Full wwPDB EM Validation Report ⓘ

Nov 8, 2022 – 06:57 AM EST

PDB ID	:	6MTD
EMDB ID	:	EMD-9240
Title	:	Rabbit 80S ribosome with eEF2 and SERBP1 (unrotated state with 40S head swivel)
Authors	:	Brown, A.; Baird, M.R.; Yip, M.C.J.; Murray, J.; Shao, S.
Deposited on	:	2018-10-19
Resolution	:	3.30 Å(reported)
Based on initial model	:	5LZV

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

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

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

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

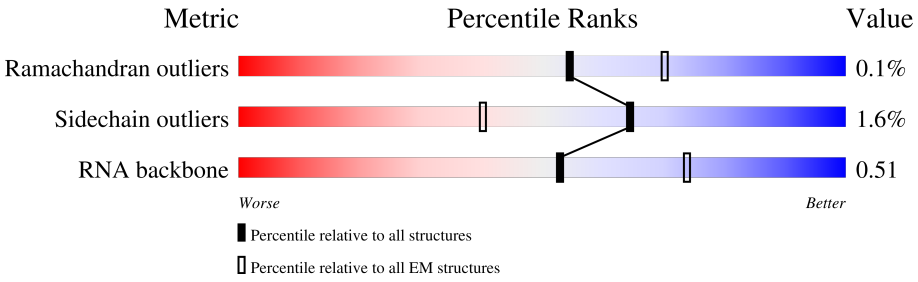
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	70% 26%
2	7	120	83% 15%
3	8	151	75% 21%
4	A	248	98%
5	B	394	98%
6	C	362	99%
7	D	293	99%
8	E	291	73% 26%

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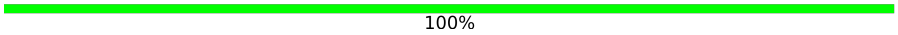
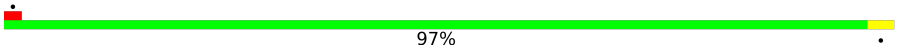
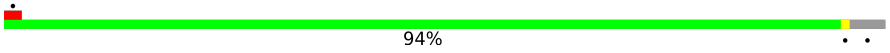
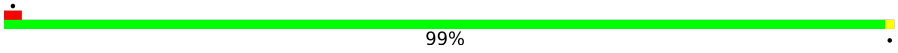
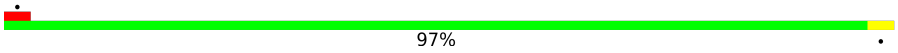
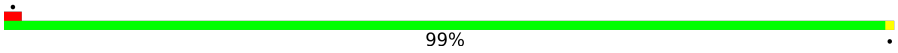
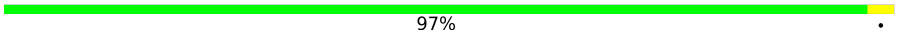
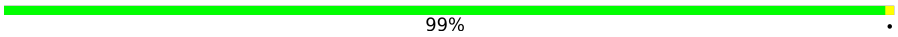
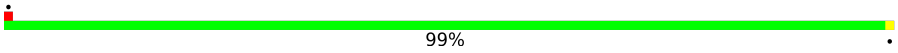
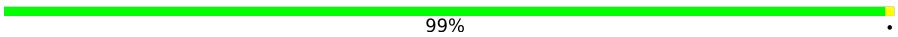
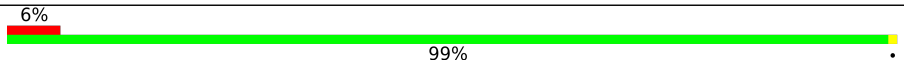
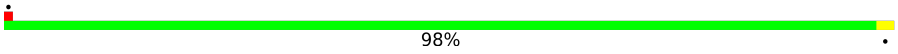
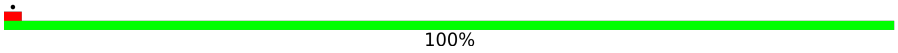
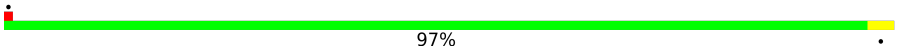
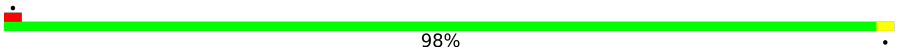
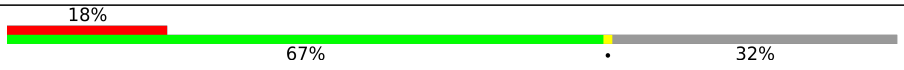
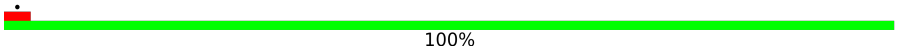
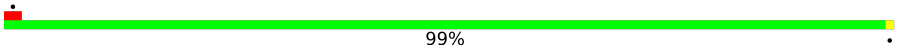
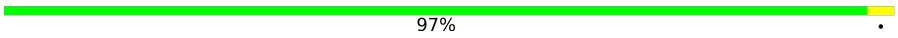
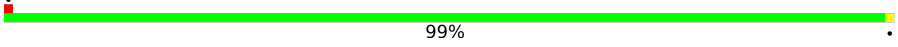
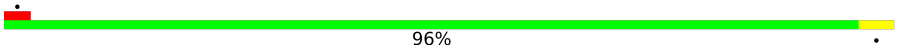
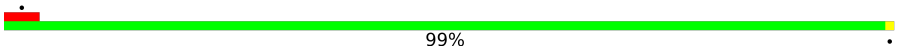
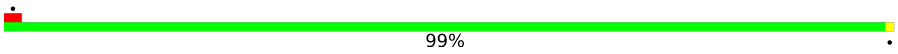
Mol	Chain	Length	Quality of chain
9	F	225	
10	G	319	
11	H	190	
12	I	214	
13	J	170	
14	L	210	
15	M	138	
16	N	203	
17	O	199	
18	P	153	
19	Q	187	
20	R	180	
21	S	176	
22	T	159	
23	U	99	
24	V	131	
25	W	157	
26	X	118	
27	Y	134	
28	Z	135	
29	a	147	
30	b	245	
31	c	98	
32	d	107	
33	e	128	

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Mol	Chain	Length	Quality of chain
34	f	109	98%
35	g	114	5% 98%
36	h	122	99%
37	i	102	98%
38	j	86	99%
39	k	69	100%
40	l	50	96%
41	m	52	96%
42	n	25	100%
43	o	103	98%
44	p	91	100%
45	r	124	97%
46	s	196	12% 99%
47	t	153	52% 95% 5%
48	u	206	96% 95% 5%
49	v	839	30% 96%
50	w	26	65% 92% 8%
51	9	1698	5% 70% 26%
52	AA	217	5% 98%
53	BB	213	99%
54	CC	221	100%
55	DD	228	7% 96%
56	EE	262	98%
57	FF	204	86% 9%
58	GG	237	11% 99%

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Mol	Chain	Length	Quality of chain
59	HH	194	9% 94% 5%
60	II	206	7% 100%
61	JJ	185	98%
62	KK	96	5% 98%
63	LL	158	6% 89% 9%
64	MM	117	40% 96%
65	NN	149	99%
66	OO	136	7% 99%
67	PP	120	9% 95% 5%
68	QQ	142	6% 97%
69	RR	132	8% 98%
70	SS	144	7% 97%
71	TT	141	99%
72	UU	100	6% 99%
73	VV	83	98%
74	WW	129	99%
75	XX	141	97%
76	YY	124	6% 99%
77	ZZ	75	9% 97%
78	aa	101	99%
79	bb	83	6% 96%
80	cc	62	8% 98%
81	dd	55	100%
82	ee	55	15% 96%
83	ff	68	35% 99%

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Mol	Chain	Length	Quality of chain
84	gg	313	9% 99%

2 Entry composition

There are 87 unique types of molecules in this entry. The entry contains 222072 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
			Total	C	N	O	P		
1	5	3597	77254	34469	14127	25061	3597	0	0

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

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

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

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

- Molecule 4 is a protein called uL2.

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

- Molecule 5 is a protein called uL3.

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

- Molecule 6 is a protein called uL4.

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

- 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	106	Total	C	N	O	S	0	0
			860	538	174	144	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 eL11.

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 uL1.

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

- Molecule 49 is a protein called eEF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	v	839	Total 6544	C 4162	N 1122	O 1216	S 44	0	0

- Molecule 50 is a protein called SERBP1.

Mol	Chain	Residues	Atoms				AltConf	Trace
50	w	26	Total 216	C 129	N 43	O 44	0	0

- Molecule 51 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	9	1698	Total 36263	C 16190	N 6509	O 11867	P 1697	0	0

- Molecule 52 is a protein called uS2.

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

- Molecule 53 is a protein called eS1.

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

- Molecule 54 is a protein called uS5.

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

- Molecule 55 is a protein called uS3.

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

- Molecule 56 is a protein called eS4.

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

- Molecule 57 is a protein called uS7.

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

- Molecule 58 is a protein called eS6.

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

- Molecule 59 is a protein called eS7.

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

- Molecule 60 is a protein called eS8.

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

- Molecule 61 is a protein called uS4.

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

- Molecule 62 is a protein called eS10.

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

- Molecule 63 is a protein called uS17.

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

- Molecule 64 is a protein called eS12.

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

- Molecule 65 is a protein called uS15.

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

- Molecule 66 is a protein called uS11.

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

- Molecule 67 is a protein called uS19.

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

- Molecule 68 is a protein called uS9.

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

- Molecule 69 is a protein called eS17.

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

- Molecule 70 is a protein called uS13.

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

- Molecule 71 is a protein called eS19.

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

- Molecule 72 is a protein called uS10.

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

- Molecule 73 is a protein called eS21.

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

- Molecule 74 is a protein called uS8.

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

- Molecule 75 is a protein called uS12.

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

- Molecule 76 is a protein called eS24.

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

- Molecule 77 is a protein called eS25.

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

- Molecule 78 is a protein called eS26.

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

- Molecule 79 is a protein called eS27.

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

- Molecule 80 is a protein called eS28.

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

- Molecule 81 is a protein called uS14.

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

- Molecule 82 is a protein called eS30.

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

- Molecule 83 is a protein called eS31.

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

- Molecule 84 is a protein called RACK1.

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

- Molecule 85 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
85	5	200	Total	Mg	0
			200	200	
85	7	7	Total	Mg	0
			7	7	
85	8	6	Total	Mg	0
			6	6	
85	A	1	Total	Mg	0
			1	1	
85	P	1	Total	Mg	0
			1	1	
85	V	1	Total	Mg	0
			1	1	
85	a	1	Total	Mg	0
			1	1	
85	g	1	Total	Mg	0
			1	1	
85	v	1	Total	Mg	0
			1	1	
85	9	73	Total	Mg	0
			73	73	
85	SS	2	Total	Mg	0
			2	2	
85	TT	1	Total	Mg	0
			1	1	
85	aa	1	Total	Mg	0
			1	1	
85	dd	1	Total	Mg	0
			1	1	

- Molecule 86 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
86	g	1	Total	Zn	0
			1	1	
86	j	1	Total	Zn	0
			1	1	
86	m	1	Total	Zn	0
			1	1	

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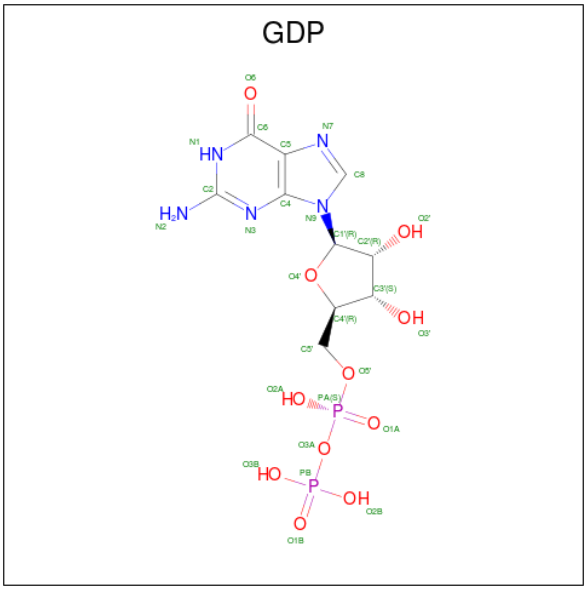
Mol	Chain	Residues	Atoms	AltConf
86	o	1	Total Zn 1 1	0
86	p	1	Total Zn 1 1	0
86	aa	1	Total Zn 1 1	0
86	dd	1	Total Zn 1 1	0
86	ff	1	Total Zn 1 1	0

- Molecule 87 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



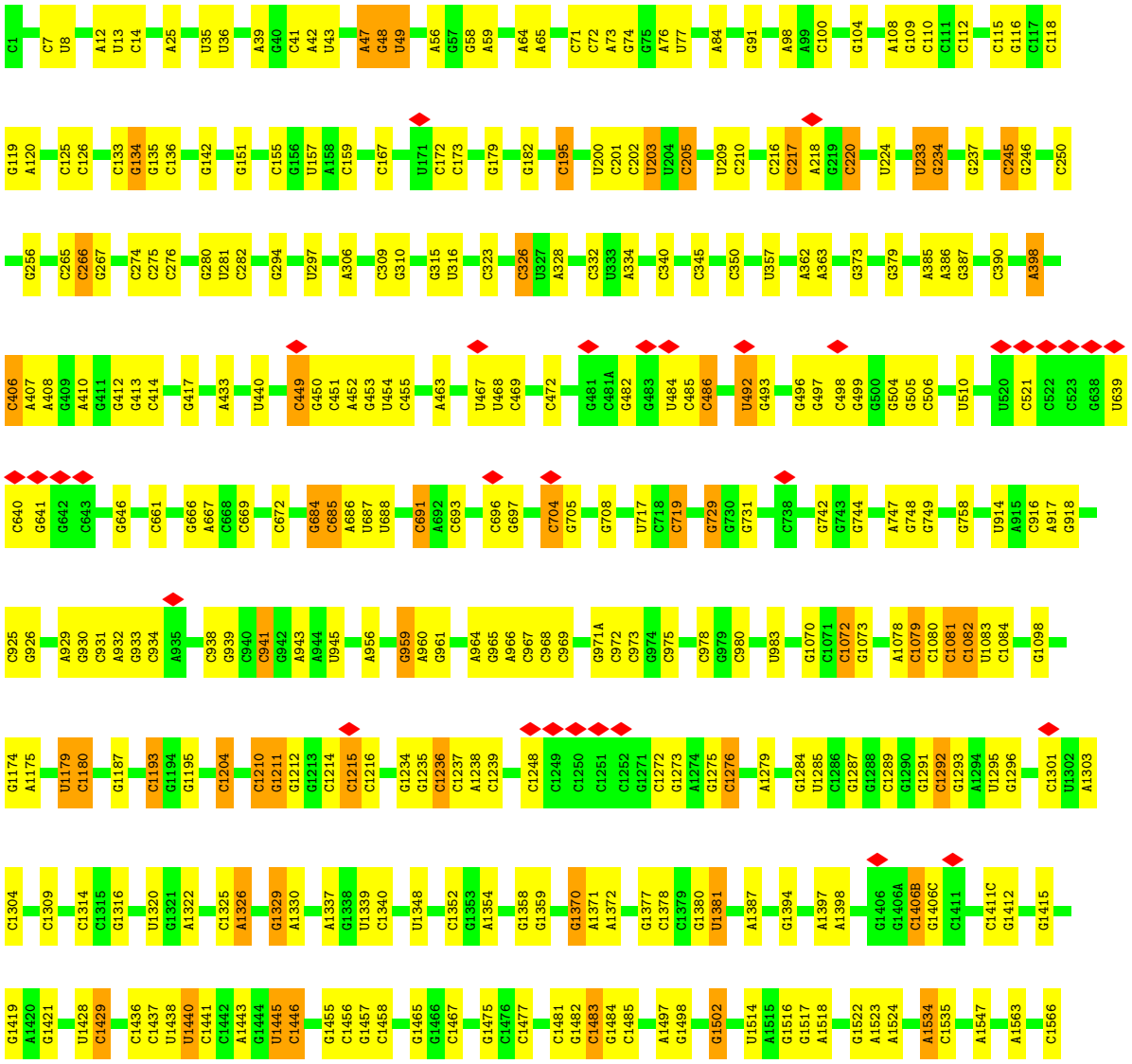
Mol	Chain	Residues	Atoms	AltConf
87	v	1	Total C N O P 28 10 5 11 2	0

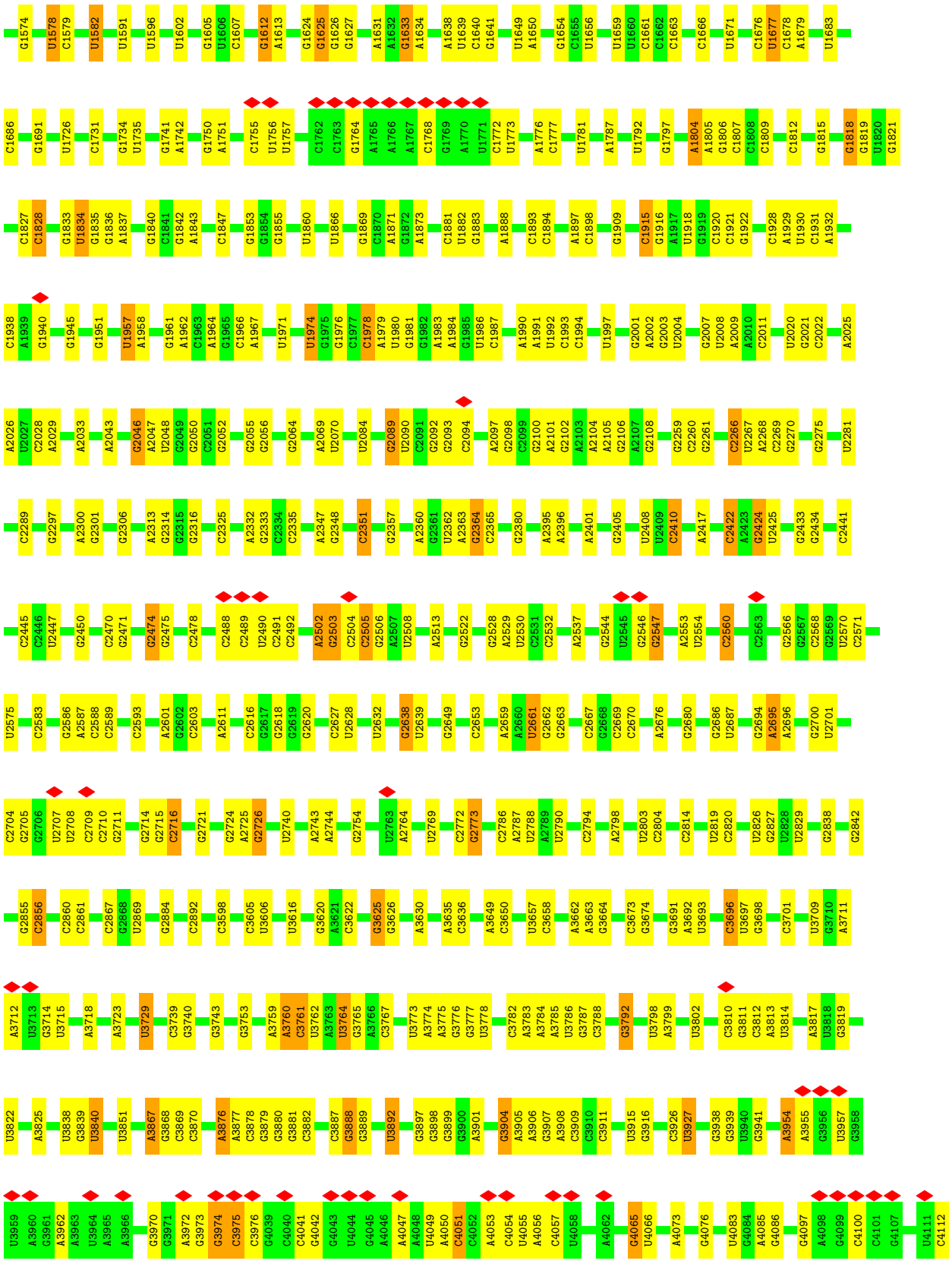
3 Residue-property plots (i)

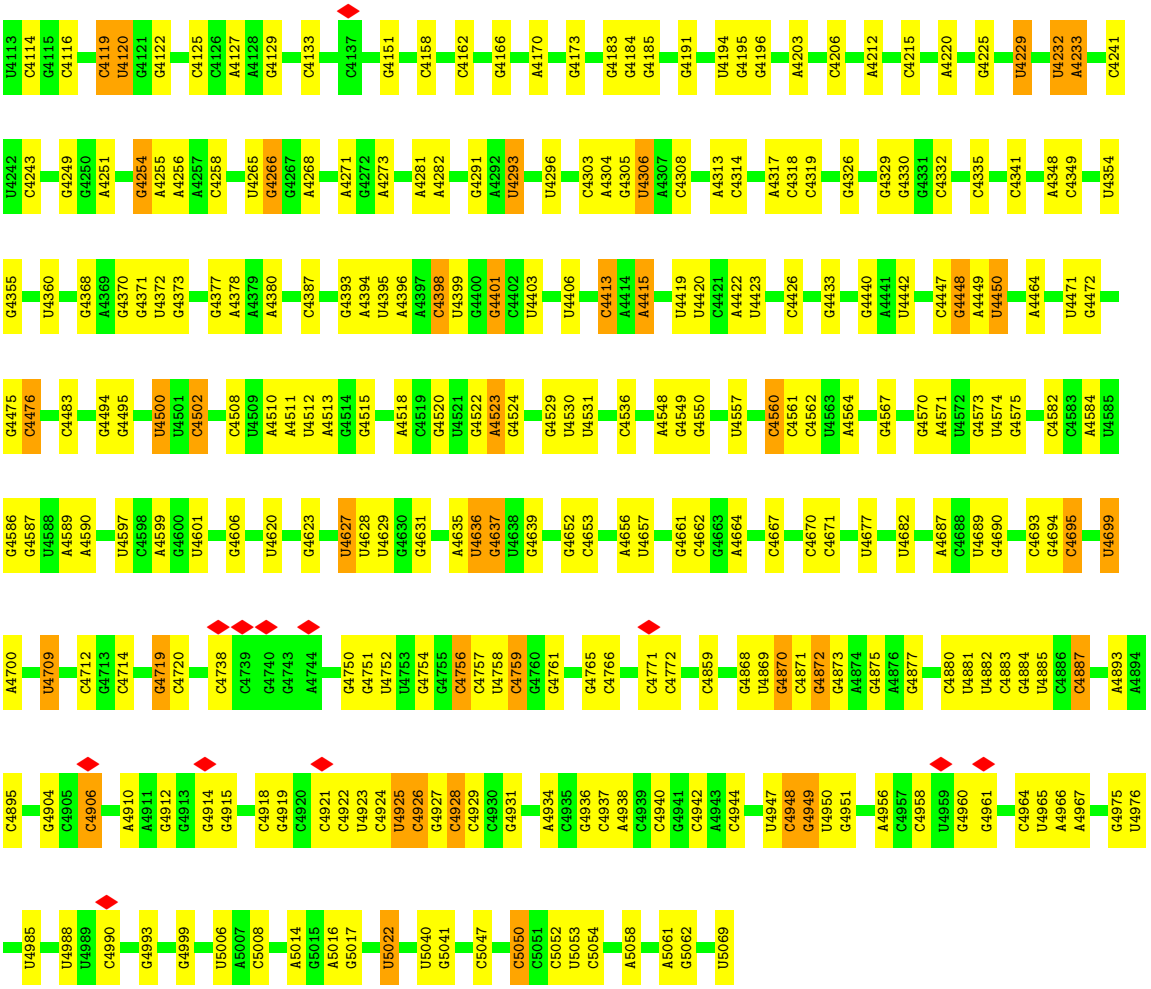
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

Chain 5:

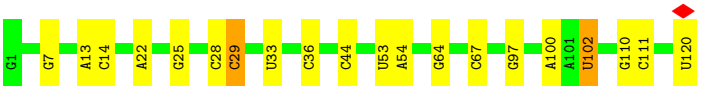



G1574 U1578 C1579 U1582 U1591 U1596 U1602 G1605 U1606 C1607 G1612 A1613 G1624 G1625 G1626 G1627 A1631 A1632 G1633 A1634 A1638 U1639 C1640 G1641 U1649 A1650 G1654 C1655 U1656 U1659 U1660 C1661 C1662 C1663 C1666 U1671 C1676 U1677 C1678 A1679 U1683
C1686 G1691 U1726 C1731 G1734 U1735 G1741 A1742 G1750 A1751 C1755 U1756 U1757 C1762 C1763 G1764 A1765 A1766 A1767 C1768 G1769 A1770 U1771 C1772 U1773 A1776 C1777 U1781 A1787 U1792 G1797 A1804 A1805 G1806 C1807 C1808 C1809 C1812 G1815 G1818 G1819 U1820 G1821
C1827 C1828 G1833 U1834 G1835 G1836 A1837 G1840 C1841 G1842 A1843 C1847 G1853 G1854 G1855 U1860 U1866 G1869 C1870 A1871 G1872 A1873 C1881 U1882 G1883 A1888 C1893 C1894 A1897 C1898 G1909 C1915 G1916 A1917 U1918 G1919 C1920 C1921 G1922 C1928 A1929 U1930 C1931 A1932
C1938 A1939 G1940 G1945 G1951 U1957 A1958 G1961 A1962 C1963 A1964 G1965 C1966 A1967 U1971 U1974 G1975 G1976 C1977 C1978 A1979 U1980 G1981 G1982 A1983 A1984 G1985 U1986 C1987 A1990 A1991 U1992 C1993 C1994 U1997 G2001 A2002 G2003 U2004 G2007 U2008 A2009 A2010 C2011 U2020 G2021 C2022 A2025
A2026 U2027 C2028 A2029 A2033 A2043 G2046 A2047 U2048 G2049 G2050 C2051 G2052 G2055 G2056 G2064 A2069 U2070 U2084 G2089 U2090 C2091 G2092 G2093 C2094 A2097 G2098 C2099 C2100 A2101 G2102 A2103 A2104 A2105 G2106 A2107 G2108 G2259 C2260 G2261 C2266 U2267 A2268 C2269 G2270 G2275 U2281
C2289 G2297 A2300 G2301 G2306 A2313 G2314 G2315 G2316 C2325 A2332 G2333 C2334 C2335 A2347 G2348 C2351 G2357 A2360 G2361 U2362 A2363 G2364 C2365 G2380 A2395 A2396 A2401 G2405 U2408 U2409 C2410 A2417 C2422 A2423 G2424 U2425 G2433 G2434 C2441
C2445 C2446 U2447 G2450 C2470 G2471 G2474 G2475 C2478 C2488 C2489 U2490 C2491 C2492 A2502 G2503 C2504 C2505 G2506 A2507 U2508 A2513 G2522 G2528 A2529 U2530 C2531 C2532 A2537 G2544 U2545 G2546 G2547 A2553 U2554 C2560 C2563 G2566 G2567 C2568 G2569 U2570 C2571
U2575 C2583 G2586 A2587 C2588 C2589 C2593 A2601 G2602 C2603 A2611 C2616 G2617 G2618 C2619 G2620 C2627 U2628 U2632 G2638 U2639 G2649 C2653 A2659 A2660 U2661 G2662 G2663 C2667 G2668 C2669 C2670 A2676 G2680 G2686 U2687 G2694 A2695 A2696 G2700 U2701
C2704 G2705 G2706 U2707 U2708 C2709 C2710 G2711 G2714 G2715 C2716 G2721 G2724 A2725 G2726 U2740 A2743 A2744 G2754 U2763 A2764 U2769 C2772 G2773 C2786 A2787 U2788 A2789 U2790 C2794 A2798 U2803 C2804 C2814 U2819 C2820 U2826 G2827 U2828 U2829 G2838 G2842
G2855 C2856 C2860 C2861 C2867 G2868 U2869 G2884 C2892 C3598 C3605 U3606 U3616 G3620 A3621 C3622 G3625 G3626 A3630 A3635 C3636 A3649 C3650 U3657 C3658 A3662 A3663 G3664 C3673 G3674 G3691 A3692 U3693 C3696 U3697 G3698 C3701 U3709 G3710 A3711
A3712 U3713 G3714 U3715 A3718 A3723 U3729 C3739 G3740 G3743 G3753 A3759 A3760 C3761 U3762 A3763 U3764 G3765 A3766 C3767 U3773 A3774 A3775 G3776 G3777 U3778 C3782 A3783 A3784 A3785 U3786 G3787 C3788 G3792 U3798 A3799 U3802 C3810 G3811 C3812 A3813 U3814 A3817 U3818 G3819
U3822 A3825 U3838 G3839 U3840 U3851 A3867 G3868 C3869 C3870 A3876 A3877 C3878 G3879 G3880 G3881 C3882 C3887 G3888 G3889 U3892 G3897 G3898 G3899 G3900 A3901 G3904 A3905 A3906 G3907 A3908 C3909 C3910 C3911 U3915 G3916 C3926 U3927 G3938 G3939 U3940 G3941 A3954 A3955 G3956 U3957 G3958
U3959 A3960 G3961 A3962 A3963 U3964 A3965 A3966 G3970 G3971 A3972 G3973 G3974 C3975 C3976 G4039 C4040 C4041 G4042 G4043 U4044 G4045 A4046 A4047 A4048 U4049 A4050 C4051 C4052 A4053 C4054 U4055 A4056 C4057 U4058 A4062 G4065 U4066 A4073 G4076 U4083 G4084 A4085 G4086 G4097 A4098 G4099 C4100 C4101 G4107 U4111 C4112



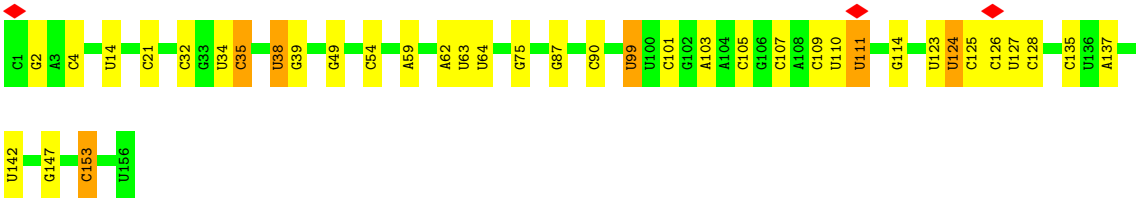
• Molecule 2: 5S rRNA

Chain 7:



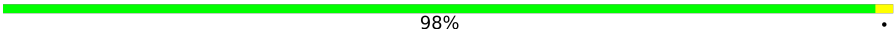
• Molecule 3: 5.8S rRNA

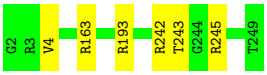
Chain 8:



• Molecule 4: uL2

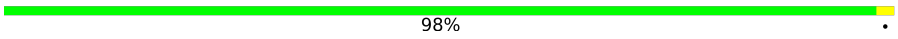
Chain A:





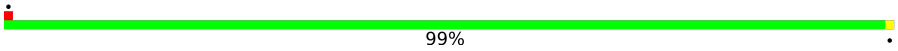
• Molecule 5: uL3

Chain B:



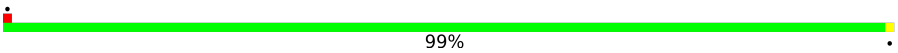
• Molecule 6: uL4

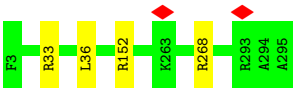
Chain C:



• Molecule 7: uL18

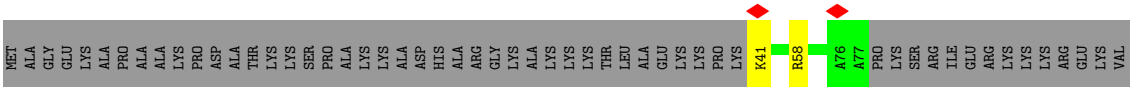
Chain D:

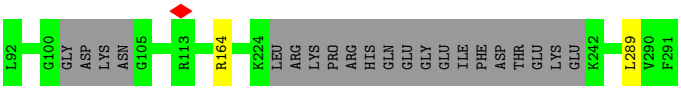




• Molecule 8: eL6

Chain E:





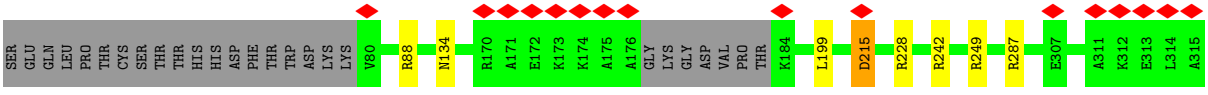
• Molecule 9: uL30

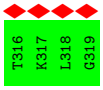
Chain F:

There are no outlier residues recorded for this chain.

• Molecule 10: eL8

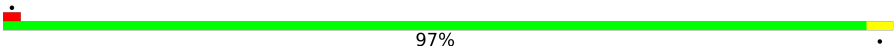
Chain G:

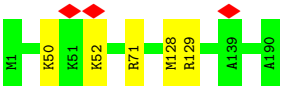




• Molecule 11: uL6

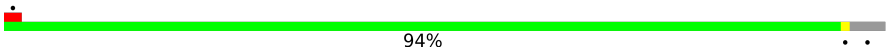
Chain H:

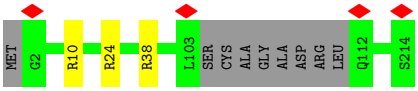




• Molecule 12: uL16

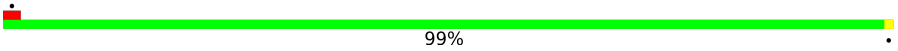
Chain I:

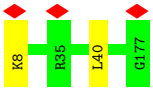




• Molecule 13: uL5

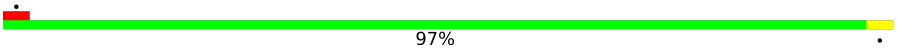
Chain J:

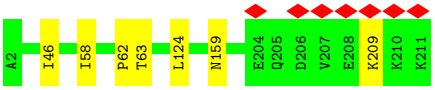




• Molecule 14: eL13

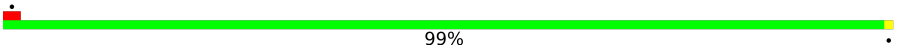
Chain L:

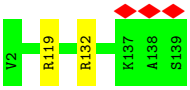




• Molecule 15: eL14

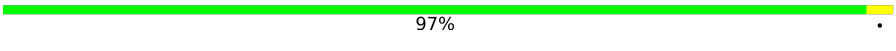
Chain M:

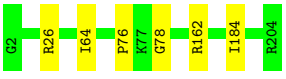




• Molecule 16: eL15

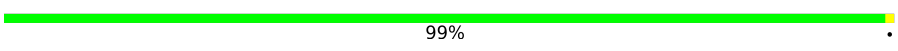
Chain N:





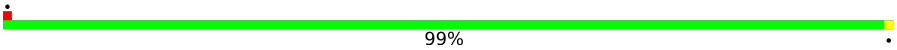
• Molecule 17: uL13

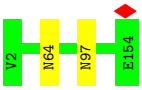
Chain O:



• Molecule 18: uL22

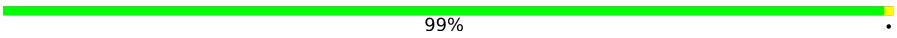
Chain P:





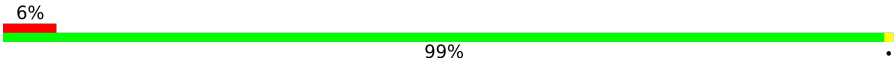
• Molecule 19: eL18

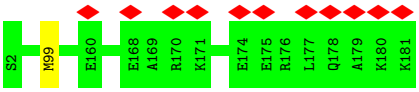
Chain Q:



• Molecule 20: eL19

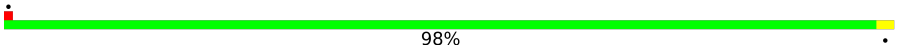
Chain R:

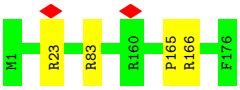




• Molecule 21: eL20

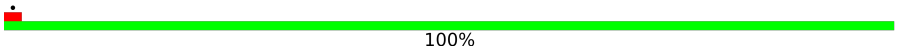
Chain S:

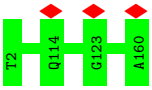




• Molecule 22: eL21

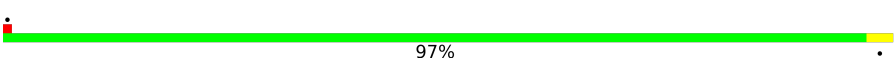
Chain T:

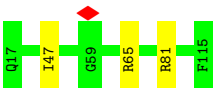




• Molecule 23: eL22

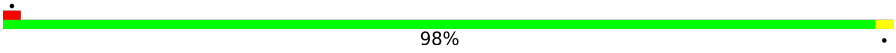
Chain U:

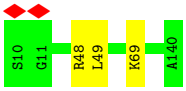




• Molecule 24: uL14

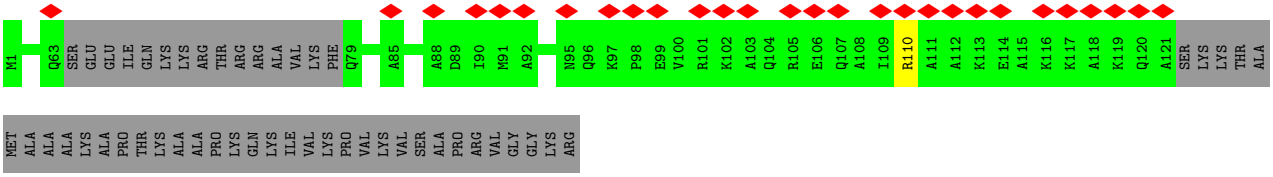
Chain V:





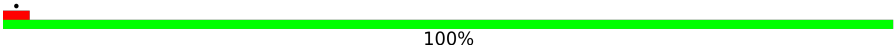
• Molecule 25: eL24

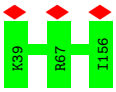
Chain W:



• Molecule 26: uL23

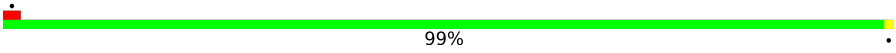
Chain X:

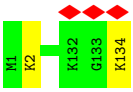




• Molecule 27: uL24

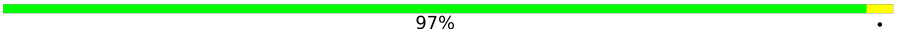
Chain Y:





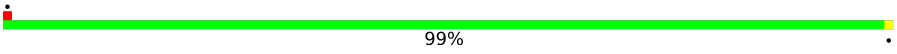
• Molecule 28: eL27

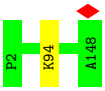
Chain Z:



• Molecule 29: uL15

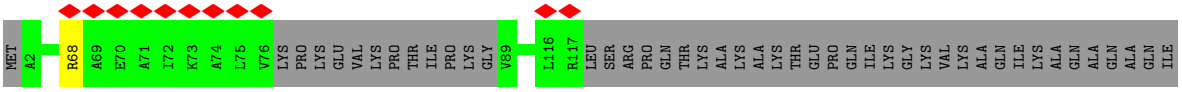
Chain a:

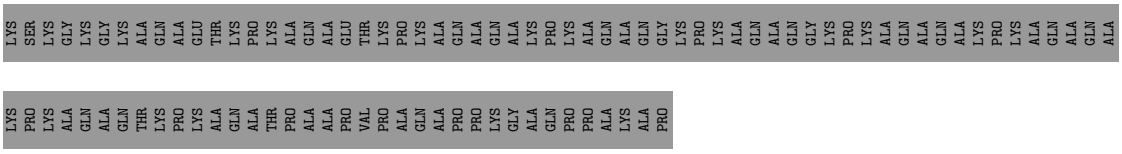




• Molecule 30: eL29

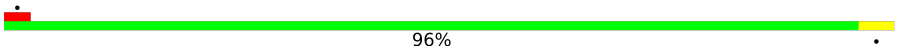
Chain b:

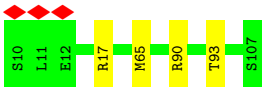




• Molecule 31: eL30

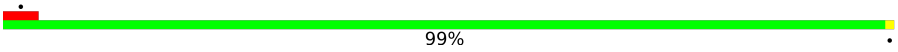
Chain c:

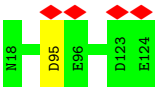




• Molecule 32: eL31

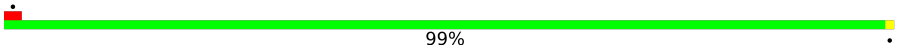
Chain d:

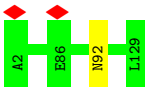




• Molecule 33: eL32

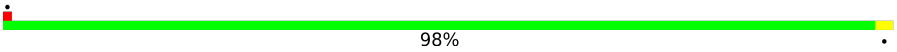
Chain e:





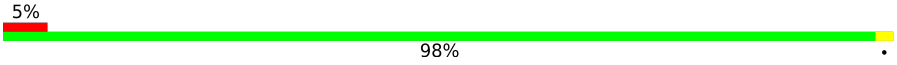
• Molecule 34: eL33

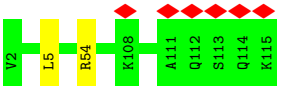
Chain f:



• Molecule 35: eL34

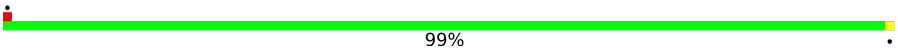
Chain g:

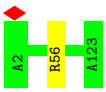




• Molecule 36: uL29

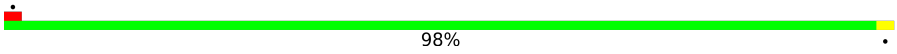
Chain h:

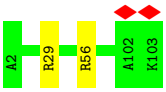




• Molecule 37: eL36

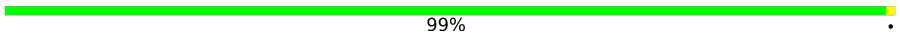
Chain i:





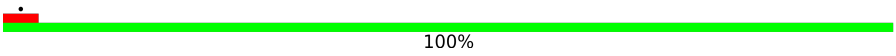
• Molecule 38: eL37

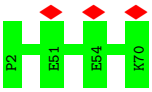
Chain j:



• Molecule 39: eL38

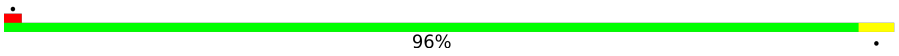
Chain k:

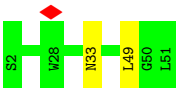




• Molecule 40: eL39

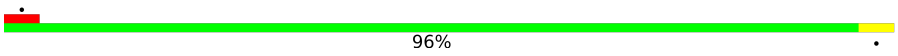
Chain l:





• Molecule 41: eL40

Chain m:

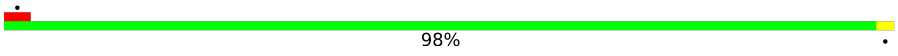


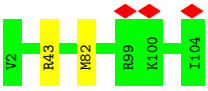
• Molecule 42: eL41

Chain n:

• Molecule 43: eL42

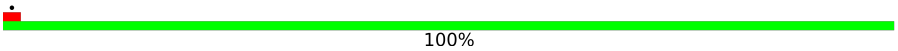
Chain o:





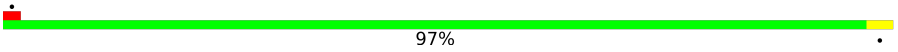
• Molecule 44: eL43

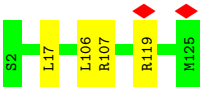
Chain p:



• Molecule 45: el28

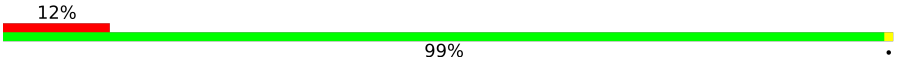
Chain r:

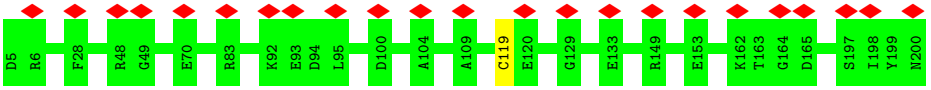




• Molecule 46: uL10

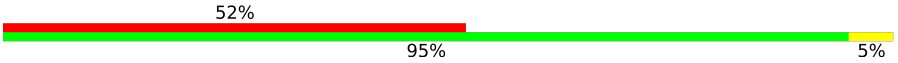
Chain s:

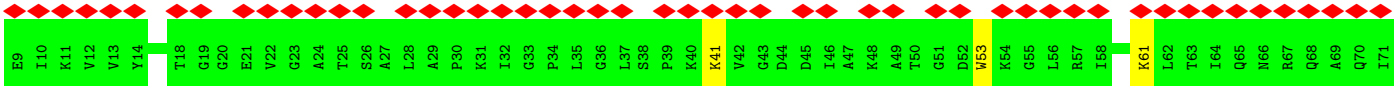


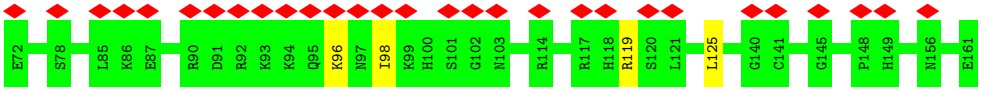


• Molecule 47: eL11

Chain t:

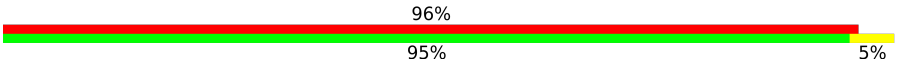


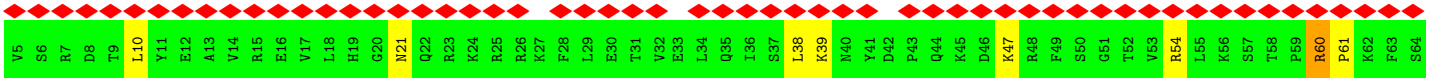


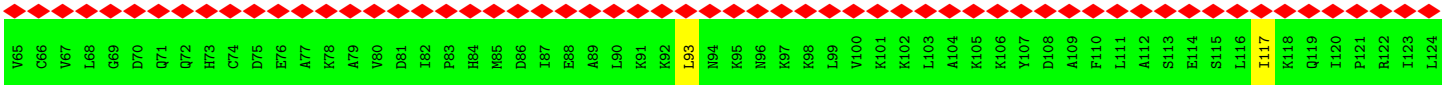


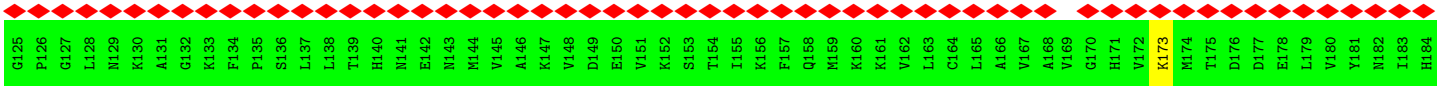
• Molecule 48: uL1

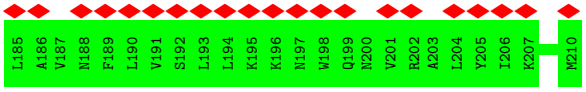
Chain u:





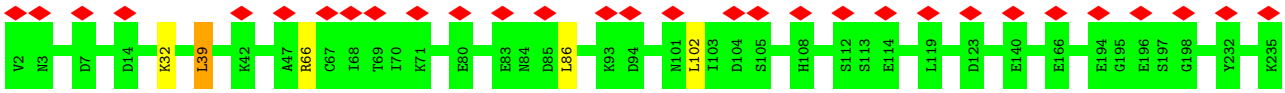


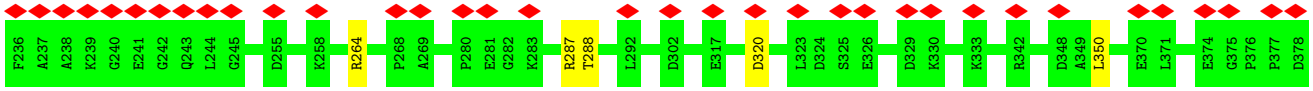


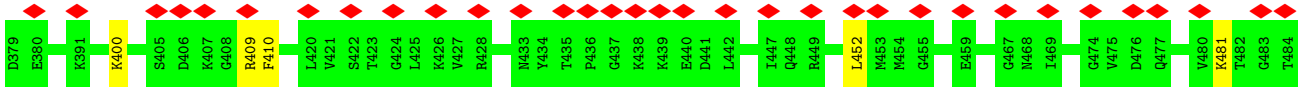


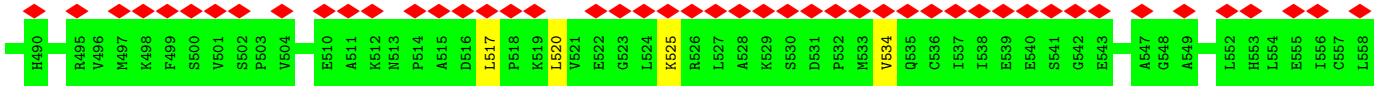
• Molecule 49: eEF2

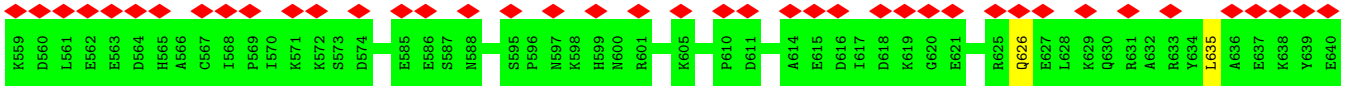
Chain v:

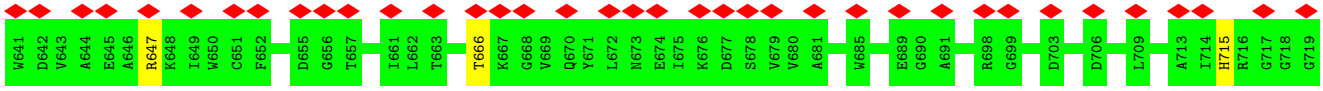


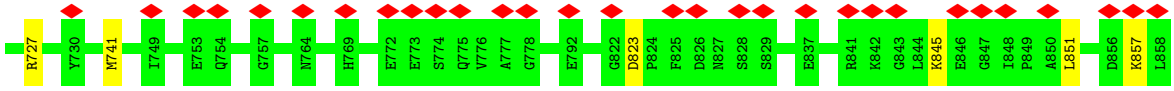






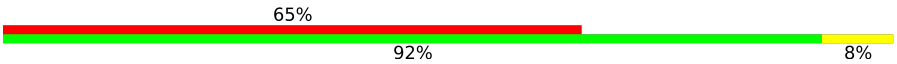


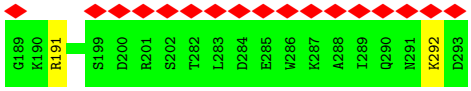




• Molecule 50: SERBP1

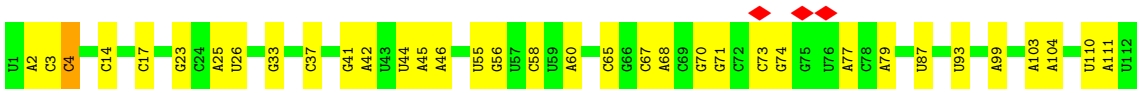
Chain w:

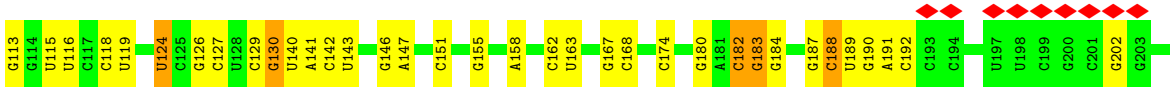


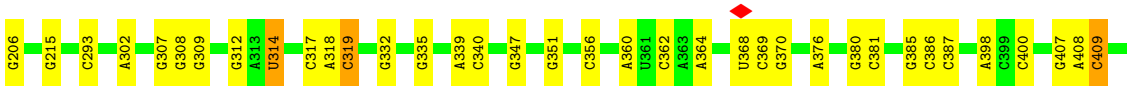


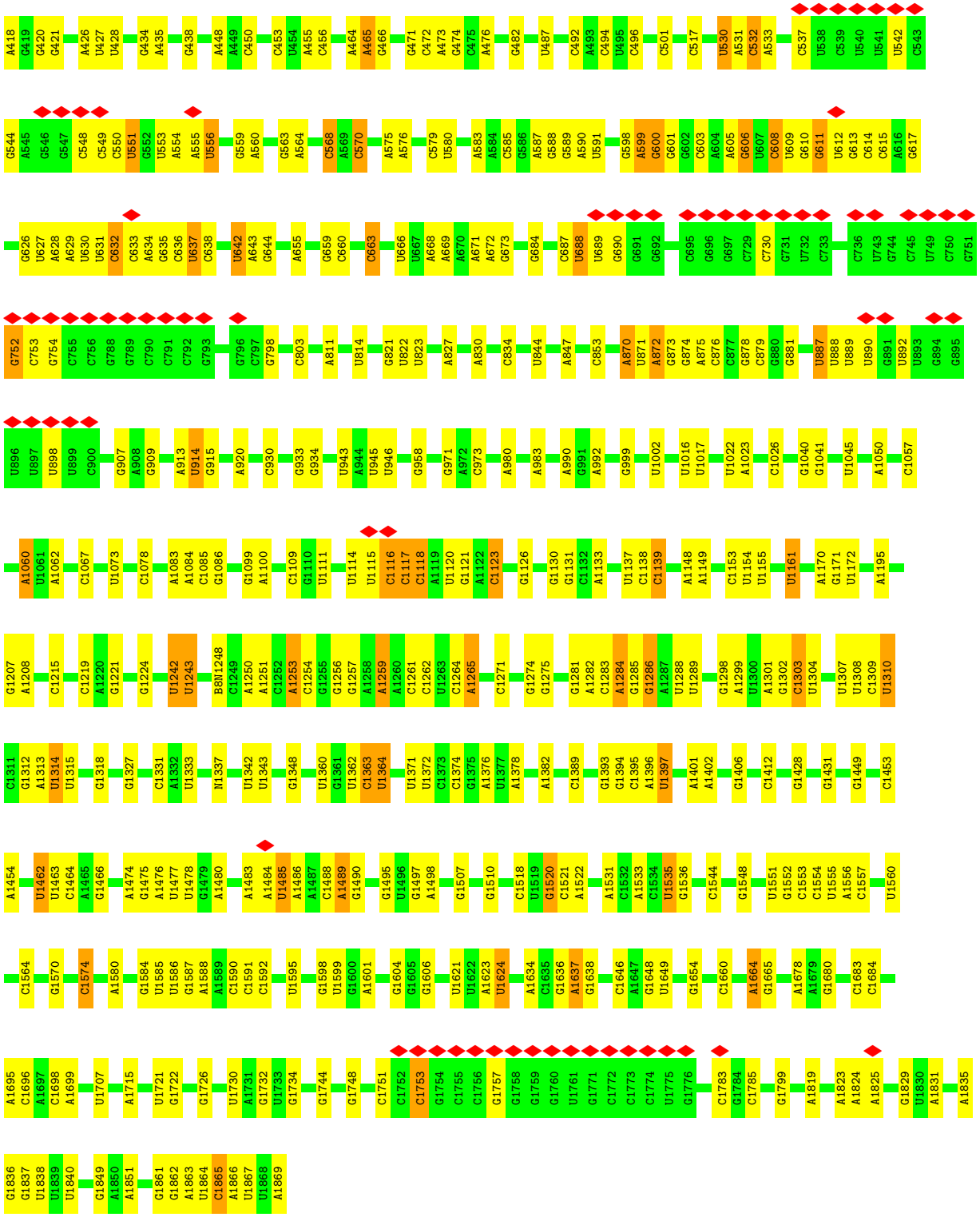
• Molecule 51: 18S rRNA

Chain 9:



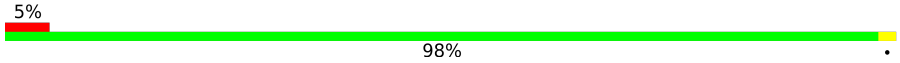


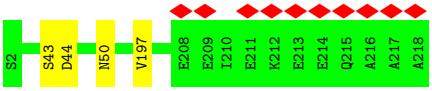




• Molecule 52: uS2

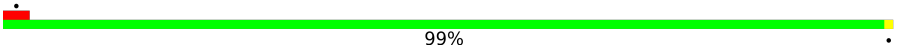
Chain AA:

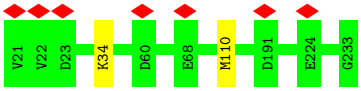




• Molecule 53: eS1

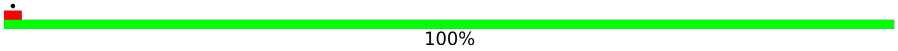
Chain BB:





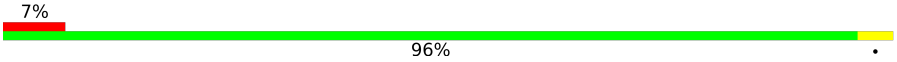
• Molecule 54: uS5

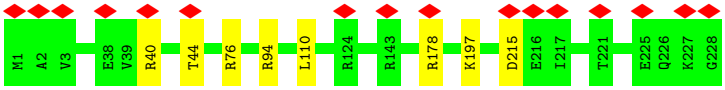
Chain CC:



• Molecule 55: uS3

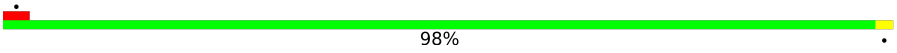
Chain DD:

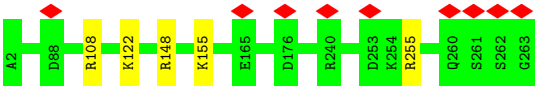




• Molecule 56: eS4

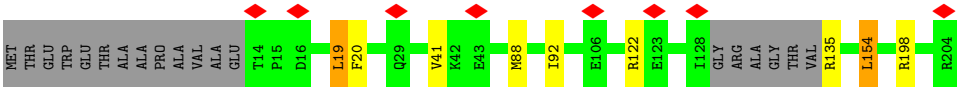
Chain EE:





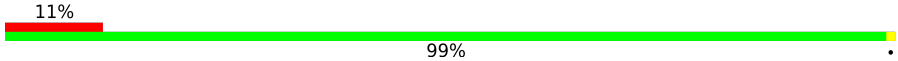
• Molecule 57: uS7

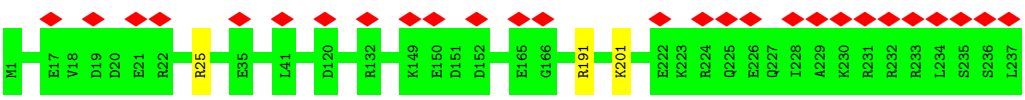
Chain FF:



• Molecule 58: eS6

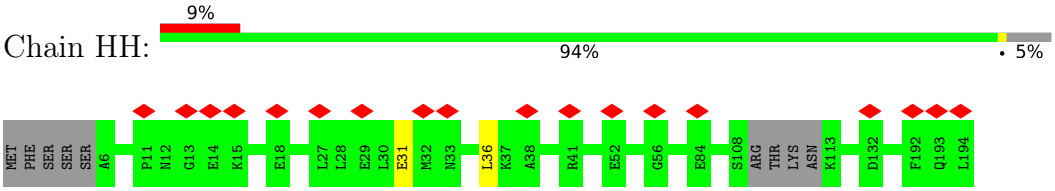
Chain GG:





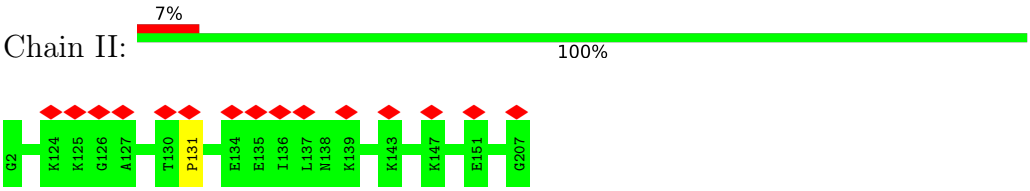
• Molecule 59: eS7

Chain HH:



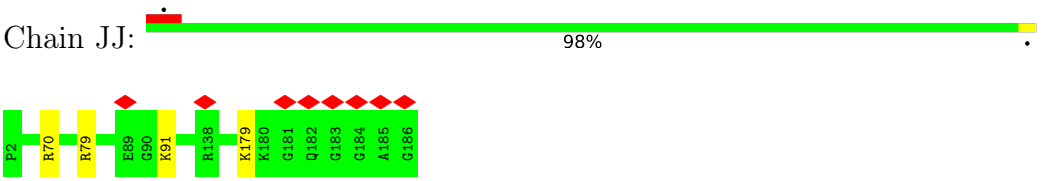
• Molecule 60: eS8

Chain II:



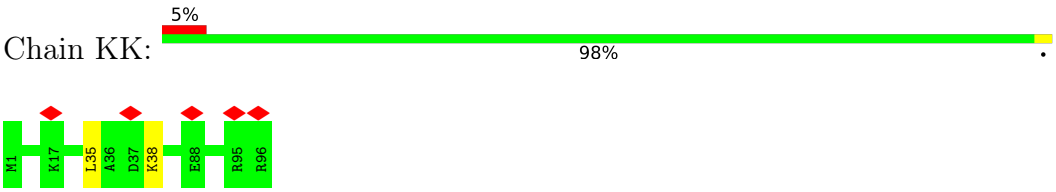
• Molecule 61: uS4

Chain JJ:



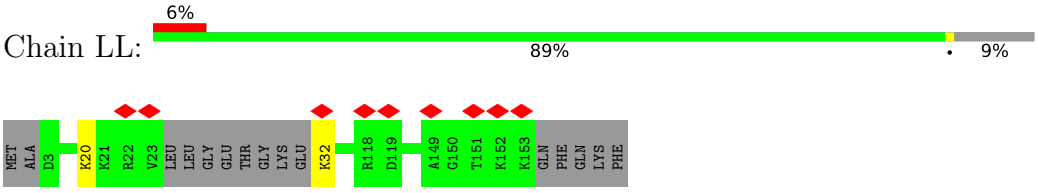
• Molecule 62: eS10

Chain KK:



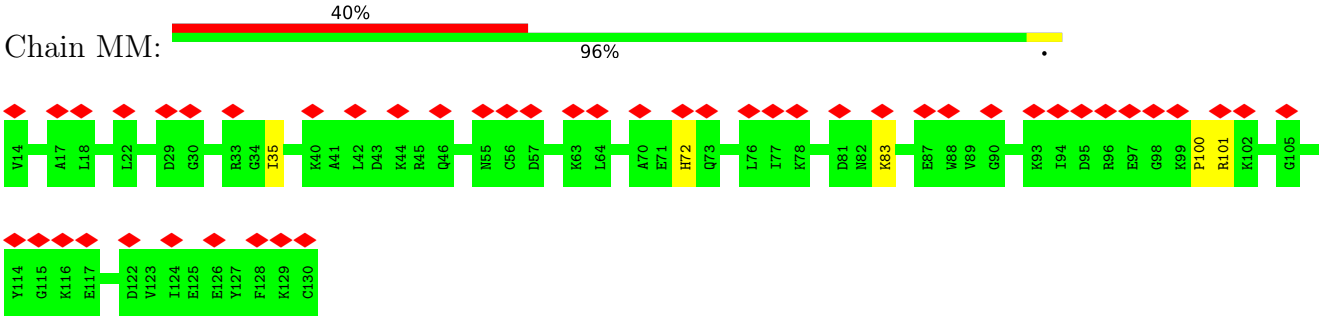
• Molecule 63: uS17

Chain LL:



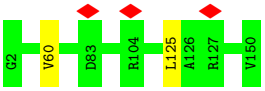
• Molecule 64: eS12

Chain MM:



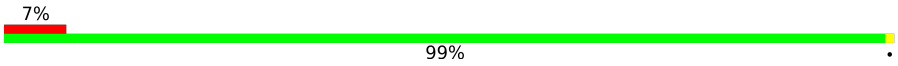
• Molecule 65: uS15

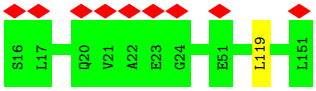
Chain NN:



• Molecule 66: uS11

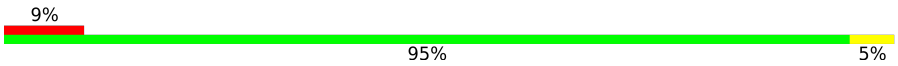
Chain OO:

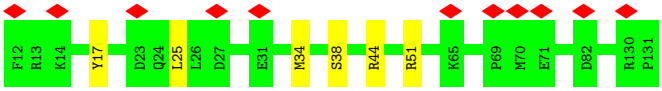




• Molecule 67: uS19

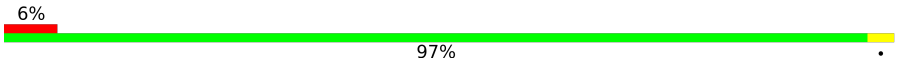
Chain PP:

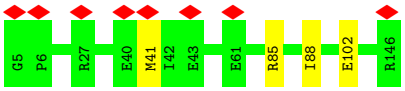




• Molecule 68: uS9

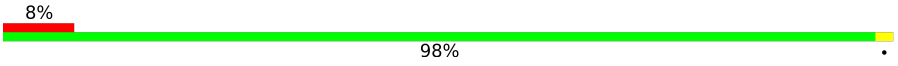
Chain QQ:

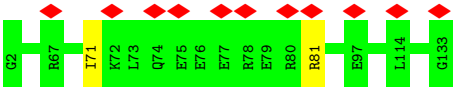




• Molecule 69: eS17

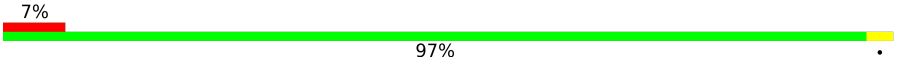
Chain RR:

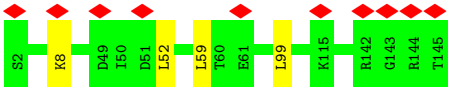




• Molecule 70: uS13

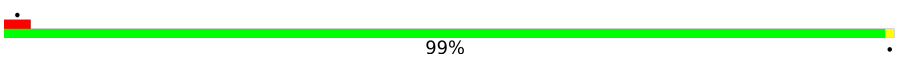
Chain SS:

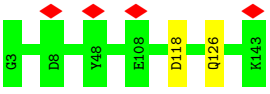




• Molecule 71: eS19

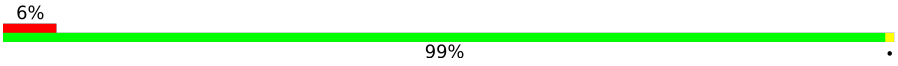
Chain TT:

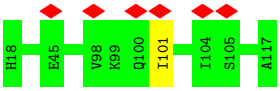




• Molecule 72: uS10

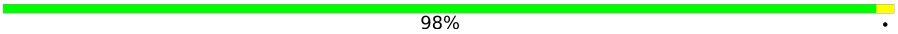
Chain UU:

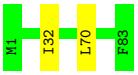




• Molecule 73: eS21

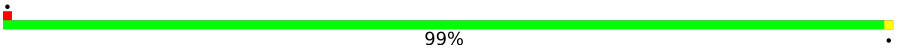
Chain VV:

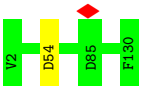




• Molecule 74: uS8

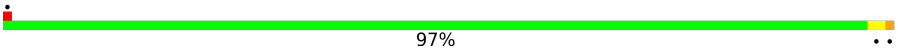
Chain WW:

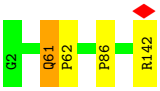




• Molecule 75: uS12

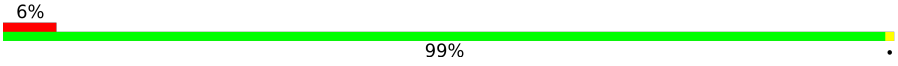
Chain XX:

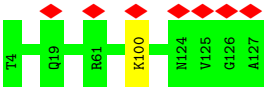




• Molecule 76: eS24

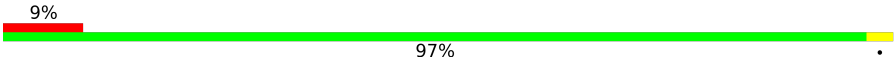
Chain YY:

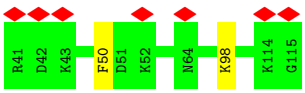




• Molecule 77: eS25

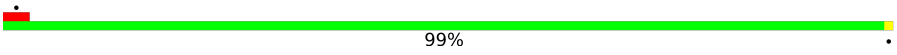
Chain ZZ:

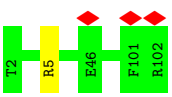




• Molecule 78: eS26

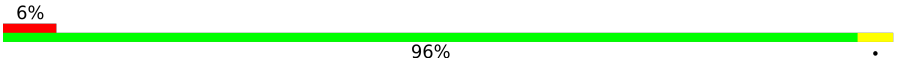
Chain aa:

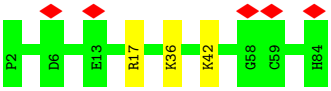




• Molecule 79: eS27

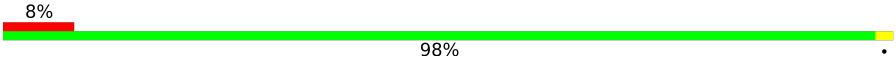
Chain bb:

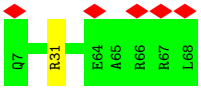




• Molecule 80: eS28

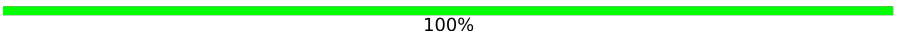
Chain cc:





• Molecule 81: uS14

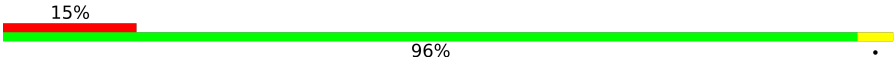
Chain dd:

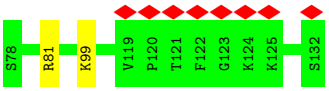


There are no outlier residues recorded for this chain.

• Molecule 82: eS30

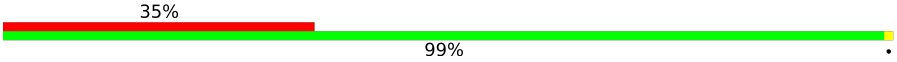
Chain ee:

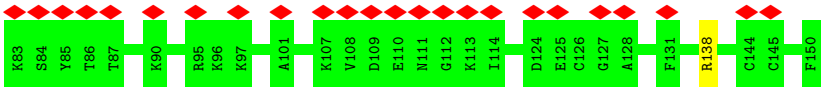




• Molecule 83: eS31

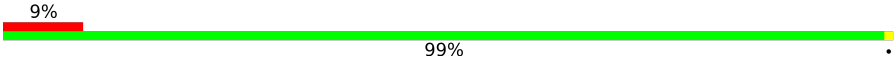
Chain ff:

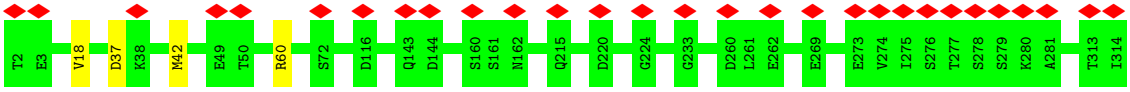




• Molecule 84: RACK1

Chain gg:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	146801	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.732	Depositor
Minimum map value	-0.379	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.09	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: B8T, DDE, UR3, ZN, P7G, 7MG, B8H, B9B, PSU, 2MG, I4U, A2M, B9H, B8Q, OMG, B8K, M7A, E7G, P4U, 5MC, GDP, MG, E6G, 4AC, BGH, 6MZ, B8W, 5MU, MLZ, OMU, B8N, OMC, MHG, 1MA

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	0.75	0/83821	1.14	578/130598 (0.4%)
2	7	0.73	0/2858	1.08	13/4455 (0.3%)
3	8	0.73	0/3559	1.15	24/5543 (0.4%)
4	A	0.48	0/1936	0.63	0/2596
5	B	0.52	0/3240	0.65	1/4339 (0.0%)
6	C	0.44	0/2927	0.58	0/3932
7	D	0.42	0/2437	0.57	0/3264
8	E	0.38	0/1762	0.60	1/2362 (0.0%)
9	F	0.46	0/1911	0.60	0/2549
10	G	0.42	0/1910	0.64	1/2569 (0.0%)
11	H	0.46	0/1535	0.67	0/2063
12	I	0.44	0/1702	0.58	0/2272
13	J	0.40	0/1385	0.65	1/1852 (0.1%)
14	L	0.42	0/1733	0.61	0/2316
15	M	0.47	0/1158	0.61	0/1547
16	N	0.51	0/1746	0.62	0/2338
17	O	0.49	0/1662	0.63	0/2222
18	P	0.46	0/1268	0.63	0/1700
19	Q	0.46	0/1539	0.65	0/2054
20	R	0.42	0/1524	0.66	2/2013 (0.1%)
21	S	0.49	0/1501	0.61	0/2012
22	T	0.46	0/1326	0.59	0/1770
23	U	0.41	0/823	0.67	0/1104
24	V	0.48	0/993	0.66	1/1332 (0.1%)
25	W	0.45	0/873	0.58	0/1158
26	X	0.40	0/984	0.59	0/1323
27	Y	0.42	0/1132	0.59	0/1504
28	Z	0.44	0/1130	0.59	0/1507
29	a	0.49	0/1191	0.59	0/1590
30	b	0.33	0/861	0.55	0/1138

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
31	c	0.45	0/771	0.62	0/1034
32	d	0.45	0/903	0.65	0/1216
33	e	0.45	0/1071	0.56	0/1429
34	f	0.49	0/895	0.60	0/1198
35	g	0.44	0/916	0.60	0/1220
36	h	0.38	0/1021	0.60	0/1348
37	i	0.39	0/841	0.58	0/1112
38	j	0.45	0/720	0.64	0/952
39	k	0.38	0/575	0.57	0/761
40	l	0.38	0/459	0.60	1/608 (0.2%)
41	m	0.45	0/425	0.67	0/561
42	n	0.34	0/240	0.60	0/305
43	o	0.42	0/855	0.55	0/1128
44	p	0.46	0/718	0.58	0/953
45	r	0.46	0/1010	0.64	1/1354 (0.1%)
46	s	0.31	0/1530	0.62	0/2064
47	t	0.30	0/1174	0.70	0/1582
48	u	0.30	0/1680	0.71	1/2255 (0.0%)
49	v	0.35	0/6651	0.72	11/8982 (0.1%)
50	w	0.34	0/218	0.60	0/287
51	9	0.75	17/40385 (0.0%)	1.93	419/62909 (0.7%)
52	AA	0.42	1/1747 (0.1%)	0.67	2/2374 (0.1%)
53	BB	0.36	0/1756	0.62	1/2350 (0.0%)
54	CC	0.41	0/1753	0.61	0/2369
55	DD	0.39	0/1796	0.67	2/2417 (0.1%)
56	EE	0.36	0/2118	0.61	0/2849
57	FF	0.36	0/1492	0.63	3/2005 (0.1%)
58	GG	0.32	0/1946	0.58	0/2590
59	HH	0.36	0/1510	0.62	0/2022
60	II	0.38	0/1715	0.61	0/2287
61	JJ	0.34	0/1550	0.55	0/2069
62	KK	0.43	0/834	0.67	1/1125 (0.1%)
63	LL	0.42	0/1195	0.56	0/1597
64	MM	0.31	0/918	0.66	0/1233
65	NN	0.37	0/1226	0.61	1/1649 (0.1%)
66	OO	0.39	0/1029	0.61	1/1380 (0.1%)
67	PP	0.36	0/1017	0.68	2/1358 (0.1%)
68	QQ	0.38	0/1146	0.63	0/1534
69	RR	0.35	0/1082	0.63	0/1452
70	SS	0.37	0/1208	0.62	0/1618
71	TT	0.36	0/1115	0.63	1/1493 (0.1%)
72	UU	0.35	0/805	0.60	0/1081
73	VV	0.40	0/643	0.63	0/860

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
74	WW	0.41	0/1051	0.64	0/1406
75	XX	0.38	0/1116	0.62	0/1490
76	YY	0.32	0/1028	0.57	0/1366
77	ZZ	0.30	0/604	0.60	0/810
78	aa	0.42	0/828	0.60	0/1109
79	bb	0.33	0/665	0.56	0/891
80	cc	0.34	0/490	0.65	0/656
81	dd	0.43	0/470	0.58	0/623
82	ee	0.36	0/447	0.61	0/587
83	ff	0.32	0/567	0.57	0/753
84	gg	0.33	0/2493	0.65	0/3394
All	All	0.62	18/234845 (0.0%)	1.17	1069/343077 (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
5	B	0	1
10	G	0	1
11	H	0	2
14	L	0	2
16	N	0	3
21	S	0	1
32	d	0	1
46	s	0	1
47	t	0	2
48	u	0	2
49	v	0	3
52	AA	0	1
56	EE	0	1
57	FF	0	2
62	KK	0	1
64	MM	0	2
67	PP	0	2
70	SS	0	1
73	VV	0	1
74	WW	0	1
75	XX	0	1
77	ZZ	0	1
84	gg	0	1
All	All	0	34

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	9	1284	A	N9-C4	41.96	1.63	1.37
51	9	1286	G	N9-C8	-31.95	1.15	1.37
51	9	1286	G	N9-C4	31.85	1.63	1.38
51	9	1284	A	N9-C8	-25.69	1.17	1.37
51	9	1284	A	N3-C4	19.97	1.46	1.34
51	9	1286	G	N3-C4	17.91	1.48	1.35
51	9	1286	G	C8-N7	16.75	1.41	1.30
51	9	1284	A	C8-N7	15.19	1.42	1.31
51	9	599	A	N9-C4	11.37	1.44	1.37
51	9	1284	A	N7-C5	-8.20	1.34	1.39
51	9	1286	G	N7-C5	-8.14	1.34	1.39
51	9	611	G	C6-O6	-7.06	1.17	1.24
51	9	611	G	C5-C6	-6.97	1.35	1.42
51	9	637	U	C2-N3	6.29	1.42	1.37
52	AA	197	VAL	C-N	-5.52	1.21	1.34
51	9	606	G	N9-C4	5.22	1.42	1.38
51	9	632	C	C4-C5	-5.08	1.38	1.43
51	9	914	U	C5-C6	-5.02	1.29	1.34

All (1069) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	9	1286	G	C4-C5-N7	-172.13	41.95	110.80
51	9	1284	A	N7-C8-N9	-146.83	40.38	113.80
51	9	1286	G	N7-C8-N9	-144.28	40.96	113.10
51	9	1284	A	C4-C5-N7	-138.38	41.51	110.70
51	9	1286	G	C8-N9-C4	-132.00	53.60	106.40
51	9	1284	A	C8-N9-C4	-129.24	54.10	105.80
51	9	1284	A	C5-N7-C8	62.20	135.00	103.90
51	9	1286	G	C5-N7-C8	60.15	134.37	104.30
51	9	1286	G	C6-C5-N7	47.27	158.76	130.40
51	9	1284	A	C6-C5-N7	36.40	157.78	132.30
51	9	1286	G	N3-C4-N9	26.11	141.66	126.00
51	9	1286	G	C8-N9-C1'	-22.90	97.23	127.00
51	9	599	A	C2-N3-C4	22.17	121.69	110.60
51	9	1284	A	N3-C4-N9	20.40	143.72	127.40
51	9	1284	A	N9-C4-C5	-19.61	97.95	105.80
51	9	632	C	N1-C2-O2	18.80	130.18	118.90
51	9	1286	G	C4-N9-C1'	18.71	150.83	126.50
51	9	1286	G	N9-C4-C5	-18.03	98.19	105.40
51	9	611	G	C4-C5-N7	17.94	117.98	110.80
51	9	1286	G	C2-N3-C4	17.22	120.51	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	9	1286	G	N3-C4-C5	-16.91	120.14	128.60
51	9	1286	G	C5-C6-N1	16.32	119.66	111.50
51	9	1284	A	C2-N3-C4	16.15	118.67	110.60
51	9	611	G	C5-C6-O6	-16.07	118.96	128.60
51	9	632	C	C5-C6-N1	15.89	128.94	121.00
51	9	1284	A	C4-N9-C1'	15.80	154.75	126.30
51	9	1284	A	C8-N9-C1'	-15.03	100.64	127.70
51	9	1284	A	C5-C6-N1	14.82	125.11	117.70
51	9	611	G	N3-C4-N9	14.53	134.72	126.00
51	9	599	A	C5-C6-N1	14.48	124.94	117.70
51	9	611	G	C6-C5-N7	-13.93	122.04	130.40
51	9	611	G	N9-C4-C5	-12.99	100.20	105.40
51	9	501	C	N1-C2-O2	12.85	126.61	118.90
51	9	612	U	C5-C4-O4	-12.79	118.23	125.90
51	9	634	A	N1-C2-N3	-12.75	122.93	129.30
51	9	914	U	C5-C4-O4	-12.66	118.31	125.90
51	9	611	G	C5-C6-N1	12.34	117.67	111.50
51	9	611	G	C5-N7-C8	-12.22	98.19	104.30
51	9	1284	A	N3-C4-C5	-12.11	118.32	126.80
51	9	501	C	C2-N1-C1'	12.07	132.08	118.80
1	5	2505	C	N1-C2-O2	11.79	125.97	118.90
51	9	914	U	C2-N1-C1'	11.71	131.75	117.70
51	9	632	C	C4-C5-C6	-11.42	111.69	117.40
51	9	599	A	N1-C6-N6	-11.37	111.78	118.60
51	9	606	G	N3-C4-N9	11.34	132.80	126.00
1	5	4056	A	OP1-P-O3'	-11.27	80.41	105.20
1	5	1079	C	N1-C2-O2	10.91	125.45	118.90
51	9	599	A	C8-N9-C4	-10.85	101.46	105.80
51	9	632	C	N3-C2-O2	-10.83	114.32	121.90
51	9	605	A	C2-N3-C4	10.81	116.01	110.60
1	5	2505	C	N3-C2-O2	-10.79	114.35	121.90
51	9	611	G	C6-N1-C2	-10.77	118.64	125.10
51	9	914	U	C6-N1-C1'	-10.69	106.23	121.20
51	9	599	A	N3-C4-C5	-10.38	119.54	126.80
51	9	501	C	N3-C2-O2	-10.26	114.72	121.90
1	5	1978	C	N1-C2-O2	10.26	125.05	118.90
51	9	1520	G	N3-C4-C5	-10.17	123.52	128.60
51	9	611	G	C8-N9-C1'	-10.14	113.81	127.00
51	9	1453	C	N1-C2-O2	10.12	124.97	118.90
51	9	1139	C	N1-C2-O2	9.96	124.88	118.90
51	9	293	C	N1-C2-O2	9.96	124.88	118.90
1	5	685	C	O5'-P-OP2	-9.83	96.85	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	v	452	LEU	CA-CB-CG	9.80	137.84	115.30
52	AA	197	VAL	C-N-CA	9.76	146.10	121.70
1	5	2814	C	N1-C2-O2	9.72	124.73	118.90
71	TT	118	ASP	CB-CG-OD1	9.61	126.95	118.30
51	9	293	C	C2-N1-C1'	9.60	129.35	118.80
51	9	1453	C	C2-N1-C1'	9.57	129.33	118.80
1	5	100	C	C2-N1-C1'	9.57	129.32	118.80
51	9	1535	U	C2-N1-C1'	9.56	129.17	117.70
1	5	4119	C	C2-N1-C1'	9.51	129.26	118.80
1	5	2814	C	N3-C2-O2	-9.50	115.25	121.90
51	9	611	G	C4-N9-C1'	9.49	138.84	126.50
51	9	314	U	N3-C2-O2	-9.45	115.58	122.20
1	5	2505	C	C6-N1-C2	-9.43	116.53	120.30
51	9	605	A	C8-N9-C4	-9.41	102.03	105.80
3	8	128	C	N1-C2-O2	9.40	124.54	118.90
51	9	1303	C	C2-N1-C1'	9.38	129.11	118.80
1	5	1612	G	N3-C4-N9	9.37	131.62	126.00
1	5	1639	U	C2-N1-C1'	9.36	128.93	117.70
51	9	1520	G	C2-N3-C4	9.29	116.55	111.90
51	9	1139	C	N3-C2-O2	-9.19	115.47	121.90
51	9	853	C	C2-N1-C1'	9.18	128.90	118.80
51	9	853	C	N1-C2-O2	9.09	124.35	118.90
51	9	1363	C	N1-C2-O2	9.08	124.35	118.90
51	9	612	U	N3-C4-O4	9.06	125.74	119.40
1	5	1079	C	N3-C2-O2	-9.05	115.57	121.90
51	9	314	U	N1-C2-O2	9.04	129.13	122.80
1	5	1236	C	C6-N1-C2	-8.95	116.72	120.30
51	9	1535	U	N1-C2-O2	8.95	129.07	122.80
1	5	4041	C	N1-C2-O2	8.91	124.25	118.90
1	5	112	C	C2-N1-C1'	8.90	128.60	118.80
1	5	1978	C	C2-N1-C1'	8.89	128.58	118.80
51	9	1520	G	C8-N9-C4	-8.82	102.87	106.40
51	9	606	G	N3-C4-C5	-8.81	124.19	128.60
1	5	4880	C	C2-N1-C1'	8.71	128.38	118.80
51	9	501	C	C6-N1-C2	-8.66	116.84	120.30
2	7	29	C	C2-N1-C1'	8.65	128.32	118.80
1	5	100	C	N1-C2-O2	8.61	124.07	118.90
1	5	2819	U	N3-C2-O2	-8.57	116.20	122.20
1	5	4119	C	N1-C2-O2	8.56	124.04	118.90
51	9	599	A	O4'-C1'-N9	8.56	115.05	108.20
51	9	1139	C	C2-N1-C1'	8.55	128.21	118.80
1	5	1381	U	N1-C2-O2	8.54	128.78	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	4056	A	OP2-P-O3'	-8.54	86.42	105.20
1	5	1079	C	C2-N1-C1'	8.51	128.16	118.80
51	9	634	A	C4-C5-C6	-8.49	112.75	117.00
1	5	1381	U	N3-C2-O2	-8.42	116.31	122.20
51	9	1271	C	N1-C2-O2	8.37	123.92	118.90
51	9	599	A	C6-N1-C2	-8.36	113.59	118.60
51	9	637	U	C2-N1-C1'	8.35	127.72	117.70
51	9	1462	U	N1-C2-O2	8.35	128.65	122.80
1	5	3788	C	N1-C2-O2	8.34	123.91	118.90
1	5	2814	C	C2-N1-C1'	8.31	127.94	118.80
1	5	4928	C	N1-C2-O2	8.31	123.89	118.90
51	9	1286	G	C5-C6-O6	-8.30	123.62	128.60
51	9	606	G	C6-C5-N7	-8.29	125.42	130.40
51	9	174	C	N3-C2-O2	-8.27	116.11	121.90
1	5	100	C	N3-C2-O2	-8.27	116.11	121.90
1	5	2505	C	C2-N1-C1'	8.24	127.86	118.80
51	9	914	U	N3-C4-O4	8.23	125.16	119.40
51	9	1624	U	N3-C2-O2	-8.22	116.45	122.20
1	5	1429	C	C2-N1-C1'	8.20	127.82	118.80
51	9	570	C	N1-C2-O2	8.17	123.80	118.90
51	9	599	A	N1-C2-N3	-8.17	125.22	129.30
51	9	501	C	C6-N1-C1'	-8.14	111.03	120.80
51	9	1284	A	N1-C2-N3	-8.14	125.23	129.30
1	5	220	C	N1-C2-O2	8.13	123.78	118.90
51	9	183	G	C2-N3-C4	8.13	115.97	111.90
1	5	521	C	N3-C2-O2	-8.11	116.22	121.90
51	9	1364	U	C2-N1-C1'	8.09	127.41	117.70
1	5	2627	C	N1-C2-O2	8.07	123.74	118.90
1	5	4928	C	N3-C2-O2	-8.04	116.27	121.90
51	9	293	C	N3-C2-O2	-8.03	116.28	121.90
51	9	630	U	O4'-C1'-N1	8.03	114.62	108.20
51	9	1343	U	N1-C2-O2	8.02	128.42	122.80
1	5	1484	G	N3-C4-N9	8.02	130.81	126.00
51	9	1462	U	N3-C2-O2	-7.98	116.61	122.20
51	9	1343	U	N3-C2-O2	-7.98	116.61	122.20
51	9	1315	U	N3-C2-O2	-7.97	116.62	122.20
51	9	1261	C	N1-C2-O2	7.97	123.68	118.90
51	9	1865	C	C6-N1-C2	-7.96	117.11	120.30
51	9	606	G	C4-N9-C1'	7.96	136.85	126.50
1	5	4880	C	N1-C2-O2	7.96	123.67	118.90
51	9	1462	U	C2-N1-C1'	7.91	127.19	117.70
51	9	611	G	N3-C2-N2	7.90	125.43	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	9	1453	C	N3-C2-O2	-7.88	116.39	121.90
51	9	632	C	C6-N1-C2	-7.85	117.16	120.30
1	5	4041	C	C6-N1-C2	-7.85	117.16	120.30
51	9	407	G	N3-C4-N9	7.83	130.70	126.00
51	9	1261	C	N3-C2-O2	-7.80	116.44	121.90
1	5	4928	C	C2-N1-C1'	7.80	127.38	118.80
51	9	1591	C	N1-C2-O2	7.79	123.58	118.90
1	5	4051	C	N1-C2-O2	7.78	123.56	118.90
1	5	4254	G	N3-C4-C5	-7.78	124.71	128.60
1	5	2819	U	N1-C2-O2	7.77	128.24	122.80
51	9	314	U	C2-N1-C1'	7.75	127.00	117.70
3	8	111	U	C2-N1-C1'	7.75	127.00	117.70
51	9	407	G	N3-C4-C5	-7.72	124.74	128.60
1	5	4759	C	N1-C2-O2	7.70	123.52	118.90
1	5	1978	C	N3-C2-O2	-7.70	116.51	121.90
51	9	853	C	N3-C2-O2	-7.69	116.52	121.90
51	9	1360	U	C5-C4-O4	7.69	130.51	125.90
1	5	4759	C	C2-N1-C1'	7.69	127.26	118.80
51	9	611	G	N7-C8-N9	7.67	116.94	113.10
51	9	1520	G	C4-N9-C1'	7.67	136.47	126.50
1	5	2022	C	N1-C2-O2	7.66	123.50	118.90
1	5	4229	U	N3-C2-O2	-7.64	116.85	122.20
1	5	4266	G	N3-C4-N9	7.63	130.58	126.00
51	9	1624	U	C2-N1-C1'	7.63	126.86	117.70
3	8	111	U	N1-C2-O2	7.62	128.13	122.80
51	9	632	C	N3-C4-C5	7.61	124.94	121.90
1	5	4709	U	N1-C2-O2	7.61	128.12	122.80
1	5	115	C	N1-C2-O2	7.60	123.46	118.90
1	5	1974	U	N3-C4-O4	7.60	124.72	119.40
1	5	77	U	N3-C2-O2	-7.59	116.89	122.20
1	5	4041	C	N3-C2-O2	-7.59	116.58	121.90
1	5	1084	C	C2-N1-C1'	7.59	127.15	118.80
1	5	1807	C	C2-N1-C1'	7.58	127.14	118.80
3	8	128	C	N3-C2-O2	-7.54	116.62	121.90
1	5	2627	C	C6-N1-C2	-7.54	117.28	120.30
51	9	427	U	C2-N1-C1'	7.53	126.74	117.70
1	5	1484	G	C4-N9-C1'	7.53	136.28	126.50
51	9	427	U	N3-C2-O2	-7.52	116.93	122.20
1	5	4560	C	N3-C2-O2	-7.50	116.65	121.90
51	9	634	A	C2-N3-C4	7.48	114.34	110.60
51	9	1016	U	N3-C2-O2	-7.47	116.97	122.20
1	5	1792	U	C2-N1-C1'	7.46	126.66	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	9	945	U	C2-N1-C1'	7.45	126.64	117.70
1	5	1484	G	N3-C4-C5	-7.45	124.88	128.60
1	5	2627	C	N3-C2-O2	-7.45	116.69	121.90
3	8	111	U	N3-C2-O2	-7.44	116.99	122.20
1	5	4924	C	N3-C2-O2	-7.43	116.70	121.90
1	5	691	C	C2-N1-C1'	7.43	126.97	118.80
51	9	319	C	O5'-P-OP1	7.43	119.61	110.70
51	9	188	C	C2-N1-C1'	7.42	126.97	118.80
51	9	1363	C	N3-C2-O2	-7.42	116.71	121.90
51	9	1535	U	N3-C2-O2	-7.42	117.01	122.20
1	5	133	C	N1-C2-O2	7.41	123.35	118.90
1	5	4360	U	N3-C2-O2	-7.41	117.01	122.20
1	5	1381	U	C2-N1-C1'	7.41	126.59	117.70
1	5	1974	U	C5-C4-O4	-7.39	121.47	125.90
51	9	638	C	C6-N1-C2	-7.39	117.34	120.30
1	5	2022	C	N3-C2-O2	-7.38	116.73	121.90
51	9	494	C	N1-C2-O2	7.38	123.33	118.90
1	5	1193	C	C2-N1-C1'	7.38	126.92	118.80
51	9	973	C	N1-C2-O2	7.37	123.32	118.90
51	9	613	G	C8-N9-C4	7.35	109.34	106.40
51	9	501	C	C5-C6-N1	7.35	124.67	121.00
51	9	130	G	C4-N9-C1'	7.34	136.04	126.50
1	5	326	C	C6-N1-C2	-7.34	117.37	120.30
51	9	1303	C	N1-C2-O2	7.32	123.29	118.90
1	5	4423	U	C2-N1-C1'	7.32	126.49	117.70
1	5	4709	U	N3-C2-O2	-7.32	117.08	122.20
51	9	605	A	N9-C4-C5	7.32	108.73	105.80
1	5	266	C	O5'-P-OP2	-7.28	99.15	105.70
1	5	2046	G	P-O3'-C3'	7.28	128.43	119.70
1	5	1429	C	N1-C2-O2	7.27	123.26	118.90
51	9	1057	C	C2-N1-C1'	7.24	126.76	118.80
1	5	1663	C	C5-C6-N1	7.22	124.61	121.00
1	5	4266	G	N3-C4-C5	-7.22	124.99	128.60
3	8	64	U	N3-C2-O2	-7.21	117.16	122.20
1	5	2814	C	C6-N1-C2	-7.18	117.43	120.30
51	9	1696	C	C2-N1-C1'	7.17	126.69	118.80
51	9	1343	U	C2-N1-C1'	7.17	126.31	117.70
1	5	1445	U	C5-C6-N1	7.17	126.28	122.70
1	5	4880	C	N3-C2-O2	-7.17	116.88	121.90
1	5	2704	C	C2-N1-C1'	7.16	126.68	118.80
2	7	29	C	N1-C2-O2	7.15	123.19	118.90
51	9	611	G	N3-C4-C5	-7.15	125.03	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	9	407	G	C4-N9-C1'	7.15	135.79	126.50
1	5	1792	U	N3-C2-O2	-7.14	117.20	122.20
51	9	1315	U	C2-N1-C1'	7.13	126.26	117.70
1	5	4667	C	C6-N1-C2	-7.12	117.45	120.30
1	5	1893	C	C2-N1-C1'	7.12	126.63	118.80
1	5	4266	G	C4-N9-C1'	7.12	135.75	126.50
1	5	4709	U	C2-N1-C1'	7.11	126.24	117.70
1	5	3636	C	N3-C2-O2	-7.09	116.94	121.90
51	9	634	A	C6-N1-C2	7.09	122.85	118.60
1	5	2661	U	P-O3'-C3'	7.09	128.21	119.70
51	9	183	G	N3-C4-C5	-7.08	125.06	128.60
51	9	188	C	N1-C2-O2	7.07	123.14	118.90
1	5	2695	A	P-O3'-C3'	7.07	128.18	119.70
1	5	1329	G	C8-N9-C4	-7.06	103.58	106.40
51	9	611	G	N1-C2-N2	-7.06	109.85	116.20
51	9	630	U	C2-N1-C1'	7.06	126.17	117.70
51	9	1389	C	C2-N1-C1'	7.06	126.56	118.80
1	5	4925	U	P-O3'-C3'	7.05	128.17	119.70
51	9	612	U	C5-C6-N1	7.04	126.22	122.70
51	9	1624	U	N1-C2-O2	7.04	127.72	122.80
1	5	1079	C	C6-N1-C2	-7.03	117.49	120.30
1	5	1612	G	C6-C5-N7	-7.03	126.18	130.40
1	5	2528	G	C4-N9-C1'	7.03	135.64	126.50
51	9	130	G	N3-C4-C5	-7.03	125.08	128.60
51	9	1751	C	N1-C2-O2	7.01	123.11	118.90
1	5	472	C	C2-N1-C1'	7.01	126.51	118.80
51	9	1485	U	C2-N1-C1'	7.00	126.11	117.70
51	9	636	C	N1-C2-O2	7.00	123.10	118.90
1	5	3788	C	N3-C2-O2	-7.00	117.00	121.90
1	5	2410	C	C2-N1-C1'	6.99	126.49	118.80
1	5	1612	G	C4-C5-N7	6.99	113.59	110.80
51	9	606	G	C8-N9-C1'	-6.98	117.92	127.00
51	9	1315	U	N1-C2-O2	6.96	127.67	122.80
1	5	1248	C	N1-C2-O2	6.96	123.08	118.90
1	5	672	C	N1-C2-O2	6.95	123.07	118.90
1	5	1792	U	N1-C2-O2	6.95	127.67	122.80
1	5	4057	C	OP1-P-OP2	6.95	130.03	119.60
1	5	4229	U	N1-C2-O2	6.95	127.67	122.80
51	9	427	U	N1-C2-O2	6.95	127.67	122.80
1	5	1612	G	C8-N9-C1'	-6.95	117.97	127.00
51	9	930	C	N1-C2-O2	6.95	123.07	118.90
1	5	1612	G	C5-C6-O6	-6.94	124.44	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	9	1485	U	C5-C6-N1	6.94	126.17	122.70
51	9	1271	C	C2-N1-C1'	6.93	126.43	118.80
51	9	124	U	N1-C2-O2	6.93	127.65	122.80
1	5	2028	C	C2-N1-C1'	6.92	126.42	118.80
1	5	1612	G	C4-N9-C1'	6.92	135.50	126.50
51	9	1298	G	N3-C4-N9	6.92	130.15	126.00
1	5	205	C	N1-C2-O2	6.91	123.05	118.90
1	5	4869	U	N3-C2-O2	-6.88	117.39	122.20
51	9	124	U	N3-C2-O2	-6.88	117.38	122.20
20	R	99	MET	CA-CB-CG	-6.88	101.61	113.30
51	9	293	C	C6-N1-C1'	-6.87	112.56	120.80
49	v	741	MET	C-N-CA	6.86	138.85	121.70
51	9	356	C	C2-N1-C1'	6.86	126.35	118.80
51	9	1303	C	C6-N1-C1'	-6.85	112.58	120.80
1	5	4948	C	C2-N1-C1'	6.84	126.32	118.80
1	5	1812	C	C2-N1-C1'	6.82	126.30	118.80
51	9	688	U	P-O3'-C3'	6.80	127.87	119.70
1	5	4254	G	C2-N3-C4	6.80	115.30	111.90
1	5	220	C	C2-N1-C1'	6.80	126.28	118.80
51	9	610	G	C5-C6-O6	-6.80	124.52	128.60
51	9	1261	C	C6-N1-C2	-6.80	117.58	120.30
1	5	217	C	N1-C2-O2	6.80	122.98	118.90
51	9	1485	U	N1-C2-O2	6.79	127.56	122.80
1	5	1339	U	C5-C6-N1	6.78	126.09	122.70
1	5	3876	A	P-O3'-C3'	6.78	127.84	119.70
1	5	4759	C	N3-C2-O2	-6.77	117.16	121.90
1	5	4502	C	N1-C2-O2	6.76	122.95	118.90
51	9	119	U	N3-C2-O2	-6.76	117.47	122.20
1	5	3636	C	N1-C2-O2	6.75	122.95	118.90
1	5	4119	C	C6-N1-C1'	-6.75	112.70	120.80
1	5	2281	U	N1-C2-O2	6.73	127.51	122.80
1	5	1612	G	N9-C4-C5	-6.73	102.71	105.40
1	5	4871	C	N1-C2-O2	6.72	122.93	118.90
51	9	537	C	C2-N1-C1'	6.72	126.19	118.80
51	9	1016	U	N1-C2-O2	6.71	127.50	122.80
1	5	100	C	C6-N1-C1'	-6.71	112.74	120.80
51	9	1360	U	N3-C4-O4	-6.70	114.71	119.40
51	9	570	C	N3-C2-O2	-6.70	117.21	121.90
51	9	1696	C	C6-N1-C2	-6.70	117.62	120.30
51	9	537	C	N1-C2-O2	6.70	122.92	118.90
51	9	1057	C	N3-C2-O2	-6.70	117.21	121.90
1	5	1340	C	C5-C6-N1	6.69	124.35	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	1882	U	C5-C4-O4	-6.69	121.89	125.90
51	9	1118	C	C2-N1-C1'	6.69	126.16	118.80
51	9	1397	U	N3-C2-O2	-6.68	117.52	122.20
51	9	823	U	N3-C2-O2	-6.68	117.52	122.20
1	5	2528	G	N3-C4-N9	6.67	130.00	126.00
51	9	1453	C	C6-N1-C1'	-6.66	112.81	120.80
51	9	1363	C	C2-N1-C1'	6.66	126.12	118.80
51	9	600	G	O5'-P-OP2	-6.65	99.72	105.70
1	5	115	C	C2-N1-C1'	6.65	126.11	118.80
51	9	980	A	C6-N1-C2	-6.65	114.61	118.60
1	5	112	C	C6-N1-C2	-6.64	117.64	120.30
51	9	1286	G	N1-C2-N3	-6.64	119.91	123.90
1	5	14	C	C5-C6-N1	6.64	124.32	121.00
51	9	1111	U	N3-C2-O2	-6.64	117.55	122.20
1	5	1429	C	C5-C6-N1	6.64	124.32	121.00
51	9	1271	C	N3-C2-O2	-6.63	117.26	121.90
1	5	1777	C	C2-N1-C1'	6.62	126.08	118.80
51	9	340	C	N1-C2-O2	6.62	122.87	118.90
1	5	2638	G	N3-C4-N9	-6.61	122.03	126.00
51	9	823	U	C2-N1-C1'	6.60	125.62	117.70
1	5	112	C	N1-C2-O2	6.60	122.86	118.90
52	AA	44	ASP	CB-CG-OD1	6.60	124.24	118.30
1	5	4925	U	OP2-P-O3'	6.59	119.70	105.20
1	5	4065	G	P-O3'-C3'	6.58	127.60	119.70
51	9	630	U	C6-N1-C1'	-6.57	112.00	121.20
51	9	1485	U	N3-C2-O2	-6.57	117.60	122.20
1	5	48	G	P-O3'-C3'	6.55	127.57	119.70
51	9	151	C	C2-N1-C1'	6.55	126.00	118.80
51	9	130	G	N3-C4-N9	6.54	129.92	126.00
1	5	217	C	C2-N1-C1'	6.53	125.98	118.80
1	5	2860	C	N1-C2-O2	6.52	122.81	118.90
1	5	4880	C	C6-N1-C1'	-6.52	112.97	120.80
1	5	3788	C	C2-N1-C1'	6.52	125.97	118.80
1	5	2505	C	C5-C6-N1	6.52	124.26	121.00
1	5	282	C	N1-C2-O2	6.51	122.81	118.90
1	5	4423	U	N3-C2-O2	-6.51	117.64	122.20
51	9	814	U	N3-C2-O2	-6.48	117.67	122.20
1	5	4360	U	N1-C2-O2	6.47	127.33	122.80
1	5	2528	G	N3-C4-C5	-6.47	125.37	128.60
1	5	4871	C	N3-C2-O2	-6.46	117.38	121.90
57	FF	88	MET	CG-SD-CE	-6.46	89.86	100.20
1	5	1484	G	C8-N9-C1'	-6.46	118.60	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	4869	U	C2-N1-C1'	6.46	125.45	117.70
51	9	1551	U	C2-N1-C1'	6.46	125.45	117.70
1	5	2627	C	C2-N1-C1'	6.45	125.90	118.80
1	5	1514	U	N1-C2-O2	6.45	127.31	122.80
1	5	2410	C	C5-C6-N1	6.45	124.22	121.00
51	9	752	G	P-O3'-C3'	6.45	127.44	119.70
51	9	1535	U	C6-N1-C1'	-6.45	112.17	121.20
1	5	1215	C	N1-C2-O2	6.45	122.77	118.90
51	9	1303	C	N3-C2-O2	-6.45	117.39	121.90
51	9	659	G	C4-N9-C1'	6.44	134.88	126.50
51	9	119	U	N1-C2-O2	6.44	127.31	122.80
51	9	453	C	C2-N1-C1'	6.43	125.88	118.80
1	5	1236	C	C5-C6-N1	6.43	124.22	121.00
51	9	1520	G	N3-C4-N9	6.43	129.86	126.00
1	5	4041	C	C2-N1-C1'	6.43	125.87	118.80
1	5	4871	C	C6-N1-C2	-6.42	117.73	120.30
51	9	914	U	C2-N3-C4	-6.42	123.15	127.00
1	5	1072	C	P-O3'-C3'	6.42	127.40	119.70
1	5	3904	G	P-O3'-C3'	6.42	127.40	119.70
51	9	1161	U	N3-C2-O2	-6.41	117.71	122.20
1	5	1514	U	C2-N1-C1'	6.41	125.39	117.70
1	5	4119	C	N3-C2-O2	-6.40	117.42	121.90
51	9	1564	C	C2-N1-C1'	6.40	125.83	118.80
1	5	4258	C	C5-C6-N1	6.39	124.19	121.00
1	5	2772	C	C2-N1-C1'	6.38	125.82	118.80
51	9	1261	C	C2-N1-C1'	6.38	125.82	118.80
1	5	2474	G	OP1-P-O3'	6.38	119.23	105.20
51	9	613	G	N7-C8-N9	-6.37	109.91	113.10
1	5	2532	C	C2-N1-C1'	6.37	125.81	118.80
51	9	853	C	C6-N1-C1'	-6.37	113.16	120.80
51	9	1271	C	C6-N1-C2	-6.37	117.75	120.30
1	5	521	C	N1-C2-O2	6.35	122.71	118.90
45	r	17	LEU	CA-CB-CG	6.34	129.89	115.30
51	9	1057	C	N1-C2-O2	6.34	122.70	118.90
51	9	183	G	C8-N9-C4	-6.33	103.87	106.40
1	5	4413	C	N1-C2-O2	6.33	122.70	118.90
51	9	1649	U	N1-C2-O2	6.33	127.23	122.80
1	5	691	C	C6-N1-C2	-6.32	117.77	120.30
1	5	4560	C	N1-C2-O2	6.32	122.69	118.90
1	5	1325	C	N1-C2-O2	6.32	122.69	118.90
1	5	2362	U	N3-C2-O2	-6.32	117.78	122.20
51	9	1111	U	N1-C2-O2	6.32	127.22	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	4423	U	N1-C2-O2	6.31	127.22	122.80
1	5	4254	G	N3-C4-N9	6.31	129.79	126.00
51	9	1591	C	N3-C2-O2	-6.31	117.48	121.90
51	9	1660	C	C2-N1-C1'	6.31	125.74	118.80
51	9	1139	C	C6-N1-C2	-6.30	117.78	120.30
51	9	556	U	O5'-P-OP2	-6.28	100.05	105.70
1	5	1656	U	N3-C2-O2	-6.27	117.81	122.20
1	5	2667	C	N1-C2-O2	6.26	122.66	118.90
1	5	691	C	C5-C6-N1	6.26	124.13	121.00
51	9	1060	A	O4'-C1'-N9	6.25	113.20	108.20
1	5	1084	C	C6-N1-C2	-6.25	117.80	120.30
1	5	3693	U	N1-C2-O2	6.25	127.17	122.80
1	5	1502	G	N3-C4-N9	-6.24	122.26	126.00
1	5	2351	C	C6-N1-C2	-6.24	117.81	120.30
2	7	29	C	C6-N1-C1'	-6.24	113.32	120.80
51	9	1453	C	C5-C6-N1	6.23	124.12	121.00
1	5	2281	U	N3-C2-O2	-6.23	117.84	122.20
1	5	2772	C	C6-N1-C2	-6.23	117.81	120.30
51	9	570	C	C2-N1-C1'	6.23	125.65	118.80
1	5	639	U	N1-C2-O2	6.22	127.16	122.80
1	5	2362	U	N1-C2-O2	6.22	127.16	122.80
51	9	579	C	N1-C2-O2	6.22	122.63	118.90
1	5	2528	G	C8-N9-C1'	-6.21	118.92	127.00
1	5	4254	G	P-O3'-C3'	6.21	127.16	119.70
3	8	4	C	C5-C6-N1	6.21	124.11	121.00
51	9	983	A	N3-C4-N9	6.21	132.37	127.40
1	5	1639	U	N1-C2-O2	6.20	127.14	122.80
1	5	1607	C	N3-C2-O2	-6.19	117.57	121.90
51	9	599	A	N9-C4-C5	6.19	108.28	105.80
1	5	233	U	C2-N1-C1'	6.19	125.12	117.70
1	5	4906	C	C2-N1-C1'	6.18	125.60	118.80
1	5	1639	U	N3-C2-O2	-6.18	117.88	122.20
51	9	1123	C	C6-N1-C2	-6.18	117.83	120.30
1	5	691	C	N1-C2-O2	6.17	122.61	118.90
1	5	1082	C	C2-N1-C1'	6.17	125.59	118.80
1	5	4266	G	C8-N9-C1'	-6.17	118.98	127.00
51	9	93	U	N3-C2-O2	-6.17	117.88	122.20
51	9	632	C	N1-C2-N3	-6.16	114.89	119.20
1	5	1325	C	N3-C2-O2	-6.16	117.59	121.90
1	5	4413	C	C2-N1-C1'	6.16	125.58	118.80
1	5	1978	C	C6-N1-C1'	-6.16	113.41	120.80
51	9	814	U	N1-C2-O2	6.16	127.11	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	4399	U	N3-C2-O2	-6.16	117.89	122.20
1	5	1686	C	C6-N1-C2	-6.15	117.84	120.30
51	9	610	G	C4-C5-N7	6.15	113.26	110.80
1	5	2020	U	N3-C2-O2	-6.15	117.90	122.20
2	7	67	C	C6-N1-C2	-6.14	117.84	120.30
51	9	605	A	N7-C8-N9	6.14	116.87	113.80
1	5	1514	U	N3-C2-O2	-6.13	117.91	122.20
1	5	1893	C	C5-C6-N1	6.13	124.07	121.00
1	5	1807	C	N1-C2-O2	6.13	122.58	118.90
51	9	606	G	N9-C4-C5	-6.13	102.95	105.40
51	9	317	C	C2-N1-C1'	6.12	125.54	118.80
1	5	1978	C	C6-N1-C2	-6.12	117.85	120.30
51	9	494	C	N3-C2-O2	-6.12	117.62	121.90
1	5	2362	U	C2-N1-C1'	6.12	125.04	117.70
1	5	4859	C	N1-C2-O2	6.10	122.56	118.90
3	8	35	C	C6-N1-C2	-6.10	117.86	120.30
1	5	4662	C	C6-N1-C2	-6.10	117.86	120.30
1	5	2020	U	N1-C2-O2	6.10	127.07	122.80
2	7	102	U	N1-C2-O2	6.10	127.07	122.80
1	5	4303	C	C2-N1-C1'	6.09	125.50	118.80
1	5	975	C	C6-N1-C2	-6.08	117.87	120.30
51	9	1453	C	C6-N1-C2	-6.08	117.87	120.30
1	5	234	G	O4'-C1'-N9	6.08	113.06	108.20
1	5	1210	C	N1-C2-O2	6.08	122.55	118.90
51	9	1172	U	N1-C2-O2	6.08	127.05	122.80
1	5	684	G	OP2-P-O3'	6.07	118.56	105.20
1	5	1485	C	N1-C2-O2	6.07	122.54	118.90
1	5	1081	C	C2-N1-C1'	6.07	125.48	118.80
1	5	3657	U	C2-N1-C1'	6.07	124.99	117.70
1	5	406	C	P-O3'-C3'	6.07	126.98	119.70
1	5	4051	C	C6-N1-C2	-6.07	117.87	120.30
51	9	635	G	C5-C6-O6	-6.07	124.96	128.60
1	5	2470	C	N1-C2-O2	6.07	122.54	118.90
51	9	1637	A	P-O3'-C3'	6.06	126.98	119.70
1	5	3739	C	N1-C2-O2	6.06	122.54	118.90
51	9	1118	C	C6-N1-C2	-6.06	117.88	120.30
51	9	634	A	N1-C6-N6	-6.06	114.96	118.60
1	5	4759	C	C6-N1-C2	-6.06	117.88	120.30
51	9	1389	C	C5-C6-N1	6.05	124.03	121.00
1	5	639	U	N3-C2-O2	-6.05	117.97	122.20
51	9	551	U	C5-C6-N1	6.04	125.72	122.70
51	9	1389	C	C6-N1-C2	-6.04	117.88	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	640	C	N1-C2-O2	6.04	122.52	118.90
51	9	407	G	C8-N9-C1'	-6.04	119.15	127.00
1	5	1081	C	N1-C2-O2	6.03	122.52	118.90
1	5	4653	C	C6-N1-C2	-6.03	117.89	120.30
51	9	666	U	C5-C6-N1	6.02	125.71	122.70
51	9	1599	U	N3-C2-O2	-6.02	117.98	122.20
1	5	4887	C	N1-C2-O2	6.02	122.51	118.90
51	9	898	U	N1-C2-O2	6.01	127.01	122.80
1	5	112	C	C6-N1-C1'	-6.01	113.59	120.80
51	9	151	C	N1-C2-O2	6.00	122.50	118.90
1	5	1429	C	C6-N1-C2	-6.00	117.90	120.30
1	5	4471	U	N3-C2-O2	-6.00	118.00	122.20
1	5	1210	C	C2-N1-C1'	6.00	125.40	118.80
1	5	1607	C	N1-C2-O2	6.00	122.50	118.90
1	5	3693	U	N3-C2-O2	-5.99	118.01	122.20
1	5	4719	G	OP1-P-O3'	5.99	118.38	105.20
51	9	599	A	N3-C4-N9	5.99	132.19	127.40
51	9	610	G	N7-C8-N9	5.98	116.09	113.10
1	5	3775	A	N7-C8-N9	5.98	116.79	113.80
51	9	914	U	O4'-C1'-N1	5.98	112.98	108.20
1	5	77	U	N1-C2-O2	5.98	126.98	122.80
1	5	1485	C	C2-N1-C1'	5.97	125.37	118.80
1	5	2772	C	C5-C6-N1	5.97	123.99	121.00
1	5	1607	C	C6-N1-C2	-5.97	117.91	120.30
51	9	1298	G	C8-N9-C1'	-5.96	119.25	127.00
1	5	115	C	N3-C2-O2	-5.96	117.73	121.90
1	5	1639	U	C6-N1-C1'	-5.96	112.86	121.20
51	9	637	U	C6-N1-C2	-5.95	117.43	121.00
1	5	220	C	N3-C2-O2	-5.95	117.73	121.90
51	9	659	G	C8-N9-C1'	-5.95	119.26	127.00
51	9	1362	U	N3-C2-O2	-5.95	118.03	122.20
1	5	4051	C	C2-N1-C1'	5.95	125.34	118.80
51	9	1535	U	C5-C6-N1	5.95	125.67	122.70
1	5	323	C	C6-N1-C2	-5.95	117.92	120.30
1	5	4712	C	C6-N1-C2	-5.94	117.92	120.30
51	9	130	G	C8-N9-C1'	-5.94	119.27	127.00
1	5	1215	C	C2-N1-C1'	5.94	125.33	118.80
1	5	112	C	C5-C6-N1	5.94	123.97	121.00
1	5	4766	C	C2-N1-C1'	5.94	125.33	118.80
1	5	3767	C	C5-C6-N1	5.94	123.97	121.00
1	5	195	C	C6-N1-C2	-5.93	117.93	120.30
66	OO	119	LEU	CA-CB-CG	5.93	128.95	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	1084	C	C5-C6-N1	5.93	123.97	121.00
1	5	1656	U	N1-C2-O2	5.93	126.95	122.80
51	9	1304	U	N1-C2-O2	5.93	126.95	122.80
1	5	1686	C	N3-C2-O2	-5.93	117.75	121.90
1	5	100	C	C6-N1-C2	-5.93	117.93	120.30
1	5	1481	C	N1-C2-O2	5.93	122.46	118.90
51	9	1364	U	N3-C2-O2	-5.93	118.05	122.20
51	9	1298	G	C4-N9-C1'	5.93	134.20	126.50
51	9	4	C	C6-N1-C2	-5.92	117.93	120.30
1	5	1276	C	C6-N1-C2	-5.92	117.93	120.30
51	9	612	U	C6-N1-C2	-5.92	117.45	121.00
1	5	1612	G	N3-C4-C5	-5.92	125.64	128.60
1	5	294	G	N3-C4-N9	5.91	129.55	126.00
51	9	55	U	C2-N1-C1'	5.91	124.79	117.70
51	9	1590	C	N1-C2-O2	5.91	122.45	118.90
1	5	4206	C	C6-N1-C2	-5.91	117.94	120.30
1	5	1248	C	N3-C2-O2	-5.90	117.77	121.90
1	5	4162	C	N3-C2-O2	-5.90	117.77	121.90
51	9	191	A	OP1-P-O3'	5.90	118.17	105.20
1	5	2089	G	P-O3'-C3'	5.90	126.78	119.70
49	v	851	LEU	CA-CB-CG	5.89	128.85	115.30
51	9	853	C	C6-N1-C2	-5.89	117.94	120.30
1	5	4051	C	C5-C6-N1	5.89	123.94	121.00
51	9	930	C	C2-N1-C1'	5.89	125.28	118.80
48	u	117	ILE	CG1-CB-CG2	-5.89	98.45	111.40
1	5	133	C	C2-N1-C1'	5.88	125.27	118.80
1	5	1882	U	N3-C4-O4	5.88	123.51	119.40
1	5	4232	U	P-O3'-C3'	5.87	126.74	119.70
1	5	1929	A	C4-N9-C1'	5.86	136.85	126.30
1	5	3954	A	P-O3'-C3'	5.86	126.73	119.70
1	5	41	C	C5-C6-N1	5.86	123.93	121.00
51	9	973	C	N3-C2-O2	-5.86	117.80	121.90
1	5	133	C	N3-C2-O2	-5.86	117.80	121.90
51	9	183	G	C4-N9-C1'	5.85	134.11	126.50
1	5	4928	C	C6-N1-C2	-5.85	117.96	120.30
1	5	4051	C	N3-C2-O2	-5.85	117.81	121.90
51	9	980	A	C5-C6-N1	5.85	120.62	117.70
3	8	99	U	C2-N1-C1'	5.84	124.71	117.70
1	5	2474	G	P-O3'-C3'	5.84	126.71	119.70
51	9	407	G	C2-N3-C4	5.84	114.82	111.90
51	9	608	C	C4-C5-C6	5.84	120.32	117.40
1	5	941	C	C6-N1-C2	-5.84	117.97	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	4206	C	C2-N1-C1'	5.83	125.22	118.80
51	9	1360	U	N3-C2-O2	-5.83	118.12	122.20
1	5	672	C	C2-N1-C1'	5.83	125.21	118.80
1	5	4560	C	C6-N1-C2	-5.83	117.97	120.30
1	5	3975	C	C6-N1-C2	-5.82	117.97	120.30
1	5	390	C	C6-N1-C2	-5.82	117.97	120.30
1	5	3926	C	C6-N1-C2	-5.82	117.97	120.30
1	5	4041	C	C5-C6-N1	5.82	123.91	121.00
1	5	4399	U	N1-C2-O2	5.82	126.87	122.80
1	5	5016	A	C5-N7-C8	-5.82	100.99	103.90
51	9	174	C	N1-C2-O2	5.82	122.39	118.90
1	5	1893	C	C6-N1-C2	-5.81	117.98	120.30
1	5	2860	C	N3-C2-O2	-5.81	117.83	121.90
51	9	870	A	P-O3'-C3'	5.81	126.67	119.70
51	9	1253	A	P-O3'-C3'	5.80	126.66	119.70
1	5	1440	U	P-O3'-C3'	5.80	126.66	119.70
1	5	4682	U	N3-C2-O2	-5.80	118.14	122.20
51	9	610	G	C6-C5-N7	-5.80	126.92	130.40
1	5	1484	G	C6-C5-N7	-5.80	126.92	130.40
1	5	2266	C	P-O3'-C3'	5.79	126.65	119.70
1	5	1289	C	C6-N1-C2	-5.79	117.98	120.30
1	5	4562	C	C6-N1-C2	-5.79	117.98	120.30
49	v	320	ASP	CB-CG-OD1	5.79	123.51	118.30
5	B	309	LEU	CA-CB-CG	5.79	128.62	115.30
51	9	1298	G	N3-C4-C5	-5.79	125.71	128.60
51	9	1389	C	N1-C2-O2	5.78	122.37	118.90
1	5	1777	C	N1-C2-O2	5.78	122.37	118.90
51	9	687	C	N1-C2-O2	5.78	122.37	118.90
51	9	1123	C	N1-C2-O2	5.78	122.37	118.90
51	9	1649	U	N3-C2-O2	-5.78	118.16	122.20
1	5	4682	U	N1-C2-O2	5.78	126.84	122.80
51	9	1259	A	C2-N3-C4	5.78	113.49	110.60
1	5	1828	C	C6-N1-C2	-5.77	117.99	120.30
1	5	1990	A	P-O3'-C3'	5.77	126.62	119.70
1	5	1481	C	C2-N1-C1'	5.77	125.14	118.80
1	5	1731	C	C2-N1-C1'	5.77	125.14	118.80
1	5	4112	C	N1-C2-O2	5.77	122.36	118.90
51	9	610	G	N3-C4-N9	5.77	129.46	126.00
1	5	1804	A	P-O3'-C3'	5.76	126.62	119.70
51	9	1161	U	N1-C2-O2	5.76	126.83	122.80
51	9	124	U	C2-N1-C1'	5.76	124.61	117.70
55	DD	110	LEU	CA-CB-CG	5.76	128.54	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	2410	C	C6-N1-C2	-5.75	118.00	120.30
1	5	4476	C	N3-C2-O2	-5.75	117.87	121.90
51	9	1485	U	C6-N1-C2	-5.75	117.55	121.00
1	5	4942	C	C2-N1-C1'	5.75	125.12	118.80
51	9	1412	C	N1-C2-O2	5.75	122.35	118.90
3	8	124	U	P-O3'-C3'	5.74	126.59	119.70
51	9	182	C	P-O3'-C3'	5.74	126.59	119.70
1	5	4758	U	C2-N1-C1'	5.74	124.58	117.70
24	V	49	LEU	CA-CB-CG	5.73	128.48	115.30
51	9	1518	C	C2-N1-C1'	5.73	125.10	118.80
51	9	958	G	O4'-C1'-N9	5.72	112.78	108.20
1	5	1440	U	N1-C2-O2	5.72	126.81	122.80
1	5	134	G	P-O3'-C3'	5.72	126.56	119.70
1	5	492	U	P-O3'-C3'	5.71	126.56	119.70
51	9	1262	C	N1-C2-O2	5.71	122.33	118.90
13	J	40	LEU	CA-CB-CG	5.71	128.43	115.30
51	9	1520	G	N7-C8-N9	5.71	115.95	113.10
51	9	585	C	N1-C2-O2	5.71	122.32	118.90
1	5	1352	C	C6-N1-C2	-5.71	118.02	120.30
51	9	1130	G	O4'-C1'-N9	5.71	112.76	108.20
51	9	1284	A	C5-C6-N6	-5.70	119.14	123.70
1	5	4233	A	O5'-P-OP1	-5.70	100.57	105.70
1	5	3911	C	C5-C6-N1	5.70	123.85	121.00
1	5	1340	C	C6-N1-C2	-5.69	118.02	120.30
1	5	4653	C	C5-C6-N1	5.69	123.84	121.00
51	9	1364	U	O4'-C1'-N1	5.69	112.75	108.20
1	5	1370	G	P-O3'-C3'	5.68	126.52	119.70
51	9	1271	C	C5-C6-N1	5.68	123.84	121.00
1	5	4926	C	C2-N1-C1'	5.68	125.05	118.80
1	5	4119	C	C6-N1-C2	-5.67	118.03	120.30
1	5	1639	U	C5-C6-N1	5.67	125.53	122.70
1	5	2351	C	C5-C6-N1	5.67	123.83	121.00
51	9	409	C	C6-N1-C2	-5.67	118.03	120.30
1	5	1193	C	N1-C2-O2	5.67	122.30	118.90
1	5	4413	C	N3-C2-O2	-5.67	117.93	121.90
51	9	1753	C	C6-N1-C2	-5.66	118.03	120.30
1	5	4752	U	N3-C2-O2	-5.66	118.24	122.20
1	5	1339	U	C2-N1-C1'	5.66	124.49	117.70
51	9	1139	C	C6-N1-C1'	-5.66	114.01	120.80
51	9	1331	C	N1-C2-O2	5.66	122.29	118.90
51	9	356	C	N1-C2-O2	5.66	122.29	118.90
51	9	1303	C	O4'-C1'-N1	5.66	112.72	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	9	1599	U	N1-C2-O2	5.65	126.76	122.80
1	5	2547	G	O5'-P-OP1	-5.65	100.62	105.70
49	v	39	LEU	CA-CB-CG	5.64	128.28	115.30
51	9	1636	G	C4-N9-C1'	5.64	133.84	126.50
1	5	133	C	C6-N1-C2	-5.64	118.04	120.30
51	9	1123	C	C5-C6-N1	5.64	123.82	121.00
1	5	49	U	N1-C2-O2	5.64	126.75	122.80
1	5	2820	C	N1-C2-O2	5.64	122.28	118.90
51	9	1397	U	N1-C2-O2	5.64	126.75	122.80
1	5	672	C	N3-C2-O2	-5.63	117.96	121.90
51	9	898	U	C2-N1-C1'	5.63	124.45	117.70
51	9	1120	U	C2-N1-C1'	5.62	124.45	117.70
1	5	941	C	C5-C6-N1	5.62	123.81	121.00
1	5	1853	G	C4-N9-C1'	5.62	133.80	126.50
51	9	1649	U	C2-N1-C1'	5.62	124.44	117.70
51	9	1707	U	N1-C2-O2	5.62	126.73	122.80
1	5	2694	G	C4-C5-N7	5.62	113.05	110.80
1	5	4119	C	C5-C6-N1	5.61	123.81	121.00
51	9	898	U	N3-C2-O2	-5.61	118.27	122.20
51	9	887	U	C2-N1-C1'	5.61	124.43	117.70
1	5	2281	U	C2-N1-C1'	5.61	124.43	117.70
51	9	409	C	C5-C6-N1	5.61	123.80	121.00
1	5	2716	C	C2-N1-C1'	5.60	124.96	118.80
1	5	4695	C	N1-C2-O2	5.60	122.26	118.90
1	5	4948	C	N1-C2-O2	5.60	122.26	118.90
1	5	640	C	C6-N1-C2	-5.60	118.06	120.30
51	9	1304	U	N3-C2-O2	-5.60	118.28	122.20
1	5	1915	C	N1-C2-O2	5.60	122.26	118.90
51	9	1412	C	C2-N1-C1'	5.59	124.95	118.80
1	5	1633	G	P-O3'-C3'	5.59	126.41	119.70
51	9	1310	U	N1-C2-O2	5.59	126.72	122.80
1	5	217	C	P-O3'-C3'	5.59	126.41	119.70
1	5	1193	C	C6-N1-C2	-5.59	118.06	120.30
1	5	2560	C	C2-N1-C1'	5.59	124.95	118.80
3	8	128	C	C2-N1-C1'	5.59	124.95	118.80
1	5	3760	A	P-O3'-C3'	5.59	126.41	119.70
1	5	4948	C	N3-C2-O2	-5.59	117.99	121.90
1	5	1978	C	C5-C6-N1	5.59	123.79	121.00
51	9	1364	U	N1-C2-O2	5.59	126.71	122.80
1	5	2856	C	N1-C2-O2	5.58	122.25	118.90
51	9	610	G	N1-C6-O6	5.57	123.24	119.90
1	5	1477	C	C2-N1-C1'	5.57	124.92	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	9	872	A	C5-C6-N1	5.57	120.48	117.70
51	9	87	U	N3-C2-O2	-5.57	118.31	122.20
1	5	282	C	N3-C2-O2	-5.56	118.01	121.90
1	5	3775	A	O4'-C1'-N9	5.56	112.64	108.20
1	5	3927	U	N3-C2-O2	-5.56	118.31	122.20
1	5	3974	G	N3-C4-C5	-5.56	125.82	128.60
1	5	2704	C	N1-C2-O2	5.55	122.23	118.90
3	8	142	U	C5-C6-N1	5.55	125.47	122.70
1	5	1686	C	N1-C2-O2	5.54	122.23	118.90
62	KK	35	LEU	CA-CB-CG	5.54	128.05	115.30
51	9	293	C	C6-N1-C2	-5.54	118.08	120.30
51	9	638	C	N3-C2-O2	-5.54	118.02	121.90
1	5	1812	C	N1-C2-O2	5.54	122.22	118.90
51	9	823	U	N1-C2-O2	5.54	126.68	122.80
1	5	4162	C	C2-N1-C1'	5.54	124.89	118.80
51	9	1016	U	C2-N1-C1'	5.54	124.34	117.70
1	5	975	C	C5-C6-N1	5.53	123.77	121.00
1	5	1578	U	N3-C2-O2	-5.53	118.33	122.20
51	9	465	A	P-O3'-C3'	5.53	126.34	119.70
1	5	1446	C	C2-N1-C1'	5.53	124.88	118.80
1	5	2570	U	N1-C2-O2	5.53	126.67	122.80
1	5	4162	C	N1-C2-O2	5.53	122.22	118.90
51	9	530	U	C2-N1-C1'	5.53	124.33	117.70
1	5	4215	C	C6-N1-C2	-5.53	118.09	120.30
1	5	4398	C	N1-C2-O2	5.53	122.22	118.90
1	5	3882	C	C2-N1-C1'	5.53	124.88	118.80
1	5	3636	C	C6-N1-C2	-5.52	118.09	120.30
1	5	2325	C	N3-C2-O2	-5.52	118.04	121.90
1	5	118	C	C2-N1-C1'	5.52	124.87	118.80
51	9	958	G	C4-N9-C1'	5.52	133.67	126.50
51	9	1363	C	P-O3'-C3'	5.52	126.32	119.70
1	5	1726	U	N3-C2-O2	-5.52	118.34	122.20
51	9	610	G	N3-C2-N2	-5.52	116.04	119.90
3	8	90	C	C2-N1-C1'	5.51	124.87	118.80
1	5	1211	G	P-O3'-C3'	5.51	126.32	119.70
51	9	1840	U	C5-C6-N1	5.51	125.46	122.70
1	5	3840	U	N3-C2-O2	-5.51	118.34	122.20
1	5	5016	A	N7-C8-N9	5.51	116.56	113.80
51	9	1574	C	N1-C2-O2	5.51	122.20	118.90
1	5	3870	C	C5-C6-N1	5.51	123.75	121.00
51	9	140	U	C2-N1-C1'	5.50	124.30	117.70
1	5	1082	C	N1-C2-O2	5.50	122.20	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	1966	C	C6-N1-C2	-5.49	118.10	120.30
1	5	2478	C	N1-C2-O2	5.49	122.19	118.90
1	5	3622	C	C6-N1-C2	-5.49	118.10	120.30
51	9	1707	U	N3-C2-O2	-5.49	118.36	122.20
1	5	4133	C	C2-N1-C1'	5.49	124.84	118.80
1	5	719	C	C2-N1-C1'	5.49	124.84	118.80
51	9	1123	C	C2-N1-C1'	5.48	124.83	118.80
1	5	640	C	N3-C2-O2	-5.48	118.06	121.90
57	FF	19	LEU	CA-CB-CG	5.48	127.91	115.30
1	5	2704	C	C5-C6-N1	5.48	123.74	121.00
1	5	1990	A	OP1-P-O3'	5.48	117.25	105.20
1	5	2502	A	OP1-P-O3'	5.48	117.25	105.20
51	9	494	C	C2-N1-C1'	5.48	124.82	118.80
1	5	641	G	C5-C6-O6	5.47	131.88	128.60
1	5	1834	U	C2-N1-C1'	5.47	124.27	117.70
1	5	3767	C	C6-N1-C2	-5.47	118.11	120.30
1	5	1429	C	C6-N1-C1'	-5.47	114.23	120.80
1	5	4502	C	N3-C2-O2	-5.47	118.07	121.90
3	8	21	C	N1-C2-O2	5.47	122.18	118.90
51	9	1304	U	C2-N1-C1'	5.47	124.26	117.70
2	7	29	C	C5-C6-N1	5.47	123.73	121.00
1	5	1440	U	N3-C2-O2	-5.46	118.38	122.20
51	9	973	C	C2-N1-C1'	5.46	124.81	118.80
51	9	4	C	C2-N1-C1'	5.46	124.80	118.80
1	5	1248	C	C2-N1-C1'	5.46	124.80	118.80
2	7	44	C	N1-C2-O2	5.45	122.17	118.90
1	5	4758	U	N1-C2-O2	5.45	126.61	122.80
51	9	1753	C	C2-N1-C1'	5.45	124.80	118.80
1	5	1179	U	C2-N1-C1'	5.45	124.24	117.70
1	5	469	C	N1-C2-O2	5.44	122.17	118.90
1	5	1406(B)	C	C6-N1-C2	-5.44	118.12	120.30
1	5	4756	C	C5-C6-N1	5.44	123.72	121.00
2	7	102	U	N3-C2-O2	-5.44	118.39	122.20
3	8	64	U	N1-C2-O2	5.44	126.61	122.80
51	9	1462	U	C5-C6-N1	5.44	125.42	122.70
1	5	294	G	N3-C4-C5	-5.44	125.88	128.60
1	5	472	C	N1-C2-O2	5.44	122.16	118.90
1	5	3657	U	N3-C2-O2	-5.44	118.39	122.20
1	5	1847	C	C2-N1-C1'	5.43	124.78	118.80
1	5	1079	C	C6-N1-C1'	-5.43	114.28	120.80
1	5	3888	G	P-O3'-C3'	5.43	126.21	119.70
1	5	4215	C	N1-C2-O2	5.43	122.16	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	1292	C	C2-N1-C1'	5.43	124.77	118.80
1	5	4906	C	N1-C2-O2	5.43	122.16	118.90
51	9	613	G	N9-C4-C5	-5.42	103.23	105.40
1	5	1309	C	C5-C6-N1	5.42	123.71	121.00
1	5	1735	U	N1-C2-O2	5.42	126.60	122.80
1	5	1807	C	C6-N1-C1'	-5.42	114.29	120.80
1	5	100	C	O4'-C1'-N1	5.42	112.54	108.20
1	5	245	C	P-O3'-C3'	5.42	126.20	119.70
51	9	663	C	C5-C6-N1	5.42	123.71	121.00
1	5	5008	C	N1-C2-O2	5.41	122.15	118.90
51	9	634	A	C4-C5-N7	5.41	113.41	110.70
1	5	332	C	C5-C6-N1	5.41	123.70	121.00
1	5	1994	C	N3-C2-O2	-5.41	118.11	121.90
1	5	4502	C	C6-N1-C2	-5.41	118.14	120.30
1	5	4758	U	N3-C2-O2	-5.41	118.41	122.20
1	5	1735	U	C5-C6-N1	5.41	125.40	122.70
1	5	2638	G	N3-C2-N2	-5.41	116.11	119.90
1	5	2560	C	N1-C2-O2	5.41	122.14	118.90
10	G	199	LEU	CA-CB-CG	5.41	127.73	115.30
1	5	1847	C	C5-C6-N1	5.40	123.70	121.00
1	5	4476	C	N1-C2-O2	5.40	122.14	118.90
1	5	4401	G	C4-N9-C1'	5.40	133.52	126.50
1	5	220	C	C5-C6-N1	5.40	123.70	121.00
1	5	2860	C	C6-N1-C2	-5.40	118.14	120.30
51	9	814	U	C2-N1-C1'	5.39	124.17	117.70
1	5	274	C	C2-N1-C1'	5.39	124.73	118.80
1	5	1309	C	C6-N1-C2	-5.39	118.14	120.30
1	5	4114	C	C6-N1-C2	-5.39	118.14	120.30
1	5	4880	C	O4'-C1'-N1	5.39	112.51	108.20
1	5	281	U	N3-C2-O2	-5.39	118.43	122.20
1	5	1406(B)	C	OP1-P-O3'	5.39	117.05	105.20
1	5	4859	C	N3-C2-O2	-5.39	118.13	121.90
1	5	2892	C	C2-N1-C1'	5.38	124.72	118.80
1	5	417	G	O4'-C1'-N9	5.38	112.50	108.20
1	5	1193	C	C5-C6-N1	5.38	123.69	121.00
1	5	2410	C	N1-C2-O2	5.38	122.13	118.90
1	5	3739	C	C2-N1-C1'	5.38	124.72	118.80
1	5	1535	C	C5-C6-N1	5.38	123.69	121.00
51	9	130	G	C2-N3-C4	5.38	114.59	111.90
51	9	453	C	C6-N1-C2	-5.37	118.15	120.30
1	5	2325	C	N1-C2-O2	5.37	122.12	118.90
1	5	3974	G	O4'-C1'-N9	5.36	112.49	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	9	580	U	N3-C2-O2	-5.36	118.45	122.20
51	9	1078	C	C2-N1-C1'	5.36	124.70	118.80
1	5	203	U	C2-N1-C1'	5.36	124.13	117.70
1	5	978	C	C2-N1-C1'	5.36	124.69	118.80
1	5	4893	A	O4'-C1'-N9	5.35	112.48	108.20
20	R	99	MET	CG-SD-CE	-5.35	91.63	100.20
1	5	449	C	P-O3'-C3'	5.35	126.12	119.70
51	9	188	C	C6-N1-C1'	-5.35	114.38	120.80
1	5	3696	C	C2-N1-C1'	5.35	124.68	118.80
1	5	684	G	P-O3'-C3'	5.35	126.12	119.70
1	5	4949	G	O4'-C1'-N9	5.34	112.47	108.20
1	5	486	C	C5-C6-N1	5.34	123.67	121.00
1	5	1079	C	C5-C6-N1	5.34	123.67	121.00
1	5	2704	C	C6-N1-C2	-5.34	118.16	120.30
1	5	4627	U	N3-C2-O2	-5.34	118.46	122.20
49	v	86	LEU	CA-CB-CG	5.34	127.58	115.30
1	5	3778	U	N1-C2-O2	5.34	126.54	122.80
51	9	606	G	N3-C2-N2	5.34	123.64	119.90
1	5	2560	C	C5-C6-N1	5.33	123.67	121.00
1	5	1579	C	C6-N1-C2	-5.33	118.17	120.30
51	9	4	C	C5-C6-N1	5.33	123.67	121.00
51	9	1117	C	C2-N1-C1'	5.33	124.67	118.80
1	5	256	G	C4-N9-C1'	5.33	133.43	126.50
1	5	959	G	P-O3'-C3'	5.33	126.09	119.70
1	5	2405	G	N3-C4-N9	5.33	129.20	126.00
51	9	1286	G	N1-C6-O6	-5.33	116.70	119.90
1	5	3904	G	OP1-P-O3'	5.32	116.91	105.20
2	7	28	C	C6-N1-C2	-5.32	118.17	120.30
2	7	36	C	C6-N1-C2	-5.32	118.17	120.30
1	5	1483	C	N1-C2-O2	5.32	122.09	118.90
3	8	38	U	C2-N1-C1'	5.32	124.08	117.70
51	9	1360	U	N1-C2-O2	5.32	126.52	122.80
57	FF	154	LEU	CA-CB-CG	5.32	127.53	115.30
1	5	4258	C	C6-N1-C2	-5.31	118.17	120.30
1	5	693	C	N1-C2-O2	5.31	122.09	118.90
67	PP	25	LEU	CA-CB-CG	5.31	127.52	115.30
1	5	323	C	C5-C6-N1	5.31	123.65	121.00
51	9	453	C	N1-C2-O2	5.31	122.08	118.90
1	5	2603	C	C5-C6-N1	5.30	123.65	121.00
51	9	943	U	C2-N1-C1'	5.30	124.06	117.70
51	9	1751	C	N3-C2-O2	-5.30	118.19	121.90
1	5	1915	C	C2-N1-C1'	5.30	124.63	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	1957	U	O4'-C1'-N1	5.29	112.43	108.20
1	5	2560	C	C6-N1-C2	-5.29	118.18	120.30
1	5	2532	C	N1-C2-O2	5.29	122.07	118.90
1	5	7	C	C5-C6-N1	5.29	123.64	121.00
51	9	1172	U	N3-C2-O2	-5.29	118.50	122.20
1	5	220	C	C6-N1-C2	-5.28	118.19	120.30
1	5	256	G	N3-C4-N9	5.28	129.17	126.00
1	5	2705	G	C4-N9-C1'	5.28	133.37	126.50
51	9	1022	U	C2-N1-C1'	5.28	124.03	117.70
51	9	1314	U	C2-N1-C1'	5.28	124.03	117.70
1	5	1180	C	N1-C2-O2	5.27	122.06	118.90
3	8	99	U	N1-C2-O2	5.27	126.49	122.80
1	5	1248	C	C6-N1-C2	-5.27	118.19	120.30
1	5	4241	C	C2-N1-C1'	5.27	124.59	118.80
51	9	930	C	N3-C2-O2	-5.26	118.22	121.90
1	5	4766	C	N1-C2-O2	5.26	122.05	118.90
1	5	14	C	C6-N1-C2	-5.25	118.20	120.30
51	9	1489	A	P-O3'-C3'	5.25	126.00	119.70
1	5	2632	U	N1-C2-O2	5.25	126.48	122.80
1	5	1329	G	N7-C8-N9	5.25	115.72	113.10
1	5	1735	U	C2-N1-C1'	5.25	124.00	117.70
1	5	5022	U	N1-C2-O2	5.25	126.47	122.80
51	9	568	C	N1-C2-O2	5.25	122.05	118.90
1	5	1339	U	C6-N1-C2	-5.25	117.85	121.00
51	9	580	U	N1-C2-O2	5.25	126.47	122.80
51	9	1590	C	C6-N1-C2	-5.25	118.20	120.30
1	5	3709	U	C2-N1-C1'	5.24	123.99	117.70
51	9	356	C	C6-N1-C1'	-5.24	114.51	120.80
51	9	1730	U	N3-C2-O2	-5.24	118.53	122.20
1	5	1406(B)	C	P-O3'-C3'	5.24	125.98	119.70
1	5	49	U	N3-C2-O2	-5.23	118.54	122.20
1	5	1485	C	N3-C2-O2	-5.23	118.24	121.90
1	5	1666	C	C6-N1-C2	-5.23	118.21	120.30
1	5	205	C	C6-N1-C2	-5.22	118.21	120.30
1	5	2814	C	C6-N1-C1'	-5.22	114.53	120.80
1	5	4631	G	N3-C4-N9	5.22	129.13	126.00
51	9	1262	C	N3-C2-O2	-5.22	118.24	121.90
1	5	1663	C	C6-N1-C2	-5.22	118.21	120.30
2	7	14	C	C5-C6-N1	5.22	123.61	121.00
51	9	1664	A	OP1-P-O3'	5.22	116.68	105.20
3	8	107	C	C6-N1-C2	-5.22	118.21	120.30
49	v	520	LEU	CA-CB-CG	5.22	127.30	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	41	C	C6-N1-C2	-5.21	118.21	120.30
1	5	294	G	C2-N3-C4	5.21	114.51	111.90
3	8	4	C	C6-N1-C2	-5.21	118.22	120.30
51	9	1242	U	N1-C2-O2	5.21	126.45	122.80
51	9	118	C	N1-C2-O2	5.21	122.03	118.90
65	NN	125	LEU	CB-CG-CD2	-5.21	102.15	111.00
3	8	54	C	N1-C2-O2	5.21	122.02	118.90
51	9	1551	U	N3-C2-O2	-5.21	118.56	122.20
1	5	326	C	C2-N1-C1'	5.21	124.53	118.80
1	5	1483	C	N3-C2-O2	-5.20	118.26	121.90
49	v	823	ASP	CB-CG-OD1	5.20	122.98	118.30
1	5	4406	U	N3-C2-O2	-5.20	118.56	122.20
51	9	752	G	OP1-P-O3'	5.20	116.63	105.20
1	5	639	U	C2-N1-C1'	5.20	123.94	117.70
1	5	704	C	C2-N1-C1'	5.20	124.52	118.80
1	5	3892	U	N3-C2-O2	-5.20	118.56	122.20
51	9	642	U	P-O3'-C3'	5.20	125.93	119.70
51	9	687	C	N3-C2-O2	-5.19	118.27	121.90
51	9	1636	G	N3-C4-C5	-5.19	126.00	128.60
1	5	390	C	C5-C6-N1	5.19	123.59	121.00
1	5	3775	A	C5-N7-C8	-5.19	101.31	103.90
1	5	2701	U	N1-C2-O2	5.19	126.43	122.80
51	9	1684	C	N1-C2-O2	5.19	122.01	118.90
51	9	1073	U	N3-C2-O2	-5.19	118.57	122.20
1	5	2593	C	C6-N1-C2	-5.18	118.23	120.30
1	5	1894	C	C6-N1-C2	-5.18	118.23	120.30
1	5	2726	G	C4-N9-C1'	5.18	133.24	126.50
1	5	4601	U	N3-C2-O2	-5.18	118.57	122.20
1	5	4667	C	N3-C2-O2	-5.18	118.27	121.90
1	5	4699	U	OP1-P-O3'	5.18	116.60	105.20
51	9	606	G	C4-C5-N7	5.18	112.87	110.80
1	5	4508	C	C5-C6-N1	5.17	123.59	121.00
1	5	1502	G	N3-C4-C5	5.17	131.19	128.60
1	5	2716	C	C6-N1-C2	-5.17	118.23	120.30
1	5	1440	U	C5-C6-N1	5.17	125.28	122.70
1	5	2325	C	C6-N1-C2	-5.17	118.23	120.30
51	9	1364	U	C6-N1-C1'	-5.17	113.97	121.20
1	5	717	U	N3-C2-O2	-5.17	118.58	122.20
1	5	1809	C	C2-N1-C1'	5.17	124.48	118.80
51	9	610	G	C4-N9-C1'	5.17	133.22	126.50
1	5	661	C	C2-N1-C1'	5.16	124.48	118.80
1	5	1204	C	N3-C2-O2	-5.16	118.29	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	4627	U	N1-C2-O2	5.16	126.41	122.80
51	9	1636	G	N3-C4-N9	5.16	129.10	126.00
1	5	4561	C	C2-N1-C1'	5.16	124.47	118.80
51	9	579	C	N3-C2-O2	-5.16	118.29	121.90
51	9	663	C	C6-N1-C2	-5.16	118.24	120.30
51	9	1116	C	N1-C2-O2	5.16	122.00	118.90
51	9	946	U	C5-C6-N1	5.16	125.28	122.70
1	5	1467	C	C6-N1-C2	-5.16	118.24	120.30
1	5	3802	U	C2-N1-C1'	5.16	123.89	117.70
51	9	1564	C	C6-N1-C2	-5.16	118.24	120.30
53	BB	34	LYS	C-N-CA	5.15	134.59	121.70
1	5	4928	C	C6-N1-C1'	-5.15	114.62	120.80
1	5	640	C	C2-N1-C1'	5.15	124.47	118.80
49	v	517	LEU	CA-CB-CG	5.15	127.15	115.30
1	5	1084	C	N1-C2-O2	5.15	121.99	118.90
1	5	2089	G	OP2-P-O3'	5.15	116.53	105.20
2	7	28	C	N1-C2-O2	5.15	121.99	118.90
1	5	2838	G	C4-N9-C1'	5.15	133.19	126.50
1	5	4662	C	C5-C6-N1	5.14	123.57	121.00
1	5	4714	C	N1-C2-O2	5.14	121.99	118.90
51	9	610	G	C5-N7-C8	-5.14	101.73	104.30
51	9	1172	U	C2-N1-C1'	5.14	123.87	117.70
1	5	4560	C	C2-N1-C1'	5.14	124.46	118.80
51	9	730	C	C5-C6-N1	5.14	123.57	121.00
1	5	1777	C	C5-C6-N1	5.14	123.57	121.00
1	5	294	G	C4-N9-C1'	5.14	133.18	126.50
1	5	2532	C	C5-C6-N1	5.14	123.57	121.00
2	7	29	C	C6-N1-C2	-5.14	118.25	120.30
1	5	4942	C	N3-C2-O2	-5.13	118.31	121.90
51	9	1310	U	N3-C2-O2	-5.13	118.61	122.20
1	5	469	C	N3-C2-O2	-5.13	118.31	121.90
3	8	153	C	C2-N1-C1'	5.13	124.45	118.80
49	v	287	ARG	CA-CB-CG	5.13	124.69	113.40
1	5	155	C	N3-C2-O2	-5.13	118.31	121.90
1	5	115	C	C6-N1-C1'	-5.12	114.65	120.80
1	5	4341	C	N1-C2-O2	5.12	121.97	118.90
1	5	4948	C	C6-N1-C1'	-5.12	114.65	120.80
51	9	142	C	N1-C2-O2	5.12	121.97	118.90
51	9	1310	U	C2-N1-C1'	5.11	123.84	117.70
1	5	1446	C	C5-C6-N1	5.11	123.56	121.00
51	9	87	U	N1-C2-O2	5.11	126.38	122.80
51	9	1660	C	N1-C2-O2	5.11	121.97	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	8	135	C	C2-N1-C1'	5.11	124.42	118.80
51	9	340	C	N3-C2-O2	-5.11	118.32	121.90
1	5	233	U	C6-N1-C1'	-5.11	114.05	121.20
51	9	1590	C	N3-C2-O2	-5.11	118.33	121.90
51	9	1265	A	N1-C6-N6	5.11	121.66	118.60
51	9	1757	G	N3-C4-C5	-5.11	126.05	128.60
1	5	4448	G	P-O3'-C3'	5.10	125.83	119.70
51	9	151	C	C6-N1-C2	-5.10	118.26	120.30
67	PP	34	MET	CA-CB-CG	5.10	121.98	113.30
1	5	217	C	N3-C2-O2	-5.10	118.33	121.90
1	5	2492	C	C5-C6-N1	5.10	123.55	121.00
1	5	3625	G	P-O3'-C3'	5.10	125.82	119.70
1	5	4557	U	C5-C6-N1	5.09	125.25	122.70
51	9	119	U	C2-N1-C1'	5.09	123.81	117.70
51	9	530	U	N1-C2-O2	5.09	126.36	122.80
1	5	1834	U	N3-C2-O2	-5.09	118.64	122.20
1	5	3876	A	OP2-P-O3'	5.09	116.39	105.20
1	5	2405	G	C6-C5-N7	-5.09	127.35	130.40
1	5	521	C	C6-N1-C2	-5.08	118.27	120.30
1	5	205	C	C5-C6-N1	5.08	123.54	121.00
1	5	1929	A	C2-N3-C4	5.08	113.14	110.60
51	9	598	G	N3-C4-N9	5.08	129.05	126.00
51	9	1303	C	C6-N1-C2	-5.08	118.27	120.30
1	5	1834	U	N1-C2-O2	5.08	126.35	122.80
1	5	2028	C	C6-N1-C1'	-5.07	114.71	120.80
1	5	2503	G	OP1-P-OP2	-5.07	111.99	119.60
51	9	915	G	O4'-C1'-N9	5.07	112.26	108.20
51	9	532	C	P-O3'-C3'	5.07	125.79	119.70
1	5	5050	C	C2-N1-C1'	5.07	124.38	118.80
1	5	3974	G	C4-N9-C1'	5.07	133.09	126.50
3	8	101	C	C2-N1-C1'	5.07	124.38	118.80
51	9	1595	U	N1-C2-O2	5.07	126.35	122.80
51	9	188	C	N3-C2-O2	-5.06	118.36	121.90
1	5	4120	U	C2-N1-C1'	5.06	123.78	117.70
51	9	853	C	O4'-C1'-N1	5.06	112.25	108.20
1	5	1929	A	C8-N9-C1'	-5.06	118.60	127.70
1	5	1179	U	N1-C2-O2	5.05	126.34	122.80
40	l	49	LEU	CA-CB-CG	5.05	126.92	115.30
1	5	47	A	OP1-P-O3'	5.05	116.31	105.20
51	9	1518	C	N1-C2-O2	5.05	121.93	118.90
3	8	99	U	N3-C2-O2	-5.05	118.67	122.20
1	5	2445	C	C6-N1-C2	-5.05	118.28	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	9	453	C	C5-C6-N1	5.05	123.52	121.00
51	9	872	A	C6-N1-C2	-5.04	115.57	118.60
1	5	2638	G	N3-C4-C5	5.04	131.12	128.60
1	5	2820	C	N3-C2-O2	-5.04	118.37	121.90
51	9	1057	C	C6-N1-C1'	-5.04	114.75	120.80
1	5	205	C	N3-C2-O2	-5.04	118.37	121.90
1	5	217	C	OP2-P-O3'	5.04	116.29	105.20
1	5	1827	C	C2-N1-C1'	5.04	124.34	118.80
1	5	1915	C	N3-C2-O2	-5.04	118.38	121.90
49	v	102	LEU	CA-CB-CG	5.04	126.88	115.30
1	5	4924	C	C6-N1-C1'	5.03	126.84	120.80
51	9	387	C	C6-N1-C2	-5.03	118.29	120.30
51	9	803	C	C6-N1-C2	-5.03	118.29	120.30
1	5	2532	C	C6-N1-C2	-5.03	118.29	120.30
1	5	4215	C	N3-C2-O2	-5.03	118.38	121.90
51	9	1592	C	C6-N1-C2	-5.03	118.29	120.30
1	5	472	C	C6-N1-C2	-5.03	118.29	120.30
1	5	1818	G	C4-N9-C1'	5.03	133.03	126.50
1	5	3761	C	N1-C2-O2	5.03	121.92	118.90
1	5	2351	C	C2-N1-C1'	5.02	124.32	118.80
1	5	2627	C	C5-C6-N1	5.02	123.51	121.00
1	5	4254	G	C4-N9-C1'	5.02	133.03	126.50
1	5	1894	C	C5-C6-N1	5.02	123.51	121.00
1	5	3927	U	N1-C2-O2	5.02	126.31	122.80
51	9	606	G	N7-C8-N9	5.02	115.61	113.10
1	5	1276	C	C2-N1-C1'	5.02	124.32	118.80
1	5	1082	C	C6-N1-C2	-5.01	118.29	120.30
51	9	14	C	C6-N1-C2	-5.01	118.30	120.30
1	5	3657	U	N1-C2-O2	5.01	126.31	122.80
51	9	730	C	C2-N1-C1'	5.01	124.31	118.80
1	5	1428	U	N1-C2-O2	5.01	126.31	122.80
1	5	1792	U	C5-C6-N1	5.01	125.20	122.70
1	5	1828	C	C5-C6-N1	5.01	123.50	121.00
51	9	870	A	OP2-P-O3'	5.01	116.22	105.20
51	9	1116	C	C2-N1-C1'	5.01	124.31	118.80
55	DD	215	ASP	CB-CG-OD1	5.01	122.81	118.30
1	5	4689	U	C5-C6-N1	5.01	125.20	122.70
1	5	4926	C	N1-C2-O2	5.01	121.90	118.90
1	5	3622	C	C5-C6-N1	5.00	123.50	121.00
1	5	1455	G	N3-C4-N9	5.00	129.00	126.00
8	E	289	LEU	CA-CB-CG	5.00	126.80	115.30

There are no chirality outliers.

All (34) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
52	AA	43	SER	Peptide
5	B	55	HIS	Peptide
56	EE	155	LYS	Peptide
57	FF	19	LEU	Peptide
57	FF	41	VAL	Peptide
10	G	215	ASP	Peptide
11	H	129	ARG	Peptide
11	H	50	LYS	Peptide
62	KK	38	LYS	Peptide
14	L	46	ILE	Peptide
14	L	62	PRO	Peptide
64	MM	100	PRO	Peptide
64	MM	72	HIS	Peptide
16	N	184	ILE	Peptide
16	N	76	PRO	Peptide
16	N	78	GLY	Peptide
67	PP	17	TYR	Peptide
67	PP	38	SER	Peptide
21	S	165	PRO	Peptide
70	SS	99	LEU	Peptide
73	VV	32	ILE	Peptide
74	WW	54	ASP	Peptide
75	XX	61	GLN	Peptide
77	ZZ	50	PHE	Peptide
32	d	95	ASP	Peptide
84	gg	37	ASP	Peptide
46	s	119	CYS	Peptide
47	t	53	TRP	Peptide
47	t	96	LYS	Peptide
48	u	38	LEU	Peptide
48	u	60	ARG	Peptide
49	v	410	PHE	Peptide
49	v	666	THR	Peptide
49	v	845	LYS	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%)	225 (92%)	21 (8%)	0	100	100
5	B	392/394 (100%)	367 (94%)	25 (6%)	0	100	100
6	C	359/362 (99%)	342 (95%)	17 (5%)	0	100	100
7	D	291/293 (99%)	277 (95%)	14 (5%)	0	100	100
8	E	208/291 (72%)	195 (94%)	13 (6%)	0	100	100
9	F	223/225 (99%)	212 (95%)	11 (5%)	0	100	100
10	G	229/319 (72%)	218 (95%)	11 (5%)	0	100	100
11	H	188/190 (99%)	179 (95%)	9 (5%)	0	100	100
12	I	201/214 (94%)	192 (96%)	9 (4%)	0	100	100
13	J	168/170 (99%)	165 (98%)	3 (2%)	0	100	100
14	L	208/210 (99%)	202 (97%)	6 (3%)	0	100	100
15	M	136/138 (99%)	125 (92%)	11 (8%)	0	100	100
16	N	201/203 (99%)	188 (94%)	13 (6%)	0	100	100
17	O	197/199 (99%)	194 (98%)	3 (2%)	0	100	100
18	P	151/153 (99%)	148 (98%)	3 (2%)	0	100	100
19	Q	185/187 (99%)	176 (95%)	9 (5%)	0	100	100
20	R	178/180 (99%)	174 (98%)	4 (2%)	0	100	100
21	S	174/176 (99%)	165 (95%)	8 (5%)	1 (1%)	25	57
22	T	157/159 (99%)	152 (97%)	5 (3%)	0	100	100
23	U	97/99 (98%)	93 (96%)	4 (4%)	0	100	100
24	V	129/131 (98%)	122 (95%)	7 (5%)	0	100	100
25	W	102/157 (65%)	97 (95%)	5 (5%)	0	100	100
26	X	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
27	Y	132/134 (98%)	128 (97%)	4 (3%)	0	100	100
28	Z	133/135 (98%)	126 (95%)	6 (4%)	1 (1%)	19	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	a	145/147 (99%)	136 (94%)	9 (6%)	0	100	100
30	b	100/245 (41%)	94 (94%)	6 (6%)	0	100	100
31	c	96/98 (98%)	90 (94%)	6 (6%)	0	100	100
32	d	105/107 (98%)	96 (91%)	9 (9%)	0	100	100
33	e	126/128 (98%)	116 (92%)	10 (8%)	0	100	100
34	f	107/109 (98%)	102 (95%)	5 (5%)	0	100	100
35	g	112/114 (98%)	109 (97%)	3 (3%)	0	100	100
36	h	120/122 (98%)	119 (99%)	1 (1%)	0	100	100
37	i	100/102 (98%)	94 (94%)	6 (6%)	0	100	100
38	j	84/86 (98%)	75 (89%)	9 (11%)	0	100	100
39	k	67/69 (97%)	64 (96%)	3 (4%)	0	100	100
40	l	48/50 (96%)	42 (88%)	6 (12%)	0	100	100
41	m	49/52 (94%)	43 (88%)	5 (10%)	1 (2%)	7	32
42	n	23/25 (92%)	23 (100%)	0	0	100	100
43	o	101/103 (98%)	96 (95%)	5 (5%)	0	100	100
44	p	89/91 (98%)	89 (100%)	0	0	100	100
45	r	122/124 (98%)	120 (98%)	2 (2%)	0	100	100
46	s	194/196 (99%)	176 (91%)	18 (9%)	0	100	100
47	t	151/153 (99%)	132 (87%)	18 (12%)	1 (1%)	22	54
48	u	204/206 (99%)	178 (87%)	24 (12%)	2 (1%)	15	46
49	v	834/839 (99%)	754 (90%)	78 (9%)	2 (0%)	47	77
50	w	22/26 (85%)	22 (100%)	0	0	100	100
52	AA	215/217 (99%)	210 (98%)	5 (2%)	0	100	100
53	BB	211/213 (99%)	203 (96%)	8 (4%)	0	100	100
54	CC	219/221 (99%)	212 (97%)	7 (3%)	0	100	100
55	DD	226/228 (99%)	216 (96%)	10 (4%)	0	100	100
56	EE	260/262 (99%)	248 (95%)	12 (5%)	0	100	100
57	FF	181/204 (89%)	165 (91%)	15 (8%)	1 (1%)	25	57
58	GG	235/237 (99%)	230 (98%)	5 (2%)	0	100	100
59	HH	181/194 (93%)	174 (96%)	7 (4%)	0	100	100
60	II	204/206 (99%)	191 (94%)	12 (6%)	1 (0%)	29	61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
61	JJ	183/185 (99%)	180 (98%)	3 (2%)	0	100	100
62	KK	94/96 (98%)	85 (90%)	9 (10%)	0	100	100
63	LL	139/158 (88%)	130 (94%)	9 (6%)	0	100	100
64	MM	115/117 (98%)	104 (90%)	11 (10%)	0	100	100
65	NN	147/149 (99%)	142 (97%)	5 (3%)	0	100	100
66	OO	134/136 (98%)	125 (93%)	9 (7%)	0	100	100
67	PP	118/120 (98%)	111 (94%)	7 (6%)	0	100	100
68	QQ	140/142 (99%)	132 (94%)	8 (6%)	0	100	100
69	RR	130/132 (98%)	126 (97%)	4 (3%)	0	100	100
70	SS	142/144 (99%)	130 (92%)	12 (8%)	0	100	100
71	TT	139/141 (99%)	131 (94%)	8 (6%)	0	100	100
72	UU	98/100 (98%)	93 (95%)	5 (5%)	0	100	100
73	VV	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
74	WW	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
75	XX	139/141 (99%)	133 (96%)	3 (2%)	3 (2%)	6	30
76	YY	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
77	ZZ	73/75 (97%)	70 (96%)	3 (4%)	0	100	100
78	aa	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
79	bb	81/83 (98%)	75 (93%)	6 (7%)	0	100	100
80	cc	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
81	dd	53/55 (96%)	51 (96%)	2 (4%)	0	100	100
82	ee	53/55 (96%)	51 (96%)	2 (4%)	0	100	100
83	ff	66/68 (97%)	59 (89%)	7 (11%)	0	100	100
84	gg	311/313 (99%)	283 (91%)	28 (9%)	0	100	100
All	All	12576/13168 (96%)	11879 (94%)	684 (5%)	13 (0%)	54	81

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
41	m	73	CYS
48	u	61	PRO
49	v	288	THR
21	S	166	ARG
49	v	481	LYS

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Mol	Chain	Res	Type
75	XX	62	PRO
47	t	98	ILE
75	XX	86	PRO
57	FF	20	PHE
48	u	60	ARG
28	Z	90	PRO
60	II	131	PRO
75	XX	61	GLN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	A	190/190 (100%)	184 (97%)	6 (3%)	39 67
5	B	342/342 (100%)	337 (98%)	5 (2%)	65 81
6	C	301/301 (100%)	296 (98%)	5 (2%)	60 78
7	D	247/247 (100%)	243 (98%)	4 (2%)	62 79
8	E	190/251 (76%)	187 (98%)	3 (2%)	62 79
9	F	196/196 (100%)	196 (100%)	0	100 100
10	G	200/272 (74%)	193 (96%)	7 (4%)	36 64
11	H	169/169 (100%)	166 (98%)	3 (2%)	59 78
12	I	175/181 (97%)	172 (98%)	3 (2%)	60 78
13	J	143/143 (100%)	142 (99%)	1 (1%)	84 90
14	L	175/175 (100%)	170 (97%)	5 (3%)	42 69
15	M	117/117 (100%)	115 (98%)	2 (2%)	60 78
16	N	171/171 (100%)	168 (98%)	3 (2%)	59 78
17	O	171/171 (100%)	170 (99%)	1 (1%)	86 91
18	P	134/134 (100%)	132 (98%)	2 (2%)	65 81
19	Q	164/164 (100%)	162 (99%)	2 (1%)	71 83
20	R	159/159 (100%)	159 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
21	S	157/157 (100%)	155 (99%)	2 (1%)	69 82
22	T	139/139 (100%)	139 (100%)	0	100 100
23	U	89/89 (100%)	86 (97%)	3 (3%)	37 65
24	V	101/101 (100%)	99 (98%)	2 (2%)	55 76
25	W	86/126 (68%)	85 (99%)	1 (1%)	71 83
26	X	106/106 (100%)	106 (100%)	0	100 100
27	Y	124/124 (100%)	122 (98%)	2 (2%)	62 79
28	Z	117/117 (100%)	114 (97%)	3 (3%)	46 71
29	a	119/119 (100%)	118 (99%)	1 (1%)	81 89
30	b	84/184 (46%)	83 (99%)	1 (1%)	71 83
31	c	84/84 (100%)	80 (95%)	4 (5%)	25 56
32	d	98/98 (100%)	98 (100%)	0	100 100
33	e	114/114 (100%)	113 (99%)	1 (1%)	78 87
34	f	88/88 (100%)	86 (98%)	2 (2%)	50 73
35	g	98/98 (100%)	96 (98%)	2 (2%)	55 76
36	h	109/109 (100%)	108 (99%)	1 (1%)	78 87
37	i	86/86 (100%)	84 (98%)	2 (2%)	50 73
38	j	73/73 (100%)	72 (99%)	1 (1%)	67 82
39	k	64/64 (100%)	64 (100%)	0	100 100
40	l	47/47 (100%)	46 (98%)	1 (2%)	53 75
41	m	47/47 (100%)	46 (98%)	1 (2%)	53 75
42	n	24/24 (100%)	24 (100%)	0	100 100
43	o	91/91 (100%)	89 (98%)	2 (2%)	52 74
44	p	74/74 (100%)	74 (100%)	0	100 100
45	r	108/108 (100%)	105 (97%)	3 (3%)	43 70
46	s	164/164 (100%)	164 (100%)	0	100 100
47	t	126/126 (100%)	122 (97%)	4 (3%)	39 67
48	u	186/186 (100%)	179 (96%)	7 (4%)	33 62
49	v	713/713 (100%)	699 (98%)	14 (2%)	55 76
50	w	23/23 (100%)	21 (91%)	2 (9%)	10 34
52	AA	180/181 (99%)	179 (99%)	1 (1%)	86 91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
53	BB	194/194 (100%)	193 (100%)	1 (0%)	88 93
54	CC	187/187 (100%)	186 (100%)	1 (0%)	88 93
55	DD	190/190 (100%)	184 (97%)	6 (3%)	39 67
56	EE	224/224 (100%)	220 (98%)	4 (2%)	59 78
57	FF	158/170 (93%)	153 (97%)	5 (3%)	39 67
58	GG	207/207 (100%)	204 (99%)	3 (1%)	67 82
59	HH	165/174 (95%)	163 (99%)	2 (1%)	71 83
60	II	178/178 (100%)	178 (100%)	0	100 100
61	JJ	161/161 (100%)	157 (98%)	4 (2%)	47 72
62	KK	87/87 (100%)	87 (100%)	0	100 100
63	LL	130/142 (92%)	128 (98%)	2 (2%)	65 81
64	MM	99/99 (100%)	96 (97%)	3 (3%)	41 68
65	NN	130/130 (100%)	129 (99%)	1 (1%)	81 89
66	OO	106/106 (100%)	106 (100%)	0	100 100
67	PP	109/109 (100%)	107 (98%)	2 (2%)	59 78
68	QQ	117/117 (100%)	113 (97%)	4 (3%)	37 65
69	RR	119/119 (100%)	117 (98%)	2 (2%)	60 78
70	SS	125/125 (100%)	122 (98%)	3 (2%)	49 73
71	TT	111/111 (100%)	110 (99%)	1 (1%)	78 87
72	UU	92/92 (100%)	91 (99%)	1 (1%)	73 85
73	VV	67/67 (100%)	66 (98%)	1 (2%)	65 81
74	WW	112/112 (100%)	112 (100%)	0	100 100
75	XX	113/113 (100%)	112 (99%)	1 (1%)	78 87
76	YY	107/107 (100%)	106 (99%)	1 (1%)	78 87
77	ZZ	66/66 (100%)	65 (98%)	1 (2%)	65 81
78	aa	88/88 (100%)	87 (99%)	1 (1%)	73 85
79	bb	75/75 (100%)	72 (96%)	3 (4%)	31 61
80	cc	55/55 (100%)	54 (98%)	1 (2%)	59 78
81	dd	48/48 (100%)	48 (100%)	0	100 100
82	ee	46/46 (100%)	44 (96%)	2 (4%)	29 59
83	ff	61/61 (100%)	60 (98%)	1 (2%)	62 79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
84	gg	272/272 (100%)	269 (99%)	3 (1%)	73 85
All	All	10962/11275 (97%)	10787 (98%)	175 (2%)	64 79

All (175) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	4	VAL
4	A	163	ARG
4	A	193	ARG
4	A	242	ARG
4	A	243	THR
4	A	245	ARG
5	B	10	ARG
5	B	24	ARG
5	B	261	ARG
5	B	262	VAL
5	B	297	LYS
6	C	38	ASN
6	C	57	LEU
6	C	188	ARG
6	C	239	LYS
6	C	258	ARG
7	D	33	ARG
7	D	36	LEU
7	D	152	ARG
7	D	268	ARG
8	E	41	LYS
8	E	58	ARG
8	E	164	ARG
10	G	88	ARG
10	G	134	ASN
10	G	215	ASP
10	G	228	ARG
10	G	242	ARG
10	G	249	ARG
10	G	287	ARG
11	H	52	LYS
11	H	71	ARG
11	H	128	MET
12	I	10	ARG
12	I	24	ARG
12	I	38	ARG

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Mol	Chain	Res	Type
13	J	8	LYS
14	L	58	ILE
14	L	63	THR
14	L	124	LEU
14	L	159	ASN
14	L	209	LYS
15	M	119	ARG
15	M	132	ARG
16	N	26	ARG
16	N	64	ILE
16	N	162	ARG
17	O	140	ARG
18	P	64	ASN
18	P	97	ASN
19	Q	78	LYS
19	Q	168	ARG
21	S	23	ARG
21	S	83	ARG
23	U	47	ILE
23	U	65	ARG
23	U	81	ARG
24	V	48	ARG
24	V	69	LYS
25	W	110	ARG
27	Y	2	LYS
27	Y	134	LYS
28	Z	60	LYS
28	Z	102	ARG
28	Z	112	ARG
29	a	94	LYS
30	b	68	ARG
31	c	17	ARG
31	c	65	MET
31	c	90	ARG
31	c	93	THR
33	e	92	ASN
34	f	16	ARG
34	f	76	ARG
35	g	5	LEU
35	g	54	ARG
36	h	56	ARG
37	i	29	ARG

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Mol	Chain	Res	Type
37	i	56	ARG
38	j	20	ARG
40	l	33	ASN
41	m	96	ARG
43	o	43	ARG
43	o	82	MET
45	r	106	LEU
45	r	107	ARG
45	r	119	ARG
47	t	41	LYS
47	t	61	LYS
47	t	119	ARG
47	t	125	LEU
48	u	10	LEU
48	u	21	ASN
48	u	39	LYS
48	u	47	LYS
48	u	54	ARG
48	u	93	LEU
48	u	173	LYS
49	v	32	LYS
49	v	39	LEU
49	v	66	ARG
49	v	264	ARG
49	v	350	LEU
49	v	400	LYS
49	v	409	ARG
49	v	525	LYS
49	v	534	VAL
49	v	626	GLN
49	v	635	LEU
49	v	647	ARG
49	v	727	ARG
49	v	857	LYS
50	w	191	ARG
50	w	292	LYS
52	AA	50	ASN
53	BB	110	MET
54	CC	248	TYR
55	DD	40	ARG
55	DD	44	THR
55	DD	76	ARG

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Mol	Chain	Res	Type
55	DD	94	ARG
55	DD	178	ARG
55	DD	197	LYS
56	EE	108	ARG
56	EE	122	LYS
56	EE	148	ARG
56	EE	255	ARG
57	FF	92	ILE
57	FF	122	ARG
57	FF	135	ARG
57	FF	154	LEU
57	FF	198	ARG
58	GG	25	ARG
58	GG	191	ARG
58	GG	201	LYS
59	HH	31	GLU
59	HH	36	LEU
61	JJ	70	ARG
61	JJ	79	ARG
61	JJ	91	LYS
61	JJ	179	LYS
63	LL	20	LYS
63	LL	32	LYS
64	MM	35	ILE
64	MM	83	LYS
64	MM	101	ARG
65	NN	60	VAL
67	PP	44	ARG
67	PP	51	ARG
68	QQ	41	MET
68	QQ	85	ARG
68	QQ	88	ILE
68	QQ	102	GLU
69	RR	71	ILE
69	RR	81	ARG
70	SS	8	LYS
70	SS	52	LEU
70	SS	59	LEU
71	TT	126	GLN
72	UU	101	ILE
73	VV	70	LEU
75	XX	142	ARG

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Mol	Chain	Res	Type
76	YY	100	LYS
77	ZZ	98	LYS
78	aa	5	ARG
79	bb	17	ARG
79	bb	36	LYS
79	bb	42	LYS
80	cc	31	ARG
82	ee	81	ARG
82	ee	99	LYS
83	ff	138	ARG
84	gg	18	VAL
84	gg	42	MET
84	gg	60	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
18	P	64	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	5	3522/3597 (97%)	832 (23%)	64 (1%)
2	7	119/120 (99%)	15 (12%)	0
3	8	149/151 (98%)	26 (17%)	1 (0%)
51	9	1675/1698 (98%)	406 (24%)	30 (1%)
All	All	5465/5566 (98%)	1279 (23%)	95 (1%)

All (1279) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	5	8	U
1	5	12	A
1	5	13	U
1	5	25	A
1	5	35	U
1	5	36	U
1	5	39	A
1	5	42	A
1	5	43	U

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Mol	Chain	Res	Type
1	5	48	G
1	5	49	U
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	74	G
1	5	76	A
1	5	84	A
1	5	91	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
1	5	142	G
1	5	151	G
1	5	157	U
1	5	159	C
1	5	167	C
1	5	172	C
1	5	173	C
1	5	179	G
1	5	182	G
1	5	195	C
1	5	200	U
1	5	201	C
1	5	202	C
1	5	203	U
1	5	205	C
1	5	209	U

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Mol	Chain	Res	Type
1	5	210	C
1	5	216	C
1	5	218	A
1	5	220	C
1	5	224	U
1	5	233	U
1	5	234	G
1	5	245	C
1	5	246	G
1	5	250	C
1	5	265	C
1	5	266	C
1	5	267	G
1	5	275	C
1	5	276	C
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	326	C
1	5	328	A
1	5	334	A
1	5	340	C
1	5	345	C
1	5	350	C
1	5	357	U
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	406	C
1	5	407	A
1	5	408	A
1	5	410	A
1	5	412	G
1	5	413	G
1	5	414	C

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Mol	Chain	Res	Type
1	5	433	A
1	5	440	U
1	5	449	C
1	5	450	G
1	5	451	C
1	5	452	A
1	5	453	G
1	5	454	U
1	5	455	C
1	5	463	A
1	5	467	U
1	5	468	U
1	5	482	G
1	5	484	U
1	5	485	C
1	5	486	C
1	5	492	U
1	5	493	G
1	5	496	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	646	G
1	5	666	G
1	5	667	A
1	5	669	C
1	5	685	C
1	5	686	A
1	5	687	U
1	5	688	U
1	5	691	C
1	5	696	C
1	5	697	G
1	5	704	C
1	5	705	G
1	5	708	G
1	5	719	C
1	5	729	2MG
1	5	731	G

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Mol	Chain	Res	Type
1	5	742	G
1	5	744	G
1	5	747	A
1	5	748	G
1	5	749	G
1	5	758	G
1	5	914	U
1	5	916	C
1	5	917	A
1	5	918	G
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	938	C
1	5	939	G
1	5	941	C
1	5	943	A
1	5	945	U
1	5	956	A
1	5	959	G
1	5	960	A
1	5	961	G
1	5	964	A
1	5	965	G
1	5	966	A
1	5	967	C
1	5	968	C
1	5	969	C
1	5	971(A)	G
1	5	972	C
1	5	973	C
1	5	980	C
1	5	983	U
1	5	1070	G
1	5	1072	C
1	5	1073	G
1	5	1078	A
1	5	1079	C

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Mol	Chain	Res	Type
1	5	1080	C
1	5	1081	C
1	5	1082	C
1	5	1083	U
1	5	1098	G
1	5	1175	A
1	5	1179	U
1	5	1180	C
1	5	1187	G
1	5	1193	C
1	5	1195	G
1	5	1204	C
1	5	1210	C
1	5	1211	G
1	5	1212	G
1	5	1214	C
1	5	1215	C
1	5	1216	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	1295	U
1	5	1296	G
1	5	1301	C
1	5	1303	A
1	5	1304	C
1	5	1314	C
1	5	1320	U
1	5	1326	A2M

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Mol	Chain	Res	Type
1	5	1330	A
1	5	1337	A
1	5	1354	A
1	5	1358	G
1	5	1359	G
1	5	1370	G
1	5	1371	A
1	5	1372	A
1	5	1377	G
1	5	1378	C
1	5	1380	G
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	1411(C)	C
1	5	1412	G
1	5	1415	G
1	5	1419	G
1	5	1421	G
1	5	1429	C
1	5	1436	C
1	5	1437	C
1	5	1438	U
1	5	1441	C
1	5	1443	A
1	5	1445	U
1	5	1446	C
1	5	1457	G
1	5	1458	C
1	5	1465	G
1	5	1475	G
1	5	1482	G
1	5	1483	C
1	5	1497	A
1	5	1498	G
1	5	1502	G
1	5	1516	G
1	5	1518	A
1	5	1523	A

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Mol	Chain	Res	Type
1	5	1534	A2M
1	5	1547	A
1	5	1563	A
1	5	1566	C
1	5	1578	U
1	5	1582	PSU
1	5	1591	U
1	5	1596	U
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	1691	G
1	5	1734	G
1	5	1741	G
1	5	1742	A
1	5	1750	G
1	5	1751	A
1	5	1755	C
1	5	1756	U
1	5	1757	U
1	5	1764	G
1	5	1768	C
1	5	1772	C

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Mol	Chain	Res	Type
1	5	1773	U
1	5	1776	A
1	5	1781	U
1	5	1787	A
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	1828	C
1	5	1833	G
1	5	1834	U
1	5	1835	G
1	5	1836	G
1	5	1837	A
1	5	1840	G
1	5	1842	G
1	5	1843	A
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	1915	C
1	5	1916	G
1	5	1918	U
1	5	1920	C
1	5	1921	C
1	5	1922	G
1	5	1928	C
1	5	1930	U
1	5	1931	C
1	5	1932	A
1	5	1938	C
1	5	1940	G
1	5	1945	G
1	5	1951	G
1	5	1957	U
1	5	1958	A

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Mol	Chain	Res	Type
1	5	1961	G
1	5	1962	A
1	5	1964	A
1	5	1967	A
1	5	1971	U
1	5	1974	U
1	5	1976	G
1	5	1978	C
1	5	1979	A
1	5	1980	U
1	5	1981	G
1	5	1983	A
1	5	1984	A
1	5	1986	U
1	5	1987	C
1	5	1991	A
1	5	1992	U
1	5	1993	C
1	5	1997	U
1	5	2001	G
1	5	2002	A
1	5	2003	G
1	5	2004	U
1	5	2007	G
1	5	2008	U
1	5	2009	A
1	5	2011	C
1	5	2021	G
1	5	2025	A
1	5	2026	A
1	5	2029	A
1	5	2033	A
1	5	2043	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	2064	G
1	5	2069	A
1	5	2070	U

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Mol	Chain	Res	Type
1	5	2084	U
1	5	2090	U
1	5	2092	G
1	5	2093	G
1	5	2094	C
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	2108	G
1	5	2259	G
1	5	2260	C
1	5	2261	G
1	5	2267	U
1	5	2268	A
1	5	2269	C
1	5	2270	G
1	5	2275	G
1	5	2289	C
1	5	2300	A
1	5	2301	G
1	5	2306	G
1	5	2313	A
1	5	2314	G
1	5	2316	G
1	5	2332	A
1	5	2333	G
1	5	2335	C
1	5	2347	A
1	5	2348	G
1	5	2351	C
1	5	2357	G
1	5	2360	A
1	5	2364	OMG
1	5	2395	A
1	5	2396	A
1	5	2408	U
1	5	2410	C

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Mol	Chain	Res	Type
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	2471	G
1	5	2474	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	2529	A
1	5	2530	U
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	2568	C
1	5	2571	C
1	5	2575	U
1	5	2583	C
1	5	2586	G
1	5	2587	A
1	5	2588	C
1	5	2589	C
1	5	2601	A
1	5	2611	A
1	5	2616	C

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Mol	Chain	Res	Type
1	5	2618	G
1	5	2620	G
1	5	2628	U
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	2676	A
1	5	2680	G
1	5	2686	G
1	5	2687	U
1	5	2695	A
1	5	2696	A
1	5	2700	G
1	5	2707	U
1	5	2708	U
1	5	2709	C
1	5	2710	C
1	5	2711	G
1	5	2714	G
1	5	2715	G
1	5	2716	C
1	5	2721	G
1	5	2724	G
1	5	2725	A
1	5	2726	G
1	5	2740	U
1	5	2743	A
1	5	2744	A
1	5	2764	A
1	5	2769	U
1	5	2773	OMG
1	5	2787	A
1	5	2788	U
1	5	2790	U
1	5	2794	C

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Mol	Chain	Res	Type
1	5	2798	A
1	5	2803	U
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	2867	C
1	5	2869	U
1	5	2884	G
1	5	3598	C
1	5	3605	C
1	5	3606	U
1	5	3616	U
1	5	3620	G
1	5	3625	G
1	5	3626	G
1	5	3630	A
1	5	3635	A
1	5	3649	A
1	5	3650	C
1	5	3658	C
1	5	3662	A
1	5	3663	A
1	5	3664	G
1	5	3673	C
1	5	3674	G
1	5	3691	G
1	5	3692	A
1	5	3696	C
1	5	3698	G
1	5	3711	A
1	5	3712	A
1	5	3714	G
1	5	3729	PSU
1	5	3740	G
1	5	3743	G
1	5	3753	G
1	5	3759	A
1	5	3760	A
1	5	3761	C

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Mol	Chain	Res	Type
1	5	3764	PSU
1	5	3765	G
1	5	3773	U
1	5	3774	A
1	5	3776	G
1	5	3777	G
1	5	3783	A
1	5	3784	A
1	5	3786	U
1	5	3787	G
1	5	3792	OMG
1	5	3798	U
1	5	3799	A
1	5	3810	C
1	5	3811	G
1	5	3812	C
1	5	3813	A
1	5	3814	U
1	5	3817	A
1	5	3819	G
1	5	3822	U
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	3881	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
1	5	3907	G
1	5	3908	A
1	5	3915	U
1	5	3916	G

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Mol	Chain	Res	Type
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	3970	G
1	5	3972	A
1	5	3973	G
1	5	3974	G
1	5	3975	C
1	5	3976	C
1	5	4042	G
1	5	4047	A
1	5	4049	U
1	5	4050	A
1	5	4051	C
1	5	4053	A
1	5	4054	C
1	5	4055	U
1	5	4066	U
1	5	4073	A
1	5	4076	G
1	5	4085	A
1	5	4086	G
1	5	4097	G
1	5	4100	C
1	5	4116	C
1	5	4119	C
1	5	4120	U
1	5	4122	G
1	5	4125	C
1	5	4127	A
1	5	4151	G
1	5	4158	C
1	5	4166	G
1	5	4170	A
1	5	4173	G
1	5	4183	G
1	5	4184	G
1	5	4191	G

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Mol	Chain	Res	Type
1	5	4195	G
1	5	4203	A
1	5	4212	A
1	5	4225	G
1	5	4229	U
1	5	4233	A
1	5	4243	C
1	5	4249	G
1	5	4251	A
1	5	4254	G
1	5	4255	A
1	5	4256	A
1	5	4265	U
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	4291	G
1	5	4293	PSU
1	5	4304	A
1	5	4305	G
1	5	4306	OMU
1	5	4308	C
1	5	4313	A
1	5	4314	C
1	5	4317	A
1	5	4318	C
1	5	4319	C
1	5	4326	G
1	5	4329	G
1	5	4330	G
1	5	4332	C
1	5	4348	A
1	5	4349	C
1	5	4354	U
1	5	4368	G
1	5	4372	U
1	5	4373	G
1	5	4377	G
1	5	4378	A

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Mol	Chain	Res	Type
1	5	4380	A
1	5	4387	C
1	5	4393	G
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	4420	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	4495	G
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	4520	G
1	5	4522	G
1	5	4523	A2M
1	5	4524	G
1	5	4548	A
1	5	4549	G
1	5	4560	C
1	5	4567	G
1	5	4570	G
1	5	4573	G
1	5	4574	U

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Mol	Chain	Res	Type
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	4629	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	4687	A
1	5	4693	C
1	5	4694	G
1	5	4695	C
1	5	4700	A
1	5	4709	U
1	5	4719	G
1	5	4720	C
1	5	4738	C
1	5	4750	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
1	5	4765	G
1	5	4771	C
1	5	4772	C
1	5	4868	G

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Mol	Chain	Res	Type
1	5	4870	OMG
1	5	4872	2MG
1	5	4873	G
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	4904	G
1	5	4906	C
1	5	4910	A
1	5	4912	G
1	5	4914	G
1	5	4915	G
1	5	4918	C
1	5	4919	G
1	5	4921	C
1	5	4922	C
1	5	4923	U
1	5	4925	U
1	5	4926	C
1	5	4927	G
1	5	4928	C
1	5	4929	C
1	5	4931	G
1	5	4934	A
1	5	4937	C
1	5	4938	A
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	4956	A
1	5	4958	C
1	5	4960	G
1	5	4961	G
1	5	4964	C

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Mol	Chain	Res	Type
1	5	4965	U
1	5	4966	A
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	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	22	A
2	7	25	G
2	7	29	C
2	7	33	U
2	7	53	U
2	7	54	A
2	7	64	G
2	7	97	G
2	7	100	A
2	7	102	U
2	7	110	G
2	7	111	C
2	7	120	U
3	8	2	G
3	8	32	C

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Mol	Chain	Res	Type
3	8	34	U
3	8	35	C
3	8	38	U
3	8	39	G
3	8	49	G
3	8	59	A
3	8	62	A
3	8	63	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	125	C
3	8	126	C
3	8	127	U
3	8	137	A
3	8	147	G
3	8	153	C
51	9	2	A
51	9	3	C
51	9	4	C
51	9	17	C
51	9	23	G
51	9	25	A
51	9	26	U
51	9	33	G
51	9	37	C
51	9	41	G
51	9	42	A
51	9	44	U
51	9	45	A
51	9	46	A
51	9	56	G
51	9	58	C
51	9	60	A
51	9	65	C

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Mol	Chain	Res	Type
51	9	67	C
51	9	68	A
51	9	70	G
51	9	71	G
51	9	73	C
51	9	74	G
51	9	77	A
51	9	79	A
51	9	99	A
51	9	103	A
51	9	104	A
51	9	110	U
51	9	111	A
51	9	113	G
51	9	115	U
51	9	116	U
51	9	124	U
51	9	126	G
51	9	127	C
51	9	129	C
51	9	130	G
51	9	141	A
51	9	143	U
51	9	146	G
51	9	147	A
51	9	155	G
51	9	158	A
51	9	162	C
51	9	163	U
51	9	167	G
51	9	168	C
51	9	180	G
51	9	183	G
51	9	184	G
51	9	187	G
51	9	188	C
51	9	189	U
51	9	190	G
51	9	192	C
51	9	202	G
51	9	206	G
51	9	215	G

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Mol	Chain	Res	Type
51	9	302	A
51	9	307	G
51	9	308	G
51	9	309	G
51	9	312	G
51	9	314	U
51	9	318	A
51	9	319	C
51	9	332	G
51	9	335	G
51	9	339	A
51	9	347	G
51	9	351	G
51	9	360	A
51	9	362	C
51	9	364	A
51	9	368	U
51	9	369	C
51	9	370	G
51	9	376	A
51	9	380	G
51	9	381	C
51	9	385	G
51	9	386	C
51	9	398	A
51	9	400	C
51	9	408	A
51	9	409	C
51	9	418	A
51	9	420	G
51	9	421	G
51	9	426	A
51	9	428	U
51	9	435	A
51	9	438	G
51	9	448	A
51	9	450	C
51	9	455	A
51	9	456	C
51	9	464	A
51	9	465	A
51	9	466	G

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Mol	Chain	Res	Type
51	9	471	G
51	9	472	C
51	9	473	A
51	9	474	G
51	9	476	A
51	9	482	G
51	9	487	U
51	9	492	C
51	9	496	C
51	9	517	C
51	9	530	U
51	9	531	A
51	9	532	C
51	9	533	A
51	9	542	U
51	9	544	G
51	9	548	C
51	9	549	C
51	9	550	C
51	9	551	U
51	9	554	A
51	9	555	A
51	9	556	U
51	9	559	G
51	9	560	A
51	9	563	G
51	9	564	A
51	9	568	C
51	9	570	C
51	9	575	A
51	9	576	A
51	9	583	A
51	9	587	A
51	9	588	G
51	9	589	G
51	9	590	A
51	9	591	U
51	9	599	A
51	9	600	G
51	9	601	G
51	9	603	C
51	9	606	G

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Mol	Chain	Res	Type
51	9	608	C
51	9	609	U
51	9	611	G
51	9	614	C
51	9	615	C
51	9	617	G
51	9	626	G
51	9	627	U
51	9	628	A
51	9	629	A
51	9	631	U
51	9	632	C
51	9	633	C
51	9	637	U
51	9	643	A
51	9	644	G
51	9	655	A
51	9	660	C
51	9	663	C
51	9	668	A
51	9	669	A
51	9	671	A
51	9	672	A
51	9	673	G
51	9	684	G
51	9	688	U
51	9	689	U
51	9	690	G
51	9	752	G
51	9	753	C
51	9	754	G
51	9	798	G
51	9	811	A
51	9	821	G
51	9	822	U
51	9	827	A
51	9	830	A
51	9	834	C
51	9	844	U
51	9	847	A
51	9	870	A
51	9	871	U

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Mol	Chain	Res	Type
51	9	872	A
51	9	873	G
51	9	874	G
51	9	875	A
51	9	876	C
51	9	878	G
51	9	879	C
51	9	881	G
51	9	887	U
51	9	888	U
51	9	889	U
51	9	890	U
51	9	892	U
51	9	907	G
51	9	909	G
51	9	913	A
51	9	914	U
51	9	920	A
51	9	933	G
51	9	934	G
51	9	971	G
51	9	990	A
51	9	992	A
51	9	999	G
51	9	1002	U
51	9	1017	U
51	9	1023	A
51	9	1026	C
51	9	1040	G
51	9	1041	G
51	9	1045	U
51	9	1050	A
51	9	1060	A
51	9	1062	A
51	9	1067	C
51	9	1083	A
51	9	1084	A
51	9	1085	C
51	9	1086	G
51	9	1099	G
51	9	1100	A
51	9	1109	C

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Mol	Chain	Res	Type
51	9	1114	U
51	9	1115	U
51	9	1116	C
51	9	1117	C
51	9	1118	C
51	9	1121	G
51	9	1123	C
51	9	1126	G
51	9	1131	G
51	9	1133	A
51	9	1138	C
51	9	1139	C
51	9	1148	A
51	9	1149	A
51	9	1153	C
51	9	1154	U
51	9	1155	U
51	9	1161	U
51	9	1170	A
51	9	1171	G
51	9	1195	A
51	9	1207	G
51	9	1208	A
51	9	1215	C
51	9	1221	G
51	9	1224	G
51	9	1242	U
51	9	1243	PSU
51	9	1250	A
51	9	1251	A
51	9	1253	A
51	9	1254	C
51	9	1256	G
51	9	1257	G
51	9	1259	A
51	9	1264	C
51	9	1265	A
51	9	1274	G
51	9	1275	G
51	9	1281	G
51	9	1282	A
51	9	1283	C

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Mol	Chain	Res	Type
51	9	1284	A
51	9	1285	G
51	9	1286	G
51	9	1288	U
51	9	1289	U
51	9	1299	A
51	9	1301	A
51	9	1302	G
51	9	1303	C
51	9	1307	U
51	9	1308	U
51	9	1309	C
51	9	1310	U
51	9	1312	G
51	9	1313	A
51	9	1314	U
51	9	1318	G
51	9	1327	G
51	9	1333	U
51	9	1342	U
51	9	1348	G
51	9	1363	C
51	9	1364	U
51	9	1371	U
51	9	1372	U
51	9	1376	A
51	9	1378	A
51	9	1382	A
51	9	1393	G
51	9	1395	C
51	9	1396	A
51	9	1397	U
51	9	1401	A
51	9	1402	A
51	9	1406	G
51	9	1428	G
51	9	1431	G
51	9	1449	G
51	9	1454	A
51	9	1462	U
51	9	1463	U
51	9	1464	C

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Mol	Chain	Res	Type
51	9	1466	G
51	9	1474	A
51	9	1475	G
51	9	1476	A
51	9	1477	U
51	9	1478	U
51	9	1480	A
51	9	1483	A
51	9	1484	A
51	9	1485	U
51	9	1486	A
51	9	1488	C
51	9	1489	A
51	9	1490	G
51	9	1495	G
51	9	1497	G
51	9	1498	A
51	9	1507	G
51	9	1510	G
51	9	1521	C
51	9	1522	A
51	9	1531	A
51	9	1533	A
51	9	1535	U
51	9	1536	G
51	9	1544	C
51	9	1548	G
51	9	1552	G
51	9	1553	C
51	9	1554	C
51	9	1555	U
51	9	1556	A
51	9	1557	C
51	9	1560	U
51	9	1570	G
51	9	1574	C
51	9	1580	A
51	9	1584	G
51	9	1585	U
51	9	1586	U
51	9	1587	G
51	9	1588	A

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Mol	Chain	Res	Type
51	9	1598	G
51	9	1601	A
51	9	1604	G
51	9	1606	G
51	9	1621	U
51	9	1623	A
51	9	1624	U
51	9	1634	A
51	9	1637	A
51	9	1638	G
51	9	1646	C
51	9	1648	G
51	9	1654	G
51	9	1664	A
51	9	1665	G
51	9	1680	G
51	9	1683	C
51	9	1695	A
51	9	1698	C
51	9	1699	A
51	9	1715	A
51	9	1721	U
51	9	1722	G
51	9	1726	G
51	9	1732	G
51	9	1734	G
51	9	1744	G
51	9	1748	G
51	9	1753	C
51	9	1783	C
51	9	1785	C
51	9	1799	G
51	9	1819	A
51	9	1823	A
51	9	1824	A
51	9	1825	A
51	9	1829	G
51	9	1831	A
51	9	1835	A
51	9	1836	G
51	9	1837	G
51	9	1838	U

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Mol	Chain	Res	Type
51	9	1849	G
51	9	1851	A
51	9	1861	G
51	9	1862	G
51	9	1863	A
51	9	1864	U
51	9	1865	C
51	9	1866	A
51	9	1867	U
51	9	1869	A

All (95) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	5	12	A
1	5	47	A
1	5	48	G
1	5	125	C
1	5	134	G
1	5	217	C
1	5	233	U
1	5	245	C
1	5	265	C
1	5	266	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	684	G
1	5	930	G
1	5	959	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

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Mol	Chain	Res	Type
1	5	1406(B)	C
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	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	3625	G
1	5	3697	U
1	5	3760	A
1	5	3876	A
1	5	3888	G
1	5	3904	G
1	5	3954	A
1	5	4053	A
1	5	4065	G
1	5	4119	C
1	5	4232	U
1	5	4254	G
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
51	9	110	U
51	9	182	C
51	9	434	G
51	9	465	A
51	9	532	C

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Mol	Chain	Res	Type
51	9	553	U
51	9	555	A
51	9	599	A
51	9	606	G
51	9	642	U
51	9	688	U
51	9	752	G
51	9	870	A
51	9	872	A
51	9	874	G
51	9	1137	U
51	9	1207	G
51	9	1253	A
51	9	1264	C
51	9	1363	C
51	9	1394	G
51	9	1395	C
51	9	1483	A
51	9	1484	A
51	9	1489	A
51	9	1520	G
51	9	1637	A
51	9	1664	A
51	9	1665	G
51	9	1835	A

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

110 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	1MA	5	1322	1,85	16,25,26	3.73	4 (25%)	18,37,40	1.68	3 (16%)
51	5MC	9	1374	51	18,22,23	3.63	7 (38%)	26,32,35	1.10	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	OMC	5	2804	1	19,22,23	2.83	7 (36%)	26,31,34	0.80	0
1	B8T	5	4671	1	19,22,23	3.01	8 (42%)	26,31,34	0.94	1 (3%)
1	B8Q	5	1456	1	17,22,23	2.70	5 (29%)	22,32,35	2.05	5 (22%)
1	MHG	5	4371	1	29,32,33	3.94	11 (37%)	34,46,49	2.38	12 (35%)
1	7MG	5	4550	1	22,26,27	3.50	10 (45%)	29,39,42	1.96	8 (27%)
1	A2M	5	3785	1	18,25,26	4.59	9 (50%)	18,36,39	2.44	3 (16%)
1	A2M	5	4571	1	18,25,26	4.79	9 (50%)	18,36,39	2.60	4 (22%)
1	PSU	5	4403	1	18,21,22	1.00	1 (5%)	22,30,33	1.73	5 (22%)
51	PSU	9	1243	51	18,21,22	1.17	1 (5%)	22,30,33	1.33	4 (18%)
1	A2M	5	2401	1,85	18,25,26	4.73	9 (50%)	18,36,39	2.66	3 (16%)
1	P7G	5	1909	1	24,28,29	4.13	11 (45%)	27,41,44	1.74	4 (14%)
1	B8H	5	3762	1	19,22,23	6.80	6 (31%)	22,32,35	2.39	5 (22%)
6	MLZ	C	333	6	8,9,10	0.84	0	4,9,11	0.70	0
1	OMG	5	1316	1	18,26,27	2.46	8 (44%)	19,38,41	1.66	4 (21%)
1	OMC	5	3887	1	19,22,23	2.83	7 (36%)	26,31,34	0.89	1 (3%)
1	A2M	5	398	1	18,25,26	4.80	9 (50%)	18,36,39	2.55	3 (16%)
1	OMC	5	2365	1	19,22,23	2.84	7 (36%)	26,31,34	0.68	0
1	P7G	5	3880	1	24,28,29	3.86	10 (41%)	27,41,44	1.60	4 (14%)
1	PSU	5	1677	1	18,21,22	1.10	3 (16%)	22,30,33	1.89	6 (27%)
1	OMG	5	373	1	18,26,27	2.49	8 (44%)	19,38,41	1.64	5 (26%)
51	4AC	9	1337	51	21,24,25	3.16	9 (42%)	29,34,37	1.13	3 (10%)
1	A2M	5	1524	1	18,25,26	4.71	9 (50%)	18,36,39	2.65	3 (16%)
1	OMG	5	3792	1	18,26,27	2.50	8 (44%)	19,38,41	1.58	4 (21%)
1	B9B	5	237	1	21,28,29	6.35	9 (42%)	23,40,43	2.26	5 (21%)
1	PSU	5	4500	1	18,21,22	1.00	1 (5%)	22,30,33	1.90	4 (18%)
1	OMG	5	1883	1	18,26,27	2.49	8 (44%)	19,38,41	1.67	4 (21%)
1	2MG	5	4872	15,1	18,26,27	2.62	7 (38%)	16,38,41	1.72	4 (25%)
1	OMC	5	4536	1	19,22,23	2.84	7 (36%)	26,31,34	0.99	1 (3%)
1	OMG	5	2424	1	18,26,27	2.53	8 (44%)	19,38,41	1.56	4 (21%)
1	OMC	5	3869	1	19,22,23	2.82	7 (36%)	26,31,34	0.70	0
1	B8W	5	4529	1,85	18,26,27	5.28	8 (44%)	21,38,41	6.32	10 (47%)
1	5MC	5	4447	1	18,22,23	3.67	7 (38%)	26,32,35	1.09	1 (3%)
1	2MG	5	729	1	18,26,27	2.45	7 (38%)	16,38,41	1.36	3 (18%)
1	A2M	5	4523	1,85	18,25,26	4.83	9 (50%)	18,36,39	2.58	3 (16%)
1	I4U	5	1659	1	21,24,25	4.92	15 (71%)	27,34,37	1.42	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	PSU	5	4442	1	18,21,22	1.07	1 (5%)	22,30,33	1.83	4 (18%)
1	OMG	5	4637	1	18,26,27	2.42	8 (44%)	19,38,41	1.52	4 (21%)
1	B8W	5	4185	1	18,26,27	5.15	8 (44%)	21,38,41	5.96	11 (52%)
1	B9B	5	1574	1	21,28,29	6.29	9 (42%)	23,40,43	2.19	6 (26%)
1	UR3	5	1866	1	19,22,23	2.54	6 (31%)	26,32,35	1.35	4 (15%)
1	2MG	5	1517	1	18,26,27	2.52	7 (38%)	16,38,41	1.63	4 (25%)
1	OMU	5	4620	1	19,22,23	2.70	7 (36%)	26,31,34	1.70	5 (19%)
51	A2M	9	1678	51	18,25,26	4.87	9 (50%)	18,36,39	2.63	3 (16%)
49	DDE	v	715	49	14,20,21	1.00	0	14,28,30	1.30	2 (14%)
1	5MU	5	4083	1	19,22,23	4.77	7 (36%)	28,32,35	3.59	10 (35%)
1	OMC	5	2422	1,85	19,22,23	2.91	7 (36%)	26,31,34	0.94	1 (3%)
1	E6G	5	4355	1	20,27,28	5.77	9 (45%)	22,39,42	2.07	7 (31%)
1	OMG	5	2050	1	18,26,27	2.45	8 (44%)	19,38,41	1.49	4 (21%)
3	OMU	8	14	1,3	19,22,23	2.79	7 (36%)	26,31,34	1.98	7 (26%)
1	B8W	5	2380	1	18,26,27	5.23	7 (38%)	21,38,41	6.10	7 (33%)
1	5MC	5	4335	1	18,22,23	3.56	7 (38%)	26,32,35	1.27	3 (11%)
1	P4U	5	1348	1,85	21,24,25	3.37	8 (38%)	27,33,36	1.43	3 (11%)
1	B8W	5	4129	1	18,26,27	5.25	8 (44%)	21,38,41	6.11	9 (42%)
1	7MG	5	2522	1	22,26,27	3.52	10 (45%)	29,39,42	1.98	8 (27%)
1	UR3	5	4530	1	19,22,23	2.65	6 (31%)	26,32,35	1.30	2 (7%)
1	OMU	5	4306	1	19,22,23	2.81	7 (36%)	26,31,34	1.76	5 (19%)
1	B8T	5	4483	1	19,22,23	3.06	8 (42%)	26,31,34	1.01	2 (7%)
1	A2M	5	3867	1	18,25,26	4.63	9 (50%)	18,36,39	2.58	3 (16%)
1	B8K	5	4690	1,11	24,28,29	5.03	17 (70%)	30,42,45	2.59	11 (36%)
1	PSU	5	1683	1	18,21,22	1.11	1 (5%)	22,30,33	1.79	4 (18%)
1	OMC	5	2861	1	19,22,23	2.88	7 (36%)	26,31,34	0.90	1 (3%)
1	OMG	5	2773	1	18,26,27	2.51	8 (44%)	19,38,41	1.49	4 (21%)
1	PSU	5	4628	1	18,21,22	1.12	2 (11%)	22,30,33	1.99	4 (18%)
1	PSU	5	3764	1	18,21,22	1.04	1 (5%)	22,30,33	1.64	4 (18%)
1	OMG	5	4196	1	18,26,27	2.47	8 (44%)	19,38,41	1.57	4 (21%)
1	OMC	5	3909	1	19,22,23	2.84	7 (36%)	26,31,34	0.73	0
1	6MZ	5	4220	1	18,25,26	2.14	4 (22%)	16,36,39	2.07	4 (25%)
1	A2M	5	1326	1	18,25,26	4.67	9 (50%)	18,36,39	2.67	3 (16%)
1	PSU	5	3729	1	18,21,22	1.03	1 (5%)	22,30,33	1.70	4 (18%)
1	M7A	5	4564	1	20,25,26	1.96	3 (15%)	28,37,40	3.86	8 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	OMG	5	4623	1	18,26,27	2.48	8 (44%)	19,38,41	1.60	4 (21%)
1	OMG	5	1625	1,85	18,26,27	2.46	8 (44%)	19,38,41	1.51	4 (21%)
1	PSU	5	4450	1,85	18,21,22	1.06	2 (11%)	22,30,33	1.92	4 (18%)
1	BGH	5	3899	1,85	25,29,30	4.22	16 (64%)	31,43,46	2.51	13 (41%)
1	UR3	5	4597	1	19,22,23	2.62	6 (31%)	26,32,35	1.32	3 (11%)
1	B8H	5	1860	1	19,22,23	6.80	6 (31%)	22,32,35	2.33	5 (22%)
1	OMG	5	4494	1	18,26,27	2.47	8 (44%)	19,38,41	1.58	4 (21%)
1	1MA	5	4415	1	16,25,26	3.94	4 (25%)	18,37,40	1.66	3 (16%)
1	A2M	5	1871	1,85	18,25,26	4.77	9 (50%)	18,36,39	2.72	3 (16%)
1	A2M	5	2363	1,85	18,25,26	4.76	9 (50%)	18,36,39	2.73	4 (22%)
1	PSU	5	3715	1	18,21,22	0.98	1 (5%)	22,30,33	1.64	4 (18%)
1	PSU	5	4531	1	18,21,22	1.03	1 (5%)	22,30,33	1.85	5 (22%)
41	MLZ	m	72	41	8,9,10	0.73	0	4,9,11	0.77	0
1	A2M	5	1534	1,85	18,25,26	4.68	9 (50%)	18,36,39	2.71	4 (22%)
1	OMG	5	2364	1	18,26,27	2.46	8 (44%)	19,38,41	1.58	4 (21%)
1	E7G	5	2297	1	24,27,28	3.48	11 (45%)	30,40,43	2.15	9 (30%)
1	7MG	5	1605	1	22,26,27	3.45	10 (45%)	29,39,42	2.04	9 (31%)
1	OMG	5	1522	1	18,26,27	2.49	8 (44%)	19,38,41	1.60	4 (21%)
1	OMG	5	4870	1	18,26,27	2.44	8 (44%)	19,38,41	1.55	3 (15%)
1	OMG	5	4370	1	18,26,27	2.52	8 (44%)	19,38,41	1.51	4 (21%)
1	B8K	5	3897	1	24,28,29	4.76	17 (70%)	30,42,45	2.56	12 (40%)
51	B8N	9	1248	51	24,29,30	2.79	7 (29%)	29,42,45	1.75	5 (17%)
1	A2M	5	3718	1	18,25,26	4.78	10 (55%)	18,36,39	2.50	3 (16%)
1	PSU	5	2508	1	18,21,22	0.98	1 (5%)	22,30,33	1.62	3 (13%)
1	PSU	5	1582	1	18,21,22	1.15	2 (11%)	22,30,33	1.70	4 (18%)
1	B8H	5	4296	1	19,22,23	6.81	6 (31%)	22,32,35	2.40	5 (22%)
1	PSU	5	4636	1	18,21,22	1.04	2 (11%)	22,30,33	1.93	4 (18%)
51	B8Q	9	1219	51	17,22,23	2.95	4 (23%)	22,32,35	2.80	7 (31%)
1	I4U	5	4194	1	21,24,25	4.96	15 (71%)	27,34,37	1.17	2 (7%)
1	5MC	5	3782	1	18,22,23	3.61	7 (38%)	26,32,35	1.11	1 (3%)
1	A2M	5	3825	1	18,25,26	4.74	7 (38%)	18,36,39	2.69	3 (16%)
1	A2M	5	3723	1	18,25,26	4.84	9 (50%)	18,36,39	2.59	3 (16%)
1	B9H	5	2786	1	20,25,26	3.15	3 (15%)	22,35,38	1.90	3 (13%)
1	B8W	5	4472	1	18,26,27	5.34	8 (44%)	21,38,41	6.01	10 (47%)
1	PSU	5	4293	1	18,21,22	1.06	1 (5%)	22,30,33	1.84	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	OMC	5	3701	1,85	19,22,23	2.79	7 (36%)	26,31,34	0.75	0
1	B9B	5	2754	1,85	21,28,29	6.35	9 (42%)	23,40,43	1.98	6 (26%)
1	E7G	5	1797	1	24,27,28	3.56	11 (45%)	30,40,43	2.18	9 (30%)

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	1MA	5	1322	1,85	-	0/3/25/26	0/3/3/3
51	5MC	9	1374	51	-	0/7/25/26	0/2/2/2
1	OMC	5	2804	1	-	0/9/27/28	0/2/2/2
1	B8T	5	4671	1	-	0/7/27/28	0/2/2/2
1	B8Q	5	1456	1	-	1/7/42/43	0/2/2/2
1	MHG	5	4371	1	-	6/16/46/47	0/3/3/3
1	7MG	5	4550	1	-	0/7/37/38	0/3/3/3
1	A2M	5	3785	1	-	3/5/27/28	0/3/3/3
1	A2M	5	4571	1	-	0/5/27/28	0/3/3/3
1	PSU	5	4403	1	-	2/7/25/26	0/2/2/2
51	PSU	9	1243	51	-	2/7/25/26	0/2/2/2
1	A2M	5	2401	1,85	-	0/5/27/28	0/3/3/3
1	P7G	5	1909	1	-	2/10/40/41	0/3/3/3
1	B8H	5	3762	1	-	3/7/25/26	0/2/2/2
6	MLZ	C	333	6	-	2/7/8/10	-
1	OMG	5	1316	1	-	0/5/27/28	0/3/3/3
1	OMC	5	3887	1	-	1/9/27/28	0/2/2/2
1	A2M	5	398	1	-	2/5/27/28	0/3/3/3
1	OMC	5	2365	1	-	0/9/27/28	0/2/2/2
1	P7G	5	3880	1	-	3/10/40/41	0/3/3/3
1	PSU	5	1677	1	-	0/7/25/26	0/2/2/2
1	OMG	5	373	1	-	1/5/27/28	0/3/3/3
51	4AC	9	1337	51	-	0/11/29/30	0/2/2/2
1	A2M	5	1524	1	-	0/5/27/28	0/3/3/3
1	OMG	5	3792	1	-	2/5/27/28	0/3/3/3
1	B9B	5	237	1	-	4/7/29/30	0/3/3/3
1	PSU	5	4500	1	-	4/7/25/26	0/2/2/2
1	OMG	5	1883	1	-	0/5/27/28	0/3/3/3
1	2MG	5	4872	15,1	-	2/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMC	5	4536	1	-	0/9/27/28	0/2/2/2
1	OMG	5	2424	1	-	2/5/27/28	0/3/3/3
1	OMC	5	3869	1	-	0/9/27/28	0/2/2/2
1	B8W	5	4529	1,85	-	2/5/27/28	0/3/3/3
1	5MC	5	4447	1	-	4/7/25/26	0/2/2/2
1	2MG	5	729	1	-	1/5/27/28	0/3/3/3
1	A2M	5	4523	1,85	-	2/5/27/28	0/3/3/3
1	I4U	5	1659	1	-	2/9/29/30	0/2/2/2
1	PSU	5	4442	1	-	0/7/25/26	0/2/2/2
1	OMG	5	4637	1	-	2/5/27/28	0/3/3/3
1	B8W	5	4185	1	-	3/5/27/28	0/3/3/3
1	B9B	5	1574	1	-	2/7/29/30	0/3/3/3
1	UR3	5	1866	1	-	2/7/25/26	0/2/2/2
1	2MG	5	1517	1	-	0/5/27/28	0/3/3/3
1	OMU	5	4620	1	-	1/9/27/28	0/2/2/2
51	A2M	9	1678	51	-	0/5/27/28	0/3/3/3
49	DDE	v	715	49	-	13/20/21/23	0/1/1/1
1	5MU	5	4083	1	-	0/7/25/26	0/2/2/2
1	OMC	5	2422	1,85	-	1/9/27/28	0/2/2/2
1	E6G	5	4355	1	-	3/6/28/29	0/3/3/3
1	OMG	5	2050	1	-	0/5/27/28	0/3/3/3
3	OMU	8	14	1,3	-	1/9/27/28	0/2/2/2
1	B8W	5	2380	1	-	5/5/27/28	0/3/3/3
1	5MC	5	4335	1	-	0/7/25/26	0/2/2/2
1	P4U	5	1348	1,85	-	4/10/29/30	0/2/2/2
1	B8W	5	4129	1	-	3/5/27/28	0/3/3/3
1	7MG	5	2522	1	-	0/7/37/38	0/3/3/3
1	UR3	5	4530	1	-	2/7/25/26	0/2/2/2
1	OMU	5	4306	1	-	0/9/27/28	0/2/2/2
1	B8T	5	4483	1	-	0/7/27/28	0/2/2/2
1	A2M	5	3867	1	-	2/5/27/28	0/3/3/3
1	B8K	5	4690	1,11	-	2/11/41/42	0/3/3/3
1	PSU	5	1683	1	-	0/7/25/26	0/2/2/2
1	OMC	5	2861	1	-	0/9/27/28	0/2/2/2
1	OMG	5	2773	1	-	2/5/27/28	0/3/3/3
1	PSU	5	4628	1	-	0/7/25/26	0/2/2/2
1	PSU	5	3764	1	-	1/7/25/26	0/2/2/2
1	OMG	5	4196	1	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMC	5	3909	1	-	0/9/27/28	0/2/2/2
1	6MZ	5	4220	1	-	0/5/27/28	0/3/3/3
1	A2M	5	1326	1	-	0/5/27/28	0/3/3/3
1	PSU	5	3729	1	-	2/7/25/26	0/2/2/2
1	M7A	5	4564	1	-	0/7/37/38	0/3/3/3
1	OMG	5	4623	1	-	0/5/27/28	0/3/3/3
1	OMG	5	1625	1,85	-	3/5/27/28	0/3/3/3
1	PSU	5	4450	1,85	-	3/7/25/26	0/2/2/2
1	BGH	5	3899	1,85	-	2/13/43/44	0/3/3/3
1	UR3	5	4597	1	-	0/7/25/26	0/2/2/2
1	B8H	5	1860	1	-	0/7/25/26	0/2/2/2
1	OMG	5	4494	1	-	1/5/27/28	0/3/3/3
1	1MA	5	4415	1	-	2/3/25/26	0/3/3/3
1	A2M	5	1871	1,85	-	0/5/27/28	0/3/3/3
1	A2M	5	2363	1,85	-	0/5/27/28	0/3/3/3
1	PSU	5	3715	1	-	0/7/25/26	0/2/2/2
1	PSU	5	4531	1	-	0/7/25/26	0/2/2/2
41	MLZ	m	72	41	-	3/7/8/10	-
1	A2M	5	1534	1,85	-	2/5/27/28	0/3/3/3
1	OMG	5	2364	1	-	2/5/27/28	0/3/3/3
1	E7G	5	2297	1	-	1/9/39/40	0/3/3/3
1	7MG	5	1605	1	-	0/7/37/38	0/3/3/3
1	OMG	5	1522	1	-	0/5/27/28	0/3/3/3
1	OMG	5	4870	1	-	3/5/27/28	0/3/3/3
1	OMG	5	4370	1	-	2/5/27/28	0/3/3/3
1	B8K	5	3897	1	-	3/11/41/42	0/3/3/3
51	B8N	9	1248	51	-	4/16/34/35	0/2/2/2
1	A2M	5	3718	1	-	0/5/27/28	0/3/3/3
1	PSU	5	2508	1	-	0/7/25/26	0/2/2/2
1	PSU	5	1582	1	-	2/7/25/26	0/2/2/2
1	B8H	5	4296	1	-	0/7/25/26	0/2/2/2
1	PSU	5	4636	1	-	3/7/25/26	0/2/2/2
51	B8Q	9	1219	51	-	1/7/42/43	0/2/2/2
1	I4U	5	4194	1	-	3/9/29/30	0/2/2/2
1	5MC	5	3782	1	-	0/7/25/26	0/2/2/2
1	A2M	5	3825	1	-	0/5/27/28	0/3/3/3
1	A2M	5	3723	1	-	0/5/27/28	0/3/3/3
1	B9H	5	2786	1	-	4/12/47/48	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	B8W	5	4472	1	-	2/5/27/28	0/3/3/3
1	PSU	5	4293	1	-	0/7/25/26	0/2/2/2
1	OMC	5	3701	1,85	-	4/9/27/28	0/2/2/2
1	B9B	5	2754	1,85	-	3/7/29/30	0/3/3/3
1	E7G	5	1797	1	-	2/9/39/40	0/3/3/3

All (766) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	2754	B9B	C2'-C1'	-18.08	1.26	1.53
1	5	1574	B9B	C2'-C1'	-17.90	1.26	1.53
1	5	237	B9B	C2'-C1'	-17.70	1.26	1.53
1	5	237	B9B	O4'-C1'	17.26	1.65	1.41
1	5	1574	B9B	O4'-C1'	16.74	1.64	1.41
1	5	2754	B9B	O4'-C1'	16.72	1.64	1.41
1	5	4523	A2M	O4'-C1'	16.62	1.64	1.41
1	5	3723	A2M	O4'-C1'	16.51	1.64	1.41
51	9	1678	A2M	O4'-C1'	16.45	1.64	1.41
1	5	398	A2M	O4'-C1'	16.32	1.63	1.41
1	5	1871	A2M	O4'-C1'	16.25	1.63	1.41
1	5	4571	A2M	O4'-C1'	16.21	1.63	1.41
1	5	3718	A2M	O4'-C1'	16.21	1.63	1.41
1	5	4355	E6G	C2'-C1'	-16.03	1.29	1.53
1	5	2363	A2M	O4'-C1'	16.02	1.63	1.41
1	5	4296	B8H	C6-C5	-15.99	1.12	1.34
1	5	3825	A2M	O4'-C1'	15.96	1.63	1.41
1	5	2401	A2M	O4'-C1'	15.91	1.63	1.41
1	5	1860	B8H	C6-C5	-15.86	1.12	1.34
1	5	3762	B8H	C6-C5	-15.84	1.12	1.34
1	5	1524	A2M	O4'-C1'	15.78	1.63	1.41
1	5	1534	A2M	O4'-C1'	15.68	1.63	1.41
1	5	1326	A2M	O4'-C1'	15.57	1.62	1.41
1	5	3867	A2M	O4'-C1'	15.31	1.62	1.41
1	5	3785	A2M	O4'-C1'	15.26	1.62	1.41
1	5	4355	E6G	O4'-C1'	15.25	1.62	1.41
1	5	1860	B8H	C4-N3	-15.07	1.10	1.38
1	5	4296	B8H	C4-N3	-15.01	1.11	1.38
1	5	3762	B8H	C4-N3	-14.67	1.11	1.38
1	5	4472	B8W	C2'-C1'	-14.66	1.31	1.53
1	5	4415	1MA	C2-N3	14.28	1.46	1.29
1	5	4529	B8W	C2'-C1'	-14.16	1.32	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	2380	B8W	C2'-C1'	-14.05	1.32	1.53
1	5	4185	B8W	C2'-C1'	-13.84	1.32	1.53
1	5	4129	B8W	C2'-C1'	-13.83	1.32	1.53
1	5	3762	B8H	C4-C5	13.74	1.83	1.44
1	5	4129	B8W	O4'-C1'	13.65	1.60	1.41
1	5	1322	1MA	C2-N3	13.57	1.45	1.29
1	5	4296	B8H	C4-C5	13.56	1.82	1.44
1	5	4472	B8W	O4'-C1'	13.51	1.59	1.41
1	5	4529	B8W	O4'-C1'	13.46	1.59	1.41
1	5	1860	B8H	C4-C5	13.38	1.82	1.44
1	5	2380	B8W	O4'-C1'	13.27	1.59	1.41
1	5	3762	B8H	C6-N1	13.19	1.69	1.36
1	5	1860	B8H	C6-N1	13.10	1.68	1.36
1	5	4185	B8W	O4'-C1'	12.93	1.59	1.41
1	5	4296	B8H	C6-N1	12.90	1.68	1.36
1	5	1909	P7G	C8-N9	11.83	1.52	1.46
1	5	4690	B8K	C3'-C4'	-11.56	1.23	1.53
1	5	1659	I4U	C3'-C2'	-11.34	1.22	1.53
1	5	3897	B8K	C3'-C4'	-11.29	1.24	1.53
1	5	4194	I4U	C3'-C2'	-11.18	1.22	1.53
1	5	4083	5MU	C2-N1	10.71	1.55	1.38
1	5	4083	5MU	C6-N1	10.57	1.56	1.38
1	5	3880	P7G	C8-N9	10.54	1.51	1.46
1	5	1659	I4U	C4-N3	10.33	1.44	1.31
1	5	3899	BGH	C3'-C4'	-10.22	1.26	1.53
1	5	4371	MHG	C8-N9	10.21	1.51	1.46
1	5	4194	I4U	C4-N3	9.86	1.44	1.31
1	5	1574	B9B	O6-C6	9.75	1.43	1.35
1	5	2754	B9B	O6-C6	9.75	1.43	1.35
1	5	1348	P4U	C4-N3	9.65	1.43	1.31
1	5	3899	BGH	O4'-C4'	9.62	1.66	1.45
1	5	237	B9B	O6-C6	9.62	1.43	1.35
1	5	4690	B8K	C8-N9	9.54	1.51	1.46
1	5	4447	5MC	C6-C5	9.49	1.50	1.34
1	5	4083	5MU	C4-C5	9.43	1.60	1.44
1	5	1909	P7G	C5-N7	9.39	1.46	1.35
1	5	2786	B9H	C2-N3	9.26	1.49	1.37
51	9	1374	5MC	C6-C5	9.20	1.49	1.34
1	5	4371	MHG	C5-N7	8.96	1.45	1.35
1	5	3782	5MC	C6-C5	8.92	1.49	1.34
1	5	4335	5MC	C6-C5	8.90	1.49	1.34
1	5	3880	P7G	C5-N7	8.66	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	4550	7MG	C8-N9	8.32	1.50	1.46
1	5	4083	5MU	C4-N3	-8.29	1.23	1.38
1	5	4194	I4U	O4'-C4'	-8.29	1.26	1.45
1	5	2522	7MG	C8-N9	8.19	1.50	1.46
51	9	1219	B8Q	C6-C5	8.18	1.51	1.33
1	5	3897	B8K	C2'-C1'	-8.16	1.27	1.53
1	5	4371	MHG	C2-N3	8.10	1.47	1.31
1	5	2297	E7G	C5-N7	8.08	1.44	1.35
1	5	1797	E7G	C5-N7	8.08	1.44	1.35
1	5	1456	B8Q	C6-C5	8.02	1.51	1.33
1	5	4690	B8K	C2'-C1'	-8.01	1.27	1.53
1	5	4355	E6G	O4'-C4'	-7.95	1.27	1.45
51	9	1248	B8N	C4-N3	-7.92	1.25	1.40
1	5	4550	7MG	C5-N7	7.82	1.44	1.35
1	5	1659	I4U	O4'-C4'	-7.80	1.27	1.45
1	5	3867	A2M	O4'-C4'	-7.75	1.27	1.45
1	5	2363	A2M	O4'-C4'	-7.70	1.27	1.45
1	5	2522	7MG	C5-N7	7.69	1.44	1.35
51	9	1678	A2M	O4'-C4'	-7.68	1.27	1.45
1	5	1605	7MG	C5-N7	7.64	1.44	1.35
1	5	1534	A2M	O4'-C4'	-7.61	1.28	1.45
1	5	1524	A2M	O4'-C4'	-7.59	1.28	1.45
1	5	2401	A2M	O4'-C4'	-7.58	1.28	1.45
1	5	4571	A2M	O4'-C4'	-7.52	1.28	1.45
1	5	3825	A2M	O4'-C4'	-7.49	1.28	1.45
1	5	1326	A2M	O4'-C4'	-7.42	1.28	1.45
1	5	3897	B8K	C8-N9	7.41	1.50	1.46
1	5	3723	A2M	O4'-C4'	-7.41	1.28	1.45
1	5	4523	A2M	O4'-C4'	-7.39	1.28	1.45
1	5	1605	7MG	C8-N9	7.34	1.50	1.46
1	5	398	A2M	O4'-C4'	-7.31	1.28	1.45
1	5	3718	A2M	O4'-C4'	-7.31	1.28	1.45
1	5	4220	6MZ	C6-N6	7.29	1.47	1.35
1	5	1871	A2M	O4'-C4'	-7.28	1.28	1.45
1	5	2754	B9B	C2-N2	7.28	1.48	1.33
1	5	2754	B9B	O4'-C4'	-7.28	1.28	1.45
1	5	237	B9B	C2-N2	7.27	1.48	1.33
1	5	2786	B9H	C2-N1	7.23	1.48	1.38
1	5	3785	A2M	O4'-C4'	-7.19	1.28	1.45
1	5	3897	B8K	O4'-C4'	7.18	1.61	1.45
51	9	1248	B8N	C6-N1	7.13	1.54	1.36
1	5	237	B9B	O4'-C4'	-7.12	1.29	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	4690	B8K	O4'-C4'	7.11	1.60	1.45
1	5	1574	B9B	O4'-C4'	-7.09	1.29	1.45
1	5	1797	E7G	C8-N9	7.09	1.49	1.46
1	5	4185	B8W	C3'-C4'	-7.02	1.35	1.53
1	5	1574	B9B	C2-N2	6.96	1.47	1.33
1	5	3782	5MC	C4-N3	6.86	1.45	1.34
1	5	2786	B9H	C6-C5	6.84	1.48	1.33
51	9	1337	4AC	C4-N3	6.75	1.44	1.32
1	5	4529	B8W	C3'-C4'	-6.73	1.35	1.53
1	5	4472	B8W	C3'-C4'	-6.71	1.35	1.53
1	5	4129	B8W	C3'-C4'	-6.70	1.35	1.53
1	5	4335	5MC	C4-N3	6.66	1.45	1.34
1	5	2380	B8W	C3'-C4'	-6.63	1.36	1.53
1	5	4530	UR3	C2-N1	6.59	1.48	1.38
1	5	4597	UR3	C2-N1	6.56	1.48	1.38
1	5	4671	B8T	C4-N3	6.55	1.44	1.32
3	8	14	OMU	C2-N3	6.54	1.49	1.38
1	5	2297	E7G	C8-N7	6.51	1.51	1.45
51	9	1374	5MC	C4-N3	6.46	1.45	1.34
1	5	1797	E7G	C8-N7	6.46	1.51	1.45
1	5	4447	5MC	C4-N3	6.45	1.45	1.34
1	5	4483	B8T	C4-N3	6.43	1.44	1.32
51	9	1219	B8Q	C2-N3	6.43	1.46	1.35
1	5	4306	OMU	C2-N3	6.38	1.49	1.38
1	5	2297	E7G	C8-N9	6.38	1.49	1.46
1	5	1866	UR3	C2-N1	6.34	1.47	1.38
3	8	14	OMU	C2-N1	6.29	1.48	1.38
1	5	4620	OMU	C2-N3	6.28	1.49	1.38
1	5	4355	E6G	O6-C6	6.27	1.40	1.35
1	5	4371	MHG	C8-N7	6.27	1.51	1.45
1	5	4371	MHG	C2-N1	6.23	1.46	1.36
1	5	2422	OMC	C2-N3	6.18	1.48	1.36
1	5	3869	OMC	C6-C5	6.18	1.49	1.35
1	5	4536	OMC	C6-C5	6.15	1.49	1.35
1	5	2804	OMC	C6-C5	6.13	1.49	1.35
1	5	2422	OMC	C6-C5	6.12	1.49	1.35
1	5	3782	5MC	C2-N3	6.12	1.48	1.36
1	5	2861	OMC	C6-C5	6.11	1.49	1.35
51	9	1374	5MC	C2-N3	6.10	1.48	1.36
1	5	4530	UR3	C6-C5	6.09	1.49	1.35
1	5	3701	OMC	C6-C5	6.08	1.49	1.35
1	5	4335	5MC	C2-N3	6.08	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	4306	OMU	C2-N1	6.07	1.48	1.38
1	5	1348	P4U	C6-C5	6.02	1.49	1.35
1	5	1517	2MG	C2-N2	6.02	1.46	1.33
51	9	1337	4AC	C6-C5	6.02	1.49	1.35
1	5	4872	2MG	C2-N2	6.01	1.46	1.33
1	5	1659	I4U	C2-N3	6.01	1.48	1.36
1	5	2861	OMC	C2-N3	6.00	1.48	1.36
1	5	3887	OMC	C6-C5	6.00	1.49	1.35
1	5	4536	OMC	C2-N3	5.99	1.48	1.36
1	5	2365	OMC	C6-C5	5.99	1.49	1.35
1	5	4447	5MC	C2-N3	5.99	1.48	1.36
1	5	3909	OMC	C6-C5	5.98	1.49	1.35
1	5	2365	OMC	C2-N3	5.97	1.48	1.36
1	5	4671	B8T	C2-N3	5.97	1.48	1.36
1	5	729	2MG	C2-N2	5.95	1.46	1.33
1	5	3909	OMC	C2-N3	5.93	1.48	1.36
1	5	4483	B8T	C2-N3	5.91	1.48	1.36
1	5	4690	B8K	C4-N9	5.91	1.44	1.37
1	5	4597	UR3	C6-C5	5.90	1.48	1.35
1	5	3887	OMC	C2-N3	5.90	1.48	1.36
1	5	2804	OMC	C2-N3	5.88	1.48	1.36
1	5	1797	E7G	C2-N3	5.87	1.47	1.33
1	5	3899	BGH	C8-N9	5.87	1.49	1.46
1	5	1866	UR3	C6-C5	5.87	1.48	1.35
51	9	1337	4AC	C2-N3	5.85	1.48	1.36
1	5	4371	MHG	C2-N2	5.84	1.46	1.33
1	5	1348	P4U	C2-N3	5.84	1.48	1.36
1	5	3897	B8K	C4-N9	5.82	1.44	1.37
1	5	4194	I4U	C6-C5	5.81	1.48	1.35
1	5	4483	B8T	C6-C5	5.81	1.48	1.35
1	5	3701	OMC	C2-N3	5.78	1.48	1.36
1	5	2422	OMC	C4-N3	5.77	1.46	1.34
1	5	2297	E7G	C2-N3	5.77	1.47	1.33
1	5	1909	P7G	C2-N1	5.76	1.47	1.33
1	5	1909	P7G	C4-N9	5.75	1.43	1.35
1	5	3869	OMC	C2-N3	5.75	1.48	1.36
1	5	2861	OMC	C4-N3	5.73	1.46	1.34
1	5	3880	P7G	C2-N1	5.72	1.47	1.33
1	5	4671	B8T	C6-C5	5.66	1.48	1.35
1	5	4194	I4U	C1'-N1	-5.66	1.31	1.47
1	5	1797	E7G	C4-N9	5.66	1.44	1.37
1	5	1456	B8Q	C2-N3	5.65	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	1659	I4U	C6-C5	5.65	1.48	1.35
1	5	3909	OMC	C4-N3	5.65	1.45	1.34
1	5	4529	B8W	C2-N2	5.63	1.45	1.33
1	5	2365	OMC	C4-N3	5.60	1.45	1.34
1	5	4620	OMU	C2-N1	5.59	1.47	1.38
1	5	1605	7MG	C2-N3	5.58	1.46	1.33
1	5	3880	P7G	C4-N9	5.57	1.43	1.35
1	5	4550	7MG	C2-N3	5.56	1.46	1.33
1	5	2522	7MG	C2-N3	5.56	1.46	1.33
1	5	2297	E7G	C4-N9	5.55	1.44	1.37
1	5	3701	OMC	C4-N3	5.55	1.45	1.34
1	5	4194	I4U	C2-N3	5.55	1.47	1.36
1	5	1909	P7G	C4-N3	5.54	1.47	1.37
1	5	4690	B8K	C2-N3	5.50	1.46	1.33
1	5	2804	OMC	C4-N3	5.49	1.45	1.34
1	5	3887	OMC	C4-N3	5.49	1.45	1.34
1	5	4083	5MU	C6-C5	5.48	1.43	1.34
1	5	4355	E6G	C2-N2	5.47	1.44	1.33
1	5	4306	OMU	C6-C5	5.46	1.47	1.35
1	5	4129	B8W	C2-N2	5.43	1.44	1.33
1	5	3880	P7G	C4-N3	5.43	1.47	1.37
1	5	3869	OMC	C4-N3	5.42	1.45	1.34
1	5	2380	B8W	C2-N2	5.41	1.44	1.33
1	5	4690	B8K	C3'-C2'	5.41	1.68	1.53
1	5	2522	7MG	C4-N3	5.38	1.47	1.34
1	5	3899	BGH	C2-N3	5.36	1.46	1.33
1	5	4690	B8K	C4-N3	5.34	1.47	1.34
1	5	1522	OMG	C2-N3	5.33	1.46	1.33
1	5	4194	I4U	C3'-C4'	5.33	1.66	1.53
1	5	1605	7MG	C4-N3	5.32	1.46	1.34
1	5	4620	OMU	C6-C5	5.31	1.47	1.35
1	5	3897	B8K	C2-N3	5.30	1.46	1.33
1	5	2424	OMG	C2-N3	5.29	1.46	1.33
1	5	2773	OMG	C2-N3	5.29	1.46	1.33
51	9	1248	B8N	C2-N1	5.29	1.54	1.39
1	5	3792	OMG	C2-N3	5.29	1.46	1.33
1	5	4185	B8W	C2-N2	5.26	1.44	1.33
1	5	4370	OMG	C2-N3	5.25	1.46	1.33
1	5	3762	B8H	C2-N3	5.25	1.47	1.38
1	5	3897	B8K	C3'-C2'	5.25	1.67	1.53
1	5	4564	M7A	C4-N9	5.24	1.47	1.38
1	5	1625	OMG	C2-N3	5.22	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	4371	MHG	C4-N3	5.21	1.46	1.34
1	5	4536	OMC	C4-N3	5.19	1.44	1.34
1	5	373	OMG	C2-N3	5.17	1.45	1.33
1	5	4472	B8W	C2-N2	5.16	1.44	1.33
1	5	4870	OMG	C2-N3	5.16	1.45	1.33
1	5	4623	OMG	C2-N3	5.14	1.45	1.33
1	5	4550	7MG	C4-N3	5.11	1.46	1.34
1	5	4296	B8H	C2-N3	5.11	1.47	1.38
1	5	4196	OMG	C2-N3	5.10	1.45	1.33
1	5	2364	OMG	C2-N3	5.09	1.45	1.33
1	5	1883	OMG	C2-N3	5.08	1.45	1.33
1	5	4494	OMG	C2-N3	5.08	1.45	1.33
1	5	3899	BGH	C4-N3	5.07	1.46	1.34
1	5	2050	OMG	C2-N3	5.07	1.45	1.33
1	5	4371	MHG	C4-N9	5.07	1.43	1.37
1	5	4637	OMG	C2-N3	5.05	1.45	1.33
1	5	1517	2MG	C4-N3	5.05	1.49	1.37
51	9	1219	B8Q	C2-N1	5.04	1.45	1.38
1	5	1316	OMG	C2-N3	5.03	1.45	1.33
1	5	3897	B8K	C4-N3	5.03	1.46	1.34
1	5	1860	B8H	C2-N3	5.03	1.46	1.38
1	5	729	2MG	C4-N3	5.01	1.49	1.37
3	8	14	OMU	C6-C5	4.98	1.46	1.35
1	5	4690	B8K	C5-N7	4.96	1.48	1.39
1	5	1659	I4U	C1'-N1	-4.95	1.33	1.47
1	5	4597	UR3	C2-N3	4.90	1.48	1.39
1	5	1605	7MG	C4-N9	4.88	1.43	1.37
1	5	3792	OMG	C4-N3	4.87	1.49	1.37
1	5	4415	1MA	C2-N1	4.83	1.44	1.35
1	5	4370	OMG	C4-N3	4.83	1.49	1.37
1	5	2773	OMG	C4-N3	4.80	1.49	1.37
1	5	1524	A2M	O3'-C3'	-4.79	1.31	1.43
1	5	3899	BGH	O4'-C1'	-4.79	1.30	1.42
1	5	2424	OMG	C4-N3	4.78	1.49	1.37
1	5	4196	OMG	C4-N3	4.75	1.48	1.37
1	5	3782	5MC	C4-N4	4.74	1.46	1.34
1	5	1883	OMG	C4-N3	4.73	1.48	1.37
1	5	398	A2M	O3'-C3'	-4.73	1.31	1.43
1	5	1797	E7G	C4-N3	4.73	1.45	1.34
1	5	4872	2MG	C2-N1	4.72	1.44	1.36
51	9	1374	5MC	C4-N4	4.72	1.46	1.34
1	5	2522	7MG	C2-N2	4.72	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	3825	A2M	O3'-C3'	-4.70	1.31	1.43
1	5	1326	A2M	O3'-C3'	-4.70	1.31	1.43
1	5	4447	5MC	C6-N1	4.69	1.46	1.38
1	5	3897	B8K	C5-N7	4.69	1.47	1.39
1	5	1883	OMG	C2-N2	4.69	1.45	1.34
1	5	1625	OMG	C4-N3	4.68	1.48	1.37
51	9	1248	B8N	C6-C5	4.68	1.41	1.34
1	5	1605	7MG	C2-N2	4.67	1.45	1.34
1	5	4447	5MC	C4-N4	4.67	1.46	1.34
1	5	373	OMG	C4-N3	4.66	1.48	1.37
51	9	1337	4AC	C7-N4	4.66	1.45	1.37
1	5	4335	5MC	C4-N4	4.66	1.46	1.34
1	5	2424	OMG	C2-N2	4.65	1.45	1.34
1	5	1522	OMG	C4-N3	4.65	1.48	1.37
1	5	2773	OMG	C2-N2	4.65	1.45	1.34
1	5	4870	OMG	C4-N3	4.65	1.48	1.37
1	5	4370	OMG	C2-N2	4.64	1.45	1.34
1	5	2364	OMG	C2-N2	4.64	1.45	1.34
1	5	4530	UR3	C2-N3	4.64	1.48	1.39
1	5	2522	7MG	C4-N9	4.63	1.43	1.37
1	5	4494	OMG	C4-N3	4.63	1.48	1.37
1	5	4637	OMG	C4-N3	4.63	1.48	1.37
1	5	373	OMG	C2-N2	4.62	1.45	1.34
1	5	4623	OMG	C2-N2	4.62	1.45	1.34
1	5	4571	A2M	O3'-C3'	-4.61	1.32	1.43
1	5	3880	P7G	C2-N2	4.61	1.45	1.34
1	5	4483	B8T	C4-N4	4.59	1.45	1.35
1	5	3867	A2M	C6-N6	4.58	1.50	1.34
1	5	4571	A2M	C6-N6	4.58	1.50	1.34
51	9	1678	A2M	O3'-C3'	-4.58	1.32	1.43
1	5	1625	OMG	C2-N2	4.57	1.45	1.34
1	5	3718	A2M	C6-N6	4.57	1.50	1.34
1	5	398	A2M	C6-N6	4.57	1.50	1.34
1	5	2050	OMG	C4-N3	4.57	1.48	1.37
1	5	4550	7MG	C2-N2	4.56	1.45	1.34
1	5	4690	B8K	O4'-C1'	4.56	1.52	1.42
1	5	4550	7MG	C4-N9	4.56	1.43	1.37
1	5	3792	OMG	C2-N2	4.56	1.45	1.34
1	5	1909	P7G	C2-N2	4.55	1.45	1.34
1	5	4623	OMG	C4-N3	4.55	1.48	1.37
1	5	4196	OMG	C2-N2	4.54	1.45	1.34
51	9	1678	A2M	C6-N6	4.54	1.50	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	3723	A2M	C6-N6	4.53	1.50	1.34
1	5	3718	A2M	O3'-C3'	-4.53	1.32	1.43
1	5	4194	I4U	C5-C4	4.52	1.49	1.43
1	5	2364	OMG	C4-N3	4.52	1.48	1.37
1	5	1326	A2M	C6-N6	4.52	1.50	1.34
1	5	4870	OMG	C2-N2	4.52	1.44	1.34
1	5	1871	A2M	C6-N6	4.52	1.50	1.34
1	5	2297	E7G	C4-N3	4.52	1.45	1.34
1	5	1534	A2M	C6-N6	4.51	1.50	1.34
1	5	3825	A2M	C6-N6	4.51	1.50	1.34
1	5	1316	OMG	C2-N2	4.51	1.44	1.34
1	5	2401	A2M	O3'-C3'	-4.50	1.32	1.43
1	5	1871	A2M	O3'-C3'	-4.50	1.32	1.43
1	5	3723	A2M	O3'-C3'	-4.49	1.32	1.43
1	5	4494	OMG	C2-N2	4.49	1.44	1.34
1	5	2401	A2M	C6-N6	4.49	1.50	1.34
1	5	1524	A2M	C6-N6	4.47	1.50	1.34
1	5	3867	A2M	O3'-C3'	-4.47	1.32	1.43
1	5	4523	A2M	C6-N6	4.47	1.50	1.34
1	5	2363	A2M	C6-N6	4.46	1.50	1.34
1	5	2363	A2M	O3'-C3'	-4.46	1.32	1.43
1	5	2050	OMG	C2-N2	4.46	1.44	1.34
1	5	3897	B8K	C2-N2	4.46	1.44	1.34
1	5	1866	UR3	C2-N3	4.45	1.47	1.39
1	5	1659	I4U	C3'-C4'	4.44	1.64	1.53
1	5	4690	B8K	C2-N2	4.44	1.44	1.34
1	5	1316	OMG	C4-N3	4.44	1.48	1.37
51	9	1374	5MC	C6-N1	4.44	1.45	1.38
1	5	1522	OMG	C2-N2	4.44	1.44	1.34
1	5	3899	BGH	C2-N2	4.42	1.44	1.34
1	5	4564	M7A	C6-N6	4.38	1.45	1.34
1	5	4690	B8K	C71-N7	4.37	1.49	1.39
1	5	1909	P7G	C8-N7	4.35	1.49	1.45
1	5	3785	A2M	C6-N6	4.34	1.49	1.34
1	5	3782	5MC	C2-N1	4.33	1.49	1.40
1	5	3899	BGH	C4-N9	4.32	1.42	1.37
1	5	3782	5MC	C6-N1	4.31	1.45	1.38
1	5	3899	BGH	O2'-C2'	-4.30	1.31	1.42
1	5	4671	B8T	C4-N4	4.30	1.44	1.35
51	9	1374	5MC	C2-N1	4.26	1.49	1.40
51	9	1337	4AC	C4-N4	4.25	1.45	1.39
1	5	4637	OMG	C2-N2	4.22	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	1348	P4U	O4-C4	4.18	1.39	1.35
1	5	1534	A2M	O3'-C3'	-4.16	1.33	1.43
1	5	1659	I4U	O4'-C1'	4.16	1.51	1.42
1	5	1348	P4U	C2-N1	4.13	1.48	1.40
1	5	1659	I4U	C5-C4	4.13	1.48	1.43
1	5	4523	A2M	O3'-C3'	-4.12	1.33	1.43
1	5	3880	P7G	C8-N7	4.07	1.49	1.45
1	5	1322	1MA	C2-N1	4.06	1.43	1.35
1	5	3897	B8K	O4'-C1'	4.05	1.51	1.42
1	5	1797	E7G	C2-N2	4.04	1.43	1.34
1	5	1348	P4U	C5-C4	4.01	1.48	1.43
1	5	237	B9B	O3'-C3'	-4.00	1.33	1.43
51	9	1337	4AC	C2-N1	4.00	1.48	1.40
1	5	2297	E7G	C2-N2	3.99	1.43	1.34
1	5	3899	BGH	C5-N7	3.99	1.46	1.39
1	5	4335	5MC	C6-N1	3.97	1.44	1.38
1	5	1517	2MG	C2-N1	3.95	1.43	1.36
1	5	4872	2MG	C6-N1	3.95	1.43	1.37
1	5	4671	B8T	C2-N1	3.94	1.48	1.40
1	5	3897	B8K	C71-N7	3.93	1.48	1.39
1	5	1909	P7G	C5-C4	3.89	1.45	1.37
1	5	2754	B9B	O3'-C3'	-3.89	1.33	1.43
1	5	2861	OMC	C4-N4	3.89	1.43	1.33
1	5	729	2MG	C2-N1	3.88	1.42	1.36
1	5	4335	5MC	C2-N1	3.87	1.48	1.40
1	5	2422	OMC	C4-N4	3.86	1.43	1.33
1	5	2365	OMC	C4-N4	3.85	1.43	1.33
1	5	4564	M7A	C5-N7	3.85	1.48	1.39
1	5	4447	5MC	C2-N1	3.82	1.48	1.40
1	5	3869	OMC	C4-N4	3.82	1.42	1.33
1	5	3785	A2M	O3'-C3'	-3.82	1.34	1.43
51	9	1337	4AC	C5-C4	3.81	1.49	1.40
1	5	4536	OMC	C4-N4	3.78	1.42	1.33
1	5	3909	OMC	C4-N4	3.76	1.42	1.33
1	5	4872	2MG	C4-N3	3.75	1.46	1.37
1	5	2422	OMC	C2-N1	3.75	1.48	1.40
1	5	1574	B9B	O3'-C3'	-3.75	1.34	1.43
1	5	2804	OMC	C4-N4	3.75	1.42	1.33
1	5	4194	I4U	C2-N1	3.75	1.48	1.40
1	5	3701	OMC	C4-N4	3.74	1.42	1.33
1	5	4129	B8W	O4'-C4'	3.74	1.53	1.45
1	5	3887	OMC	C4-N4	3.73	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	4529	B8W	O4'-C4'	3.72	1.53	1.45
1	5	4483	B8T	C2-N1	3.72	1.48	1.40
1	5	3880	P7G	C2-N3	3.72	1.46	1.37
1	5	4536	OMC	C2-N1	3.70	1.48	1.40
1	5	2380	B8W	C3'-C2'	3.64	1.63	1.53
1	5	3909	OMC	O2-C2	-3.62	1.17	1.23
1	5	2380	B8W	O4'-C4'	3.59	1.53	1.45
3	8	14	OMU	C4-N3	3.59	1.45	1.38
1	5	4472	B8W	O4'-C4'	3.58	1.53	1.45
1	5	1797	E7G	C5-C6	3.57	1.52	1.43
1	5	3880	P7G	C5-C4	3.56	1.44	1.37
1	5	3899	BGH	C5-C6	3.55	1.52	1.43
1	5	2365	OMC	C6-N1	3.55	1.46	1.38
51	9	1678	A2M	O2'-C2'	3.54	1.51	1.42
1	5	1659	I4U	C2-N1	3.54	1.47	1.40
1	5	3897	B8K	C2-N1	3.53	1.46	1.37
1	5	4194	I4U	O4'-C1'	3.53	1.50	1.42
1	5	3723	A2M	O2'-C2'	3.52	1.51	1.42
1	5	1909	P7G	C2-N3	3.52	1.46	1.37
1	5	4306	OMU	C4-N3	3.52	1.44	1.38
1	5	2297	E7G	C5-C6	3.51	1.52	1.43
1	5	4129	B8W	C3'-C2'	3.50	1.62	1.53
51	9	1243	PSU	C6-C5	3.50	1.39	1.35
1	5	4690	B8K	C2-N1	3.48	1.46	1.37
1	5	2861	OMC	C2-N1	3.47	1.47	1.40
1	5	1605	7MG	C2-N1	3.47	1.46	1.37
1	5	4185	B8W	O4'-C4'	3.47	1.52	1.45
1	5	1456	B8Q	C2-N1	3.46	1.43	1.38
1	5	4872	2MG	C5-C4	-3.45	1.34	1.43
1	5	4620	OMU	C4-N3	3.45	1.44	1.38
1	5	2424	OMG	C6-N1	3.42	1.43	1.37
1	5	3718	A2M	O2'-C2'	3.42	1.51	1.42
1	5	1797	E7G	C2-N1	3.41	1.46	1.37
1	5	2297	E7G	C2-N1	3.41	1.46	1.37
1	5	2804	OMC	C2-N1	3.40	1.47	1.40
1	5	3869	OMC	C6-N1	3.40	1.46	1.38
1	5	4690	B8K	O6-C6	-3.40	1.17	1.23
51	9	1678	A2M	C2-N3	3.40	1.37	1.32
1	5	1326	A2M	O2'-C2'	3.40	1.51	1.42
1	5	4536	OMC	C6-N1	3.39	1.46	1.38
1	5	4370	OMG	C6-N1	3.38	1.42	1.37
1	5	2522	7MG	C5-C6	3.38	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	1316	OMG	C6-N1	3.38	1.42	1.37
1	5	3825	A2M	O2'-C2'	3.38	1.51	1.42
1	5	3785	A2M	C2-N3	3.38	1.37	1.32
1	5	1534	A2M	C2-N3	3.37	1.37	1.32
1	5	4335	5MC	O2-C2	-3.37	1.17	1.23
1	5	4371	MHG	C5-C6	3.36	1.52	1.43
1	5	3701	OMC	C2-N1	3.35	1.47	1.40
1	5	4355	E6G	O2'-C2'	3.35	1.50	1.43
1	5	1582	PSU	C6-C5	3.35	1.39	1.35
1	5	3785	A2M	O2'-C2'	3.35	1.51	1.42
1	5	398	A2M	O2'-C2'	3.34	1.51	1.42
1	5	2522	7MG	C2-N1	3.34	1.45	1.37
1	5	1605	7MG	C5-C6	3.34	1.52	1.43
1	5	1683	PSU	C6-C5	3.33	1.39	1.35
1	5	2401	A2M	O2'-C2'	3.33	1.51	1.42
1	5	3887	OMC	C2-N1	3.33	1.47	1.40
1	5	4550	7MG	C5-C6	3.32	1.52	1.43
1	5	3887	OMC	O2-C2	-3.31	1.17	1.23
1	5	4194	I4U	O2'-C2'	3.31	1.50	1.43
1	5	4196	OMG	C6-N1	3.31	1.42	1.37
1	5	3887	OMC	C6-N1	3.31	1.46	1.38
1	5	2050	OMG	C6-N1	3.30	1.42	1.37
1	5	3701	OMC	C6-N1	3.30	1.45	1.38
1	5	4623	OMG	C6-N1	3.30	1.42	1.37
1	5	373	OMG	C6-N1	3.29	1.42	1.37
1	5	4571	A2M	C2-N3	3.29	1.37	1.32
1	5	2773	OMG	C6-N1	3.29	1.42	1.37
1	5	4529	B8W	C3'-C2'	3.28	1.62	1.53
1	5	4447	5MC	O2-C2	-3.28	1.17	1.23
1	5	1316	OMG	C5-C4	-3.28	1.34	1.43
1	5	3869	OMC	C2-N1	3.28	1.47	1.40
1	5	398	A2M	C2-N3	3.28	1.37	1.32
1	5	2422	OMC	C6-N1	3.26	1.45	1.38
1	5	4415	1MA	C4-N3	3.26	1.47	1.37
1	5	2861	OMC	C6-N1	3.26	1.45	1.38
1	5	1522	OMG	C6-N1	3.25	1.42	1.37
3	8	14	OMU	O4-C4	-3.24	1.18	1.24
1	5	4571	A2M	O2'-C2'	3.24	1.50	1.42
1	5	1871	A2M	O2'-C2'	3.24	1.50	1.42
1	5	1625	OMG	C6-N1	3.24	1.42	1.37
1	5	4185	B8W	C3'-C2'	3.24	1.62	1.53
1	5	4690	B8K	C5-C6	3.24	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	4483	B8T	C5-C4	3.24	1.47	1.40
1	5	4306	OMU	O4-C4	-3.24	1.18	1.24
1	5	4671	B8T	C5-C4	3.24	1.47	1.40
1	5	3764	PSU	C6-C5	3.24	1.39	1.35
1	5	2804	OMC	C6-N1	3.23	1.45	1.38
1	5	2363	A2M	O2'-C2'	3.23	1.50	1.42
1	5	2364	OMG	C6-N1	3.23	1.42	1.37
1	5	4296	B8H	O4-C4	-3.22	1.17	1.23
1	5	1860	B8H	O4-C4	-3.22	1.17	1.23
1	5	2861	OMC	O2-C2	-3.22	1.17	1.23
1	5	3899	BGH	C2-N1	3.21	1.45	1.37
1	5	4355	E6G	O3'-C3'	-3.21	1.35	1.43
51	9	1374	5MC	O2-C2	-3.21	1.17	1.23
1	5	4483	B8T	C6-N1	3.21	1.45	1.38
1	5	1524	A2M	O2'-C2'	3.19	1.50	1.42
1	5	2365	OMC	C2-N1	3.19	1.46	1.40
1	5	3867	A2M	O2'-C2'	3.18	1.50	1.42
1	5	3785	A2M	C5-C4	-3.18	1.32	1.40
1	5	2804	OMC	O2-C2	-3.18	1.17	1.23
1	5	4194	I4U	O4-C41	-3.18	1.39	1.47
1	5	4637	OMG	C6-N1	3.18	1.42	1.37
1	5	1883	OMG	C5-C4	-3.18	1.35	1.43
1	5	4494	OMG	C6-N1	3.17	1.42	1.37
1	5	4872	2MG	O6-C6	-3.17	1.16	1.23
1	5	2401	A2M	C2-N3	3.17	1.37	1.32
1	5	3909	OMC	C6-N1	3.17	1.45	1.38
1	5	1517	2MG	O6-C6	-3.16	1.16	1.23
1	5	4220	6MZ	C5-C4	-3.16	1.32	1.40
1	5	4494	OMG	C5-C4	-3.15	1.35	1.43
1	5	4550	7MG	C2-N1	3.15	1.45	1.37
1	5	4523	A2M	O2'-C2'	3.14	1.50	1.42
1	5	4371	MHG	C6-N1	3.14	1.44	1.38
1	5	3899	BGH	O6-C6	-3.13	1.17	1.23
1	5	3723	A2M	C2-N3	3.13	1.37	1.32
1	5	1534	A2M	C5-C4	-3.12	1.32	1.40
1	5	1659	I4U	O2'-C2'	3.12	1.50	1.43
1	5	4870	OMG	C6-N1	3.12	1.42	1.37
1	5	4536	OMC	O2-C2	-3.11	1.17	1.23
1	5	3909	OMC	C2-N1	3.11	1.46	1.40
1	5	1524	A2M	C2-N3	3.10	1.37	1.32
1	5	1883	OMG	C6-N1	3.10	1.42	1.37
1	5	373	OMG	C5-C4	-3.10	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	4523	A2M	C2-N3	3.09	1.37	1.32
1	5	3897	B8K	C5-C6	3.08	1.51	1.43
1	5	3869	OMC	O2-C2	-3.08	1.18	1.23
1	5	4637	OMG	C5-C4	-3.07	1.35	1.43
1	5	3792	OMG	C6-N1	3.07	1.42	1.37
1	5	2365	OMC	O2-C2	-3.06	1.18	1.23
1	5	729	2MG	O6-C6	-3.06	1.17	1.23
1	5	4620	OMU	O4-C4	-3.06	1.18	1.24
1	5	1517	2MG	C6-N1	3.06	1.42	1.37
1	5	3825	A2M	C2-N3	3.05	1.37	1.32
1	5	1659	I4U	C6-N1	3.04	1.45	1.38
1	5	2380	B8W	C5-C4	-3.04	1.32	1.40
1	5	2050	OMG	C5-C4	-3.04	1.35	1.43
1	5	4472	B8W	C5-C4	-3.03	1.32	1.40
1	5	1522	OMG	C5-C4	-3.03	1.35	1.43
1	5	1326	A2M	C2-N3	3.02	1.37	1.32
1	5	4523	A2M	C5-C4	-3.02	1.32	1.40
1	5	4293	PSU	C6-C5	3.01	1.38	1.35
1	5	1871	A2M	C5-C4	-3.01	1.33	1.40
1	5	2422	OMC	O2-C2	-3.01	1.18	1.23
1	5	3762	B8H	O4-C4	-3.01	1.17	1.23
1	5	4872	2MG	C5-C6	3.00	1.53	1.47
1	5	4472	B8W	C3'-C2'	2.99	1.61	1.53
1	5	1348	P4U	O2-C2	-2.99	1.18	1.23
1	5	4194	I4U	O2-C2	-2.99	1.18	1.23
1	5	3715	PSU	C6-C5	2.98	1.38	1.35
51	9	1337	4AC	C6-N1	2.98	1.45	1.38
1	5	2522	7MG	C6-N1	2.98	1.44	1.38
1	5	4628	PSU	C6-C5	2.98	1.38	1.35
1	5	4370	OMG	C5-C4	-2.98	1.35	1.43
1	5	2424	OMG	C5-C4	-2.98	1.35	1.43
1	5	3867	A2M	C5-C4	-2.98	1.33	1.40
1	5	3785	A2M	C3'-C4'	2.97	1.60	1.53
1	5	2364	OMG	C5-C4	-2.97	1.35	1.43
1	5	3897	B8K	C6-N1	2.97	1.44	1.38
1	5	1322	1MA	C4-N3	2.97	1.46	1.37
1	5	3729	PSU	C6-C5	2.96	1.38	1.35
1	5	4442	PSU	C6-C5	2.96	1.38	1.35
1	5	4185	B8W	C5-C4	-2.96	1.33	1.40
1	5	4355	E6G	C5-C4	-2.96	1.33	1.40
1	5	2363	A2M	C2-N3	2.95	1.36	1.32
1	5	4571	A2M	C5-C4	-2.95	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	4220	6MZ	C2-N3	2.95	1.36	1.32
1	5	2508	PSU	C6-C5	2.95	1.38	1.35
1	5	4623	OMG	C5-C4	-2.94	1.35	1.43
1	5	4483	B8T	O2-C2	-2.94	1.18	1.23
1	5	4530	UR3	C6-N1	2.94	1.45	1.38
1	5	4083	5MU	O4-C4	-2.93	1.18	1.23
1	5	3897	B8K	O6-C6	-2.93	1.18	1.23
1	5	2363	A2M	C5-C4	-2.93	1.33	1.40
1	5	1517	2MG	C5-C4	-2.93	1.35	1.43
1	5	3792	OMG	C5-C4	-2.92	1.35	1.43
1	5	4870	OMG	C5-C4	-2.92	1.35	1.43
1	5	1524	A2M	C5-C4	-2.92	1.33	1.40
1	5	1522	OMG	C5-C6	2.91	1.53	1.47
1	5	1659	I4U	O2-C2	-2.91	1.18	1.23
1	5	1605	7MG	C6-N1	2.89	1.44	1.38
1	5	4671	B8T	O2-C2	-2.89	1.18	1.23
1	5	4531	PSU	C6-C5	2.89	1.38	1.35
1	5	3718	A2M	C2-N3	2.88	1.36	1.32
1	5	2401	A2M	C5-C4	-2.88	1.33	1.40
1	5	1326	A2M	C5-C4	-2.88	1.33	1.40
1	5	1534	A2M	O2'-C2'	2.87	1.50	1.42
1	5	1871	A2M	C2-N3	2.86	1.36	1.32
1	5	1456	B8Q	O2-C2	-2.86	1.17	1.22
1	5	3782	5MC	O2-C2	-2.86	1.18	1.23
1	5	3899	BGH	C71-N7	2.86	1.46	1.39
1	5	1625	OMG	C5-C4	-2.85	1.35	1.43
1	5	3880	P7G	O6-C6	-2.84	1.19	1.23
51	9	1219	B8Q	O2-C2	-2.84	1.17	1.22
1	5	1909	P7G	O6-C6	-2.84	1.19	1.23
1	5	3825	A2M	C5-C4	-2.84	1.33	1.40
1	5	4597	UR3	C6-N1	2.82	1.44	1.38
1	5	398	A2M	C5-C4	-2.82	1.33	1.40
1	5	3723	A2M	C5-C4	-2.82	1.33	1.40
1	5	1659	I4U	O4-C4	2.82	1.40	1.35
1	5	1677	PSU	O4'-C1'	-2.82	1.39	1.43
1	5	3867	A2M	C2-N3	2.81	1.36	1.32
1	5	3718	A2M	C5-C4	-2.81	1.33	1.40
1	5	1659	I4U	O4-C41	-2.81	1.40	1.47
1	5	4529	B8W	C5-C4	-2.81	1.33	1.40
1	5	4690	B8K	C6-N1	2.80	1.44	1.38
1	5	4196	OMG	C5-C6	2.79	1.53	1.47
1	5	729	2MG	C5-C4	-2.79	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	1883	OMG	O6-C6	-2.79	1.17	1.23
51	9	1678	A2M	C5-C4	-2.77	1.33	1.40
1	5	4129	B8W	C5-C4	-2.77	1.33	1.40
1	5	4196	OMG	C5-C4	-2.76	1.36	1.43
1	5	1605	7MG	O6-C6	-2.75	1.18	1.23
1	5	3701	OMC	O2-C2	-2.75	1.18	1.23
1	5	4403	PSU	C6-C5	2.74	1.38	1.35
1	5	3792	OMG	C5-C6	2.74	1.53	1.47
1	5	4306	OMU	O2-C2	-2.73	1.18	1.23
51	9	1337	4AC	O2-C2	-2.72	1.18	1.23
1	5	2754	B9B	O2'-C2'	2.70	1.49	1.43
1	5	2297	E7G	C6-N1	2.69	1.43	1.38
1	5	4194	I4U	C6-N1	2.69	1.44	1.38
1	5	4550	7MG	C6-N1	2.68	1.43	1.38
1	5	4494	OMG	C5-C6	2.68	1.52	1.47
1	5	2773	OMG	C5-C6	2.68	1.52	1.47
1	5	2424	OMG	C5-C6	2.67	1.52	1.47
1	5	4550	7MG	O6-C6	-2.67	1.18	1.23
1	5	1797	E7G	C6-N1	2.66	1.43	1.38
1	5	2754	B9B	C5-C4	-2.66	1.33	1.40
1	5	4620	OMU	O2-C2	-2.65	1.18	1.23
1	5	2773	OMG	C5-C4	-2.65	1.36	1.43
1	5	4870	OMG	C5-C6	2.65	1.52	1.47
1	5	4371	MHG	O6-C6	-2.65	1.18	1.23
1	5	1866	UR3	C6-N1	2.65	1.44	1.38
1	5	4637	OMG	C5-C6	2.64	1.52	1.47
1	5	3899	BGH	C6-N1	2.63	1.43	1.38
1	5	4500	PSU	C6-C5	2.63	1.38	1.35
1	5	4370	OMG	C5-C6	2.63	1.52	1.47
1	5	237	B9B	O2'-C2'	2.63	1.49	1.43
1	5	4636	PSU	C6-C5	2.62	1.38	1.35
1	5	4671	B8T	C6-N1	2.62	1.44	1.38
1	5	2364	OMG	O6-C6	-2.61	1.18	1.23
1	5	1322	1MA	C5-C4	-2.61	1.36	1.43
1	5	4623	OMG	C5-C6	2.61	1.52	1.47
1	5	2522	7MG	O6-C6	-2.59	1.18	1.23
1	5	4083	5MU	O2-C2	-2.59	1.18	1.23
1	5	1517	2MG	C5-C6	2.57	1.52	1.47
1	5	1574	B9B	O2'-C2'	2.57	1.49	1.43
1	5	1316	OMG	C5-C6	2.57	1.52	1.47
1	5	4370	OMG	C2-N1	2.56	1.44	1.37
1	5	729	2MG	C6-N1	2.55	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	3792	OMG	O6-C6	-2.54	1.18	1.23
1	5	2050	OMG	C5-C6	2.54	1.52	1.47
1	5	1348	P4U	C6-N1	2.53	1.44	1.38
1	5	2773	OMG	C2-N1	2.53	1.43	1.37
1	5	373	OMG	C5-C6	2.53	1.52	1.47
1	5	2050	OMG	C2-N1	2.53	1.43	1.37
1	5	2424	OMG	C2-N1	2.52	1.43	1.37
1	5	2364	OMG	C2-N1	2.50	1.43	1.37
1	5	2050	OMG	O6-C6	-2.48	1.18	1.23
1	5	1866	UR3	O4-C4	-2.47	1.18	1.23
1	5	4494	OMG	O6-C6	-2.46	1.18	1.23
1	5	2364	OMG	C5-C6	2.46	1.52	1.47
1	5	729	2MG	C5-C6	2.45	1.52	1.47
1	5	4306	OMU	C6-N1	2.45	1.43	1.38
1	5	373	OMG	C2-N1	2.44	1.43	1.37
1	5	4450	PSU	C6-C5	2.44	1.38	1.35
1	5	1625	OMG	C2-N1	2.43	1.43	1.37
1	5	1574	B9B	C5-C4	-2.43	1.34	1.40
3	8	14	OMU	O2-C2	-2.43	1.18	1.23
1	5	4623	OMG	O6-C6	-2.43	1.18	1.23
1	5	1316	OMG	O6-C6	-2.42	1.18	1.23
1	5	3899	BGH	O5'-C5'	-2.42	1.38	1.44
1	5	2424	OMG	O6-C6	-2.42	1.18	1.23
1	5	4415	1MA	C5-C4	-2.42	1.36	1.43
1	5	1316	OMG	C2-N1	2.40	1.43	1.37
1	5	1797	E7G	O6-C6	-2.39	1.19	1.23
1	5	237	B9B	C5-C4	-2.39	1.34	1.40
1	5	4530	UR3	O4-C4	-2.39	1.18	1.23
1	5	4196	OMG	C2-N1	2.38	1.43	1.37
1	5	4623	OMG	C2-N1	2.38	1.43	1.37
1	5	4370	OMG	O6-C6	-2.38	1.18	1.23
1	5	4870	OMG	O6-C6	-2.37	1.18	1.23
1	5	4196	OMG	O6-C6	-2.37	1.18	1.23
1	5	1625	OMG	O6-C6	-2.37	1.18	1.23
1	5	3792	OMG	C2-N1	2.37	1.43	1.37
1	5	1883	OMG	C5-C6	2.36	1.52	1.47
1	5	1625	OMG	C5-C6	2.36	1.52	1.47
1	5	1522	OMG	O6-C6	-2.36	1.18	1.23
1	5	4597	UR3	O4-C4	-2.36	1.18	1.23
1	5	4494	OMG	C2-N1	2.35	1.43	1.37
1	5	373	OMG	O6-C6	-2.34	1.18	1.23
1	5	4637	OMG	C2-N1	2.34	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	4637	OMG	O6-C6	-2.32	1.18	1.23
1	5	4870	OMG	C2-N1	2.32	1.43	1.37
1	5	1866	UR3	O2-C2	-2.32	1.18	1.22
1	5	3723	A2M	C3'-C4'	2.28	1.58	1.53
1	5	2773	OMG	O6-C6	-2.27	1.18	1.23
1	5	4450	PSU	C4-C5	-2.27	1.37	1.44
1	5	4194	I4U	O4-C4	2.26	1.39	1.35
3	8	14	OMU	C6-N1	2.26	1.43	1.38
1	5	3718	A2M	C5'-C4'	2.26	1.58	1.51
51	9	1248	B8N	O2-C2	-2.25	1.18	1.22
1	5	1522	OMG	C2-N1	2.25	1.43	1.37
1	5	2297	E7G	O6-C6	-2.24	1.19	1.23
1	5	4530	UR3	O2-C2	-2.24	1.18	1.22
51	9	1678	A2M	C3'-C4'	2.23	1.58	1.53
1	5	3867	A2M	C5'-C4'	2.22	1.58	1.51
1	5	3718	A2M	C3'-C4'	2.22	1.58	1.53
51	9	1248	B8N	O4-C4	-2.21	1.18	1.23
1	5	4529	B8W	O5'-C5'	-2.21	1.39	1.44
1	5	4597	UR3	O2-C2	-2.19	1.18	1.22
1	5	3723	A2M	C5'-C4'	2.19	1.58	1.51
1	5	1534	A2M	O5'-C5'	-2.19	1.39	1.44
1	5	3785	A2M	C5'-C4'	2.17	1.58	1.51
1	5	1677	PSU	C6-C5	2.17	1.37	1.35
1	5	1871	A2M	C5'-C4'	2.17	1.58	1.51
1	5	398	A2M	C5'-C4'	2.16	1.58	1.51
1	5	4620	OMU	C6-N1	2.16	1.43	1.38
1	5	1883	OMG	C2-N1	2.16	1.43	1.37
1	5	2363	A2M	O5'-C5'	-2.16	1.39	1.44
1	5	237	B9B	C5'-C4'	2.15	1.58	1.51
1	5	4220	6MZ	C6-N1	-2.15	1.30	1.34
1	5	4636	PSU	C4-C5	-2.15	1.38	1.44
1	5	4523	A2M	C5'-C4'	2.14	1.58	1.51
1	5	1574	B9B	C5'-C4'	2.13	1.58	1.51
1	5	3867	A2M	C3'-C4'	2.12	1.58	1.53
1	5	2401	A2M	O5'-C5'	-2.12	1.39	1.44
1	5	3897	B8K	C5-C4	2.12	1.45	1.38
1	5	398	A2M	C3'-C4'	2.12	1.58	1.53
1	5	4523	A2M	C3'-C4'	2.11	1.58	1.53
1	5	1909	P7G	C6-N1	2.11	1.41	1.38
1	5	4628	PSU	O4'-C1'	-2.10	1.40	1.43
1	5	1871	A2M	C3'-C4'	2.09	1.58	1.53
1	5	4472	B8W	O5'-C5'	-2.09	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	4690	B8K	C5-C4	2.08	1.44	1.38
1	5	1534	A2M	C3'-C4'	2.07	1.58	1.53
1	5	2401	A2M	C5'-C4'	2.07	1.58	1.51
1	5	1326	A2M	C3'-C4'	2.07	1.58	1.53
1	5	4571	A2M	C5'-C4'	2.06	1.58	1.51
1	5	2754	B9B	C5'-C4'	2.05	1.58	1.51
1	5	1524	A2M	C5'-C4'	2.04	1.58	1.51
51	9	1678	A2M	C5'-C4'	2.04	1.58	1.51
1	5	1456	B8Q	C4-N3	-2.03	1.45	1.48
1	5	1326	A2M	C5'-C4'	2.03	1.57	1.51
1	5	1524	A2M	O5'-C5'	-2.03	1.39	1.44
1	5	1677	PSU	C4-C5	-2.03	1.38	1.44
1	5	1582	PSU	O4'-C1'	-2.03	1.41	1.43
1	5	4129	B8W	O5'-C5'	-2.02	1.39	1.44
51	9	1248	B8N	O4'-C1'	-2.02	1.41	1.43
1	5	2363	A2M	C5-N7	-2.02	1.32	1.39
1	5	4355	E6G	O5'-C5'	-2.02	1.39	1.44
1	5	4185	B8W	O5'-C5'	-2.01	1.39	1.44
1	5	4571	A2M	O5'-C5'	-2.01	1.39	1.44
1	5	3718	A2M	C5-N7	-2.01	1.32	1.39

All (475) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	4529	B8W	N2-C2-N3	17.01	145.51	117.79
1	5	2380	B8W	N2-C2-N3	16.88	145.29	117.79
1	5	4129	B8W	N2-C2-N3	16.74	145.07	117.79
1	5	4185	B8W	N2-C2-N3	16.50	144.68	117.79
1	5	4472	B8W	N2-C2-N3	16.34	144.42	117.79
1	5	2380	B8W	N2-C2-N1	-14.90	94.08	117.25
1	5	4529	B8W	N2-C2-N1	-14.71	94.37	117.25
1	5	4129	B8W	N2-C2-N1	-14.49	94.71	117.25
1	5	4472	B8W	N2-C2-N1	-14.38	94.89	117.25
1	5	4185	B8W	N2-C2-N1	-13.95	95.55	117.25
1	5	2380	B8W	C1'-N9-C4	13.44	150.25	126.64
1	5	4564	M7A	C5-C6-N6	13.39	146.61	123.74
1	5	4529	B8W	C1'-N9-C4	13.35	150.09	126.64
1	5	4472	B8W	C1'-N9-C4	13.13	149.71	126.64
1	5	4129	B8W	C1'-N9-C4	12.98	149.44	126.64
1	5	4083	5MU	C5-C4-N3	11.81	125.39	115.31
1	5	4185	B8W	C1'-N9-C4	11.30	146.49	126.64
1	5	4564	M7A	N6-C6-N1	-11.27	93.66	118.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	4083	5MU	C5-C6-N1	-9.34	113.73	123.34
1	5	1871	A2M	C5-C6-N6	7.80	132.21	120.35
1	5	3825	A2M	C5-C6-N6	7.77	132.16	120.35
1	5	3718	A2M	C5-C6-N6	7.72	132.08	120.35
1	5	1326	A2M	C5-C6-N6	7.68	132.03	120.35
1	5	2363	A2M	C5-C6-N6	7.63	131.94	120.35
51	9	1678	A2M	C5-C6-N6	7.57	131.85	120.35
1	5	2786	B9H	C31-N3-C2	7.49	126.57	117.21
1	5	2401	A2M	C5-C6-N6	7.46	131.69	120.35
1	5	3723	A2M	C5-C6-N6	7.45	131.67	120.35
1	5	3867	A2M	C5-C6-N6	7.37	131.55	120.35
1	5	1524	A2M	C5-C6-N6	7.36	131.53	120.35
1	5	4523	A2M	C5-C6-N6	7.35	131.53	120.35
1	5	398	A2M	C5-C6-N6	7.35	131.52	120.35
1	5	4571	A2M	C5-C6-N6	7.34	131.50	120.35
1	5	1534	A2M	C5-C6-N6	7.33	131.49	120.35
1	5	4529	B8W	O6-C6-C5	7.15	126.23	116.01
1	5	4185	B8W	O6-C6-C5	7.02	126.05	116.01
1	5	3762	B8H	C4-N3-C2	-6.98	118.31	127.35
1	5	4296	B8H	C4-N3-C2	-6.84	118.50	127.35
1	5	1860	B8H	C4-N3-C2	-6.80	118.55	127.35
51	9	1219	B8Q	C1'-N1-C2	6.61	128.14	116.99
1	5	3785	A2M	C5-C6-N6	6.43	130.13	120.35
1	5	4371	MHG	C2-N3-C4	6.18	119.70	112.04
1	5	4129	B8W	O6-C6-C5	6.08	124.71	116.01
1	5	1871	A2M	N3-C2-N1	-6.04	119.24	128.68
3	8	14	OMU	C4-N3-C2	-6.02	118.64	126.58
1	5	4296	B8H	N3-C2-N1	6.02	121.64	115.14
1	5	4690	B8K	C5-C6-N1	5.99	121.56	110.99
1	5	4472	B8W	O6-C6-C5	5.98	124.56	116.01
1	5	4690	B8K	C72-C71-N7	5.97	127.84	118.86
1	5	4564	M7A	N3-C4-N9	5.93	134.37	126.87
1	5	3762	B8H	N3-C2-N1	5.92	121.54	115.14
1	5	1909	P7G	C4-C5-N7	5.90	109.78	106.67
1	5	2401	A2M	N3-C2-N1	-5.90	119.46	128.68
1	5	3880	P7G	C4-C5-N7	5.85	109.76	106.67
1	5	1524	A2M	N3-C2-N1	-5.84	119.55	128.68
1	5	3723	A2M	N3-C2-N1	-5.84	119.55	128.68
1	5	3897	B8K	C72-C71-N7	5.80	127.59	118.86
1	5	4571	A2M	N3-C2-N1	-5.78	119.64	128.68
1	5	4564	M7A	N3-C2-N1	-5.74	119.62	128.60
1	5	2363	A2M	N3-C2-N1	-5.74	119.71	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	3899	BGH	C5-C6-N1	5.73	121.08	110.99
1	5	1534	A2M	N3-C2-N1	-5.71	119.75	128.68
1	5	3825	A2M	N3-C2-N1	-5.67	119.81	128.68
51	9	1219	B8Q	O2-C2-N3	-5.67	114.62	122.95
1	5	398	A2M	N3-C2-N1	-5.64	119.87	128.68
1	5	1797	E7G	C4-C5-N7	5.63	109.92	104.91
1	5	1326	A2M	N3-C2-N1	-5.62	119.89	128.68
51	9	1678	A2M	N3-C2-N1	-5.62	119.89	128.68
1	5	4185	B8W	N3-C2-N1	-5.59	119.77	127.22
1	5	3897	B8K	C5-C6-N1	5.59	120.84	110.99
1	5	1860	B8H	N3-C2-N1	5.58	121.17	115.14
1	5	4523	A2M	N3-C2-N1	-5.57	119.97	128.68
1	5	4355	E6G	N3-C2-N1	-5.57	119.79	127.22
1	5	4220	6MZ	N3-C2-N1	-5.55	120.00	128.68
1	5	4306	OMU	C4-N3-C2	-5.48	119.35	126.58
1	5	3785	A2M	N3-C2-N1	-5.42	120.20	128.68
1	5	3867	A2M	N3-C2-N1	-5.42	120.21	128.68
1	5	1534	A2M	N6-C6-N1	-5.37	107.43	118.57
51	9	1219	B8Q	N3-C2-N1	5.37	123.44	117.13
1	5	4628	PSU	N1-C2-N3	5.35	121.20	115.13
1	5	2401	A2M	N6-C6-N1	-5.33	107.52	118.57
1	5	4529	B8W	N3-C2-N1	-5.33	120.12	127.22
1	5	2363	A2M	N6-C6-N1	-5.32	107.53	118.57
1	5	2297	E7G	C4-C5-N7	5.32	109.64	104.91
1	5	237	B9B	N3-C2-N1	-5.31	120.14	127.22
1	5	3825	A2M	N6-C6-N1	-5.29	107.60	118.57
51	9	1219	B8Q	C6-N1-C2	-5.29	117.05	121.79
1	5	1326	A2M	N6-C6-N1	-5.28	107.61	118.57
1	5	4129	B8W	N3-C2-N1	-5.25	120.21	127.22
1	5	1456	B8Q	C31-N3-C4	5.22	122.12	114.25
1	5	4371	MHG	C4-C5-N7	5.22	109.55	104.91
1	5	4371	MHG	C5-C6-N1	5.21	120.18	110.99
1	5	1871	A2M	N6-C6-N1	-5.20	107.78	118.57
1	5	3899	BGH	C72-C71-N7	5.18	126.65	118.86
1	5	4690	B8K	C4-C5-N7	5.18	109.52	104.91
1	5	1605	7MG	C5-C6-N1	5.18	120.11	110.99
1	5	1574	B9B	O6-C6-N1	-5.15	115.68	120.12
1	5	3897	B8K	C4-C5-N7	5.15	109.49	104.91
1	5	4636	PSU	C4-N3-C2	-5.14	118.93	126.34
1	5	4083	5MU	N3-C2-N1	5.14	121.71	114.89
1	5	2754	B9B	N3-C2-N1	-5.12	120.40	127.22
51	9	1678	A2M	N6-C6-N1	-5.09	108.00	118.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	3718	A2M	N6-C6-N1	-5.08	108.02	118.57
1	5	1524	A2M	N6-C6-N1	-5.07	108.04	118.57
1	5	1797	E7G	C5-C6-N1	5.07	119.92	110.99
1	5	1322	1MA	N1-C2-N3	-5.06	120.12	126.02
1	5	4500	PSU	C4-N3-C2	-5.06	119.05	126.34
1	5	398	A2M	N6-C6-N1	-5.04	108.10	118.57
1	5	1456	B8Q	N3-C2-N1	5.04	123.06	117.13
1	5	4450	PSU	C4-N3-C2	-5.04	119.08	126.34
1	5	4620	OMU	C4-N3-C2	-5.02	119.96	126.58
1	5	2297	E7G	C5-C6-N1	5.01	119.82	110.99
1	5	1574	B9B	N3-C2-N1	-4.98	120.58	127.22
1	5	4523	A2M	N6-C6-N1	-4.98	108.24	118.57
1	5	4571	A2M	N6-C6-N1	-4.97	108.25	118.57
51	9	1219	B8Q	C31-N3-C4	4.97	121.74	114.25
1	5	3723	A2M	N6-C6-N1	-4.96	108.27	118.57
1	5	2380	B8W	N3-C2-N1	-4.95	120.62	127.22
1	5	3867	A2M	N6-C6-N1	-4.91	108.38	118.57
1	5	4472	B8W	N3-C2-N1	-4.90	120.68	127.22
1	5	4415	1MA	N1-C2-N3	-4.90	120.31	126.02
1	5	1677	PSU	C4-N3-C2	-4.89	119.29	126.34
1	5	2522	7MG	C5-C6-N1	4.89	119.61	110.99
1	5	4293	PSU	N1-C2-N3	4.87	120.65	115.13
51	9	1248	B8N	C5-C4-N3	4.86	125.18	116.17
1	5	4628	PSU	C4-N3-C2	-4.85	119.36	126.34
1	5	4550	7MG	C5-C6-N1	4.82	119.49	110.99
1	5	4083	5MU	O4-C4-C5	-4.81	119.33	124.90
1	5	4500	PSU	N1-C2-N3	4.81	120.58	115.13
1	5	4083	5MU	C4-N3-C2	-4.80	121.14	127.35
1	5	4531	PSU	N1-C2-N3	4.77	120.53	115.13
1	5	3718	A2M	N3-C2-N1	-4.76	121.23	128.68
1	5	4531	PSU	C4-N3-C2	-4.76	119.48	126.34
1	5	4293	PSU	C4-N3-C2	-4.74	119.51	126.34
1	5	3785	A2M	N6-C6-N1	-4.74	108.74	118.57
1	5	4529	B8W	C3'-C2'-C1'	4.73	108.11	100.98
1	5	4450	PSU	N1-C2-N3	4.73	120.49	115.13
1	5	4442	PSU	N1-C2-N3	4.70	120.46	115.13
1	5	237	B9B	O6-C6-N1	-4.69	116.08	120.12
1	5	4636	PSU	N1-C2-N3	4.67	120.42	115.13
1	5	237	B9B	C2-N3-C4	4.66	120.68	115.36
1	5	4442	PSU	C4-N3-C2	-4.62	119.69	126.34
1	5	2297	E7G	C2-N3-C4	4.59	120.48	112.30
1	5	1683	PSU	N1-C2-N3	4.57	120.31	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	2380	B8W	C3'-C2'-C1'	4.55	107.82	100.98
1	5	1677	PSU	N1-C2-N3	4.52	120.25	115.13
1	5	2380	B8W	O6-C6-C5	4.48	122.41	116.01
1	5	3899	BGH	C2-N3-C4	4.47	120.27	112.30
1	5	3729	PSU	N1-C2-N3	4.42	120.14	115.13
1	5	1683	PSU	C4-N3-C2	-4.40	119.99	126.34
1	5	1582	PSU	C4-N3-C2	-4.40	120.00	126.34
1	5	3715	PSU	C4-N3-C2	-4.39	120.01	126.34
1	5	4403	PSU	N1-C2-N3	4.39	120.11	115.13
1	5	1659	I4U	C5-C4-N3	-4.39	118.23	124.91
1	5	1797	E7G	C2-N3-C4	4.39	120.12	112.30
1	5	4403	PSU	C4-N3-C2	-4.38	120.02	126.34
1	5	4550	7MG	C2-N3-C4	4.38	120.10	112.30
51	9	1248	B8N	C4-N3-C2	-4.37	119.93	125.46
1	5	2522	7MG	C2-N3-C4	4.37	120.08	112.30
1	5	4355	E6G	C2-N3-C4	4.35	120.32	115.36
1	5	1582	PSU	N1-C2-N3	4.34	120.05	115.13
1	5	2508	PSU	C4-N3-C2	-4.34	120.08	126.34
1	5	3729	PSU	C4-N3-C2	-4.31	120.13	126.34
1	5	1605	7MG	C2-N3-C4	4.30	119.96	112.30
1	5	2754	B9B	C2-N3-C4	4.30	120.26	115.36
1	5	4690	B8K	C2-N3-C4	4.29	119.94	112.30
1	5	3764	PSU	C4-N3-C2	-4.20	120.28	126.34
1	5	3899	BGH	C5-C4-N9	4.17	111.76	106.35
1	5	3715	PSU	N1-C2-N3	4.16	119.84	115.13
1	5	4597	UR3	C4-N3-C2	-4.10	120.70	124.56
1	5	4220	6MZ	C9-N6-C6	-4.07	119.36	122.87
1	5	4415	1MA	C5-C6-N1	4.07	119.97	113.90
1	5	4371	MHG	C2-N1-C6	-4.07	119.80	124.48
1	5	4306	OMU	N3-C2-N1	4.05	120.27	114.89
1	5	2508	PSU	N1-C2-N3	4.03	119.70	115.13
1	5	1883	OMG	C5-C6-N1	4.03	121.06	113.95
1	5	1574	B9B	C2-N3-C4	4.02	119.95	115.36
1	5	3764	PSU	N1-C2-N3	4.02	119.68	115.13
1	5	4335	5MC	C5-C6-N1	-4.01	119.22	123.34
1	5	3897	B8K	C2-N3-C4	4.00	119.42	112.30
1	5	4129	B8W	C2-N3-C4	3.96	119.88	115.36
1	5	1517	2MG	C5-C6-N1	3.93	120.89	113.95
1	5	4083	5MU	C5M-C5-C6	-3.93	117.60	122.85
1	5	4530	UR3	C4-N3-C2	-3.93	120.87	124.56
3	8	14	OMU	C5-C4-N3	3.93	120.71	114.84
1	5	1348	P4U	C5-C4-N3	-3.89	118.99	124.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	2297	E7G	C5-C4-N3	-3.86	120.77	128.13
1	5	4872	2MG	C5-C6-N1	3.86	120.77	113.95
1	5	4447	5MC	C5-C6-N1	-3.85	119.38	123.34
1	5	1574	B9B	C1'-N9-C4	-3.82	119.93	126.64
1	5	1909	P7G	N9-C8-N7	3.81	108.82	103.38
1	5	3792	OMG	C5-C6-N1	3.81	120.67	113.95
1	5	3897	B8K	N9-C8-N7	3.78	108.41	103.33
1	5	1797	E7G	C5-C4-N3	-3.78	120.92	128.13
1	5	4872	2MG	CM2-N2-C2	-3.78	115.52	123.86
1	5	1605	7MG	C5-C4-N3	-3.78	120.93	128.13
1	5	4550	7MG	C5-C4-N3	-3.76	120.96	128.13
1	5	4196	OMG	C5-C6-N1	3.76	120.58	113.95
1	5	4083	5MU	C5M-C5-C4	3.74	122.88	118.77
1	5	3899	BGH	C4-C5-N7	3.74	108.23	104.91
1	5	1316	OMG	C5-C6-N1	3.73	120.54	113.95
1	5	4529	B8W	C2-N3-C4	3.73	119.61	115.36
1	5	4129	B8W	C3'-C2'-C1'	3.72	106.58	100.98
1	5	1860	B8H	C5-C4-N3	3.72	124.99	116.58
1	5	1522	OMG	C5-C6-N1	3.70	120.49	113.95
1	5	4472	B8W	C2-N3-C4	3.70	119.58	115.36
1	5	4296	B8H	O2-C2-N1	-3.70	118.71	122.87
1	5	1322	1MA	C5-C6-N1	3.69	119.39	113.90
1	5	2364	OMG	C5-C6-N1	3.69	120.46	113.95
1	5	4529	B8W	O6-C6-N1	-3.68	113.92	119.03
1	5	2522	7MG	C5-C4-N3	-3.67	121.14	128.13
1	5	2424	OMG	C5-C6-N1	3.67	120.42	113.95
1	5	4620	OMU	N3-C2-N1	3.66	119.75	114.89
1	5	2380	B8W	C2-N3-C4	3.66	119.54	115.36
1	5	237	B9B	N2-C2-N3	3.65	123.74	117.79
1	5	4371	MHG	C5-C4-N3	-3.65	121.18	128.13
1	5	4550	7MG	C5-C4-N9	3.64	111.08	106.35
1	5	4494	OMG	C5-C6-N1	3.62	120.35	113.95
1	5	3899	BGH	N9-C8-N7	3.62	108.18	103.33
1	5	1456	B8Q	O2-C2-N3	-3.61	117.64	122.95
1	5	4623	OMG	C5-C6-N1	3.60	120.31	113.95
1	5	2754	B9B	N2-C2-N3	3.55	123.57	117.79
1	5	4690	B8K	N9-C8-N7	3.54	108.08	103.33
1	5	1348	P4U	O2-C2-N3	-3.54	116.58	122.33
1	5	1866	UR3	C6-N1-C2	-3.53	118.63	121.79
1	5	3762	B8H	C5-C4-N3	3.53	124.56	116.58
1	5	373	OMG	C5-C6-N1	3.52	120.16	113.95
1	5	4690	B8K	C5-C4-N9	3.52	110.91	106.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	729	2MG	C5-C6-N1	3.51	120.16	113.95
1	5	4185	B8W	C2-N3-C4	3.51	119.37	115.36
3	8	14	OMU	N3-C2-N1	3.51	119.54	114.89
1	5	4370	OMG	C5-C6-N1	3.47	120.08	113.95
1	5	4637	OMG	C5-C6-N1	3.47	120.08	113.95
1	5	4870	OMG	C5-C6-N1	3.47	120.07	113.95
1	5	1625	OMG	C5-C6-N1	3.46	120.07	113.95
1	5	4185	B8W	O6-C6-N1	-3.44	114.25	119.03
1	5	4296	B8H	C5-C4-N3	3.43	124.34	116.58
1	5	3792	OMG	C2-N1-C6	-3.42	118.80	125.10
1	5	1316	OMG	C2-N1-C6	-3.41	118.81	125.10
1	5	4220	6MZ	C1'-N9-C4	-3.41	120.66	126.64
3	8	14	OMU	O4-C4-C5	-3.40	119.19	125.16
51	9	1374	5MC	C5-C6-N1	-3.37	119.87	123.34
1	5	2522	7MG	C5-C4-N9	3.36	110.71	106.35
1	5	2773	OMG	C5-C6-N1	3.36	119.89	113.95
1	5	3782	5MC	C5-C6-N1	-3.36	119.88	123.34
1	5	4564	M7A	C2-N3-C4	3.35	119.68	111.75
1	5	2050	OMG	C5-C6-N1	3.35	119.87	113.95
1	5	1883	OMG	C2-N1-C6	-3.35	118.93	125.10
1	5	4196	OMG	C2-N1-C6	-3.35	118.93	125.10
1	5	237	B9B	C3'-C2'-C1'	3.34	106.01	100.98
1	5	4185	B8W	C3'-C2'-C1'	3.33	105.99	100.98
1	5	3762	B8H	O2-C2-N1	-3.32	119.13	122.87
1	5	1522	OMG	C2-N1-C6	-3.31	119.00	125.10
1	5	4306	OMU	C5-C4-N3	3.31	119.79	114.84
51	9	1248	B8N	N3-C2-N1	3.26	121.36	116.76
1	5	1909	P7G	C71-N7-C5	3.26	132.23	124.52
1	5	2050	OMG	C2-N1-C6	-3.24	119.13	125.10
1	5	3899	BGH	C5-C4-N3	-3.23	121.98	128.13
1	5	1625	OMG	C2-N1-C6	-3.20	119.20	125.10
1	5	4371	MHG	C5-C4-N9	3.20	110.50	106.35
1	5	4637	OMG	C2-N1-C6	-3.16	119.28	125.10
1	5	1866	UR3	C1'-N1-C2	3.16	122.32	116.99
1	5	2424	OMG	C2-N1-C6	-3.15	119.30	125.10
1	5	4623	OMG	C2-N1-C6	-3.14	119.31	125.10
1	5	4620	OMU	C5-C4-N3	3.14	119.54	114.84
1	5	4690	B8K	C5-C4-N3	-3.13	122.16	128.13
1	5	2364	OMG	C2-N1-C6	-3.13	119.34	125.10
1	5	1605	7MG	C4-C5-N7	3.11	109.85	105.53
1	5	1683	PSU	O2-C2-N1	-3.11	119.37	122.79
1	5	2522	7MG	C4-C5-N7	3.10	109.84	105.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	1605	7MG	C5-C4-N9	3.09	110.36	106.35
1	5	2297	E7G	C5-C4-N9	3.08	110.34	106.35
1	5	3897	B8K	C5-C4-N9	3.07	110.33	106.35
1	5	3899	BGH	C2'-C1'-N9	-3.07	107.90	114.14
1	5	4494	OMG	C2-N1-C6	-3.06	119.47	125.10
1	5	1866	UR3	C4-N3-C2	-3.05	121.69	124.56
1	5	4371	MHG	C72-C71-N7	3.03	115.39	112.41
1	5	4450	PSU	C6-C5-C4	3.02	120.31	118.20
1	5	4370	OMG	C2-N1-C6	-3.02	119.54	125.10
1	5	4129	B8W	O6-C6-N1	-3.01	114.85	119.03
1	5	1860	B8H	O2-C2-N1	-3.01	119.48	122.87
51	9	1248	B8N	C31-N3-C4	3.01	121.74	117.31
1	5	2773	OMG	C2-N1-C6	-3.00	119.56	125.10
1	5	373	OMG	C2-N1-C6	-2.98	119.61	125.10
1	5	1883	OMG	O6-C6-C5	-2.98	118.55	124.37
1	5	4335	5MC	CM5-C5-C6	-2.98	118.88	122.85
1	5	4371	MHG	C71-C72-C73	-2.97	105.86	114.20
1	5	1797	E7G	C5-C4-N9	2.96	110.19	106.35
1	5	4690	B8K	C6-C5-C4	-2.96	116.52	122.62
1	5	4870	OMG	C2-N1-C6	-2.95	119.67	125.10
1	5	4185	B8W	C2-N1-C6	2.95	120.81	116.08
1	5	4355	E6G	O6-C6-N1	2.94	122.67	120.12
1	5	4564	M7A	C71-N7-C5	-2.94	112.72	124.01
51	9	1243	PSU	N1-C2-N3	2.93	118.45	115.13
1	5	4628	PSU	C6-N1-C2	-2.92	119.69	122.68
1	5	2754	B9B	C1'-N9-C4	-2.91	121.53	126.64
1	5	4194	I4U	C5-C4-N3	-2.90	120.50	124.91
1	5	4620	OMU	O4-C4-C5	-2.89	120.08	125.16
1	5	4550	7MG	C4-C5-N7	2.88	109.53	105.53
1	5	4530	UR3	C6-N1-C2	-2.88	119.21	121.79
1	5	4531	PSU	O2-C2-N1	-2.88	119.62	122.79
1	5	3897	B8K	C5-C4-N3	-2.86	122.67	128.13
1	5	3897	B8K	C6-C5-C4	-2.86	116.72	122.62
1	5	4597	UR3	C1'-N1-C2	2.86	121.81	116.99
1	5	4628	PSU	O2-C2-N1	-2.84	119.67	122.79
51	9	1243	PSU	C6-N1-C2	-2.84	119.78	122.68
1	5	4500	PSU	O2-C2-N1	-2.83	119.67	122.79
1	5	2297	E7G	C2-N1-C6	-2.82	119.95	125.10
1	5	1517	2MG	O6-C6-C5	-2.82	118.86	124.37
1	5	4083	5MU	O2-C2-N1	-2.82	119.04	122.79
1	5	3899	BGH	C6-C5-C4	-2.82	116.81	122.62
1	5	1605	7MG	N9-C8-N7	2.81	107.40	103.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	1316	OMG	C8-N7-C5	2.80	108.33	102.99
1	5	4637	OMG	C8-N7-C5	2.80	108.32	102.99
1	5	3729	PSU	O2-C2-N1	-2.79	119.72	122.79
1	5	1534	A2M	O4'-C1'-C2'	-2.79	101.74	106.59
51	9	1219	B8Q	C1'-N1-C6	-2.77	114.79	120.84
1	5	1797	E7G	C2-N1-C6	-2.76	120.06	125.10
1	5	1517	2MG	CM2-N2-C2	-2.76	117.77	123.86
1	5	4083	5MU	C6-N1-C2	-2.75	118.51	121.30
1	5	1605	7MG	C2-N1-C6	-2.75	120.08	125.10
1	5	4371	MHG	C21-N2-C2	-2.75	117.80	123.86
1	5	4872	2MG	C8-N7-C5	2.75	108.22	102.99
1	5	2522	7MG	N9-C8-N7	2.74	107.30	103.38
1	5	4494	OMG	C8-N7-C5	2.73	108.20	102.99
1	5	4355	E6G	N2-C2-N1	2.72	121.49	117.25
1	5	1522	OMG	C8-N7-C5	2.71	108.16	102.99
51	9	1337	4AC	C6-C5-C4	2.71	120.28	116.96
1	5	4636	PSU	O2-C2-N1	-2.70	119.81	122.79
1	5	4597	UR3	C6-N1-C2	-2.70	119.37	121.79
1	5	3729	PSU	C6-N1-C2	-2.70	119.93	122.68
1	5	2364	OMG	O6-C6-C5	-2.69	119.12	124.37
1	5	2050	OMG	C8-N7-C5	2.69	108.11	102.99
1	5	4185	B8W	O4'-C4'-C3'	-2.69	99.80	105.11
1	5	1574	B9B	N2-C2-N3	2.68	122.15	117.79
1	5	1866	UR3	O2-C2-N3	-2.67	117.57	121.34
1	5	4690	B8K	C2-N1-C6	-2.67	120.23	125.10
1	5	4529	B8W	C2-N1-C6	2.67	120.36	116.08
1	5	4442	PSU	O2-C2-N1	-2.66	119.86	122.79
1	5	1683	PSU	C6-N1-C2	-2.65	119.97	122.68
1	5	3899	BGH	C2-N1-C6	-2.65	120.27	125.10
1	5	4371	MHG	O6-C6-C5	-2.64	121.06	127.54
49	v	715	DDE	CAU-CBW-CBI	-2.64	105.96	111.20
1	5	4870	OMG	C8-N7-C5	2.64	108.02	102.99
1	5	4472	B8W	O6-C6-N1	-2.62	115.39	119.03
1	5	4620	OMU	O2-C2-N1	-2.62	119.31	122.79
1	5	1456	B8Q	C6-N1-C2	-2.61	119.45	121.79
1	5	4872	2MG	O6-C6-C5	-2.61	119.27	124.37
1	5	4306	OMU	O4-C4-C5	-2.61	120.57	125.16
1	5	3792	OMG	C8-N7-C5	2.61	107.96	102.99
1	5	3764	PSU	O2-C2-N1	-2.61	119.92	122.79
1	5	1625	OMG	O6-C6-C5	-2.61	119.28	124.37
1	5	4623	OMG	C8-N7-C5	2.60	107.95	102.99
1	5	1456	B8Q	C31-N3-C2	2.60	121.57	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	2424	OMG	O6-C6-C5	-2.58	119.33	124.37
1	5	3880	P7G	N9-C8-N7	2.58	107.06	103.38
1	5	373	OMG	CM2-O2'-C2'	-2.57	107.77	114.52
1	5	4196	OMG	C8-N7-C5	2.57	107.88	102.99
1	5	4623	OMG	O6-C6-C5	-2.57	119.36	124.37
1	5	4442	PSU	C6-N1-C2	-2.56	120.06	122.68
1	5	3764	PSU	C6-N1-C2	-2.56	120.06	122.68
1	5	3897	B8K	C2-N1-C6	-2.55	120.44	125.10
1	5	1677	PSU	O2-C2-N1	-2.55	119.98	122.79
51	9	1243	PSU	C4-N3-C2	-2.55	122.66	126.34
1	5	373	OMG	C8-N7-C5	2.54	107.84	102.99
1	5	1797	E7G	N9-C8-N7	2.53	107.00	103.38
1	5	1883	OMG	C8-N7-C5	2.53	107.81	102.99
1	5	2773	OMG	C8-N7-C5	2.53	107.81	102.99
1	5	4370	OMG	C8-N7-C5	2.53	107.81	102.99
1	5	2508	PSU	O2-C2-N1	-2.53	120.01	122.79
1	5	4083	5MU	O4-C4-N3	-2.52	115.28	120.12
1	5	4355	E6G	C2-N1-C6	2.51	120.11	116.08
1	5	2786	B9H	C1'-N1-C2	2.51	121.23	116.99
1	5	1625	OMG	C8-N7-C5	2.51	107.77	102.99
1	5	1574	B9B	C3'-C2'-C1'	2.51	104.76	100.98
1	5	2364	OMG	C8-N7-C5	2.51	107.77	102.99
3	8	14	OMU	CM2-O2'-C2'	2.50	121.10	114.52
1	5	4536	OMC	O2-C2-N3	-2.50	118.26	122.33
1	5	2424	OMG	C8-N7-C5	2.50	107.75	102.99
1	5	1316	OMG	O6-C6-C5	-2.49	119.51	124.37
1	5	3715	PSU	O2-C2-N1	-2.49	120.05	122.79
1	5	4550	7MG	N9-C8-N7	2.48	106.92	103.38
1	5	1322	1MA	C8-N7-C5	2.48	107.71	102.99
1	5	1860	B8H	O4-C4-N3	-2.47	115.38	120.12
1	5	2050	OMG	O6-C6-C5	-2.47	119.55	124.37
1	5	4472	B8W	C3'-C2'-C1'	2.47	104.69	100.98
1	5	4293	PSU	O2-C2-N1	-2.46	120.08	122.79
1	5	4196	OMG	O6-C6-C5	-2.46	119.57	124.37
3	8	14	OMU	C1'-N1-C2	2.44	121.98	117.57
49	v	715	DDE	CBW-CBI-NAD	2.43	118.38	115.28
1	5	4296	B8H	O4-C4-N3	-2.43	115.45	120.12
1	5	4293	PSU	C6-N1-C2	-2.43	120.20	122.68
1	5	1797	E7G	O6-C6-C5	-2.43	121.59	127.54
1	5	4690	B8K	O6-C6-C5	-2.43	121.59	127.54
1	5	1582	PSU	C6-N1-C2	-2.42	120.20	122.68
1	5	373	OMG	O6-C6-C5	-2.42	119.64	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	2297	E7G	O6-C6-C5	-2.41	121.62	127.54
1	5	4355	E6G	C3'-C2'-C1'	2.41	104.61	100.98
1	5	4636	PSU	C6-C5-C4	2.41	119.88	118.20
1	5	2754	B9B	C3'-C2'-C1'	2.40	104.60	100.98
51	9	1337	4AC	C5-C4-N3	-2.40	118.73	122.59
1	5	3897	B8K	O6-C6-C5	-2.40	121.66	127.54
1	5	4671	B8T	C6-C5-C4	2.40	119.89	116.96
1	5	3792	OMG	O6-C6-C5	-2.40	119.69	124.37
1	5	3897	B8K	O4'-C1'-C2'	-2.39	101.43	106.64
1	5	1582	PSU	O2-C2-N1	-2.39	120.16	122.79
1	5	4564	M7A	C5-C4-N3	-2.38	121.03	126.62
51	9	1219	B8Q	C31-N3-C2	2.38	121.25	117.79
1	5	4185	B8W	C4-C5-N7	-2.38	106.92	109.40
1	5	4415	1MA	C8-N7-C5	2.37	107.50	102.99
1	5	3762	B8H	O4-C4-N3	-2.36	115.59	120.12
1	5	4531	PSU	C6-C5-C4	2.36	119.84	118.20
1	5	1659	I4U	C5'-C4'-C3'	-2.35	106.36	115.18
1	5	1605	7MG	O6-C6-C5	-2.35	121.78	127.54
1	5	4370	OMG	O6-C6-C5	-2.35	119.78	124.37
1	5	4403	PSU	C6-N1-C2	-2.34	120.29	122.68
1	5	729	2MG	O6-C6-C5	-2.34	119.80	124.37
1	5	4371	MHG	N1-C2-N3	-2.34	120.33	123.95
1	5	4531	PSU	C6-N1-C2	-2.33	120.30	122.68
1	5	1517	2MG	C8-N7-C5	2.33	107.44	102.99
1	5	4483	B8T	O2-C2-N3	-2.33	118.54	122.33
51	9	1248	B8N	O4'-C1'-C2'	2.32	108.42	105.14
1	5	4403	PSU	O4'-C1'-C2'	2.32	108.42	105.14
1	5	4564	M7A	N9-C8-N7	-2.31	100.08	103.38
1	5	729	2MG	C8-N7-C5	2.30	107.38	102.99
1	5	4129	B8W	C2-N1-C6	2.30	119.78	116.08
51	9	1374	5MC	O2-C2-N3	-2.30	118.59	122.33
1	5	2522	7MG	C2-N1-C6	-2.30	120.91	125.10
1	5	2773	OMG	O6-C6-C5	-2.29	119.90	124.37
1	5	2297	E7G	N9-C4-N3	2.29	128.89	125.47
1	5	1797	E7G	N9-C4-N3	2.29	128.88	125.47
1	5	4306	OMU	O2-C2-N1	-2.28	119.75	122.79
1	5	2754	B9B	O6-C6-N1	-2.28	118.15	120.12
1	5	1909	P7G	C5-C4-N3	-2.28	119.98	124.00
1	5	4550	7MG	C2-N1-C6	-2.27	120.95	125.10
1	5	1348	P4U	C1'-N1-C2	2.26	123.45	118.42
1	5	3897	B8K	O3'-C3'-C4'	-2.25	104.54	111.05
1	5	3899	BGH	O6-C6-N1	-2.24	115.83	120.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	4335	5MC	C1'-N1-C6	-2.22	117.42	121.12
1	5	2363	A2M	C3'-C2'-C1'	2.22	107.06	102.89
1	5	4450	PSU	O2-C2-N1	-2.21	120.35	122.79
1	5	2297	E7G	N9-C8-N7	2.21	106.53	103.38
51	9	1243	PSU	O2-C2-N1	-2.21	120.36	122.79
1	5	4494	OMG	O6-C6-C5	-2.20	120.07	124.37
1	5	3880	P7G	C71-N7-C5	2.20	129.74	124.52
1	5	4194	I4U	O4'-C1'-C2'	-2.19	101.86	106.64
1	5	4483	B8T	C6-C5-C4	2.19	119.64	116.96
1	5	2522	7MG	O6-C6-C5	-2.19	122.17	127.54
1	5	2422	OMC	O2-C2-N3	-2.17	118.80	122.33
1	5	4637	OMG	O6-C6-C5	-2.17	120.14	124.37
1	5	1605	7MG	N9-C4-N3	2.17	128.71	125.47
1	5	3887	OMC	O2-C2-N3	-2.16	118.82	122.33
1	5	4472	B8W	O4'-C4'-C3'	-2.16	100.84	105.11
1	5	4403	PSU	O2-C2-N1	-2.16	120.42	122.79
1	5	1522	OMG	O6-C6-C5	-2.15	120.17	124.37
1	5	1677	PSU	C6-C5-C4	2.15	119.70	118.20
1	5	3899	BGH	C5'-C4'-C3'	-2.14	107.17	115.18
1	5	4472	B8W	C2-N1-C6	2.13	119.50	116.08
1	5	4529	B8W	C5'-C4'-C3'	-2.13	107.21	115.18
1	5	2786	B9H	O2-C2-N1	-2.12	117.76	122.72
1	5	4371	MHG	C71-N7-C5	2.11	129.51	124.52
1	5	4355	E6G	C61-O6-C6	-2.11	115.48	117.56
1	5	2861	OMC	C1'-N1-C2	2.10	123.11	118.42
3	8	14	OMU	O2-C2-N1	-2.10	120.00	122.79
1	5	3880	P7G	C5-C4-N3	-2.07	120.35	124.00
1	5	4550	7MG	O6-C6-C5	-2.07	122.47	127.54
1	5	4500	PSU	C6-N1-C2	-2.07	120.57	122.68
1	5	4571	A2M	C5'-C4'-C3'	-2.05	107.48	115.18
1	5	4690	B8K	C3'-C2'-C1'	2.05	105.31	101.43
1	5	4220	6MZ	C4-C5-N7	2.04	111.52	109.40
1	5	3715	PSU	C6-N1-C2	-2.03	120.60	122.68
1	5	1677	PSU	O4'-C1'-C2'	2.02	108.00	105.14
1	5	1677	PSU	C6-N1-C2	-2.02	120.61	122.68
51	9	1337	4AC	O2-C2-N3	-2.02	119.04	122.33
1	5	3899	BGH	N1-C2-N3	-2.00	119.59	123.32

There are no chirality outliers.

All (159) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	333	MLZ	N-CA-CB-CG
6	C	333	MLZ	C-CA-CB-CG
49	v	715	DDE	O-C-CA-CB
49	v	715	DDE	CA-CB-CG-ND1
49	v	715	DDE	CA-CB-CG-CD2
49	v	715	DDE	CBI-CBW-NCB-CAC
49	v	715	DDE	CBI-CBW-NCB-CAA
49	v	715	DDE	CAU-CBW-NCB-CAB
49	v	715	DDE	CAU-CBW-NCB-CAC
49	v	715	DDE	CAU-CBW-NCB-CAA
49	v	715	DDE	CAT-CAU-CBW-CBI
1	5	237	B9B	C5-C6-O6-C61
1	5	237	B9B	N1-C6-O6-C61
1	5	237	B9B	C3'-C4'-C5'-O5'
1	5	237	B9B	O4'-C4'-C5'-O5'
1	5	1348	P4U	N3-C4-O4-C41
1	5	1348	P4U	C3'-C4'-C5'-O5'
1	5	1348	P4U	O4'-C4'-C5'-O5'
1	5	1574	B9B	C5-C6-O6-C61
1	5	1574	B9B	N1-C6-O6-C61
1	5	1582	PSU	C3'-C4'-C5'-O5'
1	5	1625	OMG	C3'-C4'-C5'-O5'
1	5	1909	P7G	C72-C71-N7-C5
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	C3'-C4'-C5'-O5'
1	5	2424	OMG	O4'-C4'-C5'-O5'
1	5	2424	OMG	C3'-C4'-C5'-O5'
1	5	2773	OMG	O4'-C4'-C5'-O5'
1	5	2773	OMG	C3'-C4'-C5'-O5'
1	5	2786	B9H	C32-C31-N3-C2
1	5	3701	OMC	C2'-C1'-N1-C6
1	5	3762	B8H	O4'-C4'-C5'-O5'
1	5	3785	A2M	O4'-C4'-C5'-O5'
1	5	3792	OMG	O4'-C4'-C5'-O5'
1	5	3867	A2M	C3'-C4'-C5'-O5'
1	5	3880	P7G	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	4129	B8W	C5-C6-O6-C61
1	5	4129	B8W	N1-C6-O6-C61

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Mol	Chain	Res	Type	Atoms
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	C5-C6-O6-C61
1	5	4355	E6G	N1-C6-O6-C61
1	5	4403	PSU	O4'-C1'-C5-C4
1	5	4403	PSU	O4'-C1'-C5-C6
1	5	4415	1MA	O4'-C4'-C5'-O5'
1	5	4415	1MA	C3'-C4'-C5'-O5'
1	5	4447	5MC	C2'-C1'-N1-C6
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	4620	OMU	C1'-C2'-O2'-CM2
1	5	4637	OMG	O4'-C4'-C5'-O5'
1	5	4690	B8K	O4'-C4'-C5'-O5'
1	5	4870	OMG	O4'-C4'-C5'-O5'
1	5	4870	OMG	C3'-C4'-C5'-O5'
3	8	14	OMU	C1'-C2'-O2'-CM2
41	m	72	MLZ	N-CA-CB-CG
51	9	1248	B8N	O4'-C4'-C5'-O5'
51	9	1248	B8N	C3'-C4'-C5'-O5'
1	5	3701	OMC	C2'-C1'-N1-C2
1	5	4447	5MC	C2'-C1'-N1-C2
1	5	398	A2M	O4'-C4'-C5'-O5'
1	5	729	2MG	O4'-C4'-C5'-O5'
1	5	1582	PSU	O4'-C4'-C5'-O5'
1	5	1797	E7G	C3'-C4'-C5'-O5'
1	5	1797	E7G	O4'-C4'-C5'-O5'
1	5	2380	B8W	O4'-C4'-C5'-O5'
1	5	3729	PSU	C3'-C4'-C5'-O5'
1	5	3729	PSU	O4'-C4'-C5'-O5'
1	5	3762	B8H	C3'-C4'-C5'-O5'
1	5	3792	OMG	C3'-C4'-C5'-O5'
1	5	3867	A2M	O4'-C4'-C5'-O5'
1	5	3880	P7G	C3'-C4'-C5'-O5'
1	5	3897	B8K	C3'-C4'-C5'-O5'
1	5	4185	B8W	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	5	4194	I4U	C3'-C4'-C5'-O5'
1	5	4371	MHG	O4'-C4'-C5'-O5'
1	5	4523	A2M	C3'-C4'-C5'-O5'
1	5	4530	UR3	C3'-C4'-C5'-O5'
1	5	4636	PSU	C3'-C4'-C5'-O5'
1	5	4636	PSU	O4'-C4'-C5'-O5'
1	5	4637	OMG	C3'-C4'-C5'-O5'
1	5	4872	2MG	O4'-C4'-C5'-O5'
51	9	1243	PSU	C3'-C4'-C5'-O5'
1	5	1348	P4U	O4-C41-C42-C43
1	5	2786	B9H	O4'-C4'-C5'-O5'
1	5	3785	A2M	C3'-C4'-C5'-O5'
1	5	4530	UR3	O4'-C4'-C5'-O5'
1	5	4690	B8K	C3'-C4'-C5'-O5'
1	5	4872	2MG	C3'-C4'-C5'-O5'
51	9	1243	PSU	O4'-C4'-C5'-O5'
1	5	2380	B8W	N1-C6-O6-C61
1	5	4371	MHG	C2'-C1'-N9-C8
1	5	398	A2M	C3'-C4'-C5'-O5'
1	5	4450	PSU	C3'-C4'-C5'-O5'
1	5	4371	MHG	C75-C73-C74-C76
1	5	1625	OMG	O4'-C4'-C5'-O5'
1	5	4450	PSU	O4'-C4'-C5'-O5'
1	5	4129	B8W	O4'-C4'-C5'-O5'
1	5	4371	MHG	C3'-C4'-C5'-O5'
1	5	1909	P7G	C72-C71-N7-C8
1	5	1625	OMG	C4'-C5'-O5'-P
1	5	2754	B9B	C5-C6-O6-C61
1	5	1866	UR3	O4'-C4'-C5'-O5'
1	5	4355	E6G	O4'-C4'-C5'-O5'
41	m	72	MLZ	CD-CE-NZ-CM
1	5	2297	E7G	C72-C71-N7-C8
1	5	3701	OMC	O4'-C1'-N1-C2
1	5	2786	B9H	C3'-C4'-C5'-O5'
1	5	4447	5MC	O4'-C1'-N1-C2
51	9	1248	B8N	N3-C31-C32-C33
1	5	3701	OMC	O4'-C1'-N1-C6
1	5	4447	5MC	O4'-C1'-N1-C6
41	m	72	MLZ	C-CA-CB-CG
1	5	1534	A2M	C4'-C5'-O5'-P
1	5	3897	B8K	C4'-C5'-O5'-P
1	5	373	OMG	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
1	5	3764	PSU	C4'-C5'-O5'-P
1	5	4371	MHG	C72-C73-C74-C76
1	5	2754	B9B	C4'-C5'-O5'-P
1	5	3887	OMC	C4'-C5'-O5'-P
1	5	4870	OMG	C4'-C5'-O5'-P
49	v	715	DDE	CAT-CAU-CBW-NCB
1	5	2754	B9B	N1-C6-O6-C61
49	v	715	DDE	NAD-CBI-CBW-NCB
1	5	1659	I4U	C43-C41-O4-C4
49	v	715	DDE	OAG-CBI-CBW-NCB
1	5	4450	PSU	O4'-C1'-C5-C4
1	5	4500	PSU	O4'-C1'-C5-C4
1	5	2380	B8W	C4'-C5'-O5'-P
1	5	2786	B9H	C32-C31-N3-C4
1	5	4370	OMG	C1'-C2'-O2'-CM2
49	v	715	DDE	CE1-CAT-CAU-CBW
1	5	4370	OMG	C3'-C2'-O2'-CM2
51	9	1219	B8Q	C2'-C1'-N1-C2
1	5	3762	B8H	C4'-C5'-O5'-P
1	5	4500	PSU	C4'-C5'-O5'-P
1	5	3880	P7G	N7-C71-C72-C73
1	5	4636	PSU	O4'-C1'-C5-C6
51	9	1248	B8N	C31-C32-C33-N34
1	5	1534	A2M	O4'-C4'-C5'-O5'
1	5	1659	I4U	C42-C41-O4-C4
1	5	4194	I4U	C43-C41-O4-C4
1	5	3785	A2M	C3'-C2'-O2'-CM'
1	5	4494	OMG	C3'-C2'-O2'-CM2
1	5	1456	B8Q	O4'-C4'-C5'-O5'
1	5	1866	UR3	C3'-C4'-C5'-O5'
1	5	2422	OMC	O4'-C4'-C5'-O5'
1	5	4371	MHG	O4'-C1'-N9-C8

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 306 ligands modelled in this entry, 305 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	$\#\|Z\| > 2$
87	GDP	v	900	-	24,30,30	0.97	1 (4%)	30,47,47	1.30	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
87	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)
87	v	900	GDP	C6-N1	-2.77	1.33	1.37

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	v	900	GDP	PA-O3A-PB	-3.68	120.20	132.83
87	v	900	GDP	C3'-C2'-C1'	2.91	105.36	100.98
87	v	900	GDP	C5-C6-N1	2.53	118.42	113.95
87	v	900	GDP	C8-N7-C5	2.16	107.10	102.99
87	v	900	GDP	O6-C6-C5	-2.04	120.38	124.37

There are no chirality outliers.

There are no torsion outliers.

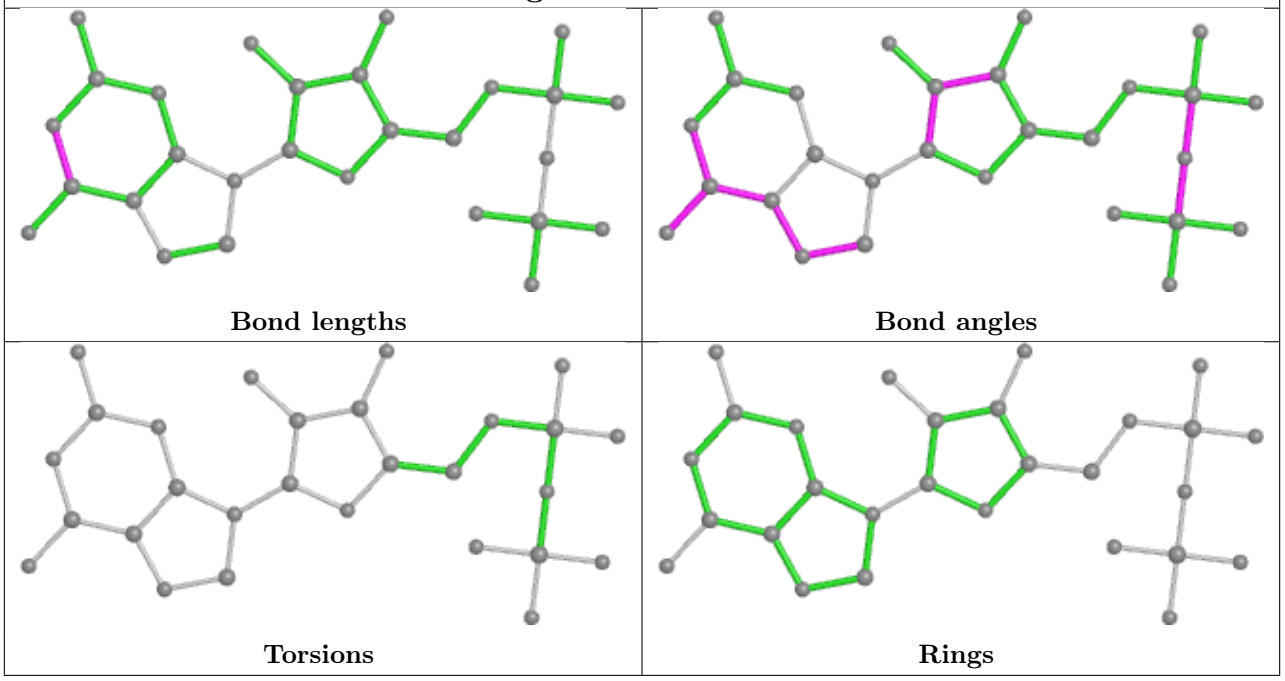
There are no ring outliers.

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 then 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.

Ligand GDP v 900



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	5	47
51	9	19
50	w	1
3	8	1

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Mol	Chain	Number of breaks
49	v	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	w	202:SER	C	282:THR	N	64.88
1	5	2113:G	O3'	2258:C	P	39.97
1	5	1252:C	O3'	1271:G	P	34.48
1	5	1406(C):G	O3'	1411:C	P	20.81
1	5	1405:C	O3'	1406:G	P	20.70
1	5	1219:G	O3'	1233:G	P	19.83
1	5	1411:C	O3'	1411(A):G	P	18.43
1	9	697:G	O3'	729:C	P	18.01
1	5	523:C	O3'	638:G	P	17.61
1	9	756:C	O3'	788:G	P	17.60
1	9	834:C	O3'	841:G	P	17.53
1	9	130:G	O3'	140:U	P	17.46
1	9	1761:U	O3'	1771:G	P	17.14
1	5	4777:C	O3'	4859:C	P	17.02
1	5	4138:C	O3'	4146:G	P	16.97
1	5	990:U	O3'	1064:G	P	16.68
1	9	323:C	O3'	329:G	P	16.58
1	5	4101:C	O3'	4107:G	P	15.93
1	5	3976:C	O3'	4039:G	P	15.04
1	5	1406:G	O3'	1406(A):G	P	14.94
1	9	1417:C	O3'	1423:C	P	14.94
1	5	1696:C	O3'	1720:C	P	14.48
1	5	5022:U	O3'	5028:G	P	14.45
1	5	760:G	O3'	904:C	P	14.02
1	5	922:C	O3'	922(A):G	P	13.55
1	5	1364:U	O3'	1368:A	P	13.55
1	5	2901:G	O3'	3597:G	P	13.23
1	5	182:G	O3'	189:G	P	12.86
1	8	79:G	O3'	85:U	P	12.75
1	5	738:C	O3'	738(A):C	P	12.46
1	v	47:ALA	C	66:ARG	N	12.04
1	5	921:C	O3'	922:C	P	11.51
1	5	922(B):C	O3'	923:C	P	8.98
1	5	4729:A	O3'	4735:G	P	8.54
1	5	1180:C	O3'	1183:C	P	8.41
1	9	225:G	O3'	287:U	P	8.05
1	5	512:U	O3'	515:C	P	8.00
1	5	738(A):C	O3'	739:G	P	7.72

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	935:A	O3'	935(A):G	P	7.65
1	5	935(A):G	O3'	936:C	P	7.35
1	9	745:C	O3'	749:U	P	6.96
1	5	3955:A	O3'	3956:G	P	6.68
1	5	500:G	O3'	504:G	P	6.36
1	5	737:C	O3'	738:C	P	6.23
1	5	481:G	O3'	481(A):C	P	5.81
1	5	480:C	O3'	481:G	P	5.65
1	5	4740:G	O3'	4743:G	P	4.97
1	9	736:C	O3'	743:U	P	4.95
1	9	1432:U	O3'	1438:A	P	4.93
1	5	1239:C	O3'	1244:G	P	4.73
1	9	309:G	O3'	310:C	P	4.66
1	9	322:C	O3'	323:C	P	4.66
1	5	170:C	O3'	171:U	P	4.49
1	5	4055:U	O3'	4056:A	P	4.39
1	5	1100:U	O3'	1168:G	P	4.38
1	5	934:C	O3'	935:A	P	4.26
1	9	304:C	O3'	305:U	P	4.14
1	9	798:G	O3'	799:U	P	4.08
1	5	3945:A	O3'	3946:G	P	3.55
1	5	1438:U	O3'	1440:U	P	3.46
1	5	3947:A	O3'	3948:C	P	3.29
1	9	903:A	O3'	904:A	P	3.25
1	5	751:G	O3'	752:G	P	3.24
1	5	4899:G	O3'	4902:C	P	3.23
1	9	1295:A	O3'	1296:U	P	3.23
1	9	902:G	O3'	903:A	P	3.22
1	5	5020:G	O3'	5021:C	P	3.21
1	9	1686:G	O3'	1687:C	P	3.20
1	5	267:G	O3'	268:G	P	3.16

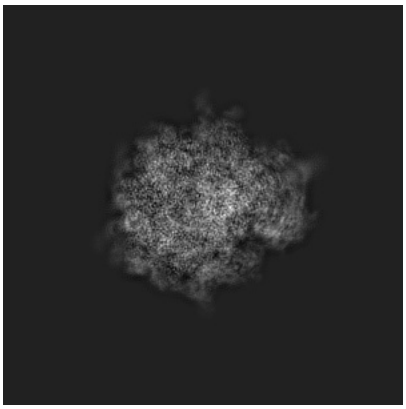
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-9240. These allow visual inspection of the internal detail of the map and identification of artifacts.

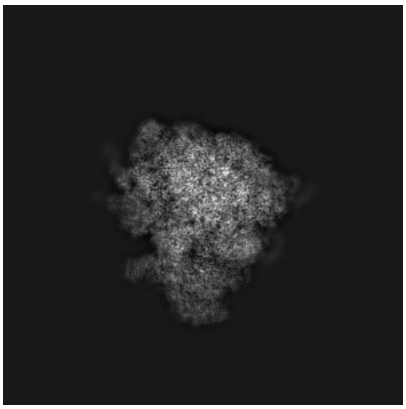
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

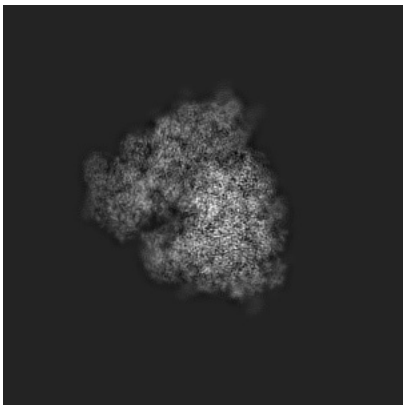
6.1.1 Primary map



X

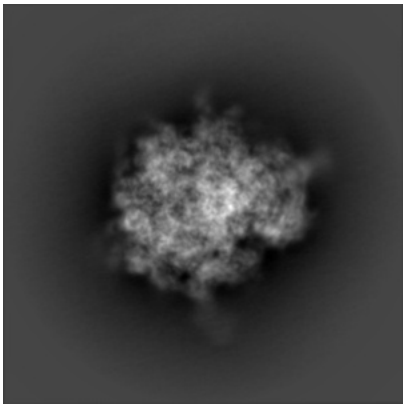


Y

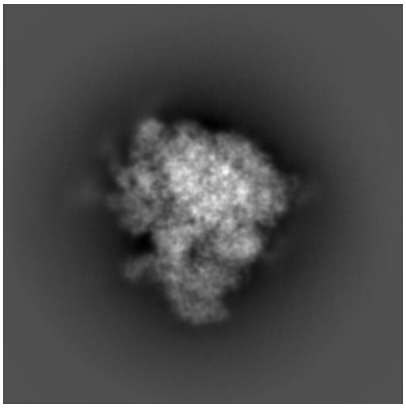


Z

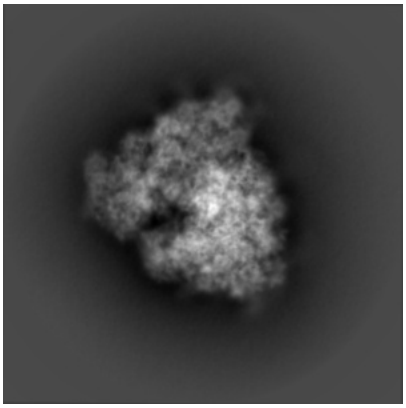
6.1.2 Raw map



X



Y

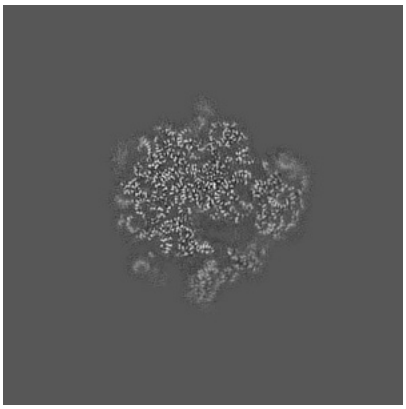


Z

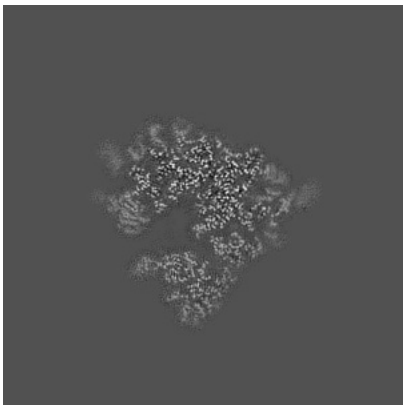
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

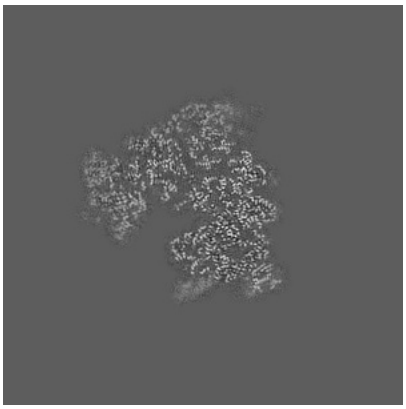
6.2.1 Primary map



X Index: 200

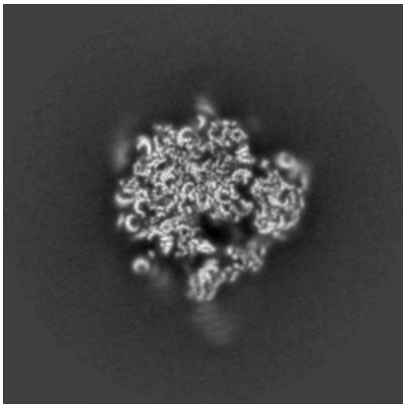


Y Index: 200

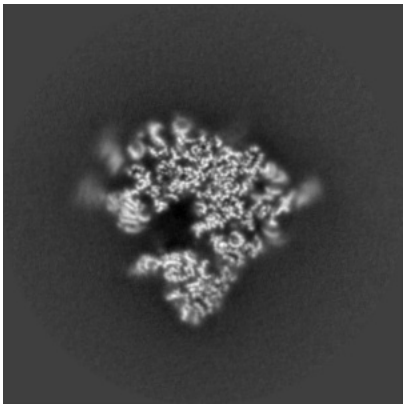


Z Index: 200

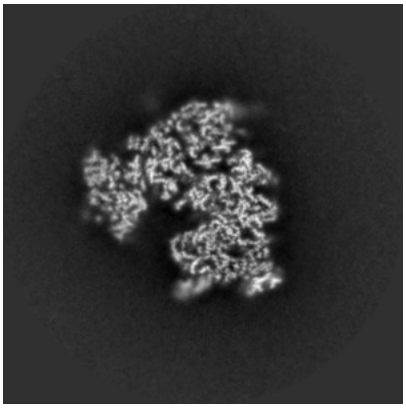
6.2.2 Raw map



X Index: 200



Y Index: 200

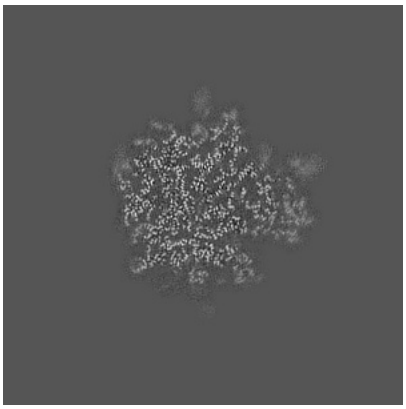


Z Index: 200

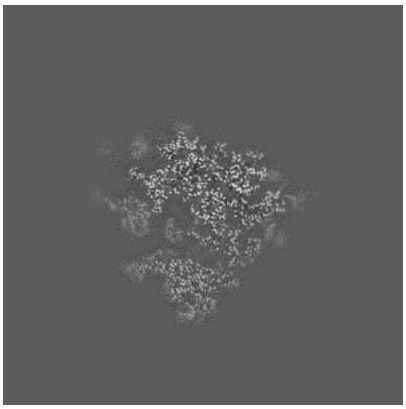
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

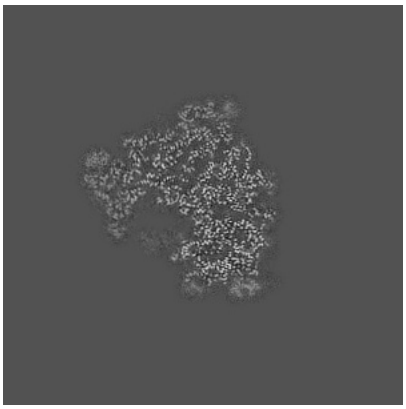
6.3.1 Primary map



X Index: 213

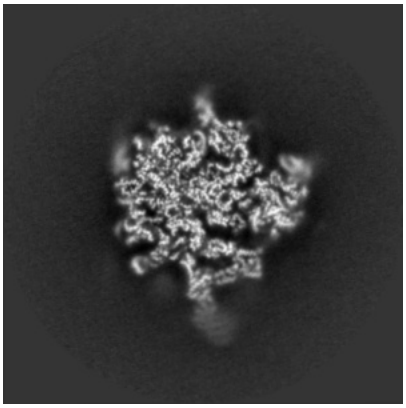


Y Index: 208

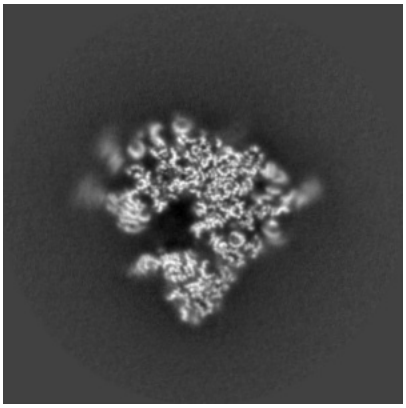


Z Index: 210

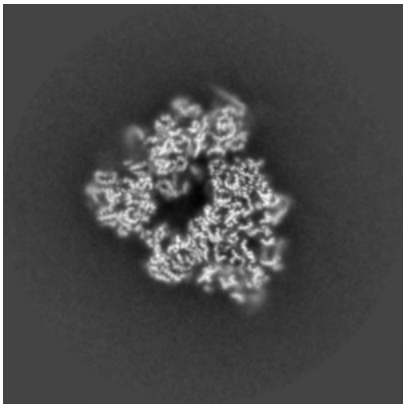
6.3.2 Raw map



X Index: 206



Y Index: 201

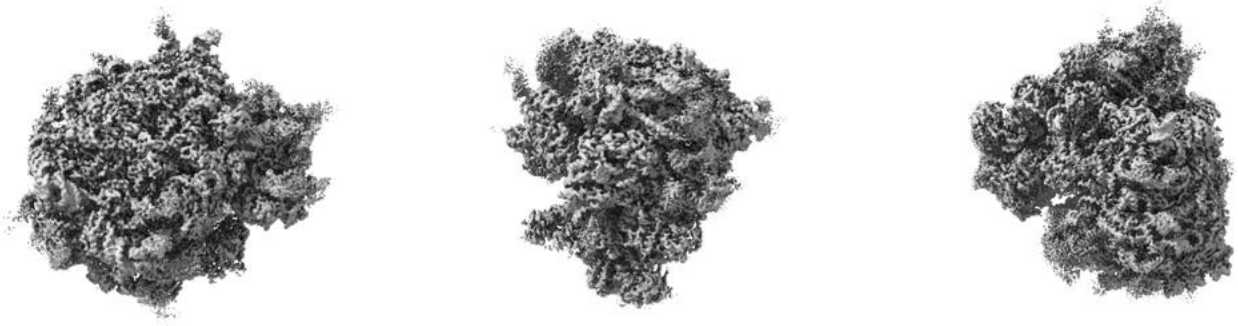


Z Index: 176

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

6.4 Orthogonal surface views (i)

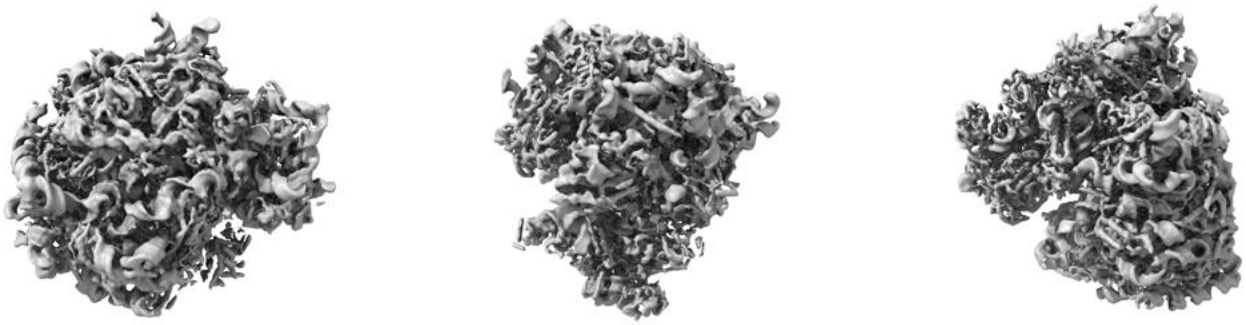
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.09. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

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

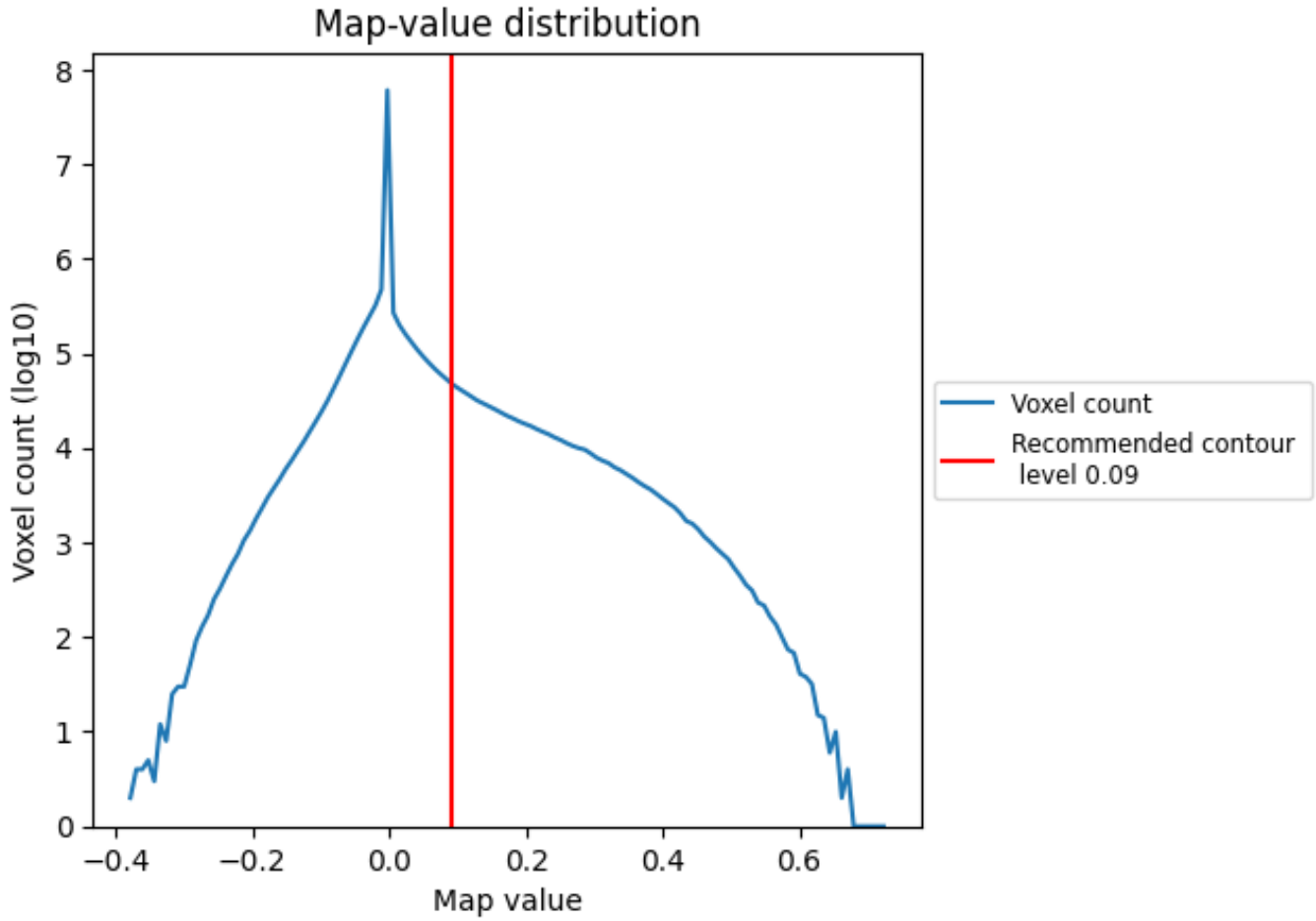
6.5 Mask visualisation (i)

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

7 Map analysis

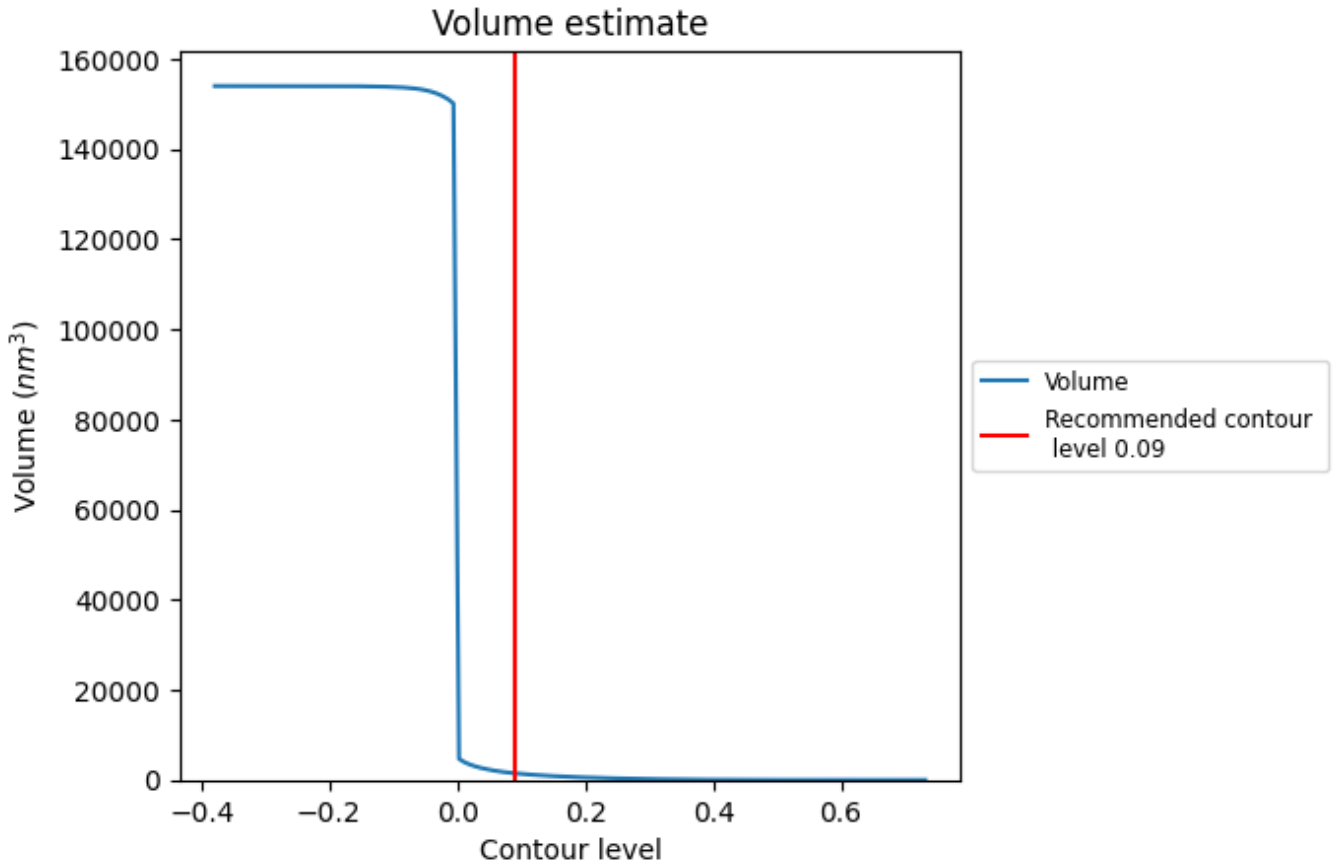
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

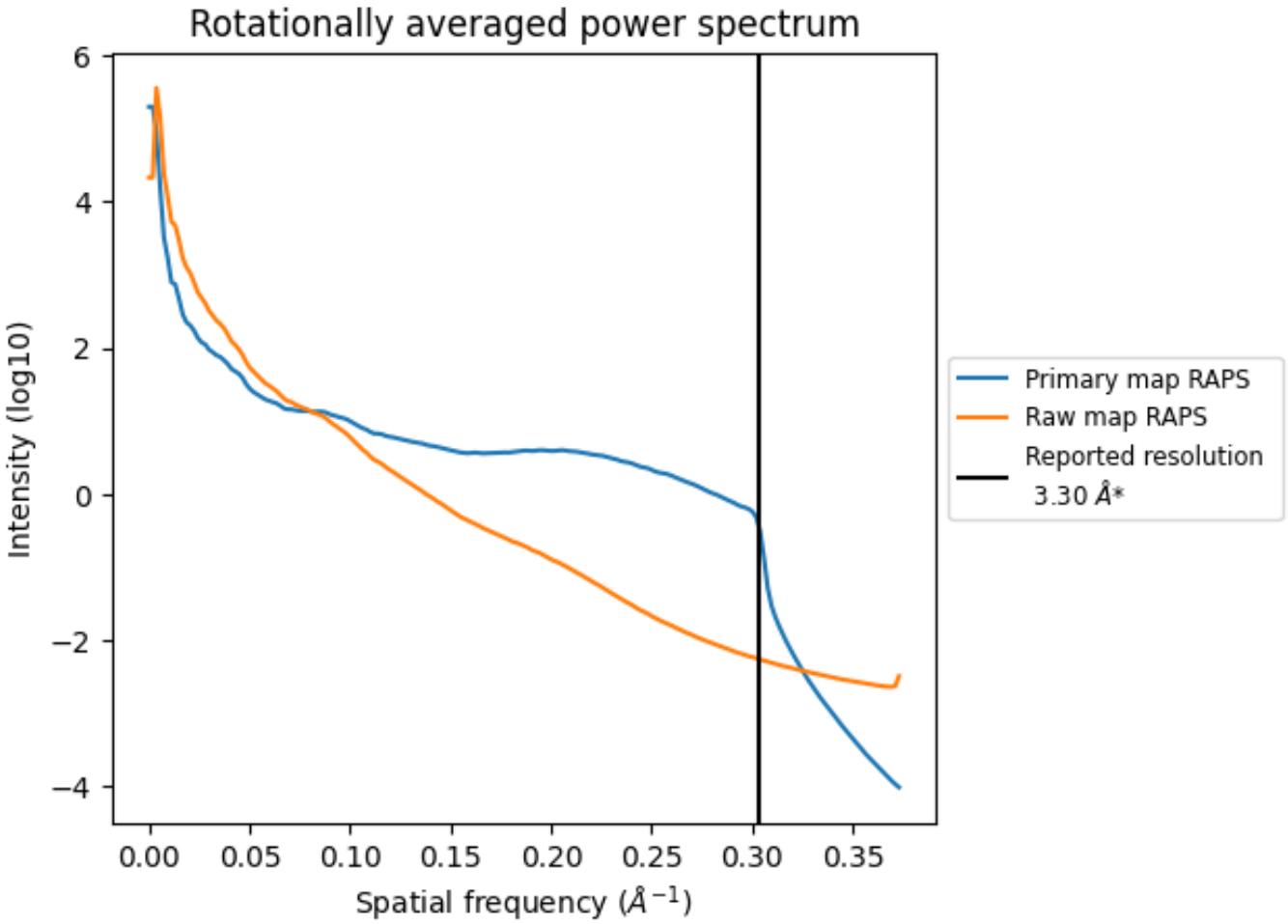
7.2 Volume estimate



The volume at the recommended contour level is 1483 nm^3; this corresponds to an approximate mass of 1340 kDa.

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

7.3 Rotationally averaged power spectrum (i)

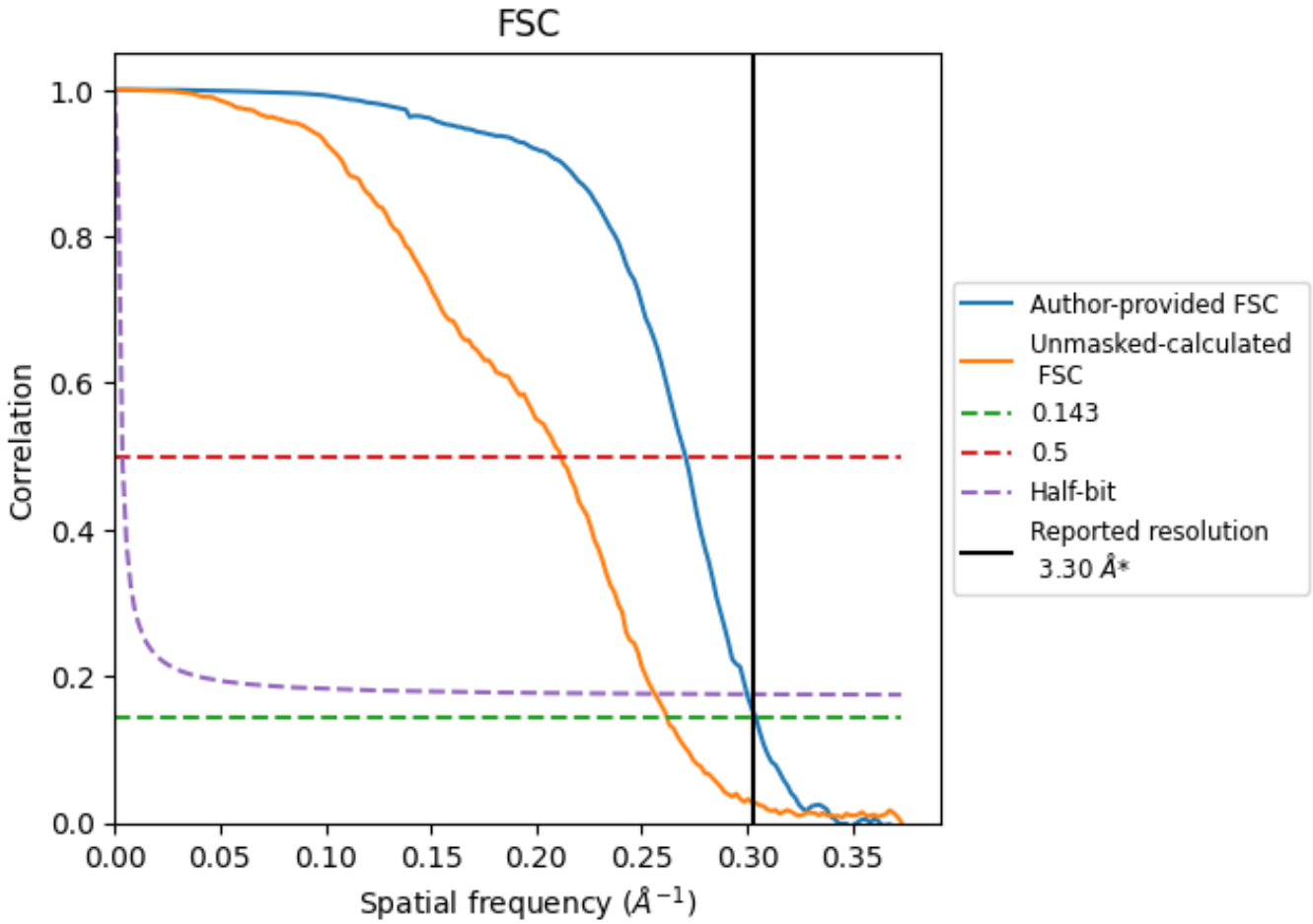


*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

8.2 Resolution estimates (i)

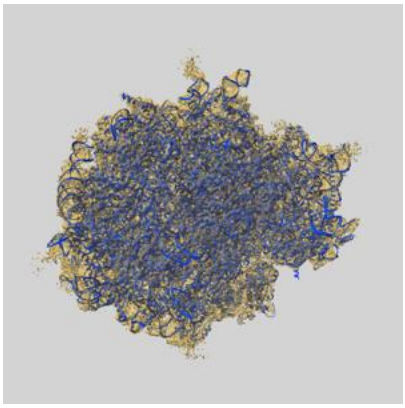
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.29	3.69	3.33
Unmasked-calculated*	3.82	4.73	3.90

*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 3.82 differs from the reported value 3.3 by more than 10 %

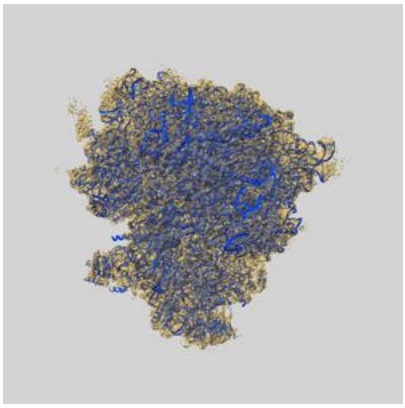
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-9240 and PDB model 6MTD. Per-residue inclusion information can be found in section 3 on page 21.

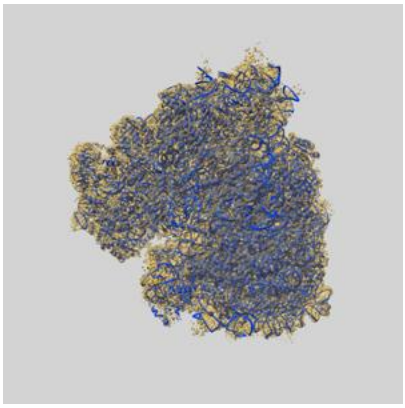
9.1 Map-model overlay



X



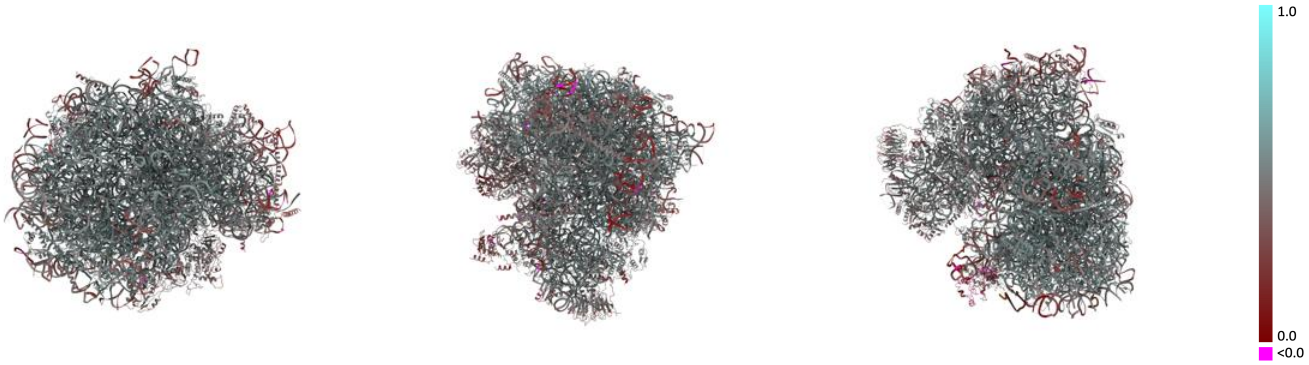
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.09 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.

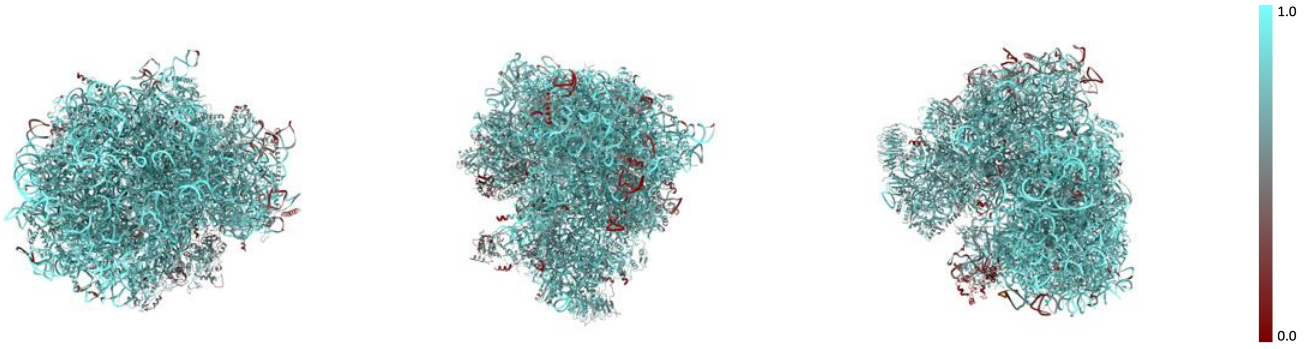
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

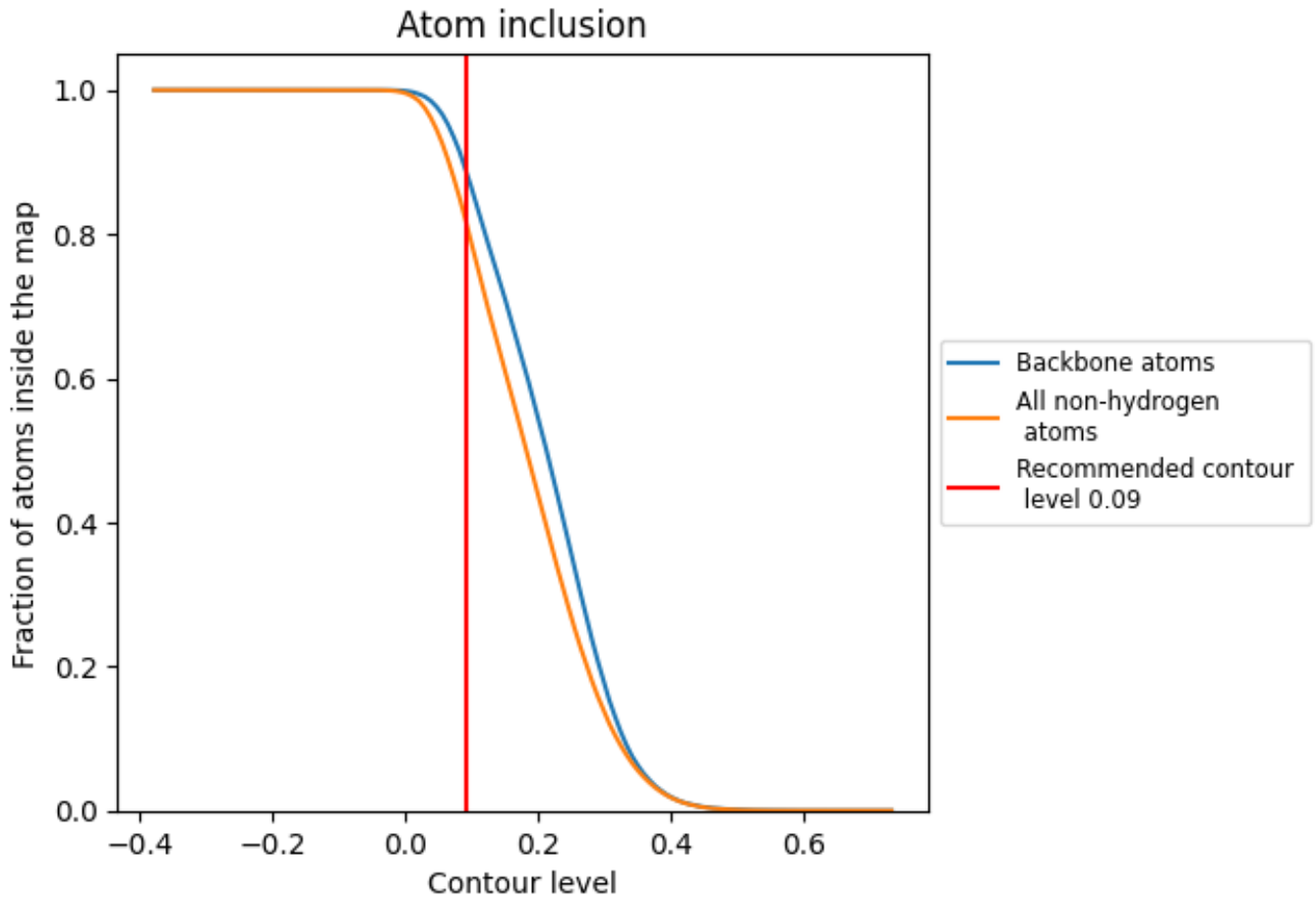
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.09).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 82% 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 (0.09) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8201	0.4860
5	0.8944	0.4930
7	0.9462	0.5210
8	0.9098	0.5010
9	0.8650	0.4680
A	0.8393	0.5480
AA	0.7711	0.4910
B	0.8666	0.5460
BB	0.7198	0.4820
C	0.8427	0.5400
CC	0.7838	0.5130
D	0.8323	0.5040
DD	0.7009	0.4740
E	0.8148	0.5160
EE	0.7289	0.4850
F	0.8247	0.5370
FF	0.6955	0.4600
G	0.7726	0.4990
GG	0.6593	0.4410
H	0.7991	0.5270
HH	0.6653	0.4530
I	0.8166	0.5310
II	0.7474	0.4970
J	0.7835	0.4970
JJ	0.7208	0.4760
KK	0.7228	0.4450
L	0.8158	0.5210
LL	0.7711	0.5210
M	0.8444	0.5210
MM	0.4206	0.2910
N	0.8765	0.5560
NN	0.7667	0.5110
O	0.8529	0.5390
OO	0.7427	0.4930
P	0.8368	0.5370

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Chain	Atom inclusion	Q-score
PP	0.7098	0.4520
Q	0.8531	0.5460
QQ	0.7363	0.4780
R	0.7828	0.5120
RR	0.6927	0.4710
S	0.8558	0.5410
SS	0.6983	0.4540
T	0.8092	0.5320
TT	0.7303	0.4610
U	0.7623	0.4700
UU	0.7274	0.4580
V	0.8205	0.5440
VV	0.7540	0.4930
W	0.6414	0.4420
WW	0.7911	0.5150
X	0.8021	0.5220
XX	0.7526	0.5140
Y	0.8145	0.5270
YY	0.6983	0.4510
Z	0.8322	0.5160
ZZ	0.6381	0.4220
a	0.8671	0.5540
aa	0.7739	0.5120
b	0.7117	0.4810
bb	0.6995	0.4820
c	0.8078	0.5110
cc	0.6596	0.4710
d	0.8133	0.5170
dd	0.8397	0.5150
e	0.8151	0.5450
ee	0.6291	0.4480
f	0.8694	0.5590
ff	0.4917	0.3380
g	0.8002	0.5260
gg	0.6683	0.4220
h	0.7926	0.5170
i	0.7990	0.5110
j	0.8722	0.5460
k	0.7271	0.4800
l	0.8173	0.5300
m	0.8345	0.5360
n	0.7615	0.5090

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Chain	Atom inclusion	Q-score
o	0.8017	0.5420
p	0.7794	0.5290
r	0.8506	0.5360
s	0.6148	0.4070
t	0.3699	0.2830
u	0.1321	0.2110
v	0.5364	0.3910
w	0.3158	0.3470