OMU	C4-N3-C2	-5.34	119.53	126.58
4	5	1605	7MG	C5-C6-N1	5.33	120.39	110.99
4	5	1326	A2M	N6-C6-N1	-5.32	107.53	118.57
4	5	4185	B8W	N3-C2-N1	-5.30	120.15	127.22
4	5	4523	A2M	N6-C6-N1	-5.30	107.58	118.57
50	9	484	A2M	N6-C6-N1	-5.27	107.64	118.57
50	9	1248	B8N	C5-C4-N3	5.25	125.89	116.17
4	5	4129	B8W	N3-C2-N1	-5.23	120.25	127.22
4	5	1574	B9B	N3-C2-N1	-5.22	120.26	127.22
50	9	568	E3C	O2-C2-N3	-5.21	115.47	122.07
4	5	3785	A2M	N6-C6-N1	-5.20	107.77	118.57
50	9	1832	6MZ	N3-C2-N1	-5.20	120.55	128.68
4	5	3867	A2M	N3-C2-N1	-5.20	120.56	128.68
4	5	1871	A2M	N6-C6-N1	-5.18	107.81	118.57
4	5	4129	B8W	O6-C6-N1	-5.18	111.84	119.03
4	5	2401	A2M	N6-C6-N1	-5.18	107.83	118.57
4	5	4628	PSU	N1-C2-N3	5.14	120.96	115.13
50	9	822	PSU	N1-C2-N3	5.13	120.95	115.13
50	9	27	A2M	N6-C6-N1	-5.13	107.93	118.57
4	5	4571	A2M	N6-C6-N1	-5.13	107.93	118.57
4	5	2363	A2M	N3-C2-N1	-5.12	120.68	128.68
4	5	4450	PSU	C4-N3-C2	-5.11	118.98	126.34
4	5	4442	PSU	C4-N3-C2	-5.10	118.99	126.34
50	9	1219	B8Q	O2-C2-N3	-5.09	115.48	122.95
4	5	4415	1MA	N1-C2-N3	-5.08	120.10	126.02
4	5	2522	7MG	C5-C6-N1	5.08	119.94	110.99
4	5	1797	E7G	C5-C6-N1	5.05	119.89	110.99
4	5	4450	PSU	N1-C2-N3	5.04	120.84	115.13
4	5	237	B9B	N3-C2-N1	-5.03	120.51	127.22
4	5	4620	OMU	C4-N3-C2	-5.02	119.96	126.58
4	5	398	A2M	N6-C6-N1	-5.01	108.18	118.57
4	5	3825	A2M	N6-C6-N1	-5.00	108.19	118.57
4	5	2754	B9B	N3-C2-N1	-5.00	120.55	127.22
4	5	4530	UR3	C4-N3-C2	-5.00	119.86	124.56
4	5	3729	PSU	N1-C2-N3	4.95	120.74	115.13
4	5	2297	E7G	C5-C6-N1	4.93	119.67	110.99
4	5	1677	PSU	C4-N3-C2	-4.91	119.27	126.34
4	5	4083	5MU	O4-C4-C5	-4.89	119.24	124.90
4	5	4355	E6G	C61-O6-C6	-4.88	112.73	117.56
4	5	4500	PSU	N1-C2-N3	4.88	120.66	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5	3718	A2M	N6-C6-N1	-4.86	108.48	118.57
4	5	4628	PSU	C4-N3-C2	-4.86	119.34	126.34
50	9	814	5MU	N3-C2-N1	4.85	121.33	114.89
4	5	4636	PSU	N1-C2-N3	4.85	120.62	115.13
4	5	3723	A2M	N6-C6-N1	-4.85	108.51	118.57
4	5	4355	E6G	N3-C2-N1	-4.83	120.78	127.22
50	9	822	PSU	C4-N3-C2	-4.80	119.42	126.34
4	5	1683	PSU	N1-C2-N3	4.80	120.57	115.13
50	9	1830	UR3	C1'-N1-C2	4.80	125.10	116.99
4	5	3899	BGH	C2-N3-C4	4.79	120.84	112.30
4	5	237	B9B	C2-N3-C4	4.78	120.82	115.36
4	5	1659	I4U	C5-C4-N3	-4.78	117.63	124.91
4	5	4083	5MU	C4-N3-C2	-4.77	121.18	127.35
4	5	4529	B8W	C3'-C2'-C1'	4.77	108.15	100.98
4	5	4550	7MG	C5-C6-N1	4.72	119.31	110.99
50	9	668	A2M	N6-C6-N1	-4.71	108.80	118.57
50	9	1219	B8Q	N3-C2-N1	4.70	122.65	117.13
4	5	4529	B8W	N3-C2-N1	-4.70	120.95	127.22
4	5	1582	PSU	N1-C2-N3	4.70	120.45	115.13
50	9	1248	B8N	C4-N3-C2	-4.69	119.53	125.46
4	5	4403	PSU	N1-C2-N3	4.68	120.44	115.13
4	5	4293	PSU	C4-N3-C2	-4.64	119.65	126.34
50	9	1081	PSU	C4-N3-C2	-4.64	119.66	126.34
4	5	1683	PSU	C4-N3-C2	-4.63	119.66	126.34
4	5	3718	A2M	N3-C2-N1	-4.62	121.46	128.68
4	5	4293	PSU	N1-C2-N3	4.59	120.33	115.13
4	5	3729	PSU	C4-N3-C2	-4.57	119.75	126.34
4	5	4472	B8W	N3-C2-N1	-4.56	121.14	127.22
50	9	119	PSU	C4-N3-C2	-4.55	119.79	126.34
4	5	4690	B8K	C2-N3-C4	4.53	120.38	112.30
50	9	814	5MU	O4-C4-C5	-4.52	119.66	124.90
50	9	1031	A2M	N6-C6-N1	-4.52	109.20	118.57
50	9	1219	B8Q	C6-N1-C2	-4.51	117.75	121.79
4	5	4472	B8W	O6-C6-C5	4.51	122.45	116.01
4	5	4531	PSU	C4-N3-C2	-4.48	119.88	126.34
4	5	1456	B8Q	N3-C2-N1	4.48	122.40	117.13
4	5	1605	7MG	C2-N3-C4	4.48	120.28	112.30
4	5	1582	PSU	C4-N3-C2	-4.47	119.90	126.34
4	5	2297	E7G	C2-N3-C4	4.45	120.22	112.30
4	5	4403	PSU	C4-N3-C2	-4.44	119.94	126.34
50	9	823	PSU	C4-N3-C2	-4.42	119.97	126.34
4	5	1574	B9B	O6-C6-N1	-4.42	116.31	120.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5	2380	B8W	C3'-C2'-C1'	4.40	107.60	100.98
4	5	2380	B8W	O6-C6-C5	4.39	122.28	116.01
4	5	1677	PSU	N1-C2-N3	4.38	120.09	115.13
50	9	1081	PSU	N1-C2-N3	4.37	120.09	115.13
4	5	2508	PSU	C4-N3-C2	-4.34	120.09	126.34
4	5	4415	1MA	C5-C6-N1	4.32	120.33	113.90
4	5	3715	PSU	N1-C2-N3	4.31	120.01	115.13
4	5	1883	OMG	C5-C6-N1	4.30	121.55	113.95
4	5	4550	7MG	C2-N3-C4	4.30	119.96	112.30
4	5	2522	7MG	C2-N3-C4	4.28	119.92	112.30
4	5	3715	PSU	C4-N3-C2	-4.27	120.19	126.34
4	5	3764	PSU	C4-N3-C2	-4.24	120.22	126.34
4	5	3899	BGH	C5-C4-N9	4.24	111.85	106.35
4	5	1909	P7G	N9-C8-N7	4.24	109.44	103.38
4	5	4531	PSU	N1-C2-N3	4.24	119.93	115.13
4	5	1348	P4U	C5-C4-N3	-4.23	118.47	124.91
4	5	4335	5MC	C5-C6-N1	-4.22	118.99	123.34
4	5	4306	OMU	N3-C2-N1	4.22	120.49	114.89
4	5	1797	E7G	C2-N3-C4	4.21	119.81	112.30
4	5	237	B9B	O6-C6-N1	-4.21	116.49	120.12
4	5	1322	1MA	C5-C6-N1	4.20	120.17	113.90
4	5	3792	OMG	C5-C6-N1	4.20	121.36	113.95
50	9	612	PSU	C4-N3-C2	-4.20	120.29	126.34
4	5	2508	PSU	N1-C2-N3	4.19	119.88	115.13
50	9	823	PSU	N1-C2-N3	4.16	119.85	115.13
50	9	1806	M7A	C71-N7-C5	-4.15	108.05	124.01
50	9	1830	UR3	C4-N3-C2	-4.14	120.67	124.56
4	5	1574	B9B	C2-N3-C4	4.14	120.08	115.36
50	9	814	5MU	C4-N3-C2	-4.06	122.09	127.35
4	5	3899	BGH	C4-C5-N7	4.03	108.50	104.91
4	5	4872	2MG	C5-C6-N1	4.01	121.04	113.95
4	5	2522	7MG	C5-C4-N3	-4.01	120.48	128.13
50	9	1219	B8Q	C31-N3-C4	4.01	120.29	114.25
4	5	1883	OMG	C2-N1-C6	-4.00	117.73	125.10
4	5	4494	OMG	C5-C6-N1	3.99	121.00	113.95
50	9	121	OMU	N3-C2-N1	3.98	120.17	114.89
50	9	1830	UR3	C6-N1-C2	-3.97	118.23	121.79
4	5	1517	2MG	C5-C6-N1	3.96	120.95	113.95
4	5	2754	B9B	C2-N3-C4	3.94	119.86	115.36
4	5	4355	E6G	O6-C6-N1	3.94	123.53	120.12
4	5	1456	B8Q	O2-C2-N3	-3.94	117.16	122.95
4	5	2424	OMG	C5-C6-N1	3.94	120.91	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5	3897	B8K	C2-N3-C4	3.93	119.30	112.30
4	5	4083	5MU	O2-C2-N1	-3.93	117.57	122.79
4	5	1522	OMG	C5-C6-N1	3.92	120.88	113.95
4	5	4296	B8H	O2-C2-N1	-3.91	118.47	122.87
4	5	4447	5MC	C5-C6-N1	-3.90	119.33	123.34
4	5	2380	B8W	C2-N3-C4	3.88	119.79	115.36
4	5	4690	B8K	C5-C4-N9	3.87	111.38	106.35
4	5	2297	E7G	C5-C4-N3	-3.87	120.75	128.13
4	5	1605	7MG	C5-C4-N3	-3.87	120.76	128.13
6	8	14	OMU	O4-C4-C5	-3.86	118.38	125.16
4	5	4597	UR3	C4-N3-C2	-3.85	120.94	124.56
4	5	4185	B8W	O6-C6-N1	-3.84	113.70	119.03
4	5	3897	B8K	N9-C8-N7	3.83	108.47	103.33
50	9	814	5MU	C1'-N1-C2	3.81	124.46	117.57
4	5	2522	7MG	C5-C4-N9	3.78	111.25	106.35
6	8	14	OMU	C5-C4-N3	3.78	120.49	114.84
4	5	4564	M7A	C2-N3-C4	3.77	120.66	111.75
4	5	4623	OMG	C5-C6-N1	3.77	120.60	113.95
50	9	612	PSU	N1-C2-N3	3.77	119.40	115.13
50	9	1243	PSU	C6-N1-C2	-3.76	118.84	122.68
4	5	4637	OMG	C5-C6-N1	3.75	120.57	113.95
50	9	116	OMU	N3-C2-N1	3.75	119.86	114.89
4	5	1797	E7G	C5-C4-N3	-3.74	121.00	128.13
4	5	4870	OMG	C5-C6-N1	3.74	120.55	113.95
4	5	4472	B8W	C3'-C2'-C1'	3.74	106.60	100.98
50	9	119	PSU	N1-C2-N3	3.74	119.36	115.13
4	5	1316	OMG	C5-C6-N1	3.73	120.54	113.95
4	5	4550	7MG	C5-C4-N9	3.72	111.17	106.35
4	5	4355	E6G	C2-N3-C4	3.72	119.60	115.36
4	5	3764	PSU	N1-C2-N3	3.72	119.34	115.13
4	5	4371	MHG	C2-N1-C6	-3.71	120.21	124.48
4	5	3762	B8H	O2-C2-N1	-3.70	118.70	122.87
50	9	644	OMG	C5-C6-N1	3.69	120.47	113.95
50	9	166	A2M	C5'-C4'-C3'	-3.69	101.36	115.18
50	9	683	OMG	C5-C6-N1	3.67	120.43	113.95
4	5	2050	OMG	C2-N1-C6	-3.64	118.39	125.10
50	9	116	OMU	C5-C4-N3	3.63	120.27	114.84
4	5	4628	PSU	O2-C2-N1	-3.63	118.79	122.79
50	9	1832	6MZ	C9-N6-C6	3.62	125.99	122.87
4	5	3792	OMG	C2-N1-C6	-3.60	118.47	125.10
4	5	4690	B8K	N9-C8-N7	3.58	108.13	103.33
4	5	4371	MHG	C5-C4-N3	-3.57	121.33	128.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5	1909	P7G	C71-N7-C5	3.57	132.97	124.52
4	5	4550	7MG	C5-C4-N3	-3.56	121.34	128.13
4	5	1348	P4U	O2-C2-N3	-3.56	116.54	122.33
4	5	1522	OMG	C2-N1-C6	-3.56	118.55	125.10
4	5	4442	PSU	O2-C2-N1	-3.56	118.87	122.79
50	9	509	OMG	C2-N1-C6	-3.56	118.55	125.10
4	5	4620	OMU	N3-C2-N1	3.56	119.61	114.89
4	5	2364	OMG	C5-C6-N1	3.55	120.22	113.95
4	5	4083	5MU	C5M-C5-C6	-3.55	118.11	122.85
4	5	237	B9B	C3'-C2'-C1'	3.54	106.31	100.98
4	5	4637	OMG	C2-N1-C6	-3.53	118.59	125.10
4	5	4296	B8H	C5-C4-N3	3.53	124.57	116.58
4	5	2754	B9B	N2-C2-N3	3.52	123.53	117.79
4	5	1860	B8H	C5-C4-N3	3.52	124.54	116.58
50	9	568	E3C	C1'-N1-C6	-3.52	113.17	120.84
4	5	237	B9B	N2-C2-N3	3.52	123.52	117.79
4	5	4623	OMG	C2-N1-C6	-3.51	118.63	125.10
4	5	1860	B8H	O2-C2-N1	-3.50	118.93	122.87
4	5	1625	OMG	C5-C6-N1	3.50	120.13	113.95
4	5	4196	OMG	C5-C6-N1	3.49	120.11	113.95
4	5	4083	5MU	C5M-C5-C4	3.49	122.61	118.77
50	9	822	PSU	O2-C2-N1	-3.48	118.96	122.79
4	5	3782	5MC	C1'-N1-C6	-3.48	115.34	121.12
4	5	1866	UR3	C6-N1-C2	-3.47	118.68	121.79
4	5	3899	BGH	N9-C8-N7	3.47	107.98	103.33
4	5	4370	OMG	C5-C6-N1	3.46	120.06	113.95
4	5	3899	BGH	C5-C4-N3	-3.46	121.54	128.13
4	5	1574	B9B	N2-C2-N3	3.46	123.43	117.79
4	5	729	2MG	C5-C6-N1	3.45	120.04	113.95
4	5	1605	7MG	C5-C4-N9	3.44	110.82	106.35
4	5	4194	I4U	C5-C4-N3	-3.44	119.67	124.91
4	5	2050	OMG	C5-C6-N1	3.44	120.03	113.95
50	9	116	OMU	O4-C4-C5	-3.44	119.11	125.16
50	9	1243	PSU	N1-C2-N3	3.43	119.01	115.13
50	9	121	OMU	C5-C4-N3	3.41	119.95	114.84
50	9	509	OMG	C5-C6-N1	3.41	119.97	113.95
4	5	4083	5MU	C1'-N1-C6	3.41	126.79	121.12
4	5	2424	OMG	C2-N1-C6	-3.40	118.83	125.10
4	5	3899	BGH	C2'-C1'-N9	-3.40	107.23	114.14
4	5	4690	B8K	C6-C5-C4	-3.39	115.64	122.62
4	5	4129	B8W	C2-N3-C4	3.38	119.22	115.36
4	5	2522	7MG	N9-C8-N7	3.38	108.21	103.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	9	568	E3C	C6-N1-C2	-3.37	118.77	121.79
4	5	4185	B8W	C3'-C2'-C1'	3.35	106.02	100.98
50	9	644	OMG	C2-N1-C6	-3.33	118.96	125.10
50	9	1842	4AC	C5-C4-N3	-3.33	117.24	122.59
4	5	3762	B8H	C5-C4-N3	3.32	124.10	116.58
4	5	1348	P4U	C1'-N1-C2	3.31	125.81	118.42
50	9	1806	M7A	C2-N3-C4	3.28	119.50	111.75
4	5	2754	B9B	C1'-N9-C4	-3.27	120.89	126.64
4	5	4370	OMG	C2-N1-C6	-3.27	119.08	125.10
4	5	4129	B8W	C4-C5-N7	-3.27	105.99	109.40
50	9	568	E3C	C32-C31-N3	3.25	120.60	112.64
4	5	2297	E7G	C5-C4-N9	3.25	110.57	106.35
4	5	4620	OMU	C5-C4-N3	3.25	119.70	114.84
4	5	4620	OMU	O4-C4-C5	-3.24	119.47	125.16
4	5	1625	OMG	C2-N1-C6	-3.23	119.14	125.10
4	5	4306	OMU	C5-C4-N3	3.23	119.67	114.84
4	5	2522	7MG	C4-C5-N7	3.22	110.01	105.53
50	9	683	OMG	C2-N1-C6	-3.22	119.17	125.10
4	5	3897	B8K	C5-C4-N9	3.21	110.51	106.35
50	9	1219	B8Q	C1'-N1-C6	-3.21	113.85	120.84
4	5	373	OMG	C5-C6-N1	3.20	119.61	113.95
4	5	4529	B8W	C2-N3-C4	3.20	119.01	115.36
4	5	4636	PSU	C6-C5-C4	3.19	120.43	118.20
4	5	4185	B8W	C2-N3-C4	3.18	118.99	115.36
4	5	4196	OMG	C2-N1-C6	-3.18	119.25	125.10
50	9	1248	B8N	C31-N3-C4	3.18	121.99	117.31
50	9	1842	4AC	C6-C5-C4	3.18	120.85	116.96
50	9	1248	B8N	N3-C2-N1	3.17	121.24	116.76
4	5	4494	OMG	C2-N1-C6	-3.17	119.26	125.10
4	5	3897	B8K	C6-C5-C4	-3.16	116.11	122.62
4	5	4450	PSU	C6-C5-C4	3.15	120.40	118.20
4	5	4083	5MU	C6-N1-C2	-3.15	118.11	121.30
4	5	1574	B9B	C1'-N9-C4	-3.14	121.13	126.64
4	5	2773	OMG	C5-C6-N1	3.13	119.49	113.95
4	5	4335	5MC	CM5-C5-C6	-3.12	118.68	122.85
4	5	2364	OMG	C2-N1-C6	-3.11	119.36	125.10
50	9	814	5MU	C6-N1-C2	-3.11	118.15	121.30
50	9	1374	5MC	C5-C6-N1	-3.10	120.15	123.34
4	5	4494	OMG	O6-C6-C5	-3.09	118.33	124.37
4	5	4564	M7A	C5-C4-N3	-3.09	119.36	126.62
50	9	814	5MU	C5M-C5-C6	-3.05	118.77	122.85
6	8	14	OMU	N3-C2-N1	3.05	118.94	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	9	121	OMU	O4-C4-C5	-3.05	119.80	125.16
4	5	4550	7MG	C4-C5-N7	3.04	109.76	105.53
4	5	237	B9B	C61-O6-C6	-3.04	111.83	117.51
4	5	1605	7MG	C4-C5-N7	3.04	109.75	105.53
4	5	4690	B8K	C5-C4-N3	-3.03	122.36	128.13
4	5	4529	B8W	O6-C6-N1	-3.02	114.84	119.03
4	5	4870	OMG	C2-N1-C6	-3.01	119.55	125.10
4	5	1517	2MG	CM2-N2-C2	-3.01	117.20	123.86
4	5	4129	B8W	C2-N1-C6	3.01	120.92	116.08
4	5	2786	B9H	O2-C2-N1	-3.01	115.67	122.72
4	5	4371	MHG	C5-C4-N9	2.99	110.23	106.35
4	5	3729	PSU	C6-N1-C2	-2.98	119.63	122.68
4	5	4872	2MG	CM2-N2-C2	-2.98	117.28	123.86
4	5	3782	5MC	C5-C6-N1	-2.97	120.28	123.34
50	9	568	E3C	C31-N3-C2	2.97	121.26	117.44
4	5	1797	E7G	C5-C4-N9	2.97	110.20	106.35
4	5	4523	A2M	O4'-C4'-C3'	-2.96	99.26	105.11
50	9	119	PSU	O2-C2-N1	-2.96	119.54	122.79
4	5	1316	OMG	C2-N1-C6	-2.96	119.66	125.10
4	5	4690	B8K	C2-N1-C6	-2.96	119.71	125.10
50	9	121	OMU	O2-C2-N1	-2.95	118.86	122.79
4	5	2364	OMG	O6-C6-C5	-2.95	118.61	124.37
4	5	4185	B8W	C2-N1-C6	2.94	120.81	116.08
4	5	4220	6MZ	C1'-N9-C4	-2.93	121.48	126.64
4	5	3729	PSU	O2-C2-N1	-2.93	119.56	122.79
4	5	1866	UR3	C1'-N1-C2	2.93	121.94	116.99
50	9	1337	4AC	C6-C5-C4	2.93	120.54	116.96
4	5	4500	PSU	O2-C2-N1	-2.93	119.57	122.79
4	5	1625	OMG	O6-C6-C5	-2.92	118.68	124.37
4	5	4620	OMU	O2-C2-N1	-2.89	118.95	122.79
4	5	1517	2MG	O6-C6-C5	-2.88	118.74	124.37
4	5	4442	PSU	C6-N1-C2	-2.88	119.74	122.68
4	5	4500	PSU	C6-C5-C4	2.87	120.21	118.20
4	5	4472	B8W	C2-N3-C4	2.87	118.64	115.36
4	5	3899	BGH	C2-N1-C6	-2.87	119.87	125.10
4	5	1797	E7G	C2-N1-C6	-2.87	119.87	125.10
4	5	4483	B8T	C6-C5-C4	2.86	120.46	116.96
4	5	2773	OMG	C2-N1-C6	-2.86	119.83	125.10
4	5	1322	1MA	C8-N7-C5	2.85	108.42	102.99
50	9	517	OMC	O2-C2-N3	-2.85	117.70	122.33
50	9	814	5MU	O2-C2-N3	-2.84	116.20	121.50
50	9	1830	UR3	O2-C2-N3	-2.84	117.34	121.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5	4371	MHG	N1-C2-N3	-2.84	119.56	123.95
4	5	4564	M7A	C71-N7-C5	-2.84	113.12	124.01
50	9	1710	OMC	O2-C2-N3	-2.84	117.72	122.33
4	5	1605	7MG	N9-C8-N7	2.83	107.43	103.38
4	5	4293	PSU	C6-N1-C2	-2.83	119.79	122.68
4	5	4623	OMG	O6-C6-C5	-2.82	118.86	124.37
4	5	1582	PSU	C6-N1-C2	-2.81	119.81	122.68
4	5	3899	BGH	C6-C5-C4	-2.80	116.85	122.62
4	5	1316	OMG	O6-C6-C5	-2.79	118.92	124.37
4	5	2297	E7G	C2-N1-C6	-2.79	120.01	125.10
4	5	3715	PSU	O2-C2-N1	-2.79	119.72	122.79
4	5	1605	7MG	C2-N1-C6	-2.79	120.02	125.10
4	5	4531	PSU	O2-C2-N1	-2.78	119.73	122.79
4	5	2522	7MG	C2-N1-C6	-2.78	120.03	125.10
4	5	373	OMG	C2-N1-C6	-2.77	119.99	125.10
50	9	1842	4AC	O2-C2-N3	-2.77	117.82	122.33
4	5	3782	5MC	C5-C4-N4	-2.77	117.33	121.48
50	9	1219	B8Q	C31-N3-C2	2.77	121.81	117.79
4	5	1683	PSU	C6-N1-C2	-2.77	119.85	122.68
4	5	4220	6MZ	C9-N6-C6	-2.73	120.52	122.87
4	5	4355	E6G	C3'-C2'-C1'	2.73	105.08	100.98
4	5	4196	OMG	O6-C6-C5	-2.72	119.06	124.37
4	5	4872	2MG	C8-N7-C5	2.72	108.16	102.99
4	5	4597	UR3	C6-N1-C2	-2.71	119.36	121.79
4	5	2050	OMG	O6-C6-C5	-2.70	119.10	124.37
4	5	3867	A2M	C3'-C2'-C1'	2.69	107.94	102.89
50	9	1842	4AC	O7-C7-CM7	-2.68	117.08	122.06
4	5	4637	OMG	C8-N7-C5	2.68	108.09	102.99
4	5	4472	B8W	O4'-C1'-C2'	-2.68	103.01	106.93
4	5	2861	OMC	O2-C2-N3	-2.68	117.98	122.33
4	5	2773	OMG	C8-N7-C5	2.68	108.09	102.99
4	5	3899	BGH	O6-C6-N1	-2.67	114.99	120.12
4	5	2754	B9B	O6-C6-N1	-2.66	117.83	120.12
4	5	4690	B8K	O6-C6-C5	-2.66	121.01	127.54
4	5	4185	B8W	C4-C5-N7	-2.66	106.62	109.40
4	5	4335	5MC	C1'-N1-C6	-2.66	116.70	121.12
4	5	3764	PSU	O2-C2-N1	-2.66	119.87	122.79
50	9	612	PSU	O2-C2-N1	-2.66	119.87	122.79
4	5	2861	OMC	C1'-N1-C2	2.64	124.32	118.42
4	5	1797	E7G	N9-C8-N7	2.63	107.14	103.38
4	5	4403	PSU	C6-N1-C2	-2.63	120.00	122.68
4	5	4450	PSU	O2-C2-N1	-2.61	119.91	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	9	509	OMG	O6-C6-C5	-2.61	119.27	124.37
4	5	4628	PSU	C6-N1-C2	-2.61	120.02	122.68
50	9	1337	4AC	C5-C4-N3	-2.59	118.42	122.59
50	9	159	A2M	O4'-C4'-C3'	-2.59	99.99	105.11
4	5	3897	B8K	C5-C4-N3	-2.59	123.20	128.13
4	5	1582	PSU	O2-C2-N1	-2.58	119.95	122.79
50	9	822	PSU	C6-N1-C2	-2.58	120.05	122.68
4	5	729	2MG	O6-C6-C5	-2.57	119.34	124.37
4	5	1522	OMG	C8-N7-C5	2.57	107.89	102.99
4	5	1522	OMG	O6-C6-C5	-2.56	119.38	124.37
4	5	1883	OMG	C8-N7-C5	2.56	107.86	102.99
4	5	3715	PSU	C6-N1-C2	-2.56	120.07	122.68
4	5	3897	B8K	O3'-C3'-C4'	-2.55	103.66	111.05
4	5	3880	P7G	N9-C8-N7	2.55	107.03	103.38
4	5	2363	A2M	C3'-C2'-C1'	2.55	107.68	102.89
50	9	668	A2M	C5'-C4'-C3'	-2.55	105.62	115.18
50	9	116	OMU	O2-C2-N1	-2.55	119.40	122.79
4	5	2773	OMG	O6-C6-C5	-2.54	119.40	124.37
4	5	4370	OMG	O6-C6-C5	-2.54	119.41	124.37
50	9	644	OMG	O6-C6-C5	-2.54	119.41	124.37
50	9	1806	M7A	C5-C4-N3	-2.53	120.69	126.62
50	9	644	OMG	C8-N7-C5	2.52	107.79	102.99
4	5	4529	B8W	C2-N1-C6	2.52	120.13	116.08
4	5	3897	B8K	C2-N1-C6	-2.51	120.51	125.10
50	9	1806	M7A	C4-N9-C1'	-2.51	120.64	126.60
4	5	2754	B9B	C3'-C2'-C1'	2.51	104.75	100.98
50	9	683	OMG	O6-C6-C5	-2.51	119.48	124.37
4	5	4293	PSU	O2-C2-N1	-2.50	120.04	122.79
4	5	4597	UR3	C1'-N1-C2	2.50	121.20	116.99
4	5	1659	I4U	C6-N1-C2	-2.50	116.16	120.49
4	5	2050	OMG	C8-N7-C5	2.49	107.74	102.99
50	9	822	PSU	O4'-C1'-C2'	2.49	108.65	105.14
4	5	2508	PSU	O2-C2-N1	-2.49	120.05	122.79
4	5	4355	E6G	N2-C2-N1	2.49	121.12	117.25
4	5	4536	OMC	C1'-N1-C2	2.48	123.96	118.42
4	5	4671	B8T	C6-C5-C4	2.48	120.00	116.96
4	5	373	OMG	C8-N7-C5	2.48	107.71	102.99
4	5	2297	E7G	N9-C8-N7	2.47	106.92	103.38
4	5	1605	7MG	O6-C6-C5	-2.47	121.47	127.54
4	5	4870	OMG	C8-N7-C5	2.45	107.66	102.99
4	5	4494	OMG	C8-N7-C5	2.45	107.65	102.99
4	5	373	OMG	O6-C6-C5	-2.43	119.62	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5	4306	OMU	O2-C2-N1	-2.43	119.56	122.79
4	5	2424	OMG	O6-C6-C5	-2.43	119.63	124.37
4	5	1883	OMG	O6-C6-C5	-2.42	119.66	124.37
50	9	1337	4AC	O7-C7-CM7	-2.41	117.58	122.06
50	9	683	OMG	C8-N7-C5	2.41	107.58	102.99
4	5	3792	OMG	C8-N7-C5	2.41	107.58	102.99
4	5	1625	OMG	C8-N7-C5	2.41	107.57	102.99
4	5	4637	OMG	O6-C6-C5	-2.40	119.68	124.37
4	5	4296	B8H	O4-C4-N3	-2.40	115.52	120.12
4	5	3792	OMG	O6-C6-C5	-2.39	119.70	124.37
4	5	2424	OMG	C8-N7-C5	2.39	107.55	102.99
4	5	1871	A2M	C3'-C2'-C1'	2.39	107.39	102.89
4	5	1797	E7G	O6-C6-C5	-2.39	121.68	127.54
4	5	1316	OMG	C8-N7-C5	2.39	107.54	102.99
4	5	4370	OMG	C8-N7-C5	2.38	107.52	102.99
4	5	4550	7MG	N9-C8-N7	2.37	106.77	103.38
4	5	3897	B8K	O6-C6-C5	-2.37	121.72	127.54
4	5	3909	OMC	O2-C2-N3	-2.37	118.48	122.33
4	5	4194	I4U	C2'-C3'-C4'	2.37	107.24	102.64
4	5	2297	E7G	O6-C6-C5	-2.37	121.74	127.54
50	9	823	PSU	C6-N1-C2	-2.36	120.27	122.68
4	5	4083	5MU	O4-C4-N3	-2.36	115.60	120.12
4	5	1517	2MG	C8-N7-C5	2.35	107.47	102.99
4	5	4415	1MA	C8-N7-C5	2.35	107.47	102.99
4	5	3782	5MC	C1'-N1-C2	2.35	123.67	118.42
4	5	4403	PSU	O4'-C1'-C2'	2.34	108.45	105.14
4	5	1456	B8Q	C1'-N1-C2	2.34	120.94	116.99
4	5	4450	PSU	C6-N1-C2	-2.33	120.30	122.68
50	9	1081	PSU	O4'-C1'-C2'	2.33	108.43	105.14
4	5	1574	B9B	C3'-C2'-C1'	2.33	104.49	100.98
50	9	1243	PSU	C4-N3-C2	-2.33	122.98	126.34
4	5	4371	MHG	O6-C6-C5	-2.33	121.83	127.54
4	5	4536	OMC	O2-C2-N3	-2.32	118.56	122.33
4	5	4403	PSU	O4-C4-N3	-2.32	115.67	120.12
4	5	2380	B8W	C2-N1-C6	2.32	119.80	116.08
50	9	509	OMG	C8-N7-C5	2.32	107.40	102.99
50	9	814	5MU	C5M-C5-C4	2.31	121.31	118.77
4	5	4623	OMG	C8-N7-C5	2.31	107.39	102.99
4	5	4194	I4U	C4'-O4'-C1'	-2.30	104.40	109.47
4	5	4523	A2M	C2'-C3'-C4'	-2.29	97.02	101.99
4	5	3880	P7G	C71-N7-C5	2.28	129.93	124.52
4	5	1683	PSU	O2-C2-N1	-2.27	120.29	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5	3899	BGH	C4'-O4'-C1'	-2.26	104.48	109.47
50	9	814	5MU	C6-C5-C4	2.26	119.92	118.03
50	9	166	A2M	C2'-C3'-C4'	2.26	106.90	101.99
4	5	1456	B8Q	C6-N1-C2	-2.26	119.77	121.79
50	9	822	PSU	C6-C5-C4	2.26	119.78	118.20
50	9	814	5MU	C1'-N1-C6	-2.25	117.38	121.12
4	5	3867	A2M	O3'-C3'-C2'	-2.25	104.77	111.17
50	9	1842	4AC	CM7-C7-N4	2.25	119.18	115.29
4	5	4690	B8K	C4'-O4'-C1'	-2.25	104.52	109.47
4	5	3897	B8K	O4'-C1'-C2'	-2.24	101.76	106.64
4	5	4220	6MZ	C4-C5-N7	2.24	111.73	109.40
4	5	4530	UR3	C3U-N3-C4	2.23	121.08	117.89
4	5	1797	E7G	N9-C4-N3	2.23	128.80	125.47
50	9	1337	4AC	N4-C4-N3	2.22	117.59	113.85
4	5	4636	PSU	C5-C6-N1	-2.22	118.79	122.11
4	5	373	OMG	CM2-O2'-C2'	-2.21	108.72	114.52
50	9	814	5MU	O4-C4-N3	-2.21	115.88	120.12
4	5	729	2MG	C8-N7-C5	2.21	107.19	102.99
4	5	4306	OMU	O4-C4-C5	-2.20	121.28	125.16
50	9	823	PSU	O2-C2-N1	-2.20	120.37	122.79
4	5	4870	OMG	O6-C6-C5	-2.20	120.07	124.37
4	5	1860	B8H	O4-C4-N3	-2.20	115.91	120.12
4	5	4129	B8W	C5-C6-N1	-2.19	119.08	123.26
4	5	4636	PSU	O2-C2-N1	-2.18	120.39	122.79
4	5	4550	7MG	N1-C2-N3	-2.17	119.26	123.32
4	5	2522	7MG	O6-C6-C5	-2.17	122.21	127.54
4	5	4690	B8K	N1-C2-N3	-2.17	119.28	123.32
50	9	1243	PSU	O2-C2-N1	-2.16	120.42	122.79
4	5	4531	PSU	C6-N1-C2	-2.15	120.48	122.68
50	9	1842	4AC	C1'-N1-C2	2.15	123.22	118.42
4	5	2297	E7G	N9-C4-N3	2.14	128.67	125.47
4	5	4494	OMG	N1-C2-N3	-2.14	119.33	123.32
4	5	3782	5MC	N4-C4-N3	2.14	122.37	118.48
4	5	2364	OMG	C8-N7-C5	2.13	107.04	102.99
4	5	4196	OMG	C8-N7-C5	2.13	107.04	102.99
4	5	4872	2MG	O6-C6-C5	-2.12	120.23	124.37
50	9	1248	B8N	O4'-C1'-C2'	2.12	108.13	105.14
4	5	4355	E6G	C2-N1-C6	2.12	119.48	116.08
4	5	1677	PSU	O4'-C1'-C2'	2.12	108.13	105.14
4	5	4530	UR3	O2-C2-N3	-2.11	118.36	121.34
4	5	3899	BGH	O4'-C4'-C3'	-2.11	100.94	105.11
4	5	3764	PSU	C6-N1-C2	-2.11	120.53	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	8	14	OMU	O2-C2-N1	-2.10	119.99	122.79
4	5	4185	B8W	C5-C6-N1	-2.10	119.25	123.26
4	5	4185	B8W	O4'-C4'-C3'	-2.10	100.96	105.11
50	9	1081	PSU	C6-N1-C2	-2.10	120.54	122.68
4	5	3867	A2M	O3'-C3'-C4'	-2.10	104.99	111.05
4	5	3899	BGH	N1-C2-N3	-2.09	119.43	123.32
4	5	4550	7MG	O6-C6-C5	-2.09	122.42	127.54
4	5	4597	UR3	C3U-N3-C2	2.09	120.97	117.31
50	9	1842	4AC	N4-C4-N3	2.08	117.35	113.85
4	5	237	B9B	C5'-C4'-C3'	-2.08	107.39	115.18
50	9	484	A2M	C5'-C4'-C3'	-2.08	107.39	115.18
4	5	4129	B8W	O4'-C4'-C3'	-2.07	101.02	105.11
4	5	3785	A2M	O3'-C3'-C4'	2.06	117.00	111.05
4	5	3762	B8H	O4-C4-N3	-2.06	116.17	120.12
4	5	4129	B8W	C3'-C2'-C1'	2.05	104.07	100.98
50	9	1248	B8N	O4-C4-N3	-2.04	116.51	119.98
4	5	2508	PSU	C6-N1-C2	-2.03	120.60	122.68
4	5	4194	I4U	O4'-C1'-C2'	-2.03	102.21	106.64
4	5	4472	B8W	C2-N1-C6	2.02	119.33	116.08
4	5	4550	7MG	C2-N1-C6	-2.02	121.41	125.10
50	9	668	A2M	C3'-C2'-C1'	2.02	106.69	102.89
4	5	3880	P7G	O4'-C1'-N9	-2.01	106.55	109.30
4	5	1316	OMG	N1-C2-N3	-2.01	119.56	123.32
4	5	2786	B9H	C32-C31-N3	2.01	116.67	112.47
4	5	2422	OMC	O2-C2-N3	-2.01	119.06	122.33
50	9	683	OMG	N2-C2-N1	2.00	120.98	116.71

There are no chirality outliers.

All (189) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	C	333	MLZ	N-CA-CB-CG
9	C	333	MLZ	C-CA-CB-CG
4	5	237	B9B	C5-C6-O6-C61
4	5	237	B9B	N1-C6-O6-C61
4	5	237	B9B	C3'-C4'-C5'-O5'
4	5	237	B9B	O4'-C4'-C5'-O5'
4	5	1348	P4U	N3-C4-O4-C41
4	5	1348	P4U	C3'-C4'-C5'-O5'
4	5	1348	P4U	O4'-C4'-C5'-O5'
4	5	1574	B9B	C5-C6-O6-C61
4	5	1574	B9B	N1-C6-O6-C61

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Mol	Chain	Res	Type	Atoms
4	5	1582	PSU	C3'-C4'-C5'-O5'
4	5	1797	E7G	O4'-C4'-C5'-O5'
4	5	1866	UR3	O4'-C4'-C5'-O5'
4	5	2364	OMG	O4'-C4'-C5'-O5'
4	5	2380	B8W	C5-C6-O6-C61
4	5	2380	B8W	N1-C6-O6-C61
4	5	2380	B8W	C3'-C4'-C5'-O5'
4	5	2424	OMG	C3'-C4'-C5'-O5'
4	5	2786	B9H	C32-C31-N3-C2
4	5	3762	B8H	O4'-C4'-C5'-O5'
4	5	3792	OMG	O4'-C4'-C5'-O5'
4	5	3792	OMG	C3'-C4'-C5'-O5'
4	5	3867	A2M	C3'-C4'-C5'-O5'
4	5	3897	B8K	O4'-C4'-C5'-O5'
4	5	3899	BGH	C3'-C4'-C5'-O5'
4	5	3899	BGH	O4'-C4'-C5'-O5'
4	5	4129	B8W	C5-C6-O6-C61
4	5	4129	B8W	N1-C6-O6-C61
4	5	4185	B8W	C5-C6-O6-C61
4	5	4185	B8W	N1-C6-O6-C61
4	5	4194	I4U	O4'-C4'-C5'-O5'
4	5	4220	6MZ	N1-C6-N6-C9
4	5	4306	OMU	C1'-C2'-O2'-CM2
4	5	4355	E6G	C5-C6-O6-C61
4	5	4355	E6G	N1-C6-O6-C61
4	5	4371	MHG	C2'-C1'-N9-C8
4	5	4371	MHG	C71-C72-C73-C75
4	5	4403	PSU	C2'-C1'-C5-C4
4	5	4403	PSU	O4'-C1'-C5-C4
4	5	4403	PSU	O4'-C1'-C5-C6
4	5	4415	1MA	C3'-C4'-C5'-O5'
4	5	4447	5MC	C2'-C1'-N1-C2
4	5	4447	5MC	C2'-C1'-N1-C6
4	5	4450	PSU	O4'-C4'-C5'-O5'
4	5	4472	B8W	C5-C6-O6-C61
4	5	4472	B8W	N1-C6-O6-C61
4	5	4500	PSU	C3'-C4'-C5'-O5'
4	5	4500	PSU	O4'-C4'-C5'-O5'
4	5	4529	B8W	C5-C6-O6-C61
4	5	4529	B8W	N1-C6-O6-C61
4	5	4636	PSU	C3'-C4'-C5'-O5'
4	5	4637	OMG	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
4	5	4870	OMG	O4'-C4'-C5'-O5'
4	5	4872	2MG	O4'-C4'-C5'-O5'
6	8	14	OMU	C1'-C2'-O2'-CM2
50	9	116	OMU	C1'-C2'-O2'-CM2
50	9	116	OMU	C3'-C4'-C5'-O5'
50	9	116	OMU	O4'-C4'-C5'-O5'
50	9	121	OMU	C3'-C4'-C5'-O5'
50	9	121	OMU	O4'-C4'-C5'-O5'
50	9	159	A2M	C3'-C4'-C5'-O5'
50	9	166	A2M	O4'-C4'-C5'-O5'
50	9	166	A2M	C3'-C4'-C5'-O5'
50	9	568	E3C	O4'-C1'-N1-C2
50	9	568	E3C	O4'-C1'-N1-C6
50	9	668	A2M	O4'-C4'-C5'-O5'
50	9	668	A2M	C3'-C4'-C5'-O5'
50	9	683	OMG	O4'-C4'-C5'-O5'
50	9	683	OMG	C3'-C4'-C5'-O5'
50	9	1243	PSU	C3'-C4'-C5'-O5'
50	9	1248	B8N	O4'-C4'-C5'-O5'
50	9	1703	OMC	O4'-C4'-C5'-O5'
50	9	1830	UR3	O4'-C1'-N1-C6
50	9	1830	UR3	O4'-C1'-N1-C2
50	9	1832	6MZ	C5-C6-N6-C9
50	9	1832	6MZ	N1-C6-N6-C9
50	9	1851	MA6	O4'-C4'-C5'-O5'
50	9	1851	MA6	C3'-C4'-C5'-O5'
4	5	398	A2M	O4'-C4'-C5'-O5'
4	5	729	2MG	O4'-C4'-C5'-O5'
4	5	1797	E7G	C3'-C4'-C5'-O5'
4	5	1866	UR3	C3'-C4'-C5'-O5'
4	5	2364	OMG	C3'-C4'-C5'-O5'
4	5	2380	B8W	O4'-C4'-C5'-O5'
4	5	2424	OMG	O4'-C4'-C5'-O5'
4	5	3729	PSU	C3'-C4'-C5'-O5'
4	5	3729	PSU	O4'-C4'-C5'-O5'
4	5	3762	B8H	C3'-C4'-C5'-O5'
4	5	3785	A2M	O4'-C4'-C5'-O5'
4	5	3785	A2M	C3'-C4'-C5'-O5'
4	5	3867	A2M	O4'-C4'-C5'-O5'
4	5	3880	P7G	C3'-C4'-C5'-O5'
4	5	3880	P7G	O4'-C4'-C5'-O5'
4	5	3897	B8K	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
4	5	4129	B8W	O4'-C4'-C5'-O5'
4	5	4194	I4U	C3'-C4'-C5'-O5'
4	5	4355	E6G	O4'-C4'-C5'-O5'
4	5	4371	MHG	O4'-C4'-C5'-O5'
4	5	4450	PSU	C3'-C4'-C5'-O5'
4	5	4523	A2M	O4'-C4'-C5'-O5'
4	5	4529	B8W	O4'-C4'-C5'-O5'
4	5	4636	PSU	O4'-C4'-C5'-O5'
4	5	4637	OMG	C3'-C4'-C5'-O5'
4	5	4870	OMG	C3'-C4'-C5'-O5'
4	5	4872	2MG	C3'-C4'-C5'-O5'
50	9	159	A2M	O4'-C4'-C5'-O5'
50	9	1243	PSU	O4'-C4'-C5'-O5'
4	5	1582	PSU	O4'-C4'-C5'-O5'
4	5	4185	B8W	O4'-C4'-C5'-O5'
4	5	4415	1MA	O4'-C4'-C5'-O5'
50	9	568	E3C	C3'-C4'-C5'-O5'
50	9	568	E3C	O4'-C4'-C5'-O5'
50	9	1248	B8N	C3'-C4'-C5'-O5'
50	9	1703	OMC	C3'-C4'-C5'-O5'
4	5	1348	P4U	O4-C41-C42-C43
4	5	4870	OMG	C3'-C2'-O2'-CM2
4	5	398	A2M	C3'-C4'-C5'-O5'
4	5	4472	B8W	O4'-C4'-C5'-O5'
4	5	3701	OMC	C2'-C1'-N1-C6
4	5	2754	B9B	O6-C61-C62-C63
50	9	1337	4AC	O4'-C4'-C5'-O5'
50	9	1851	MA6	C5-C6-N6-C9
4	5	1534	A2M	C4'-C5'-O5'-P
4	5	1625	OMG	C4'-C5'-O5'-P
4	5	1909	P7G	C72-C71-N7-C8
4	5	2754	B9B	C5-C6-O6-C61
4	5	2401	A2M	C3'-C4'-C5'-O5'
4	5	4371	MHG	C3'-C4'-C5'-O5'
50	9	1851	MA6	C4'-C5'-O5'-P
4	5	3701	OMC	C2'-C1'-N1-C2
4	5	2297	E7G	C72-C71-N7-C8
50	9	159	A2M	C4'-C5'-O5'-P
50	9	644	OMG	C4'-C5'-O5'-P
4	5	3701	OMC	C3'-C2'-O2'-CM2
4	5	3785	A2M	C3'-C2'-O2'-CM'
4	5	2786	B9H	C32-C31-N3-C4

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Mol	Chain	Res	Type	Atoms
4	5	4293	PSU	O4'-C4'-C5'-O5'
4	5	4523	A2M	C3'-C4'-C5'-O5'
4	5	4371	MHG	C71-C72-C73-C74
4	5	3701	OMC	O4'-C1'-N1-C6
4	5	2754	B9B	C4'-C5'-O5'-P
4	5	3701	OMC	O4'-C1'-N1-C2
4	5	4500	PSU	C4'-C5'-O5'-P
4	5	4447	5MC	O4'-C1'-N1-C6
50	9	1850	MA6	O4'-C4'-C5'-O5'
4	5	4447	5MC	O4'-C1'-N1-C2
4	5	1326	A2M	C4'-C5'-O5'-P
4	5	4530	UR3	C4'-C5'-O5'-P
4	5	1883	OMG	C3'-C4'-C5'-O5'
4	5	4355	E6G	C62-C61-O6-C6
4	5	729	2MG	C3'-C4'-C5'-O5'
4	5	4293	PSU	C3'-C4'-C5'-O5'
9	C	333	MLZ	CD-CE-NZ-CM
44	m	72	MLZ	CD-CE-NZ-CM
4	5	4194	I4U	C42-C41-O4-C4
4	5	1677	PSU	O4'-C1'-C5-C4
4	5	4450	PSU	O4'-C1'-C5-C4
50	9	668	A2M	C3'-C2'-O2'-CM'
4	5	3897	B8K	C4'-C5'-O5'-P
4	5	4355	E6G	C3'-C4'-C5'-O5'
4	5	3887	OMC	C4'-C5'-O5'-P
4	5	1534	A2M	O4'-C4'-C5'-O5'
4	5	1909	P7G	O4'-C4'-C5'-O5'
4	5	2861	OMC	O4'-C4'-C5'-O5'
4	5	1348	P4U	C2'-C1'-N1-C2
4	5	2363	A2M	O4'-C4'-C5'-O5'
4	5	4529	B8W	C3'-C4'-C5'-O5'
50	9	1337	4AC	C3'-C4'-C5'-O5'
4	5	1316	OMG	C1'-C2'-O2'-CM2
4	5	3785	A2M	C1'-C2'-O2'-CM'
50	9	644	OMG	C1'-C2'-O2'-CM2
50	9	1710	OMC	C1'-C2'-O2'-CM2
4	5	4371	MHG	C2'-C1'-N9-C4
50	9	1219	B8Q	C2'-C1'-N1-C2
4	5	4870	OMG	C4'-C5'-O5'-P
4	5	4620	OMU	C3'-C4'-C5'-O5'
4	5	4450	PSU	O4'-C1'-C5-C6
4	5	4636	PSU	O4'-C1'-C5-C6

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Mol	Chain	Res	Type	Atoms
50	9	814	5MU	C2'-C1'-N1-C2
4	5	1659	I4U	C42-C41-O4-C4
4	5	4194	I4U	C43-C41-O4-C4
4	5	1883	OMG	C4'-C5'-O5'-P
4	5	4523	A2M	C3'-C2'-O2'-CM'
4	5	2422	OMC	O4'-C4'-C5'-O5'
4	5	1574	B9B	O6-C61-C62-C63
4	5	3701	OMC	C4'-C5'-O5'-P
4	5	3899	BGH	C4'-C5'-O5'-P
50	9	1081	PSU	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 305 ligands modelled in this entry, 305 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
4	5	43
50	9	18
6	8	1
2	2	1
28	W	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	2113:G	O3'	2258:C	P	40.26
1	5	1252:C	O3'	1271:G	P	35.28
1	5	1405:C	O3'	1406:G	P	20.05
1	5	1219:G	O3'	1233:G	P	19.96
1	5	1406(C):G	O3'	1411:C	P	18.99
1	5	1411:C	O3'	1411(A):G	P	18.31
1	9	834:C	O3'	841:G	P	17.82
1	9	323:C	O3'	329:G	P	17.67
1	9	697:G	O3'	729:C	P	17.28
1	5	523:C	O3'	638:G	P	17.26
1	9	1761:U	O3'	1771:G	P	17.22
1	9	756:C	O3'	788:G	P	17.19
1	9	1417:C	O3'	1423:C	P	16.88
1	5	4101:C	O3'	4107:G	P	16.87
1	5	4138:C	O3'	4146:G	P	16.05
1	5	990:U	O3'	1064:G	P	15.99
1	5	1696:C	O3'	1720:C	P	15.87
1	9	130:G	O3'	140:U	P	15.86
1	5	4777:C	O3'	4859:C	P	15.85
1	5	1406:G	O3'	1406(A):G	P	15.56
1	5	760:G	O3'	904:C	P	15.37
1	5	3976:C	O3'	4039:G	P	14.31
1	5	5022:U	O3'	5028:G	P	13.97
1	5	922:C	O3'	922(A):G	P	13.56
1	5	1364:U	O3'	1368:A	P	13.45
1	8	79:G	O3'	85:U	P	13.18
1	5	738:C	O3'	738(A):C	P	12.82
1	5	2901:G	O3'	3597:G	P	12.78
1	5	182:G	O3'	189:G	P	12.60
1	5	921:C	O3'	922:C	P	11.48
1	5	4729:A	O3'	4735:G	P	10.05
1	5	922(B):C	O3'	923:C	P	9.10
1	5	1180:C	O3'	1183:C	P	8.92
1	5	738(A):C	O3'	739:G	P	8.73
1	9	225:G	O3'	287:U	P	8.33

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	935:A	O3'	935(A):G	P	7.20
1	5	481:G	O3'	481(A):C	P	6.85
1	5	512:U	O3'	515:C	P	6.78
1	9	745:C	O3'	749:U	P	6.74
1	5	737:C	O3'	738:C	P	6.37
1	5	500:G	O3'	504:G	P	6.21
1	5	480:C	O3'	481:G	P	5.99
1	5	1239:C	O3'	1244:G	P	5.62
1	9	736:C	O3'	743:U	P	5.29
1	5	935(A):G	O3'	936:C	P	4.93
1	9	322:C	O3'	323:C	P	4.92
1	9	1432:U	O3'	1438:A	P	4.81
1	5	934:C	O3'	935:A	P	4.66
1	5	4740:G	O3'	4743:G	P	4.61
1	5	170:C	O3'	171:U	P	4.59
1	5	1100:U	O3'	1168:G	P	4.20
1	9	309:G	O3'	310:C	P	4.18
1	9	304:C	O3'	305:U	P	4.17
1	9	798:G	O3'	799:U	P	4.13
1	2	16:C	O3'	18:G	P	3.88
1	5	4899:G	O3'	4902:C	P	3.28
1	5	1438:U	O3'	1440:U	P	3.27
1	5	751:G	O3'	752:G	P	3.24
1	5	5020:G	O3'	5021:C	P	3.21
1	9	902:G	O3'	903:A	P	3.20
1	9	903:A	O3'	904:A	P	3.20
1	5	267:G	O3'	268:G	P	3.17
1	9	1295:A	O3'	1296:U	P	3.17
1	W	13:ILE	C	14:TYR	N	1.18

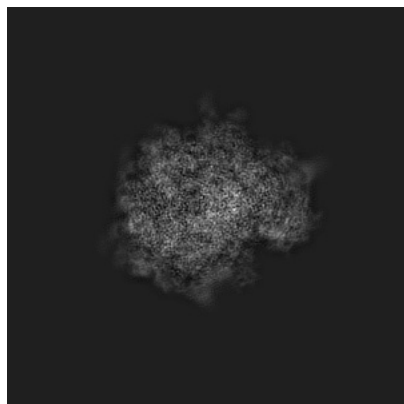
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9237. These allow visual inspection of the internal detail of the map and identification of artifacts.

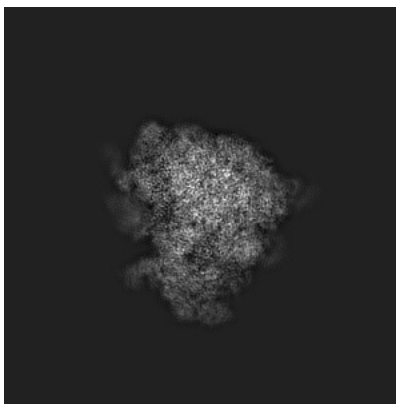
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

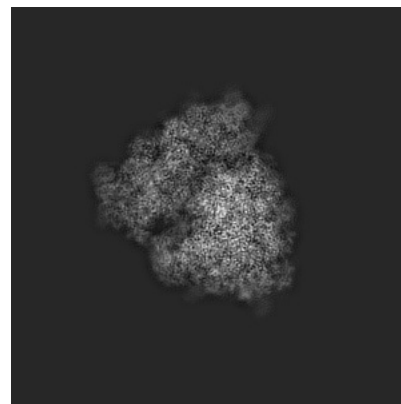
6.1.1 Primary map



X

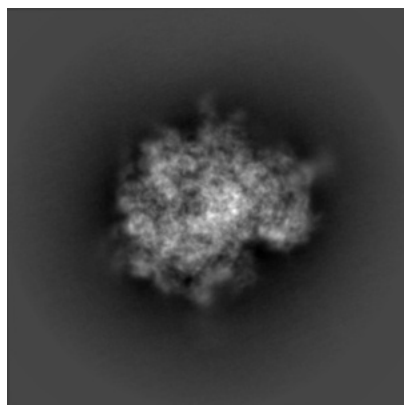


Y

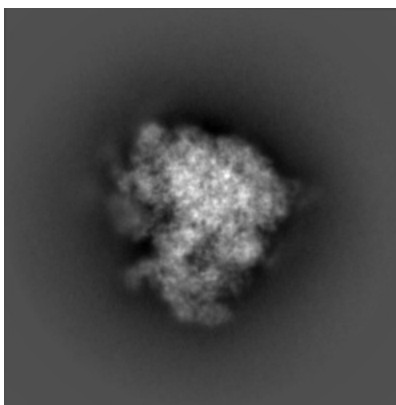


Z

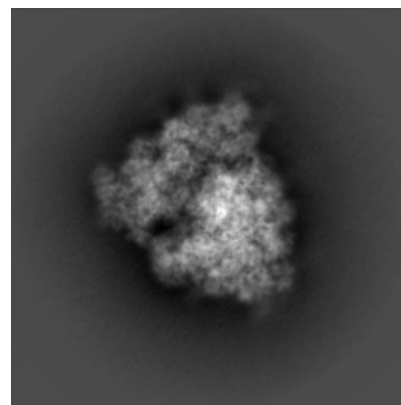
6.1.2 Raw map



X



Y

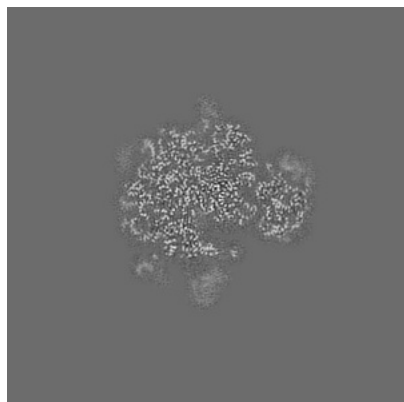


Z

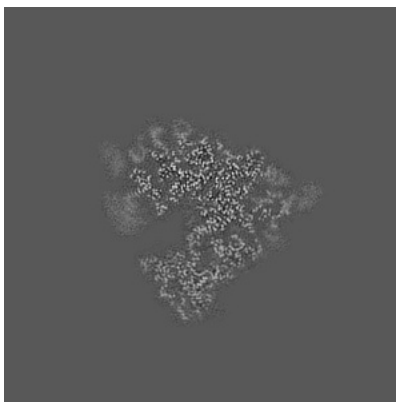
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

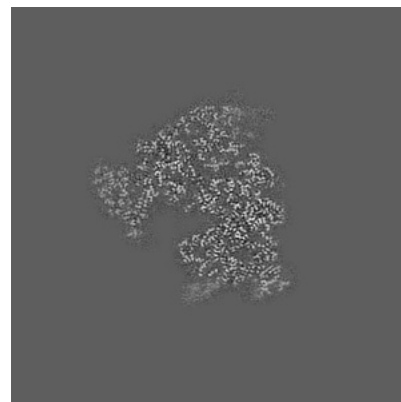
6.2.1 Primary map



X Index: 200

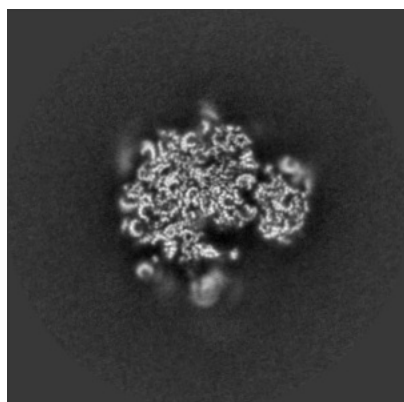


Y Index: 200

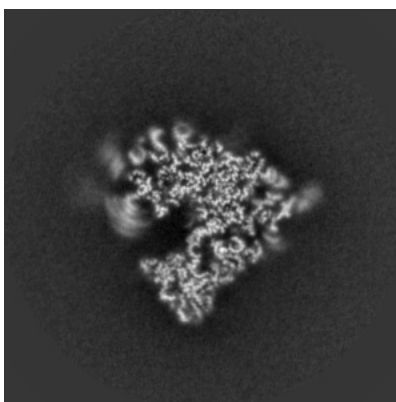


Z Index: 200

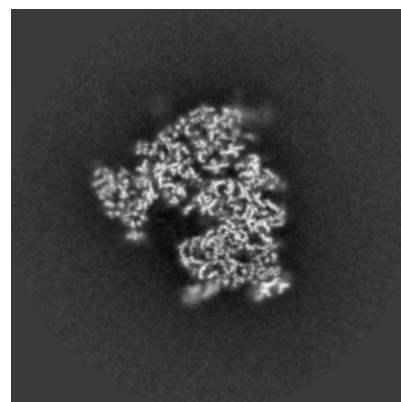
6.2.2 Raw map



X Index: 200



Y Index: 200

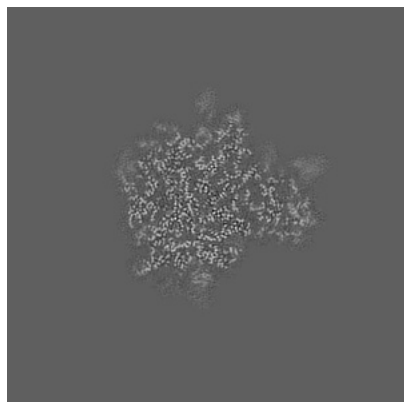


Z Index: 200

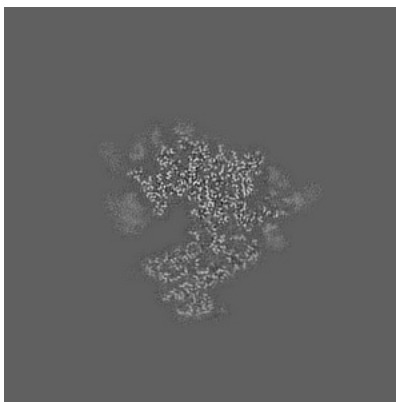
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

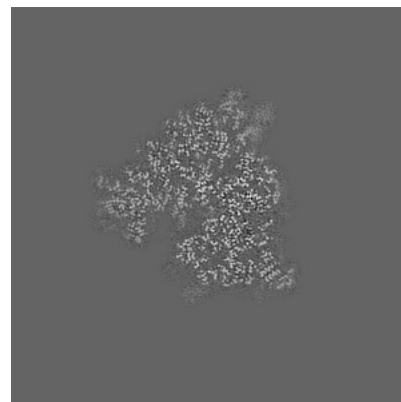
6.3.1 Primary map



X Index: 213

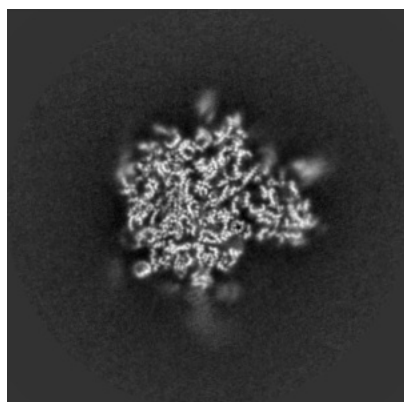


Y Index: 204

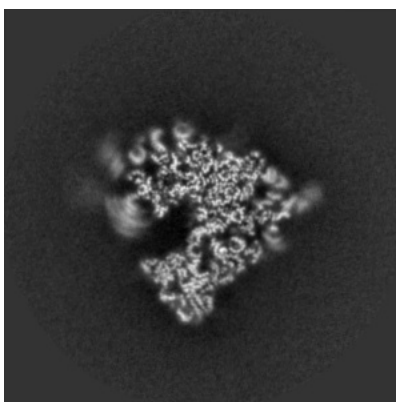


Z Index: 193

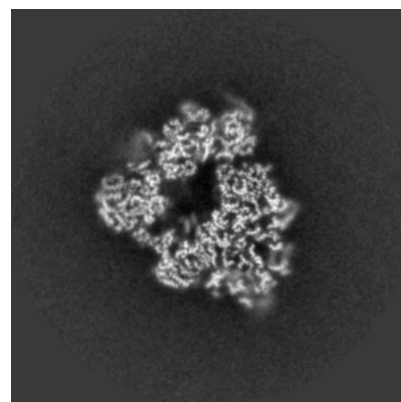
6.3.2 Raw map



X Index: 213



Y Index: 201

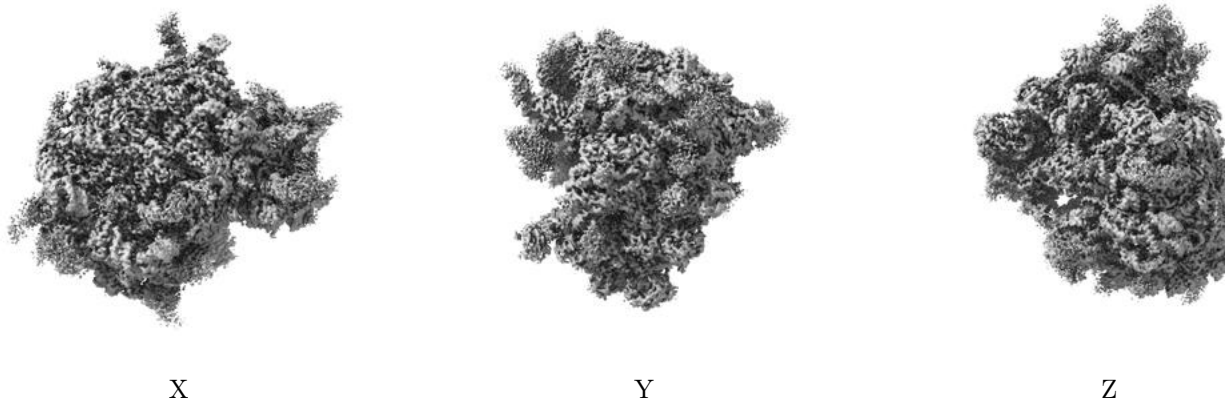


Z Index: 176

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

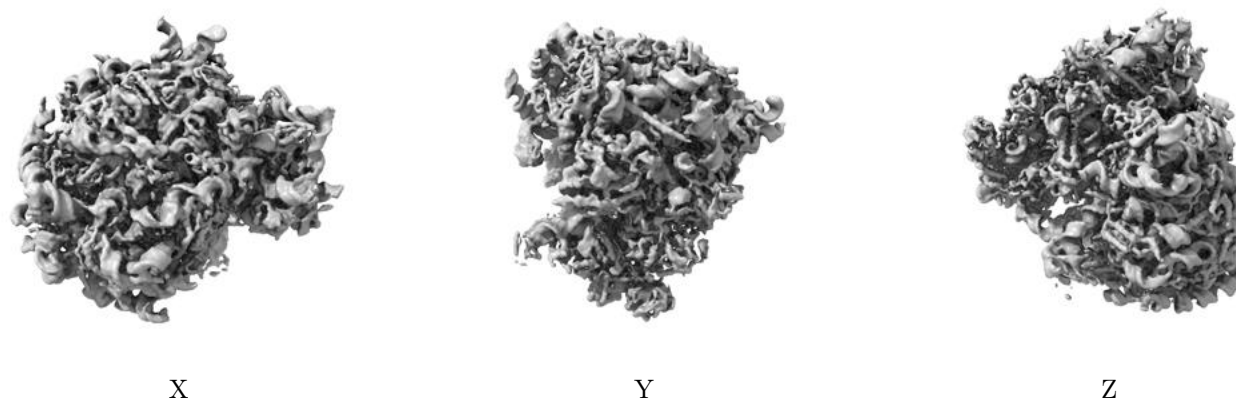
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

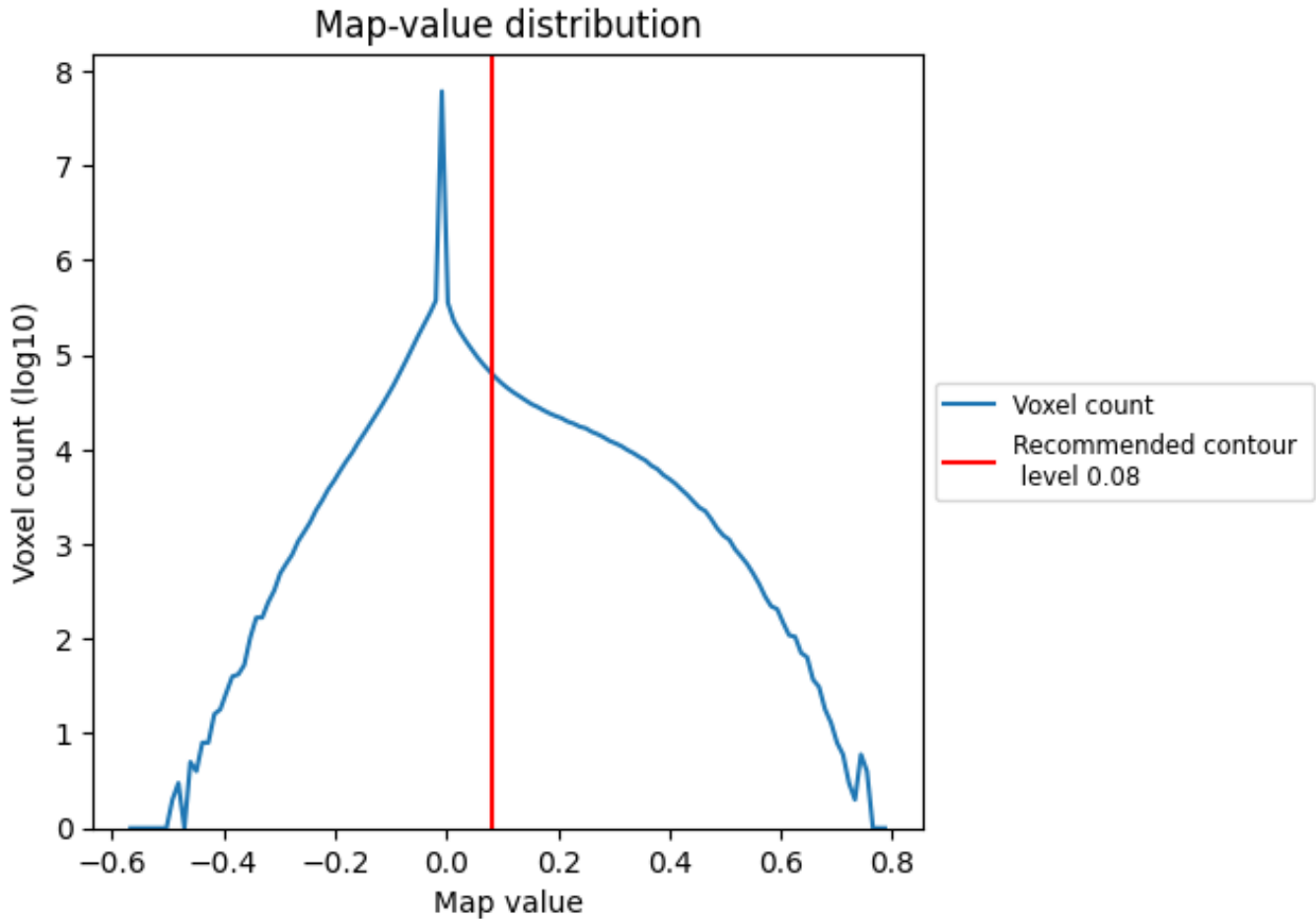
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

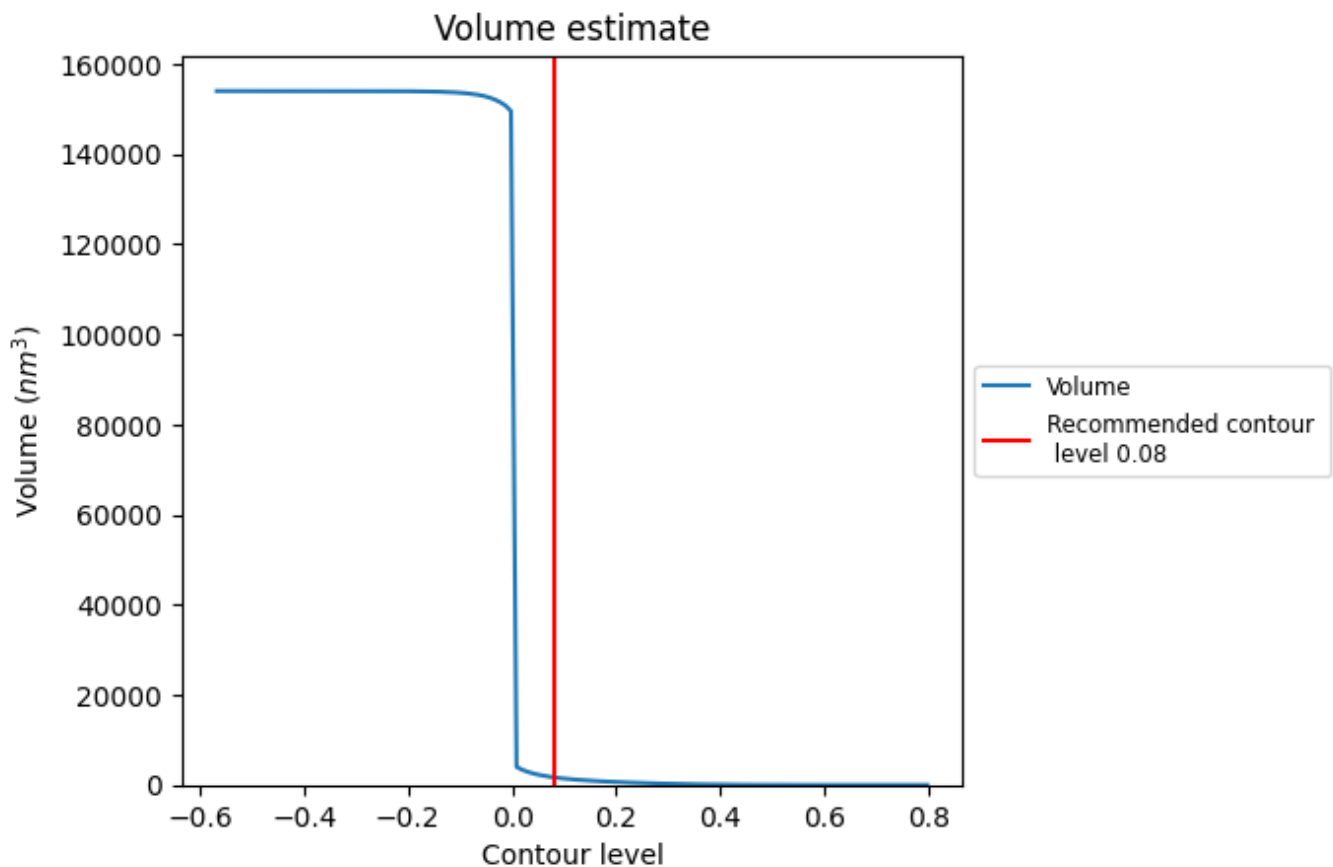
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

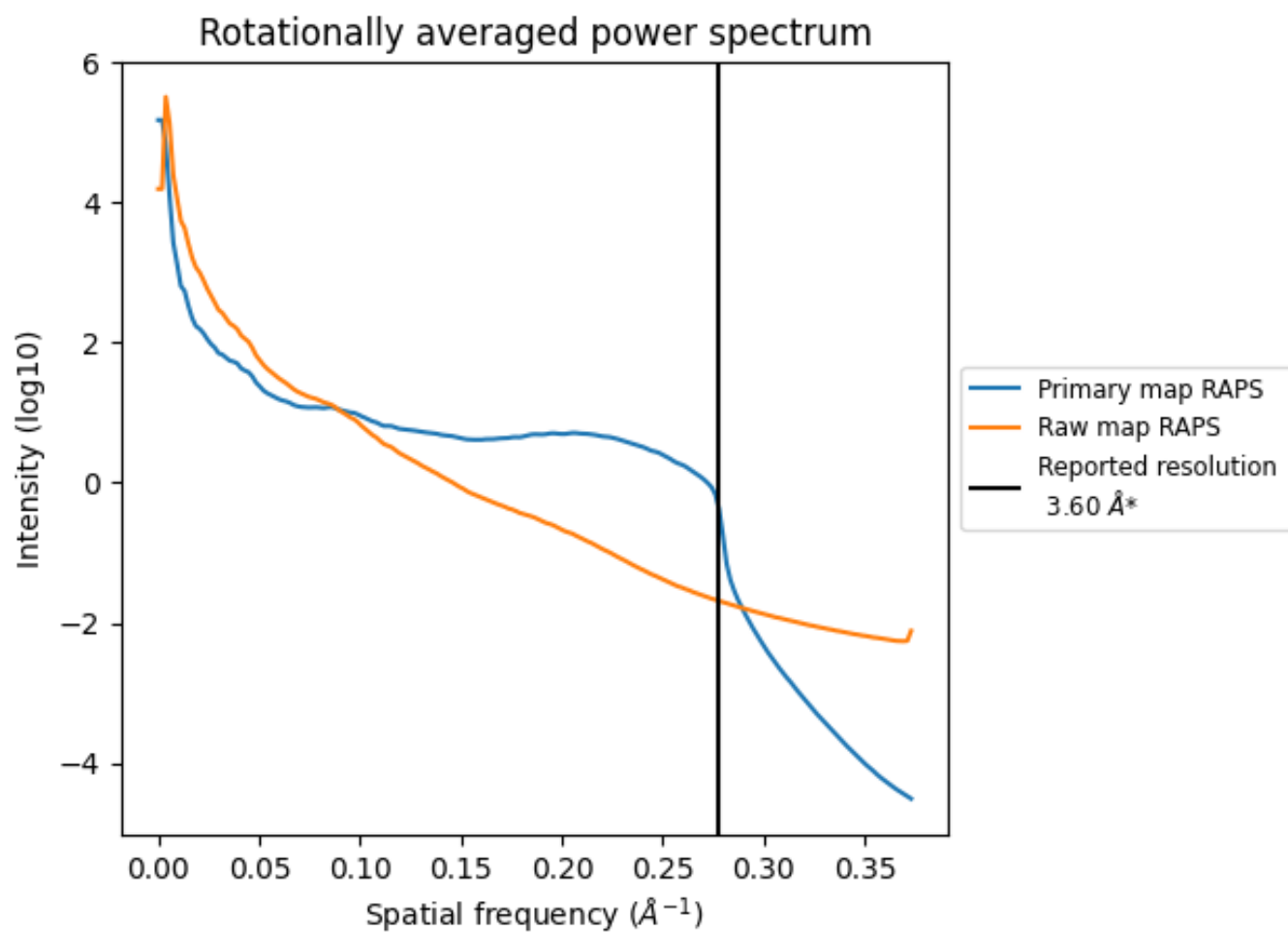
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1689 nm³; this corresponds to an approximate mass of 1525 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

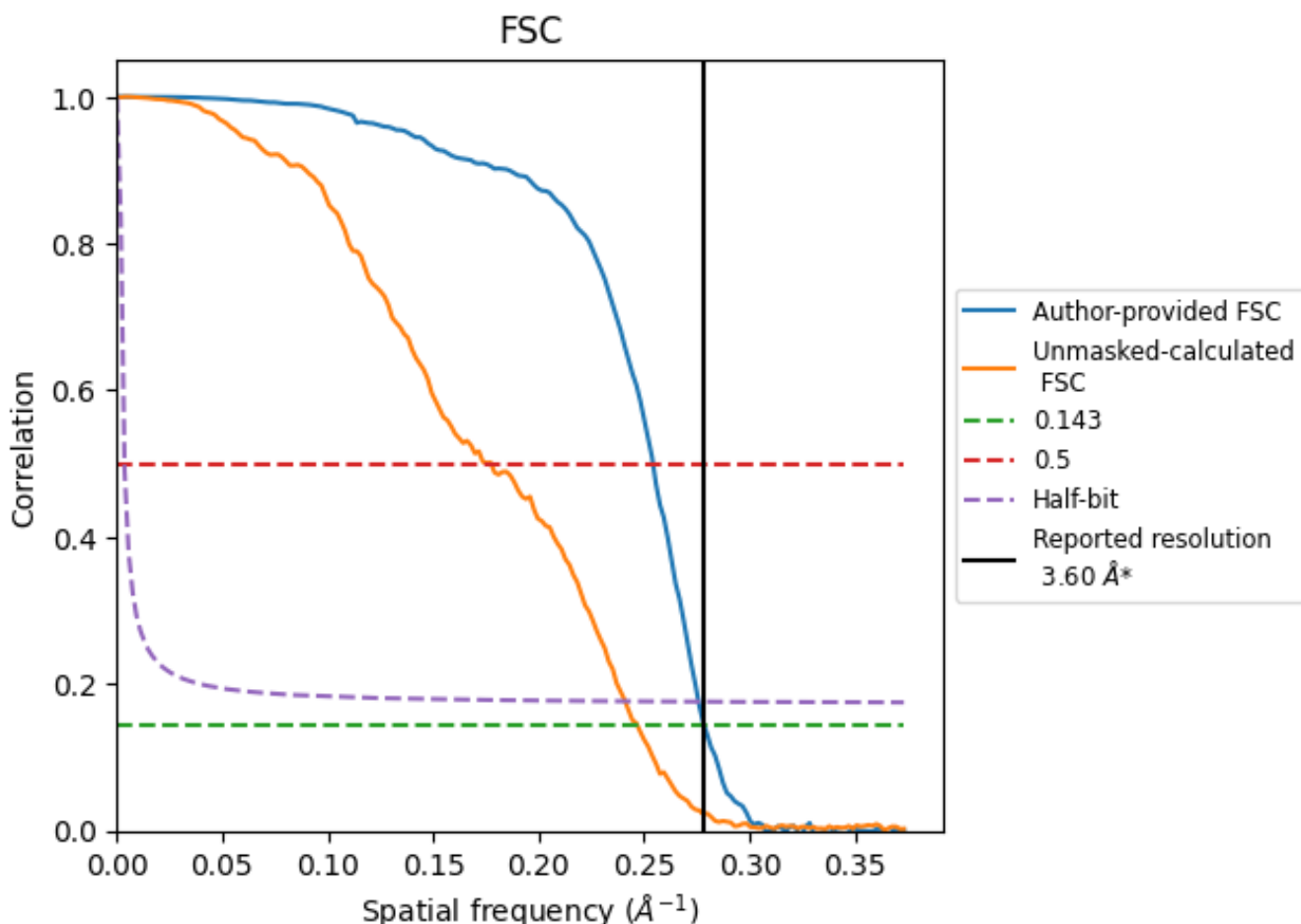


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

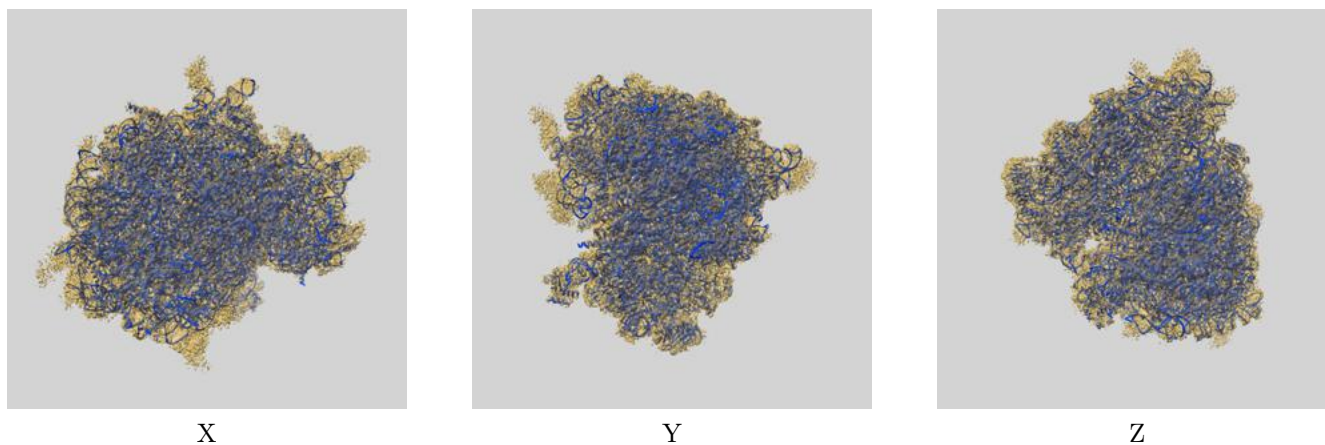
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.59	3.93	3.63
Unmasked-calculated*	4.05	5.64	4.15

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.05 differs from the reported value 3.6 by more than 10 %

9 Map-model fit [i](#)

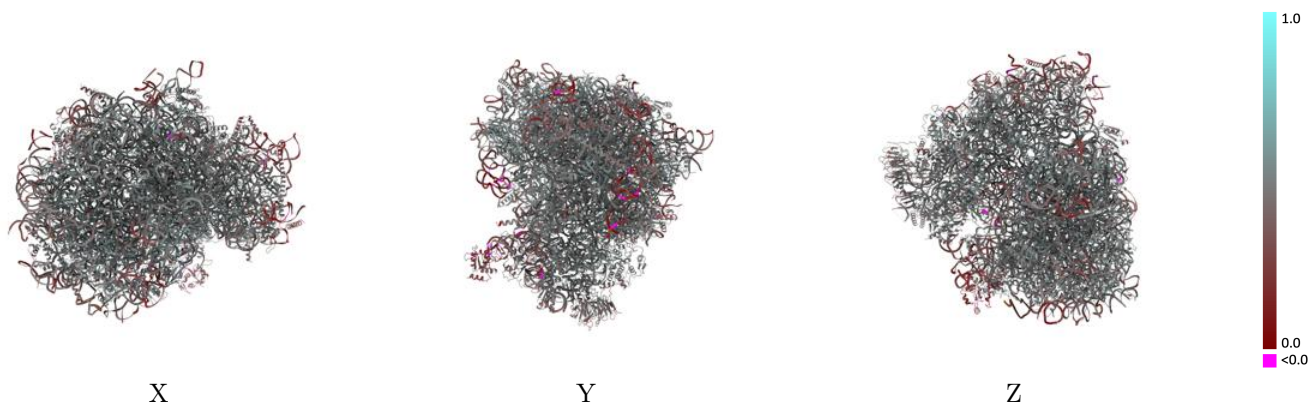
This section contains information regarding the fit between EMDB map EMD-9237 and PDB model 6MTB. Per-residue inclusion information can be found in section [3](#) on page [19](#).

9.1 Map-model overlay [i](#)



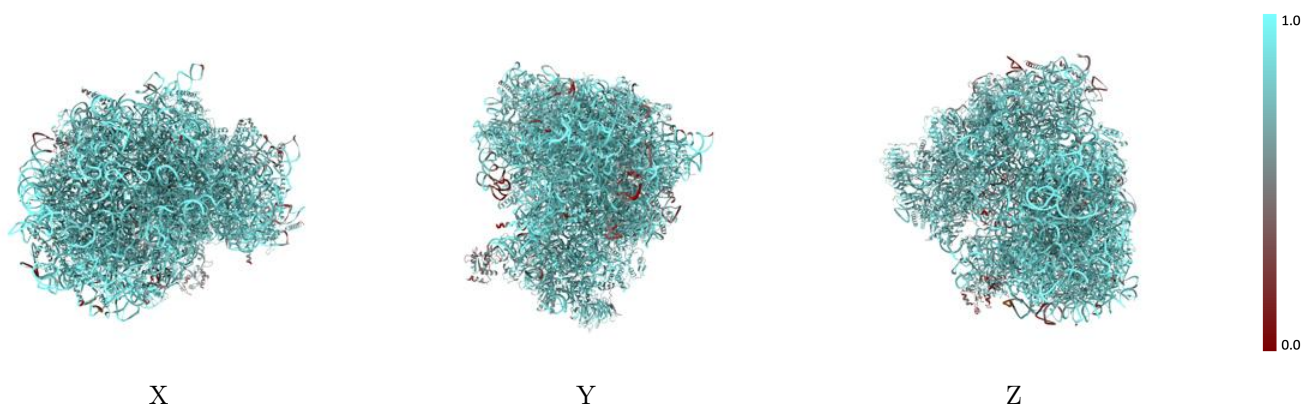
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



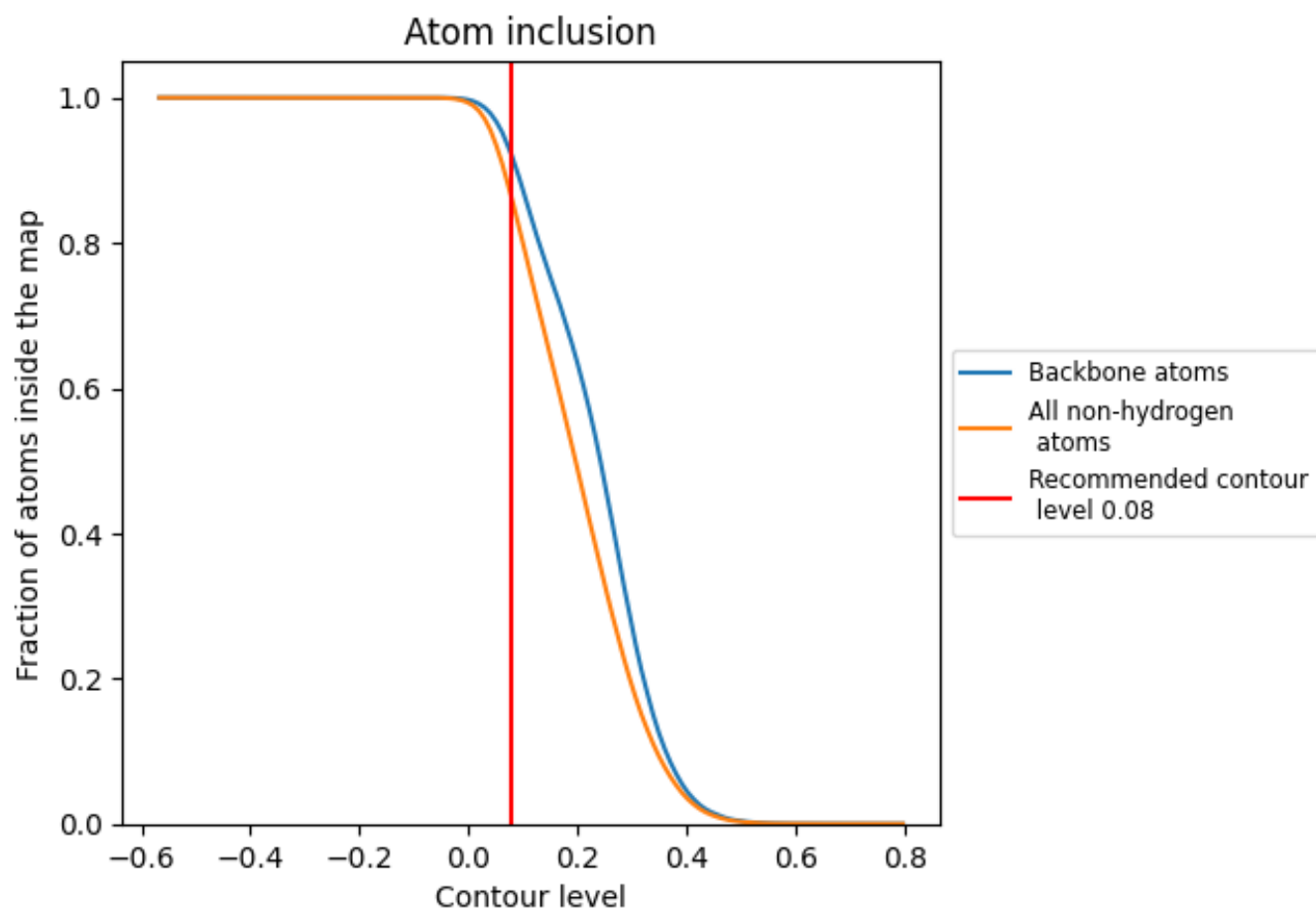
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.08).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary





















































































The table lists the average atom inclusion at the recommended contour level (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8604	 0.4680
1	 0.7919	 0.4930
2	 0.6473	 0.3510
4	 0.7520	 0.2920
5	 0.8980	 0.4560
7	 0.9423	 0.4880
8	 0.9173	 0.4670
9	 0.8913	 0.4460
A	 0.8671	 0.5320
AA	 0.8418	 0.4980
B	 0.8876	 0.5300
BB	 0.8040	 0.4950
C	 0.8585	 0.5210
CC	 0.8468	 0.5130
D	 0.8676	 0.5000
DD	 0.7606	 0.4620
E	 0.8731	 0.5070
EE	 0.8370	 0.5010
F	 0.8484	 0.5150
FF	 0.8149	 0.4790
G	 0.8027	 0.4790
GG	 0.7827	 0.4510
H	 0.8444	 0.5170
HH	 0.7420	 0.4480
I	 0.8501	 0.5210
II	 0.8033	 0.4860
J	 0.8365	 0.4920
JJ	 0.8205	 0.4880
KK	 0.7570	 0.4400
L	 0.8182	 0.4970
LL	 0.8149	 0.5110
M	 0.8644	 0.5060
MM	 0.4519	 0.2670
N	 0.8636	 0.5280
NN	 0.8199	 0.4970

















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Chain	Atom inclusion	Q-score
O	 0.8732	 0.5230
OO	 0.8004	 0.4920
P	 0.8807	 0.5300
PP	 0.7720	 0.4510
Q	 0.8663	 0.5280
QQ	 0.8086	 0.4800
R	 0.8223	 0.4840
RR	 0.7929	 0.4730
S	 0.8665	 0.5230
SS	 0.7921	 0.4650
T	 0.8496	 0.5180
TT	 0.8276	 0.4690
U	 0.7737	 0.4490
UU	 0.7390	 0.4520
V	 0.8612	 0.5280
VV	 0.8408	 0.5060
W	 0.7593	 0.4570
WW	 0.8525	 0.5180
X	 0.8372	 0.5100
XX	 0.8422	 0.5170
Y	 0.8349	 0.5040
YY	 0.8084	 0.4700
Z	 0.8667	 0.5110
ZZ	 0.7942	 0.4610
a	 0.8733	 0.5260
aa	 0.8352	 0.5200
b	 0.7669	 0.4620
bb	 0.7950	 0.4950
c	 0.8347	 0.5000
cc	 0.7638	 0.5000
d	 0.8436	 0.5110
dd	 0.8484	 0.4810
e	 0.8859	 0.5370
ee	 0.7488	 0.4780
f	 0.9050	 0.5410
ff	 0.4584	 0.1230
g	 0.8448	 0.5140
gg	 0.7357	 0.4260
h	 0.8223	 0.5000
i	 0.8354	 0.4940
j	 0.8782	 0.5240
k	 0.7612	 0.4700

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Chain	Atom inclusion	Q-score
l	 0.8759	 0.5230
m	 0.8801	 0.5120
n	 0.8119	 0.5060
o	 0.8409	 0.5270
p	 0.8229	 0.5200
r	 0.8736	 0.5220
u	 0.4502	 0.2750