



Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 04:35 am GMT

PDB ID : 6GQV
EMDB ID : EMD-0049
Title : Cryo-EM reconstruction of yeast 80S ribosome in complex with mRNA, tRNA and eEF2 (GMPPCP)
Authors : Pellegrino, S.; Yusupov, M.; Yusupova, G.; Hashem, Y.
Deposited on : 2018-06-08
Resolution : 4.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, 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

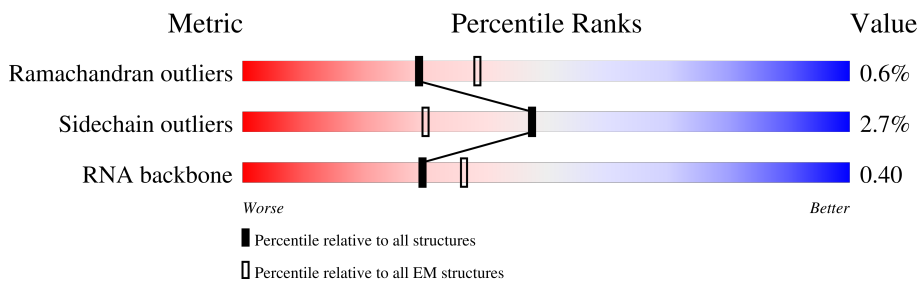
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 Å.

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



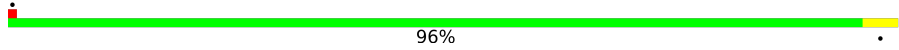

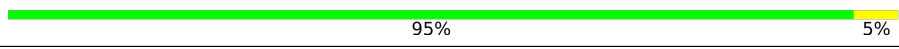
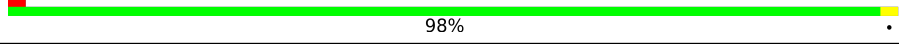
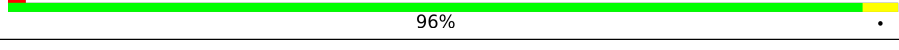
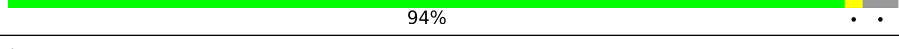
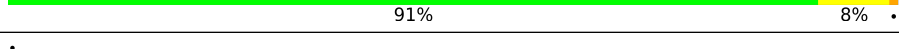
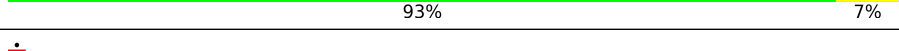
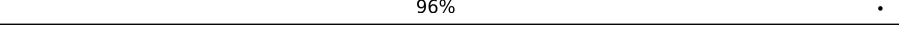
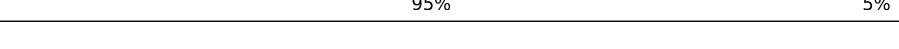
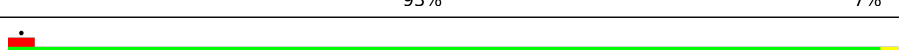
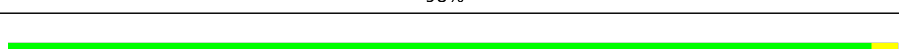
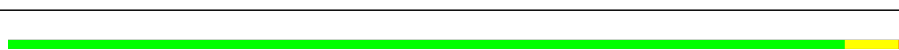
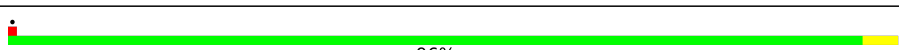
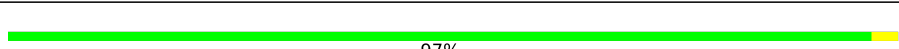
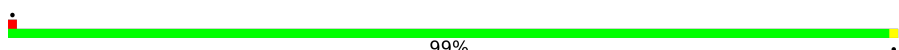

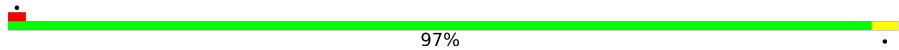
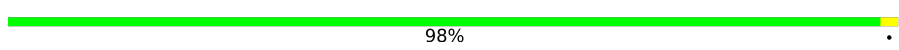
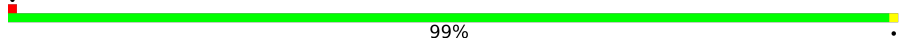
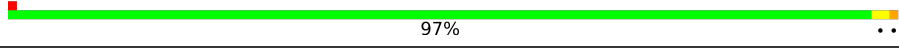
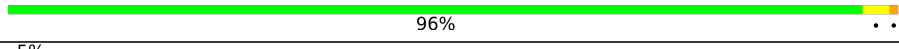
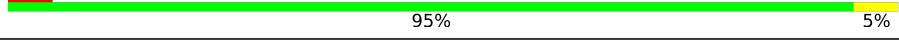
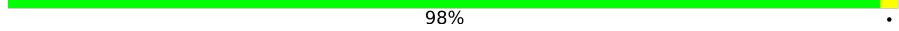

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	1	3396	
2	3	121	
3	4	158	
4	P0	189	
5	P2	94	
6	A	252	
7	B	386	
8	C	361	

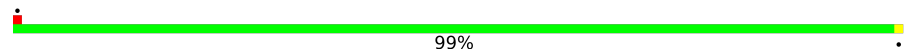
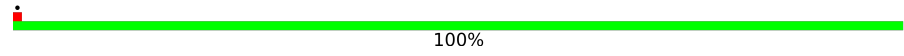
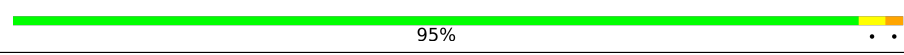
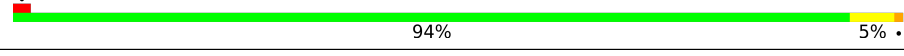
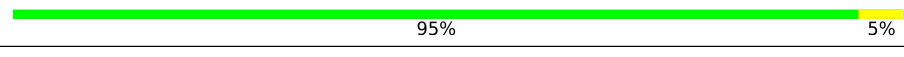
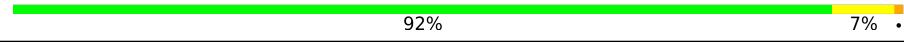
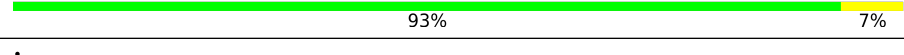
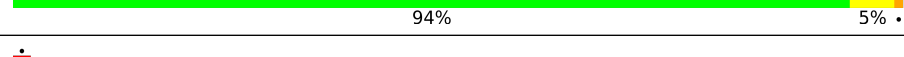
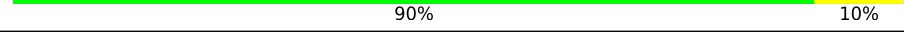
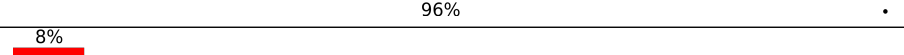
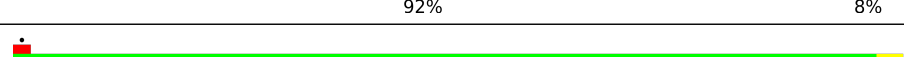
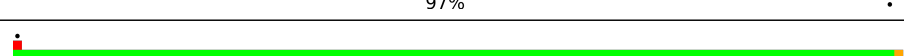
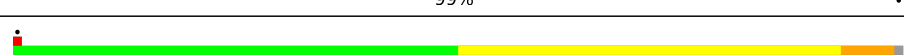
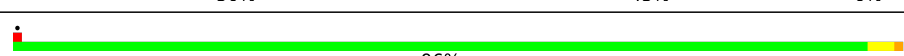
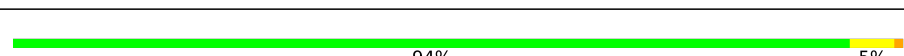
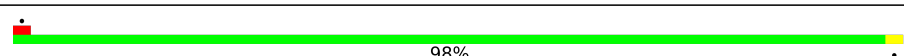
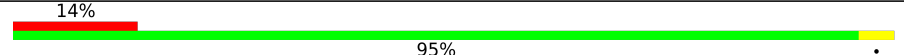
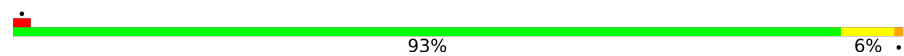
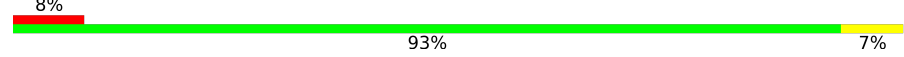
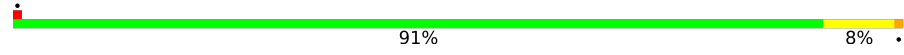
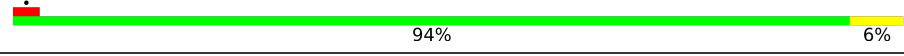
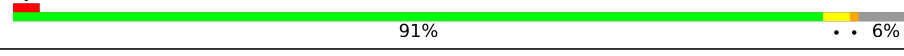
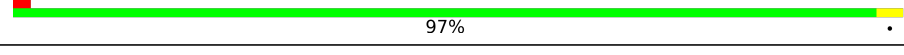


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Mol	Chain	Length	Quality of chain
9	D	296	 96%
10	E	175	 85% 5% 11%
11	F	222	 95% 5%
12	G	233	 98%
13	H	191	 96%
14	I	220	 94%
15	J	169	 91% 8%
16	L	193	 93% 7%
17	M	136	 96%
18	N	203	 95% 5%
19	O	197	 93% 7%
20	P	183	 98%
21	Q	185	 97%
22	R	188	 94% 6%
23	S	172	 96%
24	T	159	 97%
25	U	100	 99%
26	V	136	 97%
27	W	62	 97%
28	X	121	 98%
29	Y	126	 99%
30	Z	135	 97%
31	a	148	 96%
32	b	58	 5% 95% 5%
33	c	97	 98%

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Mol	Chain	Length	Quality of chain
34	d	109	 99%
35	e	127	 100%
36	f	106	 95%
37	g	112	 94%
38	h	119	 95%
39	i	99	 92%
40	j	87	 93%
41	k	77	 94%
42	l	50	 90%
43	m	52	 96%
44	n	25	 8%
45	o	105	 97%
46	p	91	 99%
47	2	1797	 50%
48	q	206	 96%
49	r	214	 94%
50	s	217	 98%
51	t	223	 14%
52	u	260	 93%
53	v	206	 8%
54	w	223	 91%
55	x	184	 94%
56	y	199	 91%
57	z	185	 97%
58	AA	105	 88%

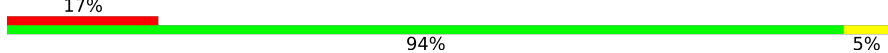
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Mol	Chain	Length	Quality of chain
59	AB	153	8% 93% 7%
60	AC	124	69% 97% .
61	AD	150	. 94% 5% .
62	AE	127	. 94% 6%
63	AF	124	6% 94% 6%
64	AG	141	11% 96% .
65	AH	125	10% 92% .. .
66	AI	145	8% 96% ..
67	AJ	143	. 98% ..
68	AK	107	12% 96% .
69	AL	87	. 93% 5% .
70	AM	129	. 97% .
71	AN	144	. 96% .
72	AO	134	. 97% .
73	AP	70	23% 96% ..
74	AQ	97	. 94% 6%
75	AR	81	. 96% .
76	AS	63	21% 97% ..
77	AT	53	. 96% .
78	AU	60	8% 93% ..
79	AV	318	12% 99% .
80	AW	37	14% 95% 5%
81	AX	837	7% 94% 5%
82	AY	76	55% 34% 11%
83	AZ	7	57% 71% 29%

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Mol	Chain	Length	Quality of chain
84	BA	204	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into three segments: a red segment on the left labeled '17%', a large green segment in the middle labeled '94%', and a small yellow segment on the right labeled '5%'.</p>

2 Entry composition

There are 86 unique types of molecules in this entry. The entry contains 212058 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 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	1	3223	68931	30790	12416	22502	3223	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	3	121	2579	1152	461	845	121	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	4	158	3353	1500	586	1109	158	0	0

- Molecule 4 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	P0	189	1473	942	257	270	4	0	0

- Molecule 5 is a protein called 60S ribosomal protein L12-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	P2	94	723	448	138	135	2	0	0

- Molecule 6 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	A	252	1914	1191	388	334	1	0	0

- Molecule 7 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	B	386	3075	1950	584	533	8	0	0

- Molecule 8 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	C	361	2748	1729	522	494	3	0	0

- Molecule 9 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	D	296	2375	1501	414	458	2	0	0

- Molecule 10 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	E	156	1239	800	222	216	1	0	0

- Molecule 11 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	F	222	1784	1151	324	308	1	0	0

- Molecule 12 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	G	233	1804	1151	323	327	3	0	0

- Molecule 13 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	H	191	1518	963	274	277	4	0	0

- Molecule 14 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	I	211	Total	C	N	O	S	0	0
			1705	1083	322	294	6		

- Molecule 15 is a protein called 60S ribosomal protein L11-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	J	169	Total	C	N	O	S	0	0
			1353	847	253	249	4		

- Molecule 16 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	L	193	Total	C	N	O	0	0
			1543	962	315	266		

- Molecule 17 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	136	Total	C	N	O	S	0	0
			1053	675	199	177	2		

- Molecule 18 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	203	Total	C	N	O	S	0	0
			1720	1077	361	281	1		

- Molecule 19 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	O	197	Total	C	N	O	S	0	0
			1555	1003	289	262	1		

- Molecule 20 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	P	183	Total	C	N	O	0	0
			1420	882	281	257		

- Molecule 21 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	Q	185	1441	908	290	241	2	0	0

- Molecule 22 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	R	188	1521	935	326	260		0	0

- Molecule 23 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	S	172	1445	930	267	244	4	0	0

- Molecule 24 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	T	159	1276	805	246	221	4	0	0

- Molecule 25 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	U	100	796	516	131	149		0	0

- Molecule 26 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	V	136	997	625	186	179	7	0	0

- Molecule 27 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	W	62	513	330	101	81	1	0	0

- Molecule 28 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	X	121	964	620	169	173	2	0	0

- Molecule 29 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	Y	126	993	625	192	176		0	0

- Molecule 30 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	Z	135	1092	710	202	180		0	0

- Molecule 31 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	a	148	1173	749	231	190	3	0	0

- Molecule 32 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	b	58	462	289	100	73		0	0

- Molecule 33 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	c	97	743	479	124	139	1	0	0

- Molecule 34 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	d	109	883	559	167	156	1	0	0

- Molecule 35 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	e	127	Total	C	N	O	S	0	0
			1020	647	205	167	1		

- Molecule 36 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	f	106	Total	C	N	O	S	0	0
			850	540	165	144	1		

- Molecule 37 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	g	112	Total	C	N	O	S	0	0
			880	545	179	152	4		

- Molecule 38 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	h	119	Total	C	N	O	S	0	0
			969	615	186	167	1		

- Molecule 39 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	i	99	Total	C	N	O	S	0	0
			771	481	156	132	2		

- Molecule 40 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	j	87	Total	C	N	O	S	0	0
			681	414	148	114	5		

- Molecule 41 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	k	77	Total	C	N	O	0	0
			612	391	115	106		

- Molecule 42 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	l	50	Total	C	N	O	S	0	0
			436	272	97	65	2		

- Molecule 43 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	m	52	Total	C	N	O	S	0	0
			417	259	86	67	5		

- Molecule 44 is a protein called 60S ribosomal protein L41-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	n	25	Total	C	N	O	S	0	0
			233	142	63	27	1		

- Molecule 45 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	o	105	Total	C	N	O	S	0	0
			847	534	170	138	5		

- Molecule 46 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	p	91	Total	C	N	O	S	0	0
			694	429	138	121	6		

- Molecule 47 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	2	1776	Total	C	N	O	P	0	0
			37845	16918	6702	12449	1776		

- Molecule 48 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	q	206	Total	C	N	O	S	0	0
			1577	1014	278	283	2		

- Molecule 49 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	r	214	Total	C	N	O	S	0	0
			1709	1084	310	311	4		

- Molecule 50 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	s	217	Total	C	N	O	S	0	0
			1635	1047	289	297	2		

- Molecule 51 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	t	223	Total	C	N	O	S	0	0
			1734	1101	313	314	6		

- Molecule 52 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	u	260	Total	C	N	O	S	0	0
			2068	1316	389	360	3		

- Molecule 53 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	v	206	Total	C	N	O	S	0	0
			1609	1007	300	299	3		

- Molecule 54 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	w	223	Total	C	N	O	S	0	0
			1790	1123	346	318	3		

- Molecule 55 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
55	x	184	Total	C	N	O	0	0
			1481	951	265	265		

- Molecule 56 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	y	188	1489	925	298	264	2	0	0

- Molecule 57 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	z	185	1494	943	289	261	1	0	0

- Molecule 58 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
58	AA	96	772	499	126	145	2	0	0

- Molecule 59 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
59	AB	153	1220	780	231	206	3	0	0

- Molecule 60 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
60	AC	124	890	560	156	172	2	0	0

- Molecule 61 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
61	AD	150	1192	759	224	207	2	0	0

- Molecule 62 is a protein called 40S ribosomal protein S14-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
62	AE	127	891	545	182	163	1	0	0

- Molecule 63 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
63	AF	124	977	622	182	166	7	0	0

- Molecule 64 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
64	AG	141	1105	708	203	194		0	0

- Molecule 65 is a protein called 40S ribosomal protein S17-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
65	AH	120	926	577	177	170	2	0	0

- Molecule 66 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
66	AI	145	1192	743	237	210	2	0	0

- Molecule 67 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
67	AJ	143	1112	694	208	208	2	0	0

- Molecule 68 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
68	AK	107	855	539	156	159	1	0	0

- Molecule 69 is a protein called 40S ribosomal protein S21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
69	AL	87	684	420	125	137	2	0	0

- Molecule 70 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	AM	129	Total	C	N	O	S	0	0
			1021	650	188	180	3		

- Molecule 71 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	AN	144	Total	C	N	O	S	0	0
			1121	708	220	191	2		

- Molecule 72 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
72	AO	134	Total	C	N	O	0	0
			1073	676	208	189		

- Molecule 73 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
73	AP	70	Total	C	N	O	0	0
			563	360	104	99		

- Molecule 74 is a protein called 40S ribosomal protein S26-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	AQ	97	Total	C	N	O	S	0	0
			769	475	160	129	5		

- Molecule 75 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	AR	81	Total	C	N	O	S	0	0
			610	382	110	113	5		

- Molecule 76 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	AS	63	Total	C	N	O	S	0	0
			497	306	99	91	1		

- Molecule 77 is a protein called 40S ribosomal protein S29-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	AT	53	Total	C	N	O	S	0	0
			442	274	92	72	4		

- Molecule 78 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	AU	60	Total	C	N	O	S	0	0
			475	299	98	77	1		

- Molecule 79 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	AV	318	Total	C	N	O	S	0	0
			2437	1541	418	470	8		

- Molecule 80 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	AW	37	Total	C	N	O	S	0	0
			287	177	57	49	4		

- Molecule 81 is a protein called Elongation factor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	AX	837	Total	C	N	O	S	0	0
			6523	4143	1120	1231	29		

- Molecule 82 is a RNA chain called Transfer RNA - Phe.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	AY	76	Total	C	N	O	P	0	0
			1626	725	293	532	76		

- Molecule 83 is a RNA chain called Messenger RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	AZ	7	Total	C	N	O	P	0	0
			144	65	21	51	7		

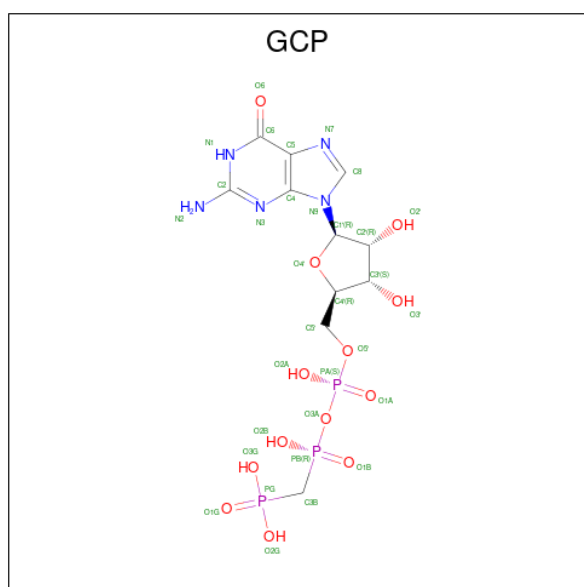
- Molecule 84 is a protein called 60S ribosomal protein L1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
84	BA	204	1609	1031	279	290	9	0	0

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

Mol	Chain	Residues	Atoms		AltConf
85	j	1	Total	Zn	0
			1	1	
85	m	1	Total	Zn	0
			1	1	
85	o	1	Total	Zn	0
			1	1	
85	p	1	Total	Zn	0
			1	1	
85	AQ	1	Total	Zn	0
			1	1	
85	AR	1	Total	Zn	0
			1	1	
85	AT	1	Total	Zn	0
			1	1	
85	AW	1	Total	Zn	0
			1	1	

- Molecule 86 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: C₁₁H₁₈N₅O₁₃P₃).



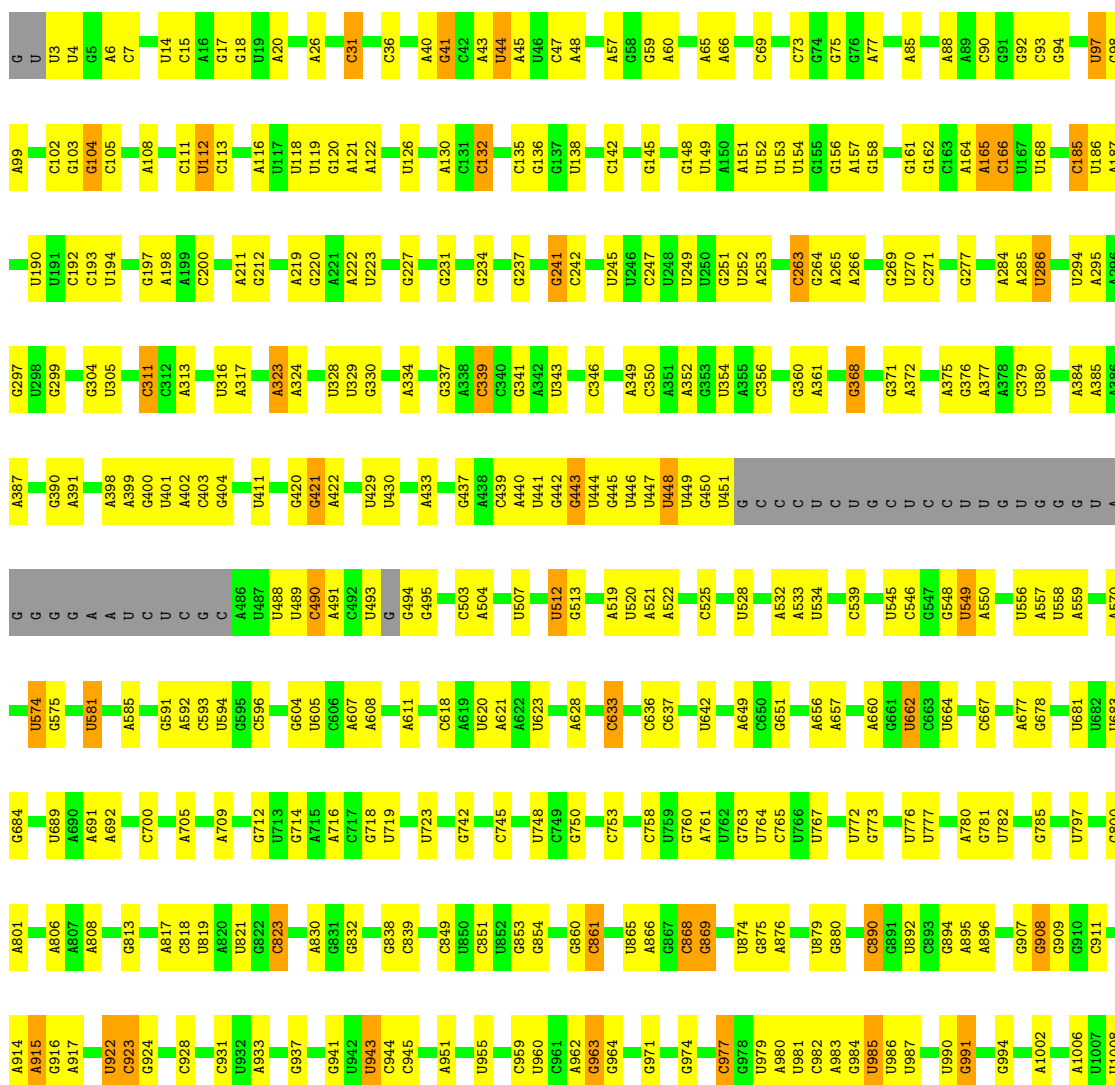
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
86	AX	1	32	11	5	13	3	0

3 Residue-property plots

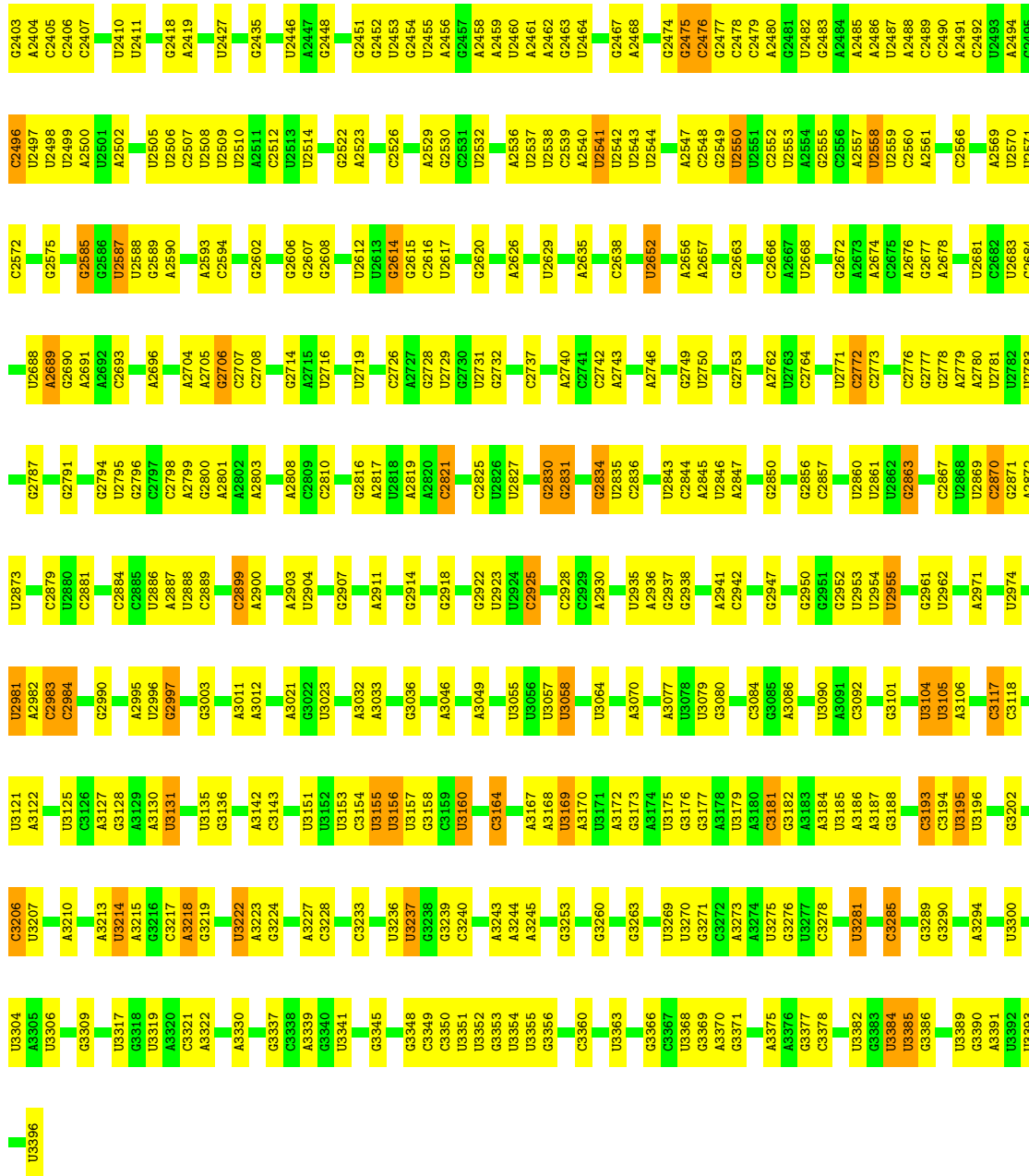
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: 25S ribosomal RNA

Chain 1: 



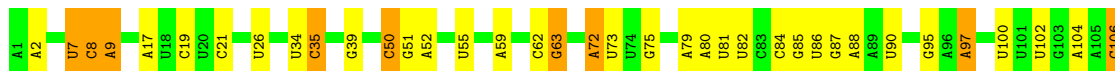
A1009	U1088	U1191	U1258	U1341	A1449	C1562	G1666	G1770	U1877	C	A2168	G2300
G1013	G1089	C1192	A1259	C1342	G1450	C1563	C1671	G1773	G1878	U	U2189	U2301
U1014	U1015	U1016	G1261	U1348	A1452	G1565	A1678	C1774	A1879	A	C2192	C2304
C1017	A1093	A1094	U1261	G1349	U1455	U1568	G1679	G1775	U1880	U	U2193	C2306
G1018	U1095	C1198	G1264	U1351	A1456	U1569	A1680	G1776	U1886	C	C2194	C2307
U1019	U1096	C1199	U1267	U1352	U1457	U1570	A1683	U1777	A1885	G	U2205	C2308
G1020	A1098	A1200	U1271	A1353	U1458	A1571	G1683	G1778	G1889	C	G2206	A2309
U1022	A1099	C1201	A1271	G1354	C1459	U1572	C1690	C1779	U1892	U	A2207	U2310
G1023	U1100	A1202	C1272	U1355	A1460	G1573	C1690	C1781	G1892	C	U2208	A2313
G1024	A1103	G1206	C1275	G1357	G1466	A1574	U1702	G1784	A1895	C	G2210	G2315
A1025	U1111	G1209	C1279	A1362	C1469	A1575	U1703	A1784	A1896	U	A2213	U2318
A1026	U1111	U1210	C1280	G1362	U1470	G1576	A1704	C1788	G1897	G	A2214	U2318
A1027	G1115	U1211	G1281	C1364	U1470	A1580	C1706	C1793	G1898	G	A2215	A2324
U1028	G1116	U1212	G1282	G1370	A1482	C1581	G1711	G1794	U1900	U	G2110	A2324
G1029	G1117	A1212	C1283	U1370	U1483	C1582	G1712	U1795	A1901	G	G2111	G2221
A1030	U1127	U1215	C1284	G1374	U1484	A1583	G1713	U1796	U1901	U	A2112	A2221
C1031	G1128	C1216	G1285	G1374	A1490	U1584	A1714	A1797	G1905	C	C2114	A2222
C1032	U1128	A1217	A1286	G1375	A1491	A1587	A1715	A1797	G1906	C	G2115	A2223
U1033	A1129	U1218	A1287	A1386	A1491	A1588	U1716	C1805	C1907	U	A2224	A2233
U1034	U1130	C1219	A1287	U1386	C1496	A1589	U1717	C1805	U1912	C	U2225	U2235
G1035	G1131	U1220	A1291	A1390	C1502	A1593	G1718	A1813	U1912	C	A2225	U2225
A1036	A1136	U1221	C1292	C1391	C1502	A1593	G1718	A1814	U1912	C	G2231	C2339
C1037	C1137	A1222	G1295	G1392	G1507	C1596	U1724	U1815	U1916	C	G2236	U2347
C1038	C1141	C1223	G1295	A1393	C1508	C1597	U1724	A1816	C1917	C	G2123	A2348
U1042	G1142	A1224	A1301	A1394	C1508	C1597	G1728	U1816	U1917	C	U2140	U2349
C1043	A1143	G1225	A1302	A1397	U1511	G1604	G1730	U1820	U1920	U	A2131	C2350
U1047	A1143	C1227	A1303	C1397	G1512	U1605	A1731	U1821	A1921	C	G2132	U2351
A1048	U1144	C1228	A1304	U1399	G1513	U1606	U1732	U1824	C1922	C	A2141	A2352
C1049	G1145	G1229	U1305	G1400	U1514	U1607	U1732	U1824	C1922	C	U2142	C2359
U1050	U1151	G1230	G1306	U1400	A1515	C1608	G1735	U1837	U1926	C	U2143	U2359
U1051	U1151	A1231	G1307	U1400	C1516	C1608	G1736	G1837	C1926	C	G2144	C2362
U1052	A1154	C1232	A1308	A1406	C1516	A1613	U1737	A1838	U1926	C	A2145	C2366
G1059	C1155	G1233	U1309	C1411	U1523	C1614	C1738	U1839	U1931	C	A2146	U2260
U1060	A1158	U1235	G1310	C1411	A1524	U1620	U1739	A1841	A1932	C	C2265	A2372
U1061	A1159	G1237	G1311	U1415	G1525	A1621	U1740	A1842	U1933	U	U2270	A2373
A1064	G1171	C1238	G1313	C1416	U1526	A1621	G1748	C1843	G1934	C	A2271	G2375
G1072	G1177	A1244	C1316	G1417	U1533	U1629	A1748	U1846	U1935	C	A2272	C2378
C1076	G1178	U1247	A1317	U1418	G1536	A1632	A1750	A1847	G1948	C	U2282	U2378
A1079	A1179	G1248	A1318	A1419	G1536	C1633	G1751	A1850	G1953	C	G2273	A2386
U1080	U1181	G1249	G1319	U1425	A1546	A1642	U1752	G1851	G1954	C	U2274	U2388
U1081	A1182	A1252	G1320	U1425	A1546	A1643	G1753	G1851	U1955	C	A2166	C2389
U1082	G1186	C1254	G1321	G1434	C1551	A1644	C1756	U1855	U1955	C	G2169	A2390
A1084	A1190	C1257	U1325	U1434	C1551	A1644	C1756	U1855	U1955	C	U2170	U2390
A1085	A1190	C1257	U1331	U1437	U1554	A1645	A1760	G1863	G1955	C	U2175	U2391
			A1332	U1438	U1555	G1646	G1761	A1864	A1955	C	C2284	C2392
			A1337	U1442	A1557	A1647	C1762	C1866	U1955	C	C2285	G2393
			C1338	U1442	A1558	A1647	C1763	C1867	U1955	C	U2286	U2393
			C1339	U1446	A1559	A1647	C1763	C1867	U1955	C	C2287	A2397
			C1340	U1447	A1560	A1647	C1763	C1867	U1955	C	G2288	A2398
				U1448	A1561	A1647	C1763	C1867	U1955	C	A2401	A2402
					A1561	A1647	C1763	C1867	U1955	C	U2184	A2402

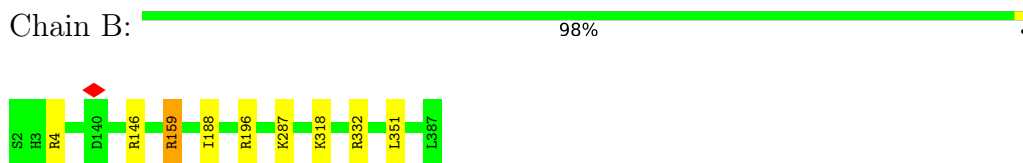
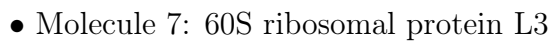
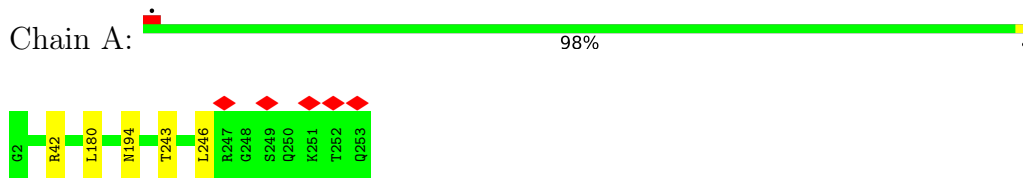
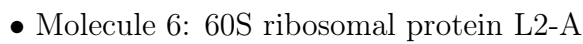
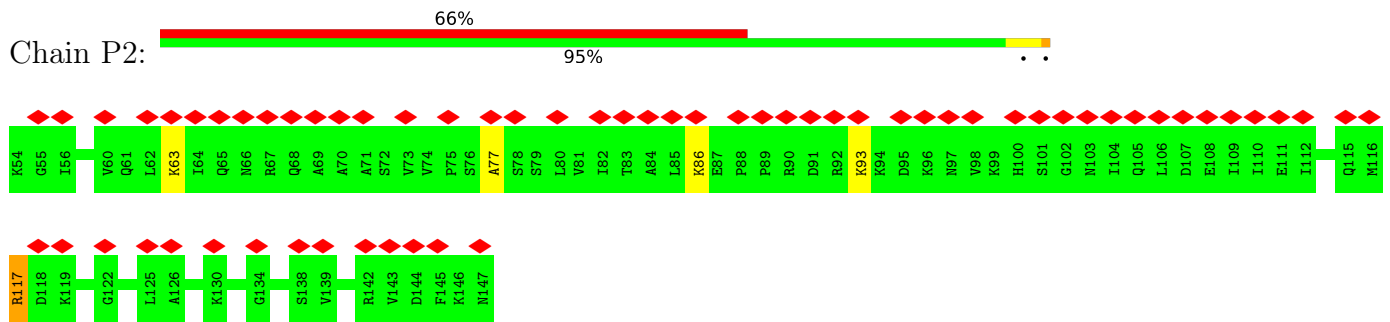
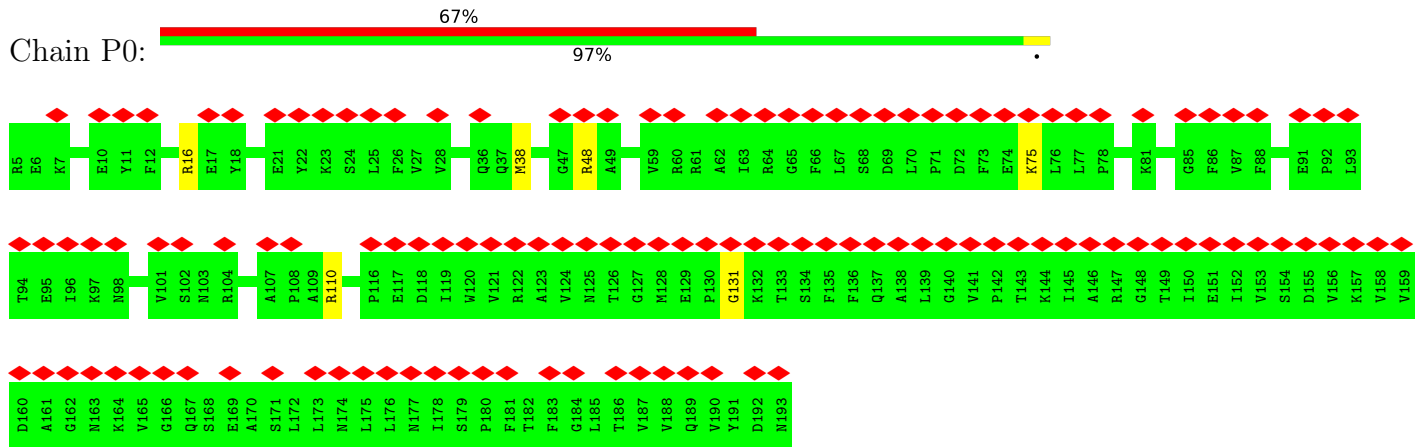
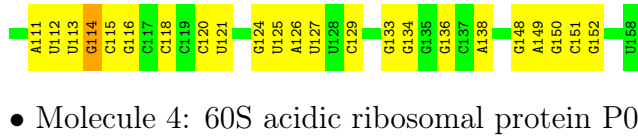


• Molecule 2: 5S ribosomal RNA



• Molecule 3: 5.8S ribosomal RNA



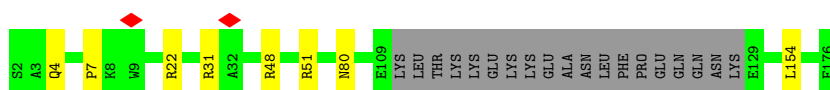
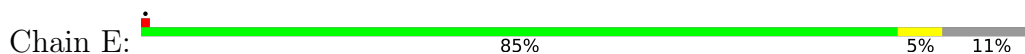




- Molecule 9: 60S ribosomal protein L5



- Molecule 10: 60S ribosomal protein L6-A



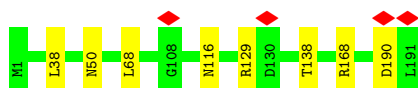
- Molecule 11: 60S ribosomal protein L7-A



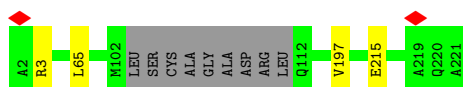
- Molecule 12: 60S ribosomal protein L8-A




- Molecule 13: 60S ribosomal protein L9-A

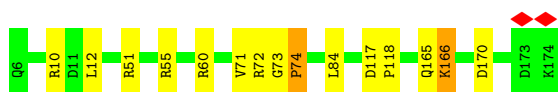


- Molecule 14: 60S ribosomal protein L10



- Molecule 15: 60S ribosomal protein L11-B

Chain J:  91% 8%



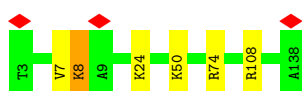
- Molecule 16: 60S ribosomal protein L13-A

Chain L:  93% 7%



- Molecule 17: 60S ribosomal protein L14-A

Chain M:  96%



- Molecule 18: 60S ribosomal protein L15-A

Chain N:  95% 5%



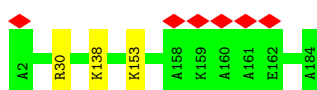
- Molecule 19: 60S ribosomal protein L16-A

Chain O:  93% 7%



- Molecule 20: 60S ribosomal protein L17-A

Chain P:  98%



- Molecule 21: 60S ribosomal protein L18-A

Chain Q:  97%



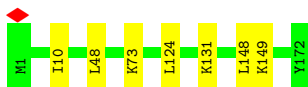
- Molecule 22: 60S ribosomal protein L19-A

Chain R:  94% 6%



- Molecule 23: 60S ribosomal protein L20-A

Chain S:  96%



- Molecule 24: 60S ribosomal protein L21-A

Chain T:  97%



- Molecule 25: 60S ribosomal protein L22-A

Chain U:  99%



- Molecule 26: 60S ribosomal protein L23-A

Chain V:  97%



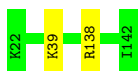
- Molecule 27: 60S ribosomal protein L24-A

Chain W:  97%



- Molecule 28: 60S ribosomal protein L25

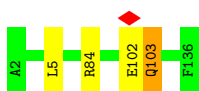
Chain X:  98%



- Molecule 29: 60S ribosomal protein L26-A



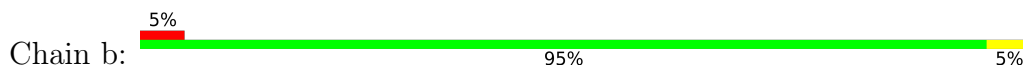
- Molecule 30: 60S ribosomal protein L27-A



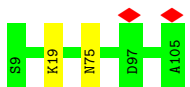
- Molecule 31: 60S ribosomal protein L28



- Molecule 32: 60S ribosomal protein L29



- Molecule 33: 60S ribosomal protein L30



- Molecule 34: 60S ribosomal protein L31-A



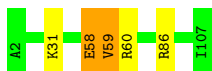
- Molecule 35: 60S ribosomal protein L32

Chain e:  100%



- Molecule 36: 60S ribosomal protein L33-A

Chain f:  95%



- Molecule 37: 60S ribosomal protein L34-A

Chain g:  94%




- Molecule 38: 60S ribosomal protein L35-A

Chain h:  95%



- Molecule 39: 60S ribosomal protein L36-A

Chain i:  92%



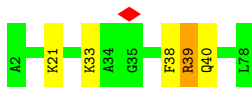
- Molecule 40: 60S ribosomal protein L37-A

Chain j:  93%




- Molecule 41: 60S ribosomal protein L38

Chain k:  94%



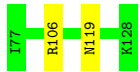
- Molecule 42: 60S ribosomal protein L39

Chain l:  90% 10%

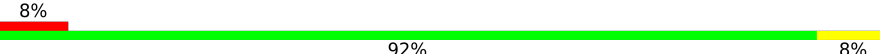


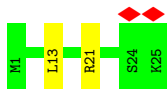
- Molecule 43: Ubiquitin-60S ribosomal protein L40

Chain m:  96%



- Molecule 44: 60S ribosomal protein L41-B

Chain n:  8% 92% 8%



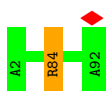
- Molecule 45: 60S ribosomal protein L42-A

Chain o:  97%



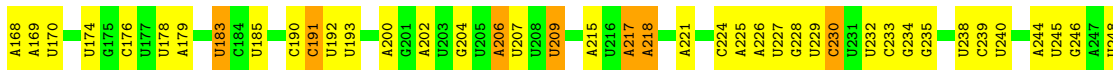
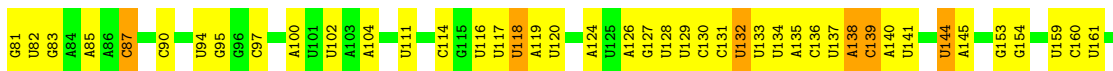
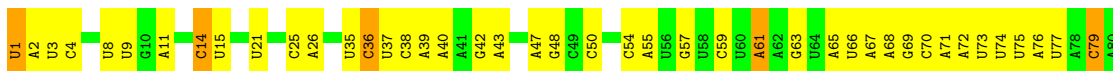
- Molecule 46: 60S ribosomal protein L43-A

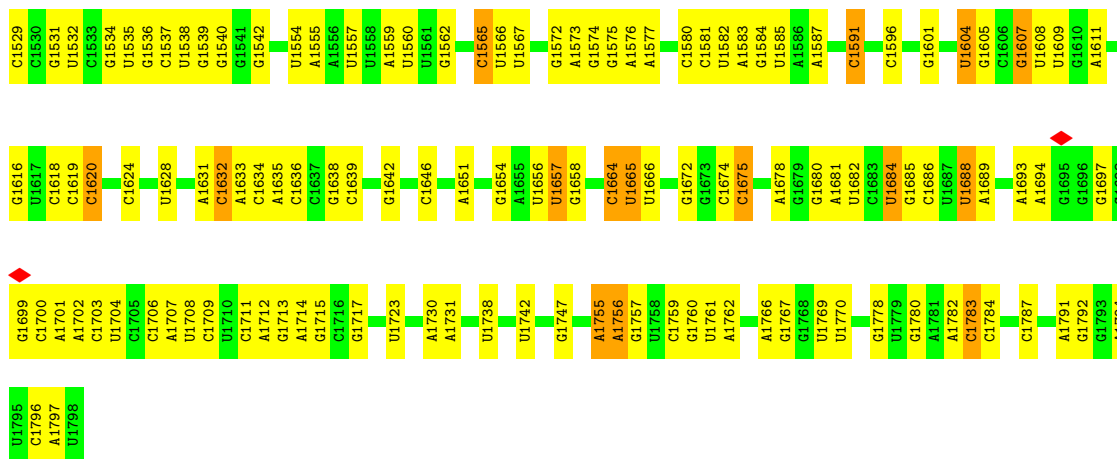
Chain p:  99%



- Molecule 47: 18S ribosomal RNA

Chain 2:  50% 43% 6%





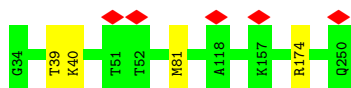
• Molecule 48: 40S ribosomal protein S0-A



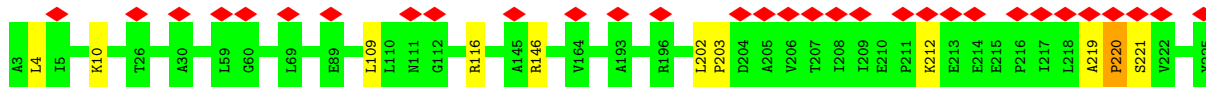
• Molecule 49: 40S ribosomal protein S1-A



• Molecule 50: 40S ribosomal protein S2

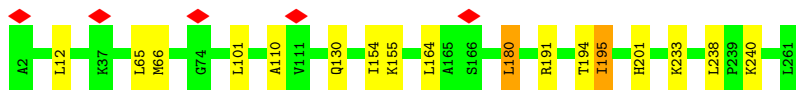


• Molecule 51: 40S ribosomal protein S3

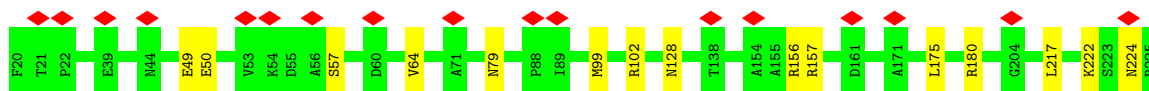
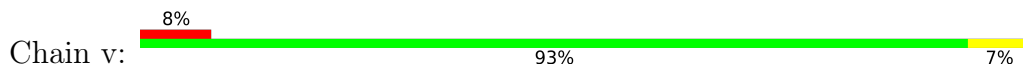


• Molecule 52: 40S ribosomal protein S4-A

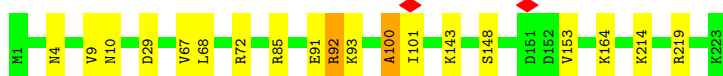
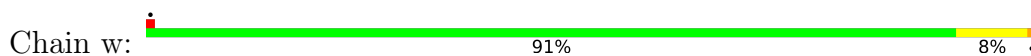




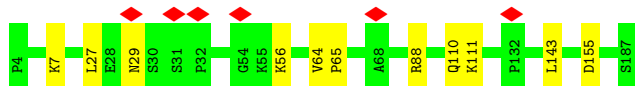
- Molecule 53: 40S ribosomal protein S5



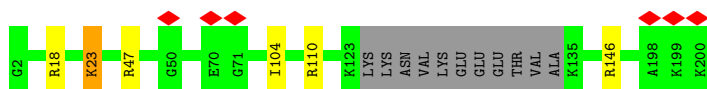
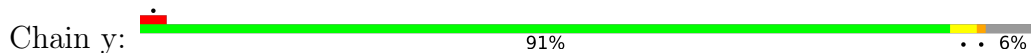
- Molecule 54: 40S ribosomal protein S6-A



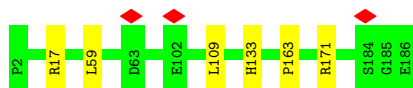
- Molecule 55: 40S ribosomal protein S7-A



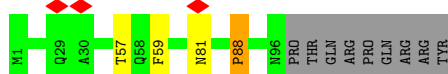
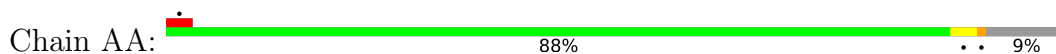
- Molecule 56: 40S ribosomal protein S8-A



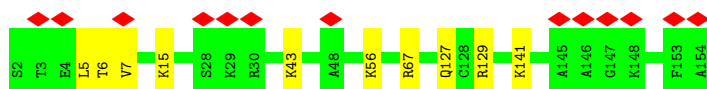
- Molecule 57: 40S ribosomal protein S9-A



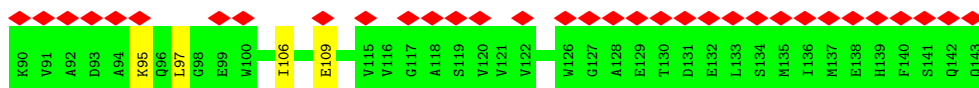
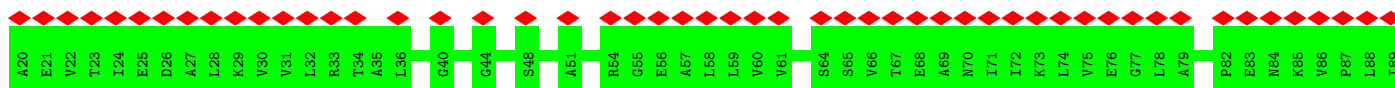
- Molecule 58: 40S ribosomal protein S10-A



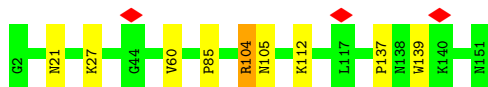
- Molecule 59: 40S ribosomal protein S11-A



- Molecule 60: 40S ribosomal protein S12



- Molecule 61: 40S ribosomal protein S13



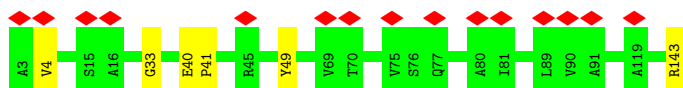
- Molecule 62: 40S ribosomal protein S14-B



- Molecule 63: 40S ribosomal protein S15

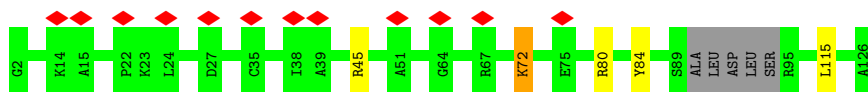


- Molecule 64: 40S ribosomal protein S16-A

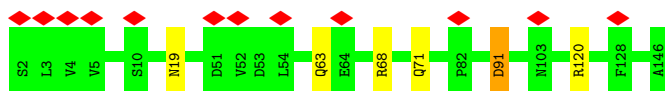


- Molecule 65: 40S ribosomal protein S17-B

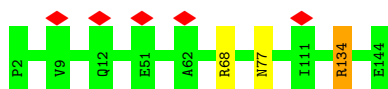




- Molecule 66: 40S ribosomal protein S18-A



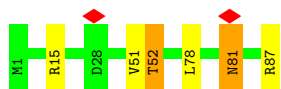
- Molecule 67: 40S ribosomal protein S19-A



- Molecule 68: 40S ribosomal protein S20



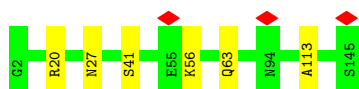
- Molecule 69: 40S ribosomal protein S21-A



- Molecule 70: 40S ribosomal protein S22-A



- Molecule 71: 40S ribosomal protein S23-A



- Molecule 72: 40S ribosomal protein S24-A

Chain AO:  97%



- Molecule 73: 40S ribosomal protein S25-A

Chain AP:  23% 96%



- Molecule 74: 40S ribosomal protein S26-B

Chain AQ:  94% 6%



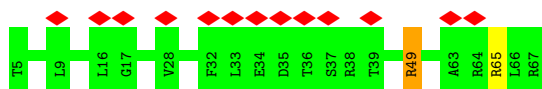
- Molecule 75: 40S ribosomal protein S27-A

Chain AR:  96%



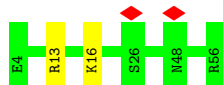
- Molecule 76: 40S ribosomal protein S28-A

Chain AS:  21% 97%



- Molecule 77: 40S ribosomal protein S29-A

Chain AT:  96%

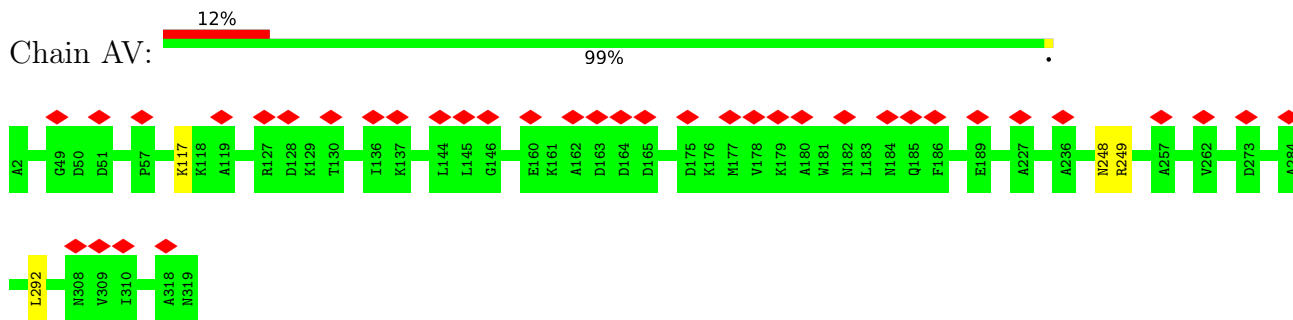


- Molecule 78: 40S ribosomal protein S30-A

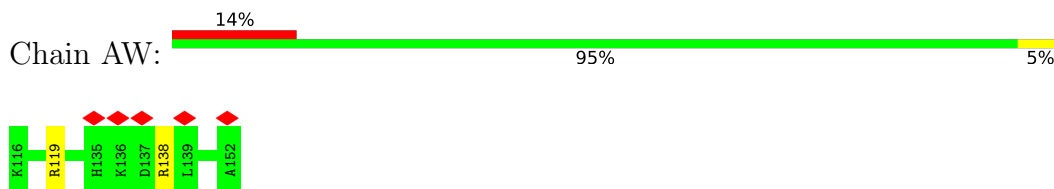
Chain AU:  8% 93%



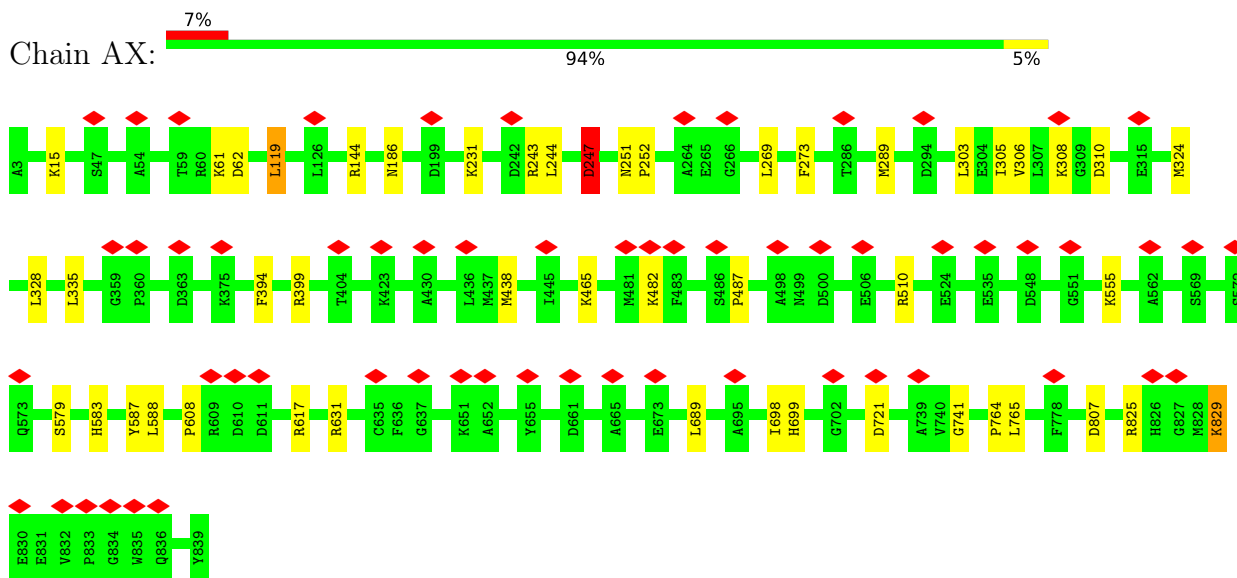
- Molecule 79: Guanine nucleotide-binding protein subunit beta-like protein



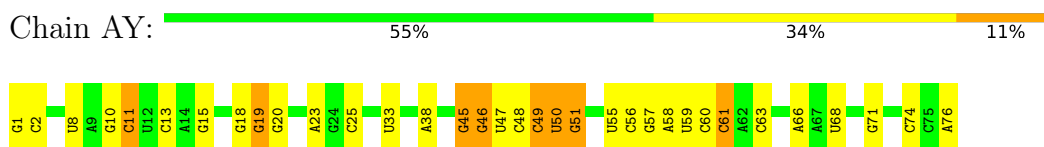
- Molecule 80: Ubiquitin-40S ribosomal protein S31



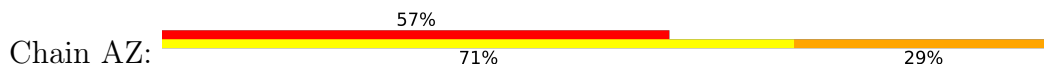
- Molecule 81: Elongation factor 2



- Molecule 82: Transfer RNA - Phe



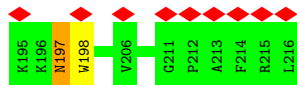
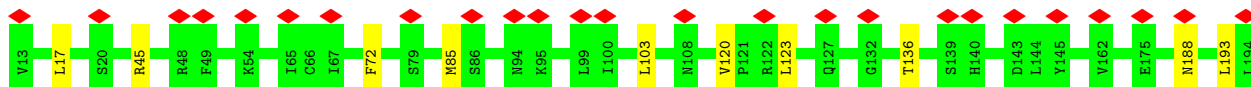
- Molecule 83: Messenger RNA





• Molecule 84: 60S ribosomal protein L1-A

Chain BA: 17% 94% 5%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	86500	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	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	0.306	Depositor
Minimum map value	-0.179	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.033	Depositor
Map size (\AA)	396.0, 396.0, 396.0	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.1, 1.1, 1.1	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: GCP, DDE, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1	0.68	1/77157 (0.0%)	1.24	613/120295 (0.5%)
2	3	0.59	0/2883	1.18	20/4491 (0.4%)
3	4	0.67	0/3746	1.26	37/5832 (0.6%)
4	P0	0.32	0/1498	0.65	1/2025 (0.0%)
5	P2	0.34	0/728	0.78	2/975 (0.2%)
6	A	0.41	0/1948	0.71	2/2617 (0.1%)
7	B	0.37	0/3146	0.67	1/4228 (0.0%)
8	C	0.38	0/2800	0.68	1/3790 (0.0%)
9	D	0.35	0/2425	0.67	2/3271 (0.1%)
10	E	0.33	0/1260	0.66	0/1694
11	F	0.39	0/1821	0.68	0/2451
12	G	0.35	0/1836	0.64	1/2481 (0.0%)
13	H	0.37	0/1539	0.71	4/2073 (0.2%)
14	I	0.39	0/1741	0.64	0/2335
15	J	0.34	0/1374	0.74	1/1842 (0.1%)
16	L	0.36	0/1568	0.67	1/2106 (0.0%)
17	M	0.32	0/1068	0.62	0/1438
18	N	0.42	0/1757	0.67	1/2354 (0.0%)
19	O	0.40	0/1585	0.66	2/2128 (0.1%)
20	P	0.37	0/1443	0.62	0/1944
21	Q	0.37	0/1465	0.66	1/1965 (0.1%)
22	R	0.32	0/1538	0.67	3/2050 (0.1%)
23	S	0.39	0/1481	0.66	1/1990 (0.1%)
24	T	0.40	0/1300	0.62	0/1743
25	U	0.35	0/812	0.64	0/1099
26	V	0.41	0/1012	0.70	0/1362
27	W	0.36	0/525	0.65	1/696 (0.1%)
28	X	0.35	0/979	0.63	0/1321
29	Y	0.33	0/1004	0.65	1/1341 (0.1%)
30	Z	0.39	0/1118	0.66	1/1497 (0.1%)
31	a	0.37	0/1204	0.69	2/1612 (0.1%)
32	b	0.34	0/473	0.60	0/629

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	c	0.33	0/751	0.62	0/1008
34	d	0.40	0/897	0.68	0/1205
35	e	0.38	0/1041	0.64	0/1394
36	f	0.40	0/868	0.67	0/1168
37	g	0.38	0/890	0.72	1/1189 (0.1%)
38	h	0.32	0/978	0.70	1/1301 (0.1%)
39	i	0.36	0/778	0.73	2/1034 (0.2%)
40	j	0.38	0/696	0.72	0/923
41	k	0.32	0/618	0.79	1/826 (0.1%)
42	l	0.35	0/443	0.75	1/588 (0.2%)
43	m	0.36	0/423	0.63	0/562
44	n	0.34	0/234	0.67	0/300
45	o	0.37	0/860	0.71	0/1136
46	p	0.46	0/701	0.68	0/934
47	2	0.56	2/42328 (0.0%)	1.28	445/65955 (0.7%)
48	q	0.33	0/1617	0.69	0/2215
49	r	0.34	0/1735	0.81	5/2335 (0.2%)
50	s	0.32	0/1665	0.68	0/2263
51	t	0.32	0/1759	0.68	0/2368
52	u	0.33	0/2109	0.77	4/2839 (0.1%)
53	v	0.31	0/1629	0.74	3/2202 (0.1%)
54	w	0.34	0/1814	0.82	2/2425 (0.1%)
55	x	0.32	0/1506	0.74	1/2028 (0.0%)
56	y	0.33	0/1514	0.67	0/2021
57	z	0.33	0/1519	0.72	0/2035
58	AA	0.32	0/789	0.70	1/1067 (0.1%)
59	AB	0.37	0/1247	0.67	1/1681 (0.1%)
60	AC	0.28	0/898	0.69	1/1220 (0.1%)
61	AD	0.33	0/1215	0.72	1/1638 (0.1%)
62	AE	0.33	0/901	0.69	0/1217
63	AF	0.35	0/998	0.77	0/1341
64	AG	0.33	0/1125	0.71	0/1510
65	AH	0.32	0/935	0.71	0/1254
66	AI	0.31	0/1211	0.69	0/1628
67	AJ	0.30	0/1130	0.63	0/1517
68	AK	0.31	0/865	0.71	1/1169 (0.1%)
69	AL	0.36	0/693	0.82	1/935 (0.1%)
70	AM	0.34	0/1038	0.66	1/1395 (0.1%)
71	AN	0.38	0/1139	0.71	0/1518
72	AO	0.33	0/1087	0.63	0/1449
73	AP	0.34	0/571	0.75	0/768
74	AQ	0.34	0/782	0.77	0/1047
75	AR	0.30	0/620	0.79	2/838 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	AS	0.29	0/499	0.73	0/670
77	AT	0.36	0/452	0.65	0/600
78	AU	0.30	0/483	0.71	1/643 (0.2%)
79	AV	0.30	0/2490	0.69	0/3389
80	AW	0.29	0/292	0.65	0/390
81	AX	0.35	0/6626	0.78	12/8970 (0.1%)
82	AY	0.57	1/1818 (0.1%)	1.42	33/2831 (1.2%)
83	AZ	0.66	1/159 (0.6%)	1.65	5/244 (2.0%)
84	BA	0.33	0/1634	0.74	2/2195 (0.1%)
All	All	0.53	5/227304 (0.0%)	1.07	1227/333053 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	P0	0	2
5	P2	0	1
7	B	0	1
8	C	0	1
9	D	0	4
10	E	0	2
11	F	0	2
12	G	0	3
14	I	0	3
15	J	0	6
16	L	0	2
17	M	0	2
18	N	0	1
19	O	0	3
22	R	0	1
23	S	0	2
30	Z	0	1
31	a	0	2
32	b	0	1
34	d	0	1
36	f	0	2
37	g	0	4
38	h	0	2
39	i	0	3
40	j	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
41	k	0	2
45	o	0	2
46	p	0	1
48	q	0	2
49	r	0	3
50	s	0	1
51	t	0	4
52	u	0	7
53	v	0	4
54	w	0	6
55	x	0	3
56	y	0	1
57	z	0	3
58	AA	0	2
59	AB	0	1
61	AD	0	2
62	AE	0	3
63	AF	0	2
64	AG	0	4
65	AH	0	1
66	AI	0	1
67	AJ	0	1
68	AK	0	2
69	AL	0	2
71	AN	0	2
73	AP	0	1
74	AQ	0	3
75	AR	0	1
76	AS	0	1
78	AU	0	1
80	AW	0	1
81	AX	0	15
84	BA	0	3
All	All	0	143

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	AY	1	G	OP3-P	-10.64	1.48	1.61
47	2	506	A	N9-C4	6.05	1.41	1.37
83	AZ	48	U	O3'-P	5.16	1.67	1.61
1	1	2149	A	N9-C4	-5.08	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	2	218	A	N9-C4	5.08	1.40	1.37

All (1227) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	2	94	U	C2-N3-C4	21.52	139.91	127.00
47	2	1706	C	N1-C2-O2	12.82	126.59	118.90
1	1	3155	U	N1-C2-O2	11.63	130.94	122.80
1	1	3155	U	C2-N1-C1'	11.51	131.52	117.70
47	2	94	U	N3-C4-C5	11.26	121.35	114.60
82	AY	45	G	OP1-P-O3'	-11.16	80.64	105.20
1	1	3155	U	N3-C2-O2	-11.11	114.42	122.20
1	1	1279	C	C5-C6-N1	11.06	126.53	121.00
47	2	1235	C	N1-C2-O2	11.02	125.51	118.90
1	1	2284	C	N1-C2-O2	10.78	125.37	118.90
47	2	1338	C	C2-N1-C1'	10.74	130.62	118.80
47	2	1235	C	C2-N1-C1'	10.69	130.56	118.80
47	2	1566	U	N3-C2-O2	-10.65	114.74	122.20
1	1	1671	C	C2-N1-C1'	10.38	130.21	118.80
47	2	1706	C	N3-C2-O2	-10.33	114.67	121.90
47	2	965	U	N3-C2-O2	-10.25	115.02	122.20
1	1	2983	C	C6-N1-C2	-10.23	116.21	120.30
47	2	1566	U	N1-C2-O2	10.08	129.86	122.80
47	2	1674	C	C2-N1-C1'	10.07	129.87	118.80
47	2	965	U	C2-N1-C1'	10.05	129.76	117.70
47	2	965	U	N1-C2-O2	9.66	129.56	122.80
47	2	841	U	N1-C2-O2	9.62	129.54	122.80
1	1	2836	C	N3-C2-O2	-9.58	115.19	121.90
47	2	841	U	N3-C2-O2	-9.56	115.50	122.20
47	2	841	U	C2-N1-C1'	9.56	129.17	117.70
1	1	3281	U	N1-C2-O2	9.51	129.46	122.80
1	1	2550	U	N3-C2-O2	-9.51	115.55	122.20
1	1	1292	C	C2-N1-C1'	9.47	129.22	118.80
1	1	823	C	C2-N1-C1'	9.45	129.20	118.80
1	1	1176	C	N3-C2-O2	-9.43	115.30	121.90
1	1	982	C	C5-C6-N1	9.42	125.71	121.00
1	1	2550	U	N1-C2-O2	9.37	129.36	122.80
3	4	21	C	N1-C2-O2	9.34	124.51	118.90
3	4	21	C	C2-N1-C1'	9.34	129.07	118.80
1	1	3281	U	N3-C2-O2	-9.30	115.69	122.20
47	2	1338	C	N1-C2-O2	9.24	124.44	118.90
1	1	2983	C	N3-C2-O2	-9.20	115.46	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1565	G	N3-C4-N9	9.17	131.50	126.00
47	2	1235	C	C6-N1-C2	-9.15	116.64	120.30
1	1	2189	U	N3-C2-O2	-9.14	115.80	122.20
1	1	2284	C	C2-N1-C1'	9.13	128.84	118.80
47	2	980	G	C4-N9-C1'	9.06	138.28	126.50
47	2	1235	C	N3-C2-O2	-9.01	115.60	121.90
1	1	1705	U	N1-C2-O2	9.00	129.10	122.80
47	2	1706	C	C2-N1-C1'	8.91	128.60	118.80
3	4	120	C	N3-C2-O2	-8.88	115.68	121.90
47	2	1174	C	C2-N1-C1'	8.88	128.56	118.80
47	2	1174	C	C6-N1-C2	-8.88	116.75	120.30
47	2	1665	U	N1-C2-O2	8.86	129.00	122.80
1	1	2189	U	N1-C2-O2	8.85	128.99	122.80
1	1	3393	U	N3-C2-O2	-8.85	116.01	122.20
1	1	2132	C	N3-C2-O2	-8.85	115.71	121.90
82	AY	46	G	OP1-P-OP2	8.79	132.78	119.60
47	2	309	C	C2-N1-C1'	8.77	128.45	118.80
47	2	1759	C	N1-C2-O2	8.77	124.16	118.90
1	1	31	C	C6-N1-C2	-8.77	116.79	120.30
1	1	2284	C	N3-C2-O2	-8.76	115.77	121.90
1	1	2836	C	N1-C2-O2	8.73	124.14	118.90
47	2	1006	C	N1-C2-O2	8.69	124.12	118.90
1	1	2899	C	C2-N1-C1'	8.65	128.31	118.80
1	1	3281	U	C2-N1-C1'	8.57	127.99	117.70
47	2	1665	U	C2-N1-C1'	8.56	127.97	117.70
1	1	1239	C	C2-N1-C1'	8.52	128.18	118.80
1	1	2899	C	N1-C2-O2	8.50	124.00	118.90
47	2	1246	C	N1-C2-O2	8.45	123.97	118.90
1	1	2132	C	N1-C2-O2	8.43	123.96	118.90
1	1	2984	C	C6-N1-C2	-8.43	116.93	120.30
47	2	1206	U	C5-C6-N1	8.43	126.91	122.70
75	AR	21	LEU	CA-CB-CG	8.42	134.66	115.30
1	1	1633	C	N1-C2-O2	8.40	123.94	118.90
1	1	2405	C	N1-C2-O2	8.39	123.93	118.90
47	2	980	G	C8-N9-C1'	-8.37	116.12	127.00
1	1	2132	C	C6-N1-C2	-8.35	116.96	120.30
47	2	1665	U	N3-C2-O2	-8.33	116.37	122.20
1	1	31	C	C5-C6-N1	8.31	125.16	121.00
1	1	1279	C	C6-N1-C2	-8.31	116.97	120.30
47	2	94	U	N1-C2-N3	8.31	119.89	114.90
1	1	955	U	N3-C2-O2	-8.31	116.39	122.20
47	2	1246	C	C2-N1-C1'	8.30	127.93	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	2	1174	C	N1-C2-O2	8.29	123.88	118.90
1	1	2359	C	C2-N1-C1'	8.27	127.89	118.80
1	1	1496	C	C2-N1-C1'	8.26	127.88	118.80
47	2	611	U	N1-C2-O2	8.25	128.58	122.80
1	1	31	C	C2-N1-C1'	8.21	127.83	118.80
1	1	3393	U	N1-C2-O2	8.20	128.54	122.80
47	2	1458	G	C4-N9-C1'	8.19	137.15	126.50
82	AY	63	C	C5-C6-N1	8.19	125.09	121.00
49	r	54	LEU	CA-CB-CG	8.18	134.12	115.30
1	1	3160	U	N3-C2-O2	-8.18	116.47	122.20
47	2	1620	C	N1-C2-O2	8.18	123.81	118.90
82	AY	50	U	C5-C6-N1	8.17	126.79	122.70
47	2	1174	C	C5-C6-N1	8.15	125.08	121.00
2	3	105	C	N1-C2-O2	8.13	123.78	118.90
47	2	302	U	N3-C2-O2	-8.12	116.52	122.20
47	2	767	U	C2-N1-C1'	8.12	127.44	117.70
1	1	2836	C	C6-N1-C2	-8.08	117.07	120.30
1	1	3214	U	C2-N1-C1'	8.07	127.39	117.70
47	2	1006	C	C6-N1-C2	-8.06	117.08	120.30
1	1	2454	G	C4-N9-C1'	8.04	136.96	126.50
47	2	611	U	N3-C2-O2	-8.01	116.59	122.20
81	AX	62	ASP	CB-CG-OD1	7.98	125.48	118.30
1	1	2984	C	C2-N1-C1'	7.96	127.56	118.80
1	1	2336	U	N3-C2-O2	-7.96	116.63	122.20
68	AK	57	ARG	C-N-CA	7.94	141.55	121.70
1	1	3160	U	N1-C2-O2	7.93	128.35	122.80
83	AZ	48	U	C1'-C2'-O2'	-7.91	86.86	110.60
47	2	411	C	N1-C2-O2	7.90	123.64	118.90
1	1	1705	U	N3-C2-O2	-7.87	116.69	122.20
47	2	1252	C	N1-C2-O2	7.84	123.61	118.90
1	1	3169	U	N1-C2-O2	7.82	128.27	122.80
37	g	81	CYS	CA-CB-SG	7.81	128.06	114.00
1	1	2984	C	C5-C6-N1	7.79	124.90	121.00
47	2	1214	U	N1-C2-O2	7.79	128.26	122.80
47	2	1338	C	C6-N1-C1'	-7.79	111.45	120.80
1	1	2983	C	N1-C2-O2	7.79	123.57	118.90
1	1	943	U	N3-C2-O2	-7.76	116.77	122.20
59	AB	5	LEU	CA-CB-CG	7.76	133.15	115.30
47	2	1458	G	N3-C4-C5	-7.74	124.73	128.60
1	1	2836	C	C2-N1-C1'	7.72	127.30	118.80
47	2	1021	C	N3-C2-O2	-7.71	116.51	121.90
47	2	1566	U	C2-N1-C1'	7.70	126.94	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	351	LEU	CA-CB-CG	7.70	133.01	115.30
47	2	1215	C	N1-C2-O2	7.70	123.52	118.90
1	1	2406	C	C6-N1-C2	-7.68	117.23	120.30
1	1	3384	U	N3-C2-O2	-7.68	116.83	122.20
1	1	3169	U	C2-N1-C1'	7.68	126.91	117.70
47	2	1214	U	C2-N1-C1'	7.67	126.91	117.70
47	2	1674	C	N1-C2-O2	7.67	123.50	118.90
1	1	2925	C	N1-C2-O2	7.66	123.50	118.90
47	2	611	U	C2-N1-C1'	7.66	126.89	117.70
2	3	39	C	N1-C2-O2	7.65	123.49	118.90
47	2	1389	C	C2-N1-C1'	7.64	127.21	118.80
1	1	2350	C	C6-N1-C2	-7.64	117.25	120.30
47	2	393	C	N1-C2-O2	7.63	123.48	118.90
47	2	1473	U	C2-N1-C1'	7.62	126.84	117.70
47	2	1657	U	C2-N1-C1'	7.61	126.83	117.70
1	1	241	G	N3-C4-C5	-7.59	124.80	128.60
1	1	2189	U	C2-N1-C1'	7.57	126.78	117.70
47	2	1332	C	C2-N1-C1'	7.55	127.11	118.80
1	1	2550	U	C2-N1-C1'	7.54	126.75	117.70
1	1	1705	U	C2-N1-C1'	7.53	126.73	117.70
47	2	1405	G	C6-C5-N7	-7.52	125.89	130.40
1	1	2950	G	N3-C4-C5	-7.52	124.84	128.60
1	1	2094	C	N3-C2-O2	-7.52	116.64	121.90
1	1	2821	C	N1-C2-O2	7.51	123.41	118.90
47	2	1006	C	N3-C2-O2	-7.51	116.64	121.90
1	1	36	C	N1-C2-O2	7.51	123.40	118.90
83	AZ	49	U	O5'-P-OP2	-7.51	98.94	105.70
47	2	1674	C	C6-N1-C1'	-7.50	111.80	120.80
1	1	3155	U	C6-N1-C1'	-7.50	110.71	121.20
1	1	3384	U	N1-C2-O2	7.50	128.05	122.80
1	1	2378	C	C2-N1-C1'	7.49	127.04	118.80
1	1	2206	G	C4-N9-C1'	7.48	136.22	126.50
1	1	263	C	C2-N1-C1'	7.47	127.01	118.80
47	2	482	U	C5-C6-N1	7.47	126.43	122.70
47	2	218	A	C2-N3-C4	7.46	114.33	110.60
47	2	1490	C	N1-C2-O2	7.46	123.37	118.90
1	1	3181	C	N1-C2-O2	7.45	123.37	118.90
47	2	1235	C	C5-C6-N1	7.45	124.73	121.00
47	2	841	U	C5-C6-N1	7.45	126.42	122.70
1	1	1671	C	N1-C2-O2	7.43	123.36	118.90
1	1	2585	G	C4-N9-C1'	7.43	136.16	126.50
47	2	1257	U	C2-N1-C1'	7.42	126.61	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	2	980	G	C6-C5-N7	-7.42	125.95	130.40
47	2	1458	G	N3-C4-N9	7.41	130.44	126.00
1	1	955	U	N1-C2-O2	7.40	127.98	122.80
47	2	411	C	C2-N1-C1'	7.40	126.94	118.80
1	1	439	C	N1-C2-O2	7.39	123.34	118.90
82	AY	45	G	OP2-P-O3'	-7.39	88.95	105.20
1	1	132	C	C2-N1-C1'	7.38	126.92	118.80
1	1	379	C	C6-N1-C2	-7.37	117.35	120.30
1	1	3156	U	P-O3'-C3'	7.36	128.53	119.70
1	1	1565	G	C4-N9-C1'	7.36	136.07	126.50
47	2	1510	U	C2-N1-C1'	7.36	126.53	117.70
1	1	3131	U	C2-N1-C1'	7.34	126.51	117.70
1	1	113	C	C2-N1-C1'	7.33	126.87	118.80
47	2	627	C	C2-N1-C1'	7.33	126.87	118.80
1	1	1671	C	C6-N1-C1'	-7.32	112.01	120.80
1	1	2879	C	C6-N1-C2	-7.32	117.37	120.30
1	1	241	G	C4-N9-C1'	7.31	136.00	126.50
1	1	982	C	C2-N1-C1'	7.31	126.84	118.80
83	AZ	47	U	C2-N1-C1'	7.30	126.47	117.70
47	2	1510	U	N1-C2-O2	7.30	127.91	122.80
1	1	1604	G	C4-N9-C1'	7.28	135.97	126.50
47	2	36	C	N1-C2-O2	7.28	123.27	118.90
47	2	706	A	P-O3'-C3'	7.28	128.43	119.70
1	1	3384	U	C2-N1-C1'	7.27	126.43	117.70
47	2	1233	G	C4-N9-C1'	7.27	135.95	126.50
47	2	1783	C	C2-N1-C1'	7.26	126.79	118.80
47	2	712	G	C8-N9-C4	-7.26	103.50	106.40
47	2	411	C	N3-C2-O2	-7.25	116.83	121.90
47	2	1755	A	P-O3'-C3'	7.24	128.39	119.70
1	1	1565	G	C8-N9-C1'	-7.24	117.59	127.00
1	1	379	C	C5-C6-N1	7.23	124.61	121.00
47	2	1642	G	N3-C4-N9	7.23	130.34	126.00
47	2	1300	A	OP1-P-O3'	7.23	121.10	105.20
54	w	29	ASP	CB-CG-OD1	7.23	124.81	118.30
1	1	868	C	C2-N1-C1'	7.22	126.74	118.80
1	1	3169	U	N3-C2-O2	-7.22	117.15	122.20
82	AY	13	C	N1-C2-O2	7.22	123.23	118.90
1	1	2476	C	C6-N1-C2	-7.21	117.42	120.30
47	2	767	U	N3-C2-O2	-7.21	117.15	122.20
3	4	21	C	N3-C2-O2	-7.20	116.86	121.90
1	1	1633	C	N3-C2-O2	-7.20	116.86	121.90
47	2	1657	U	C5-C6-N1	7.20	126.30	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2454	G	N3-C4-N9	7.18	130.31	126.00
47	2	1448	G	N3-C4-N9	7.18	130.31	126.00
1	1	2884	C	C6-N1-C2	-7.17	117.43	120.30
1	1	1292	C	C6-N1-C2	-7.17	117.43	120.30
1	1	2742	C	C6-N1-C2	-7.15	117.44	120.30
1	1	2541	U	P-O3'-C3'	7.15	128.28	119.70
1	1	2333	C	N3-C2-O2	-7.15	116.90	121.90
1	1	2405	C	N3-C2-O2	-7.15	116.90	121.90
1	1	1931	U	C2-N1-C1'	7.14	126.27	117.70
1	1	955	U	C2-N1-C1'	7.13	126.26	117.70
1	1	3135	U	N3-C2-O2	-7.13	117.21	122.20
1	1	823	C	C6-N1-C2	-7.11	117.45	120.30
1	1	1155	C	C2-N1-C1'	7.11	126.62	118.80
47	2	767	U	N1-C2-O2	7.11	127.77	122.80
9	D	137	ASP	CB-CG-OD1	7.10	124.69	118.30
47	2	519	C	N1-C2-O2	7.09	123.15	118.90
47	2	302	U	N1-C2-O2	7.08	127.76	122.80
47	2	1755	A	OP1-P-O3'	7.08	120.77	105.20
47	2	393	C	N3-C2-O2	-7.08	116.95	121.90
47	2	1620	C	N3-C2-O2	-7.07	116.95	121.90
1	1	3214	U	N1-C2-O2	7.07	127.75	122.80
1	1	823	C	C5-C6-N1	7.07	124.53	121.00
47	2	1332	C	C6-N1-C2	-7.06	117.47	120.30
1	1	241	G	N3-C4-N9	7.05	130.23	126.00
2	3	35	C	N1-C2-O2	7.05	123.13	118.90
1	1	2284	C	C6-N1-C2	-7.05	117.48	120.30
8	C	182	LEU	CA-CB-CG	7.05	131.51	115.30
47	2	1509	C	C5-C6-N1	7.04	124.52	121.00
47	2	283	U	N1-C2-O2	7.04	127.73	122.80
3	4	114	G	C6-C5-N7	-7.03	126.18	130.40
1	1	1052	U	N3-C2-O2	-7.03	117.28	122.20
47	2	691	C	C2-N1-C1'	7.02	126.53	118.80
47	2	1342	C	N1-C2-O2	7.01	123.11	118.90
47	2	1458	G	C8-N9-C1'	-7.00	117.90	127.00
47	2	488	G	O5'-P-OP1	7.00	119.09	110.70
82	AY	49	C	C5-C6-N1	7.00	124.50	121.00
1	1	2454	G	N3-C4-C5	-6.99	125.10	128.60
1	1	2454	G	C8-N9-C1'	-6.99	117.92	127.00
1	1	2585	G	N3-C4-N9	6.99	130.19	126.00
83	AZ	48	U	C2'-C3'-O3'	-6.99	94.13	109.50
3	4	114	G	C4-C5-N7	6.97	113.59	110.80
47	2	1252	C	C2-N1-C1'	6.97	126.46	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1671	C	C6-N1-C2	-6.96	117.52	120.30
47	2	1684	U	N1-C2-O2	6.96	127.67	122.80
1	1	1604	G	N3-C4-N9	6.96	130.18	126.00
3	4	120	C	C6-N1-C2	-6.95	117.52	120.30
1	1	1843	C	C2-N1-C1'	6.95	126.44	118.80
47	2	1162	C	O5'-P-OP1	6.93	119.02	110.70
1	1	3117	C	C6-N1-C2	-6.92	117.53	120.30
1	1	36	C	N3-C2-O2	-6.92	117.06	121.90
1	1	3	U	N1-C2-O2	6.91	127.64	122.80
47	2	506	A	C2-N3-C4	6.91	114.06	110.60
47	2	852	C	C6-N1-C1'	6.91	129.09	120.80
47	2	1214	U	C5-C6-N1	6.91	126.15	122.70
47	2	1657	U	N1-C2-O2	6.89	127.62	122.80
1	1	922	U	C2-N1-C1'	6.88	125.96	117.70
1	1	1931	U	N1-C2-O2	6.88	127.61	122.80
1	1	982	C	C6-N1-C2	-6.88	117.55	120.30
1	1	2716	U	N3-C2-O2	-6.88	117.39	122.20
1	1	1272	C	N1-C2-O2	6.87	123.02	118.90
47	2	1527	C	C2-N1-C1'	6.87	126.36	118.80
1	1	1574	C	N1-C2-O2	6.87	123.02	118.90
1	1	2585	G	N3-C4-C5	-6.87	125.17	128.60
47	2	1491	U	P-O3'-C3'	6.87	127.95	119.70
47	2	1214	U	N3-C2-O2	-6.87	117.39	122.20
47	2	1338	C	C5-C6-N1	6.86	124.43	121.00
1	1	2726	C	C2-N1-C1'	6.85	126.33	118.80
47	2	393	C	C6-N1-C2	-6.85	117.56	120.30
1	1	1739	U	N1-C2-O2	6.85	127.59	122.80
47	2	980	G	N3-C4-N9	6.84	130.10	126.00
47	2	1260	U	N3-C2-O2	-6.84	117.41	122.20
1	1	2925	C	N3-C2-O2	-6.83	117.12	121.90
1	1	1604	G	N3-C4-C5	-6.83	125.19	128.60
47	2	852	C	C2-N1-C1'	-6.83	111.29	118.80
47	2	230	C	N1-C2-O2	6.82	123.00	118.90
52	u	164	LEU	CA-CB-CG	6.82	130.99	115.30
47	2	1148	C	C5-C6-N1	6.82	124.41	121.00
47	2	1473	U	N1-C2-O2	6.82	127.57	122.80
47	2	1070	C	N1-C2-O2	6.81	122.98	118.90
1	1	931	C	C6-N1-C2	-6.80	117.58	120.30
47	2	1007	C	C2-N1-C1'	6.80	126.29	118.80
1	1	1579	C	N1-C2-O2	6.79	122.97	118.90
47	2	1759	C	C2-N1-C1'	6.79	126.27	118.80
47	2	1235	C	C6-N1-C1'	-6.79	112.65	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1014	U	N3-C2-O2	-6.79	117.45	122.20
82	AY	13	C	N3-C2-O2	-6.78	117.15	121.90
47	2	841	U	C6-N1-C2	-6.78	116.93	121.00
47	2	1096	C	N1-C2-O2	6.78	122.97	118.90
1	1	3160	U	C2-N1-C1'	6.77	125.83	117.70
47	2	1389	C	N1-C2-O2	6.77	122.96	118.90
47	2	1233	G	N3-C4-N9	6.75	130.05	126.00
47	2	1248	C	C2-N1-C1'	6.74	126.22	118.80
47	2	217	A	P-O3'-C3'	6.74	127.78	119.70
81	AX	269	LEU	CA-CB-CG	6.73	130.78	115.30
1	1	1739	U	N3-C2-O2	-6.73	117.49	122.20
1	1	2526	C	C2-N1-C1'	6.73	126.20	118.80
1	1	2925	C	C6-N1-C2	-6.73	117.61	120.30
47	2	1591	C	C5-C6-N1	6.72	124.36	121.00
1	1	2378	C	C6-N1-C2	-6.71	117.61	120.30
47	2	543	C	N1-C2-O2	6.71	122.92	118.90
55	x	143	LEU	CA-CB-CG	6.71	130.72	115.30
22	R	185	LEU	CA-CB-CG	6.70	130.71	115.30
47	2	144	U	P-O3'-C3'	6.70	127.74	119.70
47	2	1233	G	C8-N9-C1'	-6.70	118.30	127.00
47	2	1233	G	C6-C5-N7	-6.69	126.39	130.40
47	2	610	G	C4-N9-C1'	6.68	135.18	126.50
47	2	1620	C	C2-N1-C1'	6.68	126.14	118.80
47	2	283	U	N3-C2-O2	-6.67	117.53	122.20
47	2	433	C	C2-N1-C1'	6.67	126.14	118.80
3	4	21	C	C6-N1-C1'	-6.67	112.80	120.80
47	2	1565	C	C6-N1-C2	-6.67	117.63	120.30
1	1	2349	U	C2-N1-C1'	6.66	125.69	117.70
1	1	2884	C	C2-N1-C1'	6.65	126.12	118.80
47	2	1405	G	N3-C4-N9	6.65	129.99	126.00
1	1	2483	G	C5-C6-O6	-6.64	124.62	128.60
1	1	31	C	N1-C2-O2	6.64	122.88	118.90
1	1	618	C	C5-C6-N1	6.63	124.32	121.00
47	2	1215	C	N3-C2-O2	-6.63	117.26	121.90
47	2	541	A	P-O3'-C3'	6.62	127.65	119.70
47	2	1527	C	N1-C2-O2	6.62	122.88	118.90
1	1	2305	G	C4-N9-C1'	6.62	135.11	126.50
47	2	309	C	N1-C2-O2	6.61	122.87	118.90
47	2	1378	U	N1-C2-O2	6.61	127.43	122.80
2	3	105	C	N3-C2-O2	-6.61	117.27	121.90
47	2	1510	U	N3-C2-O2	-6.61	117.57	122.20
1	1	1907	C	N1-C2-O2	6.61	122.86	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	443	G	P-O3'-C3'	6.59	127.61	119.70
1	1	2617	U	N3-C2-O2	-6.59	117.59	122.20
3	4	118	C	C2-N1-C1'	6.59	126.05	118.80
1	1	928	C	C6-N1-C2	-6.59	117.67	120.30
47	2	1246	C	N3-C2-O2	-6.59	117.29	121.90
1	1	2846	U	C2-N1-C1'	6.58	125.60	117.70
47	2	283	U	C2-N1-C1'	6.58	125.60	117.70
47	2	1706	C	C6-N1-C2	-6.58	117.67	120.30
1	1	304	G	N3-C4-C5	-6.58	125.31	128.60
47	2	1657	U	N3-C2-O2	-6.58	117.60	122.20
5	P2	117	ARG	N-CA-C	6.57	128.75	111.00
47	2	1174	C	N3-C2-O2	-6.56	117.31	121.90
1	1	3355	U	N1-C2-O2	6.56	127.39	122.80
1	1	271	C	N1-C2-O2	6.56	122.84	118.90
2	3	39	C	N3-C2-O2	-6.55	117.31	121.90
47	2	532	U	C2-N1-C1'	6.55	125.56	117.70
1	1	1292	C	C5-C6-N1	6.54	124.27	121.00
1	1	2359	C	C5-C6-N1	6.54	124.27	121.00
47	2	1405	G	C4-C5-N7	6.52	113.41	110.80
1	1	1342	C	C5-C6-N1	6.52	124.26	121.00
47	2	1082	C	C6-N1-C2	-6.52	117.69	120.30
47	2	1350	U	N1-C2-O2	6.51	127.36	122.80
27	W	20	LEU	CA-CB-CG	6.51	130.27	115.30
1	1	985	U	N3-C2-O2	-6.51	117.65	122.20
47	2	309	C	C6-N1-C2	-6.51	117.70	120.30
1	1	823	C	N1-C2-O2	6.50	122.80	118.90
1	1	304	G	N3-C4-N9	6.50	129.90	126.00
1	1	2830	G	C4-N9-C1'	6.50	134.94	126.50
47	2	1585	U	N1-C2-O2	6.50	127.35	122.80
81	AX	244	LEU	CA-CB-CG	6.49	130.23	115.30
1	1	1014	U	N1-C2-O2	6.49	127.34	122.80
1	1	2389	C	C6-N1-C2	-6.49	117.70	120.30
47	2	1070	C	C2-N1-C1'	6.49	125.94	118.80
82	AY	50	U	C5-C4-O4	-6.49	122.01	125.90
1	1	2206	G	N3-C4-N9	6.49	129.89	126.00
47	2	1756	A	O5'-P-OP1	-6.49	99.86	105.70
1	1	1645	U	N3-C2-O2	-6.48	117.66	122.20
47	2	94	U	N3-C2-O2	-6.48	117.66	122.20
47	2	35	U	N3-C2-O2	-6.48	117.67	122.20
1	1	3300	U	N3-C2-O2	-6.47	117.67	122.20
1	1	3181	C	C2-N1-C1'	6.47	125.91	118.80
47	2	414	C	N1-C2-O2	6.46	122.78	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1565	G	N3-C4-C5	-6.46	125.37	128.60
1	1	2305	G	N3-C4-N9	6.46	129.88	126.00
47	2	1378	U	N3-C2-O2	-6.46	117.68	122.20
47	2	1006	C	C2-N1-C1'	6.46	125.90	118.80
47	2	1246	C	C6-N1-C2	-6.46	117.72	120.30
1	1	2652	U	N3-C2-O2	-6.46	117.68	122.20
1	1	1923	C	C6-N1-C2	-6.45	117.72	120.30
47	2	1220	C	N1-C2-O2	6.43	122.76	118.90
1	1	142	C	N1-C2-O2	6.43	122.76	118.90
1	1	1597	C	C2-N1-C1'	6.43	125.87	118.80
47	2	411	C	C6-N1-C2	-6.43	117.73	120.30
47	2	1399	C	P-O3'-C3'	6.42	127.41	119.70
47	2	1327	C	C6-N1-C2	-6.42	117.73	120.30
1	1	1103	A	C2-N3-C4	6.42	113.81	110.60
1	1	1923	C	C5-C6-N1	6.41	124.21	121.00
1	1	2362	C	C6-N1-C2	-6.41	117.74	120.30
3	4	114	G	P-O3'-C3'	6.41	127.39	119.70
1	1	1496	C	N1-C2-O2	6.41	122.74	118.90
1	1	839	C	C2-N1-C1'	6.40	125.84	118.80
1	1	700	C	C6-N1-C2	-6.40	117.74	120.30
1	1	1608	C	C2-N1-C1'	6.39	125.83	118.80
1	1	1239	C	N1-C2-O2	6.39	122.73	118.90
1	1	3214	U	N3-C2-O2	-6.39	117.73	122.20
47	2	821	U	N1-C2-N3	6.38	118.72	114.90
1	1	2451	G	C4-N9-C1'	6.37	134.78	126.50
1	1	1239	C	C6-N1-C1'	-6.36	113.17	120.80
47	2	1006	C	C5-C6-N1	6.34	124.17	121.00
1	1	1525	G	C4-N9-C1'	6.34	134.74	126.50
1	1	823	C	C6-N1-C1'	-6.34	113.19	120.80
1	1	439	C	C6-N1-C2	-6.33	117.77	120.30
1	1	2558	U	N3-C2-O2	-6.33	117.77	122.20
1	1	2835	U	N3-C2-O2	-6.33	117.77	122.20
47	2	1527	C	C5-C6-N1	6.33	124.17	121.00
1	1	2094	C	N1-C2-O2	6.32	122.69	118.90
1	1	421	G	N3-C4-N9	6.32	129.79	126.00
1	1	2137	U	C2-N1-C1'	6.31	125.28	117.70
1	1	3155	U	C5-C6-N1	6.31	125.86	122.70
1	1	3	U	N3-C2-O2	-6.31	117.78	122.20
1	1	1292	C	C6-N1-C1'	-6.30	113.24	120.80
47	2	376	C	C2-N1-C1'	6.30	125.73	118.80
47	2	1342	C	C2-N1-C1'	6.30	125.73	118.80
1	1	2899	C	N3-C2-O2	-6.30	117.49	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2638	C	C6-N1-C2	-6.29	117.78	120.30
47	2	302	U	C2-N1-C1'	6.29	125.25	117.70
47	2	1759	C	N3-C2-O2	-6.29	117.50	121.90
1	1	2206	G	N3-C4-C5	-6.29	125.46	128.60
47	2	777	C	N1-C2-O2	6.28	122.67	118.90
1	1	633	C	C2-N1-C1'	6.27	125.70	118.80
1	1	2835	U	C2-N1-C1'	6.26	125.21	117.70
82	AY	49	C	C6-N1-C2	-6.26	117.80	120.30
1	1	3355	U	N3-C2-O2	-6.25	117.82	122.20
1	1	2206	G	C8-N9-C1'	-6.25	118.87	127.00
47	2	476	U	N3-C2-O2	-6.25	117.82	122.20
1	1	1671	C	C5-C6-N1	6.25	124.13	121.00
1	1	1762	C	C6-N1-C2	-6.25	117.80	120.30
47	2	1527	C	C6-N1-C2	-6.25	117.80	120.30
1	1	1037	C	C2-N1-C1'	6.25	125.67	118.80
1	1	2764	C	C6-N1-C2	-6.24	117.80	120.30
47	2	191	C	O4'-C1'-N1	6.24	113.20	108.20
1	1	2585	G	C8-N9-C1'	-6.24	118.89	127.00
1	1	3206	C	N1-C2-O2	6.24	122.64	118.90
1	1	2347	U	N1-C2-O2	6.23	127.16	122.80
82	AY	49	C	C2-N1-C1'	6.23	125.65	118.80
1	1	943	U	C6-N1-C2	-6.23	117.26	121.00
1	1	2485	A	C2-N3-C4	6.23	113.71	110.60
1	1	1597	C	C6-N1-C2	-6.22	117.81	120.30
47	2	1164	G	O5'-P-OP1	6.22	118.17	110.70
1	1	596	C	C6-N1-C2	-6.22	117.81	120.30
1	1	2169	G	N3-C4-C5	-6.21	125.49	128.60
47	2	965	U	C6-N1-C1'	-6.21	112.50	121.20
47	2	1170	G	N3-C4-N9	6.21	129.73	126.00
1	1	3181	C	N3-C2-O2	-6.21	117.55	121.90
1	1	3206	C	C2-N1-C1'	6.21	125.63	118.80
1	1	439	C	N3-C2-O2	-6.20	117.56	121.90
82	AY	50	U	N3-C4-O4	6.20	123.74	119.40
1	1	2899	C	C6-N1-C1'	-6.20	113.36	120.80
1	1	1292	C	N1-C2-O2	6.20	122.62	118.90
47	2	1448	G	C4-N9-C1'	6.19	134.55	126.50
47	2	1037	C	C2-N1-C1'	6.19	125.61	118.80
54	w	91	GLU	CA-CB-CG	6.19	127.02	113.40
47	2	1591	C	C6-N1-C2	-6.19	117.82	120.30
47	2	1490	C	C6-N1-C2	-6.18	117.83	120.30
1	1	3281	U	C5-C6-N1	6.18	125.79	122.70
3	4	21	C	C6-N1-C2	-6.18	117.83	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	943	U	N1-C2-O2	6.18	127.12	122.80
1	1	3355	U	C5-C6-N1	6.18	125.79	122.70
47	2	1783	C	N1-C2-O2	6.18	122.61	118.90
2	3	81	U	N3-C2-O2	-6.17	117.88	122.20
1	1	3135	U	N1-C2-O2	6.17	127.12	122.80
1	1	3393	U	C2-N1-C1'	6.16	125.09	117.70
47	2	1664	C	C6-N1-C2	-6.16	117.83	120.30
47	2	230	C	N3-C2-O2	-6.16	117.59	121.90
47	2	1509	C	N1-C2-O2	6.16	122.59	118.90
47	2	1248	C	C6-N1-C2	-6.16	117.84	120.30
82	AY	19	G	O4'-C1'-N9	-6.15	103.28	108.20
1	1	104	G	C4-N9-C1'	6.14	134.48	126.50
1	1	1604	G	C8-N9-C1'	-6.14	119.02	127.00
1	1	3385	U	N3-C2-O2	-6.14	117.90	122.20
1	1	112	U	C2-N1-C1'	6.13	125.06	117.70
1	1	760	G	O4'-C1'-N9	6.13	113.11	108.20
47	2	1260	U	N1-C2-O2	6.13	127.09	122.80
1	1	1614	C	C2-N1-C1'	6.12	125.53	118.80
47	2	94	U	C5-C4-O4	-6.12	122.23	125.90
47	2	1399	C	OP2-P-O3'	6.12	118.67	105.20
82	AY	61	C	N1-C2-O2	6.12	122.57	118.90
47	2	1206	U	C6-N1-C2	-6.12	117.33	121.00
47	2	36	C	C2-N1-C1'	6.12	125.53	118.80
81	AX	588	LEU	CA-CB-CG	6.12	129.36	115.30
1	1	860	G	C4-N9-C1'	6.11	134.44	126.50
1	1	2884	C	C5-C6-N1	6.11	124.06	121.00
3	4	106	C	N1-C2-O2	6.11	122.56	118.90
21	Q	138	LEU	CA-CB-CG	6.11	129.34	115.30
1	1	2257	C	N1-C2-O2	6.10	122.56	118.90
47	2	489	C	C6-N1-C2	-6.10	117.86	120.30
47	2	1463	C	N1-C2-O2	6.09	122.56	118.90
1	1	185	C	C5-C6-N1	6.09	124.05	121.00
1	1	2616	C	C2-N1-C1'	6.09	125.50	118.80
2	3	18	C	C6-N1-C2	-6.09	117.86	120.30
47	2	1490	C	N3-C2-O2	-6.09	117.64	121.90
1	1	2336	U	N1-C2-O2	6.09	127.06	122.80
1	1	379	C	C2-N1-C1'	6.08	125.49	118.80
1	1	860	G	N3-C4-C5	-6.08	125.56	128.60
47	2	1289	U	N3-C2-O2	-6.08	117.94	122.20
1	1	2614	G	P-O3'-C3'	6.08	127.00	119.70
82	AY	56	C	C2-N1-C1'	6.08	125.49	118.80
4	P0	131	GLY	C-N-CA	6.08	136.89	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	2	1148	C	C6-N1-C2	-6.08	117.87	120.30
47	2	1338	C	C6-N1-C2	-6.07	117.87	120.30
1	1	1805	C	C2-N1-C1'	6.07	125.47	118.80
1	1	304	G	C4-N9-C1'	6.06	134.38	126.50
3	4	100	U	C2-N1-C1'	6.06	124.97	117.70
1	1	1311	G	N3-C4-N9	-6.06	122.37	126.00
1	1	2950	G	N3-C4-N9	6.06	129.63	126.00
47	2	610	G	C8-N9-C1'	-6.06	119.13	127.00
1	1	1837	U	P-O3'-C3'	6.05	126.96	119.70
47	2	1581	C	C6-N1-C2	-6.04	117.88	120.30
1	1	2750	U	C2-N1-C1'	6.04	124.95	117.70
1	1	3360	C	N3-C2-O2	-6.04	117.67	121.90
47	2	1	U	P-O3'-C3'	6.04	126.95	119.70
1	1	1311	G	C5-C6-O6	6.04	132.22	128.60
1	1	1262	G	N3-C4-N9	6.03	129.62	126.00
47	2	1440	C	C6-N1-C2	-6.03	117.89	120.30
1	1	2284	C	C6-N1-C1'	-6.03	113.56	120.80
1	1	2928	C	N1-C2-O2	6.03	122.52	118.90
1	1	2305	G	C8-N9-C1'	-6.03	119.17	127.00
1	1	3321	C	C5-C6-N1	6.02	124.01	121.00
47	2	990	C	C2-N1-C1'	6.02	125.42	118.80
1	1	2928	C	N3-C2-O2	-6.02	117.69	121.90
1	1	339	C	C2-N1-C1'	6.02	125.42	118.80
47	2	1609	U	N3-C2-O2	-6.02	117.99	122.20
6	A	246	LEU	CA-CB-CG	6.01	129.13	115.30
47	2	209	U	N3-C2-O2	-6.01	117.99	122.20
47	2	981	U	N3-C2-O2	-6.01	117.99	122.20
1	1	421	G	C4-N9-C1'	6.01	134.31	126.50
1	1	132	C	N1-C2-O2	6.01	122.50	118.90
1	1	2405	C	C2-N1-C1'	6.00	125.40	118.80
47	2	920	U	C5-C6-N1	6.00	125.70	122.70
1	1	1232	C	P-O3'-C3'	6.00	126.90	119.70
47	2	1684	U	N3-C2-O2	-6.00	118.00	122.20
2	3	52	G	P-O3'-C3'	5.99	126.89	119.70
47	2	646	C	C6-N1-C2	-5.99	117.90	120.30
22	R	53	LYS	CA-CB-CG	5.99	126.58	113.40
47	2	1393	C	C5-C6-N1	5.98	123.99	121.00
47	2	1440	C	O4'-C1'-N1	5.98	112.99	108.20
82	AY	49	C	N1-C2-O2	5.98	122.49	118.90
1	1	69	C	C6-N1-C2	-5.98	117.91	120.30
1	1	2347	U	N3-C2-O2	-5.98	118.02	122.20
1	1	489	U	N3-C2-O2	-5.97	118.02	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	2	1327	C	C2-N1-C1'	5.97	125.37	118.80
1	1	2925	C	C2-N1-C1'	5.97	125.36	118.80
1	1	1052	U	N1-C2-O2	5.96	126.97	122.80
1	1	3104	U	N3-C2-O2	-5.96	118.03	122.20
47	2	1033	C	N1-C2-O2	5.96	122.47	118.90
1	1	1227	C	C5-C6-N1	5.96	123.98	121.00
1	1	2638	C	N1-C2-O2	5.95	122.47	118.90
1	1	104	G	C8-N9-C1'	-5.95	119.27	127.00
47	2	1448	G	C8-N9-C1'	-5.95	119.27	127.00
1	1	2192	C	C2-N1-C1'	5.95	125.34	118.80
3	4	97	A	C8-N9-C4	-5.95	103.42	105.80
1	1	1931	U	N3-C2-O2	-5.94	118.04	122.20
1	1	1901	A	C8-N9-C4	-5.94	103.42	105.80
1	1	3193	C	P-O3'-C3'	5.94	126.82	119.70
1	1	1076	C	C2-N1-C1'	5.93	125.33	118.80
13	H	168	ARG	C-N-CA	5.93	136.53	121.70
1	1	1889	G	C4-N9-C1'	5.93	134.21	126.50
1	1	2594	C	C6-N1-C2	-5.93	117.93	120.30
82	AY	61	C	C2-N1-C1'	5.92	125.31	118.80
1	1	1458	U	N3-C2-O2	-5.92	118.06	122.20
47	2	1706	C	C6-N1-C1'	-5.92	113.70	120.80
1	1	1128	U	P-O3'-C3'	5.92	126.80	119.70
1	1	2189	U	C6-N1-C2	-5.91	117.45	121.00
1	1	2616	C	N1-C2-O2	5.91	122.45	118.90
1	1	3084	C	C2-N1-C1'	5.91	125.31	118.80
1	1	241	G	C8-N9-C1'	-5.91	119.31	127.00
47	2	1289	U	C2-N1-C1'	5.91	124.79	117.70
1	1	2169	G	N3-C4-N9	5.90	129.54	126.00
1	1	2587	U	P-O3'-C3'	5.90	126.78	119.70
47	2	1246	C	C5-C6-N1	5.90	123.95	121.00
1	1	1584	U	C2-N1-C1'	5.90	124.78	117.70
1	1	2350	C	C2-N1-C1'	5.90	125.29	118.80
82	AY	61	C	C5-C6-N1	5.90	123.95	121.00
78	AU	8	LEU	CA-CB-CG	5.90	128.86	115.30
1	1	1272	C	N3-C2-O2	-5.89	117.77	121.90
2	3	81	U	C2-N1-C1'	5.89	124.78	117.70
47	2	1152	A	N9-C4-C5	-5.89	103.44	105.80
1	1	860	G	C8-N9-C4	-5.89	104.04	106.40
47	2	1686	C	C5-C6-N1	5.89	123.95	121.00
1	1	1608	C	N1-C2-O2	5.89	122.44	118.90
1	1	2149	A	N1-C2-N3	5.89	132.25	129.30
1	1	2821	C	N3-C2-O2	-5.88	117.78	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	2	1481	C	OP1-P-O3'	5.88	118.15	105.20
47	2	1405	G	N9-C4-C5	-5.88	103.05	105.40
1	1	263	C	C6-N1-C2	-5.88	117.95	120.30
1	1	923	C	O5'-P-OP2	-5.88	100.41	105.70
47	2	217	A	OP1-P-O3'	5.88	118.12	105.20
47	2	309	C	C6-N1-C1'	-5.87	113.75	120.80
47	2	1327	C	N1-C2-O2	5.87	122.42	118.90
3	4	118	C	C6-N1-C2	-5.87	117.95	120.30
1	1	1051	U	N3-C2-O2	-5.87	118.09	122.20
1	1	97	U	P-O3'-C3'	5.87	126.74	119.70
1	1	1021	G	C4-N9-C1'	5.87	134.13	126.50
47	2	686	C	N1-C2-O2	5.86	122.42	118.90
47	2	1342	C	N3-C2-O2	-5.86	117.80	121.90
1	1	915	A	C2-N3-C4	5.85	113.53	110.60
1	1	2362	C	C5-C6-N1	5.85	123.93	121.00
47	2	1000	C	C6-N1-C2	-5.85	117.96	120.30
47	2	1327	C	C5-C6-N1	5.85	123.93	121.00
1	1	2821	C	C6-N1-C2	-5.85	117.96	120.30
47	2	723	G	C5-C6-O6	5.85	132.11	128.60
1	1	185	C	N1-C2-O2	5.85	122.41	118.90
47	2	749	U	N1-C2-O2	5.85	126.89	122.80
82	AY	51	G	N3-C4-N9	5.84	129.51	126.00
38	h	31	LEU	CA-CB-CG	5.84	128.74	115.30
47	2	1164	G	OP1-P-OP2	-5.84	110.84	119.60
47	2	1463	C	N3-C2-O2	-5.84	117.81	121.90
47	2	414	C	N3-C2-O2	-5.84	117.81	121.90
1	1	1227	C	C6-N1-C2	-5.83	117.97	120.30
23	S	124	LEU	CA-CB-CG	5.83	128.70	115.30
47	2	1591	C	C2-N1-C1'	5.83	125.21	118.80
1	1	1779	C	N1-C2-O2	5.82	122.39	118.90
47	2	1007	C	C6-N1-C2	-5.82	117.97	120.30
1	1	2189	U	C5-C6-N1	5.82	125.61	122.70
1	1	113	C	N1-C2-O2	5.82	122.39	118.90
1	1	1496	C	C6-N1-C2	-5.82	117.97	120.30
47	2	209	U	C2-N1-C1'	5.82	124.68	117.70
47	2	728	U	OP1-P-O3'	5.81	117.98	105.20
47	2	1657	U	C6-N1-C2	-5.81	117.52	121.00
16	L	51	LEU	CA-CB-CG	5.81	128.66	115.30
13	H	190	ASP	CB-CG-OD1	5.80	123.53	118.30
47	2	965	U	C6-N1-C2	-5.80	117.52	121.00
1	1	445	G	N3-C4-N9	-5.80	122.52	126.00
53	v	175	LEU	CA-CB-CG	5.80	128.63	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	2	1007	C	N1-C2-O2	5.79	122.38	118.90
1	1	2388	U	N3-C2-O2	-5.79	118.15	122.20
1	1	2359	C	C6-N1-C1'	-5.79	113.85	120.80
82	AY	13	C	C6-N1-C2	-5.79	117.99	120.30
1	1	861	C	C2-N1-C1'	5.78	125.16	118.80
47	2	206	A	P-O3'-C3'	5.78	126.64	119.70
1	1	339	C	C6-N1-C2	-5.78	117.99	120.30
47	2	1170	G	C4-N9-C1'	5.78	134.01	126.50
1	1	2706	G	P-O3'-C3'	5.78	126.63	119.70
29	Y	126	LEU	CA-CB-CG	5.78	128.59	115.30
52	u	65	LEU	CA-CB-CG	5.78	128.58	115.30
81	AX	689	LEU	CA-CB-CG	5.78	128.58	115.30
47	2	1209	C	C6-N1-C2	-5.77	117.99	120.30
1	1	3218	A	P-O3'-C3'	5.77	126.63	119.70
47	2	1581	C	C5-C6-N1	5.77	123.88	121.00
47	2	1033	C	C2-N1-C1'	5.76	125.14	118.80
2	3	69	C	C6-N1-C2	-5.76	118.00	120.30
47	2	1248	C	N1-C2-O2	5.76	122.36	118.90
1	1	2359	C	N1-C2-O2	5.76	122.36	118.90
31	a	47	LYS	C-N-CA	5.76	136.10	121.70
47	2	945	U	N1-C2-O2	5.76	126.83	122.80
1	1	1597	C	N1-C2-O2	5.75	122.35	118.90
1	1	3214	U	C6-N1-C1'	-5.75	113.15	121.20
47	2	1274	C	C2-N1-C1'	5.75	125.13	118.80
1	1	356	C	C6-N1-C2	-5.75	118.00	120.30
1	1	1342	C	C2-N1-C1'	5.75	125.12	118.80
1	1	2304	C	C6-N1-C2	-5.75	118.00	120.30
1	1	3105	U	P-O3'-C3'	5.75	126.60	119.70
3	4	21	C	C5-C6-N1	5.75	123.87	121.00
1	1	1805	C	C6-N1-C2	-5.75	118.00	120.30
47	2	476	U	N1-C2-O2	5.74	126.82	122.80
1	1	286	U	O5'-P-OP1	-5.74	100.54	105.70
2	3	28	C	C6-N1-C2	-5.74	118.00	120.30
1	1	3349	C	C2-N1-C1'	5.73	125.11	118.80
1	1	890	C	C2-N1-C1'	5.73	125.11	118.80
47	2	1116	A	P-O3'-C3'	5.73	126.58	119.70
1	1	2260	U	N3-C2-O2	-5.73	118.19	122.20
1	1	126	U	N3-C2-O2	-5.72	118.19	122.20
1	1	982	C	N1-C2-O2	5.72	122.33	118.90
1	1	2236	G	C4-N9-C1'	5.72	133.94	126.50
47	2	209	U	N1-C2-O2	5.72	126.80	122.80
47	2	726	C	C6-N1-C2	-5.72	118.01	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	2	821	U	C6-N1-C1'	5.72	129.21	121.20
61	AD	137	PRO	C-N-CA	5.71	135.98	121.70
1	1	149	U	N3-C2-O2	-5.71	118.20	122.20
1	1	2726	C	C6-N1-C2	-5.71	118.02	120.30
1	1	772	U	N3-C2-O2	-5.70	118.21	122.20
1	1	1703	U	N1-C2-O2	5.70	126.79	122.80
47	2	546	U	N3-C2-O2	-5.70	118.21	122.20
1	1	3321	C	C6-N1-C2	-5.70	118.02	120.30
1	1	2689	A	C2-N3-C4	5.69	113.45	110.60
47	2	1182	U	O5'-P-OP1	-5.69	100.58	105.70
1	1	890	C	N1-C2-O2	5.69	122.31	118.90
1	1	1155	C	C6-N1-C2	-5.69	118.03	120.30
1	1	1353	U	N1-C2-O2	5.69	126.78	122.80
1	1	1703	U	N3-C2-O2	-5.68	118.22	122.20
1	1	633	C	C6-N1-C2	-5.68	118.03	120.30
1	1	1565	G	N9-C4-C5	-5.68	103.13	105.40
47	2	1350	U	N3-C2-O2	-5.68	118.22	122.20
1	1	1525	G	C8-N9-C1'	-5.68	119.62	127.00
47	2	790	U	N3-C2-O2	-5.67	118.23	122.20
1	1	90	C	N1-C2-O2	5.67	122.30	118.90
1	1	2783	U	N3-C2-O2	-5.67	118.23	122.20
1	1	3281	U	C6-N1-C2	-5.67	117.60	121.00
47	2	536	C	C2-N1-C1'	5.67	125.04	118.80
1	1	2772	C	C2-N1-C1'	5.67	125.04	118.80
1	1	2304	C	C2-N1-C1'	5.67	125.03	118.80
2	3	78	U	N3-C2-O2	-5.66	118.23	122.20
1	1	839	C	C6-N1-C2	-5.66	118.03	120.30
1	1	2306	C	P-O3'-C3'	5.66	126.49	119.70
1	1	2984	C	N1-C2-O2	5.66	122.30	118.90
47	2	1257	U	O4'-C1'-N1	5.66	112.73	108.20
1	1	448	U	N1-C2-O2	5.66	126.76	122.80
2	3	81	U	N1-C2-O2	5.66	126.76	122.80
1	1	2406	C	C2-N1-C1'	5.66	125.02	118.80
1	1	2974	U	N3-C2-O2	-5.66	118.24	122.20
47	2	691	C	C6-N1-C2	-5.65	118.04	120.30
1	1	3222	U	N3-C2-O2	-5.65	118.25	122.20
1	1	3285	C	N1-C2-O2	5.65	122.29	118.90
47	2	1404	C	C5-C6-N1	5.64	123.82	121.00
3	4	72	A	P-O3'-C3'	5.64	126.47	119.70
1	1	1907	C	N3-C2-O2	-5.64	117.95	121.90
1	1	1671	C	N3-C2-O2	-5.63	117.96	121.90
3	4	8	C	C6-N1-C2	-5.63	118.05	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	2	376	C	C6-N1-C2	-5.63	118.05	120.30
1	1	1496	C	C6-N1-C1'	-5.63	114.04	120.80
1	1	2950	G	C4-N9-C1'	5.63	133.82	126.50
47	2	14	C	C2-N1-C1'	5.63	125.00	118.80
47	2	1257	U	C5-C6-N1	5.63	125.52	122.70
47	2	1334	U	C2-N1-C1'	5.63	124.45	117.70
60	AC	97	LEU	CA-CB-CG	5.63	128.24	115.30
82	AY	11	C	C5-C6-N1	5.63	123.81	121.00
47	2	1163	A	C2-N3-C4	5.62	113.41	110.60
58	AA	88	PRO	N-CA-CB	5.62	110.05	103.30
1	1	753	C	C6-N1-C2	-5.62	118.05	120.30
1	1	2427	U	C5-C6-N1	5.62	125.51	122.70
47	2	1473	U	C6-N1-C1'	-5.62	113.33	121.20
47	2	132	U	P-O3'-C3'	5.62	126.44	119.70
47	2	1664	C	C2-N1-C1'	5.62	124.98	118.80
1	1	368	G	N3-C4-N9	5.61	129.37	126.00
1	1	2526	C	N1-C2-O2	5.61	122.26	118.90
47	2	602	U	C2-N1-C1'	5.61	124.43	117.70
1	1	1239	C	C5-C6-N1	5.60	123.80	121.00
1	1	41	G	C4-N9-C1'	5.60	133.78	126.50
1	1	2558	U	N1-C2-O2	5.60	126.72	122.80
41	k	39	ARG	C-N-CA	5.60	135.71	121.70
1	1	142	C	N3-C2-O2	-5.60	117.98	121.90
1	1	2333	C	C6-N1-C1'	5.60	127.52	120.80
2	3	18	C	P-O3'-C3'	5.60	126.42	119.70
1	1	1843	C	C6-N1-C2	-5.60	118.06	120.30
1	1	955	U	C6-N1-C2	-5.60	117.64	121.00
1	1	3385	U	C2-N1-C1'	5.60	124.42	117.70
47	2	388	G	P-O3'-C3'	5.60	126.42	119.70
2	3	69	C	C2-N1-C1'	5.59	124.95	118.80
1	1	2835	U	N1-C2-O2	5.59	126.71	122.80
1	1	2132	C	C2-N1-C1'	5.59	124.94	118.80
1	1	2846	U	N3-C2-O2	-5.59	118.29	122.20
47	2	183	U	C5-C6-N1	5.58	125.49	122.70
1	1	922	U	N1-C2-O2	5.58	126.71	122.80
69	AL	78	LEU	CA-CB-CG	5.58	128.13	115.30
1	1	2350	C	C5-C6-N1	5.58	123.79	121.00
1	1	1238	C	C5-C6-N1	5.57	123.79	121.00
47	2	723	G	N1-C6-O6	-5.57	116.56	119.90
1	1	421	G	C8-N9-C1'	-5.57	119.76	127.00
47	2	1115	U	C2-N1-C1'	5.57	124.38	117.70
47	2	1675	C	C6-N1-C2	-5.56	118.08	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
82	AY	56	C	N1-C2-O2	5.56	122.24	118.90
47	2	728	U	P-O3'-C3'	5.56	126.37	119.70
47	2	1160	A	C5-C6-N1	5.56	120.48	117.70
1	1	132	C	C6-N1-C2	-5.56	118.08	120.30
1	1	868	C	C6-N1-C2	-5.56	118.08	120.30
47	2	1686	C	N1-C2-O2	5.55	122.23	118.90
1	1	2983	C	C5-C6-N1	5.55	123.78	121.00
1	1	2962	U	C5-C6-N1	5.55	125.47	122.70
47	2	1096	C	N3-C2-O2	-5.55	118.02	121.90
47	2	1528	U	C5-C6-N1	5.55	125.47	122.70
53	v	217	LEU	CA-CB-CG	5.55	128.06	115.30
1	1	1049	C	N1-C2-O2	5.54	122.22	118.90
1	1	651	G	N3-C4-N9	5.54	129.32	126.00
49	r	177	GLN	CA-CB-CG	5.54	125.58	113.40
1	1	1155	C	N1-C2-O2	5.53	122.22	118.90
1	1	2265	C	C2-N1-C1'	5.53	124.89	118.80
3	4	19	C	N1-C2-O2	5.53	122.22	118.90
82	AY	11	C	C2-N1-C1'	5.53	124.89	118.80
1	1	1232	C	C5-C6-N1	5.53	123.77	121.00
1	1	2638	C	N3-C2-O2	-5.53	118.03	121.90
47	2	712	G	N7-C8-N9	5.53	115.87	113.10
1	1	1141	C	C2-N1-C1'	5.53	124.88	118.80
1	1	3155	U	C6-N1-C2	-5.53	117.68	121.00
1	1	3214	U	O4'-C1'-N1	5.53	112.62	108.20
81	AX	61	LYS	C-N-CA	5.53	135.51	121.70
82	AY	2	C	C5-C6-N1	5.52	123.76	121.00
3	4	50	C	C2-N1-C1'	5.52	124.87	118.80
1	1	549	U	N1-C2-O2	5.52	126.66	122.80
47	2	1338	C	N3-C2-O2	-5.52	118.04	121.90
47	2	229	U	C2-N1-C1'	5.52	124.32	117.70
3	4	102	U	C2-N1-C1'	5.51	124.32	117.70
47	2	1674	C	C5-C6-N1	5.51	123.76	121.00
47	2	1665	U	C6-N1-C1'	-5.51	113.49	121.20
1	1	1525	G	N3-C4-N9	5.51	129.30	126.00
47	2	1273	G	P-O3'-C3'	5.51	126.31	119.70
1	1	1496	C	N3-C2-O2	-5.50	118.05	121.90
1	1	1076	C	C5-C6-N1	5.50	123.75	121.00
1	1	2288	G	C4-N9-C1'	5.50	133.66	126.50
47	2	1357	A	C4-C5-N7	5.50	113.45	110.70
70	AM	93	LEU	CA-CB-CG	5.50	127.96	115.30
81	AX	247	ASP	C-N-CA	5.50	135.46	121.70
47	2	1204	A	C2-N3-C4	5.50	113.35	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	2	1448	G	C6-C5-N7	-5.50	127.10	130.40
47	2	642	G	N3-C4-N9	5.50	129.30	126.00
47	2	1783	C	C6-N1-C2	-5.50	118.10	120.30
1	1	271	C	N3-C2-O2	-5.49	118.06	121.90
47	2	965	U	C5-C6-N1	5.49	125.45	122.70
47	2	1289	U	N1-C2-O2	5.49	126.64	122.80
47	2	602	U	N3-C2-O2	-5.49	118.36	122.20
3	4	26	U	C5-C6-N1	5.49	125.44	122.70
47	2	1684	U	C5-C6-N1	5.49	125.44	122.70
1	1	1579	C	N3-C2-O2	-5.49	118.06	121.90
1	1	1145	G	N3-C4-N9	5.49	129.29	126.00
1	1	2683	U	N1-C2-O2	5.49	126.64	122.80
1	1	2830	G	C8-N9-C1'	-5.48	119.87	127.00
47	2	1300	A	P-O3'-C3'	5.48	126.28	119.70
1	1	1342	C	C6-N1-C2	-5.48	118.11	120.30
1	1	3057	U	N3-C2-O2	-5.48	118.36	122.20
47	2	1170	G	N3-C4-C5	-5.48	125.86	128.60
1	1	1702	U	N1-C2-O2	5.47	126.63	122.80
1	1	2928	C	C6-N1-C2	-5.47	118.11	120.30
47	2	749	U	N3-C2-O2	-5.47	118.37	122.20
47	2	1604	U	C2-N1-C1'	5.47	124.26	117.70
47	2	1664	C	N1-C2-O2	5.47	122.18	118.90
1	1	439	C	C2-N1-C1'	5.47	124.81	118.80
47	2	915	A	C2-N3-C4	5.47	113.33	110.60
47	2	1688	U	N1-C2-O2	5.47	126.63	122.80
1	1	1889	G	N3-C4-N9	5.46	129.28	126.00
47	2	546	U	N1-C2-O2	5.46	126.62	122.80
1	1	126	U	N1-C2-O2	5.46	126.62	122.80
1	1	2464	U	C5-C6-N1	5.46	125.43	122.70
47	2	1580	C	C5-C6-N1	5.46	123.73	121.00
53	v	49	GLU	C-N-CA	5.46	135.35	121.70
47	2	230	C	C6-N1-C2	-5.46	118.12	120.30
1	1	1190	A	C4-N9-C1'	5.46	136.12	126.30
1	1	1765	U	O5'-P-OP2	-5.46	100.79	105.70
81	AX	303	LEU	CA-CB-CG	5.46	127.85	115.30
1	1	104	G	C6-C5-N7	-5.46	127.13	130.40
1	1	1614	C	C6-N1-C2	-5.45	118.12	120.30
1	1	3355	U	C6-N1-C2	-5.45	117.73	121.00
1	1	1228	C	C6-N1-C2	-5.45	118.12	120.30
1	1	2629	U	N3-C2-O2	-5.45	118.39	122.20
1	1	3222	U	N1-C2-O2	5.45	126.61	122.80
47	2	536	C	N1-C2-O2	5.45	122.17	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	2	627	C	N1-C2-O2	5.45	122.17	118.90
47	2	790	U	N1-C2-O2	5.45	126.61	122.80
47	2	1357	A	N9-C4-C5	-5.45	103.62	105.80
47	2	1723	U	N3-C2-O2	-5.45	118.39	122.20
1	1	3300	U	N1-C2-O2	5.44	126.61	122.80
47	2	1405	G	C4-N9-C1'	5.44	133.58	126.50
1	1	90	C	C2-N1-C1'	5.44	124.78	118.80
1	1	991	G	N3-C4-C5	-5.44	125.88	128.60
1	1	2983	C	C2-N1-C1'	5.44	124.78	118.80
1	1	421	G	N3-C4-C5	-5.44	125.88	128.60
1	1	683	U	N3-C2-O2	-5.44	118.39	122.20
1	1	2260	U	N1-C2-O2	5.44	126.61	122.80
1	1	1332	A	N3-C4-N9	5.43	131.75	127.40
81	AX	335	LEU	CA-CB-CG	5.43	127.80	115.30
9	D	83	LEU	CA-CB-CG	5.43	127.79	115.30
47	2	393	C	C2-N1-C1'	5.43	124.77	118.80
1	1	1705	U	C5-C6-N1	5.43	125.41	122.70
47	2	35	U	N1-C2-O2	5.43	126.60	122.80
1	1	1898	G	N1-C6-O6	-5.43	116.64	119.90
1	1	1901	A	C4-N9-C1'	5.43	136.07	126.30
47	2	1632	C	P-O3'-C3'	5.42	126.21	119.70
1	1	1237	G	N3-C4-N9	5.42	129.25	126.00
47	2	309	C	C5-C6-N1	5.42	123.71	121.00
1	1	977	C	C2-N1-C1'	5.42	124.76	118.80
1	1	1470	U	N3-C2-O2	-5.42	118.41	122.20
1	1	1049	C	C6-N1-C2	-5.41	118.14	120.30
1	1	2284	C	C5-C6-N1	5.41	123.71	121.00
47	2	1686	C	C6-N1-C2	-5.41	118.14	120.30
47	2	1246	C	C6-N1-C1'	-5.41	114.31	120.80
1	1	2997	G	C4-N9-C1'	5.41	133.53	126.50
1	1	3309	G	C4-N9-C1'	5.41	133.53	126.50
1	1	3206	C	N3-C2-O2	-5.40	118.12	121.90
3	4	8	C	N3-C2-O2	-5.40	118.12	121.90
1	1	323	A	P-O3'-C3'	5.40	126.18	119.70
1	1	1706	C	N1-C2-O2	5.40	122.14	118.90
1	1	2483	G	N1-C6-O6	5.40	123.14	119.90
1	1	821	U	N3-C2-O2	-5.40	118.42	122.20
1	1	1633	C	C2-N1-C1'	5.40	124.74	118.80
47	2	1389	C	N3-C2-O2	-5.40	118.12	121.90
47	2	1565	C	C2-N1-C1'	5.40	124.74	118.80
1	1	1917	C	C2-N1-C1'	5.40	124.74	118.80
1	1	1702	U	C2-N1-C1'	5.40	124.17	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	2	532	U	N1-C2-O2	5.39	126.58	122.80
1	1	618	C	C6-N1-C2	-5.39	118.14	120.30
1	1	1238	C	C6-N1-C2	-5.39	118.14	120.30
47	2	1252	C	C5-C6-N1	5.38	123.69	121.00
47	2	1164	G	O5'-P-OP2	-5.38	100.86	105.70
1	1	1049	C	N3-C2-O2	-5.38	118.14	121.90
47	2	229	U	N1-C2-O2	5.37	126.56	122.80
47	2	1674	C	C6-N1-C2	-5.37	118.15	120.30
47	2	433	C	C5-C6-N1	5.37	123.69	121.00
1	1	2149	A	N7-C8-N9	5.37	116.48	113.80
47	2	813	U	O4'-C1'-N1	5.37	112.50	108.20
47	2	1620	C	C6-N1-C2	-5.37	118.15	120.30
47	2	1163	A	OP1-P-O3'	5.37	117.00	105.20
47	2	1257	U	C6-N1-C1'	-5.36	113.69	121.20
1	1	2359	C	C6-N1-C2	-5.36	118.16	120.30
47	2	610	G	N3-C4-N9	5.36	129.21	126.00
1	1	104	G	C4-C5-N7	5.36	112.94	110.80
1	1	574	U	N1-C2-O2	5.36	126.55	122.80
82	AY	2	C	C2-N1-C1'	5.36	124.69	118.80
82	AY	56	C	C5-C6-N1	5.36	123.68	121.00
1	1	1703	U	C2-N1-C1'	5.35	124.12	117.70
1	1	1237	G	C8-N9-C1'	-5.35	120.04	127.00
1	1	2617	U	C2-N1-C1'	5.35	124.12	117.70
47	2	1138	A	P-O3'-C3'	5.35	126.12	119.70
1	1	2149	A	C2-N3-C4	-5.35	107.93	110.60
47	2	1220	C	N3-C2-O2	-5.35	118.16	121.90
1	1	943	U	C5-C6-N1	5.34	125.37	122.70
1	1	1038	C	C5-C6-N1	5.34	123.67	121.00
1	1	1230	G	N9-C4-C5	-5.34	103.26	105.40
47	2	1178	G	C4-N9-C1'	5.34	133.45	126.50
47	2	1642	G	C6-C5-N7	-5.34	127.19	130.40
1	1	574	U	C2-N1-C1'	5.34	124.11	117.70
47	2	79	C	C6-N1-C2	-5.34	118.16	120.30
1	1	1237	G	C4-N9-C1'	5.34	133.44	126.50
1	1	723	U	N3-C2-O2	-5.34	118.46	122.20
49	r	110	LEU	CA-CB-CG	5.34	127.58	115.30
1	1	311	C	N1-C2-O2	5.34	122.10	118.90
47	2	543	C	N3-C2-O2	-5.33	118.17	121.90
1	1	581	U	N1-C2-O2	5.33	126.53	122.80
13	H	138	THR	C-N-CA	5.33	135.04	121.70
47	2	833	U	N3-C4-O4	-5.33	115.67	119.40
47	2	1148	C	C2-N1-C1'	5.33	124.67	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	439	C	C5-C6-N1	5.33	123.67	121.00
1	1	623	U	N3-C2-O2	-5.33	118.47	122.20
1	1	2617	U	N1-C2-O2	5.33	126.53	122.80
2	3	18	C	C5-C6-N1	5.33	123.67	121.00
1	1	2451	G	C8-N9-C1'	-5.33	120.07	127.00
47	2	767	U	C6-N1-C1'	-5.33	113.74	121.20
2	3	35	C	N3-C2-O2	-5.33	118.17	121.90
47	2	506	A	C4-N9-C1'	5.33	135.89	126.30
1	1	1353	U	N3-C2-O2	-5.33	118.47	122.20
47	2	1214	U	C6-N1-C2	-5.32	117.81	121.00
1	1	3104	U	N1-C2-O2	5.32	126.52	122.80
47	2	646	C	C5-C6-N1	5.32	123.66	121.00
81	AX	807	ASP	CB-CG-OD1	5.32	123.09	118.30
1	1	2475	G	N3-C4-N9	5.31	129.19	126.00
1	1	1565	G	C6-C5-N7	-5.31	127.21	130.40
1	1	2899	C	C5-C6-N1	5.31	123.66	121.00
47	2	1463	C	C6-N1-C2	-5.31	118.18	120.30
47	2	1178	G	C6-C5-N7	-5.31	127.21	130.40
47	2	1178	G	C8-N9-C1'	-5.31	120.10	127.00
47	2	1665	U	C5-C6-N1	5.31	125.36	122.70
3	4	9	A	N7-C8-N9	5.31	116.45	113.80
47	2	1389	C	C6-N1-C1'	-5.31	114.43	120.80
47	2	1609	U	N1-C2-O2	5.31	126.52	122.80
1	1	1155	C	C5-C6-N1	5.30	123.65	121.00
47	2	519	C	N3-C2-O2	-5.30	118.19	121.90
1	1	869	G	N3-C4-N9	5.30	129.18	126.00
1	1	2772	C	N1-C2-O2	5.30	122.08	118.90
42	1	27	ILE	C-N-CA	5.30	134.95	121.70
47	2	433	C	N1-C2-O2	5.30	122.08	118.90
1	1	2981	U	C5-C6-N1	5.30	125.35	122.70
47	2	506	A	N3-C4-C5	-5.29	123.09	126.80
47	2	864	U	C2-N1-C1'	5.29	124.05	117.70
47	2	841	U	C6-N1-C1'	-5.29	113.80	121.20
47	2	945	U	N3-C2-O2	-5.29	118.50	122.20
47	2	87	C	C2-N1-C1'	5.28	124.61	118.80
1	1	963	G	C4-N9-C1'	5.28	133.37	126.50
47	2	851	U	C6-N1-C1'	5.28	128.59	121.20
1	1	1732	U	N1-C2-O2	5.28	126.50	122.80
1	1	2716	U	N1-C2-O2	5.28	126.50	122.80
1	1	1079	A	P-O3'-C3'	5.28	126.03	119.70
19	O	138	LEU	CA-CB-CG	5.28	127.44	115.30
1	1	2821	C	C5-C6-N1	5.28	123.64	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	2	1632	C	OP1-P-O3'	5.28	116.81	105.20
82	AY	61	C	C6-N1-C2	-5.28	118.19	120.30
1	1	2961	G	N7-C8-N9	5.27	115.73	113.10
47	2	1688	U	N3-C2-O2	-5.27	118.51	122.20
1	1	2407	C	C5-C6-N1	5.27	123.63	121.00
1	1	2526	C	C6-N1-C2	-5.26	118.19	120.30
47	2	21	U	N3-C2-O2	-5.26	118.52	122.20
1	1	2870	C	C6-N1-C2	-5.26	118.19	120.30
47	2	1596	C	C2-N1-C1'	5.26	124.59	118.80
47	2	1096	C	C2-N1-C1'	5.26	124.58	118.80
1	1	861	C	C6-N1-C2	-5.26	118.20	120.30
1	1	3164	C	C2-N1-C1'	5.26	124.58	118.80
47	2	1675	C	C2-N1-C1'	5.25	124.58	118.80
47	2	864	U	O4'-C1'-N1	5.25	112.40	108.20
82	AY	1	G	OP1-P-OP2	5.25	127.47	119.60
3	4	50	C	C6-N1-C2	-5.25	118.20	120.30
1	1	1038	C	C6-N1-C2	-5.25	118.20	120.30
1	1	2594	C	C5-C6-N1	5.25	123.62	121.00
15	J	166	LYS	C-N-CA	5.24	134.81	121.70
47	2	258	C	C6-N1-C2	-5.24	118.20	120.30
82	AY	2	C	N1-C2-O2	5.24	122.05	118.90
1	1	556	U	C5-C4-O4	-5.24	122.75	125.90
1	1	3135	U	C2-N1-C1'	5.24	123.99	117.70
3	4	63	G	N3-C4-N9	5.24	129.15	126.00
1	1	1262	G	C6-C5-N7	-5.24	127.26	130.40
31	a	47	LYS	CA-CB-CG	5.24	124.92	113.40
1	1	1889	G	N3-C4-C5	-5.24	125.98	128.60
2	3	69	C	C5-C6-N1	5.24	123.62	121.00
1	1	3131	U	C5-C6-N1	5.23	125.32	122.70
47	2	1311	U	C5-C6-N1	5.23	125.31	122.70
47	2	1448	G	N3-C2-N2	5.23	123.56	119.90
82	AY	56	C	C6-N1-C2	-5.23	118.21	120.30
1	1	354	U	C2-N1-C1'	5.23	123.97	117.70
1	1	915	A	C4-N9-C1'	5.23	135.71	126.30
1	1	1516	C	C6-N1-C2	-5.22	118.21	120.30
1	1	1249	G	N3-C4-N9	5.22	129.13	126.00
19	O	102	LEU	CA-CB-CG	5.22	127.31	115.30
3	4	114	G	C5-C6-O6	-5.22	125.47	128.60
39	i	60	LEU	CA-CB-CG	5.22	127.31	115.30
47	2	387	A	P-O3'-C3'	5.22	125.97	119.70
1	1	1871	U	N3-C2-O2	-5.22	118.55	122.20
47	2	506	A	N3-C4-N9	5.22	131.58	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	3275	U	C2-N1-C1'	5.21	123.96	117.70
1	1	943	U	C2-N1-C1'	5.21	123.95	117.70
1	1	662	U	C2-N1-C1'	5.21	123.95	117.70
1	1	1781	C	C2-N1-C1'	5.21	124.53	118.80
1	1	1764	U	OP1-P-O3'	5.21	116.66	105.20
1	1	745	C	C6-N1-C2	-5.21	118.22	120.30
47	2	1021	C	N3-C4-N4	-5.21	114.36	118.00
1	1	2708	C	C2-N1-C1'	5.21	124.53	118.80
1	1	3169	U	C6-N1-C1'	-5.21	113.91	121.20
1	1	1115	G	C4-N9-C1'	5.20	133.26	126.50
6	A	180	LEU	CA-CB-CG	5.20	127.27	115.30
1	1	489	U	N1-C2-O2	5.20	126.44	122.80
47	2	376	C	C5-C6-N1	5.20	123.60	121.00
1	1	3084	C	C6-N1-C2	-5.20	118.22	120.30
30	Z	103	GLN	CA-CB-CG	5.20	124.84	113.40
47	2	1394	G	C6-C5-N7	-5.20	127.28	130.40
81	AX	119	LEU	CA-CB-CG	5.20	127.26	115.30
1	1	1574	C	C5-C6-N1	5.20	123.60	121.00
1	1	3386	G	C4-N9-C1'	5.20	133.26	126.50
1	1	2496	C	N1-C2-O2	5.20	122.02	118.90
1	1	3195	U	N1-C2-O2	5.20	126.44	122.80
1	1	1076	C	C6-N1-C2	-5.19	118.22	120.30
1	1	3237	U	N1-C2-O2	5.19	126.43	122.80
3	4	19	C	N3-C2-O2	-5.19	118.27	121.90
3	4	55	U	N3-C2-O2	-5.19	118.57	122.20
47	2	1163	A	P-O3'-C3'	5.19	125.93	119.70
1	1	2305	G	N3-C4-C5	-5.19	126.01	128.60
47	2	587	C	C6-N1-C2	-5.19	118.23	120.30
82	AY	51	G	N9-C4-C5	-5.18	103.33	105.40
1	1	2831	G	C4-N9-C1'	5.18	133.24	126.50
47	2	602	U	N1-C2-O2	5.18	126.43	122.80
49	r	96	LEU	CA-CB-CG	5.18	127.22	115.30
1	1	1597	C	C5-C6-N1	5.18	123.59	121.00
13	H	68	LEU	CA-CB-CG	5.18	127.21	115.30
47	2	1481	C	P-O3'-C3'	5.18	125.91	119.70
75	AR	33	LEU	CA-CB-CG	5.18	127.21	115.30
47	2	1448	G	N3-C4-C5	-5.18	126.01	128.60
2	3	39	C	C2-N1-C1'	5.18	124.49	118.80
47	2	990	C	C6-N1-C2	-5.18	118.23	120.30
1	1	851	C	C2-N1-C1'	5.17	124.49	118.80
47	2	1051	G	C4-N9-C1'	5.17	133.23	126.50
1	1	963	G	C8-N9-C1'	-5.17	120.28	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	3275	U	N1-C2-O2	5.17	126.42	122.80
47	2	1404	C	C6-N1-C2	-5.17	118.23	120.30
1	1	430	U	N1-C2-O2	5.17	126.42	122.80
1	1	2666	C	C6-N1-C2	-5.17	118.23	120.30
1	1	2937	G	C4-N9-C1'	5.17	133.22	126.50
83	AZ	43	C	C6-N1-C2	-5.17	118.23	120.30
1	1	2834	G	C4-N9-C1'	5.16	133.21	126.50
47	2	1221	A	C2-N3-C4	5.16	113.18	110.60
1	1	411	U	N3-C2-O2	-5.16	118.59	122.20
1	1	1448	U	N1-C2-O2	5.16	126.41	122.80
1	1	1739	U	C2-N1-C1'	5.16	123.89	117.70
82	AY	63	C	C6-N1-C2	-5.16	118.24	120.30
84	BA	17	LEU	CA-CB-CG	5.16	127.16	115.30
1	1	2726	C	N1-C2-O2	5.16	121.99	118.90
1	1	772	U	N1-C2-O2	5.16	126.41	122.80
1	1	987	U	C2-N1-C1'	5.16	123.89	117.70
1	1	1514	G	C4-N9-C1'	5.16	133.20	126.50
22	R	44	LEU	CA-CB-CG	5.16	127.16	115.30
47	2	777	C	N3-C2-O2	-5.16	118.29	121.90
47	2	1783	C	C5-C6-N1	5.16	123.58	121.00
1	1	490	C	P-O3'-C3'	5.15	125.88	119.70
1	1	192	C	C6-N1-C2	-5.15	118.24	120.30
1	1	1584	U	N3-C2-O2	-5.15	118.59	122.20
1	1	2879	C	C5-C6-N1	5.15	123.58	121.00
47	2	1174	C	C6-N1-C1'	-5.15	114.62	120.80
1	1	1280	C	N1-C2-O2	5.15	121.99	118.90
47	2	97	C	C2-N1-C1'	5.15	124.46	118.80
3	4	9	A	C6-C5-N7	-5.14	128.70	132.30
3	4	35	C	C6-N1-C2	-5.14	118.24	120.30
1	1	3233	C	C5-C6-N1	5.14	123.57	121.00
47	2	138	A	C2-N3-C4	5.14	113.17	110.60
47	2	1404	C	N1-C2-O2	5.14	121.98	118.90
47	2	1444	A	C4-N9-C1'	5.14	135.55	126.30
1	1	945	C	C6-N1-C2	-5.13	118.25	120.30
1	1	2955	U	C5-C6-N1	5.13	125.27	122.70
1	1	1141	C	N1-C2-O2	5.13	121.98	118.90
1	1	3058	U	C2-N1-C1'	5.13	123.86	117.70
47	2	587	C	N3-C2-O2	-5.13	118.31	121.90
47	2	1257	U	C5-C4-O4	-5.13	122.82	125.90
47	2	1393	C	C6-N1-C2	-5.13	118.25	120.30
47	2	433	C	C6-N1-C2	-5.13	118.25	120.30
1	1	1279	C	C2-N1-C1'	5.12	124.44	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	839	C	C5-C6-N1	5.12	123.56	121.00
1	1	2997	G	N3-C4-C5	-5.12	126.04	128.60
1	1	1349	G	C4-N9-C1'	5.12	133.16	126.50
1	1	3064	U	N3-C2-O2	-5.12	118.61	122.20
1	1	1438	U	C2-N1-C1'	5.12	123.84	117.70
1	1	2480	A	C8-N9-C4	-5.12	103.75	105.80
2	3	18	C	C2-N1-C1'	5.12	124.43	118.80
1	1	263	C	C5-C6-N1	5.12	123.56	121.00
1	1	869	G	C8-N9-C1'	-5.12	120.35	127.00
47	2	1664	C	C5-C6-N1	5.12	123.56	121.00
1	1	908	G	N3-C4-C5	-5.12	126.04	128.60
1	1	1405	U	P-O3'-C3'	5.12	125.84	119.70
47	2	70	C	C6-N1-C2	-5.12	118.25	120.30
1	1	168	U	N3-C2-O2	-5.12	118.62	122.20
1	1	2863	G	C4-N9-C1'	5.12	133.15	126.50
47	2	1596	C	C6-N1-C1'	-5.12	114.66	120.80
1	1	868	C	C5-C6-N1	5.11	123.56	121.00
1	1	1738	C	C2-N1-C1'	5.11	124.43	118.80
39	i	43	LEU	CA-CB-CG	5.11	127.06	115.30
18	N	92	LEU	CA-CB-CG	-5.11	103.54	115.30
47	2	1007	C	C5-C6-N1	5.11	123.56	121.00
1	1	7	C	C6-N1-C2	-5.11	118.25	120.30
1	1	165	A	P-O3'-C3'	5.11	125.83	119.70
47	2	517	U	N1-C2-O2	5.11	126.38	122.80
47	2	1473	U	N3-C2-O2	-5.10	118.63	122.20
1	1	44	U	N3-C2-O2	-5.10	118.63	122.20
81	AX	765	LEU	CA-CB-CG	5.10	127.03	115.30
1	1	512	U	N1-C2-O2	5.10	126.37	122.80
47	2	431	C	C6-N1-C2	-5.10	118.26	120.30
47	2	1585	U	C2-N1-C1'	5.10	123.82	117.70
47	2	1672	G	C4-N9-C1'	5.10	133.13	126.50
1	1	1084	A	P-O3'-C3'	5.10	125.81	119.70
1	1	853	G	N3-C4-N9	5.09	129.06	126.00
1	1	2288	G	C8-N9-C1'	-5.09	120.38	127.00
1	1	2366	C	C2-N1-C1'	5.09	124.40	118.80
47	2	338	C	C2-N1-C1'	5.09	124.40	118.80
1	1	368	G	N3-C4-C5	-5.09	126.05	128.60
47	2	627	C	C6-N1-C2	-5.09	118.26	120.30
1	1	1732	U	N3-C2-O2	-5.09	118.64	122.20
47	2	1170	G	C8-N9-C1'	-5.09	120.39	127.00
1	1	1263	A	N1-C6-N6	-5.09	115.55	118.60
1	1	2406	C	C5-C6-N1	5.09	123.54	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	2	496	G	O4'-C1'-N9	5.09	112.27	108.20
1	1	1332	A	C4-N9-C1'	5.08	135.45	126.30
1	1	44	U	N1-C2-O2	5.08	126.36	122.80
1	1	334	A	O4'-C1'-N9	5.08	112.27	108.20
47	2	818	C	C6-N1-C2	-5.08	118.27	120.30
47	2	1298	U	N1-C2-O2	5.08	126.36	122.80
47	2	1607	G	C4-N9-C1'	5.08	133.11	126.50
1	1	113	C	C6-N1-C1'	-5.08	114.70	120.80
1	1	528	U	N3-C2-O2	-5.08	118.64	122.20
1	1	1279	C	C4-C5-C6	-5.08	114.86	117.40
47	2	572	C	C5-C6-N1	5.08	123.54	121.00
1	1	166	C	O4'-C1'-N1	5.08	112.26	108.20
1	1	2526	C	N3-C2-O2	-5.08	118.34	121.90
49	r	178	GLY	N-CA-C	-5.08	100.41	113.10
47	2	36	C	P-O3'-C3'	5.07	125.79	119.70
47	2	729	G	C4-N9-C1'	5.07	133.09	126.50
1	1	3130	A	C2-N3-C4	5.07	113.14	110.60
1	1	539	C	C6-N1-C2	-5.07	118.27	120.30
47	2	792	U	N1-C2-O2	5.07	126.35	122.80
47	2	849	C	C6-N1-C2	-5.07	118.27	120.30
1	1	986	U	C5-C6-N1	5.07	125.23	122.70
1	1	1230	G	C4-C5-N7	5.07	112.83	110.80
52	u	180	LEU	CA-CB-CG	5.06	126.95	115.30
84	BA	103	LEU	CA-CB-CG	5.06	126.94	115.30
1	1	1049	C	C2-N1-C1'	5.06	124.37	118.80
47	2	849	C	C5-C6-N1	5.06	123.53	121.00
1	1	963	G	N3-C4-N9	5.06	129.04	126.00
1	1	1690	C	C2-N1-C1'	5.06	124.36	118.80
47	2	747	C	C2-N1-C1'	5.06	124.36	118.80
1	1	2500	A	C2-N3-C4	5.06	113.13	110.60
1	1	2884	C	N1-C2-O2	5.06	121.93	118.90
47	2	1235	C	C2-N3-C4	5.06	122.43	119.90
3	4	63	G	N3-C4-C5	-5.05	126.07	128.60
47	2	36	C	N3-C2-O2	-5.05	118.36	121.90
82	AY	51	G	C8-N9-C1'	-5.05	120.43	127.00
1	1	931	C	N3-C2-O2	-5.05	118.36	121.90
1	1	839	C	N1-C2-O2	5.05	121.93	118.90
3	4	106	C	N3-C2-O2	-5.05	118.36	121.90
47	2	139	C	N1-C2-O2	5.05	121.93	118.90
47	2	1209	C	C5-C6-N1	5.05	123.52	121.00
1	1	1021	G	C8-N9-C1'	-5.05	120.44	127.00
1	1	1068	C	C2-N1-C1'	5.05	124.35	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	u	101	LEU	CA-CB-CG	5.05	126.91	115.30
1	1	2708	C	C6-N1-C2	-5.04	118.28	120.30
1	1	368	G	C4-N9-C1'	5.04	133.05	126.50
1	1	1872	C	N1-C2-O2	5.04	121.92	118.90
1	1	2388	U	N1-C2-O2	5.04	126.33	122.80
12	G	125	ALA	C-N-CA	5.04	134.30	121.70
1	1	3355	U	C2-N1-C1'	5.04	123.74	117.70
47	2	557	G	N3-C2-N2	-5.04	116.38	119.90
47	2	730	G	C4-N9-C1'	5.04	133.04	126.50
1	1	520	U	N1-C2-O2	5.03	126.32	122.80
1	1	3135	U	C6-N1-C2	-5.03	117.98	121.00
47	2	1565	C	C5-C6-N1	5.03	123.52	121.00
1	1	2683	U	N3-C2-O2	-5.03	118.68	122.20
1	1	1584	U	N1-C2-O2	5.03	126.32	122.80
47	2	61	A	O4'-C1'-N9	-5.03	104.17	108.20
1	1	151	A	C4-N9-C1'	5.03	135.35	126.30
47	2	118	U	P-O3'-C3'	5.03	125.73	119.70
47	2	1642	G	N9-C4-C5	-5.03	103.39	105.40
1	1	507	U	N3-C2-O2	-5.03	118.68	122.20
1	1	662	U	N3-C2-O2	-5.03	118.68	122.20
1	1	2094	C	C6-N1-C2	-5.03	118.29	120.30
47	2	305	C	N1-C2-O2	5.03	121.92	118.90
47	2	305	C	N3-C2-O2	-5.03	118.38	121.90
47	2	1342	C	C6-N1-C2	-5.03	118.29	120.30
1	1	1037	C	C5-C6-N1	5.02	123.51	121.00
1	1	2825	C	N1-C2-O2	5.02	121.91	118.90
47	2	990	C	N1-C2-O2	5.02	121.91	118.90
47	2	1528	U	N1-C2-O2	5.02	126.32	122.80
47	2	1037	C	C6-N1-C2	-5.02	118.29	120.30
47	2	1510	U	C5-C6-N1	5.02	125.21	122.70
47	2	1070	C	C6-N1-C1'	-5.02	114.78	120.80
3	4	50	C	N1-C2-O2	5.02	121.91	118.90
5	P2	86	LYS	C-N-CA	5.02	134.24	121.70
47	2	1333	C	C6-N1-C2	-5.02	118.29	120.30
1	1	656	A	N7-C8-N9	5.01	116.31	113.80
1	1	2881	C	C6-N1-C2	-5.01	118.30	120.30
47	2	707	A	C8-N9-C4	-5.01	103.79	105.80
1	1	1448	U	C2-N1-C1'	5.01	123.72	117.70
47	2	945	U	C2-N1-C1'	5.01	123.72	117.70
1	1	2137	U	C5-C6-N1	5.01	125.21	122.70
47	2	1021	C	C6-N1-C1'	5.01	126.81	120.80
47	2	1039	A	P-O3'-C3'	5.01	125.71	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	2	1206	U	N3-C4-O4	5.01	122.91	119.40
1	1	112	U	N1-C2-O2	5.01	126.31	122.80
1	1	1779	C	C5-C6-N1	5.01	123.50	121.00
1	1	2652	U	N1-C2-O2	5.01	126.31	122.80
47	2	1607	G	C8-N9-C1'	-5.01	120.49	127.00
47	2	1674	C	N3-C2-O2	-5.01	118.39	121.90
3	4	120	C	N1-C2-N3	5.01	122.71	119.20
47	2	611	U	C6-N1-C1'	-5.01	114.19	121.20
47	2	1146	G	C4-N9-C1'	5.01	133.01	126.50
1	1	448	U	N3-C2-O2	-5.00	118.70	122.20
1	1	1103	A	C4-N9-C1'	5.00	135.31	126.30
3	4	116	G	C4-N9-C1'	5.00	133.01	126.50
1	1	69	C	C6-N1-C1'	5.00	126.81	120.80
3	4	7	U	P-O3'-C3'	5.00	125.70	119.70

There are no chirality outliers.

All (143) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
58	AA	57	THR	Peptide
58	AA	59	PHE	Peptide
59	AB	6	THR	Peptide
61	AD	104	ARG	Peptide
61	AD	60	VAL	Peptide
62	AE	123	SER	Peptide
62	AE	90	ARG	Peptide
62	AE	91	THR	Peptide
63	AF	16	SER	Peptide
63	AF	47	ARG	Peptide
64	AG	33	GLY	Peptide
64	AG	4	VAL	Peptide
64	AG	40	GLU	Peptide
64	AG	49	TYR	Peptide
65	AH	84	TYR	Peptide
66	AI	91	ASP	Peptide
67	AJ	134	ARG	Peptide
68	AK	119	ALA	Peptide
68	AK	53	LYS	Peptide
69	AL	51	VAL	Peptide
69	AL	52	THR	Peptide
71	AN	113	ALA	Peptide
71	AN	41	SER	Peptide

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Mol	Chain	Res	Type	Group
73	AP	54	VAL	Peptide
74	AQ	43	ASN	Peptide
74	AQ	63	ALA	Peptide
74	AQ	9	GLY	Peptide
75	AR	80	ARG	Peptide
76	AS	49	ARG	Peptide
78	AU	3	LYS	Peptide
80	AW	119	ARG	Peptide
81	AX	144	ARG	Peptide
81	AX	247	ASP	Peptide
81	AX	251	ASN	Peptide
81	AX	273	PHE	Peptide
81	AX	305	ILE	Peptide
81	AX	394	PHE	Peptide
81	AX	482	LYS	Peptide
81	AX	487	PRO	Peptide
81	AX	579	SER	Peptide
81	AX	583	HIS	Peptide
81	AX	587	TYR	Peptide
81	AX	608	PRO	Peptide
81	AX	721	ASP	Peptide
81	AX	764	PRO	Peptide
81	AX	829	LYS	Peptide
7	B	159	ARG	Peptide
84	BA	120	VAL	Peptide
84	BA	136	THR	Peptide
84	BA	72	PHE	Peptide
8	C	93	MET	Peptide
9	D	124	GLU	Peptide
9	D	19	PRO	Peptide
9	D	281	GLU	Peptide
9	D	43	LYS	Peptide
10	E	4	GLN	Peptide
10	E	7	PRO	Peptide
11	F	157	ASN	Peptide
11	F	215	GLY	Peptide
12	G	192	GLN	Peptide
12	G	30	THR	Peptide
12	G	76	ALA	Peptide
14	I	197	VAL	Peptide
14	I	215	GLU	Peptide
14	I	65	LEU	Peptide

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Mol	Chain	Res	Type	Group
15	J	10	ARG	Peptide
15	J	117	ASP	Peptide
15	J	165	GLN	Peptide
15	J	170	ASP	Peptide
15	J	73	GLY	Peptide
15	J	74	PRO	Peptide
16	L	47	ALA	Peptide
16	L	76	THR	Peptide
17	M	7	VAL	Peptide
17	M	8	LYS	Peptide
18	N	46	ASP	Peptide
19	O	110	PRO	Peptide
19	O	36	VAL	Peptide
19	O	78	ARG	Peptide
4	P0	16	ARG	Peptide
4	P0	38	MET	Peptide
5	P2	77	ALA	Peptide
22	R	54	ALA	Peptide
23	S	148	LEU	Peptide
23	S	149	LYS	Peptide
30	Z	102	GLU	Peptide
31	a	14	HIS	Peptide
31	a	57	GLY	Peptide
32	b	41	ARG	Peptide
34	d	87	ASN	Peptide
36	f	58	GLU	Peptide
36	f	59	VAL	Peptide
37	g	65	VAL	Peptide
37	g	66	SER	Peptide
37	g	80	ARG	Peptide
37	g	82	ALA	Peptide
38	h	69	LEU	Peptide
38	h	90	ARG	Peptide
39	i	26	ILE	Peptide
39	i	52	PRO	Peptide
39	i	97	SER	Peptide
40	j	5	THR	Peptide
40	j	64	MET	Peptide
40	j	82	SER	Peptide
41	k	38	PHE	Peptide
41	k	39	ARG	Peptide
45	o	33	ALA	Peptide

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Mol	Chain	Res	Type	Group
45	o	7	THR	Peptide
46	p	84	ARG	Peptide
48	q	111	ILE	Peptide
48	q	112	THR	Peptide
49	r	177	GLN	Peptide
49	r	206	PRO	Peptide
49	r	54	LEU	Peptide
50	s	39	THR	Peptide
51	t	202	LEU	Peptide
51	t	219	ALA	Peptide
51	t	220	PRO	Peptide
51	t	221	SER	Peptide
52	u	110	ALA	Peptide
52	u	154	ILE	Peptide
52	u	191	ARG	Peptide
52	u	194	THR	Peptide
52	u	195	ILE	Peptide
52	u	201	HIS	Peptide
52	u	233	LYS	Peptide
53	v	128	ASN	Peptide
53	v	157	ARG	Peptide
53	v	57	SER	Peptide
53	v	64	VAL	Peptide
54	w	100	ALA	Peptide
54	w	148	SER	Peptide
54	w	153	VAL	Peptide
54	w	67	VAL	Peptide
54	w	9	VAL	Peptide
54	w	92	ARG	Peptide
55	x	110	GLN	Peptide
55	x	155	ASP	Peptide
55	x	64	VAL	Peptide
56	y	23	LYS	Peptide
57	z	133	HIS	Peptide
57	z	163	PRO	Peptide
57	z	171	ARG	Peptide

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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	P0	187/189 (99%)	145 (78%)	42 (22%)	0	100	100
5	P2	92/94 (98%)	64 (70%)	28 (30%)	0	100	100
6	A	250/252 (99%)	217 (87%)	33 (13%)	0	100	100
7	B	384/386 (100%)	335 (87%)	48 (12%)	1 (0%)	41	75
8	C	359/361 (99%)	305 (85%)	52 (14%)	2 (1%)	25	63
9	D	294/296 (99%)	248 (84%)	43 (15%)	3 (1%)	15	53
10	E	152/175 (87%)	137 (90%)	15 (10%)	0	100	100
11	F	220/222 (99%)	194 (88%)	25 (11%)	1 (0%)	29	67
12	G	231/233 (99%)	204 (88%)	27 (12%)	0	100	100
13	H	189/191 (99%)	168 (89%)	20 (11%)	1 (0%)	29	67
14	I	207/220 (94%)	178 (86%)	29 (14%)	0	100	100
15	J	167/169 (99%)	130 (78%)	34 (20%)	3 (2%)	8	41
16	L	191/193 (99%)	166 (87%)	23 (12%)	2 (1%)	15	53
17	M	134/136 (98%)	121 (90%)	12 (9%)	1 (1%)	22	61
18	N	201/203 (99%)	172 (86%)	29 (14%)	0	100	100
19	O	195/197 (99%)	171 (88%)	21 (11%)	3 (2%)	10	45
20	P	181/183 (99%)	161 (89%)	20 (11%)	0	100	100
21	Q	183/185 (99%)	165 (90%)	18 (10%)	0	100	100
22	R	186/188 (99%)	170 (91%)	16 (9%)	0	100	100
23	S	170/172 (99%)	151 (89%)	19 (11%)	0	100	100
24	T	157/159 (99%)	146 (93%)	11 (7%)	0	100	100
25	U	98/100 (98%)	89 (91%)	9 (9%)	0	100	100
26	V	134/136 (98%)	120 (90%)	14 (10%)	0	100	100
27	W	60/62 (97%)	57 (95%)	3 (5%)	0	100	100
28	X	119/121 (98%)	111 (93%)	8 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	Y	124/126 (98%)	115 (93%)	9 (7%)	0	100	100
30	Z	133/135 (98%)	115 (86%)	17 (13%)	1 (1%)	19	58
31	a	146/148 (99%)	118 (81%)	25 (17%)	3 (2%)	7	39
32	b	56/58 (97%)	46 (82%)	10 (18%)	0	100	100
33	c	95/97 (98%)	90 (95%)	5 (5%)	0	100	100
34	d	107/109 (98%)	95 (89%)	12 (11%)	0	100	100
35	e	125/127 (98%)	103 (82%)	22 (18%)	0	100	100
36	f	104/106 (98%)	90 (86%)	11 (11%)	3 (3%)	4	32
37	g	110/112 (98%)	98 (89%)	10 (9%)	2 (2%)	8	41
38	h	117/119 (98%)	100 (86%)	17 (14%)	0	100	100
39	i	97/99 (98%)	75 (77%)	21 (22%)	1 (1%)	15	53
40	j	85/87 (98%)	67 (79%)	16 (19%)	2 (2%)	6	36
41	k	75/77 (97%)	54 (72%)	19 (25%)	2 (3%)	5	34
42	l	48/50 (96%)	36 (75%)	11 (23%)	1 (2%)	7	39
43	m	50/52 (96%)	46 (92%)	4 (8%)	0	100	100
44	n	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
45	o	103/105 (98%)	78 (76%)	25 (24%)	0	100	100
46	p	89/91 (98%)	78 (88%)	11 (12%)	0	100	100
48	q	204/206 (99%)	162 (79%)	39 (19%)	3 (2%)	10	45
49	r	212/214 (99%)	167 (79%)	41 (19%)	4 (2%)	8	40
50	s	215/217 (99%)	187 (87%)	27 (13%)	1 (0%)	29	67
51	t	221/223 (99%)	182 (82%)	37 (17%)	2 (1%)	17	55
52	u	258/260 (99%)	195 (76%)	61 (24%)	2 (1%)	19	58
53	v	204/206 (99%)	162 (79%)	41 (20%)	1 (0%)	29	67
54	w	221/223 (99%)	167 (76%)	47 (21%)	7 (3%)	4	31
55	x	182/184 (99%)	145 (80%)	34 (19%)	3 (2%)	9	44
56	y	184/199 (92%)	148 (80%)	36 (20%)	0	100	100
57	z	183/185 (99%)	147 (80%)	36 (20%)	0	100	100
58	AA	94/105 (90%)	76 (81%)	17 (18%)	1 (1%)	14	51
59	AB	151/153 (99%)	131 (87%)	18 (12%)	2 (1%)	12	48
60	AC	122/124 (98%)	93 (76%)	27 (22%)	2 (2%)	9	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
61	AD	148/150 (99%)	118 (80%)	27 (18%)	3 (2%)	7	40
62	AE	125/127 (98%)	104 (83%)	21 (17%)	0	100	100
63	AF	122/124 (98%)	89 (73%)	33 (27%)	0	100	100
64	AG	139/141 (99%)	111 (80%)	27 (19%)	1 (1%)	22	61
65	AH	116/125 (93%)	98 (84%)	17 (15%)	1 (1%)	17	55
66	AI	143/145 (99%)	117 (82%)	24 (17%)	2 (1%)	11	46
67	AJ	141/143 (99%)	126 (89%)	15 (11%)	0	100	100
68	AK	105/107 (98%)	90 (86%)	15 (14%)	0	100	100
69	AL	85/87 (98%)	64 (75%)	19 (22%)	2 (2%)	6	36
70	AM	127/129 (98%)	115 (91%)	11 (9%)	1 (1%)	19	58
71	AN	142/144 (99%)	108 (76%)	34 (24%)	0	100	100
72	AO	132/134 (98%)	115 (87%)	17 (13%)	0	100	100
73	AP	68/70 (97%)	52 (76%)	15 (22%)	1 (2%)	10	45
74	AQ	95/97 (98%)	70 (74%)	25 (26%)	0	100	100
75	AR	79/81 (98%)	58 (73%)	21 (27%)	0	100	100
76	AS	61/63 (97%)	49 (80%)	12 (20%)	0	100	100
77	AT	51/53 (96%)	48 (94%)	3 (6%)	0	100	100
78	AU	58/60 (97%)	42 (72%)	16 (28%)	0	100	100
79	AV	316/318 (99%)	252 (80%)	64 (20%)	0	100	100
80	AW	35/37 (95%)	21 (60%)	14 (40%)	0	100	100
81	AX	834/837 (100%)	676 (81%)	155 (19%)	3 (0%)	34	71
84	BA	202/204 (99%)	153 (76%)	47 (23%)	2 (1%)	15	53
All	All	12203/12421 (98%)	10189 (84%)	1938 (16%)	76 (1%)	29	63

All (76) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
39	i	98	ARG
40	j	65	ARG
42	l	30	ARG
48	q	113	ARG
54	w	68	LEU
54	w	93	LYS
61	AD	105	ASN

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Mol	Chain	Res	Type
64	AG	41	PRO
16	L	63	VAL
16	L	77	LEU
17	M	8	LYS
31	a	78	LEU
36	f	58	GLU
36	f	60	ARG
49	r	55	LYS
49	r	62	LYS
50	s	40	LYS
52	u	195	ILE
54	w	92	ARG
55	x	111	LYS
60	AC	109	GLU
8	C	130	ALA
11	F	159	GLN
15	J	74	PRO
15	J	166	LYS
19	O	111	PRO
31	a	47	LYS
41	k	40	GLN
49	r	206	PRO
49	r	207	LEU
51	t	220	PRO
53	v	50	GLU
54	w	10	ASN
54	w	100	ALA
55	x	29	ASN
55	x	65	PRO
81	AX	698	ILE
9	D	20	PHE
9	D	261	THR
19	O	12	LYS
31	a	48	TYR
48	q	112	THR
52	u	155	LYS
59	AB	56	LYS
66	AI	91	ASP
69	AL	52	THR
69	AL	81	ASN
84	BA	197	ASN
8	C	268	ALA

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Mol	Chain	Res	Type
13	H	50	ASN
37	g	66	SER
37	g	67	LYS
41	k	33	LYS
48	q	114	SER
61	AD	139	TRP
65	AH	72	LYS
66	AI	63	GLN
19	O	37	ARG
54	w	101	ILE
61	AD	85	PRO
73	AP	97	LYS
84	BA	198	TRP
9	D	125	VAL
51	t	203	PRO
59	AB	7	VAL
40	j	6	PRO
81	AX	252	PRO
36	f	59	VAL
81	AX	741	GLY
15	J	118	PRO
30	Z	103	GLN
54	w	85	ARG
70	AM	67	GLY
7	B	188	ILE
58	AA	88	PRO
60	AC	106	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	P0	160/160 (100%)	157 (98%)	3 (2%)	57	75
5	P2	81/81 (100%)	78 (96%)	3 (4%)	34	60
6	A	193/194 (100%)	190 (98%)	3 (2%)	62	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	B	321/322 (100%)	314 (98%)	7 (2%)	52	71
8	C	288/288 (100%)	281 (98%)	7 (2%)	49	69
9	D	244/244 (100%)	241 (99%)	3 (1%)	71	84
10	E	134/152 (88%)	128 (96%)	6 (4%)	27	55
11	F	186/186 (100%)	179 (96%)	7 (4%)	33	59
12	G	187/191 (98%)	186 (100%)	1 (0%)	88	93
13	H	171/171 (100%)	168 (98%)	3 (2%)	59	77
14	I	177/186 (95%)	176 (99%)	1 (1%)	86	92
15	J	147/147 (100%)	140 (95%)	7 (5%)	25	53
16	L	154/154 (100%)	145 (94%)	9 (6%)	20	48
17	M	107/107 (100%)	103 (96%)	4 (4%)	34	60
18	N	175/175 (100%)	167 (95%)	8 (5%)	27	54
19	O	160/160 (100%)	155 (97%)	5 (3%)	40	63
20	P	140/145 (97%)	137 (98%)	3 (2%)	53	72
21	Q	150/150 (100%)	146 (97%)	4 (3%)	44	66
22	R	153/153 (100%)	144 (94%)	9 (6%)	19	48
23	S	156/156 (100%)	152 (97%)	4 (3%)	46	67
24	T	136/136 (100%)	132 (97%)	4 (3%)	42	65
25	U	87/87 (100%)	86 (99%)	1 (1%)	73	85
26	V	103/104 (99%)	99 (96%)	4 (4%)	32	58
27	W	54/54 (100%)	53 (98%)	1 (2%)	57	75
28	X	104/105 (99%)	102 (98%)	2 (2%)	57	75
29	Y	109/109 (100%)	109 (100%)	0	100	100
30	Z	115/115 (100%)	113 (98%)	2 (2%)	60	78
31	a	118/118 (100%)	117 (99%)	1 (1%)	81	89
32	b	46/46 (100%)	44 (96%)	2 (4%)	29	56
33	c	81/81 (100%)	79 (98%)	2 (2%)	47	68
34	d	94/96 (98%)	94 (100%)	0	100	100
35	e	109/109 (100%)	109 (100%)	0	100	100
36	f	90/90 (100%)	88 (98%)	2 (2%)	52	71
37	g	95/95 (100%)	94 (99%)	1 (1%)	73	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	h	104/104 (100%)	101 (97%)	3 (3%)	42	65
39	i	81/81 (100%)	78 (96%)	3 (4%)	34	60
40	j	70/70 (100%)	69 (99%)	1 (1%)	67	81
41	k	68/68 (100%)	67 (98%)	1 (2%)	65	80
42	l	45/45 (100%)	42 (93%)	3 (7%)	16	44
43	m	47/47 (100%)	45 (96%)	2 (4%)	29	56
44	n	23/23 (100%)	21 (91%)	2 (9%)	10	35
45	o	90/90 (100%)	89 (99%)	1 (1%)	73	85
46	p	71/71 (100%)	70 (99%)	1 (1%)	67	81
48	q	164/173 (95%)	158 (96%)	6 (4%)	34	60
49	r	191/191 (100%)	187 (98%)	4 (2%)	53	72
50	s	176/176 (100%)	174 (99%)	2 (1%)	73	85
51	t	182/182 (100%)	176 (97%)	6 (3%)	38	62
52	u	221/221 (100%)	215 (97%)	6 (3%)	44	66
53	v	173/173 (100%)	166 (96%)	7 (4%)	31	57
54	w	189/191 (99%)	183 (97%)	6 (3%)	39	62
55	x	165/165 (100%)	161 (98%)	4 (2%)	49	69
56	y	150/160 (94%)	144 (96%)	6 (4%)	31	57
57	z	158/158 (100%)	155 (98%)	3 (2%)	57	75
58	AA	77/98 (79%)	76 (99%)	1 (1%)	69	82
59	AB	133/134 (99%)	127 (96%)	6 (4%)	27	55
60	AC	88/100 (88%)	87 (99%)	1 (1%)	73	85
61	AD	127/127 (100%)	123 (97%)	4 (3%)	40	63
62	AE	81/96 (84%)	77 (95%)	4 (5%)	25	52
63	AF	101/104 (97%)	96 (95%)	5 (5%)	24	52
64	AG	117/117 (100%)	116 (99%)	1 (1%)	78	88
65	AH	94/113 (83%)	90 (96%)	4 (4%)	29	56
66	AI	128/128 (100%)	124 (97%)	4 (3%)	40	63
67	AJ	115/115 (100%)	112 (97%)	3 (3%)	46	67
68	AK	100/100 (100%)	99 (99%)	1 (1%)	76	86
69	AL	74/74 (100%)	71 (96%)	3 (4%)	30	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
70	AM	110/110 (100%)	108 (98%)	2 (2%)	59	77
71	AN	119/119 (100%)	115 (97%)	4 (3%)	37	61
72	AO	112/112 (100%)	108 (96%)	4 (4%)	35	61
73	AP	61/61 (100%)	59 (97%)	2 (3%)	38	62
74	AQ	83/83 (100%)	80 (96%)	3 (4%)	35	61
75	AR	70/70 (100%)	70 (100%)	0	100	100
76	AS	56/56 (100%)	54 (96%)	2 (4%)	35	61
77	AT	47/47 (100%)	45 (96%)	2 (4%)	29	56
78	AU	51/51 (100%)	47 (92%)	4 (8%)	12	39
79	AV	259/261 (99%)	255 (98%)	4 (2%)	65	80
80	AW	31/31 (100%)	30 (97%)	1 (3%)	39	62
81	AX	708/709 (100%)	687 (97%)	21 (3%)	41	64
84	BA	185/185 (100%)	179 (97%)	6 (3%)	39	62
All	All	10320/10457 (99%)	10042 (97%)	278 (3%)	48	66

All (278) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	P0	48	ARG
4	P0	75	LYS
4	P0	110	ARG
5	P2	63	LYS
5	P2	93	LYS
5	P2	117	ARG
6	A	42	ARG
6	A	194	ASN
6	A	243	THR
7	B	4	ARG
7	B	146	ARG
7	B	159	ARG
7	B	196	ARG
7	B	287	LYS
7	B	318	LYS
7	B	332	ARG
8	C	18	ASN
8	C	104	LYS
8	C	156	LEU

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Mol	Chain	Res	Type
8	C	197	ARG
8	C	221	ASN
8	C	234	ASN
8	C	346	LYS
9	D	21	ARG
9	D	224	LYS
9	D	282	ARG
10	E	22	ARG
10	E	31	ARG
10	E	48	ARG
10	E	51	ARG
10	E	80	ASN
10	E	154	LEU
11	F	105	LEU
11	F	106	LEU
11	F	128	LYS
11	F	160	ARG
11	F	172	ASN
11	F	209	ASN
11	F	231	ASN
12	G	191	ASN
13	H	38	LEU
13	H	116	ASN
13	H	129	ARG
14	I	3	ARG
15	J	12	LEU
15	J	51	ARG
15	J	55	ARG
15	J	60	ARG
15	J	71	VAL
15	J	72	ARG
15	J	84	LEU
16	L	5	LYS
16	L	35	ARG
16	L	39	ARG
16	L	42	ARG
16	L	85	LEU
16	L	157	ARG
16	L	172	LEU
16	L	180	ARG
16	L	188	ARG
17	M	24	LYS

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Mol	Chain	Res	Type
17	M	50	LYS
17	M	74	ARG
17	M	108	ARG
18	N	38	ARG
18	N	44	ARG
18	N	50	ARG
18	N	96	ARG
18	N	106	VAL
18	N	132	VAL
18	N	138	GLN
18	N	176	LYS
19	O	23	VAL
19	O	49	ARG
19	O	74	ARG
19	O	94	ARG
19	O	155	LYS
20	P	30	ARG
20	P	138	LYS
20	P	153	LYS
21	Q	11	LYS
21	Q	46	LYS
21	Q	78	ASN
21	Q	176	ARG
22	R	39	ASN
22	R	53	LYS
22	R	104	ARG
22	R	136	ARG
22	R	146	LYS
22	R	156	ASN
22	R	166	ASN
22	R	173	ARG
22	R	176	ARG
23	S	10	ILE
23	S	48	LEU
23	S	73	LYS
23	S	131	LYS
24	T	83	ARG
24	T	89	LEU
24	T	108	ARG
24	T	139	ARG
25	U	104	ARG
26	V	64	LYS

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Mol	Chain	Res	Type
26	V	69	LEU
26	V	86	ARG
26	V	109	MET
27	W	57	LYS
28	X	39	LYS
28	X	138	ARG
30	Z	5	LEU
30	Z	84	ARG
31	a	70	LYS
32	b	14	ARG
32	b	42	ASN
33	c	19	LYS
33	c	75	ASN
36	f	31	LYS
36	f	86	ARG
37	g	113	LYS
38	h	26	LYS
38	h	59	ASN
38	h	81	ARG
39	i	57	LEU
39	i	60	LEU
39	i	91	ASN
40	j	25	ARG
41	k	21	LYS
42	l	8	ARG
42	l	21	ARG
42	l	43	ASN
43	m	106	ARG
43	m	119	ASN
44	n	13	LEU
44	n	21	ARG
45	o	80	ARG
46	p	84	ARG
48	q	21	ASN
48	q	52	LYS
48	q	113	ARG
48	q	127	ARG
48	q	165	ARG
48	q	179	ARG
49	r	26	ARG
49	r	146	GLN
49	r	162	ARG

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Mol	Chain	Res	Type
49	r	166	LYS
50	s	81	MET
50	s	174	ARG
51	t	4	LEU
51	t	10	LYS
51	t	109	LEU
51	t	116	ARG
51	t	146	ARG
51	t	212	LYS
52	u	12	LEU
52	u	66	MET
52	u	130	GLN
52	u	180	LEU
52	u	238	LEU
52	u	240	LYS
53	v	79	ASN
53	v	99	MET
53	v	102	ARG
53	v	156	ARG
53	v	180	ARG
53	v	222	LYS
53	v	224	ASN
54	w	4	ASN
54	w	72	ARG
54	w	143	LYS
54	w	164	LYS
54	w	214	LYS
54	w	219	ARG
55	x	7	LYS
55	x	27	LEU
55	x	56	LYS
55	x	88	ARG
56	y	18	ARG
56	y	23	LYS
56	y	47	ARG
56	y	104	ILE
56	y	110	ARG
56	y	146	ARG
57	z	17	ARG
57	z	59	LEU
57	z	109	LEU
58	AA	81	ASN

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Mol	Chain	Res	Type
59	AB	15	LYS
59	AB	43	LYS
59	AB	67	ARG
59	AB	127	GLN
59	AB	129	ARG
59	AB	141	LYS
60	AC	95	LYS
61	AD	21	ASN
61	AD	27	LYS
61	AD	104	ARG
61	AD	112	LYS
62	AE	127	ARG
62	AE	132	ARG
62	AE	135	ARG
62	AE	136	ARG
63	AF	36	LEU
63	AF	77	ARG
63	AF	89	MET
63	AF	108	ARG
63	AF	127	ARG
64	AG	143	ARG
65	AH	45	ARG
65	AH	72	LYS
65	AH	80	ARG
65	AH	115	LEU
66	AI	19	ASN
66	AI	68	ARG
66	AI	71	GLN
66	AI	120	ARG
67	AJ	68	ARG
67	AJ	77	ASN
67	AJ	134	ARG
68	AK	102	ARG
69	AL	15	ARG
69	AL	81	ASN
69	AL	87	ARG
70	AM	15	ASN
70	AM	94	LEU
71	AN	20	ARG
71	AN	27	ASN
71	AN	56	LYS
71	AN	63	GLN

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Mol	Chain	Res	Type
72	AO	32	ARG
72	AO	68	LYS
72	AO	102	LYS
72	AO	123	LYS
73	AP	49	ARG
73	AP	97	LYS
74	AQ	5	ARG
74	AQ	10	ARG
74	AQ	51	ARG
76	AS	49	ARG
76	AS	65	ARG
77	AT	13	ARG
77	AT	16	LYS
78	AU	3	LYS
78	AU	8	LEU
78	AU	33	ARG
78	AU	53	LYS
79	AV	117	LYS
79	AV	248	ASN
79	AV	249	ARG
79	AV	292	LEU
80	AW	138	ARG
81	AX	15	LYS
81	AX	119	LEU
81	AX	186	ASN
81	AX	231	LYS
81	AX	243	ARG
81	AX	247	ASP
81	AX	289	MET
81	AX	306	VAL
81	AX	308	LYS
81	AX	310	ASP
81	AX	324	MET
81	AX	328	LEU
81	AX	399	ARG
81	AX	438	MET
81	AX	465	LYS
81	AX	510	ARG
81	AX	555	LYS
81	AX	617	ARG
81	AX	631	ARG
81	AX	825	ARG

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Mol	Chain	Res	Type
81	AX	829	LYS
84	BA	45	ARG
84	BA	85	MET
84	BA	123	LEU
84	BA	188	ASN
84	BA	193	LEU
84	BA	197	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (124) such sidechains are listed below:

Mol	Chain	Res	Type
4	P0	32	ASN
4	P0	39	HIS
4	P0	174	ASN
4	P0	189	GLN
6	A	8	GLN
6	A	97	ASN
6	A	194	ASN
6	A	233	GLN
7	B	68	HIS
7	B	173	GLN
7	B	177	HIS
7	B	243	HIS
8	C	18	ASN
8	C	48	GLN
8	C	59	GLN
8	C	221	ASN
8	C	234	ASN
8	C	260	GLN
8	C	307	GLN
9	D	39	GLN
9	D	264	GLN
10	E	80	ASN
11	F	209	ASN
11	F	225	GLN
11	F	231	ASN
11	F	237	ASN
12	G	191	ASN
12	G	240	ASN
13	H	77	ASN
13	H	116	ASN
13	H	163	GLN

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Mol	Chain	Res	Type
14	I	14	ASN
14	I	59	GLN
14	I	95	HIS
15	J	20	ASN
16	L	28	GLN
16	L	103	ASN
18	N	37	HIS
18	N	123	GLN
18	N	138	GLN
20	P	97	ASN
20	P	121	GLN
21	Q	78	ASN
22	R	39	ASN
22	R	134	HIS
22	R	156	ASN
22	R	166	ASN
24	T	54	HIS
24	T	82	ASN
27	W	33	ASN
27	W	58	HIS
27	W	59	HIS
29	Y	42	GLN
29	Y	81	GLN
30	Z	127	ASN
31	a	28	HIS
31	a	40	HIS
31	a	74	ASN
32	b	19	ASN
33	c	75	ASN
35	e	88	HIS
36	f	75	HIS
38	h	59	ASN
39	i	91	ASN
41	k	10	GLN
42	l	33	ASN
42	l	43	ASN
43	m	117	HIS
43	m	119	ASN
48	q	21	ASN
48	q	33	GLN
48	q	140	ASN
49	r	149	GLN

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Mol	Chain	Res	Type
49	r	153	HIS
49	r	199	ASN
52	u	69	HIS
52	u	231	GLN
53	v	63	GLN
53	v	79	ASN
53	v	95	ASN
53	v	103	ASN
53	v	224	ASN
54	w	4	ASN
54	w	59	GLN
54	w	176	GLN
54	w	190	GLN
56	y	103	GLN
57	z	38	ASN
57	z	176	ASN
58	AA	12	HIS
58	AA	81	ASN
59	AB	127	GLN
59	AB	138	ASN
61	AD	21	ASN
63	AF	15	HIS
64	AG	32	ASN
66	AI	19	ASN
66	AI	71	GLN
66	AI	136	GLN
67	AJ	16	ASN
67	AJ	77	ASN
69	AL	81	ASN
70	AM	15	ASN
70	AM	42	GLN
70	AM	113	HIS
71	AN	27	ASN
71	AN	63	GLN
71	AN	75	GLN
77	AT	41	GLN
78	AU	57	ASN
79	AV	17	ASN
79	AV	29	GLN
79	AV	31	ASN
79	AV	200	ASN
79	AV	248	ASN

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Mol	Chain	Res	Type
81	AX	91	GLN
81	AX	101	ASN
81	AX	108	HIS
81	AX	186	ASN
81	AX	201	GLN
81	AX	224	GLN
81	AX	800	HIS
84	BA	181	ASN
84	BA	197	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	3220/3396 (94%)	1076 (33%)	33 (1%)
2	3	120/121 (99%)	28 (23%)	3 (2%)
3	4	157/158 (99%)	47 (29%)	5 (3%)
47	2	1774/1797 (98%)	779 (43%)	38 (2%)
82	AY	75/76 (98%)	29 (38%)	0
83	AZ	6/7 (85%)	5 (83%)	2 (33%)
All	All	5352/5555 (96%)	1964 (36%)	81 (1%)

All (1964) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	4	U
1	1	6	A
1	1	14	U
1	1	15	C
1	1	17	G
1	1	18	G
1	1	20	A
1	1	26	A
1	1	31	C
1	1	40	A
1	1	41	G
1	1	43	A
1	1	44	U
1	1	45	A
1	1	47	C
1	1	48	A
1	1	57	A

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Mol	Chain	Res	Type
1	1	59	G
1	1	60	A
1	1	65	A
1	1	66	A
1	1	73	C
1	1	75	G
1	1	77	A
1	1	85	A
1	1	88	A
1	1	92	G
1	1	93	C
1	1	94	G
1	1	98	G
1	1	99	A
1	1	102	C
1	1	103	G
1	1	104	G
1	1	105	C
1	1	108	A
1	1	111	C
1	1	112	U
1	1	116	A
1	1	118	U
1	1	119	U
1	1	121	A
1	1	122	A
1	1	130	A
1	1	132	C
1	1	135	C
1	1	136	G
1	1	138	U
1	1	145	G
1	1	148	G
1	1	152	U
1	1	153	U
1	1	154	U
1	1	156	G
1	1	157	A
1	1	158	G
1	1	161	G
1	1	162	G
1	1	164	A

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Mol	Chain	Res	Type
1	1	165	A
1	1	166	C
1	1	185	C
1	1	186	U
1	1	187	A
1	1	190	U
1	1	193	C
1	1	194	U
1	1	197	G
1	1	198	A
1	1	200	C
1	1	211	A
1	1	212	G
1	1	219	A
1	1	220	G
1	1	222	A
1	1	223	U
1	1	227	G
1	1	231	G
1	1	234	G
1	1	237	G
1	1	241	G
1	1	242	C
1	1	245	U
1	1	247	C
1	1	249	U
1	1	251	G
1	1	252	U
1	1	253	A
1	1	263	C
1	1	264	G
1	1	265	A
1	1	266	A
1	1	269	G
1	1	270	U
1	1	277	G
1	1	284	A
1	1	285	A
1	1	286	U
1	1	294	U
1	1	295	A
1	1	297	G

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Mol	Chain	Res	Type
1	1	299	G
1	1	305	U
1	1	311	C
1	1	313	A
1	1	316	U
1	1	317	A
1	1	324	A
1	1	328	U
1	1	329	U
1	1	330	G
1	1	337	G
1	1	339	C
1	1	341	G
1	1	343	U
1	1	346	C
1	1	349	A
1	1	350	C
1	1	352	A
1	1	361	A
1	1	368	G
1	1	371	G
1	1	372	A
1	1	375	A
1	1	376	G
1	1	377	A
1	1	380	U
1	1	384	A
1	1	385	A
1	1	387	A
1	1	390	G
1	1	391	A
1	1	398	A
1	1	399	A
1	1	400	G
1	1	401	U
1	1	402	A
1	1	403	C
1	1	404	G
1	1	420	G
1	1	421	G
1	1	422	A
1	1	429	U

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Mol	Chain	Res	Type
1	1	433	A
1	1	437	G
1	1	440	A
1	1	441	U
1	1	442	G
1	1	443	G
1	1	444	U
1	1	446	U
1	1	447	U
1	1	448	U
1	1	449	U
1	1	450	G
1	1	451	U
1	1	488	U
1	1	490	C
1	1	491	A
1	1	493	U
1	1	494	G
1	1	495	G
1	1	503	C
1	1	504	A
1	1	512	U
1	1	513	G
1	1	519	A
1	1	521	A
1	1	522	A
1	1	525	C
1	1	532	A
1	1	533	A
1	1	534	U
1	1	545	U
1	1	546	C
1	1	548	G
1	1	549	U
1	1	550	A
1	1	557	A
1	1	558	U
1	1	559	A
1	1	570	A
1	1	574	U
1	1	575	G
1	1	581	U

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Mol	Chain	Res	Type
1	1	585	A
1	1	591	G
1	1	592	A
1	1	593	C
1	1	594	U
1	1	604	G
1	1	605	U
1	1	607	A
1	1	608	A
1	1	611	A
1	1	620	U
1	1	621	A
1	1	628	A
1	1	633	C
1	1	636	C
1	1	637	C
1	1	642	U
1	1	649	A
1	1	657	A
1	1	660	A
1	1	662	U
1	1	664	U
1	1	667	C
1	1	677	A
1	1	678	G
1	1	681	U
1	1	684	G
1	1	689	U
1	1	691	A
1	1	692	A
1	1	705	A
1	1	709	A
1	1	712	G
1	1	714	G
1	1	716	A
1	1	718	G
1	1	719	U
1	1	742	G
1	1	748	U
1	1	750	G
1	1	758	C
1	1	761	A

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Mol	Chain	Res	Type
1	1	763	G
1	1	764	U
1	1	765	C
1	1	767	U
1	1	773	G
1	1	776	U
1	1	777	U
1	1	780	A
1	1	781	G
1	1	782	U
1	1	785	G
1	1	797	U
1	1	800	G
1	1	801	A
1	1	806	A
1	1	808	A
1	1	813	G
1	1	817	A
1	1	818	C
1	1	819	U
1	1	823	C
1	1	830	A
1	1	832	G
1	1	838	G
1	1	849	C
1	1	854	G
1	1	861	C
1	1	865	U
1	1	866	A
1	1	868	C
1	1	869	G
1	1	874	U
1	1	875	G
1	1	876	A
1	1	879	U
1	1	880	G
1	1	890	C
1	1	892	U
1	1	894	G
1	1	895	A
1	1	896	A
1	1	907	G

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Mol	Chain	Res	Type
1	1	908	G
1	1	909	G
1	1	911	C
1	1	914	A
1	1	915	A
1	1	916	G
1	1	917	A
1	1	922	U
1	1	923	C
1	1	924	G
1	1	933	A
1	1	937	G
1	1	941	G
1	1	943	U
1	1	944	C
1	1	951	A
1	1	959	C
1	1	960	U
1	1	962	A
1	1	963	G
1	1	964	G
1	1	971	G
1	1	974	G
1	1	977	C
1	1	979	U
1	1	980	A
1	1	981	U
1	1	983	A
1	1	984	G
1	1	985	U
1	1	990	U
1	1	991	G
1	1	994	G
1	1	1002	A
1	1	1006	A
1	1	1008	U
1	1	1009	A
1	1	1013	G
1	1	1014	U
1	1	1015	U
1	1	1016	C
1	1	1017	C

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Mol	Chain	Res	Type
1	1	1019	G
1	1	1020	G
1	1	1021	G
1	1	1022	U
1	1	1024	G
1	1	1028	U
1	1	1029	G
1	1	1030	A
1	1	1031	C
1	1	1032	C
1	1	1033	U
1	1	1034	U
1	1	1035	G
1	1	1036	A
1	1	1037	C
1	1	1038	C
1	1	1042	U
1	1	1043	C
1	1	1047	A
1	1	1051	U
1	1	1059	G
1	1	1061	A
1	1	1064	A
1	1	1066	G
1	1	1068	C
1	1	1072	G
1	1	1080	A
1	1	1081	U
1	1	1083	G
1	1	1085	A
1	1	1088	U
1	1	1089	G
1	1	1093	A
1	1	1094	U
1	1	1095	U
1	1	1096	U
1	1	1097	G
1	1	1098	A
1	1	1100	U
1	1	1103	A
1	1	1111	U
1	1	1117	G

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Mol	Chain	Res	Type
1	1	1127	G
1	1	1129	A
1	1	1131	G
1	1	1136	A
1	1	1137	C
1	1	1143	A
1	1	1144	U
1	1	1151	U
1	1	1154	A
1	1	1155	C
1	1	1158	A
1	1	1159	A
1	1	1171	G
1	1	1172	G
1	1	1174	G
1	1	1177	G
1	1	1178	G
1	1	1180	A
1	1	1181	U
1	1	1182	A
1	1	1186	G
1	1	1190	A
1	1	1191	U
1	1	1193	A
1	1	1196	C
1	1	1197	A
1	1	1198	C
1	1	1199	C
1	1	1200	A
1	1	1201	C
1	1	1203	A
1	1	1206	G
1	1	1209	G
1	1	1210	U
1	1	1212	A
1	1	1215	U
1	1	1217	A
1	1	1218	U
1	1	1219	C
1	1	1220	U
1	1	1222	G
1	1	1224	C

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Mol	Chain	Res	Type
1	1	1225	A
1	1	1229	G
1	1	1233	G
1	1	1235	U
1	1	1236	G
1	1	1239	C
1	1	1240	A
1	1	1241	U
1	1	1244	A
1	1	1245	A
1	1	1246	G
1	1	1248	C
1	1	1249	G
1	1	1252	A
1	1	1253	U
1	1	1254	C
1	1	1257	C
1	1	1258	U
1	1	1260	A
1	1	1262	G
1	1	1263	A
1	1	1264	G
1	1	1267	U
1	1	1271	A
1	1	1272	C
1	1	1275	C
1	1	1280	C
1	1	1281	G
1	1	1282	G
1	1	1283	C
1	1	1284	C
1	1	1286	A
1	1	1287	A
1	1	1291	A
1	1	1292	C
1	1	1295	G
1	1	1301	A
1	1	1302	A
1	1	1303	A
1	1	1305	U
1	1	1307	G
1	1	1308	A

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Mol	Chain	Res	Type
1	1	1309	U
1	1	1313	G
1	1	1316	C
1	1	1318	A
1	1	1319	G
1	1	1321	G
1	1	1325	U
1	1	1331	U
1	1	1332	A
1	1	1337	A
1	1	1338	C
1	1	1340	G
1	1	1341	U
1	1	1348	U
1	1	1349	G
1	1	1350	A
1	1	1351	U
1	1	1352	A
1	1	1354	G
1	1	1355	A
1	1	1356	U
1	1	1357	G
1	1	1362	G
1	1	1364	C
1	1	1370	G
1	1	1374	G
1	1	1375	G
1	1	1386	A
1	1	1390	A
1	1	1391	C
1	1	1392	G
1	1	1394	A
1	1	1397	C
1	1	1399	A
1	1	1400	G
1	1	1406	A
1	1	1411	C
1	1	1416	C
1	1	1418	A
1	1	1419	A
1	1	1425	U
1	1	1434	G

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Mol	Chain	Res	Type
1	1	1437	C
1	1	1441	G
1	1	1442	U
1	1	1446	A
1	1	1450	G
1	1	1452	A
1	1	1455	U
1	1	1456	A
1	1	1460	A
1	1	1466	G
1	1	1469	C
1	1	1470	U
1	1	1482	A
1	1	1483	G
1	1	1484	U
1	1	1485	G
1	1	1490	A
1	1	1491	A
1	1	1496	C
1	1	1502	C
1	1	1507	G
1	1	1508	C
1	1	1511	U
1	1	1512	U
1	1	1523	U
1	1	1526	U
1	1	1533	U
1	1	1536	G
1	1	1546	A
1	1	1551	C
1	1	1554	U
1	1	1556	C
1	1	1557	A
1	1	1558	A
1	1	1559	A
1	1	1560	G
1	1	1562	C
1	1	1564	U
1	1	1565	G
1	1	1568	U
1	1	1569	U
1	1	1570	U

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Mol	Chain	Res	Type
1	1	1571	A
1	1	1572	U
1	1	1574	C
1	1	1576	G
1	1	1579	C
1	1	1580	A
1	1	1581	C
1	1	1583	A
1	1	1584	U
1	1	1587	A
1	1	1588	A
1	1	1589	A
1	1	1593	A
1	1	1596	C
1	1	1605	A
1	1	1606	U
1	1	1607	U
1	1	1613	A
1	1	1621	A
1	1	1629	U
1	1	1632	A
1	1	1633	C
1	1	1642	A
1	1	1643	A
1	1	1645	U
1	1	1647	A
1	1	1654	A
1	1	1656	A
1	1	1657	C
1	1	1666	G
1	1	1671	C
1	1	1678	G
1	1	1680	G
1	1	1683	A
1	1	1702	U
1	1	1703	U
1	1	1711	C
1	1	1713	G
1	1	1715	A
1	1	1717	U
1	1	1718	G
1	1	1724	U

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Mol	Chain	Res	Type
1	1	1728	G
1	1	1730	G
1	1	1735	G
1	1	1736	G
1	1	1738	C
1	1	1739	U
1	1	1740	U
1	1	1748	G
1	1	1749	A
1	1	1750	A
1	1	1751	G
1	1	1752	A
1	1	1754	G
1	1	1756	C
1	1	1760	A
1	1	1761	C
1	1	1764	U
1	1	1765	U
1	1	1767	C
1	1	1770	G
1	1	1773	C
1	1	1775	G
1	1	1776	G
1	1	1777	U
1	1	1779	C
1	1	1780	G
1	1	1784	G
1	1	1788	C
1	1	1793	C
1	1	1795	U
1	1	1797	A
1	1	1813	A
1	1	1815	U
1	1	1816	A
1	1	1820	U
1	1	1821	U
1	1	1824	U
1	1	1838	G
1	1	1840	U
1	1	1841	A
1	1	1842	A
1	1	1846	C

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Mol	Chain	Res	Type
1	1	1847	A
1	1	1850	A
1	1	1851	G
1	1	1855	U
1	1	1863	G
1	1	1864	A
1	1	1866	C
1	1	1868	G
1	1	1877	U
1	1	1878	G
1	1	1879	A
1	1	1880	U
1	1	1885	U
1	1	1886	A
1	1	1892	G
1	1	1895	A
1	1	1896	A
1	1	1900	A
1	1	1905	G
1	1	1906	G
1	1	1912	U
1	1	1916	U
1	1	1920	U
1	1	1922	A
1	1	1926	C
1	1	1930	A
1	1	1931	U
1	1	1932	A
1	1	1933	A
1	1	1934	G
1	1	1935	G
1	1	1948	G
1	1	1953	G
1	1	1954	G
1	1	1955	U
1	1	2095	G
1	1	2099	A
1	1	2100	A
1	1	2101	C
1	1	2102	U
1	1	2107	A
1	1	2110	G

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Mol	Chain	Res	Type
1	1	2111	G
1	1	2112	U
1	1	2114	C
1	1	2115	G
1	1	2116	G
1	1	2117	A
1	1	2122	G
1	1	2123	G
1	1	2131	A
1	1	2138	A
1	1	2139	A
1	1	2140	U
1	1	2142	A
1	1	2145	A
1	1	2148	U
1	1	2158	A
1	1	2159	U
1	1	2166	A
1	1	2169	G
1	1	2170	U
1	1	2175	U
1	1	2176	U
1	1	2180	G
1	1	2182	A
1	1	2184	U
1	1	2188	A
1	1	2192	C
1	1	2194	G
1	1	2205	U
1	1	2207	A
1	1	2209	U
1	1	2210	G
1	1	2213	A
1	1	2215	A
1	1	2221	G
1	1	2222	A
1	1	2223	A
1	1	2225	U
1	1	2231	C
1	1	2243	A
1	1	2246	G
1	1	2249	G

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Mol	Chain	Res	Type
1	1	2256	A
1	1	2257	C
1	1	2265	C
1	1	2269	U
1	1	2270	A
1	1	2271	A
1	1	2273	G
1	1	2274	U
1	1	2281	A
1	1	2282	U
1	1	2283	G
1	1	2284	C
1	1	2285	C
1	1	2286	U
1	1	2287	C
1	1	2298	U
1	1	2299	A
1	1	2301	U
1	1	2304	C
1	1	2305	G
1	1	2306	C
1	1	2307	G
1	1	2308	C
1	1	2309	A
1	1	2310	U
1	1	2313	A
1	1	2315	G
1	1	2318	U
1	1	2324	A
1	1	2334	U
1	1	2335	G
1	1	2336	U
1	1	2339	C
1	1	2347	U
1	1	2350	C
1	1	2352	A
1	1	2359	C
1	1	2372	A
1	1	2374	C
1	1	2375	G
1	1	2386	A
1	1	2391	G

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Mol	Chain	Res	Type
1	1	2393	G
1	1	2397	A
1	1	2398	A
1	1	2401	A
1	1	2402	A
1	1	2403	G
1	1	2404	A
1	1	2410	U
1	1	2411	U
1	1	2418	G
1	1	2419	A
1	1	2435	G
1	1	2446	U
1	1	2448	G
1	1	2452	G
1	1	2453	U
1	1	2455	U
1	1	2456	A
1	1	2458	A
1	1	2459	A
1	1	2460	U
1	1	2461	A
1	1	2462	A
1	1	2463	G
1	1	2467	G
1	1	2468	A
1	1	2474	G
1	1	2475	G
1	1	2476	C
1	1	2477	G
1	1	2478	C
1	1	2479	C
1	1	2482	U
1	1	2486	A
1	1	2487	U
1	1	2488	A
1	1	2489	C
1	1	2490	C
1	1	2491	A
1	1	2492	C
1	1	2494	A
1	1	2496	C

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Mol	Chain	Res	Type
1	1	2497	U
1	1	2498	U
1	1	2499	U
1	1	2502	A
1	1	2505	U
1	1	2506	U
1	1	2507	C
1	1	2508	U
1	1	2509	U
1	1	2510	U
1	1	2512	C
1	1	2514	U
1	1	2522	G
1	1	2523	A
1	1	2529	A
1	1	2530	G
1	1	2532	U
1	1	2536	A
1	1	2537	U
1	1	2538	U
1	1	2539	C
1	1	2540	A
1	1	2541	U
1	1	2542	U
1	1	2543	U
1	1	2544	U
1	1	2547	A
1	1	2548	C
1	1	2549	G
1	1	2550	U
1	1	2552	C
1	1	2553	U
1	1	2555	G
1	1	2557	A
1	1	2558	U
1	1	2559	U
1	1	2560	C
1	1	2561	A
1	1	2566	C
1	1	2569	A
1	1	2570	U
1	1	2571	U

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Mol	Chain	Res	Type
1	1	2572	C
1	1	2575	G
1	1	2585	G
1	1	2587	U
1	1	2588	U
1	1	2589	G
1	1	2590	A
1	1	2593	A
1	1	2602	G
1	1	2606	G
1	1	2607	G
1	1	2608	G
1	1	2612	U
1	1	2614	G
1	1	2615	G
1	1	2620	G
1	1	2626	A
1	1	2635	A
1	1	2652	U
1	1	2656	A
1	1	2657	A
1	1	2663	G
1	1	2668	U
1	1	2672	G
1	1	2674	A
1	1	2676	A
1	1	2677	G
1	1	2678	A
1	1	2681	U
1	1	2684	C
1	1	2688	U
1	1	2689	A
1	1	2690	G
1	1	2691	A
1	1	2693	C
1	1	2696	A
1	1	2704	A
1	1	2705	A
1	1	2707	C
1	1	2714	G
1	1	2719	U
1	1	2728	G

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Mol	Chain	Res	Type
1	1	2729	U
1	1	2731	U
1	1	2732	G
1	1	2737	C
1	1	2740	A
1	1	2743	A
1	1	2746	A
1	1	2749	G
1	1	2753	G
1	1	2762	A
1	1	2771	U
1	1	2772	C
1	1	2773	C
1	1	2776	C
1	1	2777	G
1	1	2778	G
1	1	2779	A
1	1	2780	A
1	1	2781	U
1	1	2787	G
1	1	2791	G
1	1	2794	G
1	1	2795	U
1	1	2796	G
1	1	2798	C
1	1	2799	A
1	1	2800	G
1	1	2801	A
1	1	2803	A
1	1	2808	A
1	1	2810	C
1	1	2816	G
1	1	2817	A
1	1	2819	A
1	1	2821	C
1	1	2827	U
1	1	2830	G
1	1	2831	G
1	1	2834	G
1	1	2843	U
1	1	2844	C
1	1	2845	A

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Mol	Chain	Res	Type
1	1	2847	A
1	1	2850	G
1	1	2856	G
1	1	2857	C
1	1	2860	U
1	1	2861	U
1	1	2863	G
1	1	2867	C
1	1	2869	U
1	1	2870	C
1	1	2871	G
1	1	2872	A
1	1	2873	U
1	1	2886	U
1	1	2887	A
1	1	2888	U
1	1	2889	C
1	1	2899	C
1	1	2900	A
1	1	2903	A
1	1	2904	U
1	1	2907	G
1	1	2911	A
1	1	2914	G
1	1	2918	G
1	1	2922	G
1	1	2923	U
1	1	2925	C
1	1	2930	A
1	1	2935	U
1	1	2936	A
1	1	2938	G
1	1	2941	A
1	1	2942	C
1	1	2947	G
1	1	2952	G
1	1	2953	U
1	1	2954	U
1	1	2955	U
1	1	2971	A
1	1	2982	A
1	1	2983	C

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Mol	Chain	Res	Type
1	1	2984	C
1	1	2990	G
1	1	2995	A
1	1	2996	U
1	1	2997	G
1	1	3003	G
1	1	3011	A
1	1	3012	A
1	1	3021	A
1	1	3023	U
1	1	3032	A
1	1	3033	A
1	1	3036	G
1	1	3046	A
1	1	3049	A
1	1	3055	U
1	1	3058	U
1	1	3070	A
1	1	3077	A
1	1	3079	U
1	1	3080	G
1	1	3086	A
1	1	3090	U
1	1	3092	C
1	1	3101	G
1	1	3104	U
1	1	3106	A
1	1	3117	C
1	1	3118	C
1	1	3122	A
1	1	3125	U
1	1	3127	A
1	1	3128	G
1	1	3131	U
1	1	3136	G
1	1	3142	A
1	1	3143	C
1	1	3151	U
1	1	3153	U
1	1	3154	C
1	1	3155	U
1	1	3156	U

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Mol	Chain	Res	Type
1	1	3157	U
1	1	3158	G
1	1	3160	U
1	1	3164	C
1	1	3167	A
1	1	3168	A
1	1	3169	U
1	1	3170	A
1	1	3172	A
1	1	3173	G
1	1	3175	U
1	1	3176	G
1	1	3177	G
1	1	3179	U
1	1	3181	C
1	1	3182	G
1	1	3184	A
1	1	3185	U
1	1	3186	A
1	1	3187	A
1	1	3188	G
1	1	3194	C
1	1	3195	U
1	1	3196	U
1	1	3202	G
1	1	3206	C
1	1	3207	U
1	1	3210	A
1	1	3213	A
1	1	3214	U
1	1	3215	A
1	1	3217	C
1	1	3218	A
1	1	3219	G
1	1	3222	U
1	1	3223	A
1	1	3224	G
1	1	3227	A
1	1	3228	C
1	1	3236	U
1	1	3237	U
1	1	3239	G

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Mol	Chain	Res	Type
1	1	3240	C
1	1	3243	A
1	1	3244	A
1	1	3245	A
1	1	3253	G
1	1	3260	G
1	1	3263	G
1	1	3269	U
1	1	3270	U
1	1	3271	G
1	1	3273	A
1	1	3276	G
1	1	3278	C
1	1	3281	U
1	1	3285	C
1	1	3289	G
1	1	3290	G
1	1	3294	A
1	1	3304	U
1	1	3306	U
1	1	3317	U
1	1	3319	U
1	1	3322	A
1	1	3330	A
1	1	3337	G
1	1	3339	A
1	1	3341	U
1	1	3345	G
1	1	3348	G
1	1	3350	C
1	1	3351	U
1	1	3352	U
1	1	3353	G
1	1	3354	U
1	1	3356	G
1	1	3363	U
1	1	3366	G
1	1	3368	U
1	1	3369	G
1	1	3370	A
1	1	3371	G
1	1	3375	A

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Mol	Chain	Res	Type
1	1	3377	G
1	1	3378	C
1	1	3382	U
1	1	3384	U
1	1	3385	U
1	1	3389	U
1	1	3390	G
1	1	3391	A
1	1	3396	U
2	3	7	G
2	3	10	C
2	3	11	A
2	3	13	A
2	3	17	A
2	3	19	C
2	3	29	C
2	3	32	U
2	3	38	U
2	3	41	G
2	3	44	C
2	3	52	G
2	3	53	U
2	3	54	U
2	3	55	A
2	3	65	G
2	3	69	C
2	3	70	U
2	3	73	C
2	3	74	C
2	3	76	A
2	3	77	G
2	3	89	G
2	3	93	C
2	3	112	G
2	3	113	C
2	3	117	A
2	3	121	U
3	4	2	A
3	4	8	C
3	4	9	A
3	4	17	A
3	4	34	U

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Mol	Chain	Res	Type
3	4	35	C
3	4	39	G
3	4	50	C
3	4	51	G
3	4	52	A
3	4	59	A
3	4	62	C
3	4	63	G
3	4	73	U
3	4	75	G
3	4	79	A
3	4	80	A
3	4	81	U
3	4	82	U
3	4	84	C
3	4	85	G
3	4	86	U
3	4	87	G
3	4	88	A
3	4	90	U
3	4	95	G
3	4	97	A
3	4	104	A
3	4	106	C
3	4	111	A
3	4	112	U
3	4	113	U
3	4	115	C
3	4	121	U
3	4	124	G
3	4	125	U
3	4	126	A
3	4	127	U
3	4	129	C
3	4	134	G
3	4	136	G
3	4	138	A
3	4	148	G
3	4	149	A
3	4	150	G
3	4	151	C
3	4	152	G

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Mol	Chain	Res	Type
47	2	2	A
47	2	3	U
47	2	4	C
47	2	8	U
47	2	9	U
47	2	11	A
47	2	14	C
47	2	15	U
47	2	25	C
47	2	26	A
47	2	37	U
47	2	38	C
47	2	39	A
47	2	40	A
47	2	42	G
47	2	43	A
47	2	47	A
47	2	48	G
47	2	50	C
47	2	54	C
47	2	55	A
47	2	57	G
47	2	59	C
47	2	61	A
47	2	63	G
47	2	65	A
47	2	66	U
47	2	67	A
47	2	68	A
47	2	69	G
47	2	71	A
47	2	72	A
47	2	73	U
47	2	74	U
47	2	75	U
47	2	76	A
47	2	77	U
47	2	79	C
47	2	81	G
47	2	82	U
47	2	83	G
47	2	85	A

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Mol	Chain	Res	Type
47	2	87	C
47	2	90	C
47	2	95	G
47	2	100	A
47	2	102	U
47	2	104	A
47	2	111	U
47	2	114	C
47	2	116	U
47	2	117	U
47	2	118	U
47	2	119	A
47	2	120	U
47	2	124	A
47	2	126	A
47	2	127	G
47	2	128	U
47	2	129	U
47	2	130	C
47	2	131	C
47	2	132	U
47	2	133	U
47	2	134	U
47	2	135	A
47	2	136	C
47	2	137	U
47	2	138	A
47	2	139	C
47	2	140	A
47	2	141	U
47	2	145	A
47	2	153	G
47	2	154	G
47	2	159	U
47	2	160	C
47	2	161	U
47	2	168	A
47	2	169	A
47	2	170	U
47	2	174	U
47	2	176	C
47	2	178	U

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Mol	Chain	Res	Type
47	2	179	A
47	2	183	U
47	2	185	U
47	2	190	C
47	2	191	C
47	2	192	U
47	2	193	U
47	2	200	A
47	2	202	A
47	2	204	G
47	2	207	U
47	2	209	U
47	2	215	A
47	2	217	A
47	2	218	A
47	2	221	A
47	2	224	C
47	2	225	A
47	2	226	A
47	2	227	U
47	2	228	G
47	2	230	C
47	2	232	U
47	2	233	C
47	2	234	G
47	2	235	G
47	2	238	U
47	2	239	C
47	2	240	U
47	2	244	A
47	2	245	U
47	2	246	G
47	2	248	U
47	2	250	C
47	2	256	A
47	2	260	U
47	2	261	U
47	2	262	U
47	2	266	A
47	2	270	C
47	2	272	U
47	2	274	G

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Mol	Chain	Res	Type
47	2	275	C
47	2	276	C
47	2	277	U
47	2	278	U
47	2	279	G
47	2	280	U
47	2	281	G
47	2	287	G
47	2	288	A
47	2	289	U
47	2	291	G
47	2	292	U
47	2	295	A
47	2	299	A
47	2	300	A
47	2	302	U
47	2	306	U
47	2	309	C
47	2	312	A
47	2	313	U
47	2	314	C
47	2	315	A
47	2	316	A
47	2	318	U
47	2	321	C
47	2	322	G
47	2	330	G
47	2	333	A
47	2	334	G
47	2	337	G
47	2	338	C
47	2	339	C
47	2	345	U
47	2	351	C
47	2	352	A
47	2	359	A
47	2	361	C
47	2	365	G
47	2	366	A
47	2	370	A
47	2	373	G
47	2	379	U

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Mol	Chain	Res	Type
47	2	380	U
47	2	388	G
47	2	389	G
47	2	390	G
47	2	393	C
47	2	394	C
47	2	400	A
47	2	401	A
47	2	402	C
47	2	404	G
47	2	412	A
47	2	413	U
47	2	416	A
47	2	417	A
47	2	419	G
47	2	420	A
47	2	422	G
47	2	423	G
47	2	424	C
47	2	425	A
47	2	426	G
47	2	429	G
47	2	430	G
47	2	432	G
47	2	433	C
47	2	434	G
47	2	435	C
47	2	437	A
47	2	438	A
47	2	439	U
47	2	440	U
47	2	441	A
47	2	444	C
47	2	445	A
47	2	447	U
47	2	452	A
47	2	453	U
47	2	454	U
47	2	455	C
47	2	460	A
47	2	463	U
47	2	464	A

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Mol	Chain	Res	Type
47	2	466	U
47	2	468	A
47	2	469	C
47	2	473	A
47	2	475	A
47	2	477	A
47	2	478	A
47	2	479	C
47	2	486	G
47	2	488	G
47	2	489	C
47	2	491	C
47	2	494	U
47	2	495	C
47	2	496	G
47	2	499	U
47	2	500	C
47	2	506	A
47	2	507	U
47	2	509	G
47	2	511	A
47	2	515	A
47	2	516	G
47	2	522	U
47	2	525	A
47	2	532	U
47	2	534	A
47	2	538	A
47	2	539	G
47	2	540	G
47	2	541	A
47	2	542	A
47	2	543	C
47	2	545	A
47	2	546	U
47	2	548	G
47	2	552	G
47	2	554	C
47	2	557	G
47	2	558	U
47	2	565	C
47	2	566	C

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Mol	Chain	Res	Type
47	2	567	A
47	2	568	G
47	2	572	C
47	2	578	U
47	2	579	A
47	2	580	A
47	2	582	U
47	2	583	C
47	2	592	A
47	2	594	A
47	2	595	G
47	2	597	G
47	2	606	A
47	2	610	G
47	2	611	U
47	2	619	A
47	2	620	A
47	2	623	A
47	2	624	G
47	2	630	A
47	2	635	A
47	2	637	C
47	2	639	U
47	2	640	U
47	2	653	C
47	2	654	C
47	2	655	G
47	2	656	G
47	2	657	U
47	2	658	C
47	2	677	G
47	2	679	U
47	2	680	U
47	2	681	U
47	2	686	C
47	2	687	G
47	2	692	C
47	2	693	U
47	2	695	U
47	2	696	C
47	2	697	C
47	2	698	U

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Mol	Chain	Res	Type
47	2	699	U
47	2	700	C
47	2	702	G
47	2	705	U
47	2	706	A
47	2	707	A
47	2	709	C
47	2	710	U
47	2	711	U
47	2	712	G
47	2	713	A
47	2	715	U
47	2	718	U
47	2	719	U
47	2	720	G
47	2	721	U
47	2	722	G
47	2	723	G
47	2	725	U
47	2	727	U
47	2	728	U
47	2	729	G
47	2	731	C
47	2	732	G
47	2	733	A
47	2	734	A
47	2	735	C
47	2	738	G
47	2	741	C
47	2	742	U
47	2	743	U
47	2	744	U
47	2	757	A
47	2	760	A
47	2	765	G
47	2	766	U
47	2	767	U
47	2	768	C
47	2	775	G
47	2	777	C
47	2	778	G
47	2	779	U

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Mol	Chain	Res	Type
47	2	780	A
47	2	781	U
47	2	783	G
47	2	784	C
47	2	789	A
47	2	793	A
47	2	794	U
47	2	795	U
47	2	799	A
47	2	801	G
47	2	806	A
47	2	810	G
47	2	811	A
47	2	812	A
47	2	813	U
47	2	814	A
47	2	816	G
47	2	817	A
47	2	819	G
47	2	820	U
47	2	821	U
47	2	824	G
47	2	826	U
47	2	827	C
47	2	831	U
47	2	833	U
47	2	834	G
47	2	836	U
47	2	839	U
47	2	841	U
47	2	842	C
47	2	843	U
47	2	845	G
47	2	853	G
47	2	859	A
47	2	860	U
47	2	863	A
47	2	864	U
47	2	873	U
47	2	881	A
47	2	895	G
47	2	898	A

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Mol	Chain	Res	Type
47	2	903	U
47	2	904	G
47	2	905	A
47	2	906	A
47	2	909	U
47	2	911	U
47	2	913	G
47	2	916	U
47	2	919	A
47	2	921	U
47	2	922	G
47	2	923	A
47	2	924	A
47	2	928	U
47	2	931	C
47	2	932	U
47	2	933	A
47	2	934	C
47	2	935	U
47	2	944	A
47	2	951	A
47	2	960	U
47	2	964	U
47	2	966	A
47	2	980	G
47	2	981	U
47	2	986	G
47	2	990	C
47	2	992	A
47	2	993	A
47	2	1003	A
47	2	1004	U
47	2	1005	A
47	2	1010	C
47	2	1011	G
47	2	1014	G
47	2	1016	C
47	2	1020	A
47	2	1021	C
47	2	1022	C
47	2	1023	A
47	2	1025	A

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Mol	Chain	Res	Type
47	2	1026	A
47	2	1027	A
47	2	1028	C
47	2	1030	A
47	2	1031	U
47	2	1032	G
47	2	1036	A
47	2	1040	G
47	2	1043	A
47	2	1052	U
47	2	1053	G
47	2	1056	U
47	2	1071	U
47	2	1076	A
47	2	1080	U
47	2	1082	C
47	2	1083	G
47	2	1091	A
47	2	1092	A
47	2	1097	U
47	2	1098	U
47	2	1099	U
47	2	1100	G
47	2	1108	G
47	2	1109	G
47	2	1110	G
47	2	1113	A
47	2	1117	U
47	2	1118	G
47	2	1125	A
47	2	1137	A
47	2	1138	A
47	2	1139	A
47	2	1140	G
47	2	1147	A
47	2	1149	G
47	2	1150	G
47	2	1153	G
47	2	1154	G
47	2	1155	G
47	2	1157	A
47	2	1158	C

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Mol	Chain	Res	Type
47	2	1159	C
47	2	1160	A
47	2	1162	C
47	2	1163	A
47	2	1164	G
47	2	1165	G
47	2	1166	A
47	2	1167	G
47	2	1168	U
47	2	1170	G
47	2	1171	A
47	2	1172	G
47	2	1174	C
47	2	1175	U
47	2	1179	G
47	2	1182	U
47	2	1183	A
47	2	1184	A
47	2	1185	U
47	2	1186	U
47	2	1189	A
47	2	1190	C
47	2	1192	C
47	2	1193	A
47	2	1194	A
47	2	1196	A
47	2	1199	G
47	2	1200	G
47	2	1201	G
47	2	1202	A
47	2	1203	A
47	2	1205	C
47	2	1207	C
47	2	1208	A
47	2	1209	C
47	2	1214	U
47	2	1216	C
47	2	1217	A
47	2	1219	A
47	2	1220	C
47	2	1222	C
47	2	1223	A

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Mol	Chain	Res	Type
47	2	1225	U
47	2	1226	A
47	2	1227	A
47	2	1228	G
47	2	1229	G
47	2	1230	A
47	2	1231	U
47	2	1232	U
47	2	1233	G
47	2	1234	A
47	2	1236	A
47	2	1237	G
47	2	1238	A
47	2	1239	U
47	2	1240	U
47	2	1241	G
47	2	1242	A
47	2	1243	G
47	2	1244	A
47	2	1245	G
47	2	1249	U
47	2	1250	U
47	2	1251	U
47	2	1252	C
47	2	1253	U
47	2	1255	G
47	2	1256	A
47	2	1258	U
47	2	1259	U
47	2	1260	U
47	2	1262	U
47	2	1263	G
47	2	1264	G
47	2	1266	U
47	2	1267	G
47	2	1270	G
47	2	1271	G
47	2	1273	G
47	2	1274	C
47	2	1275	A
47	2	1276	U
47	2	1284	C

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Mol	Chain	Res	Type
47	2	1285	U
47	2	1286	U
47	2	1287	A
47	2	1290	U
47	2	1293	U
47	2	1301	U
47	2	1306	C
47	2	1309	C
47	2	1312	A
47	2	1313	A
47	2	1314	U
47	2	1315	U
47	2	1320	U
47	2	1321	A
47	2	1326	A
47	2	1327	C
47	2	1328	G
47	2	1333	C
47	2	1335	U
47	2	1336	A
47	2	1339	C
47	2	1340	U
47	2	1341	A
47	2	1343	U
47	2	1344	A
47	2	1345	A
47	2	1346	A
47	2	1347	U
47	2	1348	A
47	2	1352	G
47	2	1353	U
47	2	1354	G
47	2	1355	C
47	2	1356	U
47	2	1360	A
47	2	1362	U
47	2	1363	U
47	2	1364	G
47	2	1367	G
47	2	1370	U
47	2	1371	A
47	2	1372	U

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Mol	Chain	Res	Type
47	2	1374	C
47	2	1380	U
47	2	1381	U
47	2	1382	A
47	2	1383	G
47	2	1384	A
47	2	1385	G
47	2	1386	G
47	2	1387	G
47	2	1388	A
47	2	1390	U
47	2	1391	A
47	2	1394	G
47	2	1395	G
47	2	1396	U
47	2	1398	U
47	2	1399	C
47	2	1400	A
47	2	1402	G
47	2	1406	A
47	2	1408	G
47	2	1409	G
47	2	1412	G
47	2	1413	U
47	2	1414	U
47	2	1415	U
47	2	1416	G
47	2	1419	G
47	2	1421	A
47	2	1425	A
47	2	1427	A
47	2	1428	G
47	2	1429	G
47	2	1432	U
47	2	1433	G
47	2	1434	U
47	2	1436	A
47	2	1439	C
47	2	1440	C
47	2	1443	U
47	2	1444	A
47	2	1445	G

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Mol	Chain	Res	Type
47	2	1446	A
47	2	1447	C
47	2	1448	G
47	2	1449	U
47	2	1450	U
47	2	1451	C
47	2	1454	G
47	2	1455	G
47	2	1456	C
47	2	1457	C
47	2	1458	G
47	2	1459	C
47	2	1460	A
47	2	1461	C
47	2	1466	G
47	2	1468	U
47	2	1471	A
47	2	1472	C
47	2	1473	U
47	2	1474	G
47	2	1482	C
47	2	1486	G
47	2	1487	A
47	2	1489	U
47	2	1490	C
47	2	1491	U
47	2	1492	A
47	2	1493	A
47	2	1506	G
47	2	1508	U
47	2	1509	C
47	2	1511	U
47	2	1515	A
47	2	1516	A
47	2	1517	U
47	2	1518	C
47	2	1523	G
47	2	1524	A
47	2	1525	A
47	2	1529	C
47	2	1531	G
47	2	1532	U

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Mol	Chain	Res	Type
47	2	1534	G
47	2	1535	U
47	2	1536	G
47	2	1537	C
47	2	1538	U
47	2	1539	G
47	2	1540	G
47	2	1542	G
47	2	1554	U
47	2	1555	A
47	2	1557	U
47	2	1559	A
47	2	1560	U
47	2	1562	G
47	2	1565	C
47	2	1567	U
47	2	1572	G
47	2	1573	A
47	2	1574	G
47	2	1575	G
47	2	1576	A
47	2	1577	A
47	2	1582	U
47	2	1583	A
47	2	1584	G
47	2	1587	A
47	2	1591	C
47	2	1601	G
47	2	1604	U
47	2	1605	G
47	2	1607	G
47	2	1608	U
47	2	1611	A
47	2	1616	G
47	2	1618	C
47	2	1619	C
47	2	1620	C
47	2	1624	C
47	2	1628	U
47	2	1631	A
47	2	1633	A
47	2	1634	C

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Mol	Chain	Res	Type
47	2	1635	A
47	2	1636	C
47	2	1638	G
47	2	1639	C
47	2	1646	C
47	2	1651	A
47	2	1654	G
47	2	1656	U
47	2	1657	U
47	2	1658	G
47	2	1664	C
47	2	1665	U
47	2	1666	U
47	2	1675	C
47	2	1678	A
47	2	1680	G
47	2	1681	A
47	2	1682	U
47	2	1684	U
47	2	1685	G
47	2	1688	U
47	2	1689	A
47	2	1693	A
47	2	1694	A
47	2	1697	G
47	2	1699	G
47	2	1700	C
47	2	1701	A
47	2	1702	A
47	2	1703	C
47	2	1704	U
47	2	1708	U
47	2	1709	C
47	2	1711	C
47	2	1712	A
47	2	1713	G
47	2	1714	A
47	2	1715	G
47	2	1717	G
47	2	1730	A
47	2	1731	A
47	2	1738	U

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Mol	Chain	Res	Type
47	2	1742	U
47	2	1747	G
47	2	1755	A
47	2	1756	A
47	2	1757	G
47	2	1760	G
47	2	1761	U
47	2	1762	A
47	2	1766	A
47	2	1767	G
47	2	1769	U
47	2	1770	U
47	2	1778	G
47	2	1780	G
47	2	1782	A
47	2	1783	C
47	2	1784	C
47	2	1787	C
47	2	1791	A
47	2	1792	G
47	2	1794	A
47	2	1796	C
47	2	1797	A
82	AY	8	U
82	AY	10	G
82	AY	11	C
82	AY	15	G
82	AY	18	G
82	AY	19	G
82	AY	20	G
82	AY	23	A
82	AY	25	C
82	AY	33	U
82	AY	38	A
82	AY	45	G
82	AY	46	G
82	AY	47	U
82	AY	48	C
82	AY	49	C
82	AY	50	U
82	AY	51	G
82	AY	55	U

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Mol	Chain	Res	Type
82	AY	57	G
82	AY	58	A
82	AY	59	U
82	AY	60	C
82	AY	61	C
82	AY	66	A
82	AY	68	U
82	AY	71	G
82	AY	74	C
82	AY	76	A
83	AZ	44	A
83	AZ	45	A
83	AZ	46	U
83	AZ	48	U
83	AZ	49	U

All (81) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	97	U
1	1	120	G
1	1	165	A
1	1	197	G
1	1	264	G
1	1	323	A
1	1	360	G
1	1	443	G
1	1	490	C
1	1	1015	U
1	1	1028	U
1	1	1079	A
1	1	1084	A
1	1	1128	U
1	1	1136	A
1	1	1197	A
1	1	1232	C
1	1	1405	U
1	1	1415	U
1	1	1620	U
1	1	1837	U
1	1	2270	A
1	1	2306	C

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Mol	Chain	Res	Type
1	1	2541	U
1	1	2587	U
1	1	2614	G
1	1	2706	G
1	1	2981	U
1	1	3105	U
1	1	3121	U
1	1	3156	U
1	1	3193	C
1	1	3218	A
2	3	18	C
2	3	52	G
2	3	72	A
3	4	7	U
3	4	39	G
3	4	72	A
3	4	114	G
3	4	133	G
47	2	1	U
47	2	36	C
47	2	118	U
47	2	132	U
47	2	144	U
47	2	206	A
47	2	217	A
47	2	333	A
47	2	387	A
47	2	388	G
47	2	393	C
47	2	403	G
47	2	431	C
47	2	541	A
47	2	697	C
47	2	698	U
47	2	706	A
47	2	728	U
47	2	740	A
47	2	767	U
47	2	1002	G
47	2	1039	A
47	2	1116	A
47	2	1138	A

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Mol	Chain	Res	Type
47	2	1181	U
47	2	1273	G
47	2	1347	U
47	2	1399	C
47	2	1444	A
47	2	1455	G
47	2	1481	C
47	2	1491	U
47	2	1632	C
47	2	1638	G
47	2	1680	G
47	2	1684	U
47	2	1707	A
47	2	1755	A
83	AZ	44	A
83	AZ	48	U

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

1 non-standard protein/DNA/RNA residue is 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
81	DDE	AX	699	81	14,20,21	1.95	3 (21%)	14,28,30	1.82	5 (35%)

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
81	DDE	AX	699	81	-	6/20/21/23	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	AX	699	DDE	CBI-NAD	5.57	1.46	1.32
81	AX	699	DDE	CAT-CE1	3.11	1.54	1.50
81	AX	699	DDE	OAG-CBI	-2.23	1.19	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	AX	699	DDE	CAC-NCB-CAB	3.78	118.43	108.10
81	AX	699	DDE	OAG-CBI-NAD	-2.91	117.94	123.00
81	AX	699	DDE	CBW-CBI-NAD	2.64	118.64	115.28
81	AX	699	DDE	OAG-CBI-CBW	2.31	123.41	120.49
81	AX	699	DDE	CG-ND1-CE1	2.07	109.17	103.05

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
81	AX	699	DDE	N-CA-CB-CG
81	AX	699	DDE	C-CA-CB-CG
81	AX	699	DDE	CAU-CAT-CE1-ND1
81	AX	699	DDE	CAT-CAU-CBW-CBI
81	AX	699	DDE	OAG-CBI-CBW-CAU
81	AX	699	DDE	CAU-CAT-CE1-NE2

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 9 ligands modelled in this entry, 8 are monoatomic - leaving 1 for Mogul analysis.

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
86	GCP	AX	901	-	27,34,34	1.05	3 (11%)	34,54,54	2.18	8 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	GCP	AX	901	-	-	5/15/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	AX	901	GCP	C6-N1	2.91	1.38	1.33
86	AX	901	GCP	PG-O1G	2.20	1.54	1.50
86	AX	901	GCP	PG-O3G	-2.11	1.50	1.54

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	AX	901	GCP	C5-C6-N1	-7.92	112.59	123.43
86	AX	901	GCP	C2-N1-C6	5.66	124.92	115.93
86	AX	901	GCP	O1B-PB-C3B	4.06	119.81	109.07
86	AX	901	GCP	N3-C2-N1	-3.06	123.14	127.22
86	AX	901	GCP	O1G-PG-C3B	-2.70	105.42	111.24
86	AX	901	GCP	O3G-PG-C3B	2.51	112.48	106.40
86	AX	901	GCP	C2-N3-C4	-2.42	112.59	115.36
86	AX	901	GCP	C4-C5-C6	-2.38	118.52	120.80

There are no chirality outliers.

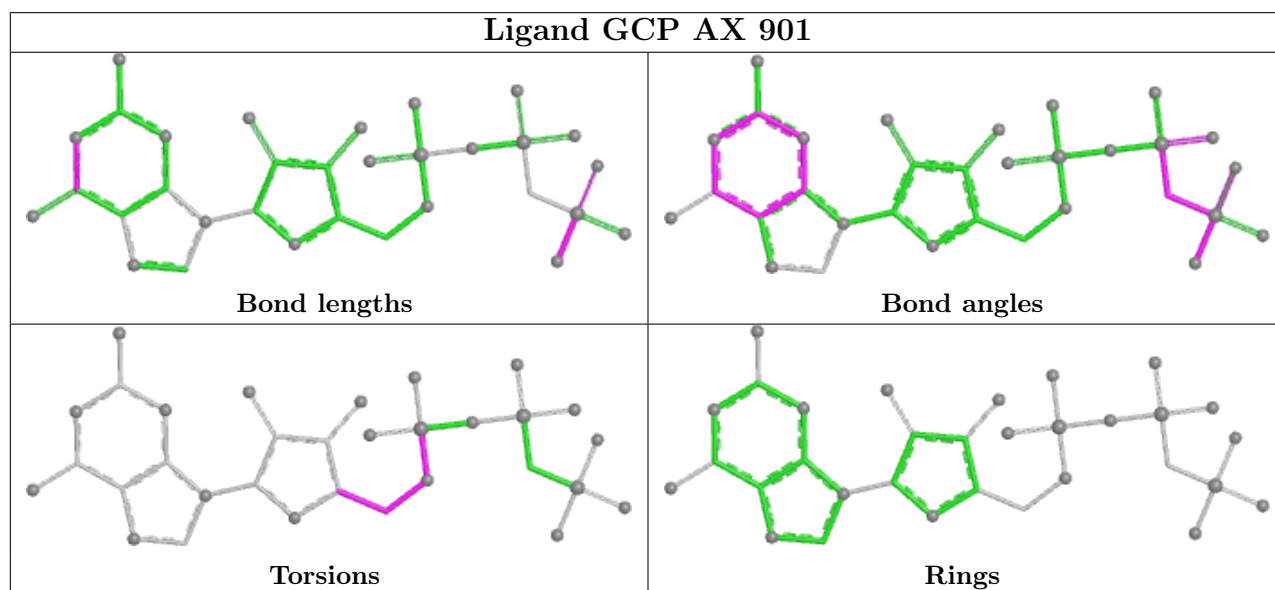
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
86	AX	901	GCP	C5'-O5'-PA-O1A
86	AX	901	GCP	C5'-O5'-PA-O2A
86	AX	901	GCP	C4'-C5'-O5'-PA
86	AX	901	GCP	C5'-O5'-PA-O3A
86	AX	901	GCP	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

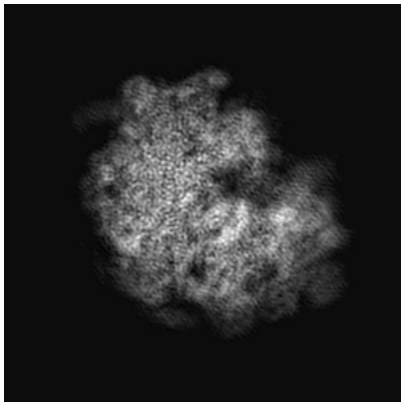
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0049. These allow visual inspection of the internal detail of the map and identification of artifacts.

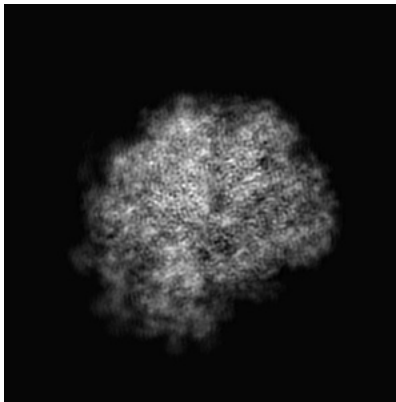
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

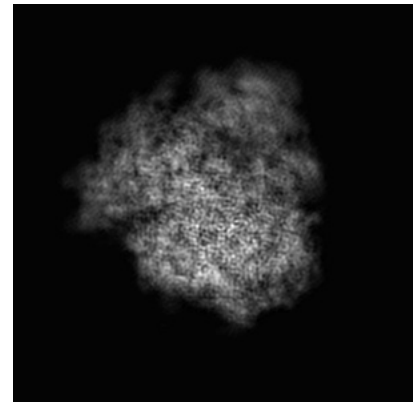
6.1.1 Primary map



X



Y

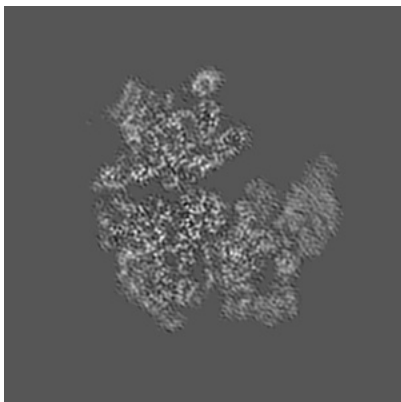


Z

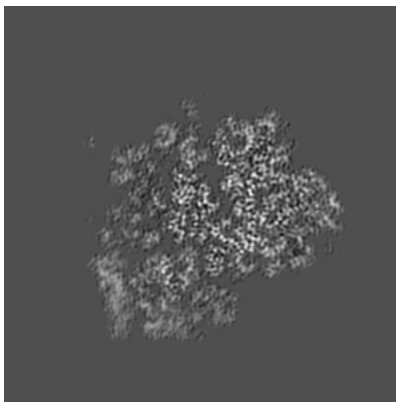
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

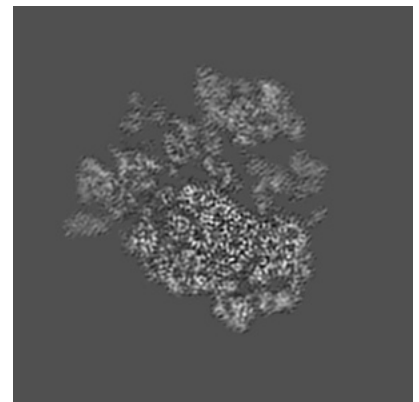
6.2.1 Primary map



X Index: 180



Y Index: 180

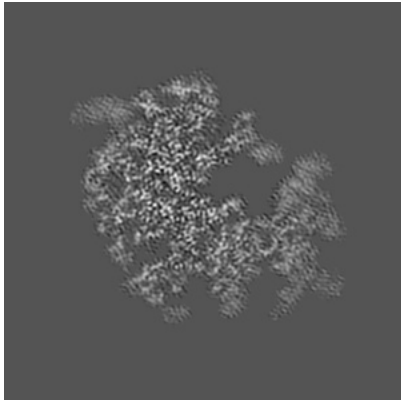


Z Index: 180

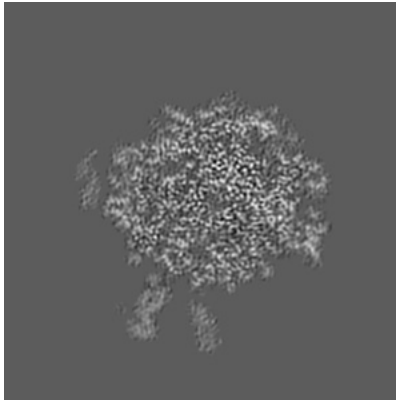
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

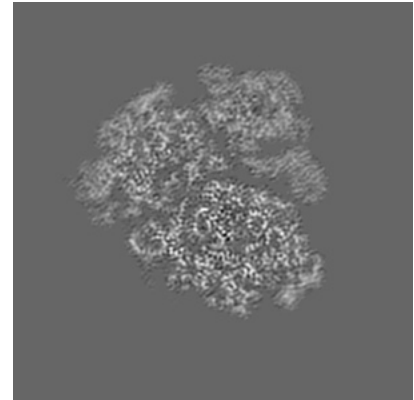
6.3.1 Primary map



X Index: 194



Y Index: 158

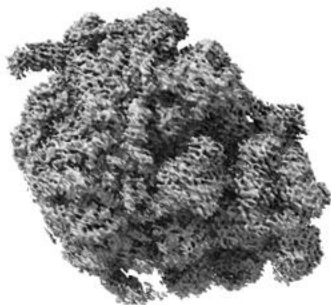


Z Index: 166

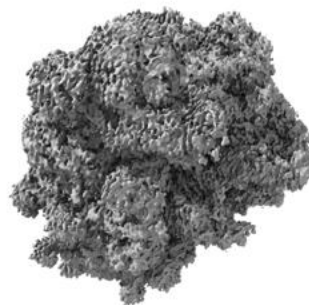
The images above show the largest variance slices of the map in three orthogonal directions.

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 0.033. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

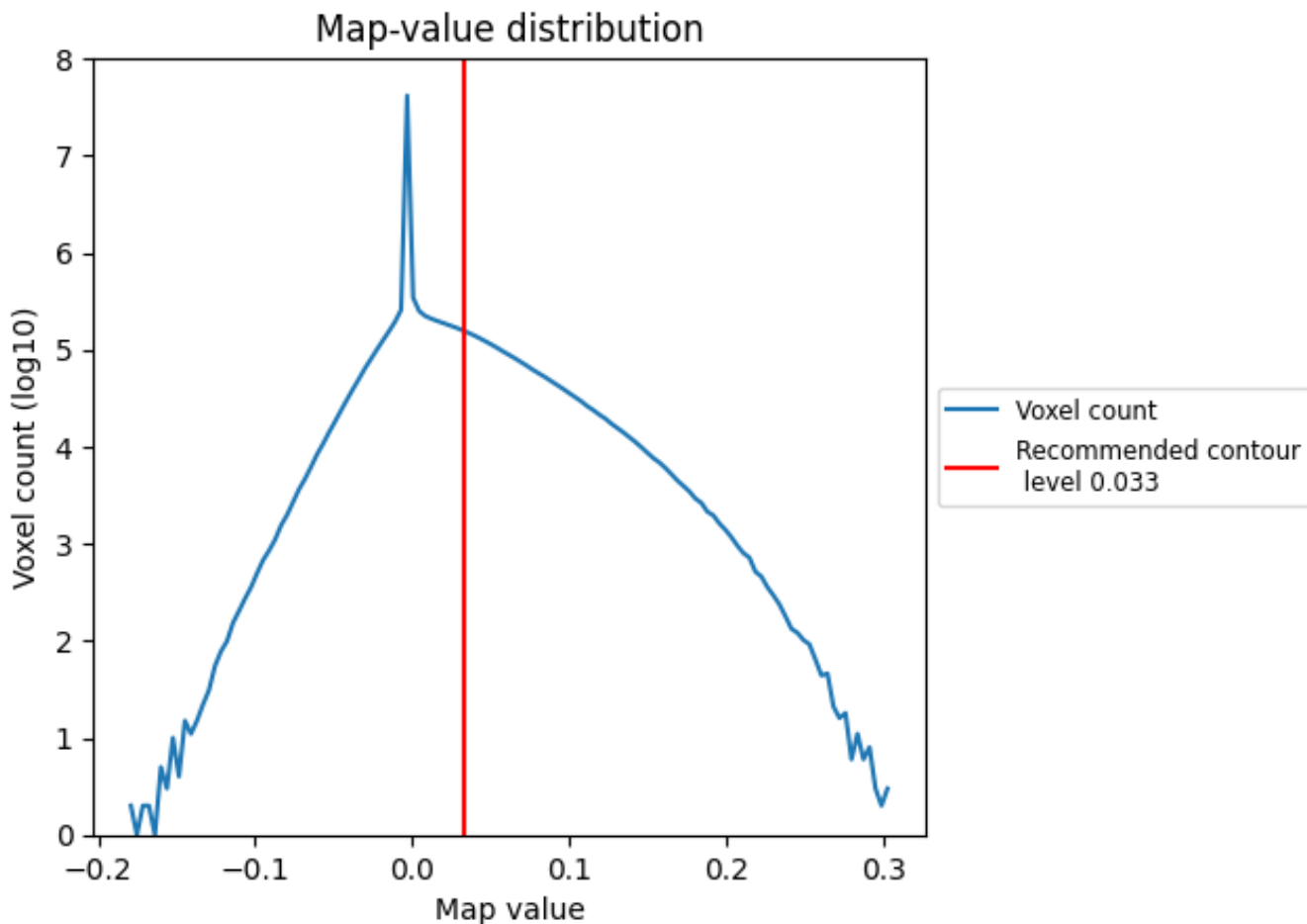
6.5 Mask visualisation

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

7 Map analysis [i](#)

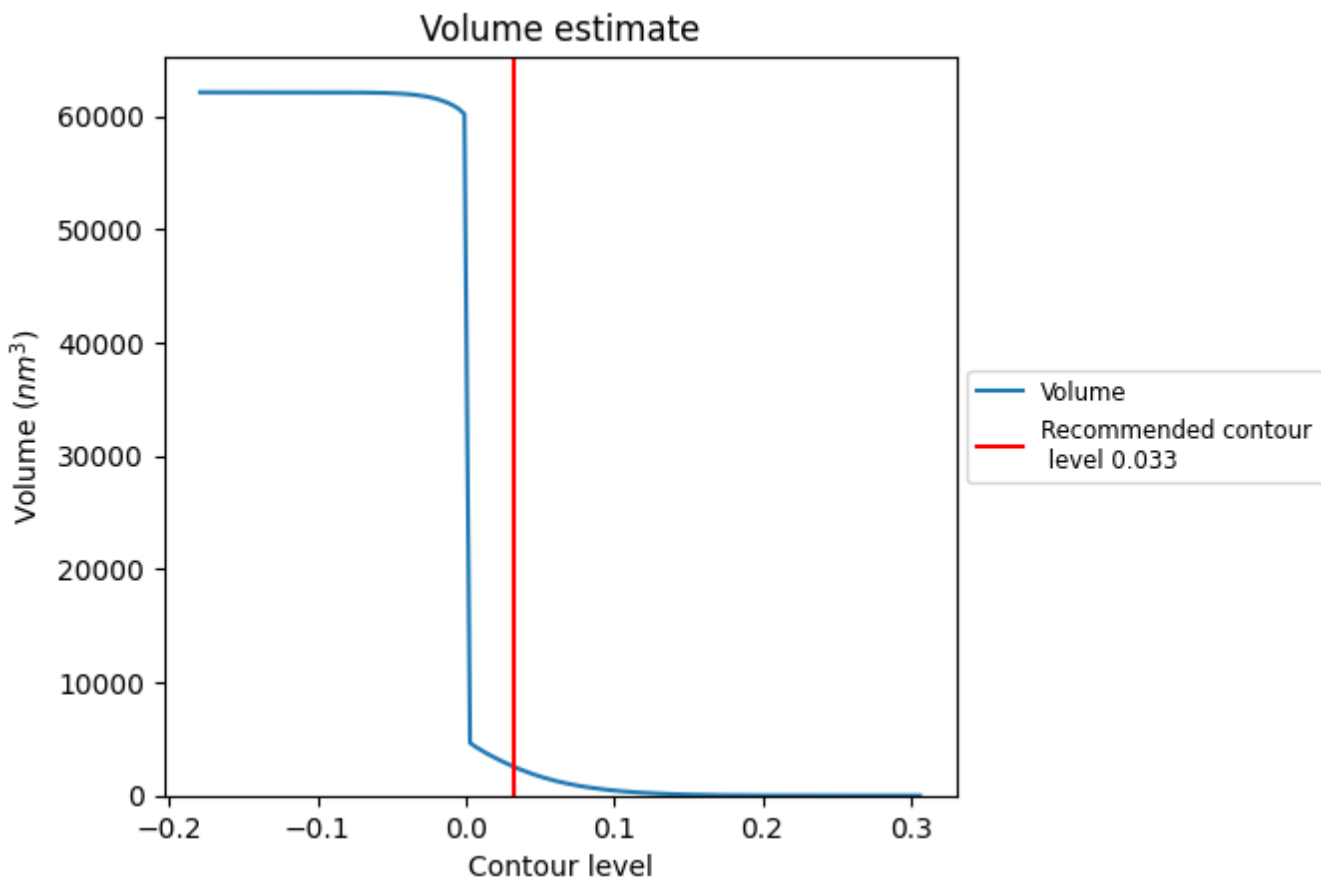
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

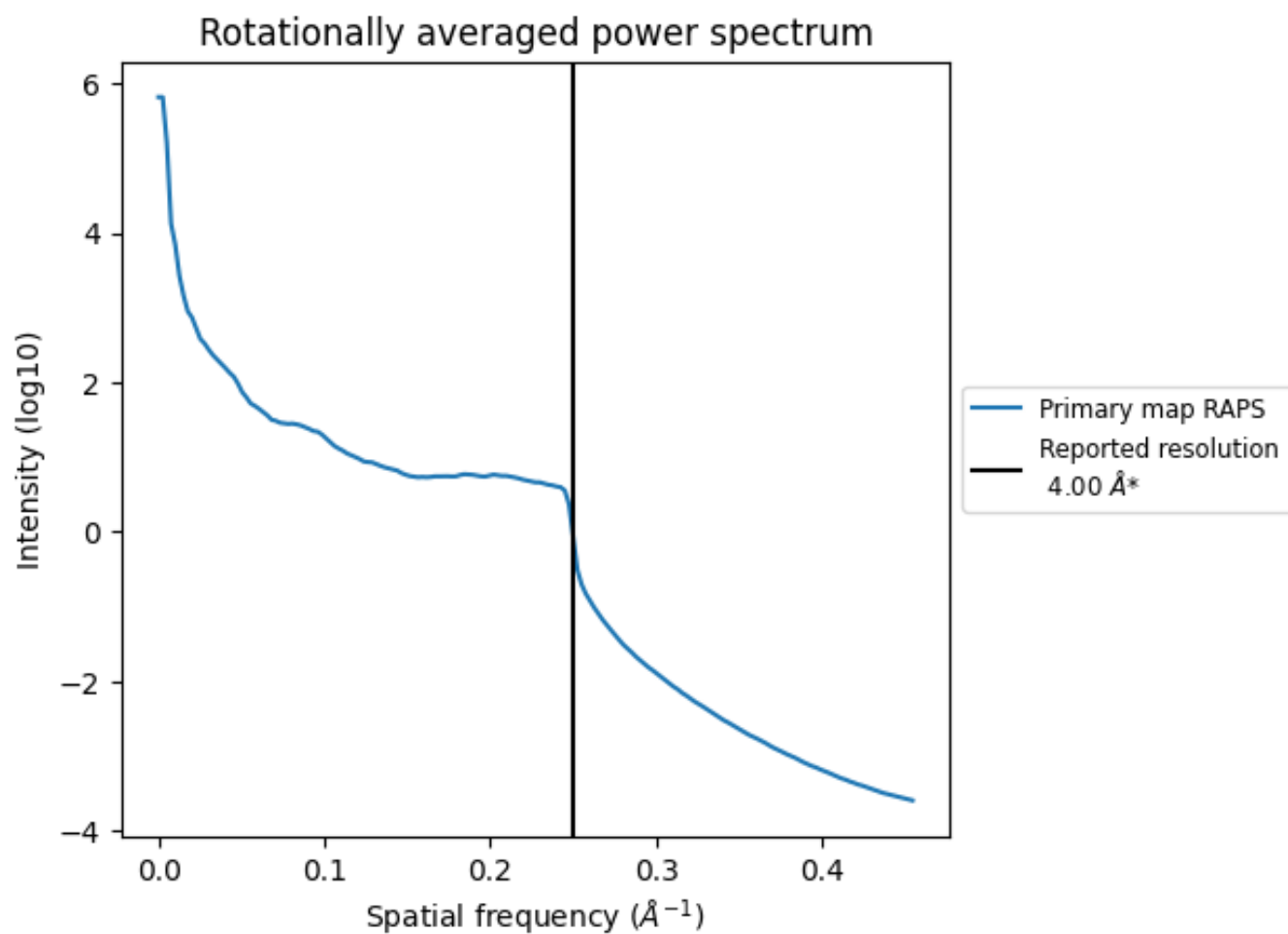
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2513 nm³; this corresponds to an approximate mass of 2270 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 0.250\AA^{-1}

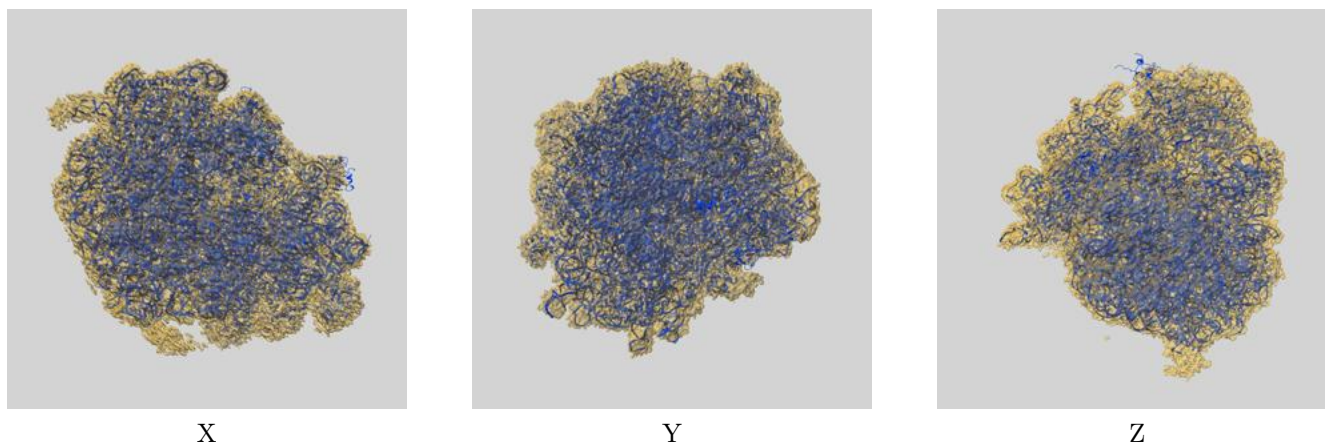
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

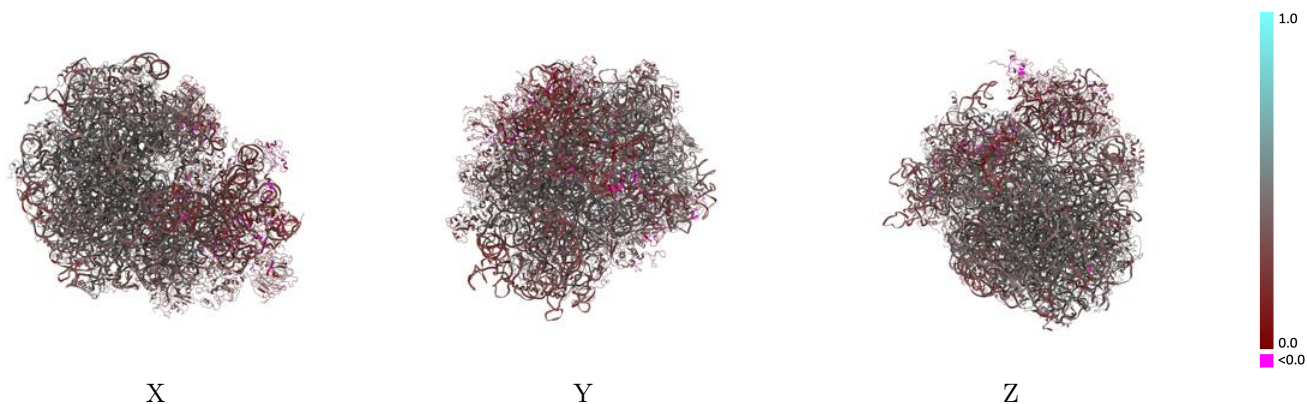
This section contains information regarding the fit between EMDB map EMD-0049 and PDB model 6GQV. Per-residue inclusion information can be found in section [3](#) on page [21](#).

9.1 Map-model overlay [i](#)



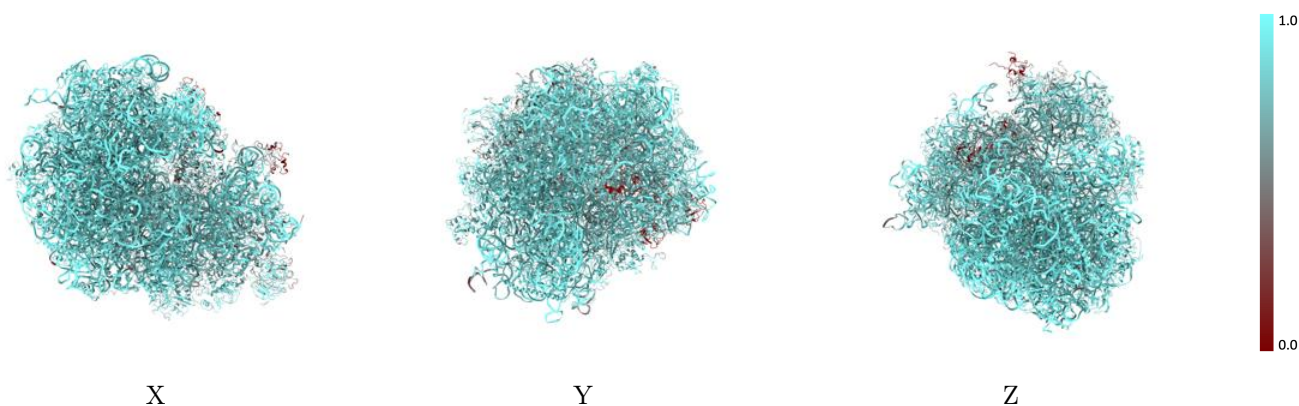
The images above show the 3D surface view of the map at the recommended contour level 0.033 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



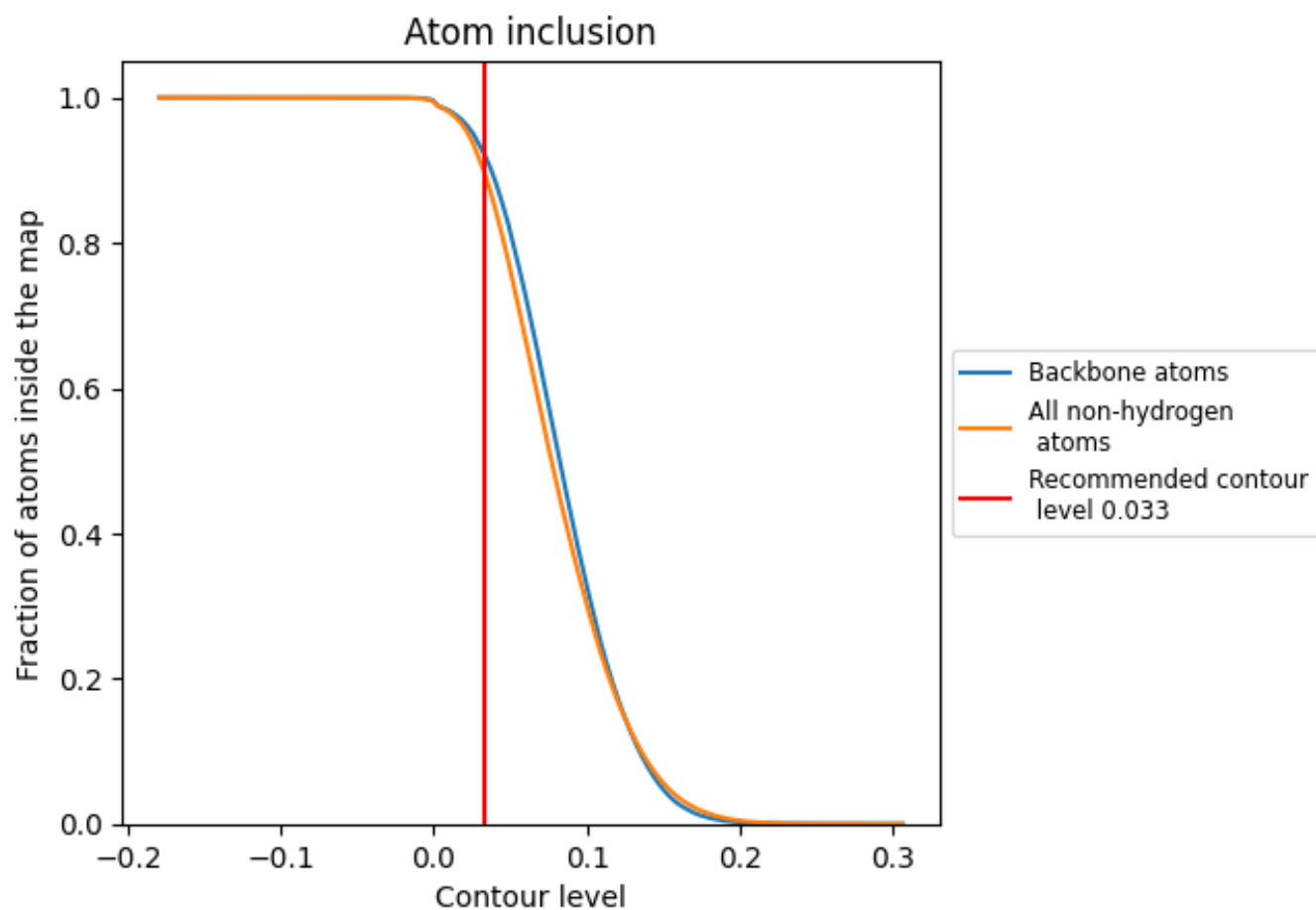
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.033).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 90% 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 (0.033) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8971	 0.3780
1	 0.9617	 0.4060
2	 0.9300	 0.3390
3	 0.9810	 0.3960
4	 0.9708	 0.4200
A	 0.8625	 0.4620
AA	 0.8668	 0.2720
AB	 0.7906	 0.3950
AC	 0.2455	 0.1250
AD	 0.8667	 0.3920
AE	 0.8886	 0.3890
AF	 0.8082	 0.2840
AG	 0.7618	 0.2500
AH	 0.7467	 0.2820
AI	 0.7790	 0.2900
AJ	 0.8076	 0.2680
AK	 0.6881	 0.2810
AL	 0.8283	 0.3480
AM	 0.8547	 0.4190
AN	 0.8108	 0.4140
AO	 0.8751	 0.3220
AP	 0.6252	 0.2320
AQ	 0.8554	 0.3750
AR	 0.8738	 0.3780
AS	 0.6373	 0.2470
AT	 0.8703	 0.3180
AU	 0.8105	 0.3710
AV	 0.7495	 0.2590
AW	 0.6643	 0.2630
AX	 0.7636	 0.3440
AY	 0.8383	 0.2940
AZ	 0.4444	 0.3240
B	 0.8997	 0.4470
BA	 0.6631	 0.2530
C	 0.9278	 0.4430



















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Chain	Atom inclusion	Q-score
D	 0.9010	 0.3750
E	 0.9093	 0.4020
F	 0.9024	 0.4280
G	 0.9018	 0.4100
H	 0.8785	 0.4080
I	 0.8959	 0.4300
J	 0.8662	 0.3700
L	 0.9233	 0.4270
M	 0.9103	 0.4030
N	 0.9071	 0.4580
O	 0.8996	 0.4250
P	 0.8983	 0.4500
P0	 0.2763	 0.1750
P2	 0.3047	 0.1930
Q	 0.9147	 0.4480
R	 0.9013	 0.4200
S	 0.9066	 0.4280
T	 0.8935	 0.4360
U	 0.8977	 0.3800
V	 0.8318	 0.4470
W	 0.8491	 0.4290
X	 0.8917	 0.4150
Y	 0.9172	 0.4220
Z	 0.9048	 0.4140
a	 0.9256	 0.4490
b	 0.8916	 0.4260
c	 0.8960	 0.4210
d	 0.8821	 0.4400
e	 0.8934	 0.4460
f	 0.9001	 0.4490
g	 0.8813	 0.4480
h	 0.8908	 0.4170
i	 0.9060	 0.4080
j	 0.9284	 0.4760
k	 0.8614	 0.3850
l	 0.8843	 0.4430
m	 0.8936	 0.4490
n	 0.7877	 0.4600
o	 0.8770	 0.4430
p	 0.8478	 0.4440
q	 0.8607	 0.3510
r	 0.8987	 0.3770

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Chain	Atom inclusion	Q-score
s	 0.8626	 0.4010
t	 0.7253	 0.2790
u	 0.8774	 0.3550
v	 0.7479	 0.2720
w	 0.8767	 0.3310
x	 0.8423	 0.3220
y	 0.8419	 0.3460
z	 0.8877	 0.3620