



Full wwPDB EM Validation Report ⓘ

Feb 3, 2025 – 11:42 PM EST

PDB ID : 6MTE
EMDB ID : EMD-9242
Title : Rabbit 80S ribosome with eEF2 and SERBP1 (rotated state)
Authors : Brown, A.; Baird, M.R.; Yip, M.C.J.; Murray, J.; Shao, S.
Deposited on : 2018-10-19
Resolution : 3.40 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.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

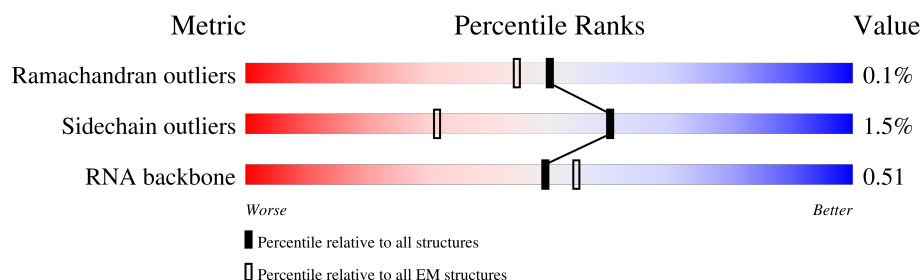
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 Å.

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



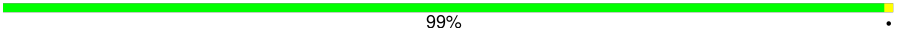


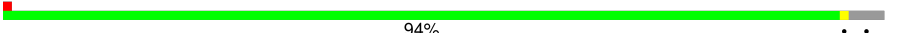
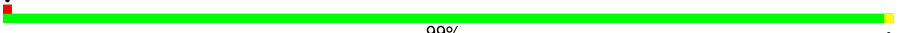
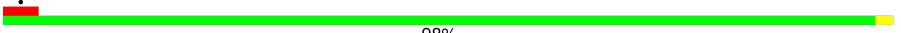









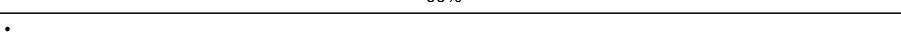
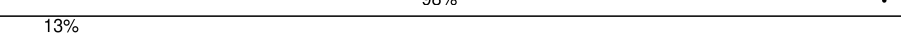

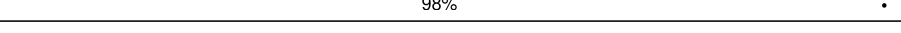
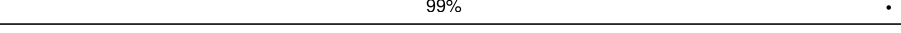
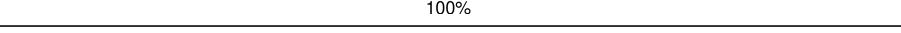
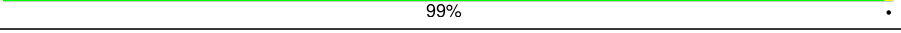

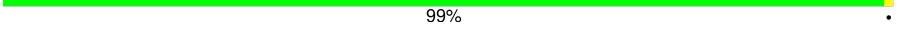
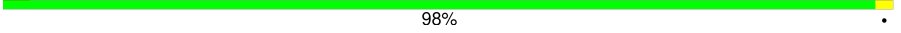
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	5	3597	
2	7	120	
3	8	151	
4	A	248	
5	B	394	
6	C	362	
7	D	293	
8	E	291	

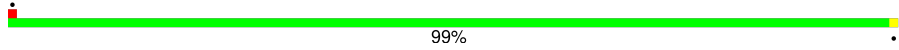
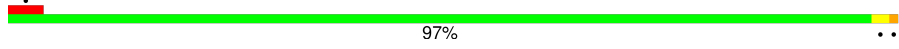
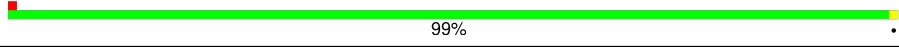
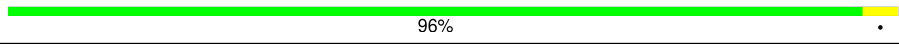
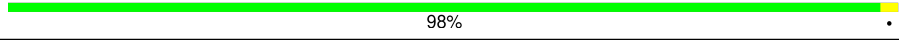
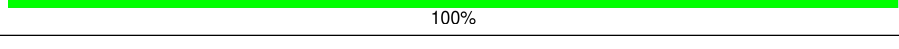
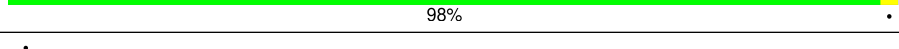
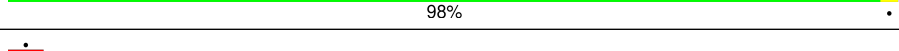
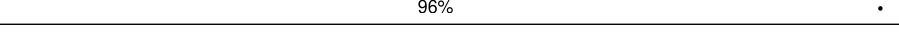
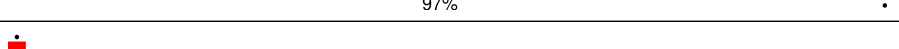
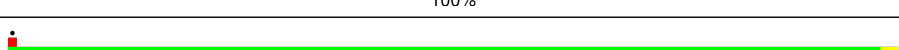
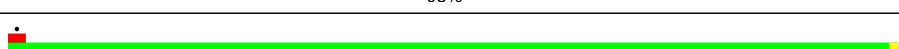
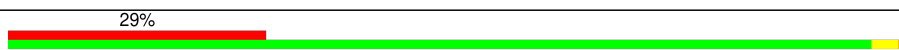
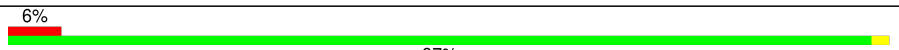
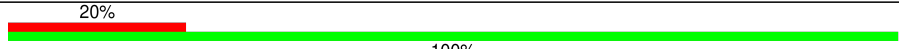

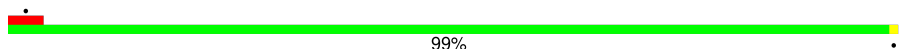
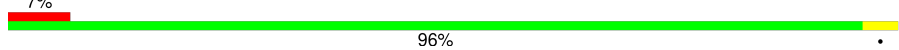
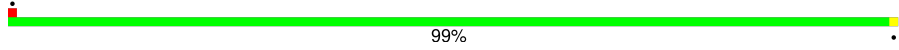
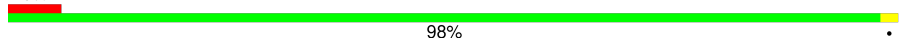
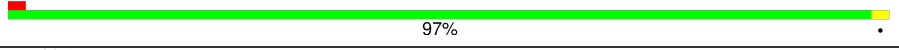
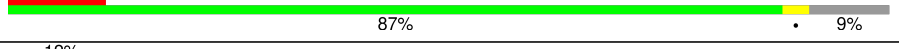
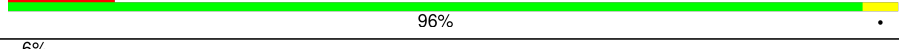
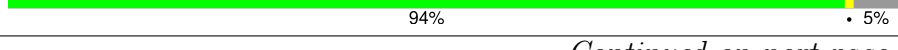

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Mol	Chain	Length	Quality of chain
9	F	225	 99%
10	G	319	 71% 27%
11	H	190	 99%
12	I	214	 94%
13	J	170	 99%
14	L	210	 98%
15	M	138	 99%
16	N	203	 97%
17	O	199	 98%
18	P	153	 98%
19	Q	187	 99%
20	R	180	 99%
21	S	176	 98%
22	T	159	 97%
23	U	99	 99%
24	V	131	 98%
25	W	157	 13% 64% 36%
26	X	118	 98%
27	Y	134	 99%
28	Z	135	 100%
29	a	147	 99%
30	b	245	 42% 58%
31	c	98	 99%
32	d	107	 98%
33	e	128	 98%

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Mol	Chain	Length	Quality of chain
34	f	109	 99%
35	g	114	 97%
36	h	122	 99%
37	i	102	 96%
38	j	86	 98%
39	k	69	 100%
40	l	50	 98%
41	m	52	 98%
42	n	25	 96%
43	o	103	 97%
44	p	91	 100%
45	r	124	 98%
46	s	196	 99%
47	t	153	 29% 97%
48	v	848	 6% 97%
49	w	55	 20% 100%
50	9	1698	 70% 26%
51	AA	217	 99%
52	BB	213	 7% 96%
53	CC	221	 99%
54	DD	228	 6% 98%
55	EE	262	 97%
56	FF	204	 11% 87% 9%
57	GG	237	 12% 96%
58	HH	194	 6% 94% 5%

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Mol	Chain	Length	Quality of chain
59	II	206	
60	JJ	185	
61	KK	96	
62	LL	158	
63	MM	117	
64	NN	149	
65	OO	136	
66	PP	125	
67	QQ	142	
68	RR	132	
69	SS	144	
70	TT	141	
71	UU	100	
72	VV	83	
73	WW	129	
74	XX	141	
75	YY	124	
76	ZZ	75	
77	aa	101	
78	bb	83	
79	cc	62	
80	dd	55	
81	ee	55	
82	ff	68	
83	gg	313	

2 Entry composition [i](#)

There are 86 unique types of molecules in this entry. The entry contains 220739 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 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	5	3597	Total	C	N	O	P	0	0
			77254	34469	14127	25061	3597		

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	7	120	Total	C	N	O	P	0	0
			2558	1141	456	842	119		

- Molecule 3 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	8	151	Total	C	N	O	P	0	0
			3209	1433	564	1062	150		

- Molecule 4 is a protein called uL2.

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

- Molecule 5 is a protein called uL3.

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

- Molecule 6 is a protein called uL4.

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

- Molecule 7 is a protein called uL18.

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

- Molecule 8 is a protein called eL6.

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

- Molecule 9 is a protein called uL30.

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

- Molecule 10 is a protein called eL8.

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

- Molecule 11 is a protein called uL6.

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

- Molecule 12 is a protein called uL16.

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

- Molecule 13 is a protein called uL5.

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

- Molecule 14 is a protein called eL13.

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

- Molecule 15 is a protein called eL14.

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

- Molecule 16 is a protein called eL15.

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

- Molecule 17 is a protein called uL13.

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

- Molecule 18 is a protein called uL22.

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

- Molecule 19 is a protein called eL18.

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

- Molecule 20 is a protein called eL19.

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

- Molecule 21 is a protein called eL20.

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

- Molecule 22 is a protein called eL21.

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

- Molecule 23 is a protein called eL22.

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

- Molecule 24 is a protein called uL14.

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

- Molecule 25 is a protein called eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	W	100	Total	C	N	O	S	0	0
			816	512	164	136	4		

- Molecule 26 is a protein called uL23.

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

- Molecule 27 is a protein called uL24.

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

- Molecule 28 is a protein called eL27.

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

- Molecule 29 is a protein called uL15.

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

- Molecule 30 is a protein called eL29.

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

- Molecule 31 is a protein called eL30.

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

- Molecule 32 is a protein called eL31.

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

- Molecule 33 is a protein called eL32.

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

- Molecule 34 is a protein called eL33.

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

- Molecule 35 is a protein called eL34.

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

- Molecule 36 is a protein called uL29.

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

- Molecule 37 is a protein called eL36.

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

- Molecule 38 is a protein called eL37.

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

- Molecule 39 is a protein called eL38.

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

- Molecule 40 is a protein called eL39.

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

- Molecule 41 is a protein called eL40.

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

- Molecule 42 is a protein called eL41.

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

- Molecule 43 is a protein called eL42.

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

- Molecule 44 is a protein called eL43.

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

- Molecule 45 is a protein called eL28.

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

- Molecule 46 is a protein called uL10.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	s	196	Total	C	N	O	S	0	0
			1507	959	263	276	9		

- Molecule 47 is a protein called uL11.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	t	153	Total	C	N	O	S	0	0
			1160	722	218	217	3		

- Molecule 48 is a protein called eEF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	v	848	Total	C	N	O	S	0	0
			6628	4211	1138	1235	44		

- Molecule 49 is a protein called SERBP1.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	w	55	Total	C	N	O	0	0
			440	263	87	90		

- 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 uS2.

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 eS1.

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 uS5.

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 uS3.

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 eS4.

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 uS7.

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 eS6.

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 eS7.

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 eS8.

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 uS4.

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 eS10.

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 uS17.

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 eS12.

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

- Molecule 64 is a protein called uS15.

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

- Molecule 65 is a protein called uS11.

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

- Molecule 66 is a protein called uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	PP	125	Total	C	N	O	S	0	0
			1025	652	192	174	7		

- Molecule 67 is a protein called uS9.

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

- Molecule 68 is a protein called eS17.

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

- Molecule 69 is a protein called uS13.

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

- Molecule 70 is a protein called eS19.

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

- Molecule 71 is a protein called uS10.

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

- Molecule 72 is a protein called eS21.

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

- Molecule 73 is a protein called uS8.

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

- Molecule 74 is a protein called uS12.

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

- Molecule 75 is a protein called eS24.

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

- Molecule 76 is a protein called eS25.

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

- Molecule 77 is a protein called eS26.

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 eS27.

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 eS28.

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 uS14.

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 eS30.

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 eS31.

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 RACK1.

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	200	Total 200	Mg 200	0
84	7	7	Total 7	Mg 7	0
84	8	6	Total 6	Mg 6	0
84	A	1	Total 1	Mg 1	0
84	P	1	Total 1	Mg 1	0
84	V	1	Total 1	Mg 1	0
84	a	1	Total 1	Mg 1	0
84	j	1	Total 1	Mg 1	0
84	v	1	Total 1	Mg 1	0
84	9	78	Total 78	Mg 78	0
84	TT	1	Total 1	Mg 1	0

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

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

- Molecule 86 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:

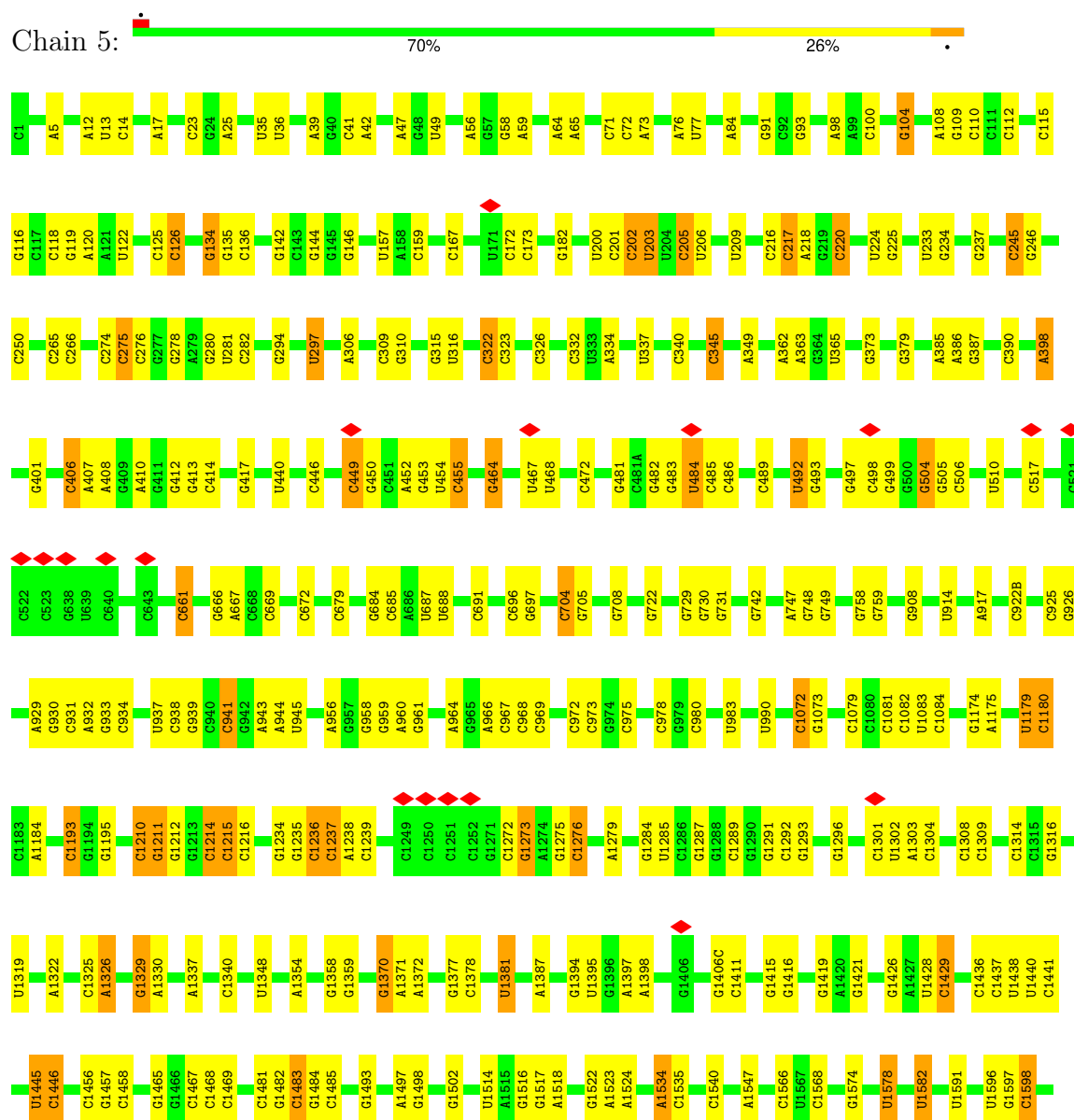
The image displays the chemical structure of GDP (Guanosine Diphosphate). It consists of a guanine base (a purine ring system with an amino group at C2 and a carbonyl group at C6) attached to a ribose sugar (a five-membered ring with hydroxyl groups at C2' and C3'). The ribose is linked to a diphosphate group via a pyrophosphate bridge. The diphosphate group consists of two phosphate groups, each with a central phosphorus atom bonded to four oxygen atoms. The structure is labeled with atom names (N1, N2, C2, C4, C5, C6, N7, C8, N9, C1' (R), C2' (R), C3' (S), C4' (R), C5') and shows the stereochemistry of the sugar and phosphate groups.

Mol	Chain	Residues	Atoms					AltConf
86	v	1	Total	C	N	O	P	0
			28	10	5	11	2	

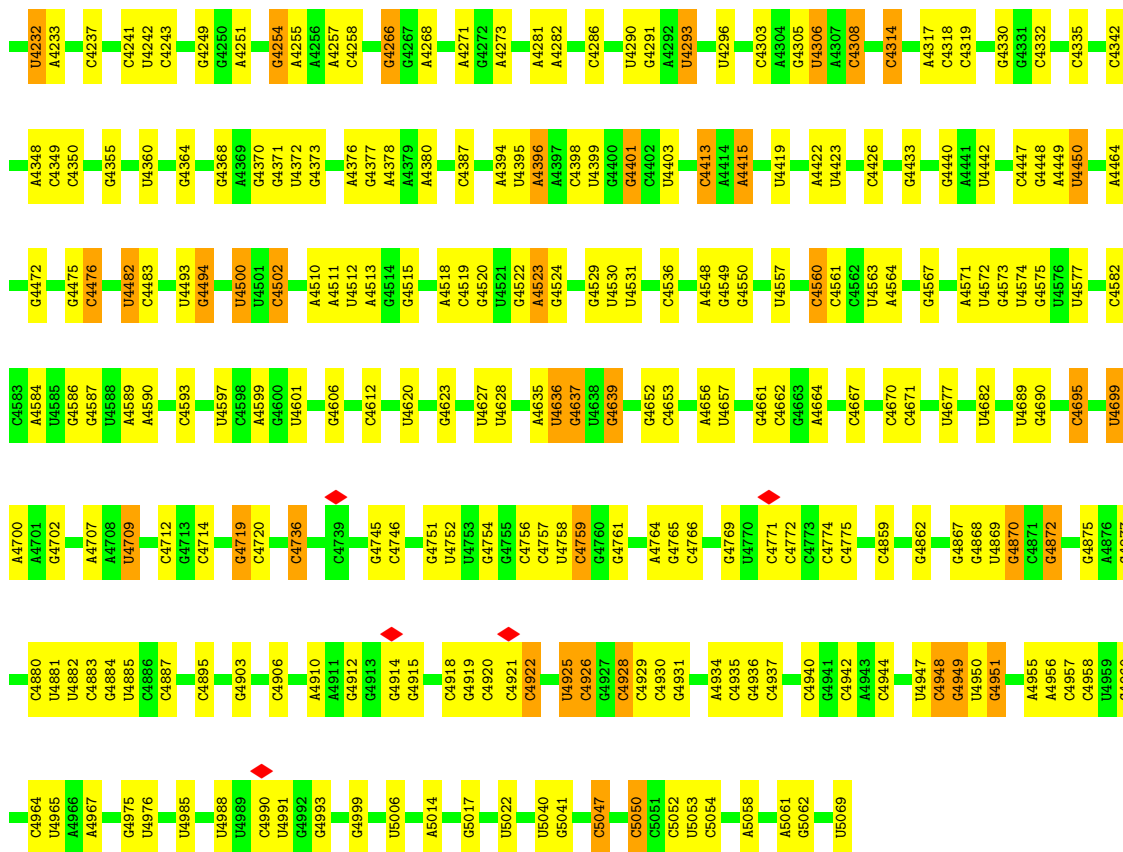
3 Residue-property plots

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.

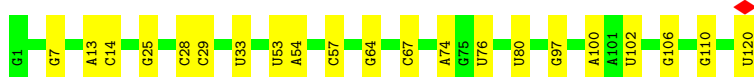
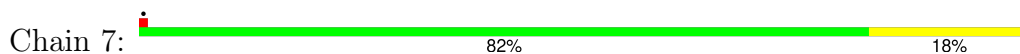
• Molecule 1: 28S rRNA



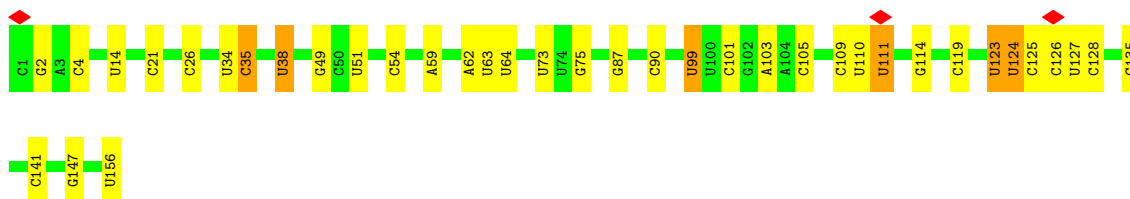
C4100	A3954	U2826	U2554	A2417	C2274	A2029	C1935	U1820	U1602
C4101	A3955	G2827	C2560	A2422	A2279	A2030	G1821	G1821	G1605
C4110	G3923	U2828	C2566	C2423	A2289	U2032	U1822	U1822	U1606
U4111	A3825	U2829	G2567	G2424	C2290	A2033	C1827	C1827	C1607
G4115	U3831	G2838	C2568	U2425	G2294	C2037	G1833	G1833	G1612
C4116	U3838	G2842	G2569	U2432	G2046	G2046	U1834	U1834	A1613
C4119	U3839	A2850	U2570	U2433	A2047	A2047	G1835	G1835	G1624
U4120	U3840	G2855	C2571	U2434	U2048	U2048	G1836	G1836	G1625
A3965	U3851	G2856	U2575	U2441	A2300	G2049	A1837	A1837	G1626
A3966	U3867	C2860	C2583	U2447	G2301	G2050	G1842	G1842	G1627
G3967	G3868	C2861	G2586	U2450	G2306	G2052	C1755	C1755	A1631
U3968	C3869	C2867	A2587	G2453	A2307	G1961	U1756	U1756	A1632
A4127	C3870	G2898	C2588	C2470	A2313	C1963	U1757	U1757	G1633
G3970	G3740	C3598	C2589	G2471	G2314	A1964	G1761	G1761	A1634
G3971	G3741	G2899	C2593	C2474	G2315	G1854	C1762	C1762	A1638
A3876	G3753	C3599	A2600	G2475	G2316	G1855	C1763	C1763	U1639
A3877	G3754	G3603	A2601	G2476	C2319	U1860	G1764	G1764	C1640
G3878	G3755	A3604	G2602	G2477	G2325	U1866	A1765	A1765	G1641
G3879	G3756	C3605	U3606	G2478	U2070	U1971	A1766	A1766	U1649
G3880	A3756	C3606	A2611	G2479	A2072	U1974	A1767	A1767	A1650
C3887	A3759	U3607	C2615	C2488	G2331	C1977	C1768	C1768	G1654
G3888	C3761	G3615	C2616	C2489	A2332	C1978	G1769	G1769	G1655
G3889	A3762	U3616	A2725	U2490	G2333	A1979	A1770	A1770	U1656
U3892	A3763	G3617	A2744	C2491	U2084	A1873	C1771	C1771	U1659
G3897	G3765	C3622	G2754	A2502	G2089	C1881	U1772	U1772	U1660
G3898	A3766	G3626	U2763	C2503	U2090	U1882	U1773	U1773	C1661
G3899	A3767	G3626	A2764	C2504	G2092	G1883	C1774	C1774	C1662
A3901	G3775	A3630	C2768	C2505	C2094	C1884	A1776	A1776	C1663
C4051	A3776	A3631	C2769	C2506	A2095	A1888	C1777	C1777	C1666
C4052	G3777	A3635	C2770	C2507	G2096	A1990	A1780	A1780	U1671
A4053	U3778	C3636	U2771	U2508	A2097	A1991	U1781	U1781	C1674
C4054	G3779	G3636	C2772	U2513	G2098	U1992	A1787	A1787	C1675
U4055	G3780	A3646	C2786	C2521	C2099	C1993	U1791	U1791	C1676
A4056	C3781	A3646	A2787	C2522	G2100	C1994	U1792	U1792	C1677
C3909	C3782	C3650	U2788	G2529	G2101	U1997	G1797	G1797	C1678
G3910	A3783	U3657	A2789	C2532	C2102	G2001	C1898	C1898	U1679
C3911	A3784	C3658	U2790	G2533	A2103	A2002	U1800	U1800	U1683
U3915	A3785	G3658	C2794	C2537	A2104	A2003	A1804	A1804	A1684
G3916	G3787	A3662	C2798	U2538	A2105	G2004	A1805	A1805	G1685
A3917	C3788	A3663	A2798	C2539	A2106	U2008	C1806	C1806	C1686
C3926	G3792	G3664	U2803	U2544	G2259	C2011	C1807	C1807	G1691
U3927	C3810	C3673	C2804	U2545	C2260	U2020	C1808	C1808	C1694
G3938	G3811	G3673	C2814	G2546	G2267	A1917	A1809	A1809	A1694
C3939	C3812	A3691	C2817	U2547	A2401	U1918	A1809	A1809	G1695
U3940	A3813	A3692	C2818	G2548	G2405	G1916	A1809	A1809	C1696
G3941	U3814	G3692	C2819	G2549	U2408	U1919	C1809	C1809	C1697
C3951	C3701	C3701	C2820	G2553	U2409	C1920	C1809	C1809	C1698
G3951	G3705	G3705	C2820	A2553	G2270	C1921	C1809	C1809	C1699
A4064	C4064	C4064	C4064	C4064	C4064	C1922	C1809	C1809	C1699
A4065	A4065	A4065	A4065	A4065	A4065	A1929	C1809	C1809	C1699
U4066	U4066	U4066	U4066	U4066	U4066	A2025	C1809	C1809	C1699
A4073	A4073	A4073	A4073	A4073	A4073	A2026	C1809	C1809	C1699
C4074	C4074	C4074	C4074	C4074	C4074	U2027	C1809	C1809	C1699
U4075	U4075	U4075	U4075	U4075	U4075	A1932	C1809	C1809	C1699
G4076	G4076	G4076	G4076	G4076	G4076	A1932	C1809	C1809	C1699
U4083	U4083	U4083	U4083	U4083	U4083	A1932	C1809	C1809	C1699
A4084	A4084	A4084	A4084	A4084	A4084	A1932	C1809	C1809	C1699
A4085	A4085	A4085	A4085	A4085	A4085	A1932	C1809	C1809	C1699
G4086	G4086	G4086	G4086	G4086	G4086	A1932	C1809	C1809	C1699
C4087	C4087	C4087	C4087	C4087	C4087	A1932	C1809	C1809	C1699
G4088	G4088	G4088	G4088	G4088	G4088	A1932	C1809	C1809	C1699
G4097	G4097	G4097	G4097	G4097	G4097	A1932	C1809	C1809	C1699



• Molecule 2: 5S rRNA



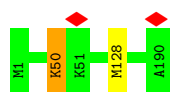
• Molecule 3: 5.8S rRNA



• Molecule 4: uL2

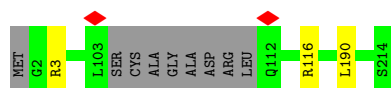


Chain H:  99%



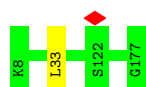
- Molecule 12: uL16

Chain I:  94%



- Molecule 13: uL5

Chain J:  99%



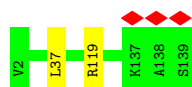
- Molecule 14: eL13

Chain L:  98%



- Molecule 15: eL14

Chain M:  99%



- Molecule 16: eL15

Chain N:  97%



- Molecule 17: uL13

Chain O:  98%



- Molecule 18: uL22

Chain P:  98% .



• Molecule 19: eL18

Chain Q:  99% .



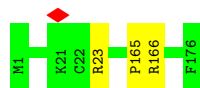
• Molecule 20: eL19

Chain R:  99% .



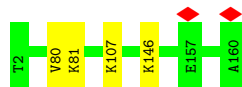
• Molecule 21: eL20

Chain S:  98% .



• Molecule 22: eL21

Chain T:  97% .



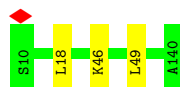
• Molecule 23: eL22

Chain U:  99% .



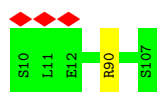
• Molecule 24: uL14

Chain V:  98% .



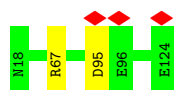
• Molecule 25: eL24

Chain c:  99% .



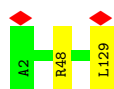
- Molecule 32: eL31

Chain d:  98% .



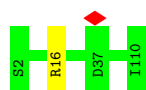
- Molecule 33: eL32

Chain e:  98% .



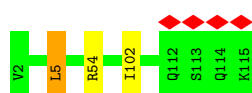
- Molecule 34: eL33

Chain f:  99% .



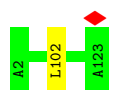
- Molecule 35: eL34

Chain g:  97% ..



- Molecule 36: uL29

Chain h:  99% .



- Molecule 37: eL36

Chain i:  96% .



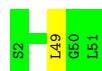
• Molecule 38: eL37

Chain j:  98%

• Molecule 39: eL38

Chain k:  100%

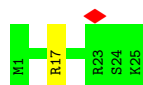
• Molecule 40: eL39

Chain l:  98%

• Molecule 41: eL40

Chain m:  98%

• Molecule 42: eL41

Chain n:  96%

• Molecule 43: eL42

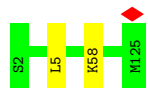
Chain o:  97%

• Molecule 44: eL43

Chain p:  100%

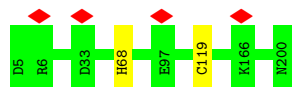
- Molecule 45: eL28

Chain r:  98%



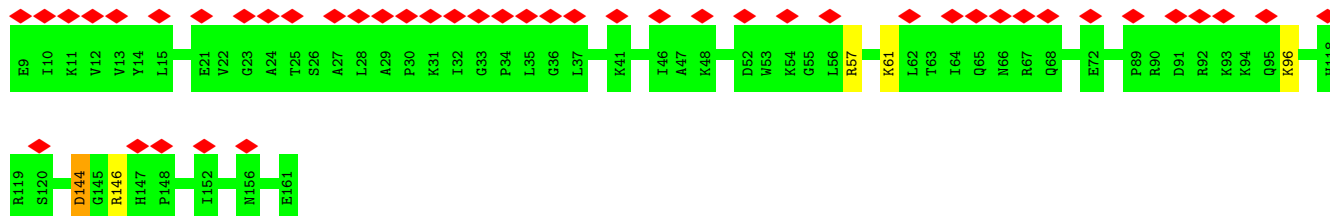
- Molecule 46: uL10

Chain s:  99%



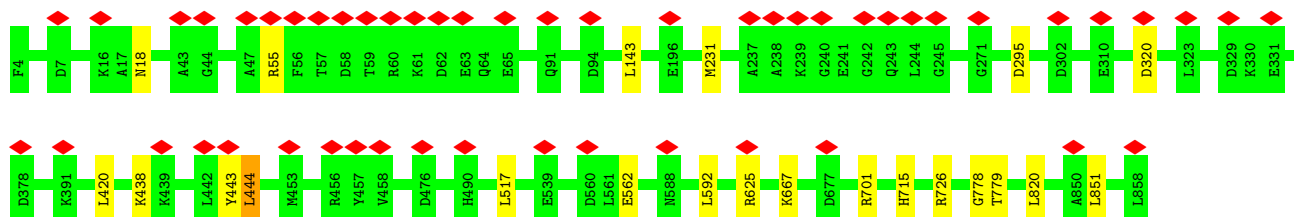
- Molecule 47: uL11

Chain t:  29% 97%



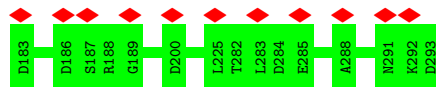
- Molecule 48: eEF2

Chain v:  6% 97%



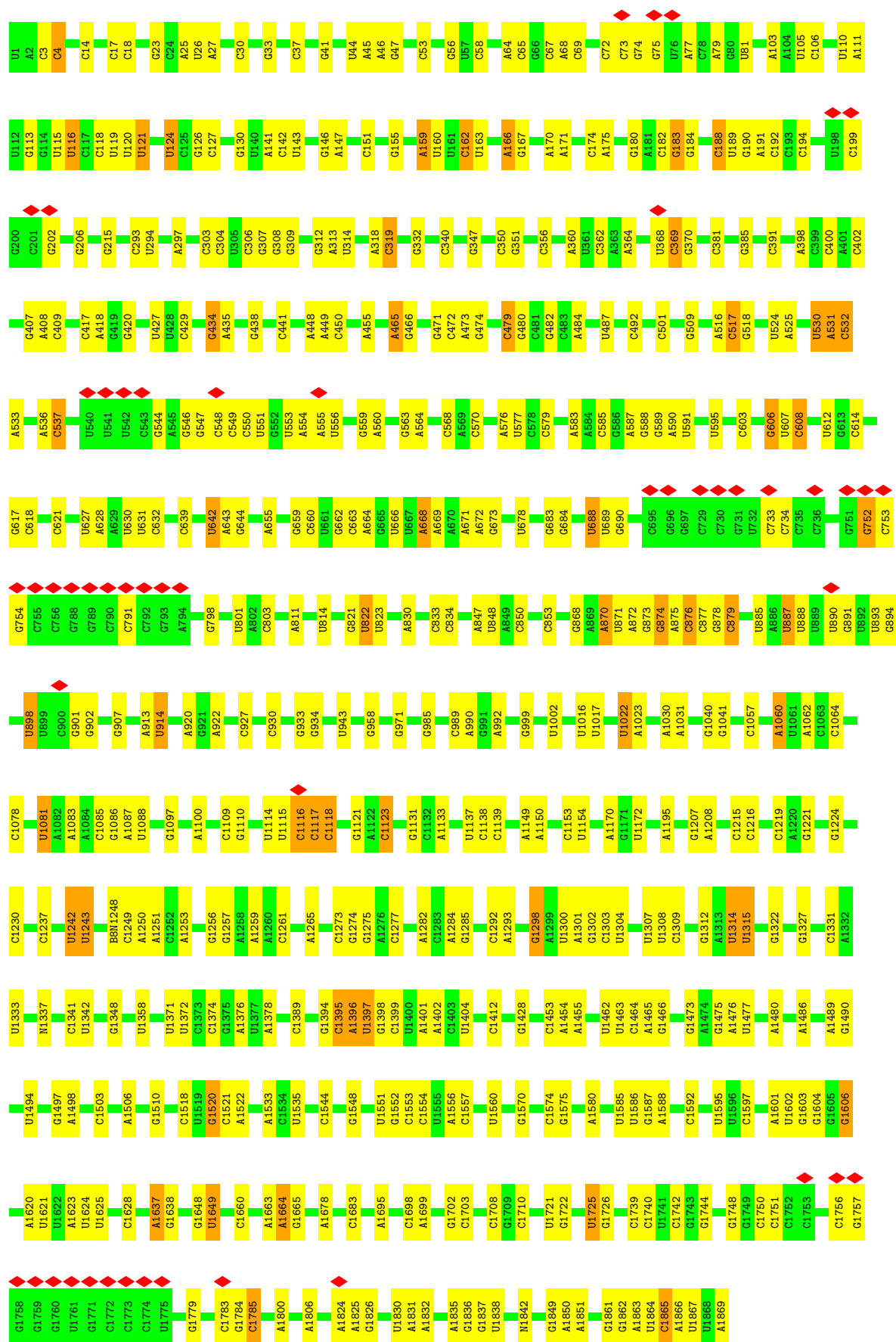
- Molecule 49: SERBP1

Chain w:  20% 100%



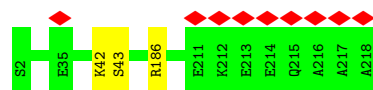
- Molecule 50: 18S rRNA

Chain 9:  70% 26%



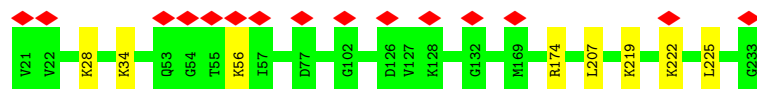
- Molecule 51: uS2

Chain AA:  99%



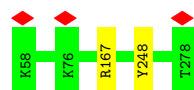
- Molecule 52: eS1

Chain BB:  96%



- Molecule 53: uS5

Chain CC:  99%



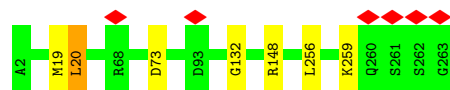
- Molecule 54: uS3

Chain DD:  98%




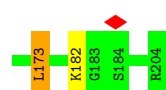
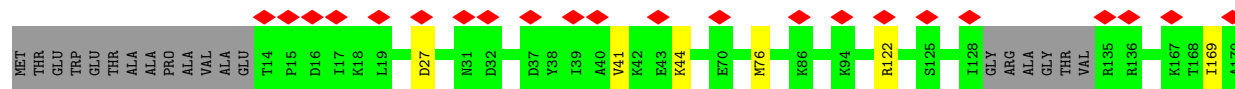
- Molecule 55: eS4

Chain EE:  97%



- Molecule 56: uS7

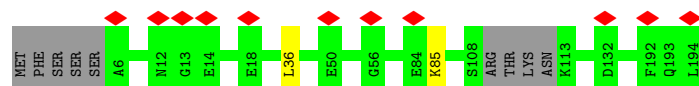
Chain FF:  87% 9%



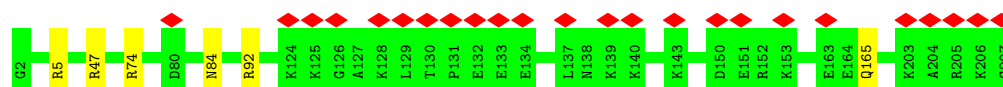
- Molecule 57: eS6



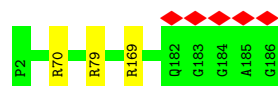
- Molecule 58: eS7



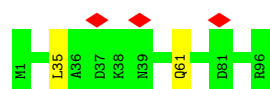
- Molecule 59: eS8



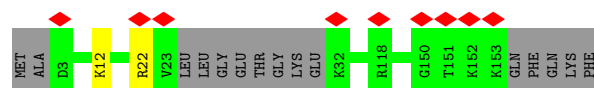
- Molecule 60: uS4



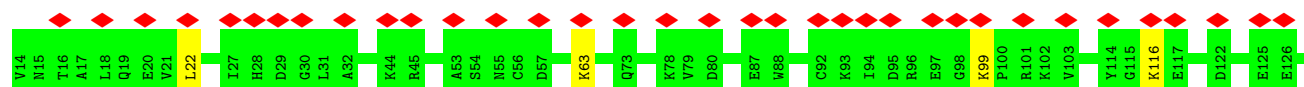
- Molecule 61: eS10



- Molecule 62: uS17

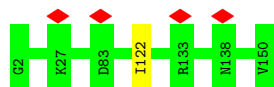


- Molecule 63: eS12

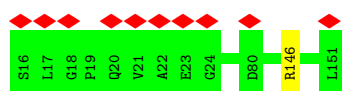




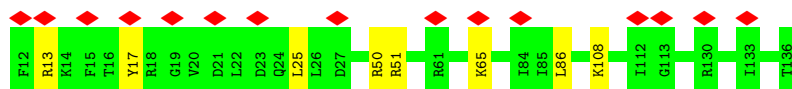
- Molecule 64: uS15



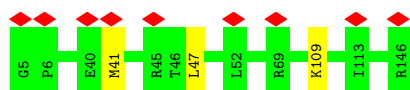
- Molecule 65: uS11



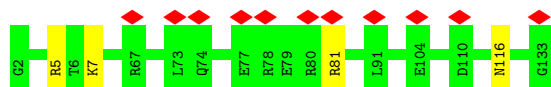
- Molecule 66: uS19



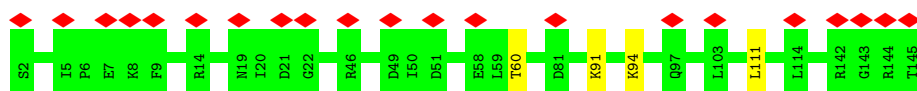
- Molecule 67: uS9



- Molecule 68: eS17



- Molecule 69: uS13



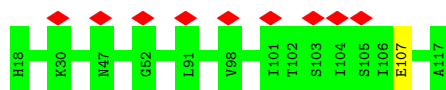
- Molecule 70: eS19

Chain TT:  7% 98%



- Molecule 71: uS10

Chain UU:  9% 99%



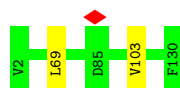
- Molecule 72: eS21

Chain VV:  98%



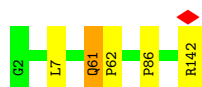
- Molecule 73: uS8

Chain WW:  98%



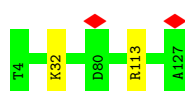
- Molecule 74: uS12

Chain XX:  96%



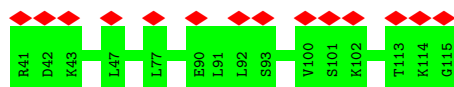
- Molecule 75: eS24

Chain YY:  98%



- Molecule 76: eS25

Chain ZZ:  19% 100%



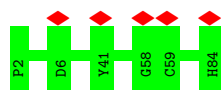
- Molecule 77: eS26

Chain aa:  99%



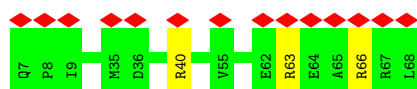
- Molecule 78: eS27

Chain bb:  100%



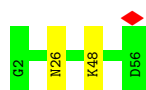
- Molecule 79: eS28

Chain cc:  95%



- Molecule 80: uS14

Chain dd:  96%



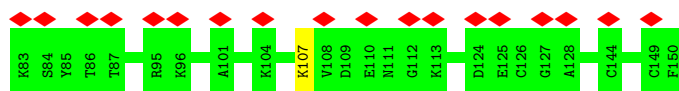
- Molecule 81: eS30

Chain ee:  95%



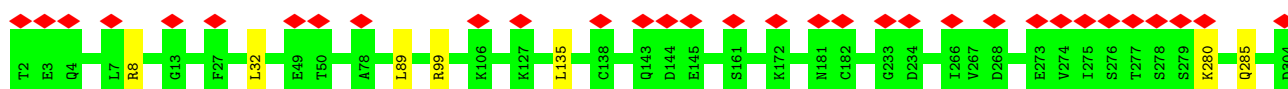
- Molecule 82: eS31

Chain ff:  99%



- Molecule 83: RACK1

Chain gg:  98%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	133480	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	104478	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.679	Depositor
Minimum map value	-0.386	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.023	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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MC, B8N, MA6, MG, OMG, E7G, 5MU, B9B, 4AC, GDP, 6MZ, M7A, B8H, 7MG, E3C, DDE, 1MA, A2M, 2MG, E6G, MHG, B9H, UR3, B8Q, B8W, PSU, BGH, ZN, OMC, P4U, P7G, B8K, OMU, B8T, MLZ, I4U

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	5	0.80	0/83819	1.15	616/130590 (0.5%)
2	7	0.79	0/2858	1.09	13/4455 (0.3%)
3	8	0.77	0/3559	1.16	39/5543 (0.7%)
4	A	0.51	0/1936	0.62	0/2596
5	B	0.49	0/3240	0.66	2/4339 (0.0%)
6	C	0.47	0/2927	0.62	2/3932 (0.1%)
7	D	0.42	0/2437	0.55	0/3264
8	E	0.39	0/1762	0.64	0/2362
9	F	0.48	0/1911	0.62	0/2549
10	G	0.41	0/1910	0.61	0/2569
11	H	0.50	1/1535 (0.1%)	0.63	0/2063
12	I	0.48	0/1702	0.60	1/2272 (0.0%)
13	J	0.38	0/1385	0.66	1/1852 (0.1%)
14	L	0.42	0/1733	0.63	2/2316 (0.1%)
15	M	0.45	0/1158	0.58	1/1547 (0.1%)
16	N	0.50	0/1746	0.62	0/2338
17	O	0.51	0/1662	0.65	0/2222
18	P	0.49	0/1268	0.61	0/1700
19	Q	0.47	0/1539	0.62	0/2054
20	R	0.41	0/1524	0.65	1/2013 (0.0%)
21	S	0.53	0/1501	0.61	0/2012
22	T	0.47	0/1326	0.57	0/1770
23	U	0.37	0/823	0.64	0/1104
24	V	0.49	0/993	0.63	1/1332 (0.1%)
25	W	0.46	0/829	0.60	0/1099
26	X	0.43	0/984	0.64	1/1323 (0.1%)
27	Y	0.45	0/1132	0.60	0/1504
28	Z	0.46	0/1130	0.59	0/1507
29	a	0.49	0/1191	0.63	0/1590
30	b	0.34	0/861	0.56	0/1138

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	c	0.42	0/771	0.60	0/1034
32	d	0.43	0/903	0.61	0/1216
33	e	0.46	0/1071	0.58	1/1429 (0.1%)
34	f	0.51	0/895	0.68	0/1198
35	g	0.46	0/916	0.63	0/1220
36	h	0.41	0/1021	0.58	0/1348
37	i	0.39	0/841	0.59	1/1112 (0.1%)
38	j	0.46	0/720	0.65	0/952
39	k	0.40	0/575	0.58	0/761
40	l	0.40	0/459	0.61	1/608 (0.2%)
41	m	0.49	0/425	0.68	0/561
42	n	0.33	0/240	0.64	0/305
43	o	0.44	0/855	0.58	1/1128 (0.1%)
44	p	0.46	0/718	0.60	0/953
45	r	0.45	0/1010	0.62	1/1354 (0.1%)
46	s	0.33	0/1530	0.59	0/2064
47	t	0.31	0/1174	0.72	1/1582 (0.1%)
48	v	0.40	0/6736	0.69	8/9094 (0.1%)
49	w	0.33	0/447	0.58	0/592
50	9	0.64	0/39723	1.15	274/61870 (0.4%)
51	AA	0.40	0/1747	0.63	0/2374
52	BB	0.37	0/1756	0.72	4/2350 (0.2%)
53	CC	0.47	0/1753	0.64	0/2369
54	DD	0.38	0/1796	0.65	0/2417
55	EE	0.38	0/2118	0.69	5/2849 (0.2%)
56	FF	0.35	0/1492	0.68	2/2005 (0.1%)
57	GG	0.32	0/1946	0.68	3/2590 (0.1%)
58	HH	0.36	0/1510	0.67	1/2022 (0.0%)
59	II	0.36	0/1715	0.65	0/2287
60	JJ	0.39	0/1550	0.63	0/2069
61	KK	0.39	0/834	0.66	1/1125 (0.1%)
62	LL	0.44	0/1195	0.59	0/1597
63	MM	0.32	0/918	0.64	1/1233 (0.1%)
64	NN	0.36	0/1226	0.58	0/1649
65	OO	0.33	0/1029	0.63	0/1380
66	PP	0.34	0/1045	0.66	2/1396 (0.1%)
67	QQ	0.32	0/1146	0.66	1/1534 (0.1%)
68	RR	0.32	0/1082	0.62	0/1452
69	SS	0.32	0/1208	0.67	0/1618
70	TT	0.30	0/1115	0.59	0/1493
71	UU	0.32	0/805	0.61	0/1081
72	VV	0.41	0/643	0.61	0/860
73	WW	0.48	0/1051	0.69	1/1406 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
74	XX	0.46	0/1116	0.64	1/1490 (0.1%)
75	YY	0.33	0/1028	0.56	0/1366
76	ZZ	0.31	0/604	0.69	0/810
77	aa	0.37	0/828	0.56	0/1109
78	bb	0.33	0/665	0.59	0/891
79	cc	0.32	0/490	0.61	0/656
80	dd	0.40	0/470	0.60	0/623
81	ee	0.36	0/447	0.54	0/587
82	ff	0.32	0/567	0.60	0/753
83	gg	0.32	0/2493	0.64	2/3394 (0.1%)
All	All	0.63	1/232799 (0.0%)	0.97	992/340171 (0.3%)

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
6	C	0	1
8	E	0	2
9	F	0	1
10	G	0	1
11	H	0	1
16	N	0	3
21	S	0	1
22	T	0	1
32	d	0	1
35	g	0	1
46	s	0	1
47	t	0	1
48	v	0	4
51	AA	0	2
54	DD	0	1
55	EE	0	1
56	FF	0	1
59	II	0	1
66	PP	0	1
69	SS	0	1
71	UU	0	1
72	VV	0	1
74	XX	0	1
83	gg	0	1
All	All	0	31

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	H	128	MET	C-N	-5.34	1.21	1.34

All (992) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	9	1116	C	N1-C2-O2	12.69	126.52	118.90
50	9	1116	C	C2-N1-C1'	11.86	131.84	118.80
1	5	4056	A	OP1-P-O3'	-11.48	79.94	105.20
50	9	501	C	N1-C2-O2	11.03	125.52	118.90
1	5	1429	C	N1-C2-O2	10.96	125.47	118.90
50	9	501	C	C2-N1-C1'	10.26	130.09	118.80
50	9	1116	C	N3-C2-O2	-10.15	114.80	121.90
50	9	356	C	N1-C2-O2	10.03	124.92	118.90
50	9	1453	C	N1-C2-O2	9.99	124.89	118.90
50	9	1016	U	N1-C2-O2	9.91	129.74	122.80
50	9	1453	C	C2-N1-C1'	9.86	129.65	118.80
50	9	1520	G	N3-C4-C5	-9.85	123.67	128.60
50	9	1139	C	N1-C2-O2	9.77	124.76	118.90
50	9	356	C	C2-N1-C1'	9.70	129.47	118.80
50	9	1016	U	C2-N1-C1'	9.65	129.28	117.70
1	5	3739	C	N1-C2-O2	9.63	124.68	118.90
1	5	217	C	N1-C2-O2	9.55	124.63	118.90
50	9	293	C	N1-C2-O2	9.50	124.60	118.90
1	5	220	C	N1-C2-O2	9.49	124.59	118.90
1	5	2814	C	N1-C2-O2	9.37	124.52	118.90
1	5	1977	C	N1-C2-O2	9.35	124.51	118.90
1	5	1639	U	C2-N1-C1'	9.33	128.90	117.70
1	5	3788	C	N1-C2-O2	9.28	124.47	118.90
1	5	2505	C	N3-C2-O2	-9.21	115.45	121.90
50	9	1139	C	N3-C2-O2	-9.18	115.47	121.90
50	9	1139	C	C2-N1-C1'	9.16	128.88	118.80
50	9	501	C	N3-C2-O2	-9.16	115.49	121.90
3	8	128	C	N1-C2-O2	9.12	124.37	118.90
50	9	1016	U	N3-C2-O2	-9.05	115.86	122.20
50	9	1303	C	N1-C2-O2	9.03	124.32	118.90
1	5	1381	U	N1-C2-O2	8.97	129.08	122.80
1	5	1236	C	C6-N1-C2	-8.81	116.78	120.30
1	5	2351	C	C6-N1-C2	-8.81	116.78	120.30
1	5	2505	C	C6-N1-C2	-8.79	116.78	120.30
1	5	1429	C	N3-C2-O2	-8.79	115.75	121.90
50	9	1303	C	C2-N1-C1'	8.68	128.34	118.80
1	5	115	C	N1-C2-O2	8.67	124.10	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	4880	C	C2-N1-C1'	8.64	128.30	118.80
1	5	2814	C	N3-C2-O2	-8.59	115.88	121.90
1	5	2274	C	C5-C6-N1	8.58	125.29	121.00
50	9	1292	C	N1-C2-O2	8.55	124.03	118.90
1	5	1381	U	N3-C2-O2	-8.51	116.25	122.20
1	5	1483	C	N1-C2-O2	8.46	123.98	118.90
1	5	4056	A	OP2-P-O3'	-8.45	86.61	105.20
1	5	112	C	C2-N1-C1'	8.40	128.04	118.80
1	5	4928	C	N1-C2-O2	8.39	123.94	118.90
1	5	217	C	C2-N1-C1'	8.39	128.03	118.80
1	5	4241	C	N1-C2-O2	8.38	123.93	118.90
1	5	2505	C	N1-C2-O2	8.36	123.92	118.90
50	9	1116	C	C6-N1-C1'	-8.35	110.78	120.80
1	5	332	C	N1-C2-O2	8.32	123.89	118.90
50	9	194	C	N3-C2-O2	-8.32	116.08	121.90
1	5	2325	C	C6-N1-C2	-8.27	116.99	120.30
1	5	4759	C	N1-C2-O2	8.25	123.85	118.90
50	9	1520	G	C8-N9-C4	-8.22	103.11	106.40
1	5	1612	G	N3-C4-N9	8.20	130.92	126.00
50	9	501	C	C6-N1-C2	-8.11	117.06	120.30
1	5	1381	U	C2-N1-C1'	8.08	127.40	117.70
1	5	1429	C	C2-N1-C1'	8.08	127.69	118.80
50	9	1242	U	N1-C2-O2	8.06	128.44	122.80
1	5	2627	C	N1-C2-O2	8.05	123.73	118.90
50	9	1624	U	C2-N1-C1'	8.05	127.36	117.70
1	5	4254	G	N3-C4-C5	-7.98	124.61	128.60
50	9	1520	G	C4-N9-C1'	7.96	136.85	126.50
50	9	293	C	N3-C2-O2	-7.94	116.34	121.90
1	5	115	C	C2-N1-C1'	7.93	127.53	118.80
50	9	356	C	N3-C2-O2	-7.91	116.36	121.90
1	5	1977	C	C2-N1-C1'	7.88	127.47	118.80
50	9	1535	U	C2-N1-C1'	7.88	127.15	117.70
1	5	4752	U	N1-C2-O2	7.86	128.30	122.80
3	8	128	C	N3-C2-O2	-7.84	116.41	121.90
1	5	3788	C	N3-C2-O2	-7.83	116.42	121.90
1	5	2819	U	N3-C2-O2	-7.82	116.73	122.20
50	9	914	U	C2-N1-C1'	7.82	127.08	117.70
1	5	3739	C	N3-C2-O2	-7.81	116.44	121.90
50	9	1520	G	C2-N3-C4	7.80	115.80	111.90
1	5	3911	C	C5-C6-N1	7.77	124.89	121.00
1	5	4928	C	C2-N1-C1'	7.77	127.34	118.80
1	5	4709	U	N1-C2-O2	7.77	128.24	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	4119	C	C2-N1-C1'	7.76	127.33	118.80
1	5	100	C	C2-N1-C1'	7.75	127.32	118.80
50	9	1453	C	N3-C2-O2	-7.72	116.49	121.90
1	5	1084	C	C2-N1-C1'	7.72	127.29	118.80
1	5	4714	C	N1-C2-O2	7.70	123.52	118.90
1	5	2008	U	N3-C2-O2	-7.67	116.83	122.20
2	7	29	C	N1-C2-O2	7.67	123.50	118.90
50	9	801	U	N3-C2-O2	-7.64	116.85	122.20
1	5	4502	C	N1-C2-O2	7.62	123.47	118.90
1	5	4869	U	N3-C2-O2	-7.62	116.87	122.20
50	9	183	G	C2-N3-C4	7.62	115.71	111.90
1	5	1445	U	C5-C6-N1	7.58	126.49	122.70
1	5	4653	C	C6-N1-C2	-7.55	117.28	120.30
50	9	1315	U	N3-C2-O2	-7.54	116.92	122.20
1	5	4759	C	C2-N1-C1'	7.54	127.09	118.80
57	GG	68	LEU	CA-CB-CG	7.53	132.62	115.30
1	5	1210	C	N1-C2-O2	7.53	123.42	118.90
50	9	1389	C	N1-C2-O2	7.51	123.41	118.90
1	5	4241	C	N3-C2-O2	-7.50	116.65	121.90
1	5	3739	C	C2-N1-C1'	7.49	127.04	118.80
1	5	4653	C	C5-C6-N1	7.47	124.73	121.00
50	9	853	C	C2-N1-C1'	7.45	127.00	118.80
52	BB	219	LYS	C-N-CA	7.45	140.33	121.70
47	t	144	ASP	CB-CG-OD1	7.45	125.00	118.30
1	5	4752	U	N3-C2-O2	-7.44	116.99	122.20
50	9	801	U	N1-C2-O2	7.43	128.00	122.80
50	9	369	C	C2-N1-C1'	7.42	126.96	118.80
1	5	4880	C	N1-C2-O2	7.41	123.35	118.90
1	5	4930	C	C2-N1-C1'	7.41	126.95	118.80
50	9	356	C	C6-N1-C1'	-7.40	111.92	120.80
50	9	1261	C	N1-C2-O2	7.37	123.32	118.90
50	9	1123	C	C2-N1-C1'	7.35	126.89	118.80
1	5	4709	U	N3-C2-O2	-7.33	117.07	122.20
3	8	119	C	N1-C2-O2	7.32	123.29	118.90
1	5	2410	C	C2-N1-C1'	7.32	126.85	118.80
50	9	293	C	C2-N1-C1'	7.32	126.85	118.80
1	5	126	C	C6-N1-C2	-7.31	117.38	120.30
50	9	1116	C	C6-N1-C2	-7.30	117.38	120.30
1	5	1483	C	N3-C2-O2	-7.29	116.80	121.90
1	5	1893	C	C2-N1-C1'	7.28	126.81	118.80
50	9	369	C	N1-C2-O2	7.25	123.25	118.90
50	9	1396	A	O4'-C1'-N9	7.24	113.99	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	217	C	N3-C2-O2	-7.22	116.85	121.90
1	5	1812	C	C2-N1-C1'	7.21	126.73	118.80
1	5	2274	C	C6-N1-C2	-7.21	117.41	120.30
1	5	4057	C	OP1-P-OP2	7.21	130.42	119.60
50	9	632	C	C6-N1-C2	-7.21	117.42	120.30
1	5	1834	U	C2-N1-C1'	7.21	126.35	117.70
1	5	1411	C	N1-C2-O2	7.20	123.22	118.90
1	5	1977	C	N3-C2-O2	-7.20	116.86	121.90
1	5	2814	C	C2-N1-C1'	7.20	126.72	118.80
1	5	4759	C	N3-C2-O2	-7.18	116.87	121.90
1	5	332	C	N3-C2-O2	-7.18	116.87	121.90
1	5	2568	C	C2-N1-C1'	7.18	126.70	118.80
50	9	570	C	N1-C2-O2	7.18	123.20	118.90
50	9	579	C	N1-C2-O2	7.14	123.18	118.90
1	5	481	G	C4-N9-C1'	7.13	135.77	126.50
1	5	1792	U	N3-C2-O2	-7.12	117.21	122.20
61	KK	35	LEU	CA-CB-CG	7.11	131.66	115.30
1	5	3636	C	N3-C2-O2	-7.11	116.92	121.90
1	5	4266	G	N3-C4-C5	-7.11	125.05	128.60
1	5	1978	C	C2-N1-C1'	7.10	126.61	118.80
1	5	2627	C	N3-C2-O2	-7.09	116.93	121.90
1	5	2046	G	P-O3'-C3'	7.08	128.20	119.70
50	9	914	U	N1-C2-O2	7.08	127.75	122.80
1	5	1656	U	N3-C2-O2	-7.05	117.26	122.20
1	5	2819	U	N1-C2-O2	7.05	127.74	122.80
1	5	115	C	N3-C2-O2	-7.05	116.97	121.90
1	5	2695	A	P-O3'-C3'	7.05	128.16	119.70
1	5	100	C	N1-C2-O2	7.03	123.12	118.90
50	9	1242	U	C2-N1-C1'	7.00	126.10	117.70
1	5	2008	U	N1-C2-O2	7.00	127.70	122.80
50	9	1277	C	C5-C6-N1	6.99	124.50	121.00
1	5	205	C	N1-C2-O2	6.98	123.09	118.90
50	9	1756	C	C2-N1-C1'	6.98	126.48	118.80
1	5	4709	U	C2-N1-C1'	6.97	126.06	117.70
52	BB	34	LYS	C-N-CA	6.97	139.12	121.70
1	5	2627	C	C6-N1-C2	-6.96	117.51	120.30
50	9	1520	G	N3-C4-N9	6.96	130.18	126.00
50	9	1595	U	N1-C2-O2	6.96	127.67	122.80
1	5	4360	U	N3-C2-O2	-6.95	117.34	122.20
1	5	4925	U	P-O3'-C3'	6.95	128.04	119.70
1	5	4948	C	C2-N1-C1'	6.90	126.39	118.80
1	5	1792	U	N1-C2-O2	6.90	127.63	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	4557	U	N3-C2-O2	-6.90	117.37	122.20
1	5	4695	C	N1-C2-O2	6.90	123.04	118.90
3	8	141	C	C6-N1-C2	-6.89	117.54	120.30
50	9	1242	U	N3-C2-O2	-6.89	117.38	122.20
1	5	1612	G	C4-N9-C1'	6.87	135.43	126.50
1	5	4286	C	N1-C2-O2	6.87	123.02	118.90
1	5	3876	A	P-O3'-C3'	6.86	127.94	119.70
50	9	1331	C	N1-C2-O2	6.86	123.02	118.90
50	9	1595	U	N3-C2-O2	-6.86	117.40	122.20
50	9	1660	C	C2-N1-C1'	6.86	126.34	118.80
1	5	3657	U	N3-C2-O2	-6.85	117.41	122.20
1	5	1483	C	C2-N1-C1'	6.85	126.33	118.80
1	5	1236	C	C5-C6-N1	6.84	124.42	121.00
1	5	1686	C	C6-N1-C2	-6.84	117.57	120.30
1	5	1966	C	C5-C6-N1	6.83	124.41	121.00
1	5	4869	U	C2-N1-C1'	6.82	125.89	117.70
1	5	4266	G	N3-C4-N9	6.81	130.09	126.00
1	5	1777	C	C2-N1-C1'	6.81	126.29	118.80
1	5	2351	C	C5-C6-N1	6.81	124.40	121.00
5	B	214	ASP	CB-CG-OD1	6.80	124.42	118.30
1	5	1484	G	N3-C4-C5	-6.80	125.20	128.60
50	9	1389	C	C2-N1-C1'	6.80	126.28	118.80
50	9	1315	U	N1-C2-O2	6.79	127.56	122.80
50	9	1453	C	C6-N1-C1'	-6.79	112.65	120.80
1	5	2325	C	C5-C6-N1	6.78	124.39	121.00
50	9	188	C	C2-N1-C1'	6.76	126.24	118.80
50	9	18	C	C5-C6-N1	6.76	124.38	121.00
1	5	77	U	N3-C2-O2	-6.76	117.47	122.20
1	5	4859	C	N1-C2-O2	6.76	122.96	118.90
50	9	183	G	N3-C4-C5	-6.75	125.22	128.60
1	5	4065	G	P-O3'-C3'	6.75	127.80	119.70
50	9	1117	C	N1-C2-O2	6.74	122.94	118.90
56	FF	27	ASP	CB-CG-OD1	6.74	124.37	118.30
1	5	1484	G	N3-C4-N9	6.74	130.04	126.00
50	9	1595	U	C2-N1-C1'	6.74	125.79	117.70
1	5	2351	C	N1-C2-O2	6.73	122.94	118.90
1	5	1671	U	N3-C2-O2	-6.73	117.49	122.20
1	5	2274	C	C2-N1-C1'	6.73	126.20	118.80
1	5	661	C	C6-N1-C2	-6.73	117.61	120.30
1	5	2704	C	C2-N1-C1'	6.73	126.20	118.80
3	8	111	U	N1-C2-O2	6.72	127.51	122.80
1	5	2539	C	C6-N1-C2	-6.72	117.61	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	4880	C	C6-N1-C1'	-6.72	112.74	120.80
2	7	67	C	C6-N1-C2	-6.72	117.61	120.30
20	R	138	LEU	CA-CB-CG	6.70	130.72	115.30
1	5	1612	G	C8-N9-C1'	-6.70	118.29	127.00
1	5	4928	C	N3-C2-O2	-6.70	117.21	121.90
1	5	220	C	C2-N1-C1'	6.69	126.16	118.80
1	5	4162	C	N3-C2-O2	-6.69	117.22	121.90
50	9	801	U	C2-N1-C1'	6.68	125.72	117.70
1	5	4162	C	C2-N1-C1'	6.68	126.14	118.80
50	9	501	C	C6-N1-C1'	-6.68	112.79	120.80
50	9	876	C	N1-C2-O2	6.68	122.91	118.90
1	5	1966	C	C6-N1-C2	-6.67	117.63	120.30
1	5	4314	C	N1-C2-O2	6.67	122.90	118.90
1	5	4926	C	C2-N1-C1'	6.67	126.14	118.80
1	5	481	G	N3-C4-N9	6.67	130.00	126.00
1	5	4758	U	N1-C2-O2	6.67	127.47	122.80
50	9	17	C	C6-N1-C2	-6.66	117.64	120.30
1	5	112	C	N1-C2-O2	6.65	122.89	118.90
1	5	1663	C	C5-C6-N1	6.65	124.33	121.00
50	9	1303	C	C6-N1-C1'	-6.65	112.82	120.80
1	5	100	C	N3-C2-O2	-6.64	117.25	121.90
1	5	4119	C	N1-C2-O2	6.64	122.88	118.90
1	5	4423	U	C2-N1-C1'	6.64	125.66	117.70
50	9	1535	U	N1-C2-O2	6.63	127.44	122.80
1	5	2502	A	P-O3'-C3'	6.62	127.65	119.70
2	7	102	U	N1-C2-O2	6.62	127.44	122.80
1	5	1325	C	N3-C2-O2	-6.62	117.26	121.90
50	9	914	U	N3-C2-O2	-6.62	117.56	122.20
50	9	876	C	C2-N1-C1'	6.62	126.08	118.80
50	9	618	C	O5'-P-OP1	-6.62	99.75	105.70
1	5	1485	C	C2-N1-C1'	6.61	126.08	118.80
3	8	64	U	N3-C2-O2	-6.60	117.58	122.20
1	5	4766	C	N1-C2-O2	6.59	122.85	118.90
1	5	220	C	N3-C2-O2	-6.58	117.29	121.90
1	5	4758	U	C2-N1-C1'	6.58	125.60	117.70
1	5	4906	C	N1-C2-O2	6.57	122.84	118.90
50	9	340	C	N1-C2-O2	6.57	122.84	118.90
1	5	4162	C	N1-C2-O2	6.55	122.83	118.90
50	9	570	C	N3-C2-O2	-6.54	117.32	121.90
1	5	4237	C	C5-C6-N1	6.54	124.27	121.00
1	5	4423	U	N3-C2-O2	-6.54	117.62	122.20
1	5	1485	C	N1-C2-O2	6.54	122.82	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	1210	C	C2-N1-C1'	6.53	125.99	118.80
1	5	1568	C	C2-N1-C1'	6.53	125.98	118.80
1	5	2325	C	C2-N1-C1'	6.53	125.98	118.80
1	5	3657	U	C2-N1-C1'	6.52	125.53	117.70
1	5	4502	C	C6-N1-C2	-6.51	117.70	120.30
50	9	1453	C	C6-N1-C2	-6.51	117.70	120.30
50	9	1303	C	N3-C2-O2	-6.50	117.35	121.90
1	5	1072	C	P-O3'-C3'	6.50	127.50	119.70
1	5	1193	C	C2-N1-C1'	6.50	125.95	118.80
50	9	1292	C	N3-C2-O2	-6.50	117.35	121.90
1	5	1656	U	N1-C2-O2	6.49	127.34	122.80
1	5	1882	U	C5-C4-O4	-6.49	122.01	125.90
1	5	1309	C	C5-C6-N1	6.48	124.24	121.00
1	5	4758	U	N3-C2-O2	-6.48	117.66	122.20
50	9	752	G	P-O3'-C3'	6.48	127.48	119.70
50	9	1172	U	N1-C2-O2	6.48	127.33	122.80
3	8	141	C	C5-C6-N1	6.48	124.24	121.00
50	9	319	C	O5'-P-OP1	6.47	118.47	110.70
50	9	1453	C	C5-C6-N1	6.47	124.24	121.00
50	9	1592	C	N3-C2-O2	-6.47	117.37	121.90
1	5	1834	U	N1-C2-O2	6.47	127.33	122.80
1	5	472	C	C2-N1-C1'	6.46	125.91	118.80
1	5	167	C	C2-N1-C1'	6.46	125.91	118.80
1	5	1671	U	N1-C2-O2	6.46	127.32	122.80
1	5	2820	C	N1-C2-O2	6.46	122.78	118.90
67	QQ	47	LEU	CA-CB-CG	6.45	130.14	115.30
1	5	2362	U	C2-N1-C1'	6.45	125.44	117.70
50	9	1395	C	OP1-P-O3'	6.45	119.39	105.20
1	5	661	C	C2-N1-C1'	6.45	125.89	118.80
50	9	1624	U	N1-C2-O2	6.45	127.31	122.80
1	5	4502	C	N3-C2-O2	-6.44	117.39	121.90
50	9	4	C	C5-C6-N1	6.43	124.22	121.00
1	5	1639	U	N1-C2-O2	6.43	127.30	122.80
1	5	1834	U	N3-C2-O2	-6.43	117.70	122.20
1	5	481	G	N3-C4-C5	-6.43	125.39	128.60
1	5	472	C	N1-C2-O2	6.42	122.75	118.90
50	9	1606	G	O4'-C1'-N9	6.42	113.34	108.20
1	5	1514	U	C2-N1-C1'	6.40	125.38	117.70
2	7	29	C	N3-C2-O2	-6.40	117.42	121.90
1	5	1308	C	C6-N1-C2	-6.39	117.74	120.30
50	9	1750	C	N1-C2-O2	6.39	122.74	118.90
1	5	1481	C	N1-C2-O2	6.39	122.73	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	4237	C	C6-N1-C2	-6.39	117.74	120.30
1	5	3778	U	N3-C2-O2	-6.39	117.73	122.20
50	9	1139	C	C6-N1-C2	-6.39	117.75	120.30
50	9	632	C	C5-C6-N1	6.38	124.19	121.00
1	5	1468	C	C6-N1-C2	-6.38	117.75	120.30
1	5	4254	G	C2-N3-C4	6.38	115.09	111.90
50	9	1123	C	C6-N1-C2	-6.38	117.75	120.30
50	9	4	C	C2-N1-C1'	6.38	125.81	118.80
1	5	2661	U	P-O3'-C3'	6.37	127.34	119.70
50	9	1412	C	C6-N1-C2	-6.35	117.76	120.30
3	8	119	C	N3-C2-O2	-6.35	117.45	121.90
1	5	1484	G	C4-N9-C1'	6.35	134.75	126.50
1	5	2351	C	N3-C2-O2	-6.34	117.46	121.90
1	5	322	C	N1-C2-O2	6.33	122.70	118.90
1	5	2072	C	C6-N1-C2	-6.33	117.77	120.30
1	5	2351	C	C2-N1-C1'	6.33	125.76	118.80
5	B	180	LEU	CA-CB-CG	6.33	129.85	115.30
1	5	2410	C	C5-C6-N1	6.33	124.16	121.00
1	5	1309	C	C6-N1-C2	-6.32	117.77	120.30
1	5	3739	C	C6-N1-C2	-6.32	117.77	120.30
1	5	1514	U	N3-C2-O2	-6.32	117.78	122.20
50	9	853	C	N3-C2-O2	-6.31	117.48	121.90
1	5	1686	C	N3-C2-O2	-6.30	117.49	121.90
1	5	2856	C	N1-C2-O2	6.30	122.68	118.90
1	5	3636	C	C6-N1-C2	-6.30	117.78	120.30
50	9	1637	A	P-O3'-C3'	6.30	127.25	119.70
1	5	2704	C	C5-C6-N1	6.29	124.14	121.00
1	5	4557	U	N1-C2-O2	6.27	127.19	122.80
1	5	1792	U	C2-N1-C1'	6.27	125.23	117.70
50	9	853	C	N1-C2-O2	6.27	122.66	118.90
50	9	1261	C	N3-C2-O2	-6.27	117.51	121.90
1	5	4232	U	P-O3'-C3'	6.27	127.22	119.70
55	EE	20	LEU	CA-CB-CG	6.26	129.70	115.30
50	9	1057	C	C2-N1-C1'	6.26	125.68	118.80
50	9	734	C	C2-N1-C1'	6.25	125.68	118.80
1	5	1612	G	C6-C5-N7	-6.25	126.65	130.40
1	5	4476	C	N3-C2-O2	-6.25	117.53	121.90
1	5	1329	G	C8-N9-C4	-6.24	103.90	106.40
1	5	1990	A	P-O3'-C3'	6.24	127.19	119.70
50	9	402	C	N1-C2-O2	6.24	122.64	118.90
50	9	1016	U	C6-N1-C1'	-6.24	112.47	121.20
1	5	2553	A	O4'-C1'-N9	6.23	113.19	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	1639	U	C6-N1-C1'	-6.23	112.48	121.20
1	5	3778	U	N1-C2-O2	6.22	127.16	122.80
50	9	688	U	P-O3'-C3'	6.22	127.17	119.70
50	9	930	C	N1-C2-O2	6.22	122.63	118.90
1	5	4926	C	N1-C2-O2	6.21	122.63	118.90
50	9	1739	C	N1-C2-O2	6.21	122.63	118.90
50	9	887	U	C2-N1-C1'	6.21	125.15	117.70
3	8	111	U	N3-C2-O2	-6.20	117.86	122.20
1	5	112	C	C6-N1-C2	-6.20	117.82	120.30
1	5	2532	C	C2-N1-C1'	6.20	125.62	118.80
50	9	1139	C	C6-N1-C1'	-6.20	113.36	120.80
48	v	320	ASP	CB-CG-OD1	6.20	123.88	118.30
50	9	1277	C	C6-N1-C2	-6.19	117.82	120.30
1	5	1289	C	C6-N1-C2	-6.19	117.82	120.30
83	gg	89	LEU	CA-CB-CG	6.19	129.54	115.30
1	5	4682	U	N1-C2-O2	6.18	127.13	122.80
1	5	323	C	C2-N1-C1'	6.18	125.60	118.80
1	5	4075	U	OP1-P-O3'	6.18	118.80	105.20
1	5	4880	C	N3-C2-O2	-6.18	117.57	121.90
48	v	444	LEU	CA-CB-CG	6.18	129.51	115.30
73	WW	69	LEU	CA-CB-CG	6.18	129.51	115.30
1	5	688	U	N3-C2-O2	-6.17	117.88	122.20
1	5	4601	U	N3-C2-O2	-6.17	117.88	122.20
48	v	851	LEU	CA-CB-CG	6.17	129.49	115.30
1	5	4350	C	C2-N1-C1'	6.17	125.58	118.80
1	5	4682	U	N3-C2-O2	-6.16	117.89	122.20
1	5	484	U	N1-C2-O2	6.16	127.11	122.80
1	5	4286	C	C2-N1-C1'	6.16	125.58	118.80
1	5	4254	G	P-O3'-C3'	6.16	127.09	119.70
1	5	1084	C	C5-C6-N1	6.16	124.08	121.00
1	5	1639	U	N3-C2-O2	-6.15	117.90	122.20
3	8	35	C	C6-N1-C2	-6.15	117.84	120.30
1	5	4413	C	N1-C2-O2	6.14	122.59	118.90
50	9	1078	C	C2-N1-C1'	6.14	125.56	118.80
50	9	1396	A	O5'-P-OP1	-6.14	100.17	105.70
6	C	150	LEU	CB-CG-CD2	-6.14	100.56	111.00
1	5	4413	C	C2-N1-C1'	6.14	125.55	118.80
1	5	3788	C	C2-N1-C1'	6.13	125.55	118.80
1	5	4667	C	C6-N1-C2	-6.13	117.85	120.30
3	8	90	C	C2-N1-C1'	6.13	125.54	118.80
1	5	517	C	C5-C6-N1	6.12	124.06	121.00
1	5	941	C	C2-N1-C1'	6.12	125.53	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	9	162	C	C6-N1-C2	-6.12	117.85	120.30
50	9	303	C	N1-C2-O2	6.12	122.57	118.90
2	7	29	C	C2-N1-C1'	6.11	125.52	118.80
2	7	102	U	N3-C2-O2	-6.11	117.92	122.20
50	9	1389	C	N3-C2-O2	-6.11	117.62	121.90
1	5	2072	C	C5-C6-N1	6.11	124.05	121.00
50	9	314	U	N3-C2-O2	-6.10	117.93	122.20
1	5	406	C	P-O3'-C3'	6.10	127.02	119.70
1	5	1210	C	N3-C2-O2	-6.10	117.63	121.90
1	5	1666	C	C6-N1-C2	-6.09	117.86	120.30
1	5	481	G	C8-N9-C1'	-6.09	119.08	127.00
50	9	479	C	P-O3'-C3'	6.09	127.00	119.70
50	9	1116	C	C5-C6-N1	6.09	124.04	121.00
50	9	1624	U	N3-C2-O2	-6.08	117.94	122.20
1	5	4266	G	C4-N9-C1'	6.08	134.41	126.50
1	5	1807	C	C2-N1-C1'	6.08	125.49	118.80
50	9	887	U	N1-C2-O2	6.08	127.06	122.80
1	5	1276	C	C6-N1-C2	-6.08	117.87	120.30
50	9	1520	G	N7-C8-N9	6.08	116.14	113.10
1	5	4303	C	N3-C2-O2	-6.07	117.65	121.90
50	9	1123	C	C5-C6-N1	6.07	124.04	121.00
1	5	1882	U	N3-C4-O4	6.07	123.65	119.40
50	9	501	C	C5-C6-N1	6.07	124.03	121.00
50	9	199	C	N1-C2-O2	6.06	122.54	118.90
1	5	1607	C	N1-C2-O2	6.06	122.53	118.90
50	9	531	A	OP1-P-O3'	6.06	118.53	105.20
1	5	1735	U	N1-C2-O2	6.05	127.04	122.80
1	5	5047	C	N3-C2-O2	-6.05	117.66	121.90
50	9	870	A	P-O3'-C3'	6.04	126.95	119.70
50	9	1123	C	N1-C2-O2	6.04	122.53	118.90
1	5	4560	C	C2-N1-C1'	6.03	125.44	118.80
52	BB	207	LEU	CA-CB-CG	6.03	129.18	115.30
1	5	1325	C	N1-C2-O2	6.03	122.52	118.90
1	5	1777	C	N1-C2-O2	6.02	122.51	118.90
1	5	2639	U	C2-N1-C1'	6.02	124.92	117.70
1	5	203	U	C2-N1-C1'	6.01	124.91	117.70
1	5	2528	G	C4-N9-C1'	6.01	134.31	126.50
3	8	21	C	C6-N1-C2	-6.00	117.90	120.30
1	5	1686	C	N1-C2-O2	6.00	122.50	118.90
1	5	3904	G	P-O3'-C3'	6.00	126.90	119.70
50	9	570	C	C2-N1-C1'	6.00	125.40	118.80
24	V	49	LEU	CA-CB-CG	6.00	129.09	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	2740	U	C2-N1-C1'	5.99	124.89	117.70
1	5	3778	U	C2-N1-C1'	5.99	124.89	117.70
1	5	1726	U	N3-C2-O2	-5.99	118.01	122.20
1	5	4928	C	C6-N1-C1'	-5.99	113.61	120.80
1	5	4075	U	P-O3'-C3'	5.98	126.88	119.70
1	5	4563	U	C5-C6-N1	5.98	125.69	122.70
50	9	1292	C	C6-N1-C2	-5.98	117.91	120.30
1	5	1893	C	C5-C6-N1	5.97	123.99	121.00
2	7	67	C	C5-C6-N1	5.97	123.98	121.00
1	5	2410	C	C6-N1-C2	-5.97	117.91	120.30
1	5	3709	U	O4'-C1'-N1	5.96	112.97	108.20
2	7	28	C	N1-C2-O2	5.96	122.48	118.90
50	9	124	U	N3-C2-O2	-5.96	118.03	122.20
1	5	517	C	C6-N1-C2	-5.96	117.92	120.30
3	8	111	U	C2-N1-C1'	5.96	124.85	117.70
1	5	2474	G	P-O3'-C3'	5.96	126.85	119.70
1	5	1598	C	N1-C2-O2	5.95	122.47	118.90
1	5	2627	C	C2-N1-C1'	5.95	125.34	118.80
1	5	2008	U	C2-N1-C1'	5.94	124.83	117.70
1	5	4243	C	C2-N1-C1'	5.94	125.33	118.80
13	J	33	LEU	CA-CB-CG	5.94	128.96	115.30
50	9	1535	U	N3-C2-O2	-5.93	118.05	122.20
1	5	1084	C	N1-C2-O2	5.93	122.46	118.90
50	9	630	U	C2-N1-C1'	5.92	124.81	117.70
1	5	4314	C	C6-N1-C2	-5.92	117.93	120.30
1	5	4719	G	OP1-P-O3'	5.92	118.22	105.20
1	5	1809	C	C6-N1-C2	-5.92	117.93	120.30
1	5	1929	A	C2-N3-C4	5.92	113.56	110.60
1	5	1809	C	C2-N1-C1'	5.91	125.30	118.80
1	5	1978	C	C5-C6-N1	5.91	123.96	121.00
50	9	914	U	C6-N1-C1'	-5.91	112.93	121.20
1	5	4752	U	C2-N1-C1'	5.91	124.79	117.70
1	5	2716	C	C6-N1-C2	-5.91	117.94	120.30
1	5	3673	C	N1-C2-O2	5.91	122.44	118.90
50	9	1261	C	C2-N1-C1'	5.91	125.30	118.80
1	5	4206	C	C2-N1-C1'	5.90	125.29	118.80
33	e	129	LEU	CA-CB-CG	5.90	128.88	115.30
50	9	632	C	C2-N1-C1'	5.90	125.29	118.80
1	5	2474	G	OP1-P-O3'	5.90	118.18	105.20
1	5	1514	U	N1-C2-O2	5.90	126.93	122.80
1	5	2716	C	N1-C2-O2	5.89	122.44	118.90
50	9	1660	C	N1-C2-O2	5.89	122.44	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	134	G	P-O3'-C3'	5.89	126.77	119.70
50	9	124	U	N1-C2-O2	5.89	126.92	122.80
57	GG	185	LEU	CA-CB-CG	5.89	128.85	115.30
48	v	420	LEU	CA-CB-CG	5.89	128.84	115.30
1	5	1237	C	C6-N1-C2	-5.88	117.95	120.30
1	5	1987	C	N1-C2-O2	5.88	122.43	118.90
1	5	2089	G	P-O3'-C3'	5.88	126.76	119.70
1	5	220	C	C5-C6-N1	5.88	123.94	121.00
1	5	77	U	N1-C2-O2	5.88	126.91	122.80
50	9	1395	C	P-O3'-C3'	5.87	126.74	119.70
1	5	3709	U	C2-N1-C1'	5.87	124.74	117.70
1	5	1807	C	N1-C2-O2	5.87	122.42	118.90
50	9	579	C	N3-C2-O2	-5.87	117.80	121.90
50	9	402	C	C6-N1-C2	-5.86	117.96	120.30
1	5	323	C	C6-N1-C2	-5.86	117.96	120.30
1	5	4206	C	C6-N1-C2	-5.86	117.96	120.30
1	5	4714	C	N3-C2-O2	-5.85	117.81	121.90
1	5	1597	G	N1-C6-O6	-5.85	116.39	119.90
1	5	1822	U	N1-C2-O2	5.84	126.89	122.80
37	i	33	LEU	CA-CB-CG	5.84	128.74	115.30
1	5	1974	U	C5-C4-O4	-5.84	122.39	125.90
1	5	4493	U	N3-C2-O2	-5.84	118.11	122.20
1	5	3636	C	N1-C2-O2	5.84	122.41	118.90
50	9	1756	C	C6-N1-C2	-5.84	117.96	120.30
1	5	2362	U	N1-C2-O2	5.84	126.89	122.80
1	5	4695	C	N3-C2-O2	-5.84	117.81	121.90
1	5	217	C	C6-N1-C2	-5.84	117.97	120.30
1	5	3954	A	P-O3'-C3'	5.84	126.70	119.70
1	5	1179	U	N1-C2-O2	5.83	126.88	122.80
50	9	1535	U	C5-C6-N1	5.83	125.61	122.70
48	v	143	LEU	CA-CB-CG	5.83	128.71	115.30
1	5	449	C	P-O3'-C3'	5.82	126.69	119.70
3	8	123	U	N1-C2-O2	5.82	126.87	122.80
1	5	1612	G	C4-C5-N7	5.82	113.13	110.80
1	5	1847	C	C5-C6-N1	5.81	123.91	121.00
50	9	1230	C	C5-C6-N1	5.81	123.91	121.00
1	5	4476	C	N1-C2-O2	5.81	122.39	118.90
3	8	119	C	C2-N1-C1'	5.81	125.19	118.80
1	5	1671	U	C2-N1-C1'	5.81	124.67	117.70
1	5	3739	C	C5-C6-N1	5.81	123.91	121.00
1	5	4360	U	N1-C2-O2	5.81	126.87	122.80
3	8	124	U	P-O3'-C3'	5.80	126.67	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	9	293	C	C6-N1-C2	-5.80	117.98	120.30
1	5	1370	G	P-O3'-C3'	5.80	126.66	119.70
1	5	688	U	N1-C2-O2	5.80	126.86	122.80
50	9	1172	U	N3-C2-O2	-5.79	118.14	122.20
50	9	1277	C	C2-N1-C1'	5.79	125.17	118.80
1	5	661	C	C5-C6-N1	5.79	123.89	121.00
1	5	417	G	O4'-C1'-N9	5.79	112.83	108.20
1	5	112	C	C5-C6-N1	5.78	123.89	121.00
1	5	337	U	N3-C2-O2	-5.78	118.15	122.20
1	5	2704	C	N1-C2-O2	5.78	122.37	118.90
1	5	1853	G	C4-N9-C1'	5.78	134.01	126.50
1	5	4303	C	C2-N1-C1'	5.78	125.16	118.80
50	9	303	C	C6-N1-C2	-5.78	117.99	120.30
1	5	100	C	C6-N1-C2	-5.77	117.99	120.30
1	5	1340	C	C5-C6-N1	5.77	123.89	121.00
1	5	1963	C	N1-C2-O2	5.77	122.36	118.90
1	5	1791	U	N1-C2-O2	5.77	126.84	122.80
1	5	2705	G	C4-N9-C1'	5.77	134.00	126.50
1	5	1411	C	C6-N1-C2	-5.77	117.99	120.30
1	5	2568	C	N1-C2-O2	5.76	122.36	118.90
3	8	21	C	N1-C2-O2	5.76	122.36	118.90
1	5	2410	C	N1-C2-O2	5.76	122.36	118.90
1	5	1411	C	C2-N1-C1'	5.75	125.13	118.80
1	5	23	C	C6-N1-C2	-5.75	118.00	120.30
1	5	4859	C	N3-C2-O2	-5.75	117.87	121.90
1	5	2266	C	P-O3'-C3'	5.75	126.60	119.70
50	9	1624	U	O4'-C1'-N1	5.75	112.80	108.20
1	5	4922	C	C6-N1-C2	-5.74	118.00	120.30
1	5	2532	C	C5-C6-N1	5.74	123.87	121.00
1	5	1179	U	C2-N1-C1'	5.73	124.58	117.70
1	5	4862	G	N1-C6-O6	-5.73	116.46	119.90
1	5	4869	U	C6-N1-C2	-5.73	117.56	121.00
1	5	1804	A	P-O3'-C3'	5.73	126.57	119.70
50	9	1725	U	C2-N1-C1'	5.73	124.57	117.70
1	5	1612	G	N3-C4-C5	-5.72	125.74	128.60
1	5	217	C	P-O3'-C3'	5.72	126.56	119.70
1	5	4766	C	N3-C2-O2	-5.72	117.90	121.90
1	5	282	C	N1-C2-O2	5.72	122.33	118.90
50	9	853	C	C6-N1-C2	-5.71	118.02	120.30
50	9	194	C	N1-C2-O2	5.71	122.33	118.90
1	5	2860	C	C6-N1-C2	-5.70	118.02	120.30
50	9	1172	U	C2-N1-C1'	5.70	124.54	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	1578	U	N3-C2-O2	-5.70	118.21	122.20
1	5	1445	U	C2-N1-C1'	5.69	124.53	117.70
1	5	1812	C	N1-C2-O2	5.69	122.31	118.90
50	9	1060	A	O4'-C1'-N9	5.69	112.75	108.20
50	9	577	U	N3-C2-O2	-5.69	118.22	122.20
1	5	4286	C	N3-C2-O2	-5.69	117.92	121.90
1	5	4949	G	O4'-C1'-N9	5.68	112.75	108.20
50	9	1649	U	N1-C2-O2	5.68	126.78	122.80
1	5	1671	U	C5-C6-N1	5.68	125.54	122.70
1	5	4254	G	N3-C4-N9	5.68	129.41	126.00
40	1	49	LEU	CA-CB-CG	5.68	128.36	115.30
1	5	1633	G	P-O3'-C3'	5.68	126.51	119.70
1	5	1929	A	C4-N9-C1'	5.67	136.51	126.30
1	5	112	C	C6-N1-C1'	-5.67	114.00	120.80
1	5	4051	C	N1-C2-O2	5.67	122.30	118.90
55	EE	256	LEU	CA-CB-CG	5.67	128.33	115.30
50	9	124	U	C2-N1-C1'	5.66	124.49	117.70
1	5	217	C	C6-N1-C1'	-5.66	114.01	120.80
1	5	3673	C	C2-N1-C1'	5.65	125.02	118.80
1	5	1607	C	N3-C2-O2	-5.65	117.94	121.90
3	8	54	C	C5-C6-N1	5.65	123.83	121.00
50	9	1016	U	C5-C6-N1	5.65	125.53	122.70
1	5	2814	C	C6-N1-C2	-5.65	118.04	120.30
1	5	2850	A	C2-N3-C4	5.65	113.42	110.60
1	5	1822	U	N3-C2-O2	-5.64	118.25	122.20
50	9	427	U	C2-N1-C1'	5.64	124.47	117.70
1	5	1535	C	N1-C2-O2	5.64	122.28	118.90
50	9	927	C	N3-C2-O2	-5.64	117.95	121.90
1	5	2072	C	C2-N1-C1'	5.63	125.00	118.80
1	5	115	C	C6-N1-C1'	-5.63	114.04	120.80
1	5	1273	G	N3-C4-N9	-5.63	122.62	126.00
50	9	1315	U	C2-N1-C1'	5.63	124.46	117.70
1	5	1827	C	N1-C2-O2	5.63	122.28	118.90
1	5	104	G	N3-C2-N2	-5.63	115.96	119.90
1	5	1429	C	C6-N1-C1'	-5.63	114.05	120.80
1	5	1395	U	N3-C2-O2	-5.63	118.26	122.20
1	5	2362	U	N3-C2-O2	-5.62	118.26	122.20
1	5	390	C	C6-N1-C2	-5.62	118.05	120.30
3	8	128	C	C2-N1-C1'	5.62	124.98	118.80
1	5	2593	C	C6-N1-C2	-5.62	118.05	120.30
1	5	1894	C	C6-N1-C2	-5.62	118.05	120.30
1	5	4413	C	N3-C2-O2	-5.62	117.97	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	9	958	G	C4-N9-C1'	5.62	133.80	126.50
56	FF	173	LEU	CA-CB-CG	5.62	128.22	115.30
57	GG	133	LEU	CA-CB-CG	5.62	128.22	115.30
1	5	245	C	P-O3'-C3'	5.62	126.44	119.70
1	5	1458	C	N1-C2-O2	5.62	122.27	118.90
45	r	5	LEU	CA-CB-CG	5.62	128.21	115.30
1	5	4662	C	C6-N1-C2	-5.61	118.06	120.30
1	5	1084	C	C6-N1-C2	-5.61	118.06	120.30
1	5	1893	C	N1-C2-O2	5.61	122.27	118.90
1	5	4314	C	N3-C2-O2	-5.61	117.98	121.90
1	5	691	C	C6-N1-C2	-5.60	118.06	120.30
1	5	1977	C	C6-N1-C1'	-5.60	114.08	120.80
50	9	1751	C	N1-C2-O2	5.60	122.26	118.90
1	5	1308	C	C5-C6-N1	5.60	123.80	121.00
1	5	2820	C	N3-C2-O2	-5.60	117.98	121.90
1	5	2867	C	C2-N1-C1'	5.59	124.95	118.80
50	9	465	A	P-O3'-C3'	5.59	126.41	119.70
50	9	930	C	C2-N1-C1'	5.59	124.95	118.80
1	5	2028	C	C2-N1-C1'	5.59	124.95	118.80
1	5	2470	C	N1-C2-O2	5.59	122.25	118.90
3	8	54	C	C6-N1-C2	-5.59	118.06	120.30
1	5	1607	C	C6-N1-C2	-5.58	118.07	120.30
1	5	4948	C	N3-C2-O2	-5.58	117.99	121.90
1	5	4964	C	N1-C2-O2	5.58	122.25	118.90
50	9	1518	C	C2-N1-C1'	5.58	124.94	118.80
1	5	205	C	N3-C2-O2	-5.58	118.00	121.90
1	5	1812	C	C6-N1-C2	-5.58	118.07	120.30
50	9	391	C	C6-N1-C2	-5.58	118.07	120.30
1	5	1381	U	C6-N1-C1'	-5.58	113.39	121.20
50	9	1740	C	N3-C2-O2	-5.58	118.00	121.90
50	9	1708	C	C6-N1-C2	-5.57	118.07	120.30
1	5	1481	C	N3-C2-O2	-5.57	118.00	121.90
1	5	1735	U	N3-C2-O2	-5.57	118.30	122.20
50	9	303	C	N3-C2-O2	-5.57	118.00	121.90
1	5	4942	C	N3-C2-O2	-5.57	118.00	121.90
50	9	1002	U	N1-C2-O2	5.57	126.69	122.80
50	9	1118	C	C2-N1-C1'	5.56	124.92	118.80
1	5	345	C	C5-C6-N1	5.56	123.78	121.00
50	9	874	G	P-O3'-C3'	5.55	126.36	119.70
1	5	3904	G	OP1-P-O3'	5.55	117.41	105.20
1	5	941	C	C6-N1-C2	-5.55	118.08	120.30
50	9	628	A	C2-N3-C4	5.55	113.37	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	1632	A	C4-N9-C1'	5.55	136.28	126.30
50	9	1389	C	C6-N1-C2	-5.55	118.08	120.30
43	o	96	ASP	CB-CG-OD1	5.54	123.29	118.30
50	9	1397	U	N1-C2-O2	5.54	126.68	122.80
1	5	4350	C	N1-C2-O2	5.53	122.22	118.90
50	9	65	C	C6-N1-C2	-5.53	118.09	120.30
50	9	1298	G	C4-N9-C1'	5.53	133.69	126.50
50	9	118	C	N1-C2-O2	5.52	122.22	118.90
3	8	99	U	N3-C2-O2	-5.52	118.33	122.20
1	5	390	C	C5-C6-N1	5.52	123.76	121.00
3	8	35	C	C5-C6-N1	5.52	123.76	121.00
1	5	978	C	C2-N1-C1'	5.51	124.86	118.80
3	8	128	C	C6-N1-C2	-5.51	118.09	120.30
50	9	183	G	C4-N9-C1'	5.50	133.65	126.50
50	9	659	G	C4-N9-C1'	5.50	133.65	126.50
50	9	1303	C	O4'-C1'-N1	5.50	112.60	108.20
1	5	2037	C	C6-N1-C2	-5.50	118.10	120.30
1	5	3831	U	C2-N1-C1'	5.50	124.29	117.70
1	5	2547	G	N3-C2-N2	-5.49	116.05	119.90
1	5	4926	C	N3-C2-O2	-5.49	118.06	121.90
50	9	1865	C	C6-N1-C2	-5.49	118.10	120.30
1	5	4399	U	N1-C2-O2	5.49	126.64	122.80
1	5	464	G	N3-C4-N9	5.49	129.29	126.00
1	5	1082	C	C2-N1-C1'	5.49	124.84	118.80
1	5	2639	U	N3-C2-O2	-5.49	118.36	122.20
50	9	434	G	P-O3'-C3'	5.48	126.28	119.70
50	9	577	U	N1-C2-O2	5.48	126.64	122.80
55	EE	19	MET	CG-SD-CE	-5.48	91.43	100.20
50	9	1592	C	N1-C2-O2	5.48	122.19	118.90
1	5	2705	G	N3-C4-N9	5.48	129.29	126.00
50	9	1664	A	P-O3'-C3'	5.47	126.27	119.70
1	5	1468	C	C5-C6-N1	5.47	123.74	121.00
1	5	4593	C	C6-N1-C2	-5.47	118.11	120.30
50	9	183	G	O4'-C1'-N9	5.47	112.58	108.20
1	5	3741	C	N3-C2-O2	-5.47	118.07	121.90
50	9	1551	U	C2-N1-C1'	5.47	124.26	117.70
1	5	1179	U	N3-C2-O2	-5.46	118.38	122.20
50	9	402	C	C5-C6-N1	5.46	123.73	121.00
50	9	1503	C	C6-N1-C2	-5.46	118.12	120.30
1	5	1180	C	N1-C2-O2	5.46	122.17	118.90
1	5	2072	C	N1-C2-O2	5.46	122.17	118.90
50	9	530	U	C2-N1-C1'	5.46	124.25	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	9	369	C	N3-C2-O2	-5.46	118.08	121.90
1	5	492	U	P-O3'-C3'	5.45	126.24	119.70
1	5	167	C	C5-C6-N1	5.45	123.73	121.00
1	5	4774	C	C6-N1-C2	-5.45	118.12	120.30
1	5	4396	A	N1-C2-N3	-5.45	126.58	129.30
50	9	369	C	C6-N1-C1'	-5.45	114.26	120.80
1	5	1193	C	N1-C2-O2	5.45	122.17	118.90
1	5	3761	C	N1-C2-O2	5.45	122.17	118.90
3	8	21	C	C5-C6-N1	5.45	123.72	121.00
50	9	1002	U	N3-C2-O2	-5.44	118.39	122.20
1	5	484	U	N3-C2-O2	-5.44	118.39	122.20
1	5	4119	C	P-O3'-C3'	5.44	126.23	119.70
50	9	151	C	C2-N1-C1'	5.44	124.78	118.80
1	5	4258	C	C5-C6-N1	5.44	123.72	121.00
1	5	4423	U	N1-C2-O2	5.43	126.60	122.80
3	8	135	C	C2-N1-C1'	5.43	124.78	118.80
1	5	322	C	C5-C6-N1	5.43	123.72	121.00
50	9	876	C	C5-C6-N1	5.43	123.72	121.00
1	5	1428	U	N1-C2-O2	5.43	126.60	122.80
48	v	444	LEU	C-N-CA	5.43	135.27	121.70
1	5	2593	C	N1-C2-O2	5.43	122.16	118.90
50	9	524	U	N3-C2-O2	-5.42	118.41	122.20
3	8	64	U	N1-C2-O2	5.42	126.59	122.80
1	5	484	U	C2-N1-C1'	5.41	124.19	117.70
1	5	4110	C	N1-C2-O2	5.41	122.15	118.90
1	5	205	C	C6-N1-C2	-5.41	118.14	120.30
50	9	1149	A	C2-N3-C4	5.41	113.30	110.60
1	5	1411	C	N3-C2-O2	-5.41	118.12	121.90
1	5	3657	U	N1-C2-O2	5.41	126.58	122.80
50	9	630	U	N1-C2-O2	5.41	126.58	122.80
50	9	887	U	N3-C2-O2	-5.40	118.42	122.20
66	PP	86	LEU	CA-CB-CG	5.40	127.72	115.30
1	5	167	C	C6-N1-C2	-5.40	118.14	120.30
1	5	941	C	C5-C6-N1	5.40	123.70	121.00
1	5	4115	G	P-O3'-C3'	5.40	126.18	119.70
2	7	76	U	N3-C2-O2	-5.40	118.42	122.20
1	5	1340	C	C6-N1-C2	-5.39	118.14	120.30
1	5	4229	U	N1-C2-O2	5.39	126.57	122.80
1	5	118	C	C2-N1-C1'	5.39	124.72	118.80
2	7	57	C	C6-N1-C2	-5.39	118.14	120.30
50	9	142	C	N1-C2-O2	5.39	122.13	118.90
50	9	663	C	C5-C6-N1	5.39	123.69	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	7	28	C	N3-C2-O2	-5.38	118.13	121.90
50	9	1117	C	N3-C2-O2	-5.38	118.13	121.90
50	9	1750	C	N3-C2-O2	-5.38	118.13	121.90
1	5	3714	G	C4-N9-C1'	5.38	133.49	126.50
50	9	850	C	N1-C2-O2	5.38	122.13	118.90
1	5	1735	U	C2-N1-C1'	5.37	124.15	117.70
1	5	49	U	N1-C2-O2	5.37	126.56	122.80
50	9	1314	U	O4'-C1'-N1	5.37	112.50	108.20
55	EE	19	MET	CA-CB-CG	-5.37	104.17	113.30
50	9	1785	C	C2-N1-C1'	5.37	124.70	118.80
1	5	1485	C	N3-C2-O2	-5.37	118.14	121.90
50	9	1520	G	C8-N9-C1'	-5.37	120.02	127.00
50	9	1412	C	C2-N1-C1'	5.36	124.70	118.80
1	5	202	C	C2-N1-C1'	5.36	124.70	118.80
1	5	1289	C	C5-C6-N1	5.36	123.68	121.00
1	5	1481	C	C2-N1-C1'	5.36	124.69	118.80
50	9	630	U	N3-C2-O2	-5.35	118.45	122.20
1	5	1777	C	C5-C6-N1	5.35	123.68	121.00
1	5	1598	C	C2-N1-C1'	5.35	124.69	118.80
50	9	570	C	C6-N1-C2	-5.35	118.16	120.30
50	9	595	U	C2-N1-C1'	5.35	124.12	117.70
1	5	323	C	C5-C6-N1	5.35	123.67	121.00
1	5	1807	C	C6-N1-C2	-5.35	118.16	120.30
1	5	1214	C	N1-C2-O2	5.34	122.11	118.90
1	5	1237	C	N1-C2-O2	5.34	122.11	118.90
48	v	592	LEU	CA-CB-CG	5.34	127.59	115.30
1	5	4919	G	N3-C4-N9	5.34	129.21	126.00
1	5	975	C	C6-N1-C2	-5.34	118.16	120.30
1	5	1894	C	C5-C6-N1	5.34	123.67	121.00
1	5	3870	C	C2-N1-C1'	5.33	124.66	118.80
50	9	733	C	N1-C2-O2	5.33	122.10	118.90
1	5	2528	G	N3-C4-C5	-5.33	125.94	128.60
3	8	4	C	C5-C6-N1	5.32	123.66	121.00
2	7	14	C	C2-N1-C1'	5.32	124.65	118.80
6	C	150	LEU	CA-CB-CG	5.32	127.54	115.30
1	5	390	C	C2-N1-C1'	5.31	124.65	118.80
50	9	927	C	N1-C2-O2	5.31	122.09	118.90
3	8	123	U	N3-C2-O2	-5.31	118.48	122.20
50	9	532	C	P-O3'-C3'	5.31	126.07	119.70
1	5	4399	U	N3-C2-O2	-5.31	118.48	122.20
1	5	4714	C	C2-N1-C1'	5.31	124.64	118.80
1	5	1974	U	N3-C4-O4	5.31	123.11	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	4922	C	C2-N1-C1'	5.31	124.64	118.80
1	5	691	C	C5-C6-N1	5.30	123.65	121.00
1	5	978	C	N1-C2-O2	5.30	122.08	118.90
50	9	958	G	O4'-C1'-N9	5.30	112.44	108.20
50	9	1022	U	C2-N1-C1'	5.30	124.06	117.70
1	5	337	U	N1-C2-O2	5.30	126.51	122.80
1	5	275	C	P-O3'-C3'	5.30	126.06	119.70
1	5	2838	G	C4-N9-C1'	5.30	133.39	126.50
1	5	4712	C	C6-N1-C2	-5.30	118.18	120.30
1	5	1915	C	C2-N1-C1'	5.29	124.62	118.80
50	9	1725	U	N1-C2-O2	5.29	126.50	122.80
15	M	37	LEU	CA-CB-CG	5.29	127.46	115.30
50	9	4	C	C6-N1-C2	-5.29	118.19	120.30
50	9	1837	G	N3-C4-N9	-5.29	122.83	126.00
1	5	2528	G	N3-C4-N9	5.29	129.17	126.00
1	5	217	C	C5-C6-N1	5.28	123.64	121.00
50	9	53	C	C6-N1-C2	-5.28	118.19	120.30
1	5	4119	C	C6-N1-C1'	-5.28	114.46	120.80
1	5	4119	C	C6-N1-C2	-5.28	118.19	120.30
50	9	105	U	N3-C2-O2	-5.28	118.50	122.20
1	5	2817	C	C6-N1-C2	-5.28	118.19	120.30
1	5	4229	U	N3-C2-O2	-5.28	118.51	122.20
3	8	26	C	C6-N1-C2	-5.28	118.19	120.30
50	9	606	G	C4-N9-C1'	5.28	133.36	126.50
1	5	1791	U	N3-C2-O2	-5.28	118.51	122.20
1	5	1993	C	N1-C2-O2	5.28	122.07	118.90
1	5	4561	C	C2-N1-C1'	5.28	124.60	118.80
50	9	848	U	N3-C2-O2	-5.28	118.51	122.20
50	9	1397	U	N3-C2-O2	-5.28	118.51	122.20
1	5	220	C	C6-N1-C2	-5.27	118.19	120.30
1	5	4199	C	N1-C2-O2	5.27	122.06	118.90
1	5	661	C	N1-C2-O2	5.27	122.06	118.90
1	5	1540	C	C6-N1-C2	-5.27	118.19	120.30
3	8	54	C	N1-C2-O2	5.27	122.06	118.90
1	5	281	U	N1-C2-O2	5.27	126.49	122.80
1	5	1674	C	C5-C6-N1	5.26	123.63	121.00
1	5	4177	C	C6-N1-C2	-5.26	118.19	120.30
1	5	4493	U	N1-C2-O2	5.26	126.48	122.80
50	9	183	G	C8-N9-C4	-5.26	104.30	106.40
50	9	791	C	N1-C2-O2	5.26	122.06	118.90
1	5	1428	U	C5-C6-N1	5.26	125.33	122.70
1	5	2405	G	C4-C5-N7	5.25	112.90	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	4243	C	N1-C2-O2	5.25	122.05	118.90
26	X	118	ASP	CB-CG-OD1	5.25	123.03	118.30
66	PP	25	LEU	CA-CB-CG	5.25	127.38	115.30
50	9	733	C	C6-N1-C2	-5.25	118.20	120.30
50	9	1756	C	N1-C2-O2	5.25	122.05	118.90
3	8	99	U	C2-N1-C1'	5.25	124.00	117.70
1	5	4759	C	C6-N1-C2	-5.25	118.20	120.30
1	5	1792	U	C5-C6-N1	5.24	125.32	122.70
1	5	1084	C	C6-N1-C1'	-5.24	114.51	120.80
1	5	2405	G	C6-C5-N7	-5.24	127.26	130.40
58	HH	36	LEU	CA-CB-CG	5.24	127.36	115.30
1	5	5050	C	C2-N1-C1'	5.24	124.56	118.80
1	5	4951	G	N3-C4-N9	5.24	129.14	126.00
1	5	704	C	C2-N1-C1'	5.23	124.56	118.80
1	5	4177	C	C2-N1-C1'	5.23	124.56	118.80
1	5	1237	C	C2-N1-C1'	5.23	124.56	118.80
1	5	4930	C	C6-N1-C1'	-5.23	114.52	120.80
1	5	1429	C	C6-N1-C2	-5.23	118.21	120.30
1	5	4942	C	N1-C2-O2	5.22	122.03	118.90
1	5	2405	G	N9-C4-C5	-5.22	103.31	105.40
1	5	3911	C	C6-N1-C2	-5.22	118.21	120.30
1	5	2615	C	C6-N1-C2	-5.22	118.21	120.30
1	5	4286	C	C6-N1-C2	-5.22	118.21	120.30
50	9	642	U	P-O3'-C3'	5.22	125.96	119.70
1	5	1428	U	C2-N1-C1'	5.22	123.96	117.70
1	5	2528	G	C8-N9-C1'	-5.22	120.22	127.00
1	5	2701	U	N1-C2-O2	5.22	126.45	122.80
1	5	294	G	C4-N9-C1'	5.21	133.28	126.50
50	9	1660	C	C6-N1-C1'	-5.21	114.54	120.80
1	5	4557	U	C2-N1-C1'	5.21	123.95	117.70
50	9	124	U	C5-C6-N1	5.21	125.31	122.70
50	9	1331	C	N3-C2-O2	-5.21	118.25	121.90
1	5	3657	U	C6-N1-C2	-5.21	117.88	121.00
3	8	21	C	C2-N1-C1'	5.21	124.53	118.80
1	5	1991	A	O5'-P-OP1	5.21	116.95	110.70
1	5	4774	C	C5-C6-N1	5.21	123.60	121.00
1	5	4918	C	N1-C2-O2	5.21	122.02	118.90
50	9	30	C	C6-N1-C2	-5.21	118.22	120.30
50	9	1261	C	C6-N1-C2	-5.21	118.22	120.30
50	9	1620	A	O4'-C1'-N9	5.21	112.36	108.20
1	5	1612	G	N9-C4-C5	-5.20	103.32	105.40
1	5	2716	C	C5-C6-N1	5.20	123.60	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	4639	G	C4-N9-C1'	5.20	133.26	126.50
14	L	124	LEU	CA-CB-CG	5.20	127.26	115.30
1	5	2716	C	C2-N1-C1'	5.20	124.52	118.80
1	5	322	C	C6-N1-C2	-5.19	118.22	120.30
50	9	579	C	C2-N1-C1'	5.19	124.51	118.80
50	9	1624	U	C6-N1-C1'	-5.19	113.93	121.20
1	5	1276	C	C5-C6-N1	5.19	123.59	121.00
50	9	199	C	N3-C2-O2	-5.19	118.27	121.90
1	5	49	U	N3-C2-O2	-5.19	118.57	122.20
1	5	322	C	C2-N1-C1'	5.19	124.50	118.80
1	5	4951	G	C4-N9-C1'	5.19	133.24	126.50
1	5	4314	C	C5-C6-N1	5.18	123.59	121.00
1	5	2705	G	C8-N9-C1'	-5.18	120.27	127.00
1	5	1484	G	C8-N9-C1'	-5.18	120.27	127.00
1	5	1893	C	C6-N1-C2	-5.18	118.23	120.30
1	5	2803	U	C5-C6-N1	5.18	125.29	122.70
1	5	3926	C	C6-N1-C2	-5.18	118.23	120.30
74	XX	7	LEU	CA-CB-CG	5.18	127.21	115.30
1	5	4254	G	C8-N9-C4	-5.17	104.33	106.40
1	5	4342	C	C6-N1-C2	-5.17	118.23	120.30
1	5	1237	C	N3-C2-O2	-5.17	118.28	121.90
1	5	4714	C	C6-N1-C2	-5.17	118.23	120.30
1	5	975	C	N1-C2-O2	5.17	122.00	118.90
1	5	2405	G	N3-C4-N9	5.17	129.10	126.00
1	5	2532	C	N1-C2-O2	5.17	122.00	118.90
3	8	101	C	C2-N1-C1'	5.16	124.48	118.80
1	5	4237	C	C2-N1-C1'	5.16	124.47	118.80
1	5	4699	U	OP1-P-O3'	5.16	116.55	105.20
3	8	90	C	C5-C6-N1	5.16	123.58	121.00
50	9	427	U	N3-C2-O2	-5.16	118.59	122.20
1	5	4880	C	O4'-C1'-N1	5.16	112.33	108.20
1	5	492	U	C2-N1-C1'	5.15	123.88	117.70
1	5	4308	C	N1-C2-O2	5.15	121.99	118.90
1	5	4396	A	C6-N1-C2	5.15	121.69	118.60
1	5	4401	G	C4-N9-C1'	5.15	133.19	126.50
50	9	18	C	C6-N1-C2	-5.15	118.24	120.30
50	9	106	C	C6-N1-C2	-5.15	118.24	120.30
50	9	1078	C	C6-N1-C2	-5.15	118.24	120.30
50	9	162	C	C5-C6-N1	5.14	123.57	121.00
1	5	3788	C	C6-N1-C2	-5.14	118.24	120.30
50	9	537	C	N1-C2-O2	5.14	121.98	118.90
1	5	281	U	N3-C2-O2	-5.14	118.60	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	1639	U	C5-C6-N1	5.14	125.27	122.70
1	5	2020	U	N3-C2-O2	-5.14	118.60	122.20
50	9	606	G	C4-C5-N7	5.14	112.85	110.80
50	9	879	C	N1-C2-O2	5.13	121.98	118.90
1	5	1216	C	N1-C2-O2	5.13	121.98	118.90
50	9	37	C	C5-C6-N1	5.13	123.57	121.00
1	5	1686	C	C5-C6-N1	5.13	123.57	121.00
1	5	4088	C	N1-C2-O2	5.13	121.98	118.90
50	9	1412	C	C5-C6-N1	5.13	123.56	121.00
1	5	1847	C	C6-N1-C2	-5.13	118.25	120.30
2	7	57	C	C5-C6-N1	5.12	123.56	121.00
1	5	294	G	N3-C4-N9	5.12	129.07	126.00
1	5	2031	C	C6-N1-C2	-5.12	118.25	120.30
1	5	4119	C	N3-C2-O2	-5.12	118.31	121.90
1	5	1446	C	C5-C6-N1	5.12	123.56	121.00
1	5	100	C	C6-N1-C1'	-5.12	114.66	120.80
1	5	122	U	N3-C2-O2	-5.12	118.62	122.20
50	9	1518	C	N3-C2-O2	-5.12	118.32	121.90
55	EE	73	ASP	CB-CG-OD1	5.12	122.91	118.30
1	5	4482	U	N1-C2-O2	5.12	126.38	122.80
1	5	4577	U	N3-C2-O2	-5.12	118.62	122.20
1	5	274	C	C2-N1-C1'	5.11	124.42	118.80
1	5	504	G	P-O3'-C3'	5.11	125.84	119.70
1	5	3714	G	C8-N9-C1'	-5.11	120.35	127.00
1	5	4859	C	C6-N1-C2	-5.11	118.25	120.30
1	5	1978	C	C6-N1-C2	-5.11	118.26	120.30
48	v	517	LEU	CA-CB-CG	5.11	127.05	115.30
1	5	4869	U	N1-C2-O2	5.11	126.38	122.80
1	5	1215	C	N1-C2-O2	5.11	121.96	118.90
1	5	4243	C	C6-N1-C2	-5.11	118.26	120.30
1	5	4759	C	C6-N1-C1'	-5.11	114.67	120.80
50	9	1551	U	N3-C2-O2	-5.11	118.63	122.20
1	5	2532	C	C6-N1-C2	-5.10	118.26	120.30
50	9	639	C	C6-N1-C2	-5.10	118.26	120.30
1	5	1458	C	N3-C2-O2	-5.10	118.33	121.90
1	5	3606	U	C2-N1-C1'	5.10	123.82	117.70
1	5	1978	C	N1-C2-O2	5.10	121.96	118.90
1	5	4215	C	C6-N1-C2	-5.10	118.26	120.30
50	9	1237	C	C6-N1-C2	-5.10	118.26	120.30
1	5	2089	G	OP2-P-O3'	5.09	116.41	105.20
50	9	659	G	C8-N9-C1'	-5.09	120.38	127.00
50	9	898	U	N3-C2-O2	-5.09	118.63	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	4476	C	C2-N1-C1'	5.09	124.40	118.80
3	8	119	C	C6-N1-C2	-5.09	118.26	120.30
1	5	41	C	C5-C6-N1	5.09	123.55	121.00
1	5	126	C	N3-C2-O2	-5.09	118.34	121.90
1	5	1990	A	OP1-P-O3'	5.09	116.39	105.20
52	BB	225	LEU	CA-CB-CG	5.09	127.00	115.30
1	5	365	U	N1-C2-O2	5.08	126.36	122.80
1	5	1694	C	C6-N1-C2	-5.08	118.27	120.30
1	5	1971	U	N1-C2-O2	5.08	126.36	122.80
1	5	4930	C	C5-C6-N1	5.08	123.54	121.00
3	8	99	U	N1-C2-O2	5.08	126.36	122.80
1	5	2568	C	C6-N1-C1'	-5.08	114.70	120.80
50	9	391	C	C2-N1-C1'	5.08	124.39	118.80
50	9	803	C	C6-N1-C2	-5.08	118.27	120.30
50	9	1628	C	N1-C2-O2	5.08	121.95	118.90
50	9	1520	G	C6-N1-C2	-5.08	122.05	125.10
1	5	3876	A	OP2-P-O3'	5.08	116.37	105.20
1	5	4612	C	N1-C2-O2	5.08	121.95	118.90
12	I	190	LEU	CA-CB-CG	5.07	126.97	115.30
50	9	1064	C	C6-N1-C2	-5.07	118.27	120.30
50	9	188	C	C6-N1-C1'	-5.07	114.72	120.80
1	5	5047	C	N1-C2-O2	5.07	121.94	118.90
50	9	105	U	N1-C2-O2	5.07	126.35	122.80
1	5	4746	C	N1-C2-O2	5.06	121.94	118.90
1	5	5047	C	C6-N1-C2	-5.06	118.28	120.30
50	9	402	C	N3-C2-O2	-5.06	118.36	121.90
83	gg	32	LEU	CA-CB-CG	5.06	126.94	115.30
50	9	479	C	C6-N1-C2	-5.06	118.28	120.30
1	5	297	U	C5-C6-N1	5.06	125.23	122.70
1	5	4560	C	N3-C2-O2	-5.06	118.36	121.90
3	8	51	U	N3-C2-O2	-5.06	118.66	122.20
3	8	90	C	C6-N1-C2	-5.06	118.28	120.30
50	9	608	C	C5-C6-N1	5.06	123.53	121.00
50	9	1725	U	N3-C2-O2	-5.06	118.66	122.20
1	5	1082	C	N1-C2-O2	5.06	121.93	118.90
1	5	1915	C	N1-C2-O2	5.06	121.93	118.90
50	9	151	C	N1-C2-O2	5.05	121.93	118.90
1	5	1884	C	N1-C2-O2	5.05	121.93	118.90
1	5	2593	C	C5-C6-N1	5.05	123.53	121.00
1	5	4689	U	C5-C6-N1	5.05	125.23	122.70
50	9	438	G	N3-C4-C5	-5.05	126.08	128.60
1	5	1807	C	C5-C6-N1	5.05	123.52	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	8	38	U	C2-N1-C1'	5.04	123.75	117.70
1	5	455	C	C2-N1-C1'	5.04	124.34	118.80
1	5	1211	G	P-O3'-C3'	5.04	125.75	119.70
1	5	4667	C	C2-N1-C1'	5.03	124.34	118.80
1	5	4951	G	C8-N9-C1'	-5.03	120.46	127.00
1	5	679	C	C6-N1-C2	-5.03	118.29	120.30
1	5	1411	C	C5-C6-N1	5.03	123.52	121.00
1	5	1991	A	O5'-P-OP2	-5.03	101.17	105.70
1	5	2701	U	N3-C2-O2	-5.03	118.68	122.20
50	9	1518	C	N1-C2-O2	5.03	121.92	118.90
1	5	4766	C	C2-N1-C1'	5.02	124.33	118.80
1	5	1467	C	C6-N1-C2	-5.02	118.29	120.30
1	5	1429	C	C5-C6-N1	5.02	123.51	121.00
1	5	4314	C	C2-N1-C1'	5.02	124.32	118.80
50	9	585	C	C2-N1-C1'	5.02	124.32	118.80
1	5	1726	U	N1-C2-O2	5.02	126.31	122.80
1	5	1735	U	C5-C6-N1	5.02	125.21	122.70
1	5	14	C	C5-C6-N1	5.01	123.51	121.00
1	5	3622	C	C6-N1-C2	-5.01	118.29	120.30
63	MM	22	LEU	CA-CB-CG	5.01	126.83	115.30
1	5	2704	C	C6-N1-C2	-5.01	118.30	120.30
14	L	155	MET	CA-CB-CG	5.01	121.82	113.30
1	5	1971	U	N3-C2-O2	-5.01	118.69	122.20
1	5	2432	U	N3-C2-O2	-5.01	118.69	122.20
50	9	585	C	C6-N1-C2	-5.01	118.30	120.30
1	5	2290	C	C6-N1-C2	-5.00	118.30	120.30
50	9	1230	C	C6-N1-C2	-5.00	118.30	120.30
1	5	1818	G	C4-N9-C1'	5.00	133.00	126.50
1	5	1977	C	C6-N1-C2	-5.00	118.30	120.30
1	5	4133	C	C2-N1-C1'	5.00	124.30	118.80
1	5	4736	C	C2-N1-C1'	5.00	124.30	118.80

There are no chirality outliers.

All (31) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
51	AA	42	LYS	Peptide
51	AA	43	SER	Peptide
6	C	73	VAL	Peptide
54	DD	153	VAL	Peptide
8	E	178	VAL	Peptide
8	E	179	THR	Peptide

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Mol	Chain	Res	Type	Group
55	EE	132	GLY	Peptide
9	F	195	THR	Peptide
56	FF	41	VAL	Peptide
10	G	215	ASP	Peptide
11	H	50	LYS	Peptide
59	II	92	ARG	Peptide
16	N	184	ILE	Peptide
16	N	76	PRO	Peptide
16	N	78	GLY	Peptide
66	PP	17	TYR	Peptide
21	S	165	PRO	Peptide
69	SS	60	THR	Peptide
22	T	80	VAL	Peptide
71	UU	107	GLU	Peptide
72	VV	32	ILE	Peptide
74	XX	61	GLN	Peptide
32	d	95	ASP	Peptide
35	g	5	LEU	Peptide
83	gg	135	LEU	Peptide
46	s	119	CYS	Peptide
47	t	96	LYS	Peptide
48	v	443	TYR	Peptide
48	v	444	LEU	Peptide
48	v	562	GLU	Peptide
48	v	820	LEU	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	
4	A	246/248 (99%)	221 (90%)	25 (10%)	0	100	100
5	B	392/394 (100%)	365 (93%)	27 (7%)	0	100	100
6	C	359/362 (99%)	339 (94%)	20 (6%)	0	100	100
7	D	291/293 (99%)	279 (96%)	12 (4%)	0	100	100
8	E	208/291 (72%)	198 (95%)	10 (5%)	0	100	100
9	F	223/225 (99%)	212 (95%)	10 (4%)	1 (0%)	30	60
10	G	229/319 (72%)	219 (96%)	10 (4%)	0	100	100
11	H	188/190 (99%)	171 (91%)	17 (9%)	0	100	100
12	I	201/214 (94%)	191 (95%)	10 (5%)	0	100	100
13	J	168/170 (99%)	160 (95%)	8 (5%)	0	100	100
14	L	208/210 (99%)	198 (95%)	8 (4%)	2 (1%)	13	39
15	M	136/138 (99%)	125 (92%)	11 (8%)	0	100	100
16	N	201/203 (99%)	190 (94%)	11 (6%)	0	100	100
17	O	197/199 (99%)	191 (97%)	6 (3%)	0	100	100
18	P	151/153 (99%)	146 (97%)	5 (3%)	0	100	100
19	Q	185/187 (99%)	177 (96%)	8 (4%)	0	100	100
20	R	178/180 (99%)	173 (97%)	5 (3%)	0	100	100
21	S	174/176 (99%)	164 (94%)	9 (5%)	1 (1%)	22	50
22	T	157/159 (99%)	153 (98%)	3 (2%)	1 (1%)	22	50
23	U	97/99 (98%)	92 (95%)	5 (5%)	0	100	100
24	V	129/131 (98%)	127 (98%)	2 (2%)	0	100	100
25	W	96/157 (61%)	89 (93%)	7 (7%)	0	100	100
26	X	116/118 (98%)	108 (93%)	8 (7%)	0	100	100
27	Y	132/134 (98%)	127 (96%)	5 (4%)	0	100	100
28	Z	133/135 (98%)	128 (96%)	5 (4%)	0	100	100
29	a	145/147 (99%)	137 (94%)	8 (6%)	0	100	100
30	b	100/245 (41%)	95 (95%)	5 (5%)	0	100	100
31	c	96/98 (98%)	88 (92%)	8 (8%)	0	100	100
32	d	105/107 (98%)	97 (92%)	8 (8%)	0	100	100
33	e	126/128 (98%)	119 (94%)	7 (6%)	0	100	100
34	f	107/109 (98%)	102 (95%)	5 (5%)	0	100	100
35	g	112/114 (98%)	108 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	h	120/122 (98%)	119 (99%)	1 (1%)	0	100	100
37	i	100/102 (98%)	97 (97%)	3 (3%)	0	100	100
38	j	84/86 (98%)	77 (92%)	7 (8%)	0	100	100
39	k	67/69 (97%)	66 (98%)	1 (2%)	0	100	100
40	l	48/50 (96%)	43 (90%)	5 (10%)	0	100	100
41	m	49/52 (94%)	46 (94%)	2 (4%)	1 (2%)	6	25
42	n	23/25 (92%)	23 (100%)	0	0	100	100
43	o	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
44	p	89/91 (98%)	87 (98%)	2 (2%)	0	100	100
45	r	122/124 (98%)	116 (95%)	6 (5%)	0	100	100
46	s	194/196 (99%)	178 (92%)	16 (8%)	0	100	100
47	t	151/153 (99%)	128 (85%)	22 (15%)	1 (1%)	19	47
48	v	843/848 (99%)	774 (92%)	68 (8%)	1 (0%)	48	78
49	w	51/55 (93%)	46 (90%)	5 (10%)	0	100	100
51	AA	215/217 (99%)	206 (96%)	9 (4%)	0	100	100
52	BB	211/213 (99%)	203 (96%)	8 (4%)	0	100	100
53	CC	219/221 (99%)	206 (94%)	13 (6%)	0	100	100
54	DD	226/228 (99%)	216 (96%)	10 (4%)	0	100	100
55	EE	260/262 (99%)	244 (94%)	16 (6%)	0	100	100
56	FF	181/204 (89%)	162 (90%)	19 (10%)	0	100	100
57	GG	235/237 (99%)	224 (95%)	11 (5%)	0	100	100
58	HH	181/194 (93%)	173 (96%)	8 (4%)	0	100	100
59	II	204/206 (99%)	185 (91%)	19 (9%)	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%)	131 (94%)	8 (6%)	0	100	100
63	MM	115/117 (98%)	101 (88%)	14 (12%)	0	100	100
64	NN	147/149 (99%)	138 (94%)	9 (6%)	0	100	100
65	OO	134/136 (98%)	123 (92%)	11 (8%)	0	100	100
66	PP	123/125 (98%)	118 (96%)	5 (4%)	0	100	100
67	QQ	140/142 (99%)	132 (94%)	8 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
68	RR	130/132 (98%)	121 (93%)	9 (7%)	0	100	100
69	SS	142/144 (99%)	135 (95%)	7 (5%)	0	100	100
70	TT	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
71	UU	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
72	VV	81/83 (98%)	76 (94%)	5 (6%)	0	100	100
73	WW	127/129 (98%)	118 (93%)	9 (7%)	0	100	100
74	XX	139/141 (99%)	132 (95%)	4 (3%)	3 (2%)	5	24
75	YY	122/124 (98%)	120 (98%)	2 (2%)	0	100	100
76	ZZ	73/75 (97%)	70 (96%)	3 (4%)	0	100	100
77	aa	99/101 (98%)	90 (91%)	9 (9%)	0	100	100
78	bb	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
79	cc	60/62 (97%)	57 (95%)	3 (5%)	0	100	100
80	dd	53/55 (96%)	48 (91%)	5 (9%)	0	100	100
81	ee	53/55 (96%)	50 (94%)	3 (6%)	0	100	100
82	ff	66/68 (97%)	55 (83%)	11 (17%)	0	100	100
83	gg	311/313 (99%)	282 (91%)	29 (9%)	0	100	100
All	All	12409/13005 (95%)	11674 (94%)	724 (6%)	11 (0%)	50	78

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	L	64	VAL
41	m	73	CYS
74	XX	62	PRO
14	L	63	THR
21	S	166	ARG
47	t	144	ASP
48	v	778	GLY
74	XX	61	GLN
74	XX	86	PRO
22	T	81	LYS
9	F	196	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	190/190 (100%)	187 (98%)	3 (2%)	58	75
5	B	342/342 (100%)	338 (99%)	4 (1%)	67	80
6	C	301/301 (100%)	297 (99%)	4 (1%)	65	78
7	D	247/247 (100%)	245 (99%)	2 (1%)	79	87
8	E	190/251 (76%)	186 (98%)	4 (2%)	48	69
9	F	196/196 (100%)	196 (100%)	0	100	100
10	G	200/272 (74%)	194 (97%)	6 (3%)	36	61
11	H	169/169 (100%)	168 (99%)	1 (1%)	84	90
12	I	175/181 (97%)	173 (99%)	2 (1%)	70	81
13	J	143/143 (100%)	143 (100%)	0	100	100
14	L	175/175 (100%)	175 (100%)	0	100	100
15	M	117/117 (100%)	116 (99%)	1 (1%)	75	86
16	N	171/171 (100%)	168 (98%)	3 (2%)	54	73
17	O	171/171 (100%)	167 (98%)	4 (2%)	45	67
18	P	134/134 (100%)	131 (98%)	3 (2%)	47	68
19	Q	164/164 (100%)	162 (99%)	2 (1%)	67	80
20	R	159/159 (100%)	158 (99%)	1 (1%)	84	90
21	S	157/157 (100%)	156 (99%)	1 (1%)	84	90
22	T	139/139 (100%)	137 (99%)	2 (1%)	62	77
23	U	89/89 (100%)	88 (99%)	1 (1%)	70	81
24	V	101/101 (100%)	99 (98%)	2 (2%)	50	70
25	W	82/126 (65%)	82 (100%)	0	100	100
26	X	106/106 (100%)	105 (99%)	1 (1%)	75	86
27	Y	124/124 (100%)	122 (98%)	2 (2%)	58	75
28	Z	117/117 (100%)	117 (100%)	0	100	100
29	a	119/119 (100%)	118 (99%)	1 (1%)	79	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	b	84/184 (46%)	82 (98%)	2 (2%)	44	66
31	c	84/84 (100%)	83 (99%)	1 (1%)	67	80
32	d	98/98 (100%)	97 (99%)	1 (1%)	73	83
33	e	114/114 (100%)	113 (99%)	1 (1%)	75	86
34	f	88/88 (100%)	87 (99%)	1 (1%)	70	81
35	g	98/98 (100%)	95 (97%)	3 (3%)	35	60
36	h	109/109 (100%)	108 (99%)	1 (1%)	75	86
37	i	86/86 (100%)	83 (96%)	3 (4%)	31	56
38	j	73/73 (100%)	71 (97%)	2 (3%)	40	63
39	k	64/64 (100%)	64 (100%)	0	100	100
40	l	47/47 (100%)	47 (100%)	0	100	100
41	m	47/47 (100%)	47 (100%)	0	100	100
42	n	24/24 (100%)	23 (96%)	1 (4%)	25	51
43	o	91/91 (100%)	89 (98%)	2 (2%)	47	68
44	p	74/74 (100%)	74 (100%)	0	100	100
45	r	108/108 (100%)	107 (99%)	1 (1%)	75	86
46	s	164/164 (100%)	163 (99%)	1 (1%)	84	90
47	t	126/126 (100%)	123 (98%)	3 (2%)	44	66
48	v	722/722 (100%)	712 (99%)	10 (1%)	62	77
49	w	46/46 (100%)	46 (100%)	0	100	100
51	AA	180/181 (99%)	179 (99%)	1 (1%)	84	90
52	BB	194/194 (100%)	190 (98%)	4 (2%)	48	69
53	CC	187/187 (100%)	185 (99%)	2 (1%)	70	81
54	DD	190/190 (100%)	186 (98%)	4 (2%)	48	69
55	EE	224/224 (100%)	221 (99%)	3 (1%)	65	78
56	FF	158/170 (93%)	152 (96%)	6 (4%)	28	54
57	GG	207/207 (100%)	199 (96%)	8 (4%)	27	53
58	HH	165/174 (95%)	164 (99%)	1 (1%)	84	90
59	II	178/178 (100%)	173 (97%)	5 (3%)	38	62
60	JJ	161/161 (100%)	158 (98%)	3 (2%)	52	71
61	KK	87/87 (100%)	86 (99%)	1 (1%)	70	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
62	LL	130/142 (92%)	128 (98%)	2 (2%)	60	76
63	MM	99/99 (100%)	96 (97%)	3 (3%)	36	61
64	NN	130/130 (100%)	129 (99%)	1 (1%)	79	87
65	OO	106/106 (100%)	105 (99%)	1 (1%)	75	86
66	PP	111/111 (100%)	106 (96%)	5 (4%)	23	50
67	QQ	117/117 (100%)	115 (98%)	2 (2%)	56	74
68	RR	119/119 (100%)	115 (97%)	4 (3%)	32	57
69	SS	125/125 (100%)	122 (98%)	3 (2%)	44	66
70	TT	111/111 (100%)	108 (97%)	3 (3%)	40	63
71	UU	92/92 (100%)	92 (100%)	0	100	100
72	VV	67/67 (100%)	66 (98%)	1 (2%)	60	76
73	WW	112/112 (100%)	111 (99%)	1 (1%)	75	86
74	XX	113/113 (100%)	112 (99%)	1 (1%)	75	86
75	YY	107/107 (100%)	105 (98%)	2 (2%)	52	71
76	ZZ	66/66 (100%)	66 (100%)	0	100	100
77	aa	88/88 (100%)	87 (99%)	1 (1%)	70	81
78	bb	75/75 (100%)	75 (100%)	0	100	100
79	cc	55/55 (100%)	52 (94%)	3 (6%)	18	44
80	dd	48/48 (100%)	46 (96%)	2 (4%)	25	51
81	ee	46/46 (100%)	43 (94%)	3 (6%)	14	39
82	ff	61/61 (100%)	60 (98%)	1 (2%)	58	75
83	gg	272/272 (100%)	268 (98%)	4 (2%)	60	76
All	All	10806/11123 (97%)	10642 (98%)	164 (2%)	60	76

All (164) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	4	VAL
4	A	163	ARG
4	A	226	ARG
5	B	10	ARG
5	B	261	ARG
5	B	262	VAL
5	B	297	LYS

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Mol	Chain	Res	Type
6	C	38	ASN
6	C	57	LEU
6	C	188	ARG
6	C	204	ARG
7	D	42	ASN
7	D	268	ARG
8	E	41	LYS
8	E	58	ARG
8	E	164	ARG
8	E	224	LYS
10	G	134	ASN
10	G	215	ASP
10	G	220	VAL
10	G	228	ARG
10	G	242	ARG
10	G	249	ARG
11	H	50	LYS
12	I	3	ARG
12	I	116	ARG
15	M	119	ARG
16	N	50	ARG
16	N	64	ILE
16	N	162	ARG
17	O	5	GLN
17	O	61	ARG
17	O	85	ARG
17	O	117	ARG
18	P	69	ARG
18	P	97	ASN
18	P	140	MET
19	Q	16	LYS
19	Q	172	ARG
20	R	170	ARG
21	S	23	ARG
22	T	107	LYS
22	T	146	LYS
23	U	81	ARG
24	V	18	LEU
24	V	46	LYS
26	X	53	ARG
27	Y	2	LYS
27	Y	124	LYS

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Mol	Chain	Res	Type
29	a	122	VAL
30	b	51	LYS
30	b	68	ARG
31	c	90	ARG
32	d	67	ARG
33	e	48	ARG
34	f	16	ARG
35	g	5	LEU
35	g	54	ARG
35	g	102	ILE
36	h	102	LEU
37	i	29	ARG
37	i	56	ARG
37	i	99	LYS
38	j	20	ARG
38	j	72	ARG
42	n	17	ARG
43	o	43	ARG
43	o	82	MET
45	r	58	LYS
46	s	68	HIS
47	t	57	ARG
47	t	61	LYS
47	t	146	ARG
48	v	18	ASN
48	v	55	ARG
48	v	231	MET
48	v	295	ASP
48	v	438	LYS
48	v	625	ARG
48	v	667	LYS
48	v	701	ARG
48	v	726	ARG
48	v	779	THR
51	AA	186	ARG
52	BB	28	LYS
52	BB	56	LYS
52	BB	174	ARG
52	BB	222	LYS
53	CC	167	ARG
53	CC	248	TYR
54	DD	45	ARG

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Mol	Chain	Res	Type
54	DD	64	ARG
54	DD	76	ARG
54	DD	113	LEU
55	EE	20	LEU
55	EE	148	ARG
55	EE	259	LYS
56	FF	44	LYS
56	FF	76	MET
56	FF	122	ARG
56	FF	169	ILE
56	FF	173	LEU
56	FF	182	LYS
57	GG	14	LYS
57	GG	22	ARG
57	GG	25	ARG
57	GG	79	LYS
57	GG	185	LEU
57	GG	203	LYS
57	GG	224	ARG
57	GG	231	ARG
58	HH	85	LYS
59	II	5	ARG
59	II	47	ARG
59	II	74	ARG
59	II	84	ASN
59	II	165	GLN
60	JJ	70	ARG
60	JJ	79	ARG
60	JJ	169	ARG
61	KK	61	GLN
62	LL	12	LYS
62	LL	22	ARG
63	MM	63	LYS
63	MM	99	LYS
63	MM	116	LYS
64	NN	122	ILE
65	OO	146	ARG
66	PP	13	ARG
66	PP	50	ARG
66	PP	51	ARG
66	PP	65	LYS
66	PP	108	LYS

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Mol	Chain	Res	Type
67	QQ	41	MET
67	QQ	109	LYS
68	RR	5	ARG
68	RR	7	LYS
68	RR	81	ARG
68	RR	116	ASN
69	SS	91	LYS
69	SS	94	LYS
69	SS	111	LEU
70	TT	43	LYS
70	TT	62	ARG
70	TT	75	MET
72	VV	70	LEU
73	WW	103	VAL
74	XX	142	ARG
75	YY	32	LYS
75	YY	113	ARG
77	aa	42	ARG
79	cc	40	ARG
79	cc	63	ARG
79	cc	66	ARG
80	dd	26	ASN
80	dd	48	LYS
81	ee	81	ARG
81	ee	99	LYS
81	ee	104	ARG
82	ff	107	LYS
83	gg	8	ARG
83	gg	99	ARG
83	gg	280	LYS
83	gg	285	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
7	D	42	ASN
15	M	48	GLN
22	T	69	GLN
55	EE	36	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	5	3520/3597 (97%)	818 (23%)	59 (1%)
2	7	119/120 (99%)	14 (11%)	0
3	8	149/151 (98%)	25 (16%)	1 (0%)
50	9	1670/1698 (98%)	388 (23%)	18 (1%)
All	All	5458/5566 (98%)	1245 (22%)	78 (1%)

All (1245) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	5	5	A
1	5	12	A
1	5	13	U
1	5	17	A
1	5	25	A
1	5	35	U
1	5	36	U
1	5	39	A
1	5	42	A
1	5	47	A
1	5	56	A
1	5	58	G
1	5	59	A
1	5	64	A
1	5	65	A
1	5	71	C
1	5	72	C
1	5	73	A
1	5	76	A
1	5	84	A
1	5	91	G
1	5	93	G
1	5	98	A
1	5	104	G
1	5	108	A
1	5	109	G
1	5	110	C
1	5	116	G
1	5	119	G
1	5	120	A
1	5	126	C
1	5	134	G
1	5	135	G
1	5	136	C

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Mol	Chain	Res	Type
1	5	142	G
1	5	144	G
1	5	146	G
1	5	157	U
1	5	159	C
1	5	172	C
1	5	173	C
1	5	182	G
1	5	200	U
1	5	201	C
1	5	202	C
1	5	203	U
1	5	205	C
1	5	206	U
1	5	209	U
1	5	216	C
1	5	218	A
1	5	220	C
1	5	224	U
1	5	225	G
1	5	233	U
1	5	234	G
1	5	246	G
1	5	250	C
1	5	265	C
1	5	266	C
1	5	275	C
1	5	276	C
1	5	278	G
1	5	280	G
1	5	297	U
1	5	306	A
1	5	309	C
1	5	310	G
1	5	315	G
1	5	316	U
1	5	322	C
1	5	326	C
1	5	334	A
1	5	340	C
1	5	345	C
1	5	349	A

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Mol	Chain	Res	Type
1	5	362	A
1	5	363	A
1	5	379	G
1	5	386	A
1	5	387	G
1	5	398	A2M
1	5	401	G
1	5	407	A
1	5	408	A
1	5	410	A
1	5	412	G
1	5	413	G
1	5	414	C
1	5	440	U
1	5	446	C
1	5	449	C
1	5	450	G
1	5	452	A
1	5	453	G
1	5	454	U
1	5	455	C
1	5	464	G
1	5	467	U
1	5	468	U
1	5	482	G
1	5	483	G
1	5	484	U
1	5	486	C
1	5	489	C
1	5	492	U
1	5	493	G
1	5	497	G
1	5	498	C
1	5	499	G
1	5	505	G
1	5	506	C
1	5	510	U
1	5	661	C
1	5	666	G
1	5	667	A
1	5	669	C
1	5	672	C

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Mol	Chain	Res	Type
1	5	684	G
1	5	685	C
1	5	687	U
1	5	696	C
1	5	697	G
1	5	704	C
1	5	705	G
1	5	708	G
1	5	722	G
1	5	730	G
1	5	731	G
1	5	742	G
1	5	747	A
1	5	748	G
1	5	749	G
1	5	758	G
1	5	759	G
1	5	908	G
1	5	914	U
1	5	917	A
1	5	922(B)	C
1	5	925	C
1	5	926	G
1	5	929	A
1	5	931	C
1	5	932	A
1	5	933	G
1	5	934	C
1	5	937	U
1	5	938	C
1	5	939	G
1	5	941	C
1	5	943	A
1	5	944	A
1	5	945	U
1	5	956	A
1	5	958	G
1	5	959	G
1	5	960	A
1	5	961	G
1	5	964	A
1	5	966	A

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Mol	Chain	Res	Type
1	5	967	C
1	5	968	C
1	5	969	C
1	5	972	C
1	5	973	C
1	5	980	C
1	5	983	U
1	5	990	U
1	5	1072	C
1	5	1073	G
1	5	1079	C
1	5	1081	C
1	5	1083	U
1	5	1175	A
1	5	1179	U
1	5	1180	C
1	5	1184	A
1	5	1193	C
1	5	1195	G
1	5	1210	C
1	5	1211	G
1	5	1212	G
1	5	1214	C
1	5	1215	C
1	5	1234	G
1	5	1235	G
1	5	1236	C
1	5	1237	C
1	5	1238	A
1	5	1239	C
1	5	1272	C
1	5	1273	G
1	5	1275	G
1	5	1276	C
1	5	1279	A
1	5	1284	G
1	5	1285	U
1	5	1287	G
1	5	1292	C
1	5	1293	G
1	5	1296	G
1	5	1301	C

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Mol	Chain	Res	Type
1	5	1302	U
1	5	1303	A
1	5	1304	C
1	5	1314	C
1	5	1319	U
1	5	1326	A2M
1	5	1329	G
1	5	1330	A
1	5	1337	A
1	5	1354	A
1	5	1358	G
1	5	1359	G
1	5	1371	A
1	5	1372	A
1	5	1377	G
1	5	1378	C
1	5	1381	U
1	5	1387	A
1	5	1394	G
1	5	1397	A
1	5	1398	A
1	5	1406(C)	G
1	5	1415	G
1	5	1416	G
1	5	1419	G
1	5	1421	G
1	5	1426	G
1	5	1429	C
1	5	1436	C
1	5	1437	C
1	5	1438	U
1	5	1441	C
1	5	1445	U
1	5	1446	C
1	5	1457	G
1	5	1465	G
1	5	1469	C
1	5	1482	G
1	5	1483	C
1	5	1493	G
1	5	1497	A
1	5	1498	G

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Mol	Chain	Res	Type
1	5	1502	G
1	5	1516	G
1	5	1518	A
1	5	1523	A
1	5	1534	A2M
1	5	1547	A
1	5	1566	C
1	5	1578	U
1	5	1582	PSU
1	5	1591	U
1	5	1596	U
1	5	1598	C
1	5	1602	U
1	5	1612	G
1	5	1613	A
1	5	1624	G
1	5	1625	OMG
1	5	1626	G
1	5	1627	G
1	5	1631	A
1	5	1633	G
1	5	1634	A
1	5	1638	A
1	5	1640	C
1	5	1641	G
1	5	1649	U
1	5	1650	A
1	5	1654	G
1	5	1661	C
1	5	1671	U
1	5	1676	C
1	5	1677	PSU
1	5	1678	C
1	5	1679	A
1	5	1684	A
1	5	1691	G
1	5	1724	G
1	5	1726	U
1	5	1734	G
1	5	1741	G
1	5	1742	A
1	5	1748	U

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Mol	Chain	Res	Type
1	5	1750	G
1	5	1752	G
1	5	1755	C
1	5	1756	U
1	5	1757	U
1	5	1761	G
1	5	1768	C
1	5	1772	C
1	5	1773	U
1	5	1775	A
1	5	1776	A
1	5	1780	A
1	5	1781	U
1	5	1787	A
1	5	1800	U
1	5	1804	A
1	5	1805	A
1	5	1806	G
1	5	1815	G
1	5	1819	G
1	5	1821	G
1	5	1822	U
1	5	1828	C
1	5	1833	G
1	5	1834	U
1	5	1835	G
1	5	1836	G
1	5	1837	A
1	5	1842	G
1	5	1855	G
1	5	1869	G
1	5	1873	A
1	5	1881	C
1	5	1888	A
1	5	1897	A
1	5	1898	C
1	5	1899	G
1	5	1917	A
1	5	1918	U
1	5	1920	C
1	5	1921	C
1	5	1922	G

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Mol	Chain	Res	Type
1	5	1930	U
1	5	1931	C
1	5	1932	A
1	5	1935	C
1	5	1938	C
1	5	1940	G
1	5	1945	G
1	5	1948	G
1	5	1957	U
1	5	1958	A
1	5	1961	G
1	5	1964	A
1	5	1967	A
1	5	1971	U
1	5	1974	U
1	5	1978	C
1	5	1979	A
1	5	1980	U
1	5	1984	A
1	5	1987	C
1	5	1991	A
1	5	1992	U
1	5	1994	C
1	5	1997	U
1	5	2001	G
1	5	2002	A
1	5	2003	G
1	5	2004	U
1	5	2008	U
1	5	2011	C
1	5	2024	G
1	5	2025	A
1	5	2026	A
1	5	2029	A
1	5	2033	A
1	5	2046	G
1	5	2047	A
1	5	2048	U
1	5	2052	G
1	5	2055	G
1	5	2056	G
1	5	2062	C

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Mol	Chain	Res	Type
1	5	2064	G
1	5	2069	A
1	5	2070	U
1	5	2072	C
1	5	2084	U
1	5	2090	U
1	5	2092	G
1	5	2093	G
1	5	2094	C
1	5	2095	A
1	5	2097	A
1	5	2098	G
1	5	2100	G
1	5	2101	A
1	5	2102	G
1	5	2104	A
1	5	2105	A
1	5	2106	G
1	5	2107	A
1	5	2108	G
1	5	2259	G
1	5	2260	C
1	5	2267	U
1	5	2268	A
1	5	2269	C
1	5	2270	G
1	5	2274	C
1	5	2279	A
1	5	2289	C
1	5	2294	G
1	5	2300	A
1	5	2301	G
1	5	2306	G
1	5	2307	A
1	5	2313	A
1	5	2314	G
1	5	2316	G
1	5	2319	C
1	5	2331	G
1	5	2333	G
1	5	2347	A
1	5	2348	G

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Mol	Chain	Res	Type
1	5	2351	C
1	5	2357	G
1	5	2360	A
1	5	2364	OMG
1	5	2370	A
1	5	2395	A
1	5	2396	A
1	5	2398	U
1	5	2408	U
1	5	2410	C
1	5	2417	A
1	5	2422	OMC
1	5	2424	OMG
1	5	2425	U
1	5	2433	G
1	5	2434	G
1	5	2441	C
1	5	2447	U
1	5	2450	G
1	5	2453	A
1	5	2471	G
1	5	2475	G
1	5	2488	C
1	5	2489	C
1	5	2490	U
1	5	2491	C
1	5	2503	G
1	5	2504	C
1	5	2505	C
1	5	2506	G
1	5	2513	A
1	5	2520	C
1	5	2529	A
1	5	2537	A
1	5	2544	G
1	5	2546	G
1	5	2547	G
1	5	2553	A
1	5	2554	U
1	5	2560	C
1	5	2566	G
1	5	2570	U

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Mol	Chain	Res	Type
1	5	2571	C
1	5	2575	U
1	5	2583	C
1	5	2586	G
1	5	2587	A
1	5	2589	C
1	5	2600	A
1	5	2602	G
1	5	2611	A
1	5	2618	G
1	5	2620	G
1	5	2627	C
1	5	2638	G
1	5	2639	U
1	5	2649	G
1	5	2653	C
1	5	2659	A
1	5	2661	U
1	5	2662	G
1	5	2663	G
1	5	2669	C
1	5	2670	C
1	5	2673	G
1	5	2676	A
1	5	2681	G
1	5	2686	G
1	5	2687	U
1	5	2695	A
1	5	2696	A
1	5	2707	U
1	5	2708	U
1	5	2709	C
1	5	2711	G
1	5	2714	G
1	5	2715	G
1	5	2716	C
1	5	2721	G
1	5	2723	U
1	5	2725	A
1	5	2726	G
1	5	2740	U
1	5	2743	A

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Mol	Chain	Res	Type
1	5	2744	A
1	5	2763	U
1	5	2764	A
1	5	2768	C
1	5	2787	A
1	5	2788	U
1	5	2790	U
1	5	2794	C
1	5	2798	A
1	5	2803	U
1	5	2814	C
1	5	2826	U
1	5	2827	G
1	5	2829	U
1	5	2842	G
1	5	2855	G
1	5	2856	C
1	5	2898	G
1	5	3598	C
1	5	3603	G
1	5	3604	A
1	5	3605	C
1	5	3606	U
1	5	3615	G
1	5	3616	U
1	5	3625	G
1	5	3626	G
1	5	3630	A
1	5	3635	A
1	5	3646	A
1	5	3650	C
1	5	3658	C
1	5	3662	A
1	5	3664	G
1	5	3673	C
1	5	3691	G
1	5	3692	A
1	5	3705	G
1	5	3711	A
1	5	3712	A
1	5	3714	G
1	5	3729	PSU

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Mol	Chain	Res	Type
1	5	3740	G
1	5	3753	G
1	5	3754	G
1	5	3756	A
1	5	3759	A
1	5	3760	A
1	5	3763	A
1	5	3765	G
1	5	3773	U
1	5	3774	A
1	5	3776	G
1	5	3777	G
1	5	3780	G
1	5	3783	A
1	5	3784	A
1	5	3786	U
1	5	3787	G
1	5	3792	OMG
1	5	3810	C
1	5	3811	G
1	5	3812	C
1	5	3814	U
1	5	3817	A
1	5	3819	G
1	5	3822	U
1	5	3824	A
1	5	3838	U
1	5	3839	G
1	5	3840	U
1	5	3851	U
1	5	3867	A2M
1	5	3868	G
1	5	3876	A
1	5	3877	A
1	5	3878	C
1	5	3879	G
1	5	3889	G
1	5	3892	U
1	5	3898	G
1	5	3901	A
1	5	3905	A
1	5	3906	A

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Mol	Chain	Res	Type
1	5	3907	G
1	5	3908	A
1	5	3915	U
1	5	3916	G
1	5	3917	A
1	5	3927	U
1	5	3938	G
1	5	3939	G
1	5	3941	G
1	5	3955	A
1	5	3957	U
1	5	3962	A
1	5	3963	A
1	5	3965	A
1	5	3966	A
1	5	3970	G
1	5	3972	A
1	5	3976	C
1	5	4042	G
1	5	4047	A
1	5	4050	A
1	5	4051	C
1	5	4052	C
1	5	4054	C
1	5	4055	U
1	5	4061	G
1	5	4065	G
1	5	4066	U
1	5	4073	A
1	5	4076	G
1	5	4083	5MU
1	5	4084	G
1	5	4085	A
1	5	4086	G
1	5	4088	C
1	5	4097	G
1	5	4116	C
1	5	4119	C
1	5	4120	U
1	5	4125	C
1	5	4127	A
1	5	4158	C

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Mol	Chain	Res	Type
1	5	4162	C
1	5	4163	U
1	5	4166	G
1	5	4168	G
1	5	4170	A
1	5	4171	C
1	5	4172	A
1	5	4173	G
1	5	4183	G
1	5	4191	G
1	5	4195	G
1	5	4212	A
1	5	4225	G
1	5	4229	U
1	5	4233	A
1	5	4242	U
1	5	4249	G
1	5	4251	A
1	5	4254	G
1	5	4255	A
1	5	4257	A
1	5	4266	G
1	5	4268	A
1	5	4271	A
1	5	4273	A
1	5	4281	A
1	5	4282	A
1	5	4290	U
1	5	4291	G
1	5	4293	PSU
1	5	4305	G
1	5	4306	OMU
1	5	4308	C
1	5	4314	C
1	5	4317	A
1	5	4318	C
1	5	4319	C
1	5	4330	G
1	5	4332	C
1	5	4348	A
1	5	4349	C
1	5	4364	G

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Mol	Chain	Res	Type
1	5	4368	G
1	5	4372	U
1	5	4373	G
1	5	4376	A
1	5	4377	G
1	5	4378	A
1	5	4380	A
1	5	4387	C
1	5	4394	A
1	5	4395	U
1	5	4396	A
1	5	4398	C
1	5	4401	G
1	5	4413	C
1	5	4415	1MA
1	5	4419	U
1	5	4422	A
1	5	4426	C
1	5	4433	G
1	5	4440	G
1	5	4448	G
1	5	4449	A
1	5	4450	PSU
1	5	4464	A
1	5	4475	G
1	5	4476	C
1	5	4482	U
1	5	4494	OMG
1	5	4500	PSU
1	5	4502	C
1	5	4510	A
1	5	4511	A
1	5	4512	U
1	5	4513	A
1	5	4515	G
1	5	4518	A
1	5	4519	C
1	5	4520	G
1	5	4522	G
1	5	4523	A2M
1	5	4524	G
1	5	4548	A

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Mol	Chain	Res	Type
1	5	4549	G
1	5	4560	C
1	5	4567	G
1	5	4572	U
1	5	4573	G
1	5	4574	U
1	5	4575	G
1	5	4582	C
1	5	4584	A
1	5	4586	G
1	5	4587	G
1	5	4589	A
1	5	4590	A
1	5	4599	A
1	5	4606	G
1	5	4627	U
1	5	4635	A
1	5	4636	PSU
1	5	4637	OMG
1	5	4639	G
1	5	4652	G
1	5	4656	A
1	5	4657	U
1	5	4661	G
1	5	4664	A
1	5	4670	C
1	5	4677	U
1	5	4695	C
1	5	4700	A
1	5	4702	G
1	5	4707	A
1	5	4709	U
1	5	4719	G
1	5	4720	C
1	5	4736	C
1	5	4745	G
1	5	4751	G
1	5	4754	G
1	5	4756	C
1	5	4757	C
1	5	4759	C
1	5	4761	G

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Mol	Chain	Res	Type
1	5	4764	A
1	5	4765	G
1	5	4769	G
1	5	4771	C
1	5	4772	C
1	5	4775	C
1	5	4867	G
1	5	4868	G
1	5	4870	OMG
1	5	4872	2MG
1	5	4875	G
1	5	4877	G
1	5	4881	U
1	5	4882	U
1	5	4883	C
1	5	4885	U
1	5	4887	C
1	5	4895	C
1	5	4903	G
1	5	4910	A
1	5	4912	G
1	5	4914	G
1	5	4915	G
1	5	4920	C
1	5	4921	C
1	5	4922	C
1	5	4925	U
1	5	4926	C
1	5	4928	C
1	5	4929	C
1	5	4931	G
1	5	4934	A
1	5	4935	C
1	5	4937	C
1	5	4940	C
1	5	4944	C
1	5	4948	C
1	5	4949	G
1	5	4950	U
1	5	4951	G
1	5	4955	A
1	5	4956	A

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Mol	Chain	Res	Type
1	5	4957	C
1	5	4958	C
1	5	4960	G
1	5	4965	U
1	5	4967	A
1	5	4975	G
1	5	4976	U
1	5	4985	U
1	5	4988	U
1	5	4990	C
1	5	4991	U
1	5	4993	G
1	5	4999	G
1	5	5006	U
1	5	5014	A
1	5	5017	G
1	5	5022	U
1	5	5040	U
1	5	5041	G
1	5	5047	C
1	5	5050	C
1	5	5052	C
1	5	5053	U
1	5	5054	C
1	5	5058	A
1	5	5061	A
1	5	5062	G
1	5	5069	U
2	7	7	G
2	7	13	A
2	7	25	G
2	7	33	U
2	7	53	U
2	7	54	A
2	7	64	G
2	7	74	A
2	7	80	U
2	7	97	G
2	7	100	A
2	7	106	G
2	7	110	G
2	7	120	U

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Mol	Chain	Res	Type
3	8	2	G
3	8	34	U
3	8	35	C
3	8	38	U
3	8	49	G
3	8	59	A
3	8	62	A
3	8	63	U
3	8	73	U
3	8	75	G
3	8	87	G
3	8	99	U
3	8	103	A
3	8	105	C
3	8	109	C
3	8	110	U
3	8	111	U
3	8	114	G
3	8	123	U
3	8	124	U
3	8	125	C
3	8	126	C
3	8	127	U
3	8	147	G
3	8	156	U
50	9	3	C
50	9	4	C
50	9	14	C
50	9	23	G
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	47	G
50	9	56	G
50	9	58	C
50	9	64	A
50	9	67	C
50	9	68	A

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Mol	Chain	Res	Type
50	9	69	C
50	9	72	C
50	9	73	C
50	9	74	G
50	9	75	G
50	9	77	A
50	9	79	A
50	9	81	U
50	9	103	A
50	9	110	U
50	9	111	A
50	9	113	G
50	9	115	U
50	9	116	OMU
50	9	120	U
50	9	121	OMU
50	9	124	U
50	9	126	G
50	9	127	C
50	9	130	G
50	9	141	A
50	9	143	U
50	9	146	G
50	9	147	A
50	9	155	G
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	170	A
50	9	171	A
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	190	G
50	9	191	A

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Mol	Chain	Res	Type
50	9	192	C
50	9	202	G
50	9	206	G
50	9	215	G
50	9	294	U
50	9	297	A
50	9	304	C
50	9	306	C
50	9	307	G
50	9	308	G
50	9	309	G
50	9	312	G
50	9	313	A
50	9	318	A
50	9	319	C
50	9	332	G
50	9	347	G
50	9	350	C
50	9	351	G
50	9	360	A
50	9	362	C
50	9	364	A
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	407	G
50	9	408	A
50	9	409	C
50	9	417	C
50	9	418	A
50	9	420	G
50	9	429	C
50	9	435	A
50	9	441	C
50	9	448	A
50	9	449	A
50	9	450	C
50	9	455	A

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Mol	Chain	Res	Type
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	480	G
50	9	482	G
50	9	487	U
50	9	492	C
50	9	516	A
50	9	517	OMC
50	9	518	G
50	9	525	A
50	9	530	U
50	9	531	A
50	9	532	C
50	9	533	A
50	9	536	A
50	9	537	C
50	9	544	G
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	563	G
50	9	564	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	603	C

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Mol	Chain	Res	Type
50	9	606	G
50	9	607	U
50	9	608	C
50	9	614	C
50	9	617	G
50	9	621	C
50	9	627	U
50	9	631	U
50	9	643	A
50	9	655	A
50	9	660	C
50	9	662	G
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	678	U
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	811	A
50	9	821	G
50	9	822	PSU
50	9	830	A
50	9	833	C
50	9	834	C
50	9	847	A
50	9	868	G
50	9	870	A
50	9	871	U
50	9	872	A
50	9	873	G
50	9	875	A
50	9	876	C

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Mol	Chain	Res	Type
50	9	877	C
50	9	878	G
50	9	879	C
50	9	885	U
50	9	887	U
50	9	888	U
50	9	890	U
50	9	891	G
50	9	893	U
50	9	894	G
50	9	898	U
50	9	901	G
50	9	902	G
50	9	907	G
50	9	913	A
50	9	914	U
50	9	920	A
50	9	922	A
50	9	933	G
50	9	934	G
50	9	943	U
50	9	971	G
50	9	985	G
50	9	989	C
50	9	990	A
50	9	992	A
50	9	999	G
50	9	1017	U
50	9	1022	U
50	9	1023	A
50	9	1030	A
50	9	1040	G
50	9	1041	G
50	9	1060	A
50	9	1062	A
50	9	1081	PSU
50	9	1083	A
50	9	1085	C
50	9	1086	G
50	9	1087	A
50	9	1088	U
50	9	1097	G

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Mol	Chain	Res	Type
50	9	1100	A
50	9	1109	C
50	9	1110	G
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	1131	G
50	9	1133	A
50	9	1138	C
50	9	1150	A
50	9	1153	C
50	9	1154	U
50	9	1170	A
50	9	1195	A
50	9	1207	G
50	9	1208	A
50	9	1215	C
50	9	1216	C
50	9	1221	G
50	9	1224	G
50	9	1242	U
50	9	1243	PSU
50	9	1249	C
50	9	1250	A
50	9	1251	A
50	9	1253	A
50	9	1256	G
50	9	1257	G
50	9	1259	A
50	9	1265	A
50	9	1273	C
50	9	1274	G
50	9	1275	G
50	9	1282	A
50	9	1284	A
50	9	1285	G
50	9	1293	A
50	9	1298	G

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Mol	Chain	Res	Type
50	9	1300	U
50	9	1301	A
50	9	1302	G
50	9	1304	U
50	9	1307	U
50	9	1308	U
50	9	1309	C
50	9	1312	G
50	9	1314	U
50	9	1315	U
50	9	1322	G
50	9	1327	G
50	9	1333	U
50	9	1341	C
50	9	1342	U
50	9	1348	G
50	9	1358	U
50	9	1371	U
50	9	1372	U
50	9	1376	A
50	9	1378	A
50	9	1395	C
50	9	1396	A
50	9	1397	U
50	9	1398	G
50	9	1399	C
50	9	1401	A
50	9	1402	A
50	9	1404	U
50	9	1428	G
50	9	1454	A
50	9	1455	A
50	9	1462	U
50	9	1463	U
50	9	1464	C
50	9	1465	A
50	9	1466	G
50	9	1473	G
50	9	1475	G
50	9	1476	A
50	9	1477	U
50	9	1480	A

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Mol	Chain	Res	Type
50	9	1486	A
50	9	1489	A
50	9	1490	G
50	9	1494	U
50	9	1497	G
50	9	1498	A
50	9	1506	A
50	9	1510	G
50	9	1521	C
50	9	1522	A
50	9	1533	A
50	9	1544	C
50	9	1548	G
50	9	1552	G
50	9	1553	C
50	9	1554	C
50	9	1556	A
50	9	1557	C
50	9	1560	U
50	9	1570	G
50	9	1574	C
50	9	1575	G
50	9	1580	A
50	9	1585	U
50	9	1586	U
50	9	1587	G
50	9	1588	A
50	9	1597	C
50	9	1601	A
50	9	1602	U
50	9	1603	G
50	9	1604	G
50	9	1606	G
50	9	1621	U
50	9	1623	A
50	9	1625	U
50	9	1637	A
50	9	1638	G
50	9	1648	G
50	9	1649	U
50	9	1663	A
50	9	1664	A

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Mol	Chain	Res	Type
50	9	1665	G
50	9	1683	C
50	9	1695	A
50	9	1698	C
50	9	1699	A
50	9	1702	G
50	9	1721	U
50	9	1722	G
50	9	1725	U
50	9	1726	G
50	9	1742	C
50	9	1744	G
50	9	1748	G
50	9	1757	G
50	9	1779	G
50	9	1783	C
50	9	1784	G
50	9	1785	C
50	9	1800	A
50	9	1824	A
50	9	1825	A
50	9	1826	G
50	9	1831	A
50	9	1835	A
50	9	1836	G
50	9	1838	U
50	9	1849	G
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 (78) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	5	12	A
1	5	125	C
1	5	134	G

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Mol	Chain	Res	Type
1	5	217	C
1	5	245	C
1	5	275	C
1	5	385	A
1	5	406	C
1	5	449	C
1	5	485	C
1	5	492	U
1	5	504	G
1	5	930	G
1	5	1072	C
1	5	1174	G
1	5	1211	G
1	5	1236	C
1	5	1238	A
1	5	1291	G
1	5	1329	G
1	5	1370	G
1	5	1440	U
1	5	1445	U
1	5	1625	OMG
1	5	1633	G
1	5	1804	A
1	5	1818	G
1	5	1979	A
1	5	1983	A
1	5	2046	G
1	5	2089	G
1	5	2266	C
1	5	2474	G
1	5	2502	A
1	5	2546	G
1	5	2587	A
1	5	2661	U
1	5	2695	A
1	5	3603	G
1	5	3625	G
1	5	3876	A
1	5	3888	G
1	5	3904	G
1	5	3954	A
1	5	4053	A

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Mol	Chain	Res	Type
1	5	4065	G
1	5	4075	U
1	5	4115	G
1	5	4119	C
1	5	4232	U
1	5	4254	G
1	5	4378	A
1	5	4448	G
1	5	4699	U
1	5	4719	G
1	5	4884	G
1	5	4925	U
1	5	4936	G
1	5	4947	U
3	8	124	U
50	9	110	U
50	9	434	G
50	9	465	A
50	9	479	C
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	1394	G
50	9	1395	C
50	9	1489	A
50	9	1520	G
50	9	1637	A
50	9	1664	A

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

138 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$
1	OMC	5	3869	1	19,22,23	2.81	7 (36%)	25,31,34	0.85	1 (4%)
1	OMG	5	4637	1	19,26,27	2.37	8 (42%)	21,38,41	1.44	4 (19%)
1	5MU	5	4083	1	19,22,23	4.71	7 (36%)	27,32,35	3.46	9 (33%)
1	5MC	5	4447	1	19,22,23	3.85	8 (42%)	26,32,35	1.13	1 (3%)
50	OMC	9	174	50	19,22,23	2.97	7 (36%)	25,31,34	0.83	1 (4%)
50	A2M	9	484	50	18,25,26	4.93	9 (50%)	20,36,39	2.67	3 (15%)
1	B8H	5	3762	1	19,22,23	6.86	6 (31%)	21,32,35	2.63	5 (23%)
1	OMC	5	3887	1	19,22,23	2.87	7 (36%)	25,31,34	0.96	1 (4%)
1	A2M	5	3825	1	18,25,26	4.93	7 (38%)	20,36,39	2.77	5 (25%)
1	B8T	5	4483	1	19,22,23	3.02	8 (42%)	25,31,34	1.07	2 (8%)
50	OMC	9	517	50	19,22,23	2.85	7 (36%)	25,31,34	0.65	0
50	5MC	9	1374	50	19,22,23	3.92	8 (42%)	26,32,35	1.35	3 (11%)
1	E7G	5	1797	1	24,27,28	3.26	11 (45%)	28,40,43	2.33	10 (35%)
1	BGH	5	3899	84,1	25,29,30	4.21	15 (60%)	30,43,46	2.68	14 (46%)
1	A2M	5	2401	84,1	18,25,26	4.91	9 (50%)	20,36,39	2.81	6 (30%)
1	MHG	5	4371	1	29,32,33	3.69	11 (37%)	34,46,49	2.43	12 (35%)
1	OMC	5	3909	1	19,22,23	2.85	7 (36%)	25,31,34	1.31	3 (12%)
1	OMG	5	1522	1	19,26,27	2.39	8 (42%)	21,38,41	1.53	4 (19%)
50	PSU	9	612	50	18,21,22	1.00	1 (5%)	21,30,33	1.87	5 (23%)
1	UR3	5	4597	1	19,22,23	2.56	7 (36%)	26,32,35	1.47	4 (15%)
1	B8H	5	4296	1	19,22,23	6.87	6 (31%)	21,32,35	2.64	5 (23%)
50	4AC	9	1842	50	21,24,25	3.11	10 (47%)	28,34,37	1.21	4 (14%)
1	5MC	5	4335	1	19,22,23	3.89	8 (42%)	26,32,35	1.19	3 (11%)
1	B8K	5	4690	1	24,28,29	4.86	17 (70%)	29,42,45	2.85	11 (37%)
50	5MU	9	814	50	19,22,23	4.93	7 (36%)	27,32,35	3.58	12 (44%)
1	B8W	5	4129	1	18,26,27	4.35	7 (38%)	17,38,41	7.37	10 (58%)
50	4AC	9	1337	50	21,24,25	3.17	9 (42%)	28,34,37	1.27	4 (14%)
1	PSU	5	2508	1	18,21,22	1.03	1 (5%)	21,30,33	1.79	4 (19%)
6	MLZ	C	333	6	8,9,10	0.84	0	4,9,11	0.70	0
1	2MG	5	729	1	18,26,27	2.46	7 (38%)	16,38,41	1.47	4 (25%)
1	OMC	5	4536	1	19,22,23	2.83	7 (36%)	25,31,34	1.07	2 (8%)
1	7MG	5	4550	1	23,26,27	3.27	10 (43%)	27,39,42	2.09	10 (37%)
1	PSU	5	3729	1	18,21,22	1.10	1 (5%)	21,30,33	1.87	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
50	OMG	9	644	50	19,26,27	2.42	8 (42%)	21,38,41	1.45	4 (19%)
50	PSU	9	1243	84,50	18,21,22	1.10	1 (5%)	21,30,33	1.97	4 (19%)
50	OMC	9	1710	50	19,22,23	2.96	7 (36%)	25,31,34	0.95	1 (4%)
1	OMC	5	2861	1	19,22,23	2.85	7 (36%)	25,31,34	0.91	1 (4%)
1	5MC	5	3782	1	19,22,23	3.69	8 (42%)	26,32,35	1.05	1 (3%)
1	PSU	5	4500	1	18,21,22	1.08	3 (16%)	21,30,33	2.06	5 (23%)
1	PSU	5	4450	84,1	18,21,22	1.09	3 (16%)	21,30,33	2.12	5 (23%)
1	OMC	5	3701	84,1	19,22,23	2.82	7 (36%)	25,31,34	0.75	0
1	I4U	5	4194	1	20,24,25	5.01	13 (65%)	27,34,37	1.82	4 (14%)
1	OMG	5	4370	1	19,26,27	2.38	8 (42%)	21,38,41	1.49	4 (19%)
1	OMC	5	2365	1	19,22,23	2.84	7 (36%)	25,31,34	0.70	0
1	PSU	5	4636	1	18,21,22	1.08	2 (11%)	21,30,33	2.12	5 (23%)
1	B9B	5	2754	84,1	20,28,29	5.07	8 (40%)	19,40,43	2.39	7 (36%)
1	P7G	5	1909	1	24,28,29	3.70	11 (45%)	25,41,44	1.28	2 (8%)
1	B8T	5	4671	1	19,22,23	3.01	8 (42%)	25,31,34	0.95	1 (4%)
1	UR3	5	1866	1	19,22,23	2.55	6 (31%)	26,32,35	1.58	5 (19%)
50	OMG	9	683	50	19,26,27	2.42	8 (42%)	21,38,41	1.50	5 (23%)
1	6MZ	5	4220	1	17,25,26	1.78	3 (17%)	15,36,39	2.07	3 (20%)
1	2MG	5	4872	1	18,26,27	2.67	7 (38%)	16,38,41	3.32	6 (37%)
50	A2M	9	668	84,50	18,25,26	4.88	7 (38%)	20,36,39	3.02	7 (35%)
1	A2M	5	3785	1	18,25,26	4.78	10 (55%)	20,36,39	3.09	5 (25%)
48	DDE	v	715	48	15,20,21	1.01	0	11,28,30	1.32	2 (18%)
50	E3C	9	568	50	19,23,24	3.37	6 (31%)	21,33,36	2.46	6 (28%)
50	6MZ	9	1832	84,50	17,25,26	1.55	3 (17%)	15,36,39	1.87	2 (13%)
1	1MA	5	4415	1	17,25,26	3.83	4 (23%)	17,37,40	1.86	3 (17%)
50	B8Q	9	1219	50	18,22,23	2.94	4 (22%)	21,32,35	2.24	7 (33%)
1	M7A	5	4564	1	19,25,26	1.61	4 (21%)	25,37,40	3.97	8 (32%)
50	PSU	9	119	50	18,21,22	0.96	1 (5%)	21,30,33	1.71	5 (23%)
1	A2M	5	2363	84,1	18,25,26	5.02	9 (50%)	20,36,39	2.82	4 (20%)
1	E6G	5	4355	1	19,27,28	4.71	7 (36%)	18,39,42	2.39	6 (33%)
50	PSU	9	823	50	18,21,22	1.11	2 (11%)	21,30,33	1.95	4 (19%)
1	B8H	5	1860	1	19,22,23	6.83	6 (31%)	21,32,35	2.39	5 (23%)
50	UR3	9	1830	50	19,22,23	2.75	7 (36%)	26,32,35	1.81	5 (19%)
1	B8W	5	2380	1	18,26,27	4.23	6 (33%)	17,38,41	7.14	9 (52%)
50	M7A	9	1806	50	19,25,26	1.62	2 (10%)	25,37,40	3.94	8 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	5	4531	1	18,21,22	1.11	3 (16%)	21,30,33	2.05	5 (23%)
1	B9H	5	2786	1	21,25,26	2.99	3 (14%)	22,35,38	1.79	3 (13%)
1	7MG	5	2522	1	23,26,27	3.24	10 (43%)	27,39,42	2.11	9 (33%)
1	A2M	5	4523	84,1	18,25,26	5.04	9 (50%)	20,36,39	2.74	5 (25%)
1	A2M	5	3867	1	18,25,26	4.91	9 (50%)	20,36,39	2.59	4 (20%)
1	PSU	5	4403	1	18,21,22	1.04	1 (5%)	21,30,33	1.99	4 (19%)
1	OMG	5	2050	1	19,26,27	2.39	8 (42%)	21,38,41	1.44	4 (19%)
1	OMG	5	2424	1	19,26,27	2.46	8 (42%)	21,38,41	1.49	4 (19%)
1	OMG	5	4196	1	19,26,27	2.36	8 (42%)	21,38,41	1.45	4 (19%)
1	OMG	5	2773	1	19,26,27	2.45	8 (42%)	21,38,41	1.48	4 (19%)
1	P7G	5	3880	1	24,28,29	3.52	10 (41%)	25,41,44	1.33	2 (8%)
50	A2M	9	1031	50	18,25,26	4.96	8 (44%)	20,36,39	2.92	5 (25%)
1	PSU	5	3764	1	18,21,22	1.05	1 (5%)	21,30,33	1.81	4 (19%)
50	MA6	9	1850	50	19,26,27	1.66	2 (10%)	18,38,41	2.85	3 (16%)
1	UR3	5	4530	1	19,22,23	2.71	7 (36%)	26,32,35	1.70	5 (19%)
1	B9B	5	1574	1	20,28,29	5.06	8 (40%)	19,40,43	2.07	6 (31%)
1	OMU	5	4620	1	19,22,23	2.74	7 (36%)	25,31,34	1.95	5 (20%)
50	A2M	9	166	50	18,25,26	5.02	9 (50%)	20,36,39	2.76	4 (20%)
1	PSU	5	1683	1	18,21,22	1.13	2 (11%)	21,30,33	1.97	4 (19%)
1	OMC	5	2422	84,1	19,22,23	2.88	7 (36%)	25,31,34	1.00	1 (4%)
1	B8W	5	4529	84,1	18,26,27	4.26	7 (38%)	17,38,41	7.41	10 (58%)
1	B9B	5	237	1	20,28,29	5.13	8 (40%)	19,40,43	2.50	5 (26%)
1	OMG	5	373	1	19,26,27	2.42	8 (42%)	21,38,41	1.63	5 (23%)
1	OMG	5	1316	1	19,26,27	2.41	8 (42%)	21,38,41	1.61	4 (19%)
1	A2M	5	3723	1	18,25,26	5.09	9 (50%)	20,36,39	2.61	4 (20%)
1	I4U	5	1659	1	20,24,25	5.00	14 (70%)	27,34,37	2.22	3 (11%)
1	A2M	5	398	1	18,25,26	5.04	9 (50%)	20,36,39	2.56	4 (20%)
1	A2M	5	1534	84,1	18,25,26	4.86	9 (50%)	20,36,39	3.01	5 (25%)
50	B8N	9	1248	84,50	25,29,30	3.09	7 (28%)	28,42,45	2.00	7 (25%)
1	2MG	5	1517	1	18,26,27	2.58	7 (38%)	16,38,41	1.83	5 (31%)
50	PSU	9	1081	50	18,21,22	1.08	2 (11%)	21,30,33	1.91	5 (23%)
1	OMG	5	2364	1	19,26,27	2.42	8 (42%)	21,38,41	1.59	4 (19%)
1	A2M	5	1524	1	18,25,26	4.94	9 (50%)	20,36,39	3.34	6 (30%)
1	7MG	5	1605	1	23,26,27	3.25	10 (43%)	27,39,42	2.18	9 (33%)
1	A2M	5	4571	1	18,25,26	4.98	8 (44%)	20,36,39	2.72	4 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
50	OMU	9	116	50	19,22,23	2.93	7 (36%)	25,31,34	1.86	5 (20%)
3	OMU	8	14	3,1	19,22,23	2.88	7 (36%)	25,31,34	1.97	7 (28%)
1	PSU	5	4442	1	18,21,22	1.08	3 (16%)	21,30,33	1.98	5 (23%)
1	OMG	5	1625	84,1	19,26,27	2.41	8 (42%)	21,38,41	1.46	4 (19%)
1	1MA	5	1322	84,1	17,25,26	3.70	4 (23%)	17,37,40	1.79	3 (17%)
50	OMU	9	121	50	19,22,23	3.00	8 (42%)	25,31,34	1.87	5 (20%)
50	PSU	9	822	50	18,21,22	1.05	2 (11%)	21,30,33	2.07	5 (23%)
1	E7G	5	2297	1	24,27,28	3.11	11 (45%)	28,40,43	2.24	9 (32%)
50	MA6	9	1851	50	19,26,27	1.69	2 (10%)	18,38,41	2.76	3 (16%)
1	PSU	5	4628	1	18,21,22	1.15	3 (16%)	21,30,33	2.23	5 (23%)
1	A2M	5	1871	84,1	18,25,26	4.92	9 (50%)	20,36,39	2.83	5 (25%)
1	PSU	5	1677	1	18,21,22	1.12	3 (16%)	21,30,33	2.04	6 (28%)
1	B8K	5	3897	1	24,28,29	4.76	17 (70%)	29,42,45	2.61	12 (41%)
50	A2M	9	159	50	18,25,26	5.06	8 (44%)	20,36,39	2.99	5 (25%)
1	OMU	5	4306	1	19,22,23	2.83	8 (42%)	25,31,34	1.86	5 (20%)
41	MLZ	m	72	41	8,9,10	0.78	0	4,9,11	0.78	0
1	OMG	5	4494	1	19,26,27	2.42	8 (42%)	21,38,41	1.51	4 (19%)
50	OMC	9	1703	50	19,22,23	2.95	7 (36%)	25,31,34	0.86	1 (4%)
50	A2M	9	27	84,50	18,25,26	4.89	8 (44%)	20,36,39	2.72	5 (25%)
1	PSU	5	1582	1	18,21,22	1.10	1 (5%)	21,30,33	1.85	4 (19%)
1	B8W	5	4185	1	18,26,27	4.27	7 (38%)	17,38,41	7.23	11 (64%)
1	B8Q	5	1456	1	18,22,23	2.75	5 (27%)	21,32,35	1.90	4 (19%)
1	OMG	5	1883	1	19,26,27	2.44	8 (42%)	21,38,41	1.61	4 (19%)
1	OMC	5	2804	1	19,22,23	2.87	7 (36%)	25,31,34	0.83	0
1	B8W	5	4472	1	18,26,27	4.25	7 (38%)	17,38,41	6.96	9 (52%)
1	PSU	5	3715	1	18,21,22	1.05	1 (5%)	21,30,33	1.83	4 (19%)
1	P4U	5	1348	84,1	21,24,25	3.28	7 (33%)	28,33,36	1.94	3 (10%)
50	A2M	9	1678	50	18,25,26	5.06	9 (50%)	20,36,39	2.86	4 (20%)
50	OMG	9	509	84,50	19,26,27	2.41	8 (42%)	21,38,41	1.40	4 (19%)
1	A2M	5	1326	1	18,25,26	4.85	10 (55%)	20,36,39	2.57	3 (15%)
1	OMG	5	4623	1	19,26,27	2.41	8 (42%)	21,38,41	1.57	4 (19%)
1	OMG	5	4870	1	19,26,27	2.41	7 (36%)	21,38,41	1.49	4 (19%)
1	A2M	5	3718	1	18,25,26	5.01	10 (55%)	20,36,39	2.49	4 (20%)
1	PSU	5	4293	1	18,21,22	1.11	2 (11%)	21,30,33	1.88	3 (14%)
1	OMG	5	3792	1	19,26,27	2.45	8 (42%)	21,38,41	1.57	4 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMC	5	3869	1	-	0/9/27/28	0/2/2/2
1	OMG	5	4637	1	-	3/5/27/28	0/3/3/3
1	5MU	5	4083	1	-	6/7/25/26	0/2/2/2
1	5MC	5	4447	1	-	4/7/25/26	0/2/2/2
50	OMC	9	174	50	-	0/9/27/28	0/2/2/2
50	A2M	9	484	50	-	0/5/27/28	0/3/3/3
1	B8H	5	3762	1	-	0/7/25/26	0/2/2/2
1	OMC	5	3887	1	-	1/9/27/28	0/2/2/2
1	A2M	5	3825	1	-	0/5/27/28	0/3/3/3
1	B8T	5	4483	1	-	2/7/27/28	0/2/2/2
50	OMC	9	517	50	-	2/9/27/28	0/2/2/2
50	5MC	9	1374	50	-	0/7/25/26	0/2/2/2
1	E7G	5	1797	1	-	3/9/39/40	0/3/3/3
1	BGH	5	3899	84,1	-	2/13/43/44	0/3/3/3
1	A2M	5	2401	84,1	-	2/5/27/28	0/3/3/3
1	MHG	5	4371	1	-	5/16/46/47	0/3/3/3
1	OMC	5	3909	1	-	1/9/27/28	0/2/2/2
1	OMG	5	1522	1	-	0/5/27/28	0/3/3/3
50	PSU	9	612	50	-	0/7/25/26	0/2/2/2
1	UR3	5	4597	1	-	0/7/25/26	0/2/2/2
1	B8H	5	4296	1	-	1/7/25/26	0/2/2/2
50	4AC	9	1842	50	-	0/11/29/30	0/2/2/2
1	5MC	5	4335	1	-	0/7/25/26	0/2/2/2
1	B8K	5	4690	1	-	0/11/41/42	0/3/3/3
50	5MU	9	814	50	-	0/7/25/26	0/2/2/2
1	B8W	5	4129	1	-	2/5/27/28	0/3/3/3
50	4AC	9	1337	50	-	0/11/29/30	0/2/2/2
1	PSU	5	2508	1	-	0/7/25/26	0/2/2/2
6	MLZ	C	333	6	-	2/7/8/10	-
1	2MG	5	729	1	-	2/5/27/28	0/3/3/3
1	OMC	5	4536	1	-	0/9/27/28	0/2/2/2
1	7MG	5	4550	1	-	0/7/37/38	0/3/3/3
1	PSU	5	3729	1	-	2/7/25/26	0/2/2/2
50	OMG	9	644	50	-	1/5/27/28	0/3/3/3
50	PSU	9	1243	84,50	-	2/7/25/26	0/2/2/2
50	OMC	9	1710	50	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMC	5	2861	1	-	0/9/27/28	0/2/2/2
1	5MC	5	3782	1	-	0/7/25/26	0/2/2/2
1	PSU	5	4500	1	-	3/7/25/26	0/2/2/2
1	PSU	5	4450	84,1	-	3/7/25/26	0/2/2/2
1	OMC	5	3701	84,1	-	4/9/27/28	0/2/2/2
1	I4U	5	4194	1	-	4/9/29/30	0/2/2/2
1	OMG	5	4370	1	-	0/5/27/28	0/3/3/3
1	OMC	5	2365	1	-	0/9/27/28	0/2/2/2
1	PSU	5	4636	1	-	4/7/25/26	0/2/2/2
1	B9B	5	2754	84,1	-	1/7/29/30	0/3/3/3
1	P7G	5	1909	1	-	3/10/40/41	0/3/3/3
1	B8T	5	4671	1	-	0/7/27/28	0/2/2/2
1	UR3	5	1866	1	-	1/7/25/26	0/2/2/2
50	OMG	9	683	50	-	2/5/27/28	0/3/3/3
1	6MZ	5	4220	1	-	0/5/27/28	0/3/3/3
1	2MG	5	4872	1	-	1/5/27/28	0/3/3/3
50	A2M	9	668	84,50	-	4/5/27/28	0/3/3/3
1	A2M	5	3785	1	-	2/5/27/28	0/3/3/3
48	DDE	v	715	48	-	15/20/21/23	0/1/1/1
50	E3C	9	568	50	-	4/9/44/45	0/2/2/2
50	6MZ	9	1832	84,50	-	2/5/27/28	0/3/3/3
1	1MA	5	4415	1	-	2/3/25/26	0/3/3/3
50	B8Q	9	1219	50	-	0/7/42/43	0/2/2/2
1	M7A	5	4564	1	-	0/7/37/38	0/3/3/3
50	PSU	9	119	50	-	2/7/25/26	0/2/2/2
1	A2M	5	2363	84,1	-	0/5/27/28	0/3/3/3
1	E6G	5	4355	1	-	5/6/28/29	0/3/3/3
50	PSU	9	823	50	-	0/7/25/26	0/2/2/2
1	B8H	5	1860	1	-	2/7/25/26	0/2/2/2
50	UR3	9	1830	50	-	4/7/25/26	0/2/2/2
1	B8W	5	2380	1	-	5/5/27/28	0/3/3/3
50	M7A	9	1806	50	-	0/7/37/38	0/3/3/3
1	PSU	5	4531	1	-	0/7/25/26	0/2/2/2
1	B9H	5	2786	1	-	3/12/47/48	0/2/2/2
1	7MG	5	2522	1	-	0/7/37/38	0/3/3/3
1	A2M	5	4523	84,1	-	2/5/27/28	0/3/3/3
1	A2M	5	3867	1	-	4/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	5	4403	1	-	2/7/25/26	0/2/2/2
1	OMG	5	2050	1	-	0/5/27/28	0/3/3/3
1	OMG	5	2424	1	-	2/5/27/28	0/3/3/3
1	OMG	5	4196	1	-	0/5/27/28	0/3/3/3
1	OMG	5	2773	1	-	0/5/27/28	0/3/3/3
1	P7G	5	3880	1	-	3/10/40/41	0/3/3/3
50	A2M	9	1031	50	-	0/5/27/28	0/3/3/3
1	PSU	5	3764	1	-	2/7/25/26	0/2/2/2
50	MA6	9	1850	50	-	1/7/29/30	0/3/3/3
1	UR3	5	4530	1	-	1/7/25/26	0/2/2/2
1	B9B	5	1574	1	-	3/7/29/30	0/3/3/3
1	OMU	5	4620	1	-	0/9/27/28	0/2/2/2
50	A2M	9	166	50	-	2/5/27/28	0/3/3/3
1	PSU	5	1683	1	-	0/7/25/26	0/2/2/2
1	OMC	5	2422	84,1	-	0/9/27/28	0/2/2/2
1	B8W	5	4529	84,1	-	2/5/27/28	0/3/3/3
1	B9B	5	237	1	-	4/7/29/30	0/3/3/3
1	OMG	5	373	1	-	1/5/27/28	0/3/3/3
1	OMG	5	1316	1	-	0/5/27/28	0/3/3/3
1	A2M	5	3723	1	-	0/5/27/28	0/3/3/3
1	I4U	5	1659	1	-	2/9/29/30	0/2/2/2
1	A2M	5	398	1	-	2/5/27/28	0/3/3/3
1	A2M	5	1534	84,1	-	1/5/27/28	0/3/3/3
50	B8N	9	1248	84,50	-	2/16/34/35	0/2/2/2
1	2MG	5	1517	1	-	0/5/27/28	0/3/3/3
50	PSU	9	1081	50	-	3/7/25/26	0/2/2/2
1	OMG	5	2364	1	-	2/5/27/28	0/3/3/3
1	A2M	5	1524	1	-	0/5/27/28	0/3/3/3
1	7MG	5	1605	1	-	0/7/37/38	0/3/3/3
1	A2M	5	4571	1	-	0/5/27/28	0/3/3/3
50	OMU	9	116	50	-	3/9/27/28	0/2/2/2
3	OMU	8	14	3,1	-	1/9/27/28	0/2/2/2
1	PSU	5	4442	1	-	0/7/25/26	0/2/2/2
1	OMG	5	1625	84,1	-	3/5/27/28	0/3/3/3
1	1MA	5	1322	84,1	-	0/3/25/26	0/3/3/3
50	OMU	9	121	50	-	2/9/27/28	0/2/2/2
50	PSU	9	822	50	-	2/7/25/26	0/2/2/2
1	E7G	5	2297	1	-	1/9/39/40	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	MA6	9	1851	50	-	3/7/29/30	0/3/3/3
1	PSU	5	4628	1	-	0/7/25/26	0/2/2/2
1	A2M	5	1871	84,1	-	0/5/27/28	0/3/3/3
1	PSU	5	1677	1	-	2/7/25/26	0/2/2/2
1	B8K	5	3897	1	-	3/11/41/42	0/3/3/3
50	A2M	9	159	50	-	3/5/27/28	0/3/3/3
1	OMU	5	4306	1	-	1/9/27/28	0/2/2/2
41	MLZ	m	72	41	-	3/7/8/10	-
1	OMG	5	4494	1	-	2/5/27/28	0/3/3/3
50	OMC	9	1703	50	-	2/9/27/28	0/2/2/2
50	A2M	9	27	84,50	-	0/5/27/28	0/3/3/3
1	PSU	5	1582	1	-	2/7/25/26	0/2/2/2
1	B8W	5	4185	1	-	4/5/27/28	0/3/3/3
1	B8Q	5	1456	1	-	2/7/42/43	0/2/2/2
1	OMG	5	1883	1	-	0/5/27/28	0/3/3/3
1	OMC	5	2804	1	-	0/9/27/28	0/2/2/2
1	B8W	5	4472	1	-	2/5/27/28	0/3/3/3
1	PSU	5	3715	1	-	0/7/25/26	0/2/2/2
1	P4U	5	1348	84,1	-	4/10/29/30	0/2/2/2
50	A2M	9	1678	50	-	0/5/27/28	0/3/3/3
50	OMG	9	509	84,50	-	0/5/27/28	0/3/3/3
1	A2M	5	1326	1	-	0/5/27/28	0/3/3/3
1	OMG	5	4623	1	-	0/5/27/28	0/3/3/3
1	OMG	5	4870	1	-	4/5/27/28	0/3/3/3
1	A2M	5	3718	1	-	0/5/27/28	0/3/3/3
1	PSU	5	4293	1	-	0/7/25/26	0/2/2/2
1	OMG	5	3792	1	-	2/5/27/28	0/3/3/3

All (930) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	237	B9B	O4'-C1'	18.41	1.65	1.40
1	5	1574	B9B	O4'-C1'	18.07	1.64	1.40
1	5	2754	B9B	O4'-C1'	18.02	1.64	1.40
1	5	3723	A2M	O4'-C1'	17.79	1.64	1.40
1	5	4523	A2M	O4'-C1'	17.66	1.64	1.40
50	9	166	A2M	O4'-C1'	17.61	1.64	1.40
50	9	1678	A2M	O4'-C1'	17.58	1.64	1.40
50	9	159	A2M	O4'-C1'	17.56	1.63	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	398	A2M	O4'-C1'	17.54	1.63	1.40
1	5	3718	A2M	O4'-C1'	17.46	1.63	1.40
1	5	2363	A2M	O4'-C1'	17.29	1.63	1.40
50	9	1031	A2M	O4'-C1'	17.25	1.63	1.40
1	5	4571	A2M	O4'-C1'	17.21	1.63	1.40
50	9	484	A2M	O4'-C1'	17.02	1.63	1.40
1	5	1871	A2M	O4'-C1'	16.98	1.63	1.40
1	5	3825	A2M	O4'-C1'	16.96	1.63	1.40
1	5	1524	A2M	O4'-C1'	16.93	1.63	1.40
50	9	27	A2M	O4'-C1'	16.84	1.63	1.40
1	5	2401	A2M	O4'-C1'	16.82	1.63	1.40
1	5	3867	A2M	O4'-C1'	16.77	1.62	1.40
1	5	1534	A2M	O4'-C1'	16.64	1.62	1.40
1	5	1326	A2M	O4'-C1'	16.51	1.62	1.40
50	9	668	A2M	O4'-C1'	16.48	1.62	1.40
1	5	4355	E6G	O4'-C1'	16.36	1.62	1.40
1	5	3785	A2M	O4'-C1'	16.27	1.62	1.40
1	5	4296	B8H	C6-C5	-16.02	1.12	1.35
1	5	3762	B8H	C6-C5	-15.66	1.12	1.35
1	5	1860	B8H	C6-C5	-15.66	1.12	1.35
1	5	4296	B8H	C4-N3	-14.97	1.10	1.38
1	5	4129	B8W	O4'-C1'	14.82	1.60	1.40
1	5	3762	B8H	C4-N3	-14.81	1.11	1.38
1	5	1860	B8H	C4-N3	-14.72	1.11	1.38
1	5	4415	1MA	C2-N3	14.45	1.46	1.28
1	5	2380	B8W	O4'-C1'	14.41	1.59	1.40
1	5	4529	B8W	O4'-C1'	14.39	1.59	1.40
1	5	4472	B8W	O4'-C1'	14.37	1.59	1.40
1	5	4185	B8W	O4'-C1'	14.34	1.59	1.40
1	5	3762	B8H	C4-C5	14.10	1.83	1.44
1	5	1322	1MA	C2-N3	14.03	1.45	1.28
1	5	1860	B8H	C4-C5	13.89	1.82	1.44
1	5	4296	B8H	C4-C5	13.79	1.82	1.44
1	5	1860	B8H	C6-N1	13.44	1.68	1.36
1	5	3762	B8H	C6-N1	13.41	1.68	1.36
1	5	4296	B8H	C6-N1	13.19	1.68	1.36
50	9	814	5MU	C2-N1	11.72	1.56	1.38
1	5	4690	B8K	C3'-C4'	-11.59	1.23	1.53
1	5	1659	I4U	C3'-C2'	-11.43	1.22	1.53
1	5	3897	B8K	C3'-C4'	-11.34	1.24	1.53
1	5	4194	I4U	C3'-C2'	-11.30	1.22	1.53
1	5	4083	5MU	C6-N1	10.53	1.55	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	1909	P7G	C8-N9	10.48	1.52	1.45
1	5	1659	I4U	C4-N3	10.48	1.44	1.31
1	5	3899	BGH	C3'-C4'	-10.40	1.26	1.53
50	9	814	5MU	C6-N1	10.32	1.55	1.38
1	5	4194	I4U	C4-N3	10.08	1.44	1.31
1	5	4083	5MU	C2-N1	9.79	1.53	1.38
1	5	1348	P4U	C4-N3	9.76	1.44	1.31
1	5	3899	BGH	O4'-C4'	9.74	1.66	1.45
50	9	814	5MU	C4-C5	9.67	1.60	1.44
1	5	4083	5MU	C4-C5	9.52	1.60	1.44
1	5	4447	5MC	C6-C5	9.51	1.50	1.34
50	9	1374	5MC	C6-C5	9.42	1.49	1.34
1	5	4371	MHG	C8-N9	9.30	1.51	1.45
1	5	3880	P7G	C8-N9	9.27	1.51	1.45
50	9	1219	B8Q	C6-C5	9.08	1.52	1.33
1	5	1456	B8Q	C6-C5	9.00	1.52	1.33
1	5	3782	5MC	C6-C5	8.95	1.49	1.34
1	5	4335	5MC	C6-C5	8.92	1.49	1.34
1	5	2786	B9H	C2-N3	8.83	1.48	1.37
1	5	4083	5MU	C4-N3	-8.52	1.22	1.38
1	5	4194	I4U	O4'-C4'	-8.44	1.26	1.45
50	9	568	E3C	C2-N3	8.41	1.48	1.37
1	5	4690	B8K	C8-N9	8.38	1.51	1.45
50	9	814	5MU	C4-N3	-8.36	1.23	1.38
1	5	3897	B8K	C2'-C1'	-8.31	1.27	1.53
50	9	1248	B8N	C4-N3	-8.29	1.25	1.40
1	5	4690	B8K	C2'-C1'	-8.25	1.27	1.53
50	9	568	E3C	C2-N1	8.23	1.49	1.38
1	5	4371	MHG	C5-N7	8.14	1.45	1.35
1	5	4371	MHG	C2-N3	8.14	1.47	1.32
1	5	1909	P7G	C5-N7	8.00	1.45	1.35
50	9	668	A2M	O4'-C4'	-7.96	1.27	1.45
1	5	4355	E6G	O4'-C4'	-7.96	1.27	1.45
1	5	1659	I4U	O4'-C4'	-7.93	1.27	1.45
1	5	3880	P7G	C5-N7	7.85	1.45	1.35
1	5	2363	A2M	O4'-C4'	-7.78	1.27	1.45
1	5	1524	A2M	O4'-C4'	-7.68	1.27	1.45
1	5	3867	A2M	O4'-C4'	-7.62	1.28	1.45
50	9	159	A2M	O4'-C4'	-7.58	1.28	1.45
1	5	1326	A2M	O4'-C4'	-7.56	1.28	1.45
50	9	484	A2M	O4'-C4'	-7.56	1.28	1.45
1	5	2401	A2M	O4'-C4'	-7.55	1.28	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	3897	B8K	O4'-C4'	7.55	1.61	1.45
50	9	1678	A2M	O4'-C4'	-7.55	1.28	1.45
1	5	3825	A2M	O4'-C4'	-7.54	1.28	1.45
1	5	4571	A2M	O4'-C4'	-7.50	1.28	1.45
1	5	4523	A2M	O4'-C4'	-7.48	1.28	1.45
1	5	398	A2M	O4'-C4'	-7.47	1.28	1.45
1	5	2786	B9H	C6-C5	7.44	1.48	1.33
50	9	1830	UR3	C2-N1	7.43	1.48	1.38
50	9	27	A2M	O4'-C4'	-7.43	1.28	1.45
1	5	1534	A2M	O4'-C4'	-7.42	1.28	1.45
50	9	1031	A2M	O4'-C4'	-7.41	1.28	1.45
1	5	3718	A2M	O4'-C4'	-7.41	1.28	1.45
1	5	1871	A2M	O4'-C4'	-7.37	1.28	1.45
50	9	1248	B8N	C6-N1	7.37	1.54	1.36
1	5	1797	E7G	C5-N7	7.37	1.44	1.35
1	5	3723	A2M	O4'-C4'	-7.30	1.28	1.45
1	5	3785	A2M	O4'-C4'	-7.28	1.28	1.45
1	5	237	B9B	O4'-C4'	-7.28	1.28	1.45
1	5	2754	B9B	C2-N2	7.25	1.48	1.33
50	9	166	A2M	O4'-C4'	-7.24	1.28	1.45
1	5	2754	B9B	O6-C6	7.24	1.43	1.34
50	9	568	E3C	C6-C5	7.23	1.48	1.33
1	5	237	B9B	C2-N2	7.23	1.48	1.33
1	5	4530	UR3	C2-N1	7.22	1.48	1.38
1	5	4335	5MC	C4-N3	7.19	1.45	1.34
1	5	4690	B8K	O4'-C4'	7.15	1.60	1.45
1	5	1574	B9B	O4'-C4'	-7.14	1.29	1.45
1	5	4550	7MG	C5-N7	7.14	1.44	1.35
1	5	2754	B9B	O4'-C4'	-7.10	1.29	1.45
1	5	1574	B9B	C2-N2	7.04	1.47	1.33
1	5	4550	7MG	C8-N9	7.02	1.50	1.45
1	5	2297	E7G	C5-N7	7.01	1.44	1.35
1	5	3782	5MC	C4-N3	7.01	1.45	1.34
1	5	4472	B8W	C3'-C4'	-6.99	1.35	1.53
1	5	2522	7MG	C8-N9	6.99	1.50	1.45
1	5	1574	B9B	O6-C6	6.99	1.43	1.34
50	9	1842	4AC	C4-N3	6.97	1.44	1.32
50	9	121	OMU	C2-N1	6.94	1.49	1.38
1	5	4185	B8W	C3'-C4'	-6.92	1.35	1.53
1	5	237	B9B	O6-C6	6.91	1.43	1.34
1	5	1797	E7G	C8-N9	6.88	1.50	1.45
1	5	2522	7MG	C5-N7	6.87	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	9	1374	5MC	C4-N3	6.87	1.45	1.34
1	5	4129	B8W	C3'-C4'	-6.85	1.35	1.53
1	5	4447	5MC	C4-N3	6.82	1.45	1.34
50	9	1337	4AC	C4-N3	6.80	1.44	1.32
50	9	116	OMU	C2-N3	6.78	1.49	1.38
50	9	116	OMU	C2-N1	6.76	1.49	1.38
1	5	1605	7MG	C5-N7	6.73	1.44	1.35
3	8	14	OMU	C2-N3	6.72	1.49	1.38
1	5	4529	B8W	C3'-C4'	-6.71	1.36	1.53
50	9	1248	B8N	C4-C5	6.68	1.62	1.47
1	5	4335	5MC	C5-C4	6.64	1.49	1.44
50	9	121	OMU	C2-N3	6.62	1.49	1.38
1	5	4306	OMU	C2-N3	6.58	1.49	1.38
1	5	4671	B8T	C4-N3	6.58	1.43	1.32
1	5	2380	B8W	C3'-C4'	-6.55	1.36	1.53
1	5	1866	UR3	C2-N1	6.53	1.47	1.38
1	5	1517	2MG	C2-N2	6.53	1.47	1.33
1	5	2786	B9H	C2-N1	6.53	1.47	1.38
1	5	4872	2MG	C2-N2	6.47	1.47	1.33
1	5	3897	B8K	C8-N9	6.44	1.50	1.45
1	5	4620	OMU	C2-N3	6.40	1.49	1.38
1	5	4483	B8T	C4-N3	6.39	1.43	1.32
50	9	1710	OMC	C2-N3	6.37	1.49	1.36
50	9	174	OMC	C2-N3	6.35	1.48	1.36
1	5	1605	7MG	C8-N9	6.31	1.50	1.45
50	9	1703	OMC	C6-C5	6.31	1.49	1.35
3	8	14	OMU	C2-N1	6.29	1.48	1.38
50	9	174	OMC	C6-C5	6.28	1.49	1.35
50	9	1710	OMC	C6-C5	6.27	1.49	1.35
1	5	2804	OMC	C6-C5	6.24	1.49	1.35
50	9	1703	OMC	C2-N3	6.24	1.48	1.36
1	5	4335	5MC	C2-N3	6.24	1.48	1.36
1	5	4597	UR3	C2-N1	6.23	1.47	1.38
1	5	4371	MHG	C2-N2	6.22	1.46	1.33
1	5	3782	5MC	C2-N3	6.22	1.48	1.36
50	9	1374	5MC	C5-C4	6.22	1.48	1.44
1	5	1659	I4U	C2-N3	6.18	1.48	1.36
1	5	4371	MHG	C2-N1	6.15	1.46	1.36
50	9	1337	4AC	C6-C5	6.15	1.49	1.35
1	5	2422	OMC	C6-C5	6.13	1.49	1.35
1	5	4447	5MC	C2-N3	6.12	1.48	1.36
1	5	4536	OMC	C2-N3	6.11	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	2422	OMC	C2-N3	6.11	1.48	1.36
50	9	517	OMC	C2-N3	6.11	1.48	1.36
50	9	1374	5MC	C2-N3	6.10	1.48	1.36
1	5	2804	OMC	C2-N3	6.09	1.48	1.36
1	5	3887	OMC	C6-C5	6.08	1.49	1.35
1	5	4671	B8T	C2-N3	6.07	1.48	1.36
1	5	3701	OMC	C6-C5	6.07	1.49	1.35
1	5	729	2MG	C2-N2	6.06	1.46	1.33
1	5	3869	OMC	C6-C5	6.06	1.49	1.35
50	9	1842	4AC	C2-N3	6.06	1.48	1.36
1	5	1348	P4U	C6-C5	6.06	1.49	1.35
1	5	3887	OMC	C2-N3	6.06	1.48	1.36
1	5	4536	OMC	C6-C5	6.06	1.49	1.35
1	5	2365	OMC	C6-C5	6.05	1.49	1.35
50	9	1830	UR3	C6-C5	6.04	1.49	1.35
1	5	2861	OMC	C6-C5	6.03	1.49	1.35
1	5	2861	OMC	C2-N3	6.03	1.48	1.36
50	9	814	5MU	C6-C5	6.03	1.44	1.34
50	9	1337	4AC	C2-N3	6.02	1.48	1.36
50	9	517	OMC	C6-C5	6.01	1.49	1.35
1	5	4194	I4U	C1'-N1	-6.00	1.30	1.47
1	5	4530	UR3	C6-C5	6.00	1.49	1.35
1	5	3909	OMC	C6-C5	5.99	1.49	1.35
1	5	2365	OMC	C2-N3	5.96	1.48	1.36
1	5	3701	OMC	C2-N3	5.96	1.48	1.36
1	5	4306	OMU	C2-N1	5.92	1.47	1.38
1	5	3869	OMC	C2-N3	5.91	1.48	1.36
1	5	1659	I4U	C6-C5	5.90	1.48	1.35
1	5	4483	B8T	C2-N3	5.87	1.48	1.36
1	5	1866	UR3	C6-C5	5.86	1.48	1.35
50	9	1219	B8Q	C2-N3	5.86	1.46	1.35
1	5	1348	P4U	C2-N3	5.86	1.48	1.36
50	9	1842	4AC	C6-C5	5.84	1.48	1.35
50	9	1703	OMC	C4-N3	5.83	1.46	1.34
1	5	4620	OMU	C2-N1	5.83	1.47	1.38
1	5	4194	I4U	C2-N3	5.82	1.47	1.36
50	9	1710	OMC	C4-N3	5.82	1.46	1.34
1	5	4597	UR3	C6-C5	5.82	1.48	1.35
1	5	2297	E7G	C8-N9	5.81	1.49	1.45
50	9	174	OMC	C4-N3	5.79	1.46	1.34
1	5	3909	OMC	C2-N3	5.79	1.47	1.36
1	5	3897	B8K	C4-N9	5.78	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	4083	5MU	C6-C5	5.76	1.44	1.34
1	5	4483	B8T	C6-C5	5.75	1.48	1.35
1	5	1909	P7G	C2-N1	5.74	1.47	1.33
1	5	2297	E7G	C2-N3	5.74	1.47	1.33
1	5	1605	7MG	C2-N3	5.72	1.47	1.33
1	5	4220	6MZ	C6-C5	-5.72	1.36	1.44
1	5	1797	E7G	C2-N3	5.69	1.47	1.33
50	9	121	OMU	C6-C5	5.69	1.48	1.35
1	5	3887	OMC	C4-N3	5.68	1.45	1.34
50	9	517	OMC	C4-N3	5.68	1.45	1.34
1	5	4671	B8T	C6-C5	5.67	1.48	1.35
1	5	3701	OMC	C4-N3	5.67	1.45	1.34
1	5	4194	I4U	C6-C5	5.65	1.48	1.35
1	5	4447	5MC	C5-C4	5.62	1.48	1.44
1	5	3880	P7G	C2-N1	5.62	1.46	1.33
1	5	4129	B8W	C2-N2	5.61	1.45	1.33
1	5	3880	P7G	C4-N3	5.61	1.47	1.37
1	5	2422	OMC	C4-N3	5.59	1.45	1.34
1	5	2365	OMC	C4-N3	5.59	1.45	1.34
1	5	4529	B8W	C2-N2	5.59	1.45	1.33
1	5	2861	OMC	C4-N3	5.57	1.45	1.34
1	5	1605	7MG	C4-N3	5.57	1.47	1.34
1	5	2804	OMC	C4-N3	5.56	1.45	1.34
1	5	4550	7MG	C2-N3	5.56	1.46	1.33
1	5	1909	P7G	C4-N3	5.53	1.46	1.37
1	5	3897	B8K	C3'-C2'	5.48	1.68	1.53
1	5	4355	E6G	C2-N2	5.48	1.44	1.33
1	5	3869	OMC	C4-N3	5.47	1.45	1.34
1	5	4306	OMU	C6-C5	5.46	1.47	1.35
1	5	2522	7MG	C4-N3	5.45	1.46	1.34
1	5	4371	MHG	C4-N3	5.44	1.46	1.34
1	5	2522	7MG	C2-N3	5.43	1.46	1.33
1	5	4185	B8W	C2-N2	5.39	1.44	1.33
1	5	3909	OMC	C4-N3	5.38	1.45	1.34
50	9	1248	B8N	C2-N1	5.38	1.55	1.39
1	5	2380	B8W	C2-N2	5.37	1.44	1.33
1	5	4550	7MG	C4-N3	5.37	1.46	1.34
1	5	3897	B8K	C2-N3	5.36	1.46	1.33
3	8	14	OMU	C6-C5	5.36	1.47	1.35
1	5	3897	B8K	C4-N3	5.36	1.46	1.34
1	5	3792	OMG	C2-N3	5.34	1.46	1.33
1	5	1860	B8H	C2-N3	5.32	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	4690	B8K	C3'-C2'	5.32	1.67	1.53
1	5	3762	B8H	C2-N3	5.32	1.47	1.38
1	5	1797	E7G	C4-N9	5.29	1.44	1.37
1	5	4536	OMC	C4-N3	5.28	1.45	1.34
50	9	116	OMU	C6-C5	5.26	1.47	1.35
1	5	4194	I4U	C3'-C4'	5.26	1.66	1.53
50	9	644	OMG	C2-N3	5.24	1.46	1.33
1	5	2773	OMG	C2-N3	5.24	1.46	1.33
1	5	3899	BGH	C2-N3	5.22	1.45	1.33
50	9	509	OMG	C2-N3	5.22	1.45	1.33
1	5	3899	BGH	C4-N3	5.22	1.46	1.34
1	5	4690	B8K	C2-N3	5.21	1.45	1.33
1	5	4620	OMU	C6-C5	5.21	1.47	1.35
1	5	4296	B8H	C2-N3	5.19	1.47	1.38
1	5	4690	B8K	C4-N9	5.19	1.44	1.37
1	5	1625	OMG	C2-N3	5.19	1.45	1.33
1	5	4870	OMG	C2-N3	5.19	1.45	1.33
1	5	2424	OMG	C2-N3	5.19	1.45	1.33
1	5	4690	B8K	C4-N3	5.17	1.46	1.34
1	5	1522	OMG	C2-N3	5.16	1.45	1.33
1	5	2364	OMG	C2-N3	5.16	1.45	1.33
50	9	1851	MA6	C6-C5	-5.15	1.37	1.44
1	5	4494	OMG	C2-N3	5.14	1.45	1.33
1	5	1883	OMG	C2-N3	5.13	1.45	1.33
1	5	1316	OMG	C2-N3	5.13	1.45	1.33
1	5	4623	OMG	C2-N3	5.12	1.45	1.33
1	5	1909	P7G	C4-N9	5.10	1.43	1.35
1	5	1456	B8Q	C2-N3	5.10	1.44	1.35
1	5	4370	OMG	C2-N3	5.10	1.45	1.33
1	5	4196	OMG	C2-N3	5.10	1.45	1.33
1	5	3899	BGH	C8-N9	5.08	1.49	1.45
1	5	1659	I4U	C1'-N1	-5.07	1.33	1.47
1	5	3880	P7G	C4-N9	5.05	1.43	1.35
1	5	2297	E7G	C4-N9	5.04	1.44	1.37
1	5	4637	OMG	C2-N3	5.04	1.45	1.33
1	5	1517	2MG	C4-N3	5.04	1.49	1.37
1	5	2050	OMG	C2-N3	5.03	1.45	1.33
1	5	729	2MG	C4-N3	5.01	1.49	1.37
1	5	373	OMG	C2-N3	5.01	1.45	1.33
1	5	3899	BGH	O4'-C1'	-4.99	1.30	1.42
1	5	4472	B8W	C2-N2	4.98	1.43	1.33
50	9	1374	5MC	C2-N1	4.94	1.50	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	3792	OMG	C4-N3	4.90	1.49	1.37
1	5	2773	OMG	C4-N3	4.90	1.49	1.37
50	9	683	OMG	C2-N3	4.87	1.45	1.33
1	5	1605	7MG	C4-N9	4.87	1.43	1.37
50	9	1832	6MZ	C6-C5	-4.85	1.37	1.44
1	5	1883	OMG	C4-N3	4.83	1.48	1.37
1	5	4335	5MC	C4-N4	4.83	1.46	1.34
50	9	509	OMG	C4-N3	4.82	1.48	1.37
1	5	4870	OMG	C4-N3	4.82	1.48	1.37
1	5	1797	E7G	C4-N3	4.82	1.45	1.34
50	9	1374	5MC	C4-N4	4.82	1.46	1.34
50	9	1850	MA6	C6-C5	-4.81	1.37	1.44
50	9	1830	UR3	C2-N3	4.80	1.48	1.39
1	5	4597	UR3	C2-N3	4.80	1.48	1.39
1	5	2424	OMG	C4-N3	4.79	1.48	1.37
1	5	3782	5MC	C4-N4	4.79	1.46	1.34
50	9	1219	B8Q	C2-N1	4.78	1.45	1.38
1	5	2364	OMG	C2-N2	4.76	1.45	1.34
1	5	1625	OMG	C4-N3	4.75	1.48	1.37
1	5	373	OMG	C2-N2	4.75	1.45	1.34
1	5	373	OMG	C4-N3	4.73	1.48	1.37
1	5	4196	OMG	C4-N3	4.73	1.48	1.37
1	5	4550	7MG	C2-N2	4.73	1.45	1.34
1	5	1605	7MG	C2-N2	4.73	1.45	1.34
1	5	2424	OMG	C2-N2	4.73	1.45	1.34
50	9	683	OMG	C2-N2	4.72	1.45	1.34
1	5	4447	5MC	C4-N4	4.72	1.46	1.34
1	5	2297	E7G	C4-N3	4.71	1.45	1.34
1	5	3867	A2M	C6-N6	4.71	1.50	1.34
1	5	1883	OMG	C2-N2	4.69	1.45	1.34
1	5	4494	OMG	C4-N3	4.68	1.48	1.37
1	5	1909	P7G	C2-N2	4.68	1.45	1.34
1	5	2522	7MG	C2-N2	4.67	1.45	1.34
50	9	644	OMG	C4-N3	4.67	1.48	1.37
1	5	3782	5MC	C5-C4	4.66	1.47	1.44
1	5	4571	A2M	C6-N6	4.66	1.50	1.34
50	9	683	OMG	C4-N3	4.66	1.48	1.37
1	5	3792	OMG	C2-N2	4.66	1.45	1.34
1	5	3825	A2M	C6-N6	4.66	1.50	1.34
1	5	3880	P7G	C2-N2	4.65	1.45	1.34
1	5	2050	OMG	C4-N3	4.64	1.48	1.37
50	9	1678	A2M	C6-N6	4.64	1.50	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	2773	OMG	C2-N2	4.64	1.45	1.34
1	5	4494	OMG	C2-N2	4.64	1.45	1.34
50	9	166	A2M	C6-N6	4.64	1.50	1.34
1	5	2364	OMG	C4-N3	4.63	1.48	1.37
1	5	4370	OMG	C4-N3	4.63	1.48	1.37
1	5	398	A2M	C6-N6	4.63	1.50	1.34
50	9	1248	B8N	C6-C5	4.63	1.41	1.35
1	5	4447	5MC	C6-N1	4.63	1.45	1.38
50	9	1031	A2M	C6-N6	4.63	1.50	1.34
50	9	668	A2M	C6-N6	4.62	1.50	1.34
1	5	3718	A2M	C6-N6	4.62	1.50	1.34
1	5	4371	MHG	C4-N9	4.62	1.43	1.37
1	5	4872	2MG	C2-N1	4.62	1.44	1.36
1	5	1316	OMG	C2-N2	4.61	1.45	1.34
50	9	27	A2M	C6-N6	4.61	1.50	1.34
1	5	1871	A2M	C6-N6	4.61	1.50	1.34
50	9	159	A2M	C6-N6	4.60	1.50	1.34
1	5	4870	OMG	C2-N2	4.60	1.44	1.34
1	5	4623	OMG	C4-N3	4.60	1.48	1.37
1	5	3723	A2M	C6-N6	4.60	1.50	1.34
1	5	4690	B8K	O4'-C1'	4.59	1.52	1.42
1	5	4623	OMG	C2-N2	4.59	1.44	1.34
1	5	4637	OMG	C4-N3	4.59	1.48	1.37
1	5	1625	OMG	C2-N2	4.58	1.44	1.34
50	9	484	A2M	C6-N6	4.58	1.50	1.34
1	5	3899	BGH	C2-N2	4.58	1.44	1.34
1	5	4523	A2M	C6-N6	4.58	1.50	1.34
1	5	1522	OMG	C2-N2	4.58	1.44	1.34
1	5	1326	A2M	C6-N6	4.57	1.50	1.34
1	5	1534	A2M	C6-N6	4.57	1.50	1.34
1	5	2363	A2M	C6-N6	4.56	1.50	1.34
1	5	2401	A2M	C6-N6	4.56	1.50	1.34
1	5	1316	OMG	C4-N3	4.56	1.48	1.37
1	5	4196	OMG	C2-N2	4.55	1.44	1.34
1	5	3897	B8K	C2-N2	4.54	1.44	1.34
1	5	1522	OMG	C4-N3	4.54	1.48	1.37
1	5	1524	A2M	C6-N6	4.53	1.50	1.34
1	5	4690	B8K	C2-N2	4.52	1.44	1.34
1	5	4370	OMG	C2-N2	4.52	1.44	1.34
1	5	4530	UR3	C2-N3	4.51	1.47	1.39
50	9	644	OMG	C2-N2	4.51	1.44	1.34
50	9	1374	5MC	C6-N1	4.50	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	1524	A2M	O3'-C3'	-4.48	1.31	1.43
1	5	4355	E6G	O6-C6	4.48	1.40	1.34
1	5	1659	I4U	C3'-C4'	4.47	1.64	1.53
1	5	3899	BGH	O2'-C2'	-4.47	1.31	1.42
1	5	2050	OMG	C2-N2	4.46	1.44	1.34
50	9	509	OMG	C2-N2	4.46	1.44	1.34
50	9	1337	4AC	C7-N4	4.43	1.46	1.37
1	5	3723	A2M	O3'-C3'	-4.42	1.32	1.43
1	5	398	A2M	O3'-C3'	-4.41	1.32	1.43
1	5	1326	A2M	O3'-C3'	-4.40	1.32	1.43
1	5	4637	OMG	C2-N2	4.39	1.44	1.34
50	9	166	A2M	O3'-C3'	-4.39	1.32	1.43
50	9	1031	A2M	O3'-C3'	-4.38	1.32	1.43
50	9	159	A2M	O3'-C3'	-4.37	1.32	1.43
1	5	3718	A2M	O3'-C3'	-4.36	1.32	1.43
1	5	4571	A2M	O3'-C3'	-4.36	1.32	1.43
50	9	1806	M7A	C6-N6	4.36	1.45	1.34
1	5	3825	A2M	O3'-C3'	-4.36	1.32	1.43
1	5	4483	B8T	C4-N4	4.35	1.45	1.36
50	9	27	A2M	O3'-C3'	-4.35	1.32	1.43
1	5	4564	M7A	C6-N6	4.35	1.45	1.34
1	5	3785	A2M	C6-N6	4.33	1.49	1.34
1	5	1871	A2M	O3'-C3'	-4.33	1.32	1.43
50	9	1337	4AC	C4-N4	4.32	1.46	1.39
1	5	4690	B8K	C71-N7	4.31	1.49	1.39
1	5	2363	A2M	O3'-C3'	-4.30	1.32	1.43
50	9	1842	4AC	C7-N4	4.28	1.45	1.37
1	5	4671	B8T	C4-N4	4.27	1.44	1.36
50	9	668	A2M	O3'-C3'	-4.25	1.32	1.43
1	5	3782	5MC	C6-N1	4.24	1.45	1.38
50	9	1678	A2M	O3'-C3'	-4.23	1.32	1.43
1	5	2401	A2M	O3'-C3'	-4.23	1.32	1.43
50	9	1850	MA6	C6-N6	4.22	1.47	1.37
1	5	3867	A2M	O3'-C3'	-4.20	1.32	1.43
1	5	4335	5MC	C6-N1	4.18	1.45	1.38
50	9	1806	M7A	C5-N7	4.18	1.49	1.39
1	5	4415	1MA	C2-N1	4.18	1.44	1.35
1	5	4335	5MC	C2-N1	4.16	1.48	1.40
50	9	1851	MA6	C6-N6	4.16	1.47	1.37
1	5	1866	UR3	C2-N3	4.15	1.47	1.39
1	5	3899	BGH	C4-N9	4.12	1.42	1.37
1	5	3782	5MC	C2-N1	4.12	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	3897	B8K	O4'-C1'	4.11	1.51	1.42
1	5	1659	I4U	O4'-C1'	4.10	1.51	1.42
1	5	2297	E7G	C2-N2	4.09	1.43	1.34
1	5	4690	B8K	C5-N7	4.08	1.47	1.39
1	5	1534	A2M	O3'-C3'	-4.07	1.32	1.43
1	5	3897	B8K	C5-N7	4.07	1.47	1.39
1	5	1348	P4U	C2-N1	4.07	1.48	1.40
1	5	4550	7MG	C4-N9	4.06	1.42	1.37
1	5	1797	E7G	C2-N2	4.05	1.43	1.34
1	5	3909	OMC	O2-C2	-4.02	1.16	1.23
1	5	2522	7MG	C4-N9	4.02	1.42	1.37
50	9	484	A2M	O3'-C3'	-4.01	1.33	1.43
1	5	4671	B8T	C2-N1	3.99	1.48	1.40
50	9	116	OMU	C4-N3	3.99	1.45	1.38
1	5	1517	2MG	C2-N1	3.98	1.43	1.36
1	5	4523	A2M	O3'-C3'	-3.98	1.33	1.43
1	5	4483	B8T	C2-N1	3.98	1.48	1.40
1	5	4872	2MG	C4-N3	3.98	1.46	1.37
1	5	1348	P4U	O4-C4	3.97	1.39	1.35
50	9	1842	4AC	C4-N4	3.96	1.45	1.39
50	9	1337	4AC	C2-N1	3.96	1.48	1.40
1	5	4447	5MC	C2-N1	3.94	1.48	1.40
3	8	14	OMU	C4-N3	3.94	1.45	1.38
50	9	1710	OMC	C2-N1	3.93	1.48	1.40
50	9	121	OMU	C4-N3	3.89	1.45	1.38
50	9	174	OMC	C2-N1	3.87	1.48	1.40
1	5	3897	B8K	C71-N7	3.86	1.48	1.39
50	9	1703	OMC	C2-N1	3.85	1.48	1.40
50	9	174	OMC	C4-N4	3.84	1.43	1.33
1	5	2422	OMC	C4-N4	3.82	1.43	1.33
50	9	1842	4AC	C2-N1	3.81	1.48	1.40
1	5	4872	2MG	C6-N1	3.79	1.43	1.37
1	5	237	B9B	O3'-C3'	-3.79	1.33	1.43
50	9	1710	OMC	C4-N4	3.78	1.43	1.33
50	9	1703	OMC	C4-N4	3.78	1.43	1.33
1	5	2365	OMC	C4-N4	3.76	1.43	1.33
1	5	2861	OMC	C4-N4	3.76	1.43	1.33
1	5	3723	A2M	O2'-C2'	3.75	1.51	1.42
1	5	3701	OMC	C4-N4	3.74	1.43	1.33
1	5	2422	OMC	C2-N1	3.74	1.47	1.40
1	5	3909	OMC	C2-N1	3.73	1.47	1.40
1	5	3880	P7G	C2-N3	3.73	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	4536	OMC	C2-N1	3.73	1.47	1.40
1	5	729	2MG	C2-N1	3.71	1.42	1.36
1	5	3869	OMC	C4-N4	3.71	1.42	1.33
1	5	3887	OMC	C4-N4	3.70	1.42	1.33
1	5	1909	P7G	C2-N3	3.69	1.46	1.37
1	5	4194	I4U	C2-N1	3.69	1.47	1.40
1	5	3867	A2M	O2'-C2'	3.68	1.51	1.42
1	5	2804	OMC	C4-N4	3.67	1.42	1.33
1	5	4306	OMU	C4-N3	3.67	1.44	1.38
1	5	2380	B8W	O4'-C4'	3.66	1.53	1.45
50	9	517	OMC	C4-N4	3.65	1.42	1.33
1	5	4129	B8W	O4'-C4'	3.65	1.53	1.45
1	5	4529	B8W	O4'-C4'	3.65	1.53	1.45
1	5	3887	OMC	C2-N1	3.64	1.47	1.40
1	5	1797	E7G	C5-C6	3.64	1.52	1.43
1	5	2754	B9B	O3'-C3'	-3.62	1.34	1.43
50	9	1678	A2M	O2'-C2'	3.62	1.51	1.42
1	5	3909	OMC	C4-N4	3.62	1.42	1.33
50	9	174	OMC	C6-N1	3.61	1.46	1.38
1	5	4536	OMC	C4-N4	3.60	1.42	1.33
1	5	2380	B8W	C3'-C2'	3.59	1.63	1.53
50	9	1243	PSU	C6-C5	3.57	1.39	1.35
50	9	484	A2M	O2'-C2'	3.57	1.51	1.42
1	5	4872	2MG	C5-C4	-3.57	1.34	1.43
1	5	4371	MHG	C5-C6	3.56	1.52	1.43
50	9	1337	4AC	C5-C4	3.56	1.48	1.41
1	5	2297	E7G	C5-C6	3.56	1.52	1.43
1	5	3899	BGH	C5-C6	3.56	1.52	1.43
1	5	1322	1MA	C2-N1	3.55	1.43	1.35
1	5	1574	B9B	O3'-C3'	-3.55	1.34	1.43
1	5	4564	M7A	C5-N7	3.55	1.47	1.39
1	5	3785	A2M	O2'-C2'	3.55	1.51	1.42
1	5	3897	B8K	C2-N1	3.55	1.46	1.37
1	5	4129	B8W	C3'-C2'	3.54	1.63	1.53
1	5	3785	A2M	O3'-C3'	-3.54	1.34	1.43
1	5	398	A2M	O2'-C2'	3.54	1.51	1.42
1	5	4194	I4U	O4'-C1'	3.53	1.50	1.42
1	5	1605	7MG	C5-C6	3.52	1.52	1.43
50	9	166	A2M	O2'-C2'	3.52	1.51	1.42
1	5	4415	1MA	C4-N3	3.52	1.48	1.37
1	5	4620	OMU	C4-N3	3.52	1.44	1.38
1	5	2365	OMC	C6-N1	3.52	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	4185	B8W	O4'-C4'	3.50	1.52	1.45
50	9	517	OMC	C2-N1	3.50	1.47	1.40
50	9	517	OMC	C6-N1	3.50	1.46	1.38
1	5	2861	OMC	C2-N1	3.49	1.47	1.40
1	5	1326	A2M	O2'-C2'	3.49	1.51	1.42
50	9	1710	OMC	C6-N1	3.49	1.46	1.38
1	5	1534	A2M	C2-N3	3.48	1.37	1.32
1	5	2522	7MG	C2-N1	3.48	1.46	1.37
1	5	2401	A2M	O2'-C2'	3.47	1.51	1.42
1	5	4690	B8K	O6-C6	-3.47	1.17	1.23
50	9	1678	A2M	C2-N3	3.47	1.37	1.32
1	5	1797	E7G	C8-N7	3.46	1.52	1.45
1	5	3718	A2M	O2'-C2'	3.46	1.51	1.42
50	9	668	A2M	O2'-C2'	3.45	1.51	1.42
1	5	1605	7MG	C2-N1	3.45	1.46	1.37
1	5	4371	MHG	C8-N7	3.44	1.52	1.45
1	5	2522	7MG	C5-C6	3.43	1.52	1.43
1	5	4550	7MG	C5-C6	3.43	1.52	1.43
50	9	159	A2M	O2'-C2'	3.42	1.51	1.42
1	5	1883	OMG	C5-C4	-3.42	1.34	1.43
1	5	3869	OMC	C2-N1	3.42	1.47	1.40
1	5	1871	A2M	O2'-C2'	3.41	1.51	1.42
1	5	3899	BGH	C2-N1	3.40	1.45	1.37
1	5	2804	OMC	C2-N1	3.40	1.47	1.40
1	5	4355	E6G	O2'-C2'	3.39	1.51	1.43
1	5	2297	E7G	C2-N1	3.38	1.45	1.37
50	9	668	A2M	C1'-N9	-3.38	1.41	1.49
1	5	2804	OMC	C6-N1	3.38	1.46	1.38
1	5	1316	OMG	C5-C4	-3.38	1.34	1.43
1	5	4447	5MC	O2-C2	-3.38	1.17	1.23
50	9	27	A2M	C2-N3	3.37	1.37	1.32
50	9	683	OMG	C6-N1	3.37	1.43	1.37
1	5	1797	E7G	C2-N1	3.37	1.45	1.37
1	5	4571	A2M	O2'-C2'	3.36	1.50	1.42
1	5	1659	I4U	C2-N1	3.36	1.47	1.40
50	9	644	OMG	C6-N1	3.36	1.42	1.37
1	5	2773	OMG	C6-N1	3.36	1.42	1.37
50	9	159	A2M	C2-N3	3.36	1.37	1.32
1	5	2861	OMC	O2-C2	-3.36	1.17	1.23
1	5	3785	A2M	C2-N3	3.35	1.37	1.32
1	5	3869	OMC	C6-N1	3.35	1.46	1.38
50	9	166	A2M	C2-N3	3.35	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	3825	A2M	O2'-C2'	3.35	1.50	1.42
1	5	4472	B8W	O4'-C4'	3.35	1.52	1.45
1	5	4571	A2M	C2-N3	3.35	1.37	1.32
1	5	2297	E7G	C8-N7	3.34	1.51	1.45
1	5	1456	B8Q	C2-N1	3.34	1.43	1.38
1	5	2363	A2M	O2'-C2'	3.34	1.50	1.42
1	5	3701	OMC	C2-N1	3.34	1.47	1.40
1	5	4550	7MG	C2-N1	3.34	1.45	1.37
1	5	2401	A2M	C1'-N9	-3.33	1.41	1.49
1	5	4335	5MC	O2-C2	-3.33	1.17	1.23
50	9	1842	4AC	C5-C4	3.33	1.48	1.41
1	5	1534	A2M	O2'-C2'	3.33	1.50	1.42
1	5	4185	B8W	C3'-C2'	3.33	1.62	1.53
1	5	2424	OMG	C6-N1	3.32	1.42	1.37
1	5	398	A2M	C2-N3	3.32	1.37	1.32
50	9	1081	PSU	C6-C5	3.32	1.39	1.35
1	5	3887	OMC	C6-N1	3.31	1.46	1.38
1	5	1683	PSU	C6-C5	3.30	1.38	1.35
1	5	3701	OMC	C6-N1	3.30	1.46	1.38
1	5	4690	B8K	C2-N1	3.30	1.45	1.37
1	5	3897	B8K	C5-C6	3.30	1.51	1.43
1	5	2050	OMG	C5-C4	-3.30	1.34	1.43
1	5	3729	PSU	C6-C5	3.29	1.38	1.35
50	9	1703	OMC	C6-N1	3.29	1.45	1.38
1	5	4523	A2M	C2-N3	3.29	1.37	1.32
1	5	4370	OMG	C6-N1	3.28	1.42	1.37
1	5	3899	BGH	C5-N7	3.28	1.46	1.39
1	5	4194	I4U	O4-C41	-3.28	1.39	1.47
50	9	1031	A2M	O2'-C2'	3.28	1.50	1.42
1	5	4623	OMG	C6-N1	3.27	1.42	1.37
1	5	4494	OMG	C5-C4	-3.27	1.35	1.43
50	9	509	OMG	C6-N1	3.27	1.42	1.37
1	5	4620	OMU	O4-C4	-3.26	1.18	1.24
1	5	3764	PSU	C6-C5	3.26	1.38	1.35
1	5	1524	A2M	O2'-C2'	3.26	1.50	1.42
1	5	4523	A2M	O2'-C2'	3.26	1.50	1.42
1	5	373	OMG	C5-C4	-3.26	1.35	1.43
50	9	823	PSU	C6-C5	3.26	1.38	1.35
1	5	2365	OMC	C2-N1	3.24	1.46	1.40
50	9	668	A2M	C2-N3	3.24	1.37	1.32
1	5	1582	PSU	C6-C5	3.23	1.38	1.35
1	5	1860	B8H	O4-C4	-3.23	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	4536	OMC	C6-N1	3.23	1.45	1.38
1	5	2365	OMC	O2-C2	-3.23	1.17	1.23
1	5	4293	PSU	C6-C5	3.22	1.38	1.35
1	5	3723	A2M	C2-N3	3.21	1.37	1.32
1	5	2804	OMC	O2-C2	-3.21	1.17	1.23
1	5	4355	E6G	O3'-C3'	-3.21	1.35	1.43
50	9	484	A2M	C2-N3	3.21	1.37	1.32
1	5	1659	I4U	O4-C41	-3.21	1.40	1.47
1	5	4296	B8H	O4-C4	-3.20	1.17	1.23
1	5	3715	PSU	C6-C5	3.20	1.38	1.35
1	5	2363	A2M	C2-N3	3.20	1.37	1.32
1	5	1326	A2M	C2-N3	3.19	1.37	1.32
1	5	1524	A2M	C1'-N9	-3.19	1.42	1.49
1	5	2422	OMC	C6-N1	3.19	1.45	1.38
1	5	4194	I4U	O2'-C2'	3.19	1.50	1.43
1	5	373	OMG	C6-N1	3.19	1.42	1.37
1	5	4529	B8W	C3'-C2'	3.18	1.62	1.53
1	5	4637	OMG	C5-C4	-3.17	1.35	1.43
1	5	4483	B8T	O2-C2	-3.16	1.17	1.23
1	5	1316	OMG	C6-N1	3.16	1.42	1.37
1	5	4494	OMG	C6-N1	3.16	1.42	1.37
1	5	2364	OMG	C6-N1	3.15	1.42	1.37
50	9	1703	OMC	O2-C2	-3.15	1.17	1.23
1	5	3887	OMC	O2-C2	-3.15	1.17	1.23
50	9	683	OMG	C5-C4	-3.15	1.35	1.43
3	8	14	OMU	O4-C4	-3.15	1.18	1.24
1	5	4306	OMU	O4-C4	-3.15	1.18	1.24
1	5	2401	A2M	C2-N3	3.14	1.37	1.32
1	5	4623	OMG	C5-C4	-3.14	1.35	1.43
1	5	3909	OMC	C6-N1	3.14	1.45	1.38
50	9	119	PSU	C6-C5	3.13	1.38	1.35
1	5	4690	B8K	C5-C6	3.13	1.51	1.43
1	5	4870	OMG	C6-N1	3.13	1.42	1.37
1	5	2508	PSU	C6-C5	3.13	1.38	1.35
1	5	2861	OMC	C6-N1	3.13	1.45	1.38
1	5	4872	2MG	C5-C6	3.12	1.53	1.47
1	5	3825	A2M	C2-N3	3.12	1.36	1.32
1	5	4536	OMC	O2-C2	-3.12	1.17	1.23
1	5	1517	2MG	C5-C4	-3.12	1.35	1.43
1	5	3762	B8H	O4-C4	-3.12	1.17	1.23
1	5	1522	OMG	C5-C4	-3.11	1.35	1.43
1	5	1625	OMG	C6-N1	3.11	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	9	568	E3C	C4-N3	3.11	1.53	1.48
1	5	2364	OMG	C5-C4	-3.10	1.35	1.43
50	9	159	A2M	C1'-N9	-3.08	1.42	1.49
1	5	729	2MG	C5-C4	-3.08	1.35	1.43
1	5	2050	OMG	C6-N1	3.08	1.42	1.37
50	9	1031	A2M	C2-N3	3.07	1.36	1.32
1	5	3867	A2M	C2-N3	3.07	1.36	1.32
1	5	2422	OMC	O2-C2	-3.07	1.18	1.23
50	9	822	PSU	C6-C5	3.07	1.38	1.35
1	5	4531	PSU	C6-C5	3.07	1.38	1.35
50	9	116	OMU	O4-C4	-3.07	1.18	1.24
1	5	1522	OMG	C6-N1	3.06	1.42	1.37
50	9	1337	4AC	C6-N1	3.06	1.45	1.38
1	5	1909	P7G	C5-C4	3.06	1.44	1.36
1	5	3897	B8K	O6-C6	-3.05	1.17	1.23
50	9	1374	5MC	O2-C2	-3.05	1.18	1.23
1	5	2424	OMG	C5-C4	-3.05	1.35	1.43
1	5	1322	1MA	C4-N3	3.05	1.46	1.37
1	5	4371	MHG	C6-N1	3.04	1.44	1.38
1	5	1883	OMG	C6-N1	3.04	1.42	1.37
1	5	4220	6MZ	C2-N3	3.03	1.36	1.32
1	5	4637	OMG	C6-N1	3.03	1.42	1.37
1	5	2363	A2M	C1'-N9	-3.03	1.42	1.49
1	5	1871	A2M	C1'-N9	-3.03	1.42	1.49
1	5	4442	PSU	C6-C5	3.03	1.38	1.35
1	5	4370	OMG	C5-C4	-3.02	1.35	1.43
1	5	1871	A2M	C2-N3	3.02	1.36	1.32
1	5	3880	P7G	C5-C4	3.02	1.44	1.36
1	5	3718	A2M	C2-N3	3.02	1.36	1.32
1	5	3792	OMG	C6-N1	3.02	1.42	1.37
1	5	4196	OMG	C6-N1	3.01	1.42	1.37
50	9	644	OMG	C5-C4	-3.01	1.35	1.43
1	5	4671	B8T	O2-C2	-3.01	1.18	1.23
1	5	1659	I4U	O2-C2	-3.00	1.18	1.23
50	9	1842	4AC	C6-N1	3.00	1.45	1.38
1	5	3785	A2M	C3'-C4'	3.00	1.60	1.53
50	9	27	A2M	O2'-C2'	2.99	1.50	1.42
1	5	4483	B8T	C6-N1	2.99	1.45	1.38
1	5	1659	I4U	C6-N1	2.99	1.45	1.38
1	5	3785	A2M	C1'-N9	-2.99	1.42	1.49
50	9	121	OMU	O4-C4	-2.99	1.18	1.24
1	5	4571	A2M	C1'-N9	-2.99	1.42	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	9	568	E3C	C6-N1	2.98	1.45	1.38
1	5	3825	A2M	C1'-N9	-2.98	1.42	1.49
1	5	2522	7MG	C6-N1	2.97	1.44	1.38
1	5	1659	I4U	O2'-C2'	2.97	1.50	1.43
1	5	4870	OMG	C5-C4	-2.97	1.35	1.43
1	5	3792	OMG	C5-C4	-2.97	1.35	1.43
1	5	1524	A2M	C2-N3	2.96	1.36	1.32
1	5	3899	BGH	O6-C6	-2.95	1.18	1.23
1	5	4628	PSU	C6-C5	2.95	1.38	1.35
1	5	4483	B8T	C5-C4	2.94	1.47	1.41
1	5	4083	5MU	O2-C2	-2.94	1.17	1.23
50	9	1031	A2M	C1'-N9	-2.93	1.42	1.49
1	5	3867	A2M	C1'-N9	-2.92	1.42	1.49
1	5	3782	5MC	O2-C2	-2.91	1.18	1.23
1	5	4403	PSU	C6-C5	2.91	1.38	1.35
50	9	27	A2M	C1'-N9	-2.91	1.42	1.49
1	5	4306	OMU	O2-C2	-2.91	1.17	1.23
1	5	4671	B8T	C5-C4	2.91	1.47	1.41
1	5	3869	OMC	O2-C2	-2.90	1.18	1.23
1	5	4196	OMG	C5-C4	-2.90	1.35	1.43
1	5	1517	2MG	C6-N1	2.90	1.42	1.37
50	9	517	OMC	O2-C2	-2.89	1.18	1.23
50	9	1710	OMC	O2-C2	-2.88	1.18	1.23
1	5	1625	OMG	C5-C4	-2.87	1.36	1.43
1	5	2773	OMG	C5-C4	-2.87	1.36	1.43
1	5	4083	5MU	O4-C4	-2.87	1.18	1.23
50	9	1842	4AC	O2-C2	-2.87	1.18	1.23
1	5	1326	A2M	C1'-N9	-2.86	1.42	1.49
1	5	1456	B8Q	O2-C2	-2.86	1.17	1.22
1	5	3899	BGH	C71-N7	2.86	1.45	1.39
1	5	1348	P4U	O2-C2	-2.86	1.18	1.23
1	5	1534	A2M	C1'-N9	-2.86	1.42	1.49
1	5	2773	OMG	C5-C6	2.86	1.53	1.47
1	5	4530	UR3	C6-N1	2.85	1.44	1.38
1	5	4472	B8W	C1'-N9	-2.85	1.42	1.49
1	5	3792	OMG	C5-C6	2.85	1.53	1.47
1	5	1517	2MG	O6-C6	-2.85	1.16	1.23
50	9	121	OMU	O2-C2	-2.84	1.18	1.23
1	5	3899	BGH	C6-N1	2.84	1.44	1.38
1	5	3723	A2M	C1'-N9	-2.84	1.42	1.49
1	5	2424	OMG	C5-C6	2.84	1.53	1.47
1	5	4550	7MG	C6-N1	2.84	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	9	174	OMC	O2-C2	-2.83	1.18	1.23
1	5	1522	OMG	C5-C6	2.83	1.53	1.47
1	5	4872	2MG	O6-C6	-2.82	1.16	1.23
1	5	1605	7MG	C6-N1	2.82	1.44	1.38
1	5	1677	PSU	O4'-C1'	-2.81	1.40	1.43
1	5	3897	B8K	C6-N1	2.81	1.44	1.38
1	5	4194	I4U	O2-C2	-2.81	1.18	1.23
1	5	1348	P4U	C6-N1	2.81	1.44	1.38
50	9	484	A2M	C1'-N9	-2.81	1.43	1.49
50	9	1337	4AC	O2-C2	-2.80	1.18	1.23
50	9	683	OMG	C5-C6	2.80	1.53	1.47
50	9	509	OMG	C5-C6	2.79	1.52	1.47
1	5	3701	OMC	O2-C2	-2.79	1.18	1.23
50	9	814	5MU	O4-C4	-2.79	1.18	1.23
1	5	4185	B8W	C1'-N9	-2.78	1.43	1.49
1	5	4620	OMU	O2-C2	-2.78	1.18	1.23
1	5	1909	P7G	C8-N7	2.78	1.50	1.45
1	5	4472	B8W	C3'-C2'	2.77	1.60	1.53
1	5	4500	PSU	C6-C5	2.76	1.38	1.35
1	5	398	A2M	C1'-N9	-2.76	1.43	1.49
50	9	509	OMG	C5-C4	-2.75	1.36	1.43
50	9	1830	UR3	C6-N1	2.75	1.44	1.38
3	8	14	OMU	O2-C2	-2.74	1.18	1.23
1	5	1322	1MA	C5-C4	-2.74	1.36	1.43
1	5	729	2MG	O6-C6	-2.73	1.17	1.23
1	5	3718	A2M	C1'-N9	-2.72	1.43	1.49
50	9	644	OMG	C5-C6	2.70	1.52	1.47
50	9	1678	A2M	C1'-N9	-2.70	1.43	1.49
1	5	1605	7MG	O6-C6	-2.70	1.18	1.23
50	9	1219	B8Q	O2-C2	-2.70	1.17	1.22
1	5	4597	UR3	C6-N1	2.70	1.44	1.38
1	5	4636	PSU	C6-C5	2.70	1.38	1.35
1	5	4671	B8T	C6-N1	2.68	1.44	1.38
1	5	1625	OMG	C5-C6	2.66	1.52	1.47
50	9	166	A2M	C1'-N9	-2.65	1.43	1.49
50	9	814	5MU	O2-C2	-2.65	1.18	1.23
1	5	2773	OMG	C2-N1	2.64	1.44	1.37
1	5	4550	7MG	O6-C6	-2.64	1.18	1.23
1	5	1866	UR3	C6-N1	2.64	1.44	1.38
1	5	4523	A2M	C1'-N9	-2.63	1.43	1.49
1	5	2050	OMG	C5-C6	2.63	1.52	1.47
1	5	1316	OMG	C5-C6	2.62	1.52	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	4870	OMG	C5-C6	2.62	1.52	1.47
1	5	3880	P7G	O6-C6	-2.62	1.19	1.23
1	5	4196	OMG	C5-C6	2.62	1.52	1.47
50	9	121	OMU	C6-N1	2.61	1.44	1.38
1	5	4637	OMG	C5-C6	2.60	1.52	1.47
50	9	612	PSU	C6-C5	2.60	1.38	1.35
50	9	116	OMU	O2-C2	-2.59	1.18	1.23
1	5	2424	OMG	C2-N1	2.59	1.43	1.37
1	5	1797	E7G	C6-N1	2.58	1.43	1.38
50	9	683	OMG	C2-N1	2.56	1.43	1.37
1	5	2754	B9B	O2'-C2'	2.56	1.49	1.43
1	5	4355	E6G	C1'-N9	-2.56	1.43	1.49
1	5	1517	2MG	C5-C6	2.55	1.52	1.47
50	9	1832	6MZ	C2-N3	2.55	1.36	1.32
1	5	4690	B8K	C6-N1	2.55	1.43	1.38
1	5	4370	OMG	C2-N1	2.54	1.43	1.37
50	9	509	OMG	C2-N1	2.54	1.43	1.37
1	5	2050	OMG	C2-N1	2.54	1.43	1.37
1	5	4370	OMG	C5-C6	2.54	1.52	1.47
1	5	4371	MHG	O6-C6	-2.54	1.18	1.23
1	5	1883	OMG	O6-C6	-2.53	1.17	1.23
1	5	1574	B9B	C1'-N9	-2.53	1.43	1.49
1	5	729	2MG	C6-N1	2.53	1.41	1.37
50	9	644	OMG	C2-N1	2.53	1.43	1.37
1	5	2522	7MG	O6-C6	-2.52	1.18	1.23
1	5	237	B9B	O2'-C2'	2.51	1.49	1.43
1	5	2364	OMG	C2-N1	2.51	1.43	1.37
1	5	4194	I4U	C6-N1	2.51	1.44	1.38
1	5	1866	UR3	O4-C4	-2.51	1.18	1.23
1	5	2380	B8W	C1'-N9	-2.50	1.43	1.49
1	5	1574	B9B	O2'-C2'	2.50	1.49	1.43
1	5	4415	1MA	C5-C4	-2.50	1.36	1.43
1	5	4623	OMG	C5-C6	2.49	1.52	1.47
1	5	1625	OMG	C2-N1	2.48	1.43	1.37
1	5	2297	E7G	C6-N1	2.47	1.43	1.38
1	5	4623	OMG	C2-N1	2.47	1.43	1.37
1	5	2364	OMG	C5-C6	2.47	1.52	1.47
1	5	4450	PSU	C6-C5	2.47	1.38	1.35
1	5	4637	OMG	C2-N1	2.44	1.43	1.37
50	9	159	A2M	C5'-C4'	2.44	1.58	1.51
1	5	729	2MG	C5-C6	2.43	1.52	1.47
1	5	373	OMG	C5-C6	2.43	1.52	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	373	OMG	C2-N1	2.42	1.43	1.37
1	5	3897	B8K	C5-C4	2.42	1.45	1.37
50	9	116	OMU	C6-N1	2.41	1.43	1.38
1	5	1909	P7G	O6-C6	-2.41	1.19	1.23
1	5	4494	OMG	C2-N1	2.41	1.43	1.37
1	5	4450	PSU	C4-C5	-2.40	1.37	1.44
50	9	1830	UR3	O4-C4	-2.40	1.18	1.23
1	5	4494	OMG	C5-C6	2.39	1.52	1.47
1	5	1883	OMG	C5-C6	2.39	1.52	1.47
1	5	4306	OMU	C6-N1	2.38	1.43	1.38
1	5	3792	OMG	C2-N1	2.38	1.43	1.37
3	8	14	OMU	C6-N1	2.38	1.43	1.38
1	5	4530	UR3	O4-C4	-2.37	1.18	1.23
1	5	4870	OMG	C2-N1	2.37	1.43	1.37
1	5	4597	UR3	O4-C4	-2.36	1.18	1.23
50	9	1678	A2M	C5'-C4'	2.35	1.58	1.51
1	5	4529	B8W	C1'-N9	-2.35	1.44	1.49
1	5	3723	A2M	C3'-C4'	2.34	1.58	1.53
1	5	4220	6MZ	C6-N1	-2.34	1.30	1.34
1	5	1677	PSU	C4-C5	-2.33	1.37	1.44
1	5	3792	OMG	O6-C6	-2.33	1.17	1.23
1	5	1316	OMG	C2-N1	2.33	1.43	1.37
1	5	2754	B9B	C1'-N9	-2.32	1.44	1.49
1	5	4597	UR3	O2-C2	-2.32	1.18	1.22
1	5	4530	UR3	O2-C2	-2.31	1.18	1.22
1	5	1797	E7G	O6-C6	-2.31	1.19	1.23
50	9	1678	A2M	C3'-C4'	2.30	1.58	1.53
1	5	1522	OMG	C2-N1	2.30	1.43	1.37
50	9	484	A2M	C3'-C4'	2.30	1.58	1.53
50	9	1248	B8N	O4-C4	-2.30	1.18	1.23
1	5	4628	PSU	C4-C5	-2.29	1.38	1.44
50	9	1830	UR3	O2-C2	-2.29	1.18	1.22
1	5	237	B9B	C1'-N9	-2.29	1.44	1.49
1	5	1683	PSU	C4-C5	-2.29	1.38	1.44
1	5	4636	PSU	C4-C5	-2.29	1.38	1.44
1	5	1326	A2M	C3'-C4'	2.28	1.58	1.53
1	5	4523	A2M	C5'-C4'	2.28	1.58	1.51
1	5	4500	PSU	C4-C5	-2.28	1.38	1.44
1	5	1534	A2M	C3'-C4'	2.28	1.58	1.53
1	5	4129	B8W	O6-C6	2.27	1.41	1.35
1	5	2297	E7G	O6-C6	-2.27	1.19	1.23
1	5	2364	OMG	O6-C6	-2.27	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	4196	OMG	C2-N1	2.26	1.43	1.37
1	5	1866	UR3	O2-C2	-2.26	1.18	1.22
50	9	121	OMU	C5-C4	2.26	1.48	1.43
1	5	3723	A2M	C5'-C4'	2.26	1.58	1.51
1	5	1574	B9B	C5'-C4'	2.25	1.58	1.51
1	5	3867	A2M	C3'-C4'	2.25	1.58	1.53
1	5	4530	UR3	C4-N3	2.25	1.45	1.40
1	5	4571	A2M	C5'-C4'	2.24	1.58	1.51
1	5	1883	OMG	C2-N1	2.23	1.43	1.37
1	5	2363	A2M	C5'-C4'	2.22	1.58	1.51
1	5	3867	A2M	C5'-C4'	2.22	1.58	1.51
1	5	3880	P7G	C8-N7	2.22	1.49	1.45
1	5	2050	OMG	O6-C6	-2.21	1.18	1.23
1	5	2424	OMG	O6-C6	-2.21	1.18	1.23
1	5	4185	B8W	O6-C6	2.21	1.41	1.35
1	5	2401	A2M	C5'-C4'	2.20	1.58	1.51
1	5	3718	A2M	C5'-C4'	2.20	1.58	1.51
1	5	2754	B9B	C5'-C4'	2.20	1.58	1.51
1	5	4637	OMG	O6-C6	-2.19	1.18	1.23
50	9	484	A2M	C5'-C4'	2.19	1.58	1.51
1	5	2363	A2M	C5-N7	-2.18	1.32	1.39
1	5	4529	B8W	O6-C6	2.16	1.41	1.35
1	5	2401	A2M	C3'-C4'	2.16	1.58	1.53
50	9	27	A2M	C5'-C4'	2.16	1.58	1.51
50	9	166	A2M	C5'-C4'	2.15	1.58	1.51
1	5	398	A2M	C3'-C4'	2.15	1.58	1.53
1	5	4523	A2M	C3'-C4'	2.15	1.58	1.53
50	9	1842	4AC	O7-C7	-2.15	1.18	1.23
1	5	4370	OMG	O6-C6	-2.15	1.18	1.23
1	5	1871	A2M	C5'-C4'	2.14	1.58	1.51
1	5	1871	A2M	C3'-C4'	2.14	1.58	1.53
1	5	4690	B8K	C5-C4	2.13	1.44	1.37
1	5	4293	PSU	C4-C5	-2.13	1.38	1.44
50	9	644	OMG	O6-C6	-2.13	1.18	1.23
1	5	1524	A2M	C5'-C4'	2.12	1.57	1.51
1	5	1316	OMG	O6-C6	-2.12	1.18	1.23
1	5	4628	PSU	O4'-C1'	-2.11	1.40	1.43
1	5	1326	A2M	C5'-C4'	2.10	1.57	1.51
1	5	3785	A2M	C5-N7	-2.10	1.32	1.39
1	5	1677	PSU	C6-C5	2.10	1.37	1.35
1	5	1522	OMG	O6-C6	-2.10	1.18	1.23
1	5	4306	OMU	C5-C4	2.10	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	9	509	OMG	O6-C6	-2.09	1.18	1.23
50	9	166	A2M	C3'-C4'	2.09	1.58	1.53
1	5	4623	OMG	O6-C6	-2.08	1.18	1.23
50	9	823	PSU	C4-C5	-2.08	1.38	1.44
1	5	4620	OMU	C6-N1	2.08	1.43	1.38
1	5	4442	PSU	C4-C5	-2.08	1.38	1.44
1	5	3718	A2M	C5-N7	-2.07	1.32	1.39
50	9	568	E3C	O2-C2	-2.07	1.18	1.22
1	5	3718	A2M	C3'-C4'	2.06	1.58	1.53
1	5	1909	P7G	C6-N1	2.06	1.41	1.38
1	5	4472	B8W	C4-N3	-2.06	1.32	1.35
1	5	4494	OMG	O6-C6	-2.06	1.18	1.23
1	5	4597	UR3	C4-N3	2.06	1.44	1.40
1	5	398	A2M	C5'-C4'	2.06	1.57	1.51
50	9	1248	B8N	O2-C2	-2.06	1.18	1.22
1	5	373	OMG	O6-C6	-2.06	1.18	1.23
1	5	237	B9B	C5'-C4'	2.05	1.57	1.51
1	5	3785	A2M	C5'-C4'	2.05	1.57	1.51
50	9	683	OMG	O6-C6	-2.05	1.18	1.23
1	5	4531	PSU	C4-C5	-2.04	1.38	1.44
50	9	822	PSU	O4'-C1'	-2.04	1.41	1.43
50	9	1081	PSU	C4-C5	-2.04	1.38	1.44
1	5	1326	A2M	C5-N7	-2.04	1.32	1.39
1	5	4196	OMG	O6-C6	-2.04	1.18	1.23
1	5	4531	PSU	O4'-C1'	-2.04	1.41	1.43
1	5	4500	PSU	O4'-C1'	-2.03	1.41	1.43
1	5	4450	PSU	O4'-C1'	-2.03	1.41	1.43
1	5	1625	OMG	O6-C6	-2.03	1.18	1.23
50	9	1832	6MZ	C6-N1	-2.03	1.31	1.34
1	5	1524	A2M	C3'-C4'	2.02	1.58	1.53
1	5	1534	A2M	C5-N7	-2.02	1.32	1.39
1	5	4564	M7A	C5-C6	-2.02	1.35	1.40
1	5	4442	PSU	O4'-C1'	-2.02	1.41	1.43
1	5	1456	B8Q	C4-N3	-2.01	1.45	1.48
1	5	1659	I4U	C5-C4	2.01	1.48	1.43
50	9	1031	A2M	C5'-C4'	2.01	1.57	1.51
1	5	4564	M7A	C8-N9	-2.01	1.40	1.45
1	5	2773	OMG	O6-C6	-2.01	1.18	1.23
50	9	1830	UR3	C4-N3	2.01	1.44	1.40
1	5	4129	B8W	C1'-N9	-2.00	1.45	1.49

All (643) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	4529	B8W	N2-C2-N3	17.85	145.65	117.79
1	5	4129	B8W	N2-C2-N3	17.71	145.43	117.79
1	5	4185	B8W	N2-C2-N3	17.48	145.08	117.79
1	5	2380	B8W	N2-C2-N3	17.43	145.01	117.79
1	5	4472	B8W	N2-C2-N3	16.65	143.78	117.79
1	5	4529	B8W	N2-C2-N1	-15.38	94.16	117.22
1	5	2380	B8W	N2-C2-N1	-15.28	94.31	117.22
1	5	4129	B8W	N2-C2-N1	-15.07	94.62	117.22
1	5	4185	B8W	N2-C2-N1	-14.83	94.98	117.22
1	5	4472	B8W	N2-C2-N1	-14.53	95.44	117.22
1	5	2380	B8W	C1'-N9-C4	13.57	150.49	126.64
1	5	4129	B8W	C1'-N9-C4	13.54	150.43	126.64
1	5	4529	B8W	C1'-N9-C4	13.10	149.66	126.64
1	5	4564	M7A	C5-C6-N6	13.00	145.83	123.75
1	5	4472	B8W	C1'-N9-C4	12.87	149.25	126.64
50	9	1806	M7A	C5-C6-N6	12.85	145.58	123.75
1	5	4185	B8W	C1'-N9-C4	11.74	147.27	126.64
50	9	814	5MU	C5-C4-N3	11.38	125.21	115.32
1	5	4083	5MU	C5-C4-N3	11.09	124.96	115.32
1	5	4564	M7A	N6-C6-N1	-10.77	94.38	118.38
50	9	1806	M7A	N6-C6-N1	-10.77	94.39	118.38
1	5	4872	2MG	N1-C2-N2	9.78	126.54	116.56
1	5	4083	5MU	C5-C6-N1	-9.47	113.02	123.31
50	9	814	5MU	C5-C6-N1	-9.25	113.27	123.31
50	9	1850	MA6	N1-C6-N6	-9.01	106.42	116.83
1	5	1659	I4U	O4-C4-C5	8.71	121.63	115.45
50	9	1851	MA6	N1-C6-N6	-8.60	106.90	116.83
1	5	4529	B8W	O6-C6-C5	8.43	128.24	116.72
1	5	1524	A2M	C4'-O4'-C1'	-8.18	102.44	109.92
1	5	4129	B8W	O6-C6-C5	8.14	127.84	116.72
50	9	1031	A2M	C5-C6-N6	8.04	132.56	120.31
50	9	484	A2M	C5-C6-N6	8.02	132.53	120.31
50	9	159	A2M	C5-C6-N6	7.92	132.38	120.31
1	5	1871	A2M	C5-C6-N6	7.88	132.31	120.31
1	5	4472	B8W	C4'-O4'-C1'	-7.87	102.72	109.92
1	5	1348	P4U	O4-C4-C5	7.82	121.00	115.45
1	5	1524	A2M	C5-C6-N6	7.79	132.19	120.31
1	5	4185	B8W	C4'-O4'-C1'	-7.79	102.79	109.92
1	5	3825	A2M	C5-C6-N6	7.77	132.15	120.31
1	5	2380	B8W	C4'-O4'-C1'	-7.73	102.84	109.92
50	9	166	A2M	C5-C6-N6	7.66	131.98	120.31
1	5	4571	A2M	C5-C6-N6	7.63	131.93	120.31
1	5	4185	B8W	O6-C6-C5	7.58	127.08	116.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	1534	A2M	C5-C6-N6	7.56	131.83	120.31
1	5	3718	A2M	C5-C6-N6	7.54	131.80	120.31
50	9	668	A2M	C5-C6-N6	7.54	131.79	120.31
1	5	3867	A2M	C5-C6-N6	7.53	131.79	120.31
1	5	2363	A2M	C5-C6-N6	7.52	131.77	120.31
1	5	3723	A2M	C5-C6-N6	7.52	131.77	120.31
1	5	2401	A2M	C5-C6-N6	7.49	131.73	120.31
1	5	4523	A2M	C5-C6-N6	7.41	131.61	120.31
1	5	398	A2M	C5-C6-N6	7.40	131.59	120.31
1	5	1326	A2M	C5-C6-N6	7.38	131.56	120.31
50	9	27	A2M	C5-C6-N6	7.36	131.52	120.31
50	9	1678	A2M	C5-C6-N6	7.29	131.41	120.31
1	5	3762	B8H	C4-N3-C2	-7.14	117.98	127.34
1	5	4296	B8H	C4-N3-C2	-7.10	118.03	127.34
1	5	4194	I4U	O4-C4-C5	7.10	120.49	115.45
1	5	2401	A2M	N3-C2-N1	-7.05	119.10	128.67
50	9	166	A2M	N3-C2-N1	-7.04	119.11	128.67
1	5	1871	A2M	N3-C2-N1	-7.04	119.12	128.67
1	5	4296	B8H	N3-C2-N1	6.98	121.97	115.22
1	5	3785	A2M	C5-C6-N6	6.94	130.88	120.31
1	5	3762	B8H	N3-C2-N1	6.91	121.90	115.22
1	5	4571	A2M	N3-C2-N1	-6.72	119.55	128.67
50	9	1031	A2M	N3-C2-N1	-6.71	119.56	128.67
1	5	3723	A2M	N3-C2-N1	-6.69	119.58	128.67
1	5	1524	A2M	N3-C2-N1	-6.64	119.66	128.67
1	5	4523	A2M	N3-C2-N1	-6.60	119.71	128.67
1	5	1534	A2M	N3-C2-N1	-6.58	119.74	128.67
50	9	1850	MA6	N3-C2-N1	-6.56	119.76	128.67
1	5	4690	B8K	C72-C71-N7	6.54	128.45	118.80
50	9	1678	A2M	N3-C2-N1	-6.53	119.80	128.67
50	9	484	A2M	N3-C2-N1	-6.52	119.82	128.67
1	5	398	A2M	N3-C2-N1	-6.52	119.83	128.67
50	9	1851	MA6	N3-C2-N1	-6.49	119.86	128.67
50	9	27	A2M	N3-C2-N1	-6.48	119.88	128.67
1	5	1326	A2M	N3-C2-N1	-6.48	119.88	128.67
1	5	4371	MHG	C2-N3-C4	6.47	120.10	112.00
1	5	3785	A2M	N3-C2-N1	-6.45	119.92	128.67
1	5	1860	B8H	C4-N3-C2	-6.43	118.92	127.34
1	5	2363	A2M	N3-C2-N1	-6.42	119.96	128.67
1	5	3825	A2M	N3-C2-N1	-6.41	119.97	128.67
1	5	2786	B9H	C31-N3-C2	6.40	125.16	117.29
50	9	159	A2M	N3-C2-N1	-6.40	119.98	128.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	9	1832	6MZ	N3-C2-N1	-6.39	120.00	128.67
1	5	1797	E7G	C4-C5-N7	6.35	110.09	104.94
50	9	668	A2M	N3-C2-N1	-6.31	120.10	128.67
1	5	4220	6MZ	N3-C2-N1	-6.24	120.21	128.67
50	9	568	E3C	C1'-N1-C2	6.20	127.20	117.04
1	5	4529	B8W	C4'-O4'-C1'	-6.14	104.30	109.92
1	5	3867	A2M	N3-C2-N1	-6.12	120.36	128.67
1	5	4690	B8K	C5-C6-N1	6.12	121.71	110.94
50	9	668	A2M	C4'-O4'-C1'	-6.04	104.40	109.92
50	9	1806	M7A	N3-C2-N1	-6.03	119.45	128.58
1	5	2297	E7G	C4-C5-N7	5.90	109.72	104.94
1	5	3785	A2M	C4'-O4'-C1'	-5.81	104.61	109.92
1	5	4690	B8K	C4-C5-N7	5.79	109.61	104.93
3	8	14	OMU	C4-N3-C2	-5.78	119.43	126.61
1	5	4306	OMU	C4-N3-C2	-5.78	119.44	126.61
1	5	4564	M7A	N3-C2-N1	-5.78	119.83	128.58
1	5	4620	OMU	C4-N3-C2	-5.77	119.44	126.61
1	5	1860	B8H	N3-C2-N1	5.77	120.80	115.22
1	5	4628	PSU	N1-C2-N3	5.76	121.25	115.17
1	5	237	B9B	N3-C2-N1	-5.74	119.92	127.21
1	5	3899	BGH	C5-C6-N1	5.72	121.01	110.94
1	5	3897	B8K	C72-C71-N7	5.72	127.24	118.80
1	5	4185	B8W	N3-C2-N1	-5.72	119.94	127.21
1	5	4129	B8W	N3-C2-N1	-5.71	119.95	127.21
1	5	4472	B8W	O6-C6-C5	5.66	124.46	116.72
1	5	4564	M7A	N3-C4-N9	5.61	133.90	126.88
50	9	121	OMU	C4-N3-C2	-5.61	119.65	126.61
1	5	3897	B8K	C5-C6-N1	5.60	120.79	110.94
1	5	4355	E6G	N3-C2-N1	-5.58	120.12	127.21
1	5	4529	B8W	N3-C2-N1	-5.54	120.16	127.21
1	5	4872	2MG	N2-C2-N3	-5.54	113.46	120.51
1	5	237	B9B	O6-C6-N1	-5.53	115.50	120.23
1	5	3718	A2M	N3-C2-N1	-5.50	121.21	128.67
1	5	4450	PSU	C4-N3-C2	-5.47	118.83	126.37
50	9	1678	A2M	C4'-O4'-C1'	-5.47	104.91	109.92
50	9	116	OMU	C4-N3-C2	-5.46	119.83	126.61
1	5	4371	MHG	C4-C5-N7	5.45	109.36	104.94
1	5	2754	B9B	N3-C2-N1	-5.39	120.36	127.21
1	5	3899	BGH	C72-C71-N7	5.37	126.72	118.80
1	5	4636	PSU	C4-N3-C2	-5.36	118.99	126.37
1	5	3897	B8K	C4-C5-N7	5.35	109.25	104.93
1	5	4129	B8W	C61-O6-C6	5.33	122.87	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	1534	A2M	C4'-O4'-C1'	-5.30	105.07	109.92
1	5	4628	PSU	C4-N3-C2	-5.29	119.08	126.37
1	5	1677	PSU	C4-N3-C2	-5.28	119.10	126.37
50	9	159	A2M	C4'-O4'-C1'	-5.28	105.09	109.92
50	9	1243	PSU	N1-C2-N3	5.27	120.72	115.17
1	5	4403	PSU	N1-C2-N3	5.26	120.71	115.17
1	5	4500	PSU	C4-N3-C2	-5.21	119.20	126.37
1	5	1605	7MG	C5-C6-N1	5.21	120.10	110.94
1	5	4371	MHG	C5-C6-N1	5.19	120.08	110.94
1	5	3785	A2M	O4'-C1'-N9	5.19	115.62	108.75
50	9	1248	B8N	C5-C4-N3	5.18	125.55	116.15
50	9	822	PSU	N1-C2-N3	5.17	120.62	115.17
1	5	1524	A2M	N6-C6-N1	-5.17	107.30	118.33
1	5	1574	B9B	N3-C2-N1	-5.16	120.66	127.21
50	9	822	PSU	C4-N3-C2	-5.15	119.28	126.37
1	5	1797	E7G	C5-C6-N1	5.14	119.98	110.94
1	5	2380	B8W	N3-C2-N1	-5.13	120.68	127.21
50	9	159	A2M	N6-C6-N1	-5.13	107.37	118.33
1	5	4636	PSU	N1-C2-N3	5.13	120.58	115.17
1	5	4531	PSU	C4-N3-C2	-5.13	119.31	126.37
1	5	1534	A2M	N6-C6-N1	-5.11	107.42	118.33
1	5	4531	PSU	N1-C2-N3	5.11	120.56	115.17
1	5	2401	A2M	N6-C6-N1	-5.11	107.42	118.33
50	9	1031	A2M	N6-C6-N1	-5.11	107.43	118.33
1	5	4500	PSU	N1-C2-N3	5.10	120.55	115.17
50	9	814	5MU	N3-C2-N1	5.09	121.52	114.89
1	5	3825	A2M	N6-C6-N1	-5.07	107.50	118.33
1	5	4472	B8W	N3-C2-N1	-5.06	120.78	127.21
1	5	4129	B8W	O4'-C1'-N9	5.04	115.42	108.75
50	9	484	A2M	N6-C6-N1	-5.02	107.60	118.33
1	5	1871	A2M	N6-C6-N1	-5.01	107.63	118.33
1	5	4442	PSU	N1-C2-N3	5.00	120.45	115.17
1	5	1322	1MA	N1-C2-N3	-4.99	119.66	125.90
50	9	1219	B8Q	O2-C2-N3	-4.99	115.95	122.95
50	9	166	A2M	N6-C6-N1	-4.98	107.69	118.33
1	5	4450	PSU	N1-C2-N3	4.97	120.41	115.17
1	5	4550	7MG	C5-C6-N1	4.97	119.68	110.94
1	5	4571	A2M	N6-C6-N1	-4.96	107.74	118.33
1	5	2297	E7G	C5-C6-N1	4.95	119.66	110.94
1	5	4293	PSU	C4-N3-C2	-4.95	119.55	126.37
50	9	1081	PSU	N1-C2-N3	4.94	120.38	115.17
50	9	668	A2M	N6-C6-N1	-4.93	107.79	118.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	4185	B8W	O4'-C1'-N9	4.92	115.28	108.75
1	5	4415	1MA	N1-C2-N3	-4.90	119.77	125.90
1	5	4442	PSU	C4-N3-C2	-4.90	119.63	126.37
50	9	823	PSU	C4-N3-C2	-4.90	119.63	126.37
1	5	1683	PSU	N1-C2-N3	4.88	120.32	115.17
50	9	814	5MU	O4-C4-C5	-4.87	119.35	124.92
50	9	1830	UR3	C4-N3-C2	-4.87	120.66	124.58
1	5	3867	A2M	N6-C6-N1	-4.87	107.94	118.33
1	5	2363	A2M	N6-C6-N1	-4.85	107.97	118.33
1	5	237	B9B	C2-N3-C4	4.85	120.71	115.48
50	9	823	PSU	N1-C2-N3	4.85	120.28	115.17
1	5	2522	7MG	C5-C6-N1	4.84	119.46	110.94
50	9	1806	M7A	N3-C4-N9	4.84	132.93	126.88
1	5	1683	PSU	C4-N3-C2	-4.82	119.73	126.37
1	5	4293	PSU	N1-C2-N3	4.80	120.23	115.17
1	5	3785	A2M	N6-C6-N1	-4.79	108.10	118.33
50	9	27	A2M	N6-C6-N1	-4.78	108.13	118.33
1	5	4523	A2M	N6-C6-N1	-4.77	108.14	118.33
1	5	398	A2M	N6-C6-N1	-4.77	108.14	118.33
1	5	1677	PSU	N1-C2-N3	4.75	120.18	115.17
1	5	3899	BGH	C2-N3-C4	4.75	120.48	112.30
1	5	1326	A2M	N6-C6-N1	-4.74	108.20	118.33
1	5	3729	PSU	N1-C2-N3	4.73	120.16	115.17
1	5	3715	PSU	N1-C2-N3	4.72	120.15	115.17
50	9	612	PSU	C4-N3-C2	-4.70	119.90	126.37
50	9	1678	A2M	N6-C6-N1	-4.69	108.31	118.33
50	9	1248	B8N	C4-N3-C2	-4.69	119.85	125.62
1	5	3729	PSU	C4-N3-C2	-4.68	119.92	126.37
50	9	1243	PSU	C4-N3-C2	-4.68	119.92	126.37
1	5	4403	PSU	C4-N3-C2	-4.67	119.93	126.37
1	5	2508	PSU	C4-N3-C2	-4.66	119.95	126.37
1	5	4415	1MA	C5-C6-N1	4.66	120.64	113.95
1	5	4597	UR3	C4-N3-C2	-4.65	120.84	124.58
1	5	3718	A2M	N6-C6-N1	-4.65	108.40	118.33
1	5	1659	I4U	C5-C4-N3	-4.65	118.04	124.86
1	5	3723	A2M	N6-C6-N1	-4.65	108.40	118.33
1	5	4083	5MU	N3-C2-N1	4.64	120.93	114.89
1	5	1582	PSU	N1-C2-N3	4.63	120.06	115.17
1	5	4529	B8W	C61-O6-C6	4.62	122.03	116.65
1	5	3764	PSU	N1-C2-N3	4.61	120.03	115.17
50	9	1081	PSU	C4-N3-C2	-4.60	120.03	126.37
50	9	1219	B8Q	C1'-N1-C2	4.60	124.57	117.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	1605	7MG	C2-N3-C4	4.60	120.22	112.30
50	9	814	5MU	C4-N3-C2	-4.59	121.32	127.34
50	9	612	PSU	N1-C2-N3	4.59	120.01	115.17
1	5	4530	UR3	C4-N3-C2	-4.59	120.89	124.58
1	5	3715	PSU	C4-N3-C2	-4.58	120.07	126.37
1	5	4690	B8K	C2-N3-C4	4.56	120.15	112.30
1	5	3764	PSU	C4-N3-C2	-4.55	120.11	126.37
50	9	568	E3C	O2-C2-N3	-4.54	116.29	122.10
1	5	4185	B8W	C61-O6-C6	4.54	121.94	116.65
1	5	4550	7MG	C2-N3-C4	4.53	120.10	112.30
1	5	2297	E7G	C2-N3-C4	4.52	120.09	112.30
1	5	2508	PSU	N1-C2-N3	4.52	119.93	115.17
1	5	1797	E7G	C2-N3-C4	4.50	120.06	112.30
50	9	568	E3C	C4-N3-C2	-4.46	113.96	122.00
1	5	1456	B8Q	C31-N3-C4	4.46	122.47	114.76
50	9	1219	B8Q	N3-C2-N1	4.45	123.36	117.16
1	5	3880	P7G	C4-C5-N7	4.43	109.69	106.71
1	5	4355	E6G	C4'-O4'-C1'	-4.40	105.90	109.92
1	5	4529	B8W	O4'-C1'-N9	4.40	114.58	108.75
1	5	4472	B8W	O4'-C1'-N9	4.39	114.56	108.75
1	5	3899	BGH	C4-C5-N7	4.37	108.46	104.93
1	5	2522	7MG	C2-N3-C4	4.36	119.81	112.30
1	5	2363	A2M	C4'-O4'-C1'	-4.35	105.94	109.92
50	9	1830	UR3	C1'-N1-C2	4.32	124.11	117.04
1	5	1582	PSU	C4-N3-C2	-4.31	120.43	126.37
50	9	1031	A2M	C4'-O4'-C1'	-4.31	105.98	109.92
1	5	4083	5MU	O4-C4-C5	-4.30	119.99	124.92
1	5	1456	B8Q	N3-C2-N1	4.24	123.06	117.16
1	5	4371	MHG	N1-C2-N2	4.24	120.89	116.56
1	5	3899	BGH	C5-C4-N9	4.23	111.76	106.33
1	5	4355	E6G	C2-N3-C4	4.21	120.02	115.48
1	5	1909	P7G	C4-C5-N7	4.20	109.54	106.71
1	5	2380	B8W	O6-C6-C5	4.19	122.44	116.72
50	9	121	OMU	N3-C2-N1	4.15	120.29	114.89
1	5	3897	B8K	C2-N3-C4	4.14	119.44	112.30
50	9	1219	B8Q	C31-N3-C4	4.12	121.90	114.76
1	5	4129	B8W	C2-N3-C4	4.11	119.92	115.48
1	5	4690	B8K	N9-C8-N7	4.08	108.70	103.31
1	5	4872	2MG	CM2-N2-C2	-4.08	114.88	123.65
50	9	119	PSU	N1-C2-N3	4.08	119.47	115.17
50	9	1850	MA6	C2-N1-C6	4.07	120.83	116.84
1	5	4690	B8K	C5-C4-N9	4.07	111.55	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	3899	BGH	N9-C8-N7	4.06	108.66	103.31
1	5	4129	B8W	C4'-O4'-C1'	-4.05	106.21	109.92
1	5	4083	5MU	C4-N3-C2	-4.04	122.04	127.34
1	5	1605	7MG	C5-C4-N3	-4.04	120.55	128.13
50	9	568	E3C	C6-N1-C2	-4.03	118.51	121.80
50	9	1851	MA6	C2-N1-C6	4.03	120.79	116.84
50	9	568	E3C	C31-N3-C2	4.02	122.54	117.49
1	5	2754	B9B	N2-C2-N3	4.00	124.04	117.79
1	5	4306	OMU	N3-C2-N1	4.00	120.10	114.89
1	5	4620	OMU	N3-C2-N1	4.00	120.09	114.89
1	5	1322	1MA	C5-C6-N1	3.99	119.69	113.95
1	5	4296	B8H	O2-C2-N1	-3.94	118.80	122.78
1	5	2754	B9B	C2-N3-C4	3.94	119.73	115.48
1	5	2297	E7G	C5-C4-N3	-3.91	120.79	128.13
1	5	1517	2MG	N1-C2-N2	3.91	120.55	116.56
1	5	1574	B9B	C2-N3-C4	3.89	119.67	115.48
3	8	14	OMU	C5-C4-N3	3.89	120.24	114.80
1	5	4371	MHG	C5-C4-N3	-3.88	120.85	128.13
1	5	1348	P4U	C5-C4-N3	-3.87	119.18	124.86
1	5	2522	7MG	C4-C5-N7	3.84	109.91	105.38
1	5	2380	B8W	C2-N3-C4	3.82	119.61	115.48
1	5	4529	B8W	C2-N3-C4	3.82	119.60	115.48
1	5	1797	E7G	C5-C4-N3	-3.81	120.97	128.13
1	5	1883	OMG	C5-C6-N1	3.81	121.34	114.07
1	5	3897	B8K	N9-C8-N7	3.80	108.32	103.31
3	8	14	OMU	N3-C2-N1	3.80	119.83	114.89
1	5	1456	B8Q	O2-C2-N3	-3.80	117.62	122.95
1	5	1866	UR3	C6-N1-C2	-3.79	118.70	121.80
1	5	1860	B8H	C5-C4-N3	3.79	124.89	116.55
50	9	119	PSU	C4-N3-C2	-3.78	121.16	126.37
1	5	4371	MHG	C2-N1-C6	-3.78	119.98	124.55
1	5	4620	OMU	C5-C4-N3	3.78	120.09	114.80
1	5	4083	5MU	O2-C2-N1	-3.74	117.93	122.80
50	9	1374	5MC	O2-C2-N3	-3.71	116.49	122.33
1	5	3909	OMC	O2-C2-N3	-3.69	116.51	122.33
1	5	237	B9B	N2-C2-N3	3.68	123.53	117.79
1	5	1605	7MG	C4-C5-N7	3.68	109.72	105.38
50	9	116	OMU	C5-C4-N3	3.67	119.95	114.80
1	5	4550	7MG	C5-C4-N9	3.67	111.04	106.33
1	5	3762	B8H	C5-C4-N3	3.67	124.62	116.55
1	5	4523	A2M	C4'-O4'-C1'	-3.67	106.57	109.92
1	5	2522	7MG	C5-C4-N3	-3.65	121.28	128.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	9	116	OMU	N3-C2-N1	3.63	119.62	114.89
1	5	4472	B8W	C2-N3-C4	3.62	119.39	115.48
50	9	121	OMU	C5-C4-N3	3.62	119.87	114.80
50	9	1248	B8N	N3-C2-N1	3.62	121.14	116.72
1	5	2364	OMG	C5-C6-N1	3.60	120.95	114.07
1	5	1316	OMG	C2-N1-C6	-3.60	118.52	125.11
1	5	4335	5MC	C5-C6-N1	-3.60	119.40	123.31
1	5	4530	UR3	C5-C4-N3	3.60	119.78	115.04
1	5	4550	7MG	C5-C4-N3	-3.58	121.40	128.13
1	5	1574	B9B	C1'-N9-C4	-3.58	120.34	126.64
1	5	2380	B8W	O4'-C1'-N9	3.57	113.47	108.75
1	5	2522	7MG	C5-C4-N9	3.57	110.90	106.33
1	5	4296	B8H	C5-C4-N3	3.56	124.39	116.55
50	9	1806	M7A	C4-N9-C1'	-3.55	118.35	126.63
1	5	1316	OMG	C5-C6-N1	3.55	120.85	114.07
1	5	4185	B8W	C2-N3-C4	3.54	119.30	115.48
1	5	4306	OMU	C5-C4-N3	3.54	119.75	114.80
1	5	1883	OMG	C2-N1-C6	-3.53	118.64	125.11
1	5	3825	A2M	C4'-O4'-C1'	-3.52	106.70	109.92
1	5	3762	B8H	O2-C2-N1	-3.51	119.23	122.78
1	5	4447	5MC	C5-C6-N1	-3.50	119.52	123.31
1	5	4628	PSU	O2-C2-N1	-3.49	119.19	122.79
1	5	3792	OMG	C5-C6-N1	3.49	120.72	114.07
50	9	1830	UR3	C5-C4-N3	3.48	119.63	115.04
1	5	4872	2MG	C5-C6-N1	3.48	120.70	114.07
50	9	1830	UR3	C6-N1-C2	-3.47	118.96	121.80
1	5	4550	7MG	C4-C5-N7	3.47	109.47	105.38
1	5	4564	M7A	C2-N3-C4	3.45	120.27	111.83
1	5	1517	2MG	C5-C6-N1	3.42	120.60	114.07
1	5	1534	A2M	O4'-C1'-C2'	-3.42	100.77	106.61
1	5	2754	B9B	C4'-O4'-C1'	-3.42	106.79	109.92
1	5	1860	B8H	O2-C2-N1	-3.41	119.33	122.78
1	5	3909	OMC	C1'-N1-C2	3.41	125.97	118.44
1	5	2786	B9H	C4-N3-C2	-3.40	115.87	122.00
1	5	4597	UR3	C5-C4-N3	3.40	119.52	115.04
1	5	1866	UR3	C4-N3-C2	-3.40	121.84	124.58
1	5	3899	BGH	C5-C4-N3	-3.39	121.76	128.13
1	5	4872	2MG	C8-N7-C5	3.39	108.32	102.55
1	5	1866	UR3	C1'-N1-C2	3.39	122.59	117.04
50	9	814	5MU	C5M-C5-C6	-3.39	118.27	122.85
1	5	4623	OMG	C2-N1-C6	-3.38	118.92	125.11
1	5	3792	OMG	C2-N1-C6	-3.37	118.94	125.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	2364	OMG	C2-N1-C6	-3.36	118.95	125.11
50	9	1248	B8N	C1'-C5-C4	3.35	122.70	117.61
1	5	1522	OMG	C2-N1-C6	-3.35	118.98	125.11
1	5	4530	UR3	C1'-N1-C2	3.34	122.51	117.04
1	5	4371	MHG	C5-C4-N9	3.34	110.61	106.33
1	5	4370	OMG	C2-N1-C6	-3.34	119.00	125.11
1	5	4690	B8K	C6-C5-C4	-3.33	116.54	122.40
1	5	2050	OMG	C8-N7-C5	3.32	108.20	102.55
1	5	4623	OMG	C5-C6-N1	3.32	120.40	114.07
1	5	4355	E6G	O6-C6-N1	3.32	123.06	120.23
1	5	1522	OMG	C8-N7-C5	3.31	108.19	102.55
1	5	1522	OMG	C5-C6-N1	3.30	120.36	114.07
50	9	644	OMG	C2-N1-C6	-3.30	119.08	125.11
1	5	2050	OMG	C2-N1-C6	-3.29	119.09	125.11
1	5	2424	OMG	C5-C6-N1	3.29	120.34	114.07
1	5	4623	OMG	C8-N7-C5	3.29	108.14	102.55
50	9	116	OMU	O4-C4-C5	-3.28	119.50	125.16
3	8	14	OMU	O4-C4-C5	-3.28	119.50	125.16
1	5	4450	PSU	C6-C5-C4	3.28	120.39	118.17
1	5	4637	OMG	C8-N7-C5	3.28	108.14	102.55
1	5	4620	OMU	O4-C4-C5	-3.28	119.51	125.16
1	5	4494	OMG	C5-C6-N1	3.28	120.33	114.07
1	5	3899	BGH	C2'-C1'-N9	-3.28	107.47	114.14
50	9	822	PSU	O2-C2-N1	-3.28	119.41	122.79
1	5	4403	PSU	C6-N1-C2	-3.27	119.66	122.69
1	5	4690	B8K	C5-C4-N3	-3.27	122.00	128.13
1	5	4083	5MU	C5M-C5-C6	-3.26	118.44	122.85
1	5	373	OMG	C5-C6-N1	3.25	120.27	114.07
1	5	1316	OMG	C8-N7-C5	3.25	108.08	102.55
1	5	2754	B9B	C1'-N9-C4	-3.24	120.94	126.64
1	5	1683	PSU	O2-C2-N1	-3.24	119.45	122.79
1	5	2773	OMG	C8-N7-C5	3.24	108.07	102.55
1	5	3792	OMG	C8-N7-C5	3.23	108.04	102.55
50	9	1806	M7A	C2-N3-C4	3.22	119.70	111.83
1	5	2424	OMG	C8-N7-C5	3.22	108.03	102.55
1	5	2297	E7G	C5-C4-N9	3.21	110.45	106.33
1	5	4870	OMG	C5-C6-N1	3.20	120.17	114.07
1	5	4637	OMG	C2-N1-C6	-3.19	119.27	125.11
1	5	4196	OMG	C5-C6-N1	3.19	120.16	114.07
1	5	2773	OMG	C5-C6-N1	3.19	120.16	114.07
50	9	509	OMG	C2-N1-C6	-3.19	119.27	125.11
1	5	4370	OMG	C5-C6-N1	3.19	120.15	114.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	1605	7MG	C5-C4-N9	3.19	110.42	106.33
1	5	1582	PSU	C6-N1-C2	-3.17	119.75	122.69
50	9	683	OMG	C5-C6-N1	3.17	120.12	114.07
1	5	4530	UR3	C6-N1-C2	-3.17	119.21	121.80
1	5	1625	OMG	C2-N1-C6	-3.17	119.31	125.11
1	5	3897	B8K	C5-C4-N9	3.17	110.39	106.33
1	5	4083	5MU	C5M-C5-C4	3.16	122.16	118.78
1	5	4220	6MZ	C1'-N9-C4	-3.16	121.08	126.64
50	9	509	OMG	C8-N7-C5	3.16	107.93	102.55
1	5	1797	E7G	C5-C4-N9	3.16	110.38	106.33
1	5	4870	OMG	C8-N7-C5	3.16	107.92	102.55
50	9	644	OMG	C5-C6-N1	3.15	120.09	114.07
1	5	2424	OMG	C2-N1-C6	-3.15	119.35	125.11
1	5	1625	OMG	C8-N7-C5	3.14	107.90	102.55
1	5	2401	A2M	C4'-O4'-C1'	-3.14	107.05	109.92
50	9	644	OMG	C8-N7-C5	3.14	107.90	102.55
1	5	373	OMG	C8-N7-C5	3.13	107.89	102.55
1	5	4531	PSU	C6-C5-C4	3.13	120.29	118.17
1	5	1871	A2M	C4'-O4'-C1'	-3.13	107.06	109.92
1	5	4494	OMG	C8-N7-C5	3.13	107.88	102.55
1	5	3897	B8K	C5-C4-N3	-3.13	122.25	128.13
50	9	683	OMG	C8-N7-C5	3.13	107.87	102.55
1	5	4564	M7A	C5-C4-N3	-3.12	119.34	126.56
1	5	4194	I4U	C5-C4-N3	-3.12	120.28	124.86
1	5	4196	OMG	C2-N1-C6	-3.12	119.40	125.11
50	9	1219	B8Q	C6-N1-C2	-3.12	119.25	121.80
1	5	4628	PSU	C6-N1-C2	-3.12	119.80	122.69
1	5	4196	OMG	C8-N7-C5	3.11	107.85	102.55
1	5	4637	OMG	C5-C6-N1	3.11	120.00	114.07
1	5	1456	B8Q	C6-N1-C2	-3.11	119.26	121.80
50	9	612	PSU	O2-C2-N1	-3.10	119.59	122.79
1	5	3782	5MC	C5-C6-N1	-3.10	119.95	123.31
1	5	2754	B9B	O6-C6-N1	-3.09	117.58	120.23
1	5	4494	OMG	C2-N1-C6	-3.08	119.47	125.11
1	5	1348	P4U	O2-C2-N3	-3.08	117.48	122.33
1	5	729	2MG	C5-C6-N1	3.07	119.93	114.07
1	5	4636	PSU	O2-C2-N1	-3.07	119.62	122.79
1	5	4870	OMG	C2-N1-C6	-3.06	119.50	125.11
1	5	3897	B8K	C6-C5-C4	-3.06	117.02	122.40
1	5	2773	OMG	C2-N1-C6	-3.05	119.52	125.11
1	5	1625	OMG	C5-C6-N1	3.05	119.89	114.07
1	5	4306	OMU	O2-C2-N1	-3.05	118.83	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	9	568	E3C	C1'-N1-C6	-3.04	114.28	120.78
1	5	1866	UR3	C5-C4-N3	3.04	119.04	115.04
1	5	2522	7MG	N9-C8-N7	3.03	107.67	103.37
1	5	3899	BGH	C6-C5-C4	-3.03	117.07	122.40
1	5	1883	OMG	O6-C6-C5	-3.03	118.32	124.32
1	5	4500	PSU	O2-C2-N1	-3.02	119.67	122.79
50	9	1248	B8N	O4-C4-C5	-3.02	117.36	122.58
50	9	509	OMG	C5-C6-N1	3.01	119.82	114.07
50	9	1374	5MC	C5-C6-N1	-3.01	120.04	123.31
50	9	1248	B8N	C31-N3-C4	3.01	121.43	117.18
1	5	373	OMG	C2-N1-C6	-3.00	119.63	125.11
1	5	1866	UR3	O2-C2-N3	-2.99	117.19	121.33
1	5	1883	OMG	C8-N7-C5	2.99	107.64	102.55
1	5	4370	OMG	C8-N7-C5	2.99	107.64	102.55
50	9	119	PSU	C6-N1-C2	-2.99	119.92	122.69
50	9	1337	4AC	C5-C4-N3	-2.98	117.93	122.60
1	5	2364	OMG	C8-N7-C5	2.98	107.62	102.55
1	5	2050	OMG	C5-C6-N1	2.98	119.75	114.07
1	5	1322	1MA	C8-N7-C5	2.95	107.56	102.55
1	5	4450	PSU	O2-C2-N1	-2.94	119.76	122.79
50	9	119	PSU	O2-C2-N1	-2.94	119.76	122.79
50	9	814	5MU	C1'-N1-C2	2.93	122.85	117.59
50	9	1243	PSU	C6-N1-C2	-2.92	119.98	122.69
1	5	729	2MG	C8-N7-C5	2.92	107.52	102.55
1	5	4531	PSU	O2-C2-N1	-2.91	119.78	122.79
1	5	3729	PSU	C6-N1-C2	-2.90	120.00	122.69
1	5	4415	1MA	C8-N7-C5	2.89	107.47	102.55
1	5	1582	PSU	O2-C2-N1	-2.89	119.81	122.79
1	5	4690	B8K	C2-N1-C6	-2.88	119.89	125.11
1	5	4636	PSU	C6-C5-C4	2.87	120.11	118.17
1	5	1909	P7G	N9-C8-N7	2.87	107.43	103.37
1	5	1797	E7G	C2-N1-C6	-2.87	119.92	125.11
1	5	3729	PSU	O2-C2-N1	-2.86	119.83	122.79
50	9	1243	PSU	O2-C2-N1	-2.86	119.84	122.79
1	5	1517	2MG	C8-N7-C5	2.86	107.41	102.55
50	9	814	5MU	O2-C2-N3	-2.84	116.25	121.49
50	9	683	OMG	C2-N1-C6	-2.82	119.94	125.11
1	5	3897	B8K	O4'-C1'-C2'	-2.82	100.58	106.62
50	9	1842	4AC	C6-C5-C4	2.82	120.40	117.00
1	5	1683	PSU	C6-N1-C2	-2.82	120.08	122.69
50	9	814	5MU	C5M-C5-C4	2.82	121.79	118.78
1	5	3715	PSU	O2-C2-N1	-2.82	119.89	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	2364	OMG	O6-C6-C5	-2.81	118.75	124.32
1	5	2297	E7G	C2-N1-C6	-2.81	120.02	125.11
1	5	4403	PSU	O2-C2-N1	-2.81	119.89	122.79
1	5	4355	E6G	C61-O6-C6	-2.80	113.71	117.32
1	5	1605	7MG	N9-C8-N7	2.80	107.34	103.37
1	5	4536	OMC	O2-C2-N3	-2.80	117.92	122.33
1	5	3899	BGH	C2-N1-C6	-2.80	120.04	125.11
50	9	1081	PSU	C6-N1-C2	-2.79	120.10	122.69
50	9	116	OMU	C1'-N1-C2	2.79	122.60	117.59
50	9	823	PSU	O2-C2-N1	-2.77	119.93	122.79
1	5	2422	OMC	O2-C2-N3	-2.77	117.96	122.33
50	9	1842	4AC	C5-C4-N3	-2.75	118.29	122.60
1	5	4335	5MC	CM5-C5-C6	-2.74	119.14	122.85
1	5	1605	7MG	C2-N1-C6	-2.74	120.14	125.11
1	5	4442	PSU	C6-N1-C2	-2.74	120.15	122.69
1	5	3764	PSU	O2-C2-N1	-2.73	119.97	122.79
1	5	373	OMG	CM2-O2'-C2'	-2.73	107.47	114.47
50	9	121	OMU	O4-C4-C5	-2.71	120.48	125.16
1	5	4083	5MU	O4-C4-N3	-2.70	115.05	120.11
1	5	3880	P7G	N9-C8-N7	2.70	107.19	103.37
1	5	1517	2MG	O6-C6-C5	-2.69	118.98	124.32
1	5	1797	E7G	N9-C8-N7	2.69	107.19	103.37
1	5	4564	M7A	C4-N9-C1'	-2.68	120.38	126.63
50	9	1081	PSU	O2-C2-N1	-2.67	120.04	122.79
1	5	2786	B9H	O2-C2-N1	-2.66	116.86	122.78
1	5	1574	B9B	O6-C6-N1	-2.66	117.96	120.23
1	5	2380	B8W	C61-O6-C6	-2.65	113.56	116.65
1	5	4129	B8W	C4-C5-N7	-2.64	106.55	109.34
1	5	4671	B8T	C6-C5-C4	2.64	120.18	117.00
1	5	4442	PSU	O2-C2-N1	-2.64	120.07	122.79
1	5	3762	B8H	O4-C4-N3	-2.62	115.18	120.11
50	9	1710	OMC	O2-C2-N3	-2.62	118.20	122.33
50	9	1337	4AC	C6-C5-C4	2.62	120.16	117.00
1	5	1524	A2M	O4'-C1'-N9	2.62	112.22	108.75
1	5	4620	OMU	O2-C2-N1	-2.62	119.39	122.80
1	5	4355	E6G	N2-C2-N1	2.62	121.14	117.22
1	5	1677	PSU	O2-C2-N1	-2.61	120.09	122.79
1	5	1659	I4U	C5'-C4'-C3'	-2.60	105.86	115.21
1	5	3897	B8K	C2-N1-C6	-2.60	120.40	125.11
50	9	814	5MU	C6-N1-C2	-2.59	118.72	121.30
1	5	4185	B8W	O4'-C4'-C3'	-2.59	100.02	105.15
1	5	3764	PSU	C6-N1-C2	-2.59	120.29	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	1316	OMG	O6-C6-C5	-2.59	119.19	124.32
1	5	3715	PSU	C6-N1-C2	-2.58	120.30	122.69
50	9	27	A2M	C3'-C2'-C1'	2.58	107.75	102.81
1	5	4483	B8T	O2-C2-N3	-2.57	118.28	122.33
1	5	4690	B8K	O6-C6-C5	-2.57	121.31	127.62
50	9	668	A2M	O4'-C1'-N9	-2.56	105.35	108.75
1	5	4500	PSU	C6-N1-C2	-2.56	120.31	122.69
50	9	1806	M7A	C71-N7-C5	-2.56	112.77	123.44
1	5	1860	B8H	O4-C4-N3	-2.55	115.32	120.11
1	5	4494	OMG	O6-C6-C5	-2.54	119.29	124.32
1	5	4623	OMG	O6-C6-C5	-2.53	119.30	124.32
50	9	1832	6MZ	C6-C5-C4	-2.51	115.01	117.68
1	5	1574	B9B	N2-C2-N3	2.51	121.70	117.79
1	5	4530	UR3	O2-C2-N3	-2.51	117.87	121.33
50	9	823	PSU	C6-N1-C2	-2.50	120.37	122.69
1	5	4306	OMU	O4-C4-C5	-2.50	120.85	125.16
1	5	4483	B8T	C6-C5-C4	2.49	120.00	117.00
50	9	814	5MU	O4-C4-N3	-2.49	115.43	120.11
50	9	166	A2M	C5'-C4'-C3'	-2.47	106.34	115.21
1	5	4370	OMG	O6-C6-C5	-2.45	119.46	124.32
1	5	373	OMG	O6-C6-C5	-2.45	119.47	124.32
1	5	1605	7MG	N9-C4-N3	2.44	129.04	125.46
1	5	4185	B8W	C4-C5-N7	-2.44	106.76	109.34
1	5	3723	A2M	C4'-O4'-C1'	-2.43	107.70	109.92
1	5	2522	7MG	C2-N1-C6	-2.43	120.71	125.11
50	9	1842	4AC	O7-C7-CM7	-2.42	117.74	122.05
50	9	822	PSU	O4'-C1'-C2'	2.42	108.50	105.15
50	9	644	OMG	O6-C6-C5	-2.42	119.53	124.32
3	8	14	OMU	C1'-N1-C2	2.42	121.94	117.59
50	9	1806	M7A	C5-C4-N3	-2.41	120.99	126.56
1	5	4296	B8H	O4-C4-N3	-2.41	115.59	120.11
1	5	4550	7MG	N9-C8-N7	2.40	106.78	103.37
1	5	4628	PSU	C6-C5-C4	2.40	119.79	118.17
1	5	4597	UR3	C1'-N1-C2	2.40	120.96	117.04
48	v	715	DDE	CAU-CBW-CBI	-2.40	106.53	111.22
1	5	3887	OMC	O2-C2-N3	-2.39	118.56	122.33
1	5	1797	E7G	O6-C6-C5	-2.39	121.75	127.62
1	5	4529	B8W	C4-C5-N7	-2.38	106.82	109.34
50	9	668	A2M	C3'-C2'-C1'	2.38	107.36	102.81
50	9	27	A2M	C4'-O4'-C1'	-2.38	107.75	109.92
1	5	2508	PSU	O2-C2-N1	-2.37	120.34	122.79
1	5	4472	B8W	O4'-C4'-C3'	-2.37	100.45	105.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	4690	B8K	C3'-C2'-C1'	2.36	105.92	101.46
1	5	2297	E7G	N9-C8-N7	2.35	106.70	103.37
1	5	4371	MHG	C21-N2-C2	-2.35	118.59	123.65
1	5	4293	PSU	C6-N1-C2	-2.35	120.51	122.69
50	9	121	OMU	C1'-N1-C2	2.34	121.80	117.59
3	8	14	OMU	CM2-O2'-C2'	2.34	120.49	114.47
1	5	2754	B9B	O4'-C1'-N9	2.34	111.85	108.75
1	5	3897	B8K	O6-C6-C5	-2.34	121.88	127.62
50	9	822	PSU	C6-N1-C2	-2.34	120.52	122.69
1	5	4531	PSU	C6-N1-C2	-2.34	120.52	122.69
1	5	2522	7MG	O6-C6-C5	-2.33	121.89	127.62
1	5	4550	7MG	O6-C6-C5	-2.33	121.89	127.62
1	5	3792	OMG	O6-C6-C5	-2.33	119.69	124.32
50	9	1219	B8Q	C31-N3-C2	2.33	121.36	117.70
1	5	4371	MHG	O6-C6-C5	-2.33	121.90	127.62
50	9	814	5MU	C6-C5-C4	2.32	119.94	118.02
50	9	159	A2M	O4'-C4'-C3'	-2.32	100.54	105.15
50	9	1337	4AC	O7-C7-CM7	-2.32	117.92	122.05
1	5	4194	I4U	O4'-C1'-C2'	-2.30	101.69	106.62
1	5	4597	UR3	C6-N1-C2	-2.30	119.92	121.80
1	5	4371	MHG	C71-C72-C73	-2.29	108.00	114.13
1	5	2297	E7G	O6-C6-C5	-2.29	122.00	127.62
50	9	1374	5MC	O2-C2-N1	2.29	123.39	118.90
1	5	2424	OMG	O6-C6-C5	-2.28	119.79	124.32
1	5	3718	A2M	C4'-O4'-C1'	-2.28	107.84	109.92
1	5	729	2MG	O6-C6-C5	-2.27	119.82	124.32
1	5	3899	BGH	C5'-C4'-C3'	-2.27	107.04	115.21
1	5	4550	7MG	C2-N1-C6	-2.27	121.00	125.11
1	5	1605	7MG	O6-C6-C5	-2.26	122.06	127.62
1	5	2508	PSU	C6-N1-C2	-2.26	120.60	122.69
1	5	2297	E7G	N9-C4-N3	2.25	128.76	125.46
50	9	683	OMG	O6-C6-C5	-2.25	119.86	124.32
1	5	4550	7MG	C6-C5-C4	-2.25	118.45	122.40
1	5	2773	OMG	O6-C6-C5	-2.25	119.87	124.32
1	5	1625	OMG	O6-C6-C5	-2.24	119.87	124.32
1	5	2050	OMG	O6-C6-C5	-2.24	119.87	124.32
1	5	729	2MG	CM2-N2-C2	-2.23	118.85	123.65
50	9	509	OMG	O6-C6-C5	-2.22	119.91	124.32
1	5	3897	B8K	O3'-C3'-C4'	-2.22	104.70	111.08
1	5	2861	OMC	O2-C2-N3	-2.22	118.83	122.33
1	5	4872	2MG	O6-C6-C5	-2.22	119.93	124.32
1	5	4335	5MC	C1'-N1-C6	-2.21	117.51	121.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	4536	OMC	C1'-N1-C2	2.21	123.33	118.44
1	5	3869	OMC	O2-C2-N3	-2.21	118.85	122.33
1	5	4220	6MZ	C9-N6-C6	-2.20	120.81	122.85
50	9	1248	B8N	O4'-C1'-C2'	2.20	108.19	105.15
1	5	3909	OMC	C1'-N1-C6	-2.19	116.10	120.78
50	9	1703	OMC	O2-C2-N3	-2.18	118.89	122.33
1	5	4371	MHG	N1-C2-N3	-2.18	120.01	123.68
1	5	4442	PSU	O4'-C1'-C2'	2.18	108.17	105.15
1	5	1677	PSU	C6-N1-C2	-2.18	120.67	122.69
50	9	612	PSU	C6-N1-C2	-2.18	120.67	122.69
1	5	1797	E7G	N9-C4-N3	2.17	128.64	125.46
50	9	668	A2M	C5'-C4'-C3'	-2.17	107.39	115.21
50	9	1830	UR3	O2-C2-N3	-2.17	118.33	121.33
1	5	4550	7MG	N1-C2-N3	-2.16	119.37	123.32
50	9	1219	B8Q	C1'-N1-C6	-2.15	116.17	120.78
1	5	4571	A2M	C5'-C4'-C3'	-2.15	107.46	115.21
1	5	2401	A2M	C2'-C1'-N9	-2.15	107.79	112.56
1	5	4196	OMG	O6-C6-C5	-2.14	120.08	124.32
1	5	4636	PSU	C6-N1-C2	-2.13	120.71	122.69
1	5	1517	2MG	CM2-N2-C2	-2.13	119.07	123.65
1	5	4194	I4U	C2'-C3'-C4'	2.13	106.72	102.61
1	5	4870	OMG	O6-C6-C5	-2.13	120.11	124.32
1	5	1524	A2M	C2'-C1'-N9	-2.12	107.84	112.56
1	5	237	B9B	C1'-N9-C4	-2.12	122.91	126.64
1	5	4450	PSU	C5-C6-N1	-2.12	119.19	122.14
48	v	715	DDE	CAC-NCB-CBW	2.12	115.60	110.52
50	9	1031	A2M	C5'-C4'-C3'	-2.12	107.58	115.21
1	5	4523	A2M	O4'-C1'-N9	2.12	111.56	108.75
3	8	14	OMU	O2-C2-N1	-2.12	120.04	122.80
1	5	1522	OMG	O6-C6-C5	-2.11	120.13	124.32
1	5	1871	A2M	C2'-C1'-N9	-2.11	107.88	112.56
50	9	1842	4AC	N4-C4-N3	2.10	117.28	113.87
1	5	4371	MHG	N9-C4-N3	2.10	128.54	125.46
50	9	612	PSU	O4'-C1'-C2'	2.10	108.05	105.15
1	5	1677	PSU	C6-C5-C4	2.09	119.58	118.17
50	9	683	OMG	N1-C2-N3	-2.08	119.50	123.32
1	5	1797	E7G	C6-C5-C4	-2.08	118.74	122.40
1	5	1677	PSU	O4'-C1'-C2'	2.08	108.03	105.15
1	5	3825	A2M	C5'-C4'-C3'	-2.07	107.75	115.21
50	9	1081	PSU	O4'-C1'-C2'	2.07	108.01	105.15
1	5	3867	A2M	C3'-C2'-C1'	2.06	106.75	102.81
1	5	4637	OMG	O6-C6-C5	-2.05	120.25	124.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	2522	7MG	C6-C5-C4	-2.04	118.81	122.40
1	5	2401	A2M	C3'-C2'-C1'	2.04	106.72	102.81
50	9	174	OMC	O2-C2-N3	-2.04	119.11	122.33
1	5	3899	BGH	O4'-C4'-C3'	-2.04	101.10	105.15
1	5	3899	BGH	O6-C6-C5	-2.04	122.62	127.62
1	5	4500	PSU	C6-C5-C4	2.03	119.54	118.17
1	5	3899	BGH	N1-C2-N3	-2.02	119.63	123.32
1	5	4564	M7A	N9-C8-N7	2.02	106.23	103.37
1	5	398	A2M	C4'-O4'-C1'	-2.02	108.08	109.92
50	9	119	PSU	O4-C4-N3	-2.01	116.33	120.11
50	9	1337	4AC	O2-C2-N3	-2.01	119.16	122.33
1	5	1574	B9B	C4'-O4'-C1'	-2.00	108.09	109.92

There are no chirality outliers.

All (211) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	5	237	B9B	C5-C6-O6-C61
1	5	237	B9B	N1-C6-O6-C61
1	5	237	B9B	O4'-C4'-C5'-O5'
1	5	1348	P4U	N3-C4-O4-C41
1	5	1582	PSU	O4'-C4'-C5'-O5'
1	5	2364	OMG	O4'-C4'-C5'-O5'
1	5	2364	OMG	C3'-C4'-C5'-O5'
1	5	2380	B8W	C5-C6-O6-C61
1	5	2380	B8W	N1-C6-O6-C61
1	5	3701	OMC	C2'-C1'-N1-C2
1	5	3701	OMC	C2'-C1'-N1-C6
1	5	3792	OMG	O4'-C4'-C5'-O5'
1	5	3897	B8K	O4'-C4'-C5'-O5'
1	5	3899	BGH	C3'-C4'-C5'-O5'
1	5	3899	BGH	O4'-C4'-C5'-O5'
1	5	4083	5MU	C2'-C1'-N1-C2
1	5	4083	5MU	C2'-C1'-N1-C6
1	5	4129	B8W	C5-C6-O6-C61
1	5	4129	B8W	N1-C6-O6-C61
1	5	4185	B8W	C5-C6-O6-C61
1	5	4185	B8W	N1-C6-O6-C61
1	5	4194	I4U	O4'-C4'-C5'-O5'
1	5	4355	E6G	O4'-C4'-C5'-O5'
1	5	4355	E6G	C5-C6-O6-C61
1	5	4355	E6G	N1-C6-O6-C61

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Mol	Chain	Res	Type	Atoms
1	5	4403	PSU	O4'-C1'-C5-C4
1	5	4403	PSU	O4'-C1'-C5-C6
1	5	4447	5MC	C2'-C1'-N1-C6
1	5	4450	PSU	O4'-C4'-C5'-O5'
1	5	4472	B8W	C5-C6-O6-C61
1	5	4472	B8W	N1-C6-O6-C61
1	5	4500	PSU	C3'-C4'-C5'-O5'
1	5	4500	PSU	O4'-C4'-C5'-O5'
1	5	4523	A2M	O4'-C4'-C5'-O5'
1	5	4529	B8W	C5-C6-O6-C61
1	5	4529	B8W	N1-C6-O6-C61
1	5	4637	OMG	C1'-C2'-O2'-CM2
1	5	4870	OMG	O4'-C4'-C5'-O5'
1	5	4870	OMG	C3'-C4'-C5'-O5'
3	8	14	OMU	C1'-C2'-O2'-CM2
6	C	333	MLZ	N-CA-CB-CG
6	C	333	MLZ	C-CA-CB-CG
41	m	72	MLZ	N-CA-CB-CG
41	m	72	MLZ	CD-CE-NZ-CM
48	v	715	DDE	O-C-CA-CB
48	v	715	DDE	CA-CB-CG-CD2
48	v	715	DDE	CAU-CAT-CE1-ND1
48	v	715	DDE	CBI-CBW-NCB-CAB
48	v	715	DDE	CBI-CBW-NCB-CAC
48	v	715	DDE	CBI-CBW-NCB-CAA
48	v	715	DDE	CAU-CBW-NCB-CAB
48	v	715	DDE	CAU-CBW-NCB-CAC
48	v	715	DDE	CAU-CBW-NCB-CAA
48	v	715	DDE	CAT-CAU-CBW-CBI
48	v	715	DDE	CAT-CAU-CBW-NCB
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	O4'-C4'-C5'-O5'
50	9	568	E3C	O4'-C1'-N1-C2
50	9	568	E3C	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	1850	MA6	C5-C6-N6-C10
50	9	1851	MA6	O4'-C4'-C5'-O5'
1	5	4447	5MC	C2'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
1	5	237	B9B	C3'-C4'-C5'-O5'
1	5	398	A2M	O4'-C4'-C5'-O5'
1	5	1582	PSU	C3'-C4'-C5'-O5'
1	5	1625	OMG	C3'-C4'-C5'-O5'
1	5	1797	E7G	O4'-C4'-C5'-O5'
1	5	2380	B8W	C3'-C4'-C5'-O5'
1	5	2380	B8W	O4'-C4'-C5'-O5'
1	5	2424	OMG	O4'-C4'-C5'-O5'
1	5	2424	OMG	C3'-C4'-C5'-O5'
1	5	3729	PSU	O4'-C4'-C5'-O5'
1	5	3880	P7G	O4'-C4'-C5'-O5'
1	5	4185	B8W	O4'-C4'-C5'-O5'
1	5	4415	1MA	C3'-C4'-C5'-O5'
1	5	4636	PSU	C3'-C4'-C5'-O5'
1	5	4636	PSU	O4'-C4'-C5'-O5'
1	5	4637	OMG	O4'-C4'-C5'-O5'
50	9	121	OMU	C3'-C4'-C5'-O5'
50	9	159	A2M	O4'-C4'-C5'-O5'
50	9	159	A2M	C3'-C4'-C5'-O5'
50	9	166	A2M	C3'-C4'-C5'-O5'
50	9	1081	PSU	O4'-C4'-C5'-O5'
50	9	1851	MA6	C3'-C4'-C5'-O5'
50	9	1830	UR3	O4'-C1'-N1-C6
1	5	1348	P4U	C3'-C4'-C5'-O5'
1	5	1348	P4U	O4'-C4'-C5'-O5'
1	5	2401	A2M	C3'-C4'-C5'-O5'
1	5	3764	PSU	C3'-C4'-C5'-O5'
1	5	3764	PSU	O4'-C4'-C5'-O5'
1	5	3792	OMG	C3'-C4'-C5'-O5'
1	5	3867	A2M	O4'-C4'-C5'-O5'
1	5	3867	A2M	C3'-C4'-C5'-O5'
1	5	4355	E6G	C3'-C4'-C5'-O5'
1	5	4371	MHG	O4'-C4'-C5'-O5'
1	5	4415	1MA	O4'-C4'-C5'-O5'
1	5	4450	PSU	C3'-C4'-C5'-O5'
50	9	119	PSU	O4'-C4'-C5'-O5'
50	9	166	A2M	O4'-C4'-C5'-O5'
50	9	568	E3C	C3'-C4'-C5'-O5'
50	9	568	E3C	O4'-C4'-C5'-O5'
50	9	668	A2M	O4'-C4'-C5'-O5'
50	9	683	OMG	O4'-C4'-C5'-O5'
50	9	1703	OMC	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
50	9	1830	UR3	O4'-C4'-C5'-O5'
1	5	4371	MHG	C2'-C1'-N9-C8
1	5	3897	B8K	C3'-C4'-C5'-O5'
1	5	4194	I4U	C3'-C4'-C5'-O5'
50	9	517	OMC	C3'-C4'-C5'-O5'
50	9	668	A2M	C3'-C4'-C5'-O5'
1	5	1574	B9B	O6-C61-C62-C63
1	5	1456	B8Q	C3'-C4'-C5'-O5'
1	5	1797	E7G	C3'-C4'-C5'-O5'
1	5	3729	PSU	C3'-C4'-C5'-O5'
1	5	3785	A2M	O4'-C4'-C5'-O5'
1	5	3785	A2M	C3'-C4'-C5'-O5'
1	5	4523	A2M	C3'-C4'-C5'-O5'
50	9	1243	PSU	O4'-C4'-C5'-O5'
1	5	1348	P4U	O4-C41-C42-C43
1	5	1456	B8Q	O4'-C4'-C5'-O5'
1	5	1625	OMG	O4'-C4'-C5'-O5'
1	5	3880	P7G	C3'-C4'-C5'-O5'
1	5	4637	OMG	C3'-C4'-C5'-O5'
50	9	517	OMC	O4'-C4'-C5'-O5'
50	9	1081	PSU	C3'-C4'-C5'-O5'
1	5	1909	P7G	C72-C71-N7-C8
1	5	2297	E7G	C72-C71-N7-C8
1	5	4355	E6G	C62-C61-O6-C6
1	5	1574	B9B	O4'-C4'-C5'-O5'
1	5	4371	MHG	C3'-C4'-C5'-O5'
1	5	4494	OMG	O4'-C4'-C5'-O5'
50	9	1830	UR3	C3'-C4'-C5'-O5'
1	5	2786	B9H	C32-C31-N3-C2
48	v	715	DDE	N-CA-CB-CG
1	5	398	A2M	C3'-C4'-C5'-O5'
1	5	1909	P7G	O4'-C4'-C5'-O5'
1	5	4494	OMG	C3'-C4'-C5'-O5'
50	9	683	OMG	C3'-C4'-C5'-O5'
1	5	4483	B8T	C3'-C4'-C5'-O5'
48	v	715	DDE	NAD-CBI-CBW-NCB
1	5	4083	5MU	C3'-C4'-C5'-O5'
1	5	4483	B8T	O4'-C4'-C5'-O5'
50	9	822	PSU	C3'-C4'-C5'-O5'
41	m	72	MLZ	C-CA-CB-CG
50	9	1248	B8N	N3-C31-C32-C33
1	5	2786	B9H	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
48	v	715	DDE	C-CA-CB-CG
48	v	715	DDE	CA-CB-CG-ND1
50	9	1851	MA6	C5-C6-N6-C10
1	5	1625	OMG	C4'-C5'-O5'-P
50	9	159	A2M	C4'-C5'-O5'-P
1	5	4083	5MU	O4'-C1'-N1-C6
50	9	644	OMG	C4'-C5'-O5'-P
1	5	1909	P7G	C72-C71-N7-C5
1	5	4371	MHG	C72-C71-N7-C5
1	5	1677	PSU	O4'-C1'-C5-C4
1	5	1860	B8H	O4'-C1'-C5-C4
50	9	1248	B8N	O4'-C1'-C5-C4
1	5	4083	5MU	O4'-C4'-C5'-O5'
50	9	119	PSU	C3'-C4'-C5'-O5'
50	9	1703	OMC	C3'-C4'-C5'-O5'
1	5	4371	MHG	C72-C71-N7-C8
1	5	1797	E7G	C72-C71-N7-C8
1	5	3887	OMC	C4'-C5'-O5'-P
1	5	4447	5MC	O4'-C1'-N1-C6
1	5	729	2MG	O4'-C4'-C5'-O5'
1	5	4872	2MG	O4'-C4'-C5'-O5'
1	5	2401	A2M	O4'-C4'-C5'-O5'
1	5	4447	5MC	O4'-C1'-N1-C2
1	5	3701	OMC	O4'-C1'-N1-C6
1	5	4870	OMG	C3'-C2'-O2'-CM2
1	5	3897	B8K	C4'-C5'-O5'-P
50	9	1081	PSU	C4'-C5'-O5'-P
1	5	1574	B9B	C62-C61-O6-C6
1	5	373	OMG	C4'-C5'-O5'-P
1	5	2754	B9B	C4'-C5'-O5'-P
1	5	4500	PSU	C4'-C5'-O5'-P
1	5	4870	OMG	C4'-C5'-O5'-P
50	9	822	PSU	O4'-C4'-C5'-O5'
1	5	3867	A2M	C1'-C2'-O2'-CM'
50	9	668	A2M	C1'-C2'-O2'-CM'
1	5	2380	B8W	C4'-C5'-O5'-P
1	5	4530	UR3	C4'-C5'-O5'-P
1	5	4083	5MU	O4'-C1'-N1-C2
50	9	1243	PSU	C3'-C4'-C5'-O5'
1	5	1677	PSU	O4'-C1'-C5-C6
1	5	1860	B8H	O4'-C1'-C5-C6
1	5	4636	PSU	O4'-C1'-C5-C6

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Mol	Chain	Res	Type	Atoms
1	5	2786	B9H	C32-C31-N3-C4
50	9	668	A2M	C3'-C2'-O2'-CM'
1	5	3701	OMC	O4'-C1'-N1-C2
1	5	1659	I4U	C42-C41-O4-C4
1	5	1659	I4U	C43-C41-O4-C4
1	5	4194	I4U	C42-C41-O4-C4
1	5	4194	I4U	C43-C41-O4-C4
1	5	4296	B8H	C3'-C4'-C5'-O5'
1	5	4450	PSU	C2'-C1'-C5-C6
1	5	4636	PSU	C2'-C1'-C5-C6
1	5	4185	B8W	C3'-C4'-C5'-O5'
1	5	729	2MG	C3'-C4'-C5'-O5'
1	5	1866	UR3	O4'-C4'-C5'-O5'
1	5	3880	P7G	C72-C71-N7-C5
1	5	1534	A2M	C4'-C5'-O5'-P
1	5	3867	A2M	C4'-C5'-O5'-P
1	5	3909	OMC	C2'-C1'-N1-C2
1	5	4306	OMU	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 307 ligands modelled in this entry, 306 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z > 2$
86	GDP	v	900	-	25,30,30	0.90	1 (4%)	30,47,47	1.39	5 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	GDP	v	900	-	-	0/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	v	900	GDP	C6-N1	-2.51	1.34	1.37

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	v	900	GDP	C4'-O4'-C1'	-3.68	106.56	109.92
86	v	900	GDP	C8-N7-C5	2.86	107.41	102.55
86	v	900	GDP	C5-C6-N1	2.28	118.42	114.07
86	v	900	GDP	O4'-C1'-N9	2.22	111.69	108.75
86	v	900	GDP	O6-C6-C5	-2.04	120.27	124.32

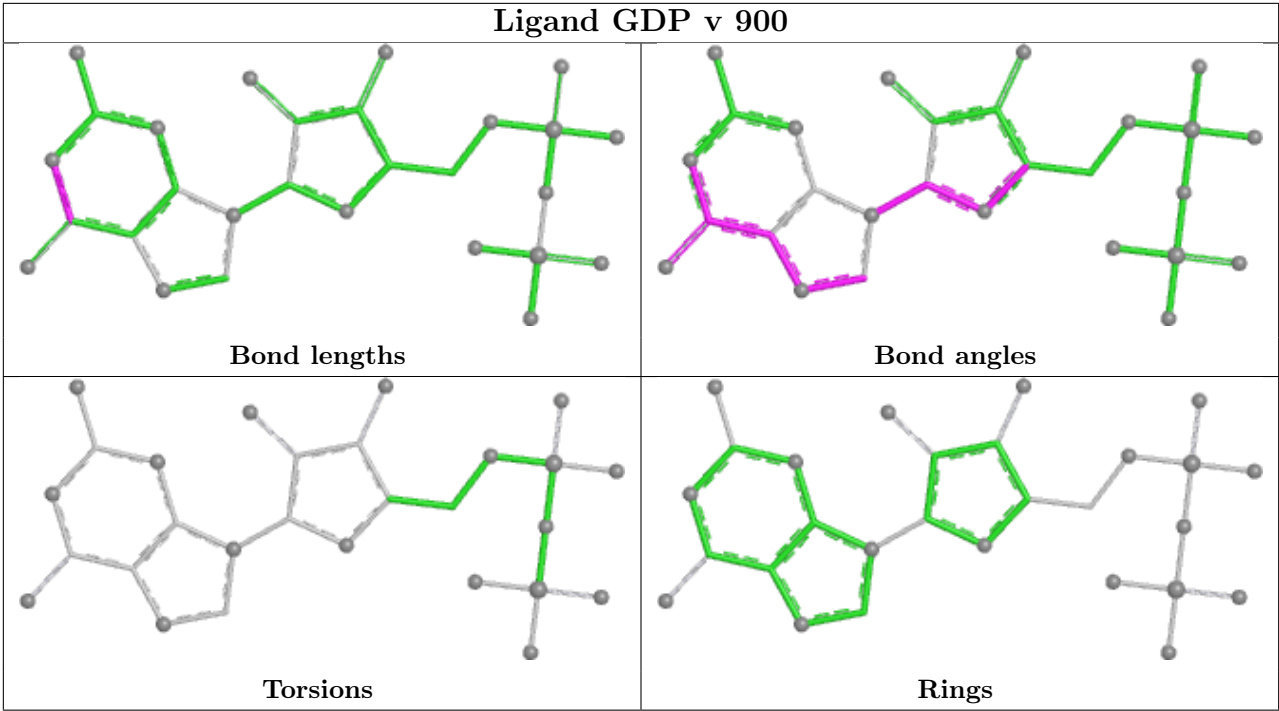
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	5	49
50	9	18
49	w	1
48	v	1
3	8	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	w	225:LEU	C	282:THR	N	57.95
1	5	2113:G	O3'	2258:C	P	39.61
1	5	1252:C	O3'	1271:G	P	35.94
1	5	1405:C	O3'	1406:G	P	22.80
1	5	1406(C):G	O3'	1411:C	P	20.78
1	5	1406:G	O3'	1406(A):G	P	20.04
1	5	1219:G	O3'	1233:G	P	19.33

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	9	1761:U	O3'	1771:G	P	18.12
1	5	523:C	O3'	638:G	P	17.67
1	9	834:C	O3'	841:G	P	17.65
1	5	1411:C	O3'	1411(A):G	P	17.43
1	5	4138:C	O3'	4146:G	P	17.42
1	9	697:G	O3'	729:C	P	17.13
1	9	756:C	O3'	788:G	P	17.03
1	5	990:U	O3'	1064:G	P	16.93
1	5	4101:C	O3'	4107:G	P	16.67
1	9	323:C	O3'	329:G	P	16.66
1	v	47:ALA	C	55:ARG	N	16.62
1	5	3976:C	O3'	4039:G	P	15.89
1	9	130:G	O3'	140:U	P	15.53
1	9	1417:C	O3'	1423:C	P	15.32
1	5	4777:C	O3'	4859:C	P	14.68
1	5	5022:U	O3'	5028:G	P	14.56
1	5	1696:C	O3'	1720:C	P	14.38
1	5	760:G	O3'	904:C	P	14.02
1	5	1364:U	O3'	1368:A	P	13.67
1	5	922:C	O3'	922(A):G	P	13.19
1	5	737:C	O3'	738:C	P	13.16
1	5	2901:G	O3'	3597:G	P	12.84
1	5	182:G	O3'	189:G	P	12.76
1	5	970:G	O3'	971:U	P	12.41
1	5	971:U	O3'	971(A):G	P	12.06
1	8	79:G	O3'	85:U	P	12.06
1	5	934:C	O3'	935:A	P	11.68
1	5	481:G	O3'	481(A):C	P	11.01
1	5	921:C	O3'	922:C	P	10.36
1	9	745:C	O3'	749:U	P	9.60
1	5	4729:A	O3'	4735:G	P	9.45
1	5	1180:C	O3'	1183:C	P	8.76
1	9	225:G	O3'	287:U	P	7.98
1	5	738(A):C	O3'	739:G	P	6.89
1	5	512:U	O3'	515:C	P	6.76
1	5	935:A	O3'	935(A):G	P	6.65
1	9	1432:U	O3'	1438:A	P	6.59
1	5	480:C	O3'	481:G	P	6.54
1	5	500:G	O3'	504:G	P	6.11
1	5	3955:A	O3'	3956:G	P	5.97
1	5	922(B):C	O3'	923:C	P	5.49
1	9	798:G	O3'	799:U	P	5.40

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	3945:A	O3'	3946:G	P	4.92
1	5	1239:C	O3'	1244:G	P	4.90
1	5	1100:U	O3'	1168:G	P	4.87
1	9	322:C	O3'	323:C	P	4.79
1	9	304:C	O3'	305:U	P	4.65
1	9	736:C	O3'	743:U	P	4.64
1	5	4740:G	O3'	4743:G	P	4.62
1	5	170:C	O3'	171:U	P	4.58
1	5	4899:G	O3'	4902:C	P	3.71
1	9	309:G	O3'	310:C	P	3.69
1	5	738:C	O3'	738(A):C	P	3.66
1	5	4055:U	O3'	4056:A	P	3.51
1	5	5020:G	O3'	5021:C	P	3.47
1	5	3947:A	O3'	3948:C	P	3.25
1	5	751:G	O3'	752:G	P	3.24
1	9	902:G	O3'	903:A	P	3.24
1	5	1438:U	O3'	1440:U	P	3.23
1	9	903:A	O3'	904:A	P	3.22
1	5	267:G	O3'	268:G	P	3.19
1	9	1295:A	O3'	1296:U	P	3.17
1	5	935(A):G	O3'	936:C	P	3.16

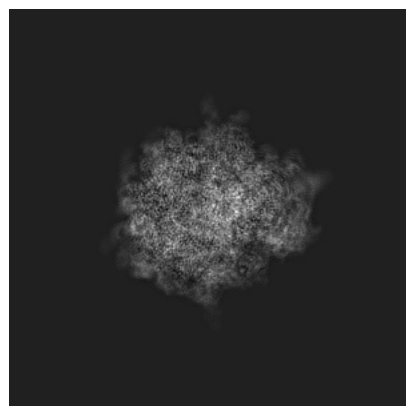
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9242. These allow visual inspection of the internal detail of the map and identification of artifacts.

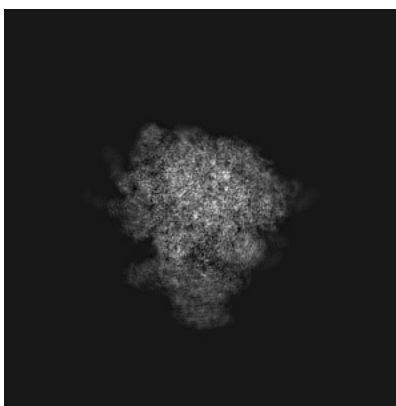
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

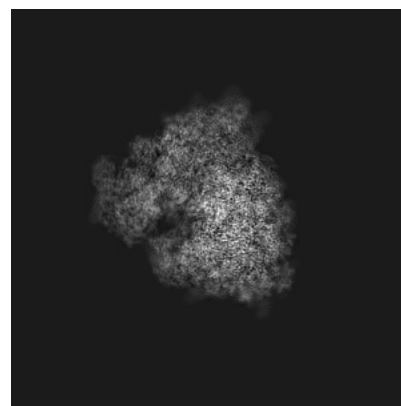
6.1.1 Primary map



X

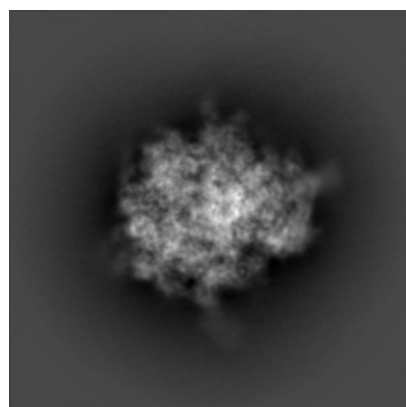


Y

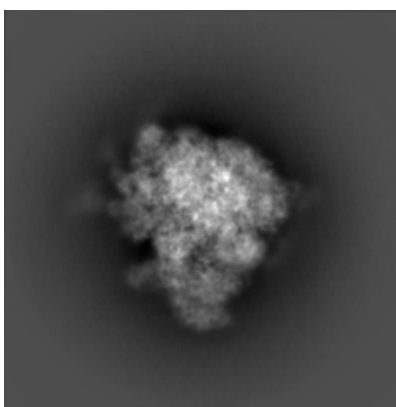


Z

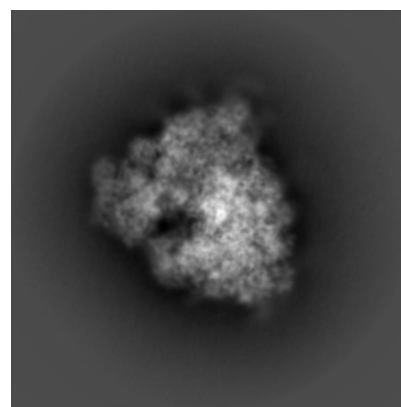
6.1.2 Raw map



X



Y

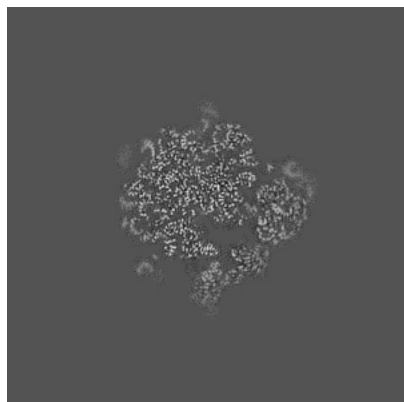


Z

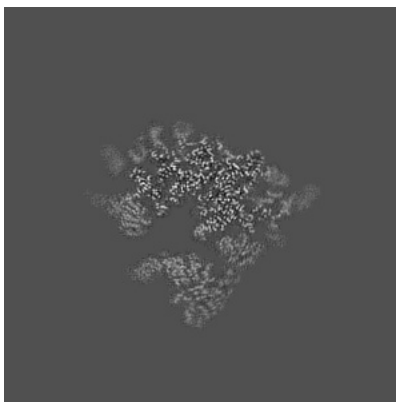
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

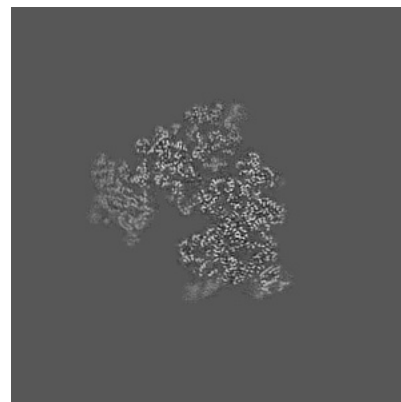
6.2.1 Primary map



X Index: 200

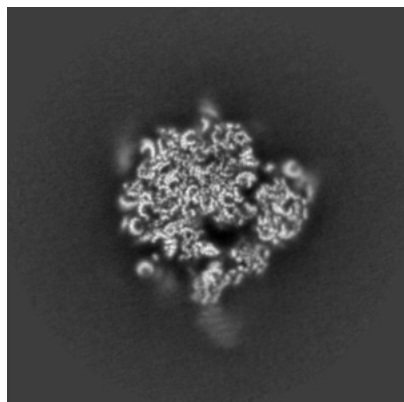


Y Index: 200

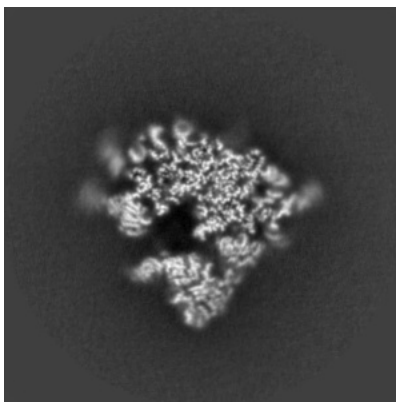


Z Index: 200

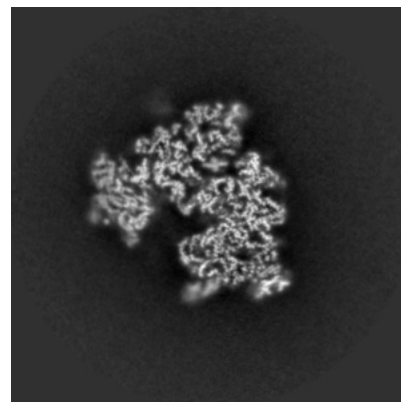
6.2.2 Raw map



X Index: 200



Y Index: 200

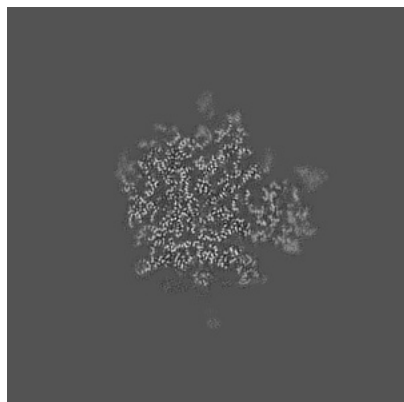


Z Index: 200

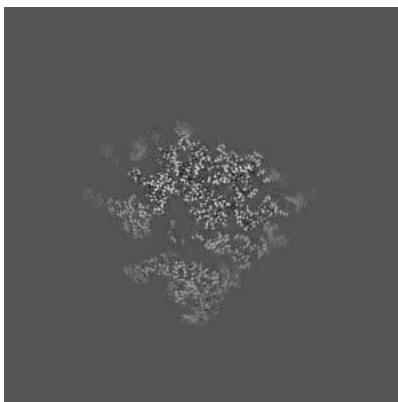
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

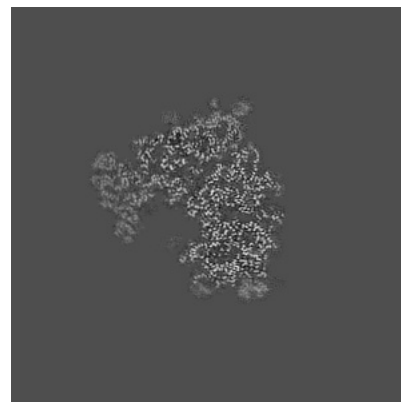
6.3.1 Primary map



X Index: 213

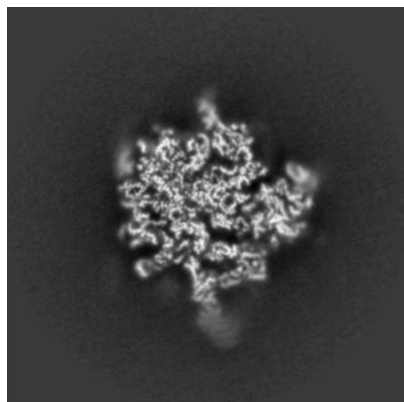


Y Index: 206

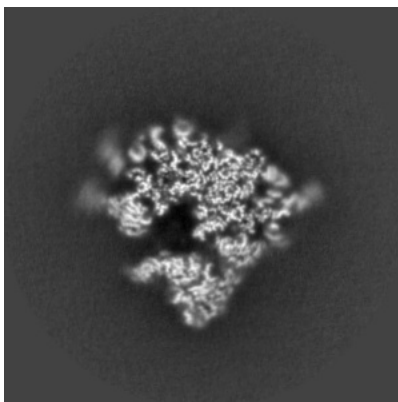


Z Index: 210

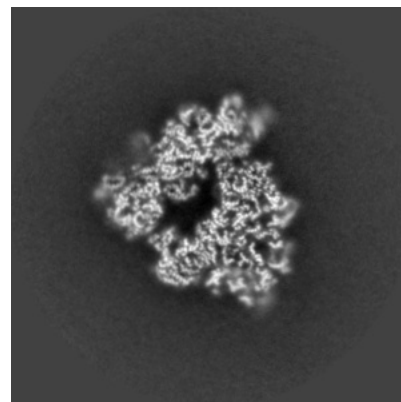
6.3.2 Raw map



X Index: 206



Y Index: 201

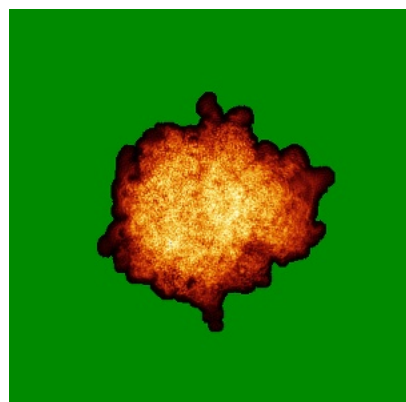


Z Index: 176

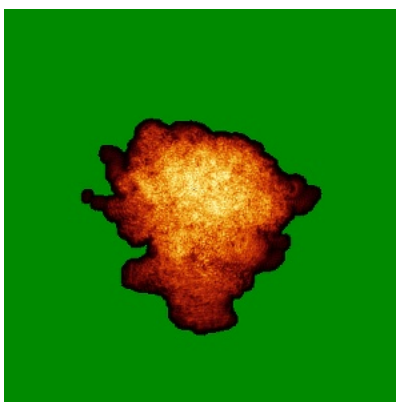
The images above show the largest variance slices of the map in three orthogonal directions.

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

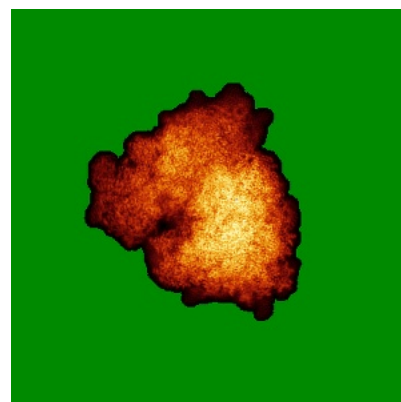
6.4.1 Primary map



X

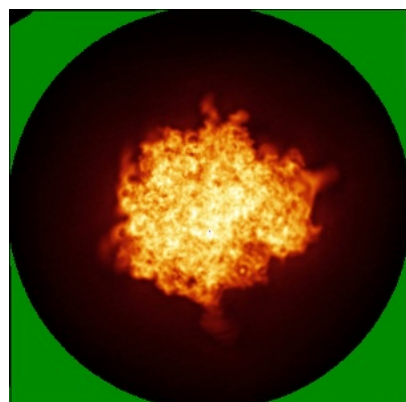


Y

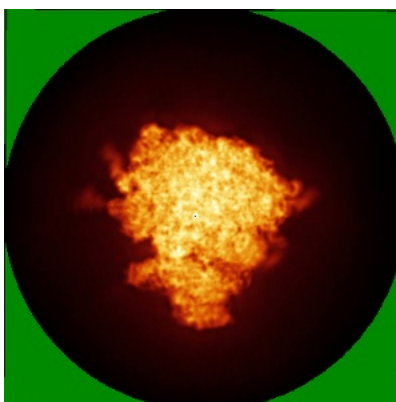


Z

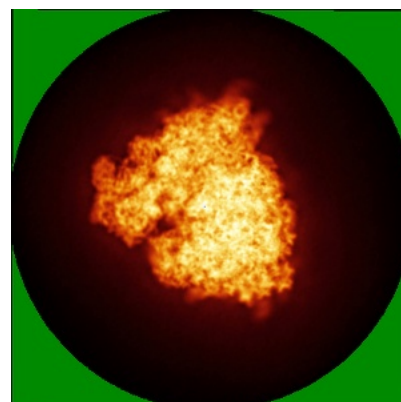
6.4.2 Raw map



X



Y

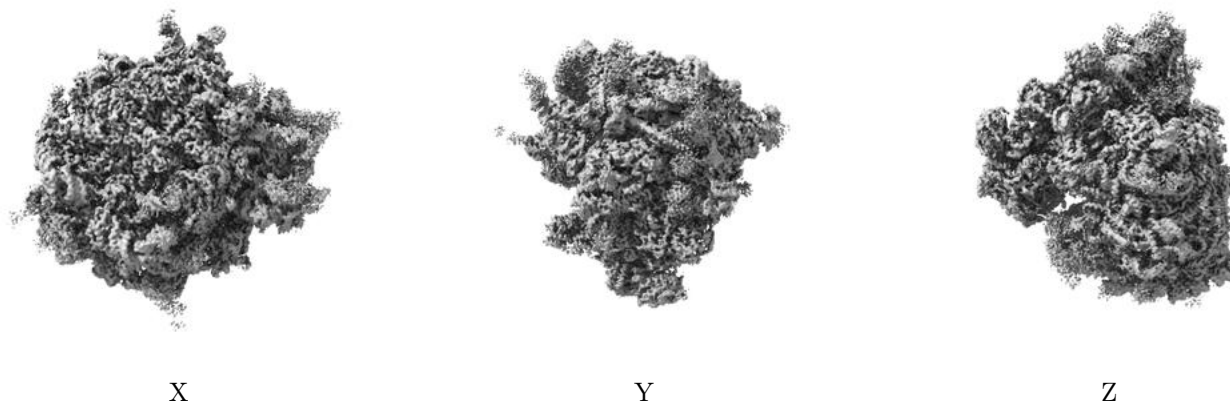


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

6.5.2 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.

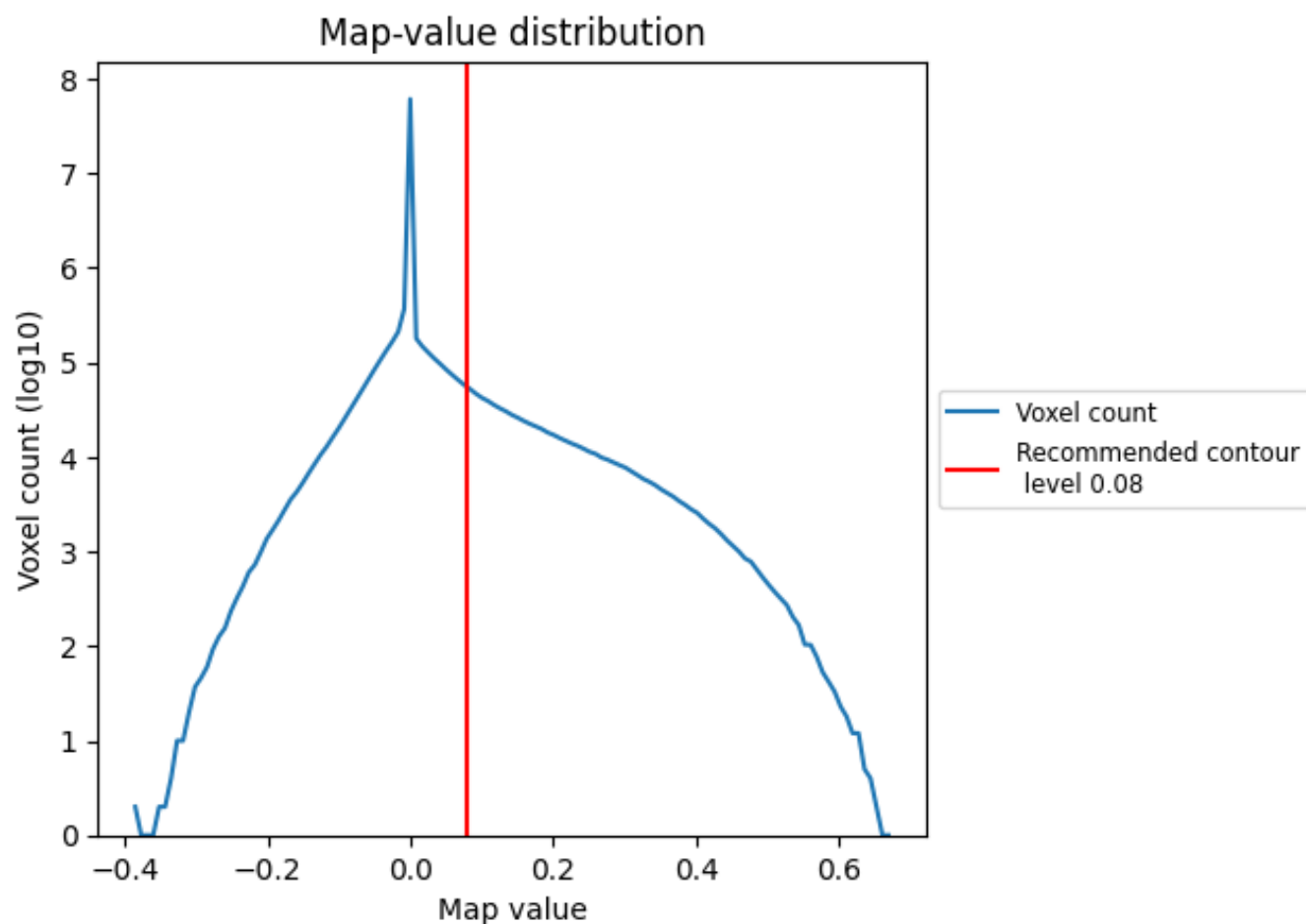
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

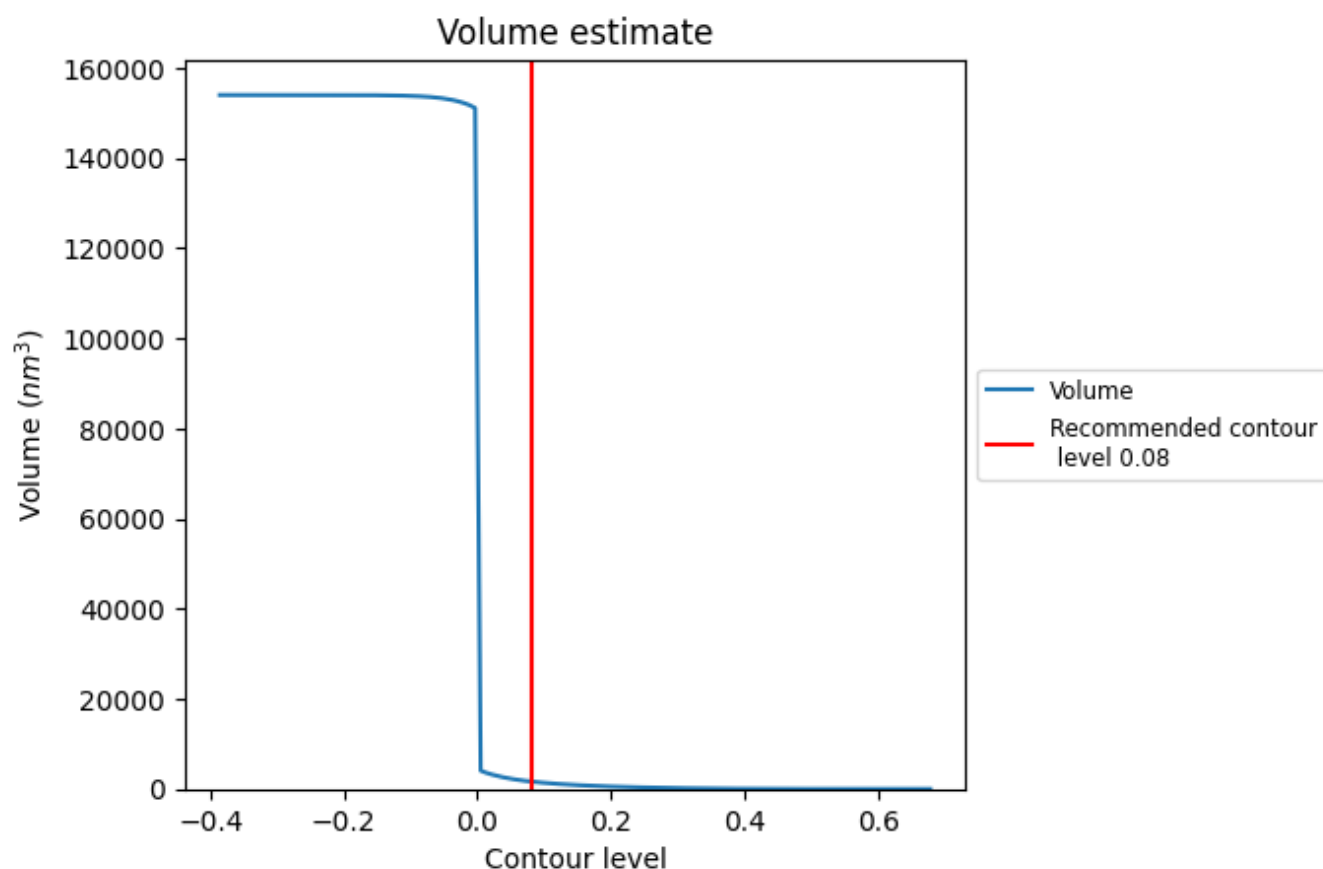
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

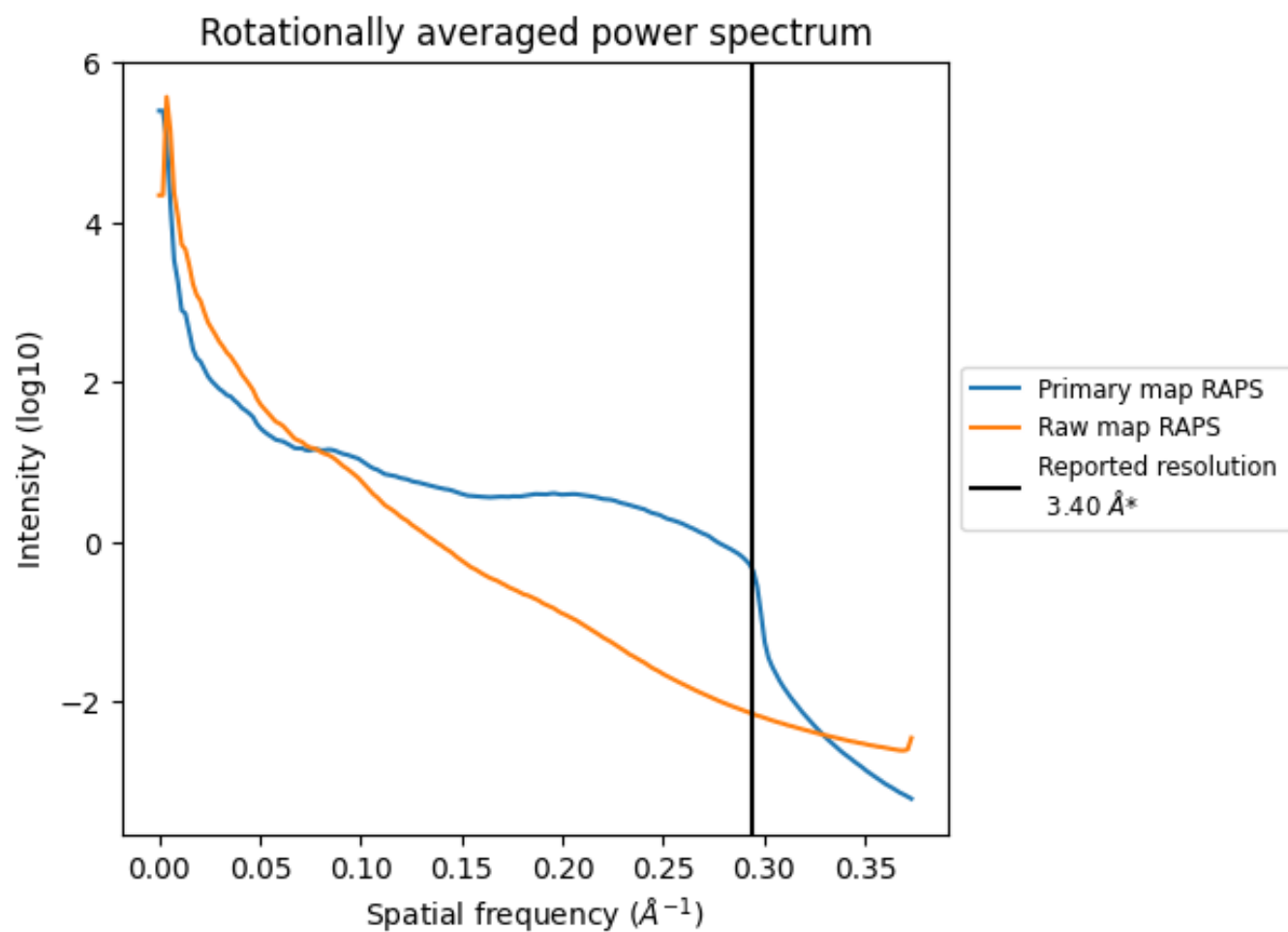
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1651 nm³; this corresponds to an approximate mass of 1492 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

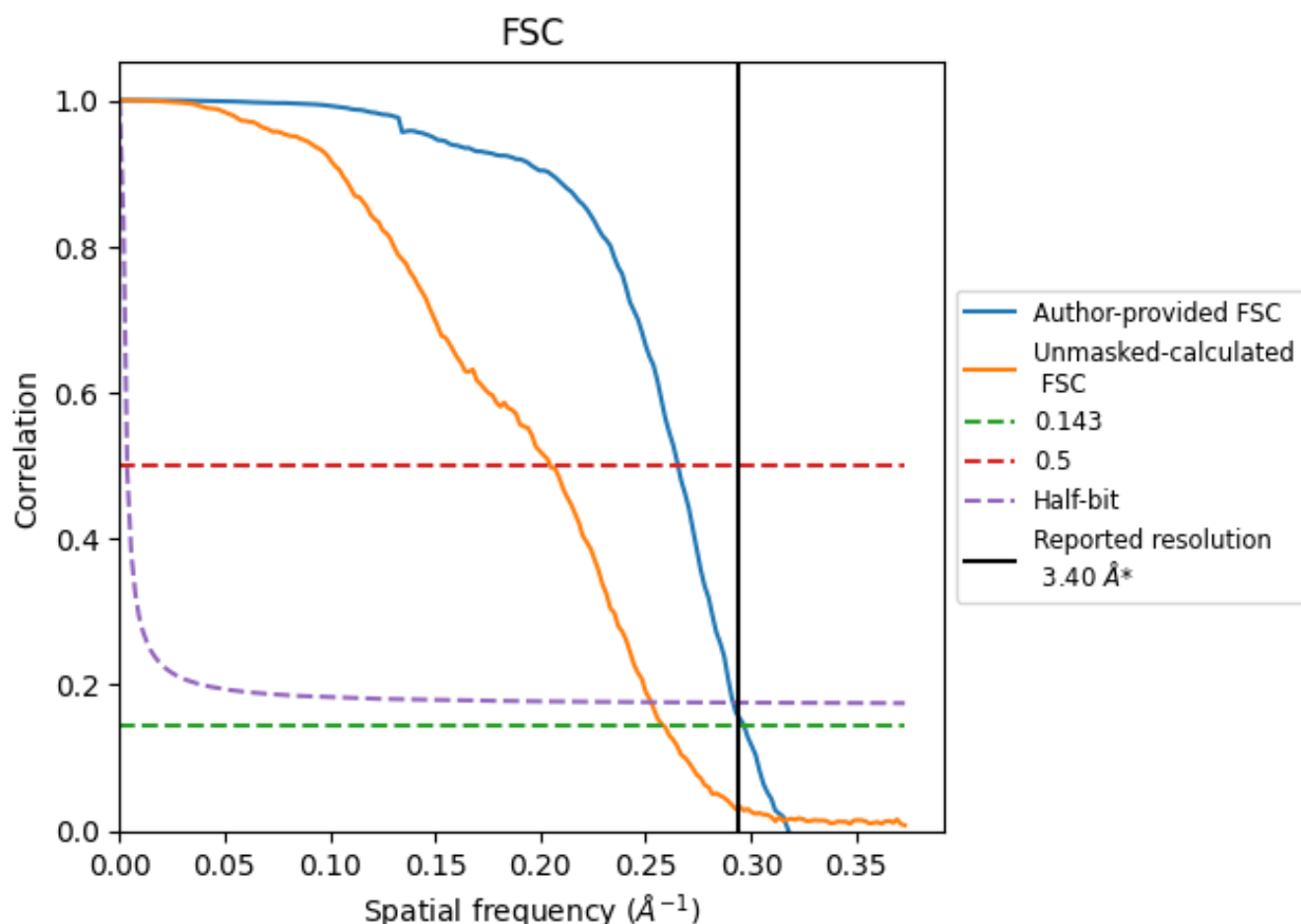


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 0.294 Å⁻¹

8.2 Resolution estimates [i](#)

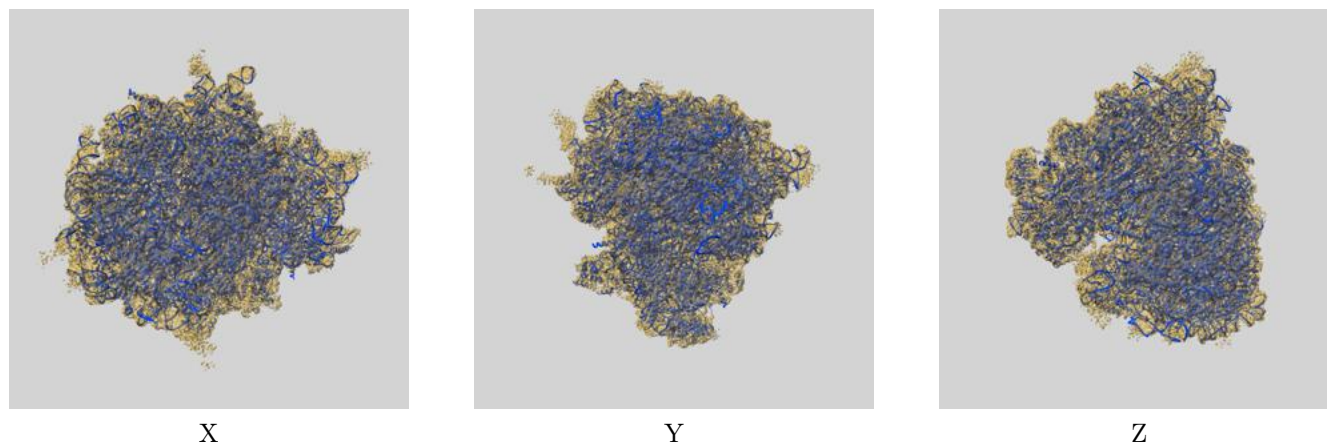
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.37	3.77	3.43
Unmasked-calculated*	3.86	4.89	3.96

*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 3.86 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

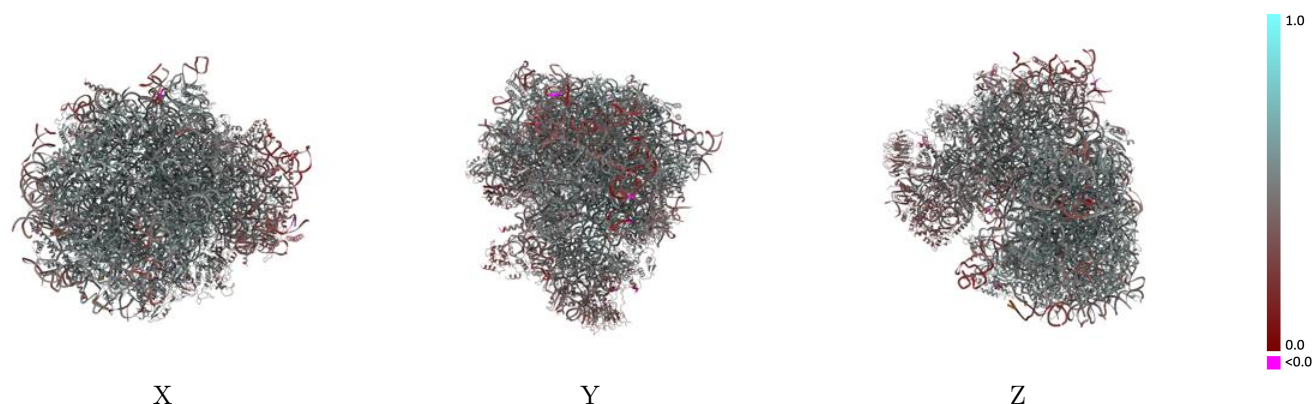
This section contains information regarding the fit between EMDB map EMD-9242 and PDB model 6MTE. Per-residue inclusion information can be found in [section 3](#) on [page 20](#).

9.1 Map-model overlay [i](#)



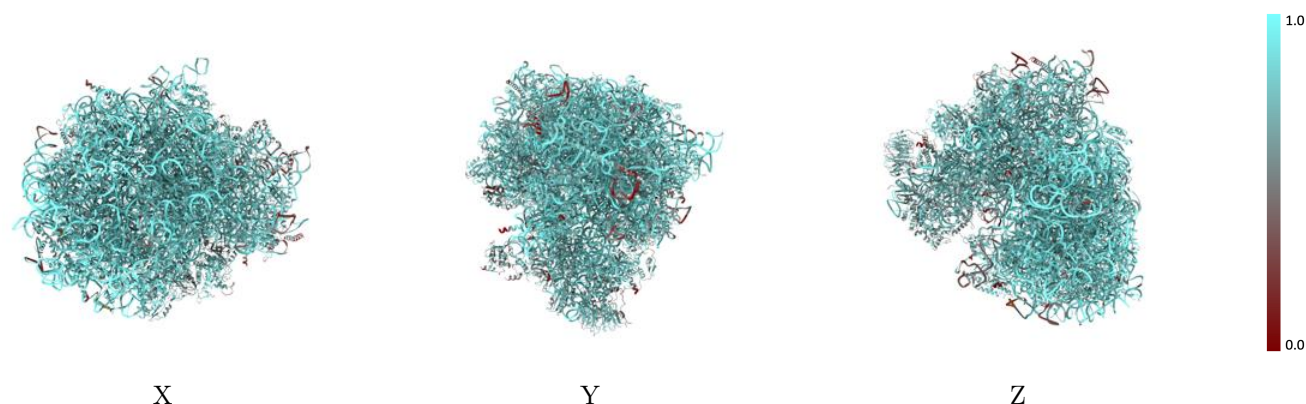
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



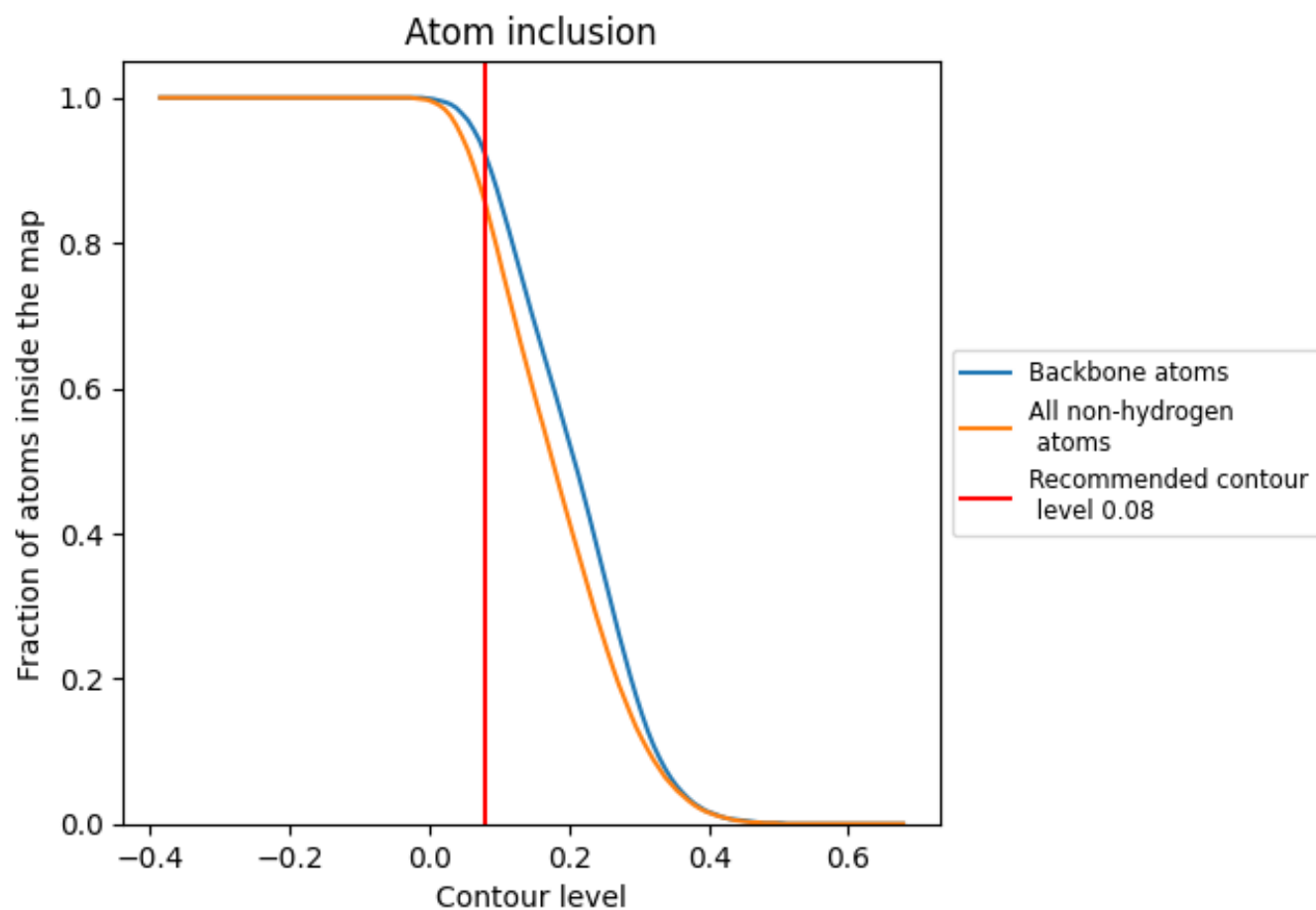
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 85% 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	 0.8540	 0.4760
5	 0.9160	 0.4870
7	 0.9630	 0.5120
8	 0.9260	 0.4850
9	 0.8930	 0.4420
A	 0.8580	 0.5490
AA	 0.7840	 0.4740
B	 0.8840	 0.5420
BB	 0.7010	 0.4310
C	 0.8660	 0.5310
CC	 0.8250	 0.5120
D	 0.8470	 0.5020
DD	 0.7130	 0.4450
E	 0.8540	 0.5080
EE	 0.7990	 0.4840
F	 0.8580	 0.5320
FF	 0.6030	 0.3480
G	 0.7970	 0.4890
GG	 0.6660	 0.3620
H	 0.8510	 0.5290
HH	 0.7240	 0.4390
I	 0.8530	 0.5330
II	 0.7240	 0.4290
J	 0.8260	 0.4880
JJ	 0.8100	 0.4880
KK	 0.7510	 0.4370
L	 0.8290	 0.5080
LL	 0.7740	 0.4820
M	 0.8610	 0.5280
MM	 0.5280	 0.2930
N	 0.8910	 0.5470
NN	 0.7690	 0.4710
O	 0.8740	 0.5320
OO	 0.7360	 0.4470
P	 0.8560	 0.5340

















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Chain	Atom inclusion	Q-score
PP	 0.6710	 0.3650
Q	 0.8590	 0.5360
QQ	 0.6820	 0.3980
R	 0.8140	 0.5060
RR	 0.6740	 0.4170
S	 0.8830	 0.5440
SS	 0.6520	 0.3520
T	 0.8360	 0.5270
TT	 0.6810	 0.3710
U	 0.8010	 0.4710
UU	 0.7160	 0.4240
V	 0.8540	 0.5480
VV	 0.8140	 0.4980
W	 0.6740	 0.4520
WW	 0.8450	 0.5270
X	 0.8250	 0.5210
XX	 0.8390	 0.5340
Y	 0.8440	 0.5140
YY	 0.7620	 0.4410
Z	 0.8460	 0.5110
ZZ	 0.5710	 0.3140
a	 0.8810	 0.5420
aa	 0.7650	 0.4840
b	 0.7370	 0.4590
bb	 0.7340	 0.4710
c	 0.8090	 0.4910
cc	 0.5720	 0.3790
d	 0.8320	 0.5150
dd	 0.8230	 0.4670
e	 0.8550	 0.5450
ee	 0.7440	 0.4750
f	 0.8910	 0.5500
ff	 0.5900	 0.3200
g	 0.8280	 0.5230
gg	 0.6550	 0.3720
h	 0.8330	 0.5160
i	 0.8180	 0.4960
j	 0.9040	 0.5430
k	 0.8020	 0.4920
l	 0.8430	 0.5220
m	 0.8660	 0.5360
n	 0.7570	 0.5070

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Chain	Atom inclusion	Q-score
o	 0.8400	 0.5420
p	 0.8040	 0.5270
r	 0.8780	 0.5310
s	 0.7500	 0.4490
t	 0.5360	 0.3330
v	 0.7430	 0.4550
w	 0.6220	 0.4480