Full wwPDB EM Validation Report (i)

Nov 20, 2022 – 04:35 am GMT

PDB ID	:	6GQ1
EMDB ID	:	EMD-0047
Title	:	Cryo-EM reconstruction of yeast 80S ribosome in complex with mRNA, tRNA and eEF2 (GMPPCP/sordarin)
Authors	:	Pellegrino, S.; Demeshkina, N.; Mancera-Martinez, E.; Melnikov, S.; Simonetti, A.; Myasnikov, A.; Yusupov, M.; Yusupova, G.; Hashem, Y.
Deposited on	:	2018-06-07
Resolution	:	4.40 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 (i) 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 (1)) were used in the production of this report:

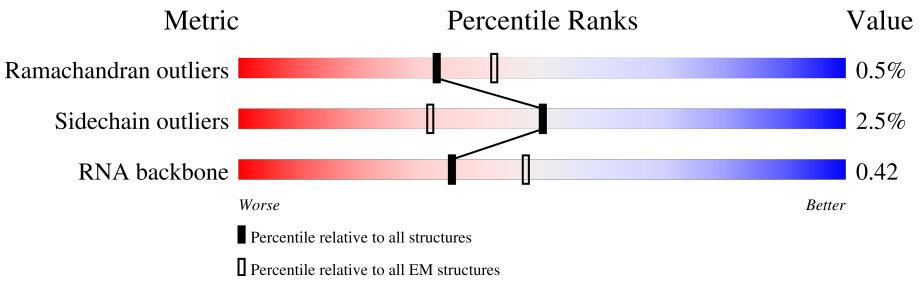
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 4.40 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	1	3396	60% 31% • 5%
2	3	121	67% 30% •
3	4	158	65% 33% •
4	P0	189	80% 97% •
5	P2	94	84% 95% 5%
6	A	252	6% 98% •
7	B	386	98% •
8	C	361	98% •

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Mol	Chain	Length	Quality of chain
9	D	296	5% 97%
10	E	175	86% 11%
11	F	222	95% 5%
12	G	233	95% 5%
13	H	191	5% 95% 5%
14	I	220	6% 91% 5%
15	J	169	8% 96%
16	L	193	96%
17	M	136	97%
18	N	203	96%
19	O	197	95% 5%
20	P	183	6% 97%
21	Q	185	96%
22	R	188	97%
23	S	172	97%
24	T	159	93% 7%
25	U	100	98%
26	V	136	7% 97%
27	W	63	95% 5%
28	X	121	100%
29	Y	126	98%
30	Z	135	96%
31	a	148	99%
32	b	58	7% 95% 5%
33	c	97	97%

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Mol	Chain	Length	Quality of chain
34	d	109	7% 98%
35	e	127	94% 6%
36	f	106	93% 6%
37	g	112	91% 8%
38	h	119	95% 5%
39	i	99	5% 95% 5%
40	j	87	97%
41	k	77	9% 96%
42	l	50	92% 6%
43	m	52	98%
44	n	25	20% 96%
45	o	105	6% 96%
46	p	91	100%
47	2	1797	57% 37% 5%
48	q	206	7% 97%
49	r	214	5% 93% 7%
50	s	217	98%
51	t	223	36% 95% 5%
52	u	260	5% 93% 6%
53	v	206	40% 98%
54	w	223	9% 93% 6%
55	x	184	9% 97%
56	y	199	9% 92% 6%
57	z	185	5% 96%
58	AA	105	16% 86% 5% 9%

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Mol	Chain	Length	Quality of chain
59	AB	153	14% 97%
60	AC	124	88% 96%
61	AD	150	7% 94% 5%
62	AE	127	98%
63	AF	124	27% 91% 9%
64	AG	141	32% 96%
65	AH	125	32% 93%
66	AI	145	31% 95% 5%
67	AJ	143	25% 97%
68	AK	107	52% 95% 5%
69	AL	87	9% 95% 5%
70	AM	129	96%
71	AN	144	10% 94% 6%
72	AO	134	8% 96%
73	AP	70	50% 96%
74	AQ	97	9% 87% 12%
75	AR	81	5% 94% 6%
76	AS	63	49% 100%
77	AT	53	13% 96%
78	AU	60	17% 95% 5%
79	AV	318	44% 98%
80	AW	37	70% 95% 5%
81	AX	76	9% 47% 50%
82	AY	8	75% 38% 62%
83	AZ	840	13% 95% 5%

2 Entry composition (i)

There are 86 unique types of molecules in this entry. The entry contains 210540 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 Saccharomyces cerevisiae S288C 35S pre-ribosomal RNA (RDN37-1), miscRNA.

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 5.8S 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 5S 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
			Total	C	N	O	S		
14	I	211	1705	1083	322	294	6	0	0

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

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

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

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

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

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

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

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

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

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

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

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

- 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		
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		
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	1003	628	189	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	63	521	336	102	82	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		
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		
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		
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
			Total	C	N	O	S		
35	e	127	1020	647	205	167	1	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	n	25	227	139	60	27	1	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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		
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
			Total	C	N	O	S		
70	AM	129	1021	650	188	180	3	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 81 is a RNA chain called Transfer RNA - Phe.

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

- Molecule 82 is a RNA chain called Messenger RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
82	AY	8	164	74	23	59	8	0	0

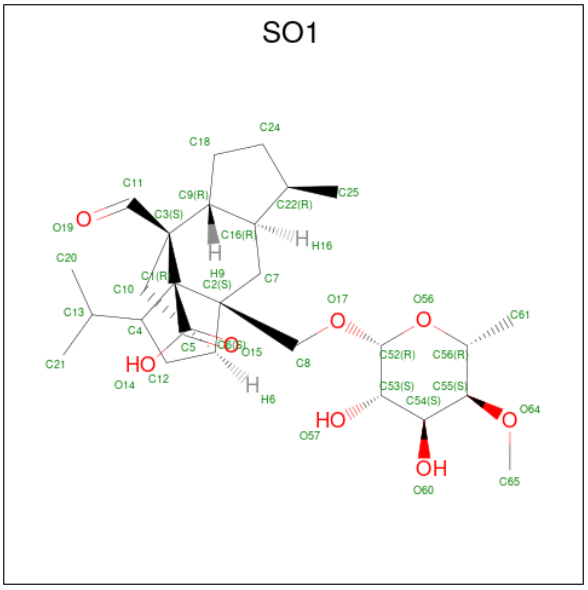
- Molecule 83 is a protein called Elongation factor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
83	AZ	840	6551	4161	1124	1237	29	0	0

- Molecule 84 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

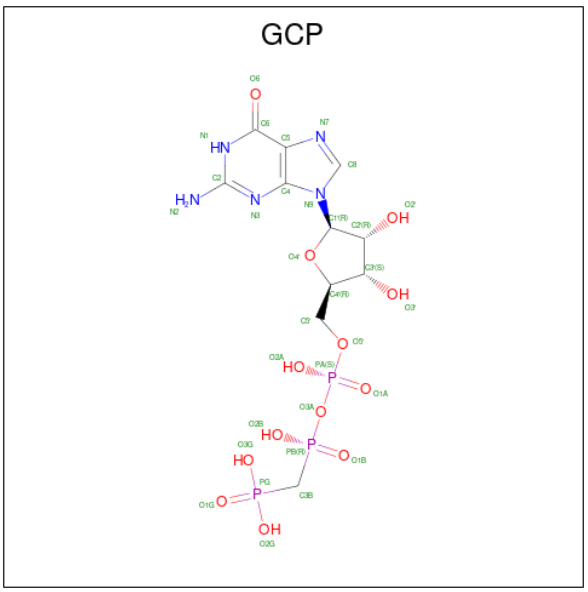
- Molecule 85 is [1R-(1.ALPHA.,3A.BETA.,4.BETA.,4A.BETA.,7.BETA.,7A.ALPHA.,8A.BETA.)]8A-[(6-DEOXY-4-O-METHYL-BETA-D-ALTROPYRANOSYLOXY)METHYL]-4-FORMYL-4,4A,5,6,7,7A,8,8A-OCTAHYDRO-7-METHYL-3-(1-METHYLETHYL)-1,4-METHANO-S-INDACENE-3A(1H)-CARBOXYLIC ACID (three-letter code: SO1) (formula: $C_{27}H_{42}O_8$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
85	AZ	1	35	27	8	0

- Molecule 86 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-

letter code: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).



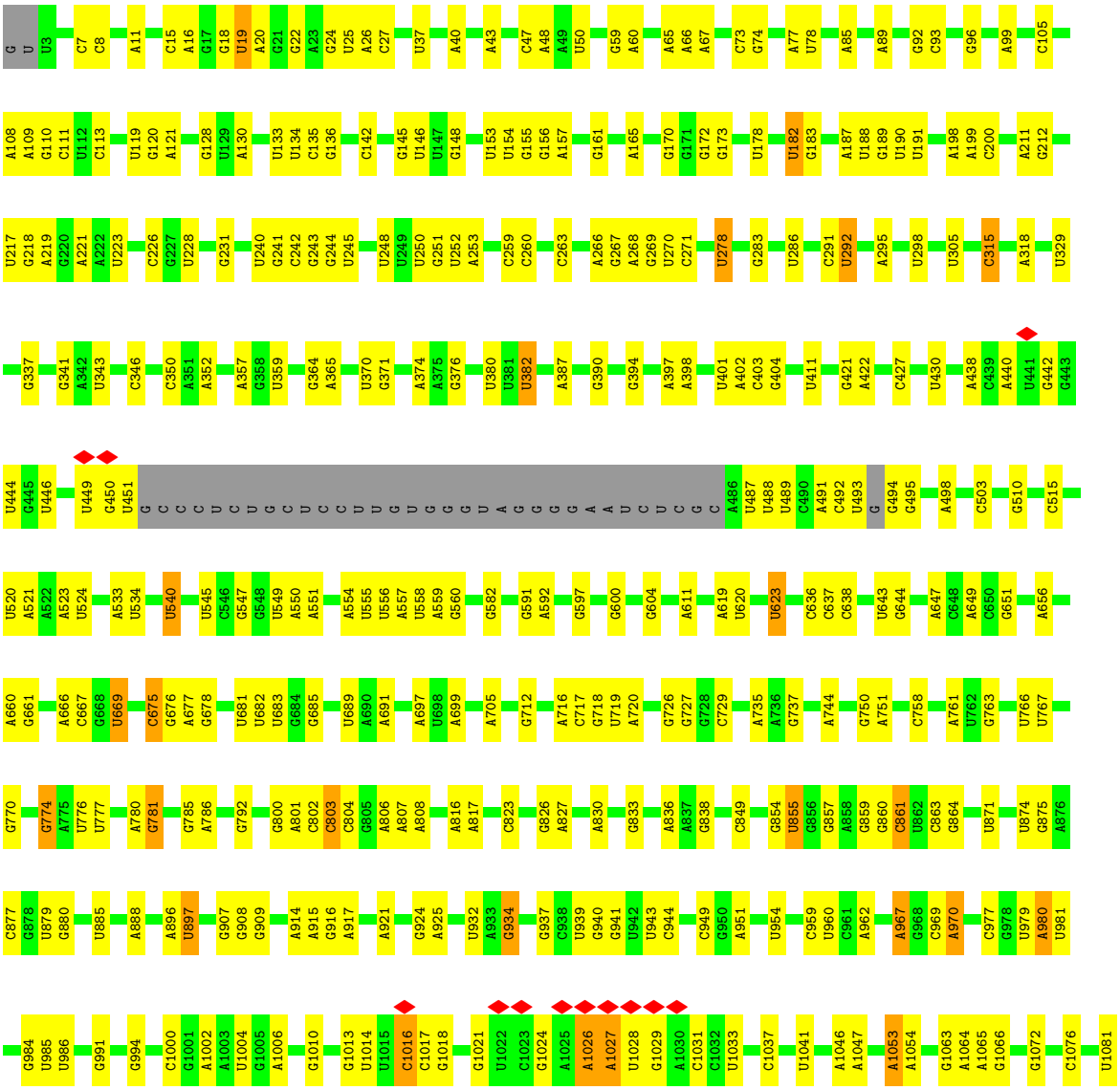
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
86	AZ	1	32	11	5	13	3	0

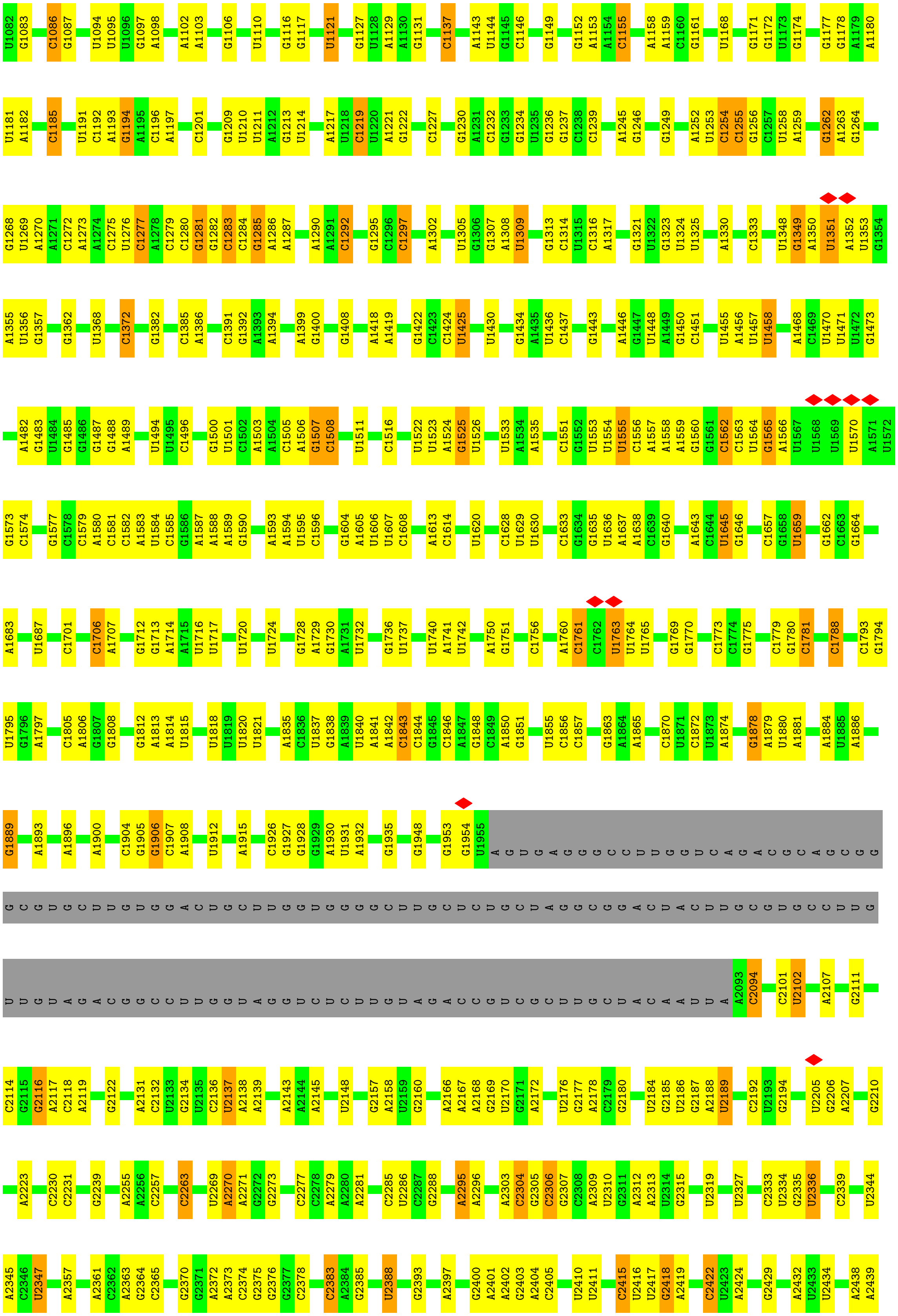
3 Residue-property plots (i)

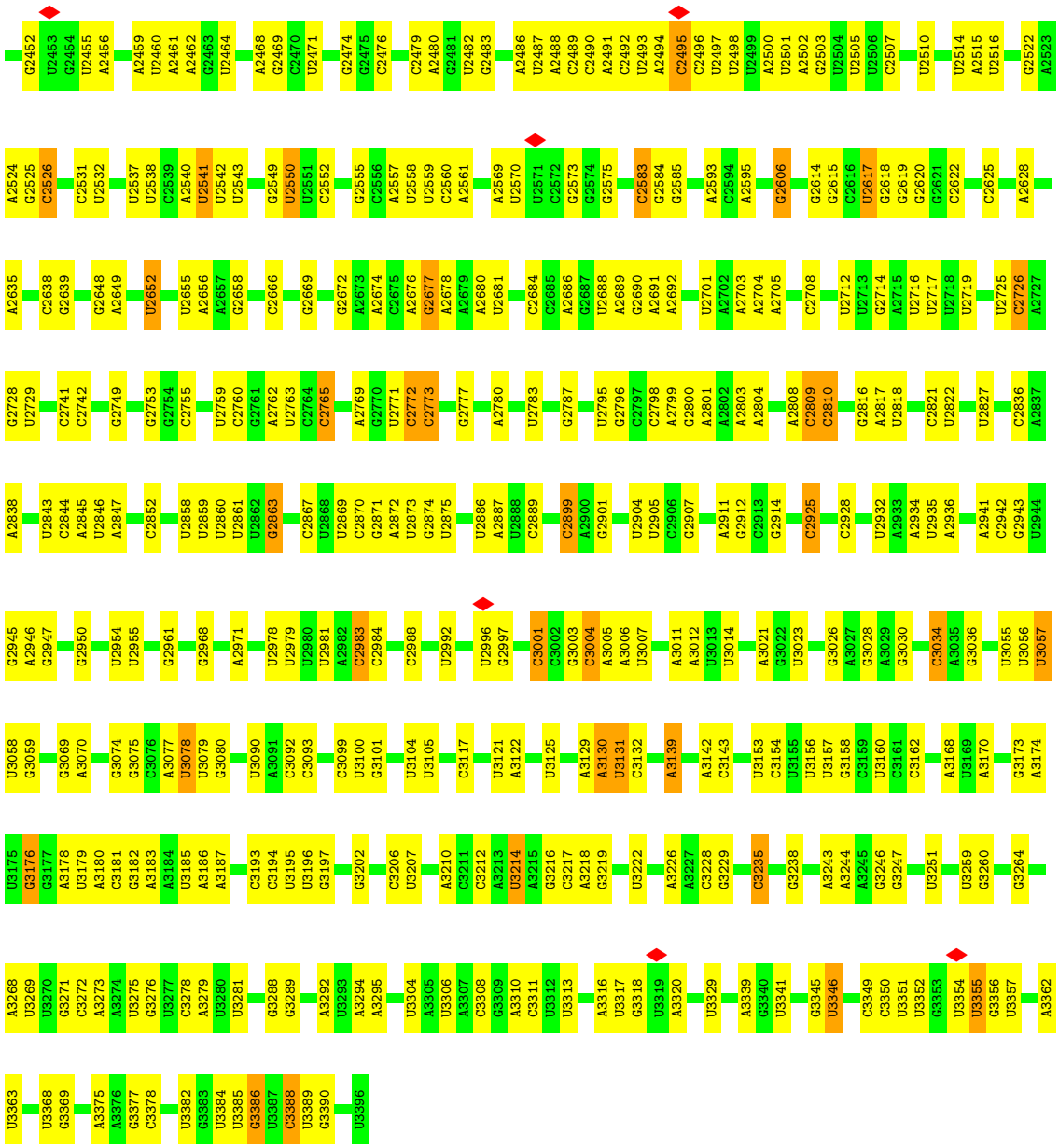
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Saccharomyces cerevisiae S288C 35S pre-ribosomal RNA (RDN37-1), miscRNA

Chain 1: 60% 31% 5%

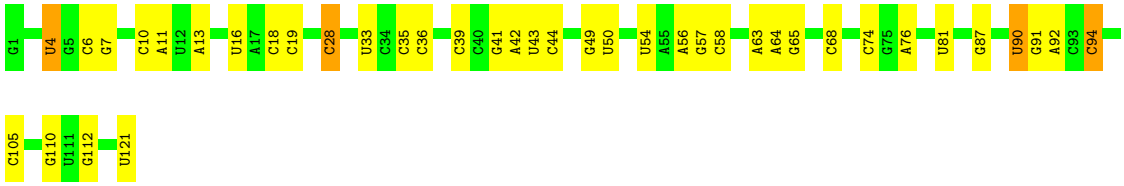



U1082 G1083 C1086 G1087 U1094 U1095 U1096 G1097 A1098 A1102 A1103 G1106 U1110 G1116 G1117 U1121 G1127 U1128 A1129 A1130 G1131 C1137 A1143 U1144 G1145 C1146 G1149 G1152 A1153 A1154 C1155 A1158 A1159 C1160 G1161 U1168 G1171 G1172 U1173 G1174 G1177 G1178 A1179 A1180
U1181 A1182 C1185 U1191 C1192 A1193 G1194 A1195 C1196 A1197 C1201 G1209 U1210 U1211 A1212 G1213 U1214 A1217 U1218 C1219 U1220 A1221 G1222 C1227 G1230 A1231 C1232 G1233 G1234 U1235 G1236 G1237 C1238 C1239 A1245 G1246 G1249 A1252 U1253 C1254 C1255 G1256 C1257 U1258 A1259 G1262 A1263 G1264
G1268 U1269 A1270 A1271 C1272 A1273 A1274 C1275 U1276 C1277 A1278 C1279 C1280 G1281 G1282 C1283 C1284 G1285 A1286 A1287 A1290 A1291 C1292 G1295 C1296 C1297 A1302 U1305 G1306 G1307 A1308 U1309 G1313 C1314 U1315 C1316 A1317 G1321 U1322 G1323 U1324 U1325 A1330 C1333 U1348 G1349 A1350 U1351 A1352 U1353 G1354
A1355 U1356 G1357 G1362 U1368 C1372 G1382 C1385 A1386 C1391 G1392 A1393 A1394 A1399 G1400 G1408 A1418 A1419 G1422 C1423 C1424 U1425 U1430 G1434 A1435 U1436 C1437 G1443 A1446 G1447 U1448 A1449 G1450 C1451 U1455 A1456 U1457 U1458 A1468 C1469 U1470 U1471 U1472 G1473
A1482 G1483 U1484 G1485 G1486 G1487 G1488 A1489 U1494 U1495 C1496 G1500 U1501 C1502 A1503 A1504 C1505 A1506 G1507 C1508 U1511 C1516 U1522 U1523 A1524 G1525 U1526 U1533 A1534 A1535 C1551 G1552 U1553 U1554 U1555 C1556 A1557 A1558 A1559 G1560 G1561 C1562 C1563 U1564 G1565 A1566 U1567 U1568 U1569 U1570 A1571 U1572
G1573 C1574 G1577 C1578 C1579 A1580 C1581 C1582 A1583 U1584 C1585 G1586 A1587 A1588 A1589 G1590 A1593 A1594 U1595 C1596 G1604 A1605 U1606 U1607 C1608 A1613 C1614 U1620 C1628 U1629 U1630 C1633 G1634 G1635 U1636 A1637 A1638 C1639 G1640 A1643 C1644 U1645 G1646 C1657 G1658 U1659 G1662 C1663 G1664
A1683 U1687 C1701 C1706 A1707 G1712 G1713 A1714 A1715 U1716 U1717 U1720 U1724 G1728 A1729 G1730 A1731 U1732 G1736 U1737 U1740 A1741 U1742 A1750 G1751 C1756 A1760 C1761 C1762 U1763 U1764 U1765 G1769 G1770 C1773 C1774 G1775 C1779 G1780 C1781 C1788 C1793 G1794
U1795 G1796 A1797 C1805 A1806 G1807 G1808 G1812 A1813 A1814 U1815 U1818 U1819 U1820 U1821 A1835 C1836 U1837 G1838 A1839 U1840 A1841 A1842 C1843 C1844 G1845 C1846 A1847 G1848 C1849 A1850 G1851 U1855 C1856 C1857 G1863 A1864 A1865 C1870 U1871 C1872 U1873 A1874 G1878 A1879 U1880 A1881 A1884 U1885 A1886
G1889 A1893 A1896 A1900 C1904 G1905 G1906 C1907 A1908 U1912 A1915 C1926 G1927 G1928 G1929 A1930 U1931 A1932 G1935 G1948 G1953 G1954 U1955 A G U G A G G G C C U U G G U C A G A C G C A G C G
G C G U G C U U G U G G A C U G C U U G G U G G G G C U U G C U C U G C U A G G C G G A C U A C U U G C G U G C C U U G
U U G U A G A C G G C C U U G G U A G G U C U C U U G U A G A C C G U C G G C U U G C U A C A A U U A A2093 C2094 C2101 U2102 A2107 G2111
C2114 G2115 G2116 A2117 C2118 A2119 G2122 A2131 C2132 U2133 G2134 U2135 C2136 U2137 A2138 A2139 A2143 A2144 A2145 U2148 G2157 A2158 U2159 G2160 A2166 A2167 A2168 G2169 U2170 G2171 A2172 U2176 G2177 A2178 C2179 G2180 U2184 G2185 U2186 G2187 A2188 U2189 C2192 U2193 G2194 U2205 G2206 A2207 G2210
A2223 C2230 C2231 G2239 A2255 A2256 C2257 C2263 U2269 A2270 A2271 G2272 G2273 C2277 C2278 A2279 A2280 A2281 C2285 U2286 C2287 G2288 A2295 A2296 A2303 C2304 G2305 C2306 G2307 C2308 A2309 U2310 G2311 A2312 A2313 U2314 G2315 U2319 U2327 C2333 U2334 G2335 U2336 C2339 U2344
A2345 C2346 U2347 A2357 A2361 C2362 A2363 G2364 C2365 G2370 G2371 A2372 A2373 C2374 G2375 G2376 G2377 C2378 C2383 A2384 G2385 U2388 G2393 A2397 G2400 A2401 G2402 G2403 A2404 C2405 U2410 U2411 C2415 U2416 U2417 G2418 A2419 C2422 U2423 A2424 G2429 A2432 U2433 U2434 A2438 A2439



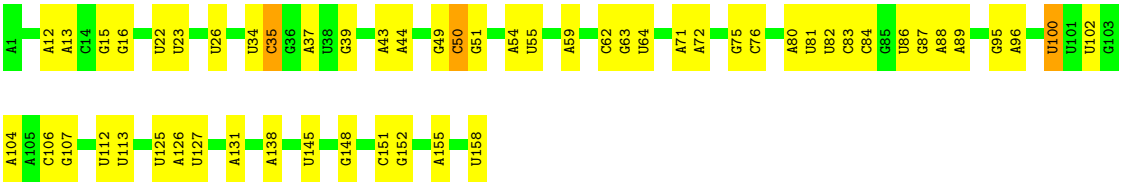
- Molecule 2: 5.8S ribosomal RNA

Chain 3:



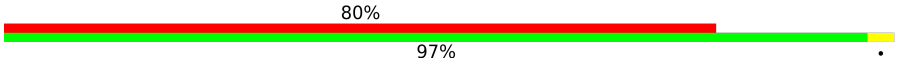
- Molecule 3: 5S ribosomal RNA

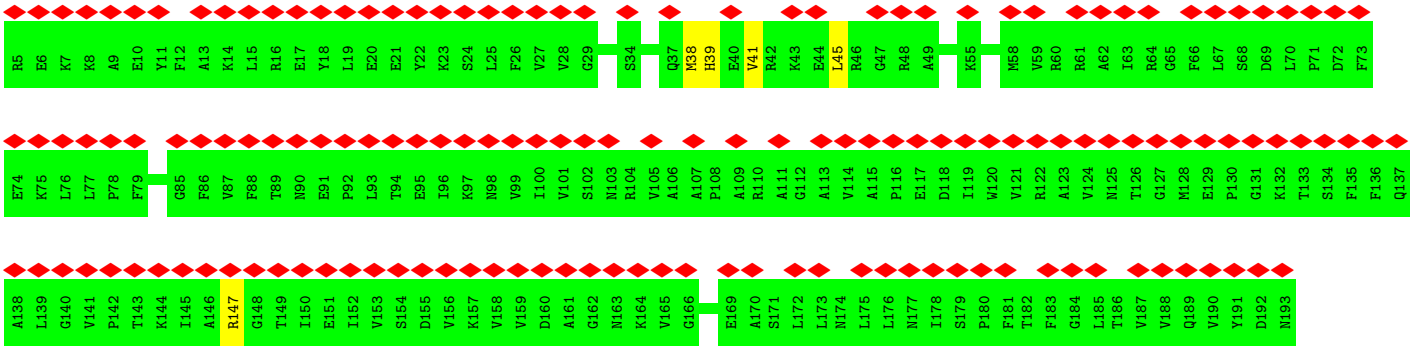
Chain 4:



- Molecule 4: 60S acidic ribosomal protein P0

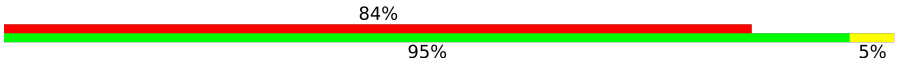
Chain P0:

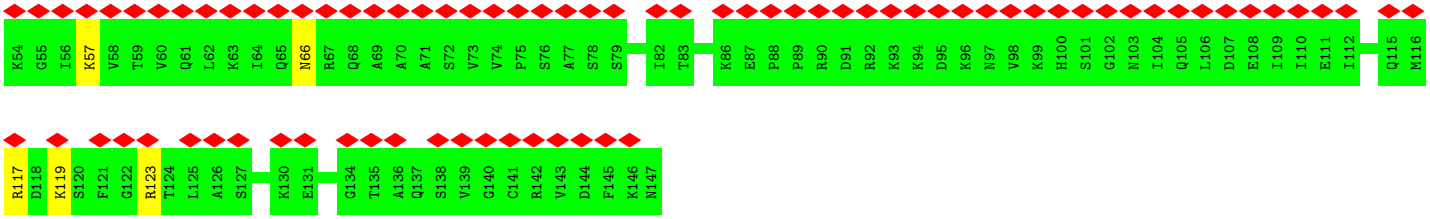




- Molecule 5: 60S ribosomal protein L12-A

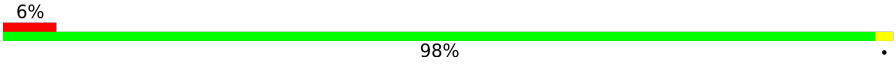
Chain P2:

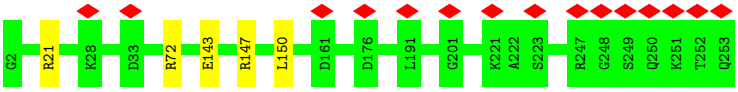




- Molecule 6: 60S ribosomal protein L2-A

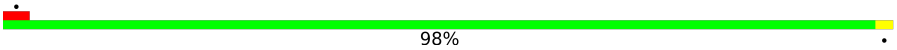
Chain A:

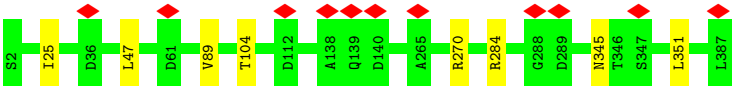




- Molecule 7: 60S ribosomal protein L3

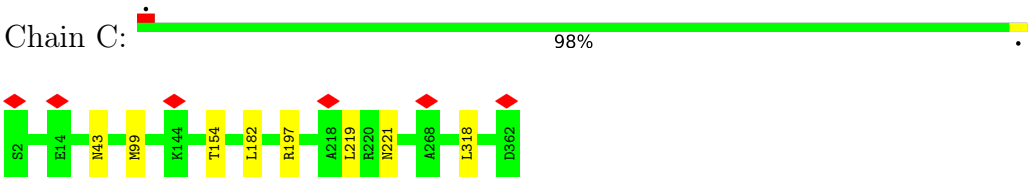
Chain B:





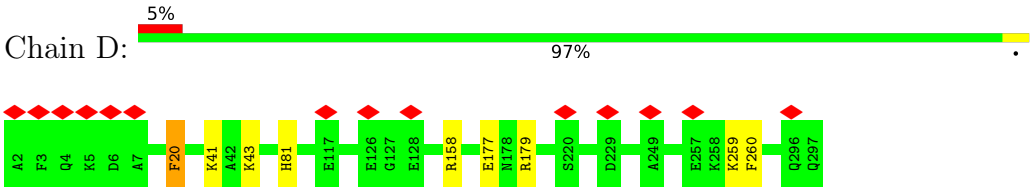
- Molecule 8: 60S ribosomal protein L4-A

Chain C:



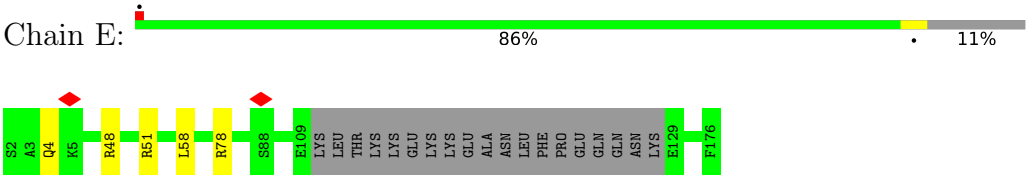
• Molecule 9: 60S ribosomal protein L5

Chain D:



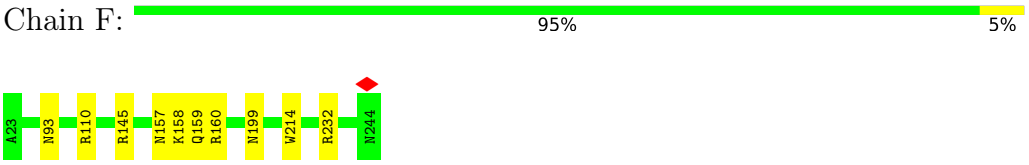
• Molecule 10: 60S ribosomal protein L6-A

Chain E:



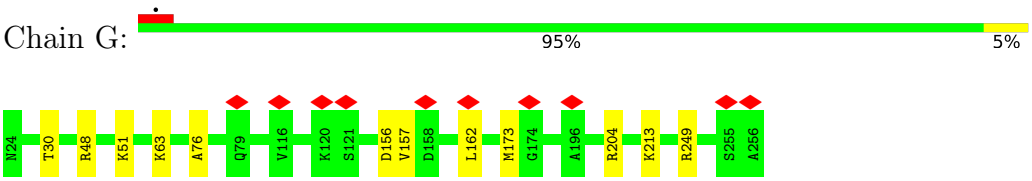
• Molecule 11: 60S ribosomal protein L7-A

Chain F:



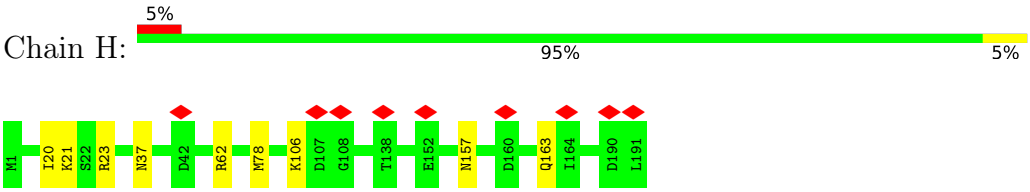
• Molecule 12: 60S ribosomal protein L8-A

Chain G:



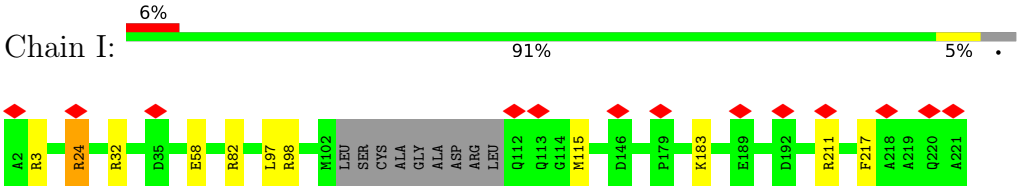
• Molecule 13: 60S ribosomal protein L9-A

Chain H:



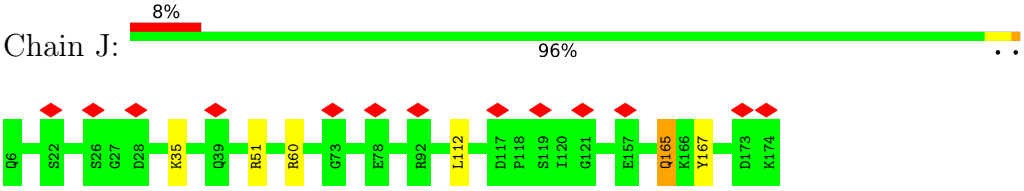
• Molecule 14: 60S ribosomal protein L10

Chain I:



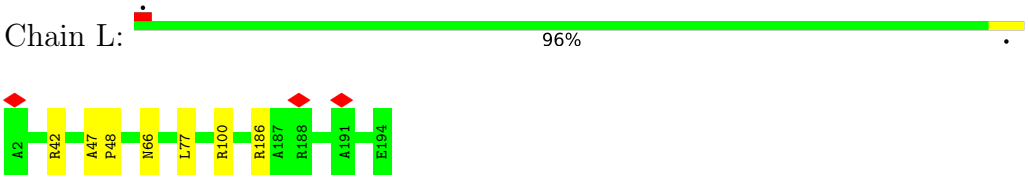
• Molecule 15: 60S ribosomal protein L11-B

Chain J:



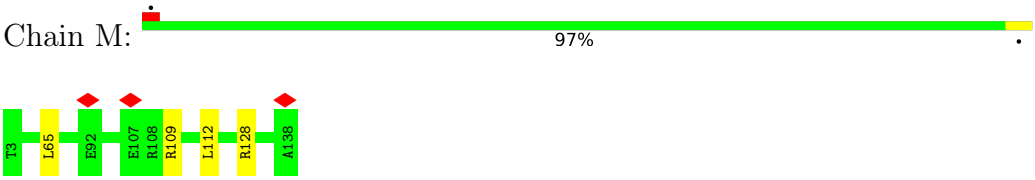
• Molecule 16: 60S ribosomal protein L13-A

Chain L:



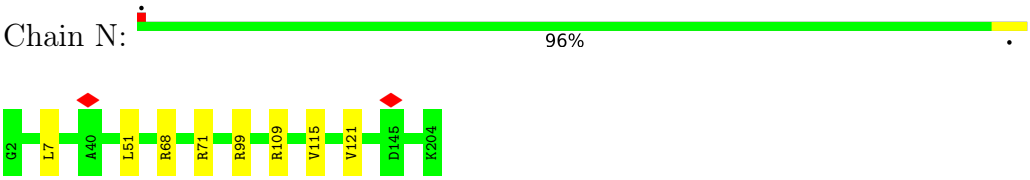
• Molecule 17: 60S ribosomal protein L14-A

Chain M:



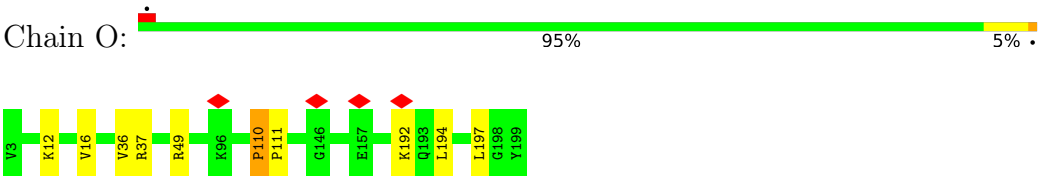
• Molecule 18: 60S ribosomal protein L15-A

Chain N:



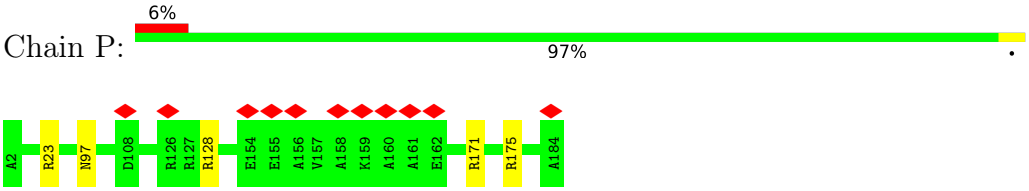
• Molecule 19: 60S ribosomal protein L16-A

Chain O:



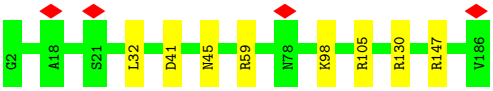
• Molecule 20: 60S ribosomal protein L17-A

Chain P:



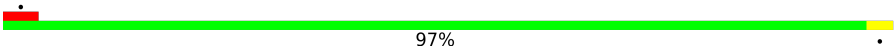
• Molecule 21: 60S ribosomal protein L18-A

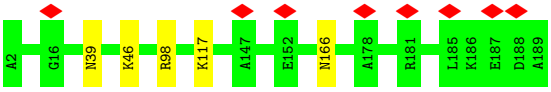
Chain Q:



• Molecule 22: 60S ribosomal protein L19-A

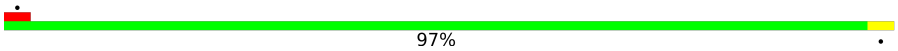
Chain R:

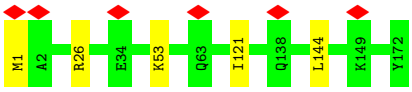




• Molecule 23: 60S ribosomal protein L20-A

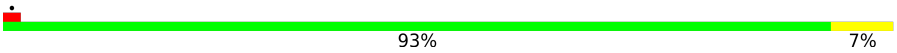
Chain S:

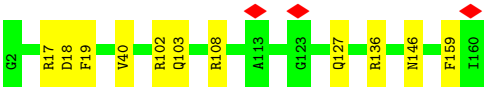




• Molecule 24: 60S ribosomal protein L21-A

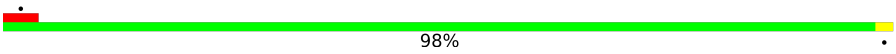
Chain T:

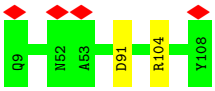




• Molecule 25: 60S ribosomal protein L22-A

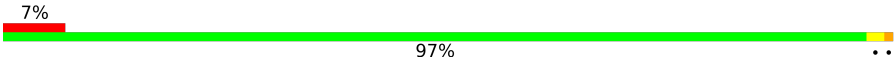
Chain U:

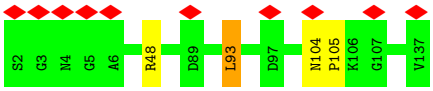




• Molecule 26: 60S ribosomal protein L23-A

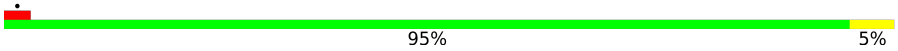
Chain V:

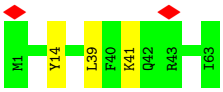




• Molecule 27: 60S ribosomal protein L24-A

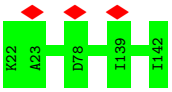
Chain W:





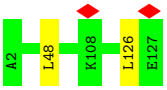
• Molecule 28: 60S ribosomal protein L25

Chain X: 100%



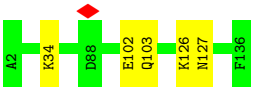
• Molecule 29: 60S ribosomal protein L26-A

Chain Y: 98%



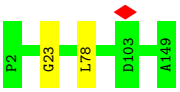
• Molecule 30: 60S ribosomal protein L27-A

Chain Z: 96%



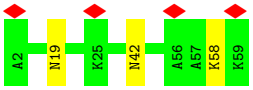
• Molecule 31: 60S ribosomal protein L28

Chain a: 99%



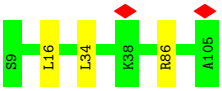
• Molecule 32: 60S ribosomal protein L29

Chain b: 7% 95% 5%



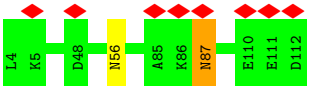
• Molecule 33: 60S ribosomal protein L30

Chain c: 97%



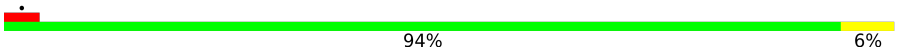
• Molecule 34: 60S ribosomal protein L31-A

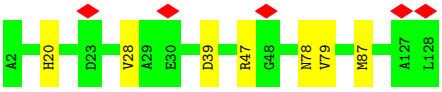
Chain d: 7% 98%



- Molecule 35: 60S ribosomal protein L32

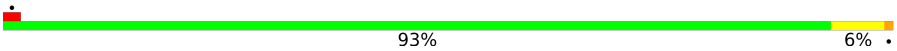
Chain e:

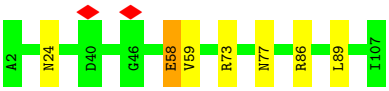




- Molecule 36: 60S ribosomal protein L33-A

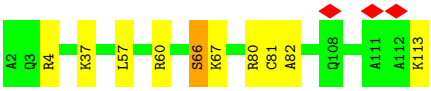
Chain f:





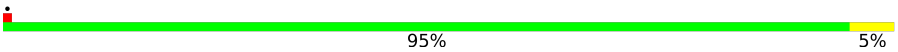
- Molecule 37: 60S ribosomal protein L34-A

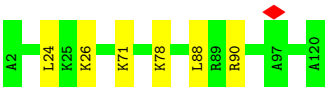
Chain g:



- Molecule 38: 60S ribosomal protein L35-A

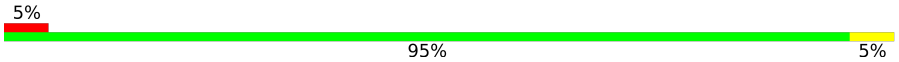
Chain h:

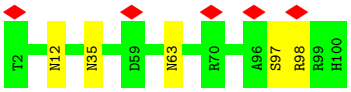




- Molecule 39: 60S ribosomal protein L36-A

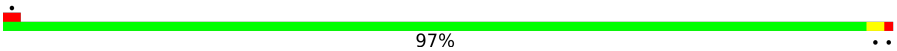
Chain i:

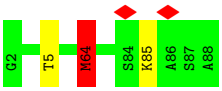




- Molecule 40: 60S ribosomal protein L37-A

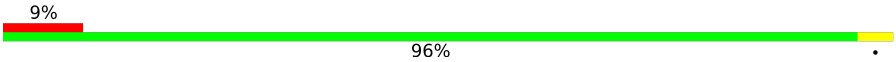
Chain j:

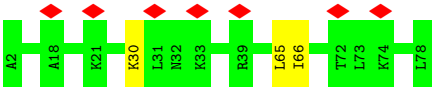




- Molecule 41: 60S ribosomal protein L38

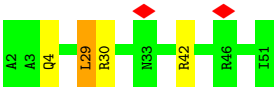
Chain k:





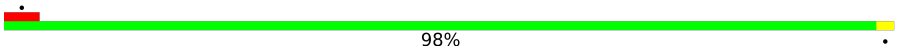
• Molecule 42: 60S ribosomal protein L39

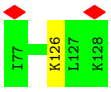
Chain l:



• Molecule 43: Ubiquitin-60S ribosomal protein L40

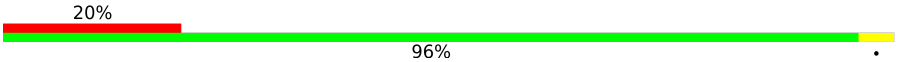
Chain m:

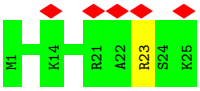




• Molecule 44: 60S ribosomal protein L41-B

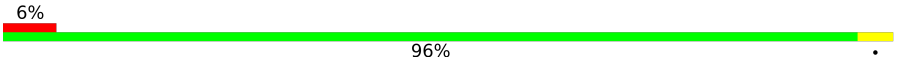
Chain n:

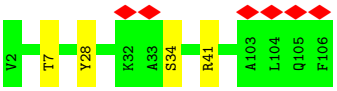




• Molecule 45: 60S ribosomal protein L42-A

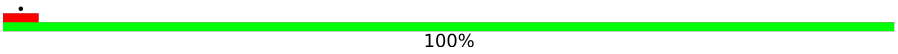
Chain o:

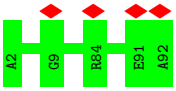




• Molecule 46: 60S ribosomal protein L43-A

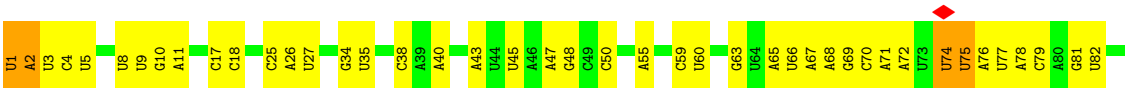
Chain p:

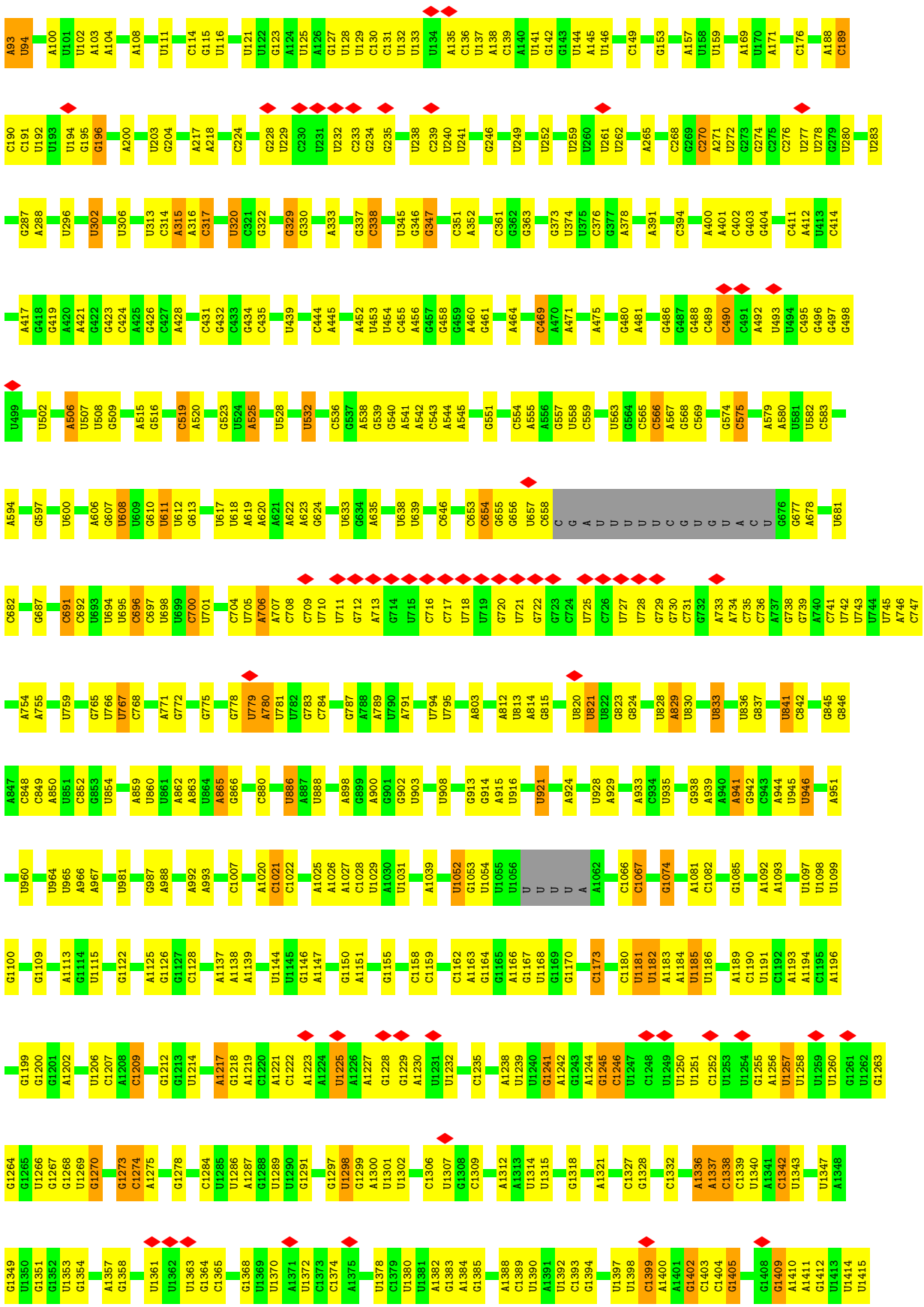




• Molecule 47: 18S ribosomal RNA

Chain 2:




A93 U94 A100 U101 U102 A103 A104 A108 U111 C114 G115 U116 U121 U122 G123 A124 U125 A126 G127 U128 U129 C130 C131 U132 U133 U134 A135 C136 U137 A138 C139 A140 U141 G142 G143 U144 A145 U146 C149 G153 A157 U158 U159 A169 U170 A171 C176 A188 C189
C190 C191 U192 U193 U194 G195 G196 A200 U203 G204 A217 A218 C224 G228 U229 C230 U231 U232 C233 G234 G235 U238 C239 U240 U241 G246 U249 U252 U259 U260 U261 U262 A265 C268 C269 C270 A271 U272 G273 G274 C275 C276 U277 U278 G279 U280 U283
G287 A288 U296 U302 U306 U313 C314 A315 A316 G317 U320 C321 G322 G329 G330 A333 G337 G338 U345 G346 G347 C351 A352 C361 G362 G363 G373 U374 U375 C376 G377 A378 A391 C394 A400 A401 C402 G403 G404 C411 A412 U413 C414
A417 G418 G419 A420 A421 G422 G423 C424 A425 G426 C427 A428 C431 G432 C433 G434 C435 U439 C444 A445 A452 U453 U454 C455 A456 G457 G458 G459 A460 G461 A464 C469 A470 A471 A475 G480 A481 G486 G487 G488 C489 C490 C491 A492 U493 U494 C495 G496 G497 G498
U499 U502 A506 U507 U508 G509 A515 G516 C519 A520 G523 U524 A525 U528 U532 C536 G537 A538 G539 G540 A541 A542 C543 A544 A545 G551 C554 A555 A556 G557 U558 C559 U563 G564 C565 C566 A567 G568 C569 G574 C575 A579 A580 U581 U582 C583
A594 G597 U600 A606 G607 U608 U609 G610 U611 U612 G613 U617 U618 A619 A620 A621 A622 A623 G624 U633 G634 A635 U638 U639 C646 C653 C654 G655 G656 U657 C658 C G A U U U U C G U G U A C U G676 G677 A678 U681
C682 G687 C691 C692 U693 U694 U695 C696 C697 U698 U699 C700 U701 C704 U705 A706 A707 C708 C709 U710 U711 G712 A713 G714 U715 C716 C717 U718 U719 G720 U721 G722 G723 C724 U725 C726 U727 U728 G729 G730 C731 G732 A733 A734 C735 C736 A737 G738 G739 A740 C741 U742 U743 U744 U745 A746 C747
A754 A755 U759 G765 U766 U767 C768 A771 G772 G775 G778 U779 A780 U781 U782 G783 C784 G787 A788 A789 U790 A791 U794 U795 A803 A812 U813 A814 G815 U820 U821 U822 G823 G824 U828 A829 U830 U833 U836 G837 U841 C842 G845 G846
A847 C848 C849 A850 U851 C852 G853 U854 A859 U860 U861 A862 A863 U864 A865 G866 C880 U886 A887 U888 A898 G899 A900 G901 G902 U903 U908 G913 G914 A915 U916 U921 A924 U928 A929 A933 C934 U935 G938 A939 A940 A941 G942 G943 A944 U945 U946 A951
U960 U964 U965 A966 A967 U981 G987 A988 A992 A993 C1007 A1020 C1021 C1022 A1025 A1026 A1027 C1028 U1029 A1030 U1031 A1039 U1052 G1053 U1054 U1055 U1056 U U U U A A1062 C1066 C1067 G1074 A1081 C1082 G1085 A1092 A1093 U1097 U1098 U1099
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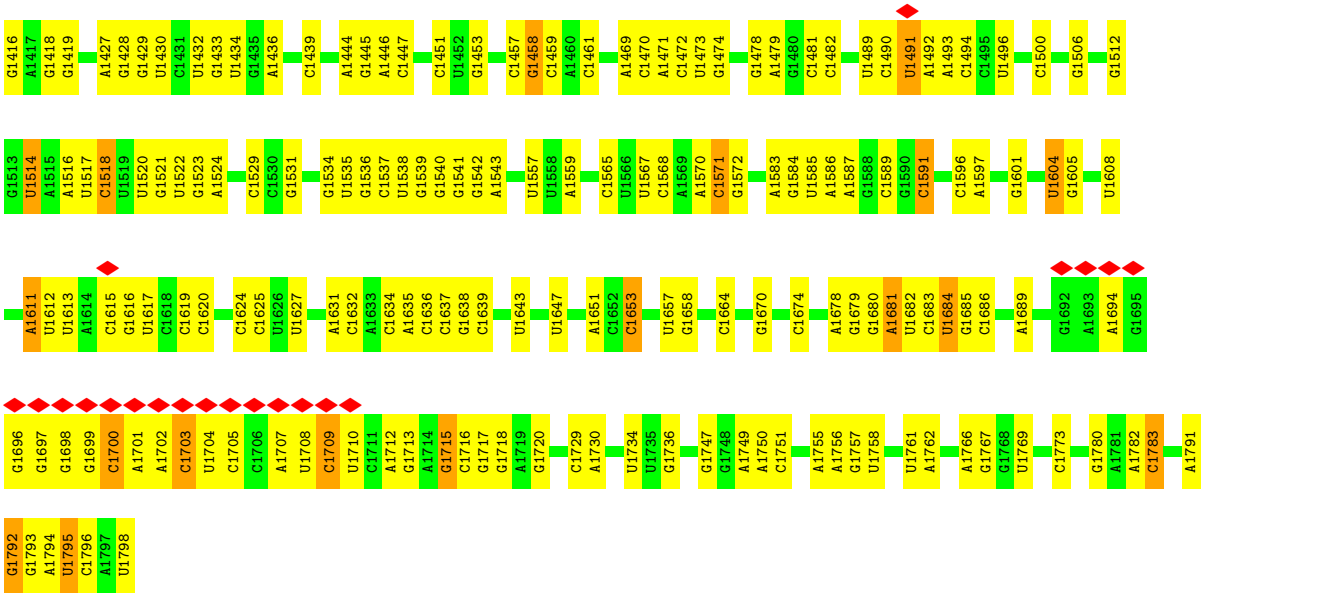
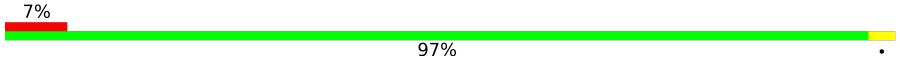
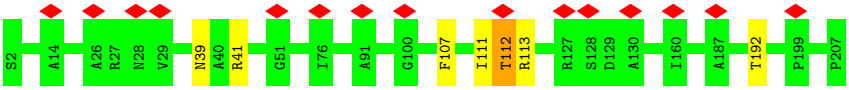
G1199 G1200 G1201 A1202 U1206 C1207 A1208 C1209 G1212 G1213 U1214 A1217 G1218 A1219 C1220 A1221 C1222 A1223 A1224 U1225 A1226 A1227 G1228 G1229 A1230 U1231 U1232 C1235 A1238 U1239 U1240 G1241 A1242 G1243 A1244 G1245 C1246 U1247 C1248 U1249 U1250 U1251 C1252 U1253 U1254 G1255 A1256 U1257 U1258 U1259 U1260 G1261 U1262 G1263
G1264 G1265 U1266 G1267 G1268 U1269 G1270 G1273 C1274 A1275 G1278 C1284 U1285 U1286 A1287 G1288 U1289 U1290 G1291 G1297 U1298 G1299 A1300 U1301 U1302 C1306 U1307 G1308 C1309 A1312 A1313 U1314 U1315 G1318 A1321 C1327 G1328 C1332 A1336 A1337 C1338 C1339 U1340 A1341 C1342 U1343 U1347 A1348
G1349 U1350 G1351 G1352 U1353 G1354 A1357 G1358 U1361 U1362 U1363 G1364 C1365 G1368 U1369 U1370 A1371 U1372 C1373 C1374 A1375 U1378 C1379 U1380 U1381 A1382 G1383 A1384 G1385 A1388 C1389 U1390 A1391 U1392 C1393 G1394 U1397 U1398 C1399 A1400 A1401 G1402 C1403 C1404 G1405 G1408 G1409 A1410 A1411 G1412 U1413 U1414 U1415



- Molecule 48: 40S ribosomal protein S0-A

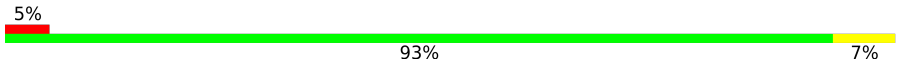
Chain q:

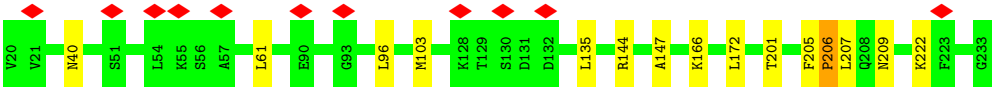




- Molecule 49: 40S ribosomal protein S1-A

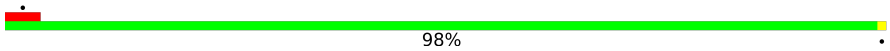
Chain r:





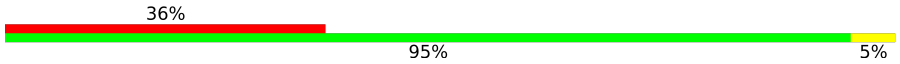
- Molecule 50: 40S ribosomal protein S2

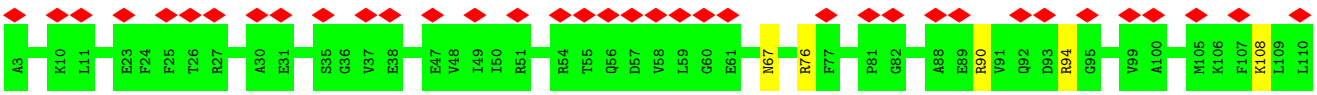
Chain s:

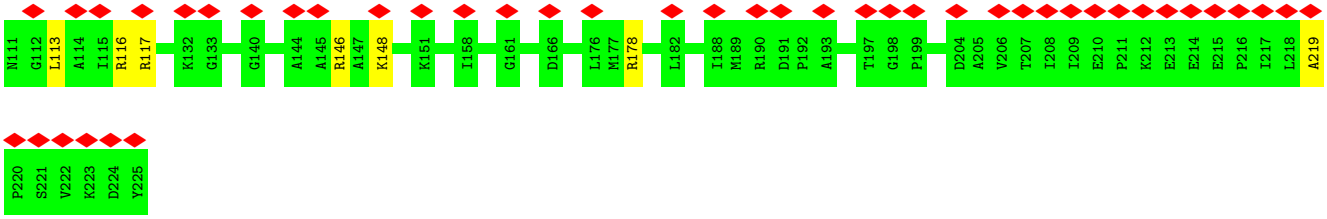


- Molecule 51: 40S ribosomal protein S3

Chain t:

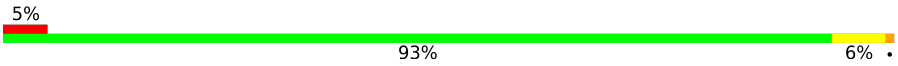


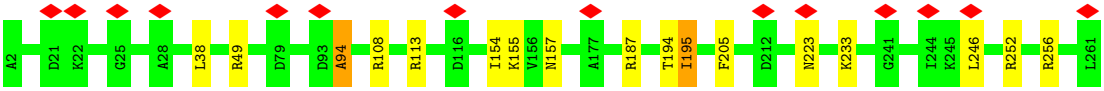




• Molecule 52: 40S ribosomal protein S4-A

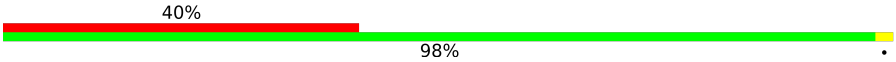
Chain u:

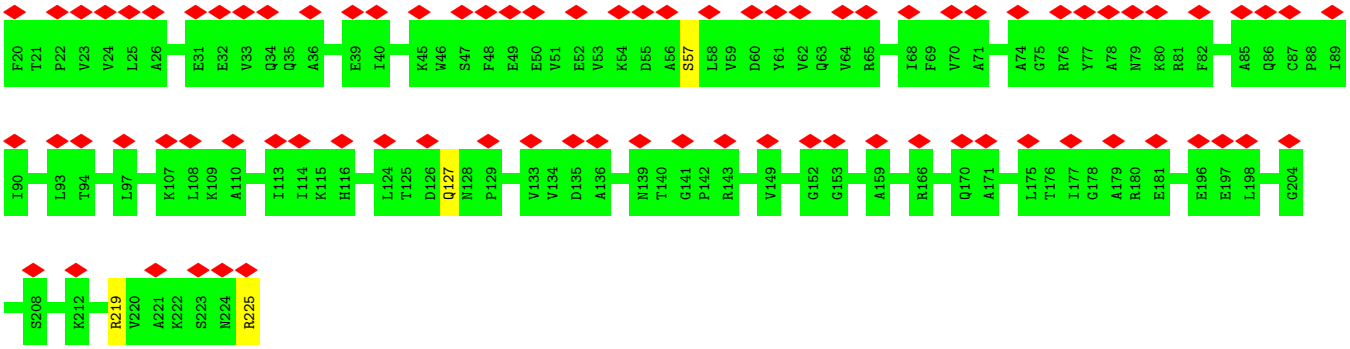




• Molecule 53: 40S ribosomal protein S5

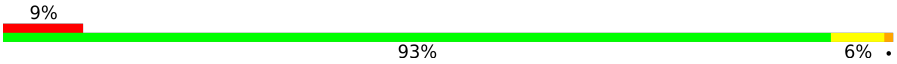
Chain v:

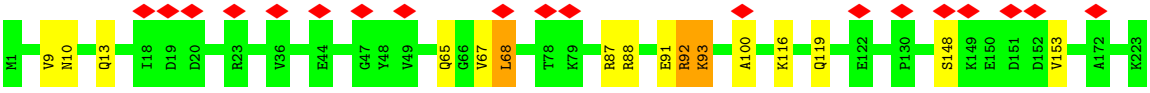




• Molecule 54: 40S ribosomal protein S6-A

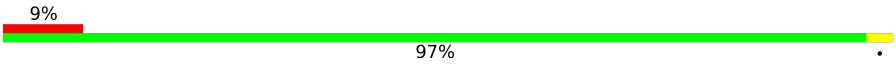
Chain w:

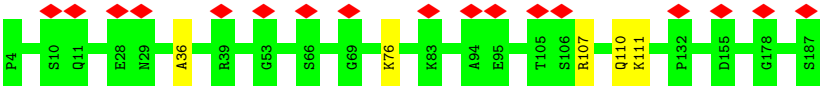




• Molecule 55: 40S ribosomal protein S7-A

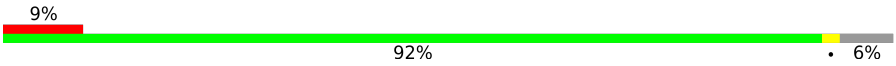
Chain x:

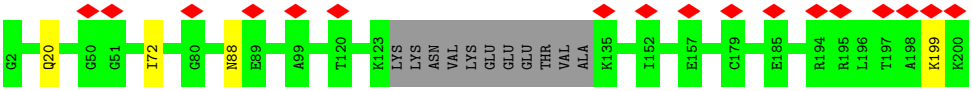




• Molecule 56: 40S ribosomal protein S8-A

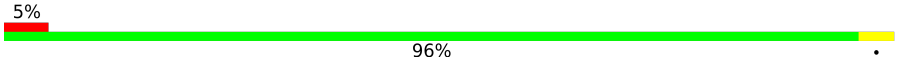
Chain y:

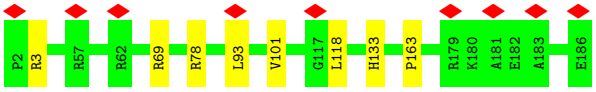




• Molecule 57: 40S ribosomal protein S9-A

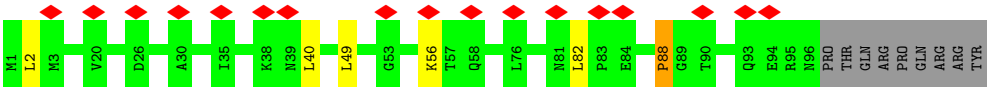
Chain z:





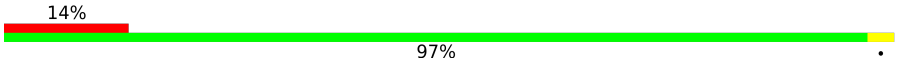
• Molecule 58: 40S ribosomal protein S10-A

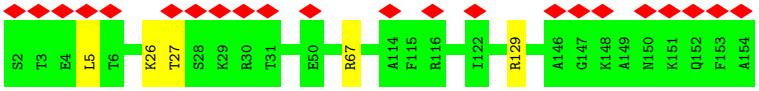
Chain AA:



• Molecule 59: 40S ribosomal protein S11-A

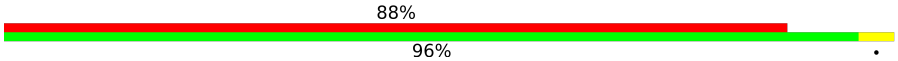
Chain AB:

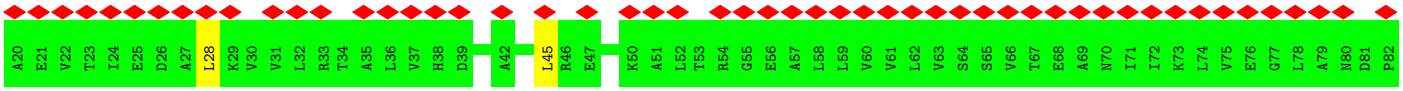


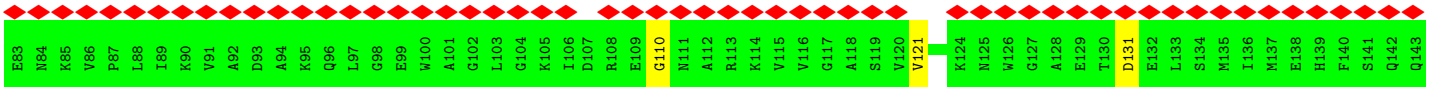


• Molecule 60: 40S ribosomal protein S12

Chain AC:

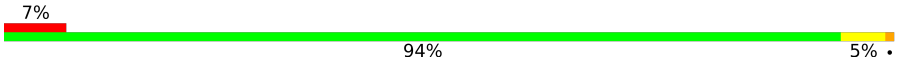


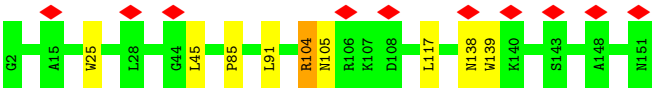




• Molecule 61: 40S ribosomal protein S13

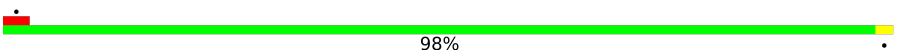
Chain AD:

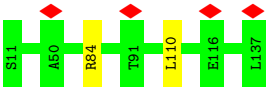




• Molecule 62: 40S ribosomal protein S14-B

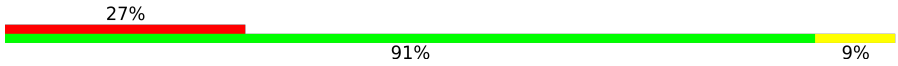
Chain AE:

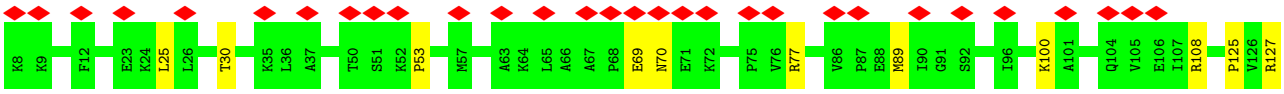




- Molecule 63: 40S ribosomal protein S15

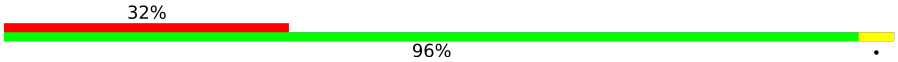
Chain AF:

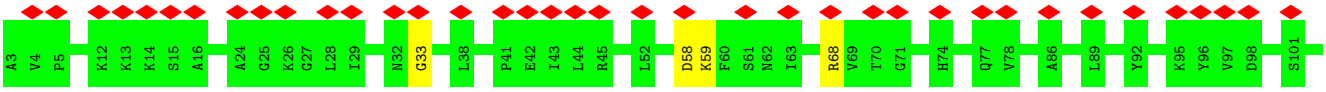


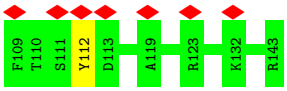


- Molecule 64: 40S ribosomal protein S16-A

Chain AG:

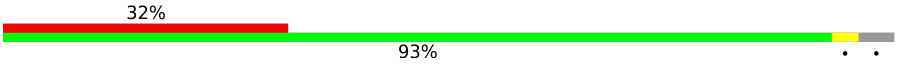


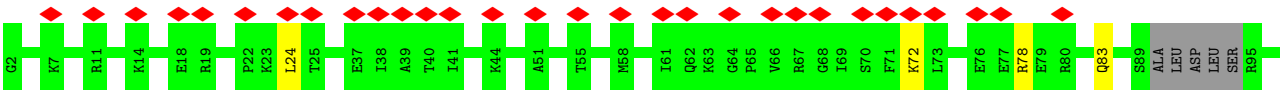


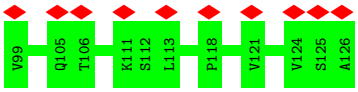


- Molecule 65: 40S ribosomal protein S17-B

Chain AH:

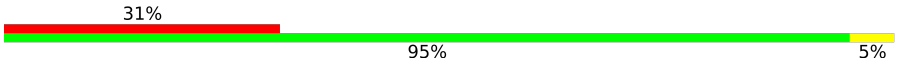


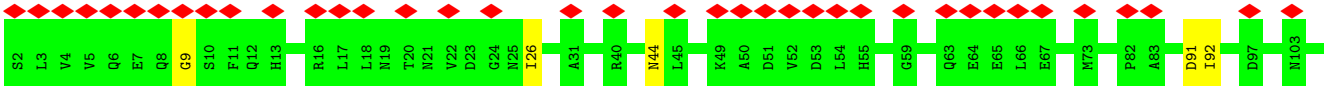


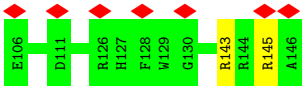


- Molecule 66: 40S ribosomal protein S18-A

Chain AI:

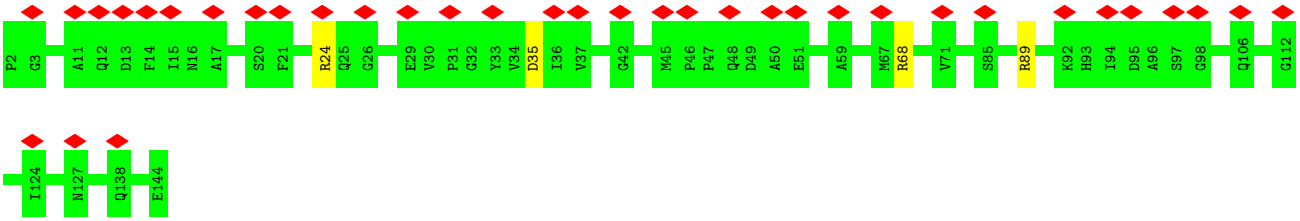






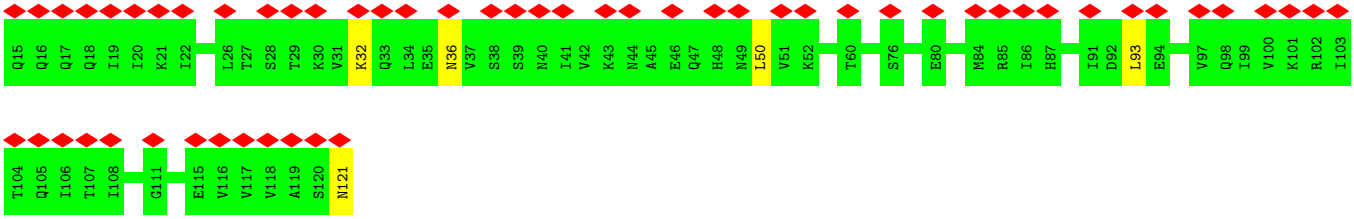
- Molecule 67: 40S ribosomal protein S19-A

Chain AJ: 25% 97%



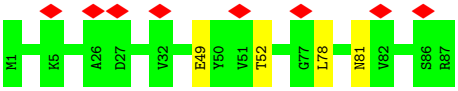
• Molecule 68: 40S ribosomal protein S20

Chain AK: 52% 95% 5%



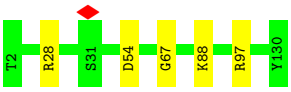
• Molecule 69: 40S ribosomal protein S21-A

Chain AL: 9% 95% 5%



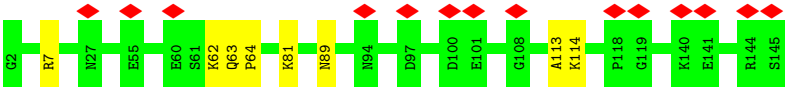
• Molecule 70: 40S ribosomal protein S22-A

Chain AM: 96%



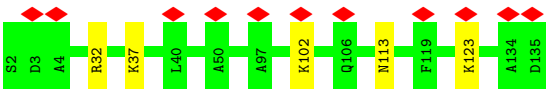
• Molecule 71: 40S ribosomal protein S23-A

Chain AN: 10% 94% 6%



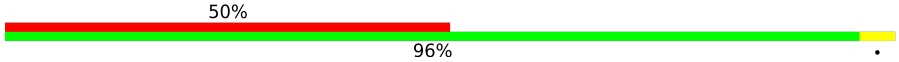
• Molecule 72: 40S ribosomal protein S24-A

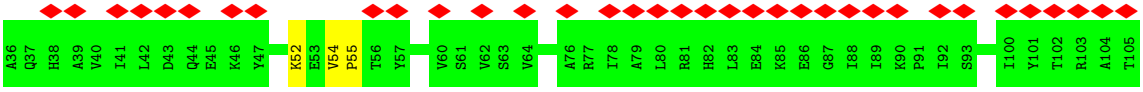
Chain AO: 8% 96%



- Molecule 73: 40S ribosomal protein S25-A

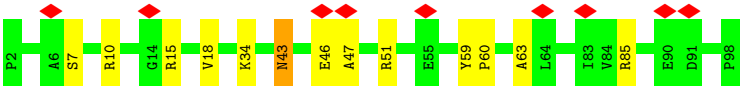
Chain AP:





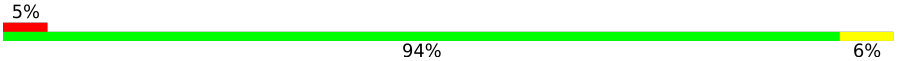
- Molecule 74: 40S ribosomal protein S26-B

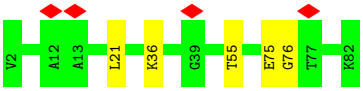
Chain AQ:



- Molecule 75: 40S ribosomal protein S27-A

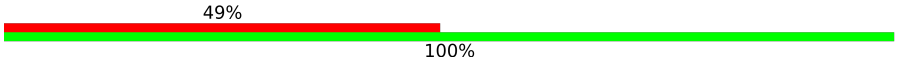
Chain AR:

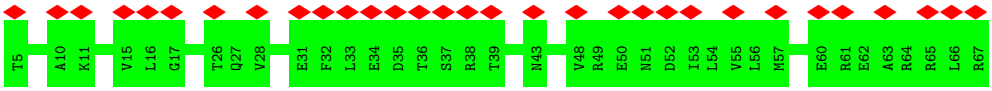




- Molecule 76: 40S ribosomal protein S28-A

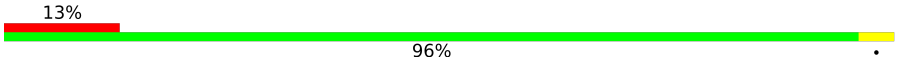
Chain AS:

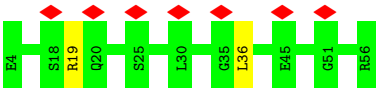




- Molecule 77: 40S ribosomal protein S29-A

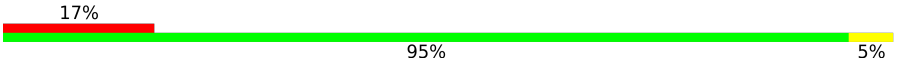
Chain AT:

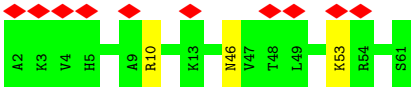




- Molecule 78: 40S ribosomal protein S30-A

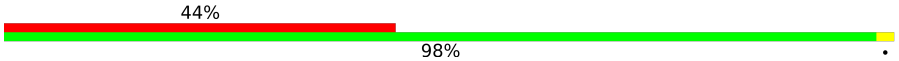
Chain AU:

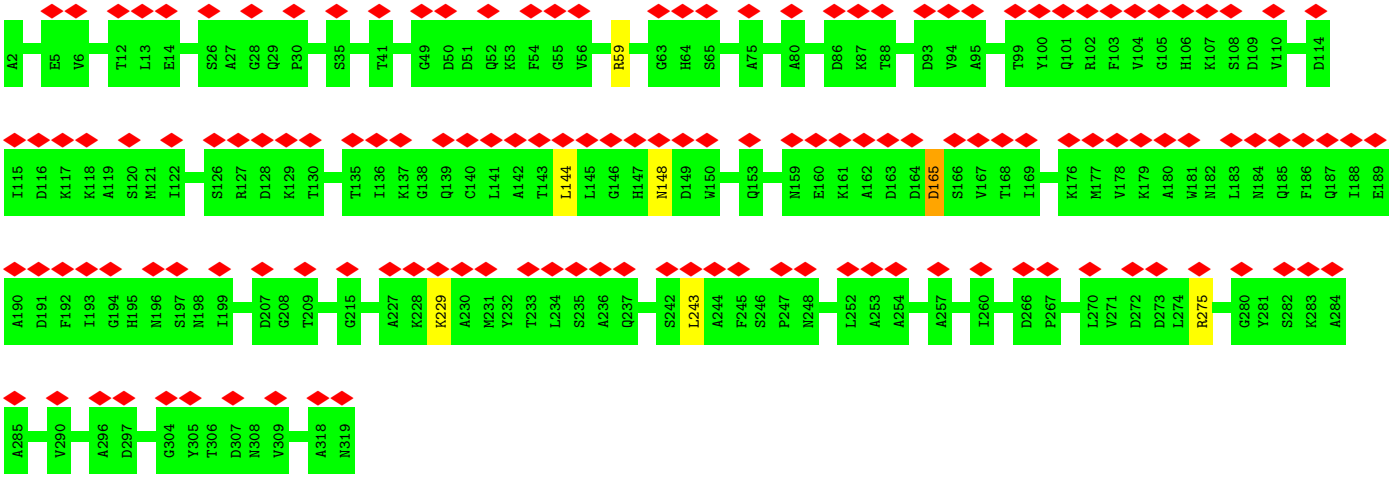




- Molecule 79: Guanine nucleotide-binding protein subunit beta-like protein

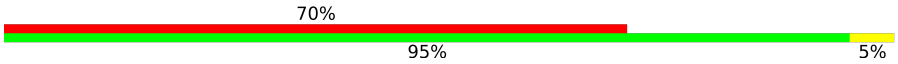
Chain AV:

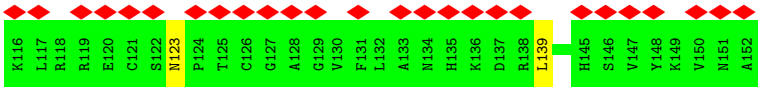




- Molecule 80: Ubiquitin-40S ribosomal protein S31

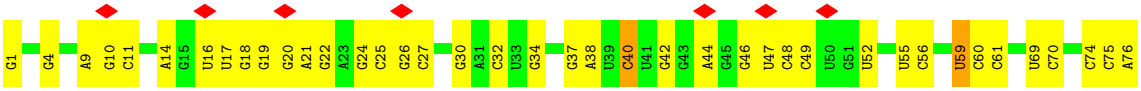
Chain AW:





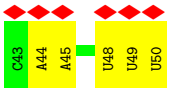
- Molecule 81: Transfer RNA - Phe

Chain AX:



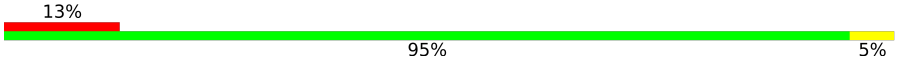
- Molecule 82: Messenger RNA

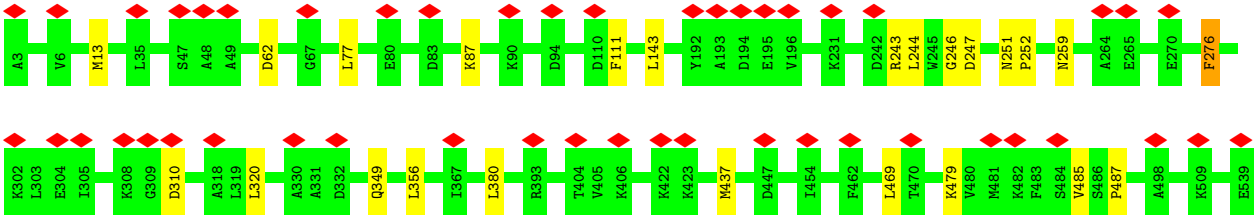
Chain AY:

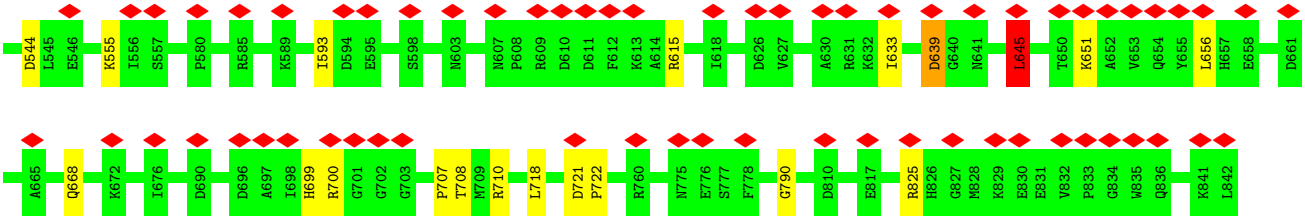


- Molecule 83: Elongation factor 2

Chain AZ:






D544
L545
E546
K555
I556
S557
P580
R585
K589
I593
D594
E595
S598
N603
N607
P608
R609
D610
D611
F612
K613
A614
R615
I618
D626
V627
A630
R631
K632
I633
D639
G640
N641
L645
T650
K651
A652
V653
Q654
Y655
L656
H657
E658
D661
A665
Q668
K672
I676
D690
D696
A697
I698
H699
R700
G701
G702
G703
P707
T708
W709
R710
L718
D721
P722
R760
N775
E776
S777
F778
G790
D810
E817
R825
H826
G827
N828
K829
E830
E831
V832
P833
G834
W835
Q836
K841
L842

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	189700	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	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	0.347	Depositor
Minimum map value	-0.197	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	396.0, 396.0, 396.0	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: SO1, ZN, GCP, DDE

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	0.64	0/77157	1.21	496/120295 (0.4%)
2	3	0.54	0/2883	1.17	23/4491 (0.5%)
3	4	0.61	0/3746	1.13	14/5832 (0.2%)
4	P0	0.31	0/1498	0.67	1/2025 (0.0%)
5	P2	0.28	0/728	0.68	0/975
6	A	0.43	0/1948	0.72	1/2617 (0.0%)
7	B	0.37	0/3146	0.65	1/4228 (0.0%)
8	C	0.35	0/2800	0.66	3/3790 (0.1%)
9	D	0.34	0/2425	0.62	0/3271
10	E	0.31	0/1260	0.62	0/1694
11	F	0.37	0/1821	0.66	0/2451
12	G	0.34	0/1836	0.64	1/2481 (0.0%)
13	H	0.34	0/1539	0.64	0/2073
14	I	0.37	0/1741	0.67	0/2335
15	J	0.32	0/1374	0.73	1/1842 (0.1%)
16	L	0.35	0/1568	0.65	0/2106
17	M	0.31	0/1068	0.62	1/1438 (0.1%)
18	N	0.41	0/1757	0.69	1/2354 (0.0%)
19	O	0.39	0/1585	0.66	2/2128 (0.1%)
20	P	0.35	0/1443	0.62	0/1944
21	Q	0.34	0/1465	0.65	2/1965 (0.1%)
22	R	0.32	0/1538	0.61	0/2050
23	S	0.36	0/1481	0.65	1/1990 (0.1%)
24	T	0.36	0/1300	0.68	2/1743 (0.1%)
25	U	0.35	0/812	0.67	1/1099 (0.1%)
26	V	0.38	0/1018	0.71	1/1369 (0.1%)
27	W	0.36	0/533	0.70	1/707 (0.1%)
28	X	0.36	0/979	0.66	0/1321
29	Y	0.31	0/1004	0.68	2/1341 (0.1%)
30	Z	0.36	0/1118	0.66	2/1497 (0.1%)
31	a	0.36	0/1204	0.65	0/1612
32	b	0.28	0/473	0.63	0/629

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	c	0.35	0/751	0.67	1/1008 (0.1%)
34	d	0.36	0/897	0.63	0/1205
35	e	0.32	0/1041	0.61	0/1394
36	f	0.40	0/868	0.70	1/1168 (0.1%)
37	g	0.37	0/890	0.72	2/1189 (0.2%)
38	h	0.31	0/978	0.66	2/1301 (0.2%)
39	i	0.32	0/778	0.66	0/1034
40	j	0.40	0/696	0.74	1/923 (0.1%)
41	k	0.29	0/618	0.66	1/826 (0.1%)
42	l	0.45	0/443	0.83	1/588 (0.2%)
43	m	0.35	0/423	0.63	0/562
44	n	0.28	0/228	0.60	0/293
45	o	0.35	0/860	0.65	0/1136
46	p	0.39	0/701	0.68	0/934
47	2	0.53	0/42328	1.23	349/65955 (0.5%)
48	q	0.31	0/1617	0.63	0/2215
49	r	0.33	0/1735	0.78	3/2335 (0.1%)
50	s	0.32	0/1665	0.67	1/2263 (0.0%)
51	t	0.32	0/1759	0.69	1/2368 (0.0%)
52	u	0.33	0/2109	0.76	3/2839 (0.1%)
53	v	0.30	0/1629	0.67	0/2202
54	w	0.33	0/1814	0.77	2/2425 (0.1%)
55	x	0.33	0/1506	0.73	0/2028
56	y	0.33	0/1514	0.68	0/2021
57	z	0.33	0/1519	0.70	3/2035 (0.1%)
58	AA	0.33	0/789	0.75	4/1067 (0.4%)
59	AB	0.34	0/1247	0.66	1/1681 (0.1%)
60	AC	0.29	0/898	0.72	2/1220 (0.2%)
61	AD	0.32	0/1215	0.70	1/1638 (0.1%)
62	AE	0.32	0/901	0.64	0/1217
63	AF	0.36	0/998	0.74	1/1341 (0.1%)
64	AG	0.30	0/1125	0.73	0/1510
65	AH	0.30	0/935	0.67	1/1254 (0.1%)
66	AI	0.29	0/1211	0.68	1/1628 (0.1%)
67	AJ	0.32	0/1130	0.67	1/1517 (0.1%)
68	AK	0.30	0/865	0.71	2/1169 (0.2%)
69	AL	0.38	0/693	0.78	1/935 (0.1%)
70	AM	0.36	0/1038	0.68	2/1395 (0.1%)
71	AN	0.36	0/1139	0.72	0/1518
72	AO	0.31	0/1087	0.63	0/1449
73	AP	0.32	0/571	0.73	0/768
74	AQ	0.36	0/782	0.82	2/1047 (0.2%)
75	AR	0.38	0/620	0.81	0/838

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
76	AS	0.30	0/499	0.69	0/670
77	AT	0.32	0/452	0.63	1/600 (0.2%)
78	AU	0.29	0/483	0.59	0/643
79	AV	0.30	0/2490	0.70	3/3389 (0.1%)
80	AW	0.30	0/292	0.65	0/390
81	AX	0.52	1/1818 (0.1%)	1.34	25/2831 (0.9%)
82	AY	0.30	0/181	0.97	0/278
83	AZ	0.35	0/6655	0.76	11/9009 (0.1%)
All	All	0.51	1/225729 (0.0%)	1.04	987/330942 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	P0	0	2
5	P2	0	1
6	A	0	1
7	B	0	1
9	D	0	5
10	E	0	1
11	F	0	3
12	G	0	3
13	H	0	2
14	I	0	2
15	J	0	1
16	L	0	1
19	O	0	2
21	Q	0	1
24	T	0	2
26	V	0	2
27	W	0	1
31	a	0	1
34	d	0	2
35	e	0	2
36	f	0	1
37	g	0	3
38	h	0	1
39	i	0	3
40	j	0	1
42	l	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
45	o	0	3
48	q	0	4
49	r	0	4
51	t	0	1
52	u	0	5
53	v	0	2
54	w	0	11
55	x	0	2
56	y	0	1
57	z	0	2
59	AB	0	1
60	AC	0	1
61	AD	0	3
63	AF	0	2
64	AG	0	3
65	AH	0	2
66	AI	0	1
69	AL	0	2
71	AN	0	1
72	AO	0	1
73	AP	0	1
74	AQ	0	7
75	AR	0	2
79	AV	0	1
83	AZ	0	14
All	All	0	123

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	AX	1	G	OP3-P	-10.59	1.48	1.61

All (987) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	2	94	U	C2-N3-C4	22.19	140.31	127.00
47	2	654	C	N1-C2-O2	13.09	126.75	118.90
47	2	654	C	C2-N1-C1'	12.26	132.29	118.80
47	2	94	U	N3-C4-C5	12.07	121.84	114.60
47	2	453	U	C2-N1-C1'	11.67	131.70	117.70
1	1	2094	C	N1-C2-O2	11.61	125.86	118.90
47	2	654	C	N3-C2-O2	-11.54	113.83	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	2	453	U	N1-C2-O2	11.35	130.75	122.80
47	2	767	U	N1-C2-O2	11.23	130.66	122.80
47	2	453	U	N3-C2-O2	-11.06	114.46	122.20
47	2	767	U	N3-C2-O2	-10.92	114.56	122.20
47	2	1342	C	N1-C2-O2	10.74	125.35	118.90
47	2	490	C	N3-C2-O2	-10.56	114.50	121.90
47	2	767	U	C2-N1-C1'	10.53	130.33	117.70
1	1	2094	C	N3-C2-O2	-10.42	114.60	121.90
1	1	2836	C	N1-C2-O2	10.37	125.12	118.90
47	2	654	C	C6-N1-C2	-10.20	116.22	120.30
1	1	1856	C	N3-C2-O2	-10.18	114.78	121.90
1	1	3235	C	N3-C2-O2	-10.06	114.86	121.90
1	1	2230	C	N1-C2-O2	9.75	124.75	118.90
1	1	1155	C	N3-C2-O2	-9.43	115.30	121.90
1	1	1137	C	N1-C2-O2	9.37	124.52	118.90
47	2	1052	U	N3-C2-O2	-9.36	115.65	122.20
47	2	1246	C	N1-C2-O2	9.33	124.50	118.90
47	2	1052	U	N1-C2-O2	9.23	129.26	122.80
1	1	823	C	C2-N1-C1'	9.20	128.92	118.80
1	1	1496	C	C2-N1-C1'	9.16	128.87	118.80
47	2	490	C	N1-C2-O2	9.09	124.35	118.90
1	1	1763	U	N1-C2-O2	9.05	129.13	122.80
47	2	1389	C	C6-N1-C2	-9.04	116.69	120.30
1	1	2405	C	N1-C2-O2	9.03	124.32	118.90
1	1	3355	U	N1-C2-O2	8.84	128.99	122.80
1	1	1281	G	C8-N9-C1'	-8.84	115.51	127.00
47	2	1342	C	C2-N1-C1'	8.84	128.52	118.80
1	1	1645	U	N3-C2-O2	-8.83	116.02	122.20
25	U	91	ASP	CB-CG-OD1	8.83	126.25	118.30
1	1	1309	U	N1-C2-O2	8.82	128.98	122.80
1	1	1194	G	N3-C4-N9	8.71	131.23	126.00
47	2	1374	C	C6-N1-C2	-8.70	116.82	120.30
1	1	2783	U	N3-C2-O2	-8.69	116.11	122.20
1	1	1309	U	N3-C2-O2	-8.69	116.12	122.20
1	1	1194	G	C8-N9-C1'	-8.66	115.74	127.00
1	1	3235	C	N1-C2-O2	8.64	124.09	118.90
1	1	1763	U	N3-C2-O2	-8.58	116.19	122.20
47	2	94	U	C2-N1-C1'	8.57	127.98	117.70
67	AJ	35	ASP	CB-CG-OD1	8.55	126.00	118.30
83	AZ	62	ASP	CB-CG-OD1	8.55	125.99	118.30
1	1	3355	U	C2-N1-C1'	8.55	127.95	117.70
1	1	1281	G	C4-N9-C1'	8.53	137.59	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	2	1246	C	C2-N1-C1'	8.54	128.19	118.80
2	3	94	C	C2-N1-C1'	8.53	128.18	118.80
1	1	1194	G	C4-N9-C1'	8.43	137.46	126.50
1	1	1645	U	N1-C2-O2	8.43	128.70	122.80
1	1	1280	C	N3-C2-O2	-8.39	116.03	121.90
1	1	1281	G	N3-C4-N9	8.39	131.03	126.00
1	1	3355	U	N3-C2-O2	-8.34	116.36	122.20
47	2	1342	C	N3-C2-O2	-8.32	116.08	121.90
1	1	78	U	N3-C2-O2	-8.30	116.39	122.20
59	AB	5	LEU	CA-CB-CG	8.28	134.35	115.30
4	P0	45	LEU	CA-CB-CG	8.27	134.32	115.30
1	1	524	U	N1-C2-O2	8.26	128.59	122.80
47	2	1389	C	N3-C2-O2	-8.26	116.11	121.90
47	2	1393	C	C5-C6-N1	8.24	125.12	121.00
1	1	2836	C	C2-N1-C1'	8.24	127.86	118.80
47	2	908	U	N1-C2-O2	8.21	128.54	122.80
1	1	226	C	N3-C2-O2	-8.20	116.16	121.90
47	2	1389	C	N1-C2-O2	8.20	123.82	118.90
47	2	190	C	N3-C2-O2	-8.19	116.17	121.90
1	1	1763	U	C2-N1-C1'	8.18	127.51	117.70
47	2	908	U	N3-C2-O2	-8.18	116.48	122.20
47	2	497	G	N3-C4-N9	8.15	130.89	126.00
65	AH	24	LEU	CA-CB-CG	8.14	134.03	115.30
47	2	1246	C	N3-C2-O2	-8.12	116.22	121.90
47	2	532	U	N3-C2-O2	-8.11	116.52	122.20
47	2	908	U	C2-N1-C1'	8.09	127.41	117.70
47	2	1653	C	C2-N1-C1'	8.09	127.69	118.80
37	g	81	CYS	CA-CB-SG	8.08	128.54	114.00
1	1	2652	U	N3-C2-O2	-8.06	116.56	122.20
1	1	1219	C	N1-C2-O2	8.05	123.73	118.90
1	1	3023	U	N3-C2-O2	-8.03	116.58	122.20
47	2	654	C	C6-N1-C1'	-8.02	111.18	120.80
1	1	292	U	C2-N1-C1'	8.00	127.31	117.70
1	1	2230	C	N3-C2-O2	-8.00	116.30	121.90
1	1	1856	C	N1-C2-O2	7.93	123.66	118.90
1	1	1857	C	C2-N1-C1'	7.93	127.52	118.80
1	1	2531	C	N1-C2-O2	7.90	123.64	118.90
47	2	965	U	C2-N1-C1'	7.89	127.17	117.70
1	1	2405	C	N3-C2-O2	-7.89	116.38	121.90
47	2	1571	C	N3-C2-O2	-7.88	116.38	121.90
47	2	1389	C	C2-N1-C1'	7.88	127.46	118.80
47	2	75	U	O5'-P-OP1	-7.87	98.61	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
81	AX	59	U	N1-C2-O2	7.86	128.30	122.80
1	1	1706	C	N1-C2-O2	7.85	123.61	118.90
1	1	2230	C	C2-N1-C1'	7.85	127.44	118.80
47	2	682	C	N1-C2-O2	7.81	123.59	118.90
47	2	431	C	C6-N1-C2	-7.80	117.18	120.30
47	2	1571	C	N1-C2-O2	7.80	123.58	118.90
1	1	3214	U	N1-C2-O2	7.80	128.26	122.80
1	1	1149	G	N3-C4-N9	-7.80	121.32	126.00
42	l	29	LEU	CA-CB-CG	7.80	133.23	115.30
1	1	2836	C	N3-C2-O2	-7.79	116.45	121.90
1	1	2305	G	N3-C4-C5	-7.77	124.72	128.60
47	2	1700	C	N1-C2-O2	7.76	123.56	118.90
81	AX	40	C	C2-N1-C1'	7.75	127.32	118.80
1	1	823	C	C6-N1-C2	-7.75	117.20	120.30
47	2	431	C	C2-N1-C1'	7.71	127.29	118.80
47	2	829	A	O4'-C1'-N9	7.71	114.37	108.20
81	AX	59	U	C2-N1-C1'	7.71	126.95	117.70
1	1	1551	C	N3-C2-O2	-7.71	116.50	121.90
1	1	3235	C	C6-N1-C2	-7.71	117.22	120.30
1	1	2765	C	C5-C6-N1	7.69	124.84	121.00
47	2	302	U	C2-N1-C1'	7.69	126.92	117.70
1	1	2132	C	C6-N1-C2	-7.66	117.23	120.30
47	2	646	C	C6-N1-C2	-7.65	117.24	120.30
1	1	1837	U	C2-N1-C1'	7.64	126.87	117.70
1	1	524	U	N3-C2-O2	-7.62	116.86	122.20
1	1	1281	G	N9-C4-C5	-7.61	102.36	105.40
47	2	498	G	N7-C8-N9	7.60	116.90	113.10
47	2	302	U	N1-C2-O2	7.55	128.09	122.80
1	1	638	C	C5-C6-N1	7.55	124.78	121.00
1	1	861	C	C2-N1-C1'	7.54	127.09	118.80
1	1	3034	C	N1-C2-O2	7.54	123.42	118.90
27	W	39	LEU	CA-CB-CG	7.53	132.61	115.30
47	2	1783	C	C5-C6-N1	7.51	124.76	121.00
1	1	1281	G	C6-C5-N7	-7.50	125.90	130.40
47	2	489	C	N1-C2-O2	7.49	123.39	118.90
47	2	1052	U	C2-N1-C1'	7.48	126.68	117.70
47	2	1773	C	C2-N1-C1'	7.48	127.03	118.80
1	1	2765	C	C6-N1-C2	-7.48	117.31	120.30
47	2	176	C	N1-C2-O2	7.47	123.38	118.90
47	2	453	U	C6-N1-C1'	-7.46	110.76	121.20
1	1	2263	C	C2-N1-C1'	7.43	126.97	118.80
1	1	3214	U	N3-C2-O2	-7.41	117.01	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	2	302	U	N3-C2-O2	-7.41	117.02	122.20
47	2	82	U	C2-N1-C1'	7.40	126.58	117.70
6	A	150	LEU	CA-CB-CG	7.39	132.30	115.30
1	1	19	U	C2-N1-C1'	7.38	126.55	117.70
69	AL	78	LEU	CA-CB-CG	7.37	132.25	115.30
1	1	1496	C	C6-N1-C2	-7.35	117.36	120.30
1	1	2333	C	N3-C2-O2	-7.34	116.76	121.90
1	1	2677	G	C4-N9-C1'	7.34	136.05	126.50
47	2	946	U	N1-C2-O2	7.31	127.92	122.80
1	1	2652	U	N1-C2-O2	7.29	127.90	122.80
1	1	1372	C	N1-C2-O2	7.28	123.27	118.90
1	1	1487	G	N3-C4-N9	-7.27	121.64	126.00
1	1	2783	U	N1-C2-O2	7.26	127.88	122.80
1	1	1137	C	N3-C2-O2	-7.26	116.82	121.90
7	B	351	LEU	CA-CB-CG	7.24	131.96	115.30
1	1	1525	G	C4-N9-C1'	7.22	135.89	126.50
1	1	1585	C	C2-N1-C1'	7.21	126.73	118.80
47	2	682	C	N3-C2-O2	-7.21	116.86	121.90
47	2	469	C	N1-C2-O2	7.20	123.22	118.90
47	2	70	C	C2-N1-C1'	7.20	126.72	118.80
1	1	1659	U	N3-C2-O2	-7.20	117.16	122.20
60	AC	28	LEU	CA-CB-CG	7.18	131.82	115.30
81	AX	59	U	N3-C2-O2	-7.18	117.17	122.20
1	1	1507	G	C4-N9-C1'	7.17	135.81	126.50
47	2	1470	C	C6-N1-C2	-7.16	117.44	120.30
1	1	2489	C	N1-C2-O2	7.16	123.20	118.90
47	2	706	A	P-O3'-C3'	7.14	128.27	119.70
47	2	94	U	N3-C2-O2	-7.14	117.20	122.20
1	1	1194	G	C6-C5-N7	-7.13	126.12	130.40
47	2	489	C	C6-N1-C2	-7.12	117.45	120.30
47	2	532	U	N1-C2-O2	7.11	127.77	122.80
1	1	2305	G	N3-C4-N9	7.10	130.26	126.00
1	1	1281	G	C4-C5-N7	7.10	113.64	110.80
1	1	1280	C	C6-N1-C2	-7.09	117.47	120.30
1	1	142	C	N1-C2-O2	7.08	123.15	118.90
1	1	3023	U	C2-N1-C1'	7.08	126.19	117.70
1	1	2415	C	C6-N1-C2	-7.07	117.47	120.30
81	AX	56	C	C2-N1-C1'	7.05	126.56	118.80
1	1	1155	C	N1-C2-O2	7.04	123.12	118.90
2	3	81	U	C2-N1-C1'	7.03	126.14	117.70
1	1	260	C	N3-C2-O2	-7.02	116.99	121.90
47	2	228	G	N3-C4-N9	7.00	130.20	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	19	U	N1-C2-O2	7.00	127.70	122.80
47	2	828	U	N3-C2-O2	-6.99	117.31	122.20
47	2	1674	C	C2-N1-C1'	6.99	126.49	118.80
47	2	654	C	C5-C6-N1	6.99	124.49	121.00
57	z	93	LEU	CA-CB-CG	6.97	131.34	115.30
1	1	1121	U	C2-N1-C1'	6.97	126.06	117.70
81	AX	40	C	N1-C2-O2	6.96	123.07	118.90
1	1	2606	G	N3-C4-N9	6.95	130.17	126.00
1	1	1297	C	N1-C2-O2	6.94	123.06	118.90
1	1	524	U	C2-N1-C1'	6.93	126.02	117.70
1	1	2336	U	N3-C2-O2	-6.92	117.35	122.20
47	2	841	U	C5-C6-N1	6.91	126.16	122.70
1	1	2305	G	C4-N9-C1'	6.91	135.48	126.50
1	1	1496	C	N1-C2-O2	6.90	123.04	118.90
47	2	767	U	C6-N1-C1'	-6.90	111.54	121.20
1	1	2550	U	N3-C2-O2	-6.90	117.37	122.20
29	Y	126	LEU	CA-CB-CG	6.89	131.16	115.30
47	2	1338	C	P-O3'-C3'	6.89	127.97	119.70
47	2	1470	C	C5-C6-N1	6.89	124.45	121.00
47	2	1458	G	C4-N9-C1'	6.89	135.46	126.50
3	4	100	U	C2-N1-C1'	6.89	125.96	117.70
1	1	1194	G	N9-C4-C5	-6.88	102.65	105.40
81	AX	56	C	C5-C6-N1	6.88	124.44	121.00
1	1	1857	C	C6-N1-C2	-6.88	117.55	120.30
1	1	2677	G	N3-C4-C5	-6.87	125.17	128.60
1	1	2950	G	C4-N9-C1'	6.87	135.43	126.50
1	1	1551	C	N1-C2-O2	6.86	123.02	118.90
47	2	1185	U	C2-N1-C1'	6.86	125.93	117.70
47	2	1783	C	C2-N1-C1'	6.86	126.34	118.80
1	1	1564	U	C5-C6-N1	6.85	126.13	122.70
47	2	498	G	N1-C2-N2	-6.85	110.03	116.20
1	1	2950	G	N3-C4-C5	-6.84	125.18	128.60
47	2	532	U	C2-N1-C1'	6.84	125.91	117.70
1	1	934	G	C4-N9-C1'	6.84	135.39	126.50
83	AZ	77	LEU	CA-CB-CG	6.84	131.03	115.30
1	1	1297	C	C2-N1-C1'	6.83	126.32	118.80
1	1	3023	U	N1-C2-O2	6.83	127.58	122.80
47	2	489	C	N3-C2-O2	-6.83	117.12	121.90
1	1	1137	C	C2-N1-C1'	6.83	126.31	118.80
1	1	1349	G	C4-N9-C1'	6.83	135.38	126.50
1	1	2263	C	C5-C6-N1	6.82	124.41	121.00
1	1	3034	C	N3-C2-O2	-6.82	117.13	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	Y	48	LEU	CA-CB-CG	6.82	130.98	115.30
47	2	176	C	N3-C2-O2	-6.81	117.13	121.90
83	AZ	143	LEU	CA-CB-CG	6.81	130.96	115.30
1	1	2230	C	C6-N1-C2	-6.79	117.58	120.30
47	2	270	C	C2-N1-C1'	6.79	126.27	118.80
40	j	64	MET	CA-CB-CG	6.79	124.84	113.30
1	1	1878	G	C4-N9-C1'	6.77	135.31	126.50
1	1	1907	C	N1-C2-O2	6.76	122.96	118.90
1	1	2498	U	C2-N1-C1'	6.76	125.81	117.70
1	1	1781	C	C2-N1-C1'	6.76	126.23	118.80
1	1	2606	G	N3-C4-C5	-6.75	125.22	128.60
47	2	82	U	N1-C2-O2	6.75	127.52	122.80
47	2	1257	U	N3-C2-O2	-6.74	117.48	122.20
1	1	2102	U	N3-C2-O2	-6.72	117.49	122.20
1	1	1458	U	N3-C2-O2	-6.71	117.50	122.20
1	1	823	C	C5-C6-N1	6.71	124.36	121.00
47	2	17	C	C5-C6-N1	6.71	124.35	121.00
1	1	1275	C	C6-N1-C2	-6.70	117.62	120.30
47	2	646	C	C5-C6-N1	6.70	124.35	121.00
47	2	946	U	C2-N1-C1'	6.69	125.73	117.70
8	C	219	LEU	CA-CB-CG	6.69	130.69	115.30
1	1	1562	C	N1-C2-O2	6.69	122.91	118.90
1	1	2583	C	C2-N1-C1'	6.68	126.15	118.80
1	1	1168	U	N3-C2-O2	-6.68	117.52	122.20
47	2	946	U	N3-C2-O2	-6.68	117.53	122.20
47	2	1173	C	C2-N1-C1'	6.68	126.15	118.80
1	1	1659	U	N1-C2-O2	6.66	127.46	122.80
8	C	182	LEU	CA-CB-CG	6.66	130.62	115.30
1	1	1525	G	C8-N9-C1'	-6.66	118.34	127.00
47	2	1715	G	C4-N9-C1'	6.66	135.16	126.50
1	1	3078	U	P-O3'-C3'	6.65	127.68	119.70
1	1	2405	C	C2-N1-C1'	6.64	126.11	118.80
1	1	1496	C	C5-C6-N1	6.64	124.32	121.00
1	1	2846	U	N3-C2-O2	-6.64	117.55	122.20
1	1	2102	U	N1-C2-O2	6.61	127.42	122.80
47	2	1327	C	C2-N1-C1'	6.60	126.06	118.80
47	2	1715	G	N3-C4-N9	6.60	129.96	126.00
47	2	842	C	C6-N1-C2	-6.59	117.66	120.30
1	1	2677	G	N3-C4-N9	6.59	129.95	126.00
47	2	1222	C	N1-C2-O2	6.58	122.85	118.90
47	2	1540	G	C4-N9-C1'	6.58	135.06	126.50
47	2	94	U	N1-C2-N3	6.58	118.85	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	2132	C	N3-C2-O2	-6.57	117.30	121.90
47	2	376	C	C2-N1-C1'	6.57	126.03	118.80
1	1	2415	C	C2-N1-C1'	6.57	126.02	118.80
47	2	2	A	O5'-P-OP1	-6.57	99.79	105.70
47	2	1332	C	C2-N1-C1'	6.54	126.00	118.80
47	2	296	U	N1-C2-O2	6.54	127.38	122.80
1	1	1219	C	N3-C2-O2	-6.54	117.32	121.90
1	1	2773	C	C6-N1-C2	-6.54	117.69	120.30
1	1	2378	C	C2-N1-C1'	6.53	125.98	118.80
1	1	1659	U	C2-N1-C1'	6.53	125.53	117.70
2	3	81	U	N1-C2-O2	6.52	127.37	122.80
81	AX	40	C	C6-N1-C2	-6.51	117.69	120.30
1	1	3346	U	C2-N1-C1'	6.51	125.51	117.70
47	2	1374	C	N3-C2-O2	-6.51	117.34	121.90
1	1	1292	C	C2-N1-C1'	6.50	125.95	118.80
1	1	1590	G	N3-C4-N9	6.50	129.90	126.00
1	1	2867	C	N3-C2-O2	-6.50	117.35	121.90
47	2	320	U	N1-C2-O2	6.50	127.35	122.80
49	r	61	LEU	CA-CB-CG	6.50	130.25	115.30
1	1	1525	G	N3-C4-N9	6.49	129.89	126.00
47	2	1709	C	N1-C2-O2	6.49	122.79	118.90
58	AA	88	PRO	N-CA-CB	6.49	111.08	103.30
47	2	431	C	N1-C2-O2	6.48	122.79	118.90
1	1	2765	C	C2-N1-C1'	6.47	125.92	118.80
1	1	1227	C	C5-C6-N1	6.47	124.23	121.00
1	1	1507	G	N3-C4-N9	6.46	129.88	126.00
1	1	2846	U	C2-N1-C1'	6.46	125.45	117.70
47	2	497	G	N9-C4-C5	-6.45	102.82	105.40
1	1	492	C	C2-N1-C1'	6.44	125.89	118.80
47	2	1734	U	N3-C2-O2	-6.43	117.70	122.20
81	AX	56	C	C6-N1-C2	-6.43	117.73	120.30
1	1	1027	A	C2-N3-C4	6.43	113.81	110.60
1	1	1309	U	C2-N1-C1'	6.43	125.41	117.70
47	2	1697	G	C4-N9-C1'	6.43	134.85	126.50
1	1	1219	C	C6-N1-C2	-6.42	117.73	120.30
47	2	1389	C	C5-C6-N1	6.42	124.21	121.00
1	1	1590	G	C4-N9-C1'	6.42	134.85	126.50
1	1	1194	G	N3-C2-N2	6.41	124.39	119.90
1	1	1277	C	N1-C2-O2	6.41	122.75	118.90
1	1	1706	C	N3-C2-O2	-6.41	117.41	121.90
1	1	623	U	N1-C2-O2	6.41	127.28	122.80
47	2	700	C	N1-C2-O2	6.39	122.74	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	3	94	C	C6-N1-C2	-6.39	117.74	120.30
47	2	296	U	N3-C2-O2	-6.39	117.73	122.20
1	1	2347	U	N1-C2-O2	6.38	127.27	122.80
1	1	2726	C	C2-N1-C1'	6.38	125.82	118.80
3	4	64	U	N3-C2-O2	-6.38	117.73	122.20
81	AX	25	C	N1-C2-O2	6.38	122.73	118.90
1	1	623	U	N3-C2-O2	-6.37	117.74	122.20
2	3	81	U	N3-C2-O2	-6.37	117.74	122.20
47	2	1029	U	N3-C2-O2	-6.37	117.74	122.20
54	w	68	LEU	CA-CB-CG	6.37	129.94	115.30
47	2	1393	C	C6-N1-C2	-6.36	117.75	120.30
1	1	1234	G	C5-C6-O6	6.36	132.42	128.60
47	2	70	C	N1-C2-O2	6.36	122.72	118.90
1	1	3181	C	C2-N1-C1'	6.36	125.79	118.80
1	1	492	C	C5-C6-N1	6.36	124.18	121.00
1	1	2617	U	N3-C2-O2	-6.36	117.75	122.20
47	2	1624	C	C2-N1-C1'	6.35	125.79	118.80
47	2	583	C	C6-N1-C2	-6.35	117.76	120.30
1	1	278	U	N1-C2-O2	6.35	127.24	122.80
1	1	1121	U	N1-C2-O2	6.34	127.24	122.80
1	1	2383	C	N1-C2-O2	6.34	122.71	118.90
1	1	2531	C	N3-C2-O2	-6.34	117.46	121.90
1	1	2638	C	N1-C2-O2	6.34	122.71	118.90
47	2	1620	C	N1-C2-O2	6.34	122.70	118.90
1	1	1507	G	C8-N9-C1'	-6.33	118.78	127.00
47	2	1653	C	C6-N1-C2	-6.32	117.77	120.30
47	2	1773	C	N1-C2-O2	6.31	122.69	118.90
1	1	638	C	C6-N1-C2	-6.30	117.78	120.30
1	1	1843	C	N1-C2-O2	6.30	122.68	118.90
1	1	2347	U	C2-N1-C1'	6.30	125.27	117.70
47	2	608	U	N3-C2-O2	-6.30	117.79	122.20
47	2	656	G	N3-C4-C5	-6.30	125.45	128.60
81	AX	32	C	N1-C2-O2	6.29	122.68	118.90
1	1	1194	G	C4-C5-N7	6.29	113.31	110.80
47	2	431	C	C5-C6-N1	6.29	124.14	121.00
47	2	411	C	C2-N1-C1'	6.28	125.71	118.80
1	1	3214	U	C2-N1-C1'	6.28	125.23	117.70
2	3	94	C	C5-C6-N1	6.28	124.14	121.00
1	1	1155	C	C6-N1-C2	-6.28	117.79	120.30
47	2	35	U	N3-C2-O2	-6.27	117.81	122.20
47	2	696	C	N1-C2-O2	6.27	122.66	118.90
81	AX	70	C	C5-C6-N1	6.26	124.13	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	27	C	N1-C2-O2	6.26	122.66	118.90
47	2	317	C	C5-C6-N1	6.26	124.13	121.00
1	1	1262	G	C4-N9-C1'	6.26	134.64	126.50
47	2	583	C	C2-N1-C1'	6.26	125.68	118.80
1	1	1349	G	N3-C4-N9	6.25	129.75	126.00
1	1	8	C	C5-C6-N1	6.24	124.12	121.00
1	1	19	U	N3-C2-O2	-6.24	117.83	122.20
47	2	1439	C	C5-C6-N1	6.24	124.12	121.00
50	s	235	LEU	CA-CB-CG	6.24	129.64	115.30
1	1	1333	C	C2-N1-C1'	6.24	125.66	118.80
47	2	1246	C	C6-N1-C2	-6.23	117.81	120.30
47	2	94	U	C5-C4-O4	-6.23	122.16	125.90
1	1	1372	C	N3-C2-O2	-6.23	117.54	121.90
58	AA	2	LEU	CA-CB-CG	6.22	129.61	115.30
52	u	38	LEU	CA-CB-CG	6.22	129.60	115.30
1	1	3057	U	N1-C2-O2	6.22	127.15	122.80
47	2	453	U	C5-C6-N1	6.21	125.81	122.70
1	1	2132	C	N1-C2-O2	6.21	122.63	118.90
1	1	2846	U	N1-C2-O2	6.21	127.14	122.80
1	1	1857	C	N3-C2-O2	-6.20	117.56	121.90
83	AZ	639	ASP	CB-CG-OD1	6.20	123.88	118.30
47	2	633	U	N3-C2-O2	-6.20	117.86	122.20
1	1	382	U	C2-N1-C1'	6.19	125.12	117.70
1	1	2498	U	N1-C2-O2	6.19	127.13	122.80
1	1	2677	G	C8-N9-C1'	-6.18	118.97	127.00
83	AZ	320	LEU	CA-CB-CG	6.17	129.50	115.30
1	1	492	C	C6-N1-C2	-6.17	117.83	120.30
1	1	855	U	C2-N1-C1'	6.17	125.10	117.70
47	2	1591	C	C6-N1-C2	-6.16	117.84	120.30
1	1	986	U	N3-C2-O2	-6.16	117.89	122.20
1	1	430	U	N1-C2-O2	6.15	127.11	122.80
1	1	669	U	C2-N1-C1'	6.15	125.08	117.70
1	1	1275	C	N1-C2-O2	6.14	122.59	118.90
47	2	836	U	C5-C6-N1	6.14	125.77	122.70
1	1	2418	G	C4-N9-C1'	6.14	134.48	126.50
1	1	669	U	N1-C2-O2	6.13	127.09	122.80
47	2	1518	C	N1-C2-O2	6.13	122.58	118.90
1	1	2550	U	N1-C2-O2	6.13	127.09	122.80
1	1	1590	G	C8-N9-C1'	-6.12	119.04	127.00
79	AV	144	LEU	CA-CB-CG	6.12	129.39	115.30
1	1	3001	C	C2-N1-C1'	6.12	125.53	118.80
1	1	1121	U	N3-C2-O2	-6.12	117.92	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	2763	U	N3-C2-O2	-6.11	117.92	122.20
47	2	1697	G	N3-C4-N9	6.11	129.67	126.00
1	1	3388	C	C6-N1-C2	-6.10	117.86	120.30
47	2	1342	C	C6-N1-C2	-6.10	117.86	120.30
47	2	1700	C	N3-C2-O2	-6.09	117.63	121.90
47	2	497	G	C8-N9-C1'	-6.09	119.08	127.00
47	2	608	U	N1-C2-O2	6.09	127.06	122.80
47	2	1029	U	N1-C2-O2	6.08	127.06	122.80
2	3	4	U	C2-N1-C1'	6.08	124.99	117.70
47	2	528	U	N1-C2-O2	6.08	127.05	122.80
1	1	78	U	N1-C2-O2	6.07	127.05	122.80
1	1	1555	U	N1-C2-O2	6.07	127.05	122.80
1	1	1907	C	N3-C2-O2	-6.07	117.65	121.90
47	2	1168	U	N3-C2-O2	-6.07	117.95	122.20
1	1	2531	C	C2-N1-C1'	6.06	125.47	118.80
1	1	2622	C	C6-N1-C2	-6.05	117.88	120.30
1	1	2899	C	C2-N1-C1'	6.05	125.45	118.80
1	1	2383	C	C6-N1-C2	-6.04	117.88	120.30
1	1	954	U	N3-C2-O2	-6.04	117.97	122.20
1	1	1645	U	C2-N1-C1'	6.04	124.95	117.70
47	2	1342	C	C6-N1-C1'	-6.03	113.56	120.80
47	2	1518	C	C2-N1-C1'	6.03	125.43	118.80
47	2	1337	A	O4'-C1'-N9	6.03	113.02	108.20
1	1	2383	C	N3-C2-O2	-6.02	117.69	121.90
1	1	3057	U	N3-C2-O2	-6.01	117.99	122.20
47	2	1729	C	C2-N1-C1'	6.01	125.41	118.80
1	1	3131	U	C2-N1-C1'	6.00	124.90	117.70
1	1	3346	U	N3-C2-O2	-6.00	118.00	122.20
1	1	3346	U	N1-C2-O2	6.00	127.00	122.80
1	1	2983	C	N1-C2-O2	5.99	122.50	118.90
1	1	1507	G	O5'-P-OP2	-5.99	100.31	105.70
1	1	2763	U	N1-C2-O2	5.99	126.99	122.80
81	AX	25	C	N3-C2-O2	-5.99	117.71	121.90
1	1	2541	U	P-O3'-C3'	5.99	126.89	119.70
1	1	3034	C	C6-N1-C2	-5.99	117.90	120.30
1	1	1037	C	C2-N1-C1'	5.98	125.38	118.80
1	1	1604	G	C4-N9-C1'	5.98	134.28	126.50
47	2	1336	A	C8-N9-C4	-5.98	103.41	105.80
47	2	489	C	C5-C6-N1	5.98	123.99	121.00
1	1	1608	C	C2-N1-C1'	5.98	125.38	118.80
1	1	2666	C	N1-C2-O2	5.97	122.48	118.90
1	1	3057	U	C2-N1-C1'	5.97	124.87	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	1555	U	N3-C2-O2	-5.97	118.02	122.20
1	1	1878	G	C8-N9-C1'	-5.97	119.23	127.00
21	Q	41	ASP	CB-CG-OD1	5.97	123.67	118.30
2	3	4	U	N3-C2-O2	-5.97	118.02	122.20
47	2	734	A	C2-N3-C4	5.97	113.58	110.60
1	1	669	U	N3-C2-O2	-5.96	118.03	122.20
68	AK	50	LEU	CA-CB-CG	5.95	128.98	115.30
1	1	1889	G	C4-N9-C1'	5.95	134.23	126.50
2	3	105	C	N1-C2-O2	5.95	122.47	118.90
47	2	1214	U	N1-C2-O2	5.95	126.96	122.80
1	1	1137	C	C6-N1-C2	-5.94	117.92	120.30
1	1	492	C	N1-C2-O2	5.94	122.47	118.90
47	2	1703	C	N1-C2-O2	5.94	122.47	118.90
47	2	1729	C	N1-C2-O2	5.94	122.46	118.90
47	2	1751	C	C2-N1-C1'	5.94	125.33	118.80
1	1	1508	C	C6-N1-C1'	5.94	127.92	120.80
1	1	1496	C	C6-N1-C1'	-5.93	113.68	120.80
47	2	528	U	N3-C2-O2	-5.93	118.05	122.20
70	AM	54	ASP	CB-CG-OD1	5.93	123.64	118.30
1	1	1168	U	N1-C2-O2	5.93	126.95	122.80
1	1	2726	C	N1-C2-O2	5.93	122.46	118.90
47	2	908	U	C5-C6-N1	5.93	125.67	122.70
47	2	18	C	C6-N1-C2	-5.93	117.93	120.30
47	2	1624	C	C6-N1-C2	-5.93	117.93	120.30
47	2	1273	G	P-O3'-C3'	5.92	126.81	119.70
15	J	112	LEU	CA-CB-CG	5.92	128.92	115.30
1	1	1279	C	C5-C6-N1	5.92	123.96	121.00
47	2	1115	U	C2-N1-C1'	5.92	124.80	117.70
1	1	1149	G	N3-C4-C5	5.91	131.56	128.60
1	1	1516	C	N1-C2-O2	5.91	122.45	118.90
1	1	1806	A	N7-C8-N9	5.91	116.75	113.80
1	1	142	C	N3-C2-O2	-5.91	117.77	121.90
3	4	64	U	C2-N1-C1'	5.91	124.79	117.70
1	1	863	C	C2-N1-C1'	5.90	125.29	118.80
47	2	656	G	C4-N9-C1'	5.90	134.17	126.50
47	2	1697	G	C8-N9-C1'	-5.90	119.33	127.00
1	1	1565	G	N3-C4-N9	5.89	129.54	126.00
1	1	2606	G	C4-N9-C1'	5.89	134.16	126.50
47	2	759	U	N3-C2-O2	-5.89	118.07	122.20
47	2	611	U	P-O3'-C3'	5.89	126.77	119.70
1	1	1349	G	C8-N9-C1'	-5.89	119.34	127.00
47	2	1374	C	C5-C6-N1	5.88	123.94	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	823	C	C6-N1-C1'	-5.88	113.75	120.80
47	2	902	G	C6-C5-N7	-5.87	126.88	130.40
47	2	1439	C	C6-N1-C2	-5.87	117.95	120.30
1	1	2263	C	C6-N1-C2	-5.87	117.95	120.30
3	4	26	U	C5-C6-N1	5.87	125.63	122.70
47	2	1173	C	C6-N1-C2	-5.87	117.95	120.30
47	2	497	G	C4-N9-C1'	5.87	134.13	126.50
51	t	113	LEU	CA-CB-CG	5.87	128.79	115.30
47	2	1332	C	C6-N1-C2	-5.86	117.95	120.30
1	1	2773	C	N3-C2-O2	-5.86	117.80	121.90
1	1	1907	C	C6-N1-C2	-5.86	117.96	120.30
47	2	1270	G	C8-N9-C1'	5.86	134.62	127.00
63	AF	69	GLU	C-N-CA	5.86	136.35	121.70
1	1	855	U	N3-C2-O2	-5.86	118.10	122.20
47	2	1773	C	C6-N1-C2	-5.85	117.96	120.30
47	2	394	C	C6-N1-C2	-5.85	117.96	120.30
1	1	2388	U	N3-C2-O2	-5.85	118.11	122.20
47	2	575	C	N1-C2-O2	5.85	122.41	118.90
1	1	1507	G	N3-C4-C5	-5.85	125.68	128.60
47	2	1458	G	C8-N9-C1'	-5.85	119.40	127.00
1	1	934	G	C8-N9-C1'	-5.84	119.40	127.00
1	1	2347	U	N3-C2-O2	-5.84	118.11	122.20
1	1	1280	C	N1-C2-O2	5.84	122.40	118.90
1	1	292	U	C5-C6-N1	5.83	125.62	122.70
1	1	2493	U	C2-N1-C1'	5.83	124.69	117.70
47	2	1066	C	N3-C2-O2	-5.82	117.83	121.90
47	2	1409	G	O4'-C1'-N9	5.82	112.85	108.20
1	1	1351	U	C2-N1-C1'	5.81	124.67	117.70
47	2	1327	C	C6-N1-C2	-5.81	117.98	120.30
47	2	1715	G	C8-N9-C1'	-5.81	119.45	127.00
1	1	1239	C	C2-N1-C1'	5.81	125.19	118.80
1	1	380	U	C2-N1-C1'	5.81	124.67	117.70
47	2	1783	C	C6-N1-C2	-5.81	117.98	120.30
1	1	2950	G	N3-C4-N9	5.80	129.48	126.00
1	1	1843	C	C2-N1-C1'	5.79	125.17	118.80
1	1	2305	G	C8-N9-C1'	-5.79	119.47	127.00
1	1	2189	U	N1-C2-O2	5.79	126.85	122.80
47	2	489	C	C2-N1-C1'	5.79	125.17	118.80
1	1	8	C	C2-N1-C1'	5.79	125.16	118.80
30	Z	103	GLN	CA-CB-CG	5.79	126.13	113.40
47	2	38	C	C6-N1-C2	-5.79	117.99	120.30
3	4	64	U	N1-C2-O2	5.78	126.85	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	2	453	U	C6-N1-C2	-5.78	117.53	121.00
79	AV	165	ASP	CB-CG-OD1	5.78	123.50	118.30
47	2	296	U	C2-N1-C1'	5.78	124.64	117.70
47	2	1458	G	N3-C4-N9	5.78	129.47	126.00
47	2	1225	U	N1-C2-O2	5.78	126.84	122.80
1	1	2822	U	N3-C2-O2	-5.78	118.16	122.20
1	1	3004	C	P-O3'-C3'	5.78	126.63	119.70
18	N	51	LEU	CA-CB-CG	5.78	128.58	115.30
1	1	2495	C	N1-C2-O2	5.77	122.36	118.90
1	1	2306	C	P-O3'-C3'	5.77	126.62	119.70
1	1	2943	G	N3-C4-N9	5.76	129.46	126.00
1	1	2263	C	N1-C2-O2	5.76	122.36	118.90
1	1	804	C	C6-N1-C2	-5.75	118.00	120.30
1	1	3181	C	N1-C2-O2	5.75	122.35	118.90
1	1	2822	U	N1-C2-O2	5.74	126.82	122.80
1	1	885	U	N3-C2-O2	-5.74	118.18	122.20
1	1	1234	G	N1-C6-O6	-5.74	116.45	119.90
47	2	1591	C	C5-C6-N1	5.74	123.87	121.00
1	1	1857	C	N1-C2-O2	5.74	122.34	118.90
47	2	347	G	C4-N9-C1'	5.74	133.96	126.50
47	2	1565	C	C6-N1-C2	-5.74	118.01	120.30
1	1	1016	C	C6-N1-C2	-5.73	118.01	120.30
47	2	519	C	C6-N1-C2	-5.73	118.01	120.30
1	1	2726	C	N3-C2-O2	-5.73	117.89	121.90
1	1	3105	U	N3-C2-O2	-5.73	118.19	122.20
47	2	1298	U	P-O3'-C3'	5.73	126.57	119.70
47	2	833	U	N3-C4-O4	-5.73	115.39	119.40
1	1	3078	U	OP2-P-O3'	5.72	117.79	105.20
1	1	2836	C	C6-N1-C1'	-5.72	113.94	120.80
2	3	4	U	N1-C2-O2	5.72	126.80	122.80
47	2	768	C	N1-C2-O2	5.72	122.33	118.90
1	1	3130	A	O4'-C1'-N9	5.71	112.77	108.20
1	1	1779	C	C6-N1-C2	-5.71	118.02	120.30
47	2	1246	C	C6-N1-C1'	-5.71	113.95	120.80
1	1	1086	C	C6-N1-C2	-5.71	118.02	120.30
1	1	1562	C	N3-C2-O2	-5.70	117.91	121.90
2	3	28	C	N1-C2-O2	5.70	122.32	118.90
47	2	1734	U	N1-C2-O2	5.70	126.79	122.80
47	2	780	A	O5'-P-OP1	-5.69	100.58	105.70
47	2	1029	U	C2-N1-C1'	5.69	124.53	117.70
52	u	94	ALA	C-N-CA	5.69	135.93	121.70
3	4	50	C	C6-N1-C2	-5.69	118.02	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	2	828	U	N1-C2-O2	5.69	126.78	122.80
47	2	1115	U	N3-C2-O2	-5.69	118.22	122.20
47	2	315	A	P-O3'-C3'	5.68	126.52	119.70
1	1	774	G	C4-N9-C1'	5.68	133.88	126.50
47	2	17	C	C2-N1-C1'	5.68	125.05	118.80
47	2	1342	C	C5-C6-N1	5.68	123.84	121.00
1	1	2583	C	N1-C2-O2	5.67	122.30	118.90
1	1	1779	C	N1-C2-O2	5.67	122.30	118.90
1	1	2950	G	C8-N9-C4	-5.67	104.13	106.40
2	3	94	C	C6-N1-C1'	-5.67	113.99	120.80
47	2	1585	U	N1-C2-O2	5.67	126.77	122.80
83	AZ	645	LEU	CA-CB-CG	5.67	128.34	115.30
1	1	2189	U	C2-N1-C1'	5.67	124.50	117.70
1	1	861	C	C6-N1-C2	-5.66	118.03	120.30
1	1	3104	U	N3-C2-O2	-5.66	118.23	122.20
47	2	1608	U	C2-N1-C1'	5.66	124.49	117.70
1	1	278	U	N3-C2-O2	-5.66	118.24	122.20
1	1	1283	C	P-O3'-C3'	5.66	126.49	119.70
47	2	18	C	C5-C6-N1	5.66	123.83	121.00
81	AX	44	A	C2-N3-C4	5.66	113.43	110.60
1	1	2102	U	C2-N1-C1'	5.65	124.48	117.70
1	1	7	C	N3-C2-O2	-5.65	117.94	121.90
47	2	965	U	C6-N1-C1'	-5.65	113.28	121.20
2	3	58	C	C2-N1-C1'	5.65	125.02	118.80
47	2	108	A	N7-C8-N9	5.65	116.63	113.80
1	1	1086	C	C2-N1-C1'	5.65	125.01	118.80
47	2	320	U	N3-C2-O2	-5.65	118.25	122.20
1	1	1565	G	N3-C4-C5	-5.65	125.78	128.60
47	2	35	U	N1-C2-O2	5.65	126.75	122.80
47	2	908	U	C6-N1-C2	-5.64	117.61	121.00
74	AQ	18	VAL	C-N-CA	5.64	135.81	121.70
47	2	320	U	C2-N1-C1'	5.64	124.47	117.70
81	AX	32	C	N3-C2-O2	-5.64	117.95	121.90
1	1	3386	G	C4-N9-C1'	5.64	133.83	126.50
47	2	1674	C	C6-N1-C2	-5.64	118.05	120.30
47	2	1491	U	P-O3'-C3'	5.63	126.46	119.70
1	1	2230	C	C5-C6-N1	5.63	123.81	121.00
47	2	841	U	C2-N1-C1'	5.63	124.45	117.70
47	2	1270	G	C4-N9-C1'	-5.63	119.19	126.50
1	1	1281	G	C5-C6-O6	-5.62	125.23	128.60
1	1	2726	C	C6-N1-C2	-5.62	118.05	120.30
81	AX	40	C	C5-C6-N1	5.62	123.81	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	2	74	U	OP1-P-O3'	5.62	117.57	105.20
1	1	774	G	C8-N9-C1'	-5.62	119.69	127.00
1	1	8	C	C6-N1-C2	-5.61	118.06	120.30
2	3	18	C	C2-N1-C1'	5.61	124.98	118.80
47	2	1611	A	P-O3'-C3'	5.61	126.44	119.70
1	1	1856	C	C6-N1-C2	-5.61	118.06	120.30
47	2	1620	C	C2-N1-C1'	5.61	124.97	118.80
36	f	89	LEU	CA-CB-CG	5.61	128.19	115.30
47	2	270	C	N1-C2-O2	5.61	122.26	118.90
47	2	1067	C	C5-C6-N1	5.61	123.80	121.00
3	4	55	U	N3-C2-O2	-5.61	118.28	122.20
47	2	633	U	N1-C2-O2	5.61	126.72	122.80
47	2	1289	U	N3-C2-O2	-5.61	118.28	122.20
83	AZ	356	LEU	CA-CB-CG	5.60	128.19	115.30
1	1	855	U	N1-C2-O2	5.60	126.72	122.80
1	1	1279	C	C6-N1-C2	-5.60	118.06	120.30
1	1	986	U	N1-C2-O2	5.59	126.72	122.80
49	r	96	LEU	CA-CB-CG	5.59	128.17	115.30
47	2	1128	C	C6-N1-C2	-5.59	118.06	120.30
1	1	1604	G	C8-N9-C1'	-5.59	119.73	127.00
1	1	226	C	N1-C2-N3	5.59	123.11	119.20
1	1	774	G	N3-C4-N9	5.59	129.35	126.00
47	2	376	C	C5-C6-N1	5.59	123.79	121.00
47	2	779	U	P-O3'-C3'	5.58	126.40	119.70
47	2	497	G	C4-C5-N7	5.58	113.03	110.80
3	4	50	C	C2-N1-C1'	5.58	124.94	118.80
47	2	1494	C	C2-N1-C1'	5.58	124.94	118.80
47	2	1514	U	N1-C2-O2	5.58	126.70	122.80
1	1	781	G	N3-C4-C5	-5.58	125.81	128.60
47	2	74	U	P-O3'-C3'	5.58	126.39	119.70
47	2	411	C	C6-N1-C2	-5.57	118.07	120.30
47	2	1700	C	C2-N1-C1'	5.57	124.93	118.80
1	1	540	U	N3-C2-O2	-5.57	118.30	122.20
1	1	1585	C	N1-C2-O2	5.56	122.24	118.90
47	2	941	A	P-O3'-C3'	5.56	126.37	119.70
81	AX	1	G	OP1-P-OP2	5.56	127.94	119.60
1	1	1292	C	N1-C2-O2	5.55	122.23	118.90
24	T	19	PHE	C-N-CA	5.55	135.57	121.70
1	1	2378	C	C6-N1-C2	-5.54	118.08	120.30
47	2	1684	U	N1-C2-O2	5.54	126.68	122.80
58	AA	49	LEU	CA-CB-CG	5.54	128.04	115.30
68	AK	93	LEU	CA-CB-CG	5.54	128.03	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	2	1585	U	N3-C2-O2	-5.53	118.33	122.20
1	1	259	C	N1-C2-O2	5.53	122.22	118.90
1	1	1878	G	N3-C4-N9	5.53	129.32	126.00
1	1	3355	U	C6-N1-C1'	-5.53	113.46	121.20
47	2	569	C	N1-C2-O2	5.52	122.21	118.90
47	2	1405	G	C4-C5-N7	5.52	113.01	110.80
1	1	675	C	C2-N1-C1'	5.52	124.87	118.80
1	1	1255	C	C5-C6-N1	5.52	123.76	121.00
61	AD	45	LEU	CA-CB-CG	5.52	127.99	115.30
47	2	196	G	N1-C2-N2	-5.51	111.24	116.20
47	2	376	C	C6-N1-C2	-5.51	118.09	120.30
1	1	967	A	N7-C8-N9	5.51	116.55	113.80
57	z	101	VAL	C-N-CA	5.51	135.47	121.70
1	1	142	C	C6-N1-C2	-5.50	118.10	120.30
1	1	934	G	N3-C4-C5	-5.50	125.85	128.60
1	1	1907	C	C2-N1-C1'	5.50	124.85	118.80
1	1	2210	G	N3-C4-C5	-5.50	125.85	128.60
47	2	497	G	C6-C5-N7	-5.50	127.10	130.40
47	2	1399	C	P-O3'-C3'	5.50	126.30	119.70
1	1	1053	A	P-O3'-C3'	5.50	126.30	119.70
47	2	1270	G	N3-C4-N9	-5.50	122.70	126.00
1	1	1487	G	C5-C6-O6	5.50	131.90	128.60
47	2	176	C	C2-N1-C1'	5.50	124.85	118.80
47	2	780	A	C2-N3-C4	5.50	113.35	110.60
1	1	1805	C	C6-N1-C2	-5.50	118.10	120.30
1	1	7	C	N1-C2-O2	5.49	122.19	118.90
1	1	1211	U	N3-C2-O2	-5.49	118.36	122.20
47	2	921	U	C2-N1-C1'	5.49	124.29	117.70
47	2	1632	C	N1-C2-O2	5.49	122.19	118.90
79	AV	243	LEU	CA-CB-CG	5.48	127.91	115.30
1	1	524	U	C5-C6-N1	5.48	125.44	122.70
1	1	315	C	C2-N1-C1'	5.48	124.83	118.80
1	1	1262	G	C8-N9-C1'	-5.48	119.88	127.00
47	2	1585	U	C2-N1-C1'	5.48	124.27	117.70
1	1	1706	C	C2-N1-C1'	5.47	124.82	118.80
47	2	1327	C	C5-C6-N1	5.47	123.74	121.00
83	AZ	718	LEU	CA-CB-CG	5.47	127.89	115.30
1	1	1275	C	N3-C2-O2	-5.47	118.07	121.90
19	O	194	LEU	CA-CB-CG	5.47	127.88	115.30
12	G	162	LEU	CA-CB-CG	5.46	127.87	115.30
1	1	2772	C	N1-C2-O2	5.46	122.18	118.90
3	4	55	U	N1-C2-O2	5.46	126.62	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	3	94	C	N1-C2-O2	5.46	122.17	118.90
1	1	2606	G	C8-N9-C1'	-5.45	119.91	127.00
47	2	229	U	C5-C6-N1	5.45	125.43	122.70
1	1	877	C	N1-C2-O2	5.45	122.17	118.90
1	1	2836	C	C6-N1-C2	-5.45	118.12	120.30
47	2	302	U	C5-C6-N1	5.45	125.42	122.70
1	1	2192	C	C2-N1-C1'	5.45	124.79	118.80
1	1	3176	G	O5'-P-OP1	-5.45	100.80	105.70
1	1	1843	C	N3-C2-O2	-5.44	118.09	121.90
1	1	1878	G	N3-C4-C5	-5.44	125.88	128.60
1	1	2189	U	N3-C2-O2	-5.44	118.39	122.20
1	1	2516	U	N3-C2-O2	-5.44	118.39	122.20
1	1	1565	G	C4-N9-C1'	5.44	133.57	126.50
1	1	2617	U	N1-C2-O2	5.44	126.61	122.80
47	2	469	C	N3-C2-O2	-5.44	118.09	121.90
1	1	1633	C	N1-C2-O2	5.44	122.16	118.90
47	2	1604	U	C5-C6-N1	5.43	125.42	122.70
47	2	1620	C	C6-N1-C2	-5.43	118.13	120.30
1	1	954	U	N1-C2-O2	5.43	126.60	122.80
1	1	2137	U	C2-N1-C1'	5.43	124.22	117.70
1	1	3311	C	C2-N1-C1'	5.43	124.78	118.80
26	V	93	LEU	CA-CB-CG	5.43	127.79	115.30
47	2	1225	U	N3-C2-O2	-5.43	118.40	122.20
47	2	1066	C	N1-C2-O2	5.43	122.16	118.90
1	1	1277	C	N3-C2-O2	-5.43	118.10	121.90
1	1	370	U	C2-N1-C1'	5.42	124.21	117.70
1	1	3105	U	N1-C2-O2	5.42	126.59	122.80
1	1	1194	G	N1-C2-N2	-5.42	111.32	116.20
1	1	2137	U	N3-C2-O2	-5.42	118.41	122.20
81	AX	56	C	N1-C2-O2	5.42	122.15	118.90
1	1	3001	C	C6-N1-C2	-5.42	118.13	120.30
1	1	1275	C	C5-C6-N1	5.41	123.71	121.00
1	1	1349	G	N3-C4-C5	-5.41	125.89	128.60
47	2	1155	G	N3-C4-N9	5.41	129.25	126.00
1	1	2961	G	C6-C5-N7	-5.41	127.15	130.40
47	2	79	C	C6-N1-C2	-5.41	118.14	120.30
47	2	1147	A	N7-C8-N9	5.41	116.50	113.80
1	1	2304	C	N1-C2-O2	5.41	122.15	118.90
74	AQ	60	PRO	C-N-CA	5.41	135.22	121.70
1	1	2336	U	N1-C2-O2	5.40	126.58	122.80
1	1	1732	U	N1-C2-O2	5.40	126.58	122.80
1	1	1732	U	N3-C2-O2	-5.40	118.42	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	2810	C	C6-N1-C2	-5.40	118.14	120.30
47	2	70	C	C6-N1-C2	-5.40	118.14	120.30
77	AT	36	LEU	CA-CB-CG	5.40	127.72	115.30
1	1	540	U	N1-C2-O2	5.40	126.58	122.80
2	3	68	C	C6-N1-C2	-5.40	118.14	120.30
47	2	1021	C	N3-C2-O2	-5.40	118.12	121.90
1	1	315	C	C6-N1-C2	-5.40	118.14	120.30
1	1	2809	C	C6-N1-C2	-5.40	118.14	120.30
23	S	144	LEU	CA-CB-CG	5.40	127.71	115.30
1	1	940	G	N3-C4-N9	-5.39	122.76	126.00
1	1	1219	C	C5-C6-N1	5.39	123.70	121.00
1	1	3132	C	C5-C6-N1	5.39	123.69	121.00
1	1	3311	C	N1-C2-O2	5.39	122.13	118.90
19	O	197	LEU	CA-CB-CG	5.39	127.69	115.30
41	k	65	LEU	CA-CB-CG	5.39	127.69	115.30
47	2	1624	C	N1-C2-O2	5.39	122.13	118.90
1	1	969	C	C5-C6-N1	5.39	123.69	121.00
83	AZ	247	ASP	C-N-CA	5.39	135.17	121.70
1	1	969	C	C6-N1-C2	-5.38	118.15	120.30
1	1	1026	A	C8-N9-C4	-5.38	103.65	105.80
1	1	2495	C	C2-N1-C1'	5.38	124.72	118.80
1	1	2666	C	N3-C2-O2	-5.38	118.13	121.90
47	2	1620	C	N3-C2-O2	-5.38	118.13	121.90
21	Q	32	LEU	CA-CB-CG	5.37	127.65	115.30
1	1	1425	U	N3-C2-O2	-5.37	118.44	122.20
1	1	3235	C	C2-N1-C1'	5.37	124.70	118.80
1	1	3251	U	N3-C2-O2	-5.37	118.44	122.20
47	2	965	U	N1-C2-O2	5.36	126.56	122.80
1	1	271	C	C6-N1-C2	-5.36	118.16	120.30
47	2	1653	C	C6-N1-C1'	-5.36	114.37	120.80
24	T	18	ASP	CB-CG-OD1	5.36	123.12	118.30
1	1	2132	C	C2-N1-C1'	5.35	124.69	118.80
38	h	24	LEU	CA-CB-CG	5.34	127.59	115.30
47	2	1245	G	O5'-P-OP1	-5.34	100.89	105.70
47	2	196	G	N1-C6-O6	-5.34	116.70	119.90
47	2	1773	C	N3-C2-O2	-5.34	118.16	121.90
1	1	2925	C	C6-N1-C2	-5.34	118.17	120.30
1	1	2684	C	C2-N1-C1'	5.34	124.67	118.80
1	1	2347	U	C5-C6-N1	5.33	125.36	122.70
47	2	1529	C	C5-C6-N1	5.33	123.67	121.00
47	2	833	U	C5-C4-O4	5.33	129.10	125.90
54	w	92	ARG	C-N-CA	5.33	135.02	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
81	AX	44	A	C4-N9-C1'	5.33	135.89	126.30
1	1	1614	C	C6-N1-C2	-5.33	118.17	120.30
1	1	1906	G	N3-C4-N9	5.32	129.19	126.00
1	1	2742	C	C2-N1-C1'	5.32	124.66	118.80
47	2	1458	G	C6-C5-N7	-5.32	127.21	130.40
47	2	82	U	C6-N1-C1'	-5.32	113.75	121.20
47	2	656	G	N3-C4-N9	5.32	129.19	126.00
47	2	1674	C	N1-C2-O2	5.32	122.09	118.90
47	2	1604	U	C2-N1-C1'	5.32	124.08	117.70
1	1	2763	U	C2-N1-C1'	5.31	124.07	117.70
47	2	1783	C	N1-C2-O2	5.31	122.09	118.90
1	1	2137	U	N1-C2-O2	5.31	126.51	122.80
1	1	226	C	C6-N1-C2	-5.30	118.18	120.30
1	1	1314	C	N1-C2-O2	5.30	122.08	118.90
47	2	1168	U	N1-C2-O2	5.30	126.51	122.80
47	2	525	A	N9-C4-C5	-5.30	103.68	105.80
1	1	1788	C	C2-N1-C1'	5.29	124.62	118.80
47	2	1627	U	N3-C2-O2	-5.29	118.50	122.20
47	2	1751	C	C6-N1-C2	-5.29	118.18	120.30
1	1	1870	C	N3-C2-O2	-5.29	118.20	121.90
1	1	2773	C	N1-C2-O2	5.29	122.07	118.90
1	1	1254	C	O4'-C1'-N1	5.29	112.43	108.20
47	2	1500	C	N1-C2-O2	5.29	122.07	118.90
1	1	651	G	C6-C5-N7	-5.28	127.23	130.40
1	1	2870	C	C6-N1-C2	-5.28	118.19	120.30
47	2	1697	G	N3-C4-C5	-5.28	125.96	128.60
47	2	93	A	C4-N9-C1'	5.28	135.80	126.30
47	2	82	U	N3-C2-O2	-5.28	118.51	122.20
47	2	1540	G	C8-N9-C1'	-5.28	120.14	127.00
1	1	2415	C	C5-C6-N1	5.27	123.64	121.00
1	1	1837	U	C6-N1-C1'	-5.27	113.82	121.20
1	1	803	C	C6-N1-C2	-5.26	118.19	120.30
47	2	1715	G	C6-C5-N7	-5.26	127.24	130.40
2	3	43	U	C2-N1-C1'	5.26	124.01	117.70
1	1	2550	U	C2-N1-C1'	5.26	124.01	117.70
1	1	823	C	N1-C2-O2	5.26	122.05	118.90
1	1	3251	U	N1-C2-O2	5.26	126.48	122.80
3	4	145	U	C2-N1-C1'	5.26	124.01	117.70
47	2	1181	U	P-O3'-C3'	5.26	126.01	119.70
81	AX	52	U	N3-C2-O2	-5.26	118.52	122.20
83	AZ	310	ASP	CB-CG-OD2	5.26	123.03	118.30
47	2	1182	U	C5-C6-N1	5.25	125.33	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	1255	C	C2-N1-C1'	5.25	124.58	118.80
47	2	317	C	C6-N1-C2	-5.25	118.20	120.30
47	2	1405	G	C6-C5-N7	-5.25	127.25	130.40
1	1	271	C	N1-C2-O2	5.25	122.05	118.90
47	2	497	G	N3-C2-N2	5.25	123.57	119.90
47	2	1643	U	N1-C2-O2	5.25	126.47	122.80
1	1	1779	C	C5-C6-N1	5.25	123.62	121.00
1	1	2498	U	C5-C6-N1	5.24	125.32	122.70
47	2	1540	G	N3-C4-C5	-5.24	125.98	128.60
1	1	897	U	C2-N1-C1'	5.24	123.98	117.70
47	2	498	G	C8-N9-C4	-5.24	104.31	106.40
47	2	1632	C	N3-C2-O2	-5.23	118.24	121.90
1	1	934	G	N3-C4-N9	5.23	129.14	126.00
1	1	2652	U	C2-N1-C1'	5.23	123.98	117.70
38	h	88	LEU	CA-CB-CG	5.23	127.33	115.30
81	AX	44	A	N3-C4-N9	5.23	131.58	127.40
1	1	781	G	C2-N3-C4	5.22	114.51	111.90
1	1	3139	A	N3-C4-N9	5.22	131.57	127.40
1	1	980	A	P-O3'-C3'	5.22	125.96	119.70
1	1	2983	C	N3-C2-O2	-5.22	118.25	121.90
1	1	182	U	N1-C2-O2	5.21	126.45	122.80
47	2	516	G	N3-C4-N9	5.21	129.13	126.00
1	1	411	U	N3-C2-O2	-5.21	118.55	122.20
1	1	2319	U	N3-C2-O2	-5.21	118.55	122.20
58	AA	40	LEU	CA-CB-CG	5.21	127.29	115.30
1	1	27	C	N3-C2-O2	-5.21	118.25	121.90
1	1	1906	G	C8-N9-C1'	-5.21	120.23	127.00
2	3	35	C	C6-N1-C2	-5.21	118.22	120.30
1	1	1889	G	C8-N9-C1'	-5.21	120.23	127.00
1	1	781	G	C4-N9-C1'	5.21	133.27	126.50
47	2	414	C	N3-C2-O2	-5.20	118.26	121.90
47	2	1795	U	C5-C6-N1	5.20	125.30	122.70
1	1	1027	A	C4-N9-C1'	5.20	135.65	126.30
47	2	190	C	N1-C2-O2	5.20	122.02	118.90
47	2	865	A	P-O3'-C3'	5.20	125.93	119.70
70	AM	28	ARG	C-N-CD	-5.20	109.17	120.60
1	1	1857	C	C6-N1-C1'	-5.19	114.57	120.80
47	2	981	U	N3-C2-O2	-5.19	118.56	122.20
47	2	821	U	N1-C2-O2	5.19	126.43	122.80
47	2	1684	U	N3-C2-O2	-5.18	118.57	122.20
47	2	17	C	C6-N1-C2	-5.18	118.23	120.30
47	2	1402	G	N3-C4-N9	5.18	129.11	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	2	1653	C	N1-C2-O2	5.18	122.01	118.90
81	AX	70	C	C6-N1-C2	-5.18	118.23	120.30
1	1	1285	G	C8-N9-C4	-5.18	104.33	106.40
1	1	2418	G	C8-N9-C1'	-5.18	120.27	127.00
1	1	3104	U	N1-C2-O2	5.18	126.43	122.80
3	4	35	C	N3-C2-O2	-5.18	118.27	121.90
47	2	338	C	C2-N1-C1'	5.18	124.50	118.80
1	1	2277	C	C6-N1-C2	-5.18	118.23	120.30
47	2	270	C	C5-C6-N1	5.18	123.59	121.00
1	1	1333	C	N1-C2-O2	5.18	122.01	118.90
1	1	1585	C	C6-N1-C1'	-5.18	114.59	120.80
1	1	2422	C	C6-N1-C2	-5.17	118.23	120.30
47	2	149	C	C2-N1-C1'	5.17	124.49	118.80
47	2	1514	U	N3-C2-O2	-5.17	118.58	122.20
47	2	1274	C	P-O3'-C3'	5.17	125.90	119.70
1	1	1254	C	N3-C2-O2	-5.17	118.28	121.90
47	2	696	C	N3-C2-O2	-5.17	118.28	121.90
1	1	2405	C	C6-N1-C2	-5.16	118.23	120.30
3	4	50	C	N3-C2-O2	-5.16	118.29	121.90
47	2	1	U	N3-C2-O2	-5.16	118.59	122.20
47	2	583	C	C5-C6-N1	5.16	123.58	121.00
1	1	2708	C	C2-N1-C1'	5.16	124.47	118.80
47	2	1674	C	N3-C2-O2	-5.15	118.29	121.90
1	1	1906	G	C4-N9-C1'	5.15	133.20	126.50
1	1	651	G	C4-C5-N7	5.15	112.86	110.80
1	1	2422	C	C2-N1-C1'	5.15	124.46	118.80
47	2	1144	U	N3-C2-O2	-5.15	118.60	122.20
1	1	3306	U	C2-N1-C1'	5.15	123.88	117.70
1	1	1425	U	N1-C2-O2	5.14	126.40	122.80
47	2	317	C	N1-C2-O2	5.14	121.99	118.90
47	2	842	C	C5-C6-N1	5.14	123.57	121.00
81	AX	25	C	C6-N1-C2	-5.14	118.24	120.30
47	2	747	C	N1-C2-O2	5.14	121.98	118.90
1	1	370	U	N3-C2-O2	-5.14	118.60	122.20
81	AX	52	U	N1-C2-O2	5.14	126.39	122.80
1	1	1761	C	C6-N1-C2	-5.13	118.25	120.30
1	1	1372	C	C2-N1-C1'	5.13	124.44	118.80
47	2	506	A	C2-N3-C4	5.13	113.17	110.60
66	AI	26	ILE	CG1-CB-CG2	-5.13	100.11	111.40
47	2	1274	C	N1-C2-O2	5.12	121.97	118.90
1	1	2765	C	N1-C2-O2	5.12	121.97	118.90
47	2	196	G	N3-C2-N2	5.12	123.48	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	r	135	LEU	CA-CB-CG	5.12	127.07	115.30
1	1	1279	C	N1-C2-O2	5.12	121.97	118.90
1	1	3386	G	C8-N9-C1'	-5.12	120.35	127.00
81	AX	52	U	C2-N1-C1'	5.12	123.84	117.70
1	1	2928	C	N3-C2-O2	-5.11	118.32	121.90
1	1	986	U	C2-N1-C1'	5.11	123.83	117.70
47	2	1146	G	C4-N9-C1'	5.11	133.15	126.50
2	3	35	C	N1-C2-O2	5.10	121.96	118.90
47	2	563	U	N3-C2-O2	-5.10	118.63	122.20
3	4	50	C	N1-C2-O2	5.10	121.96	118.90
1	1	2943	G	N3-C4-C5	-5.10	126.05	128.60
30	Z	102	GLU	C-N-CA	5.10	134.45	121.70
1	1	1185	C	C6-N1-C2	-5.10	118.26	120.30
1	1	1590	G	C6-C5-N7	-5.10	127.34	130.40
1	1	2836	C	C5-C6-N1	5.10	123.55	121.00
2	3	36	C	N1-C2-O2	5.10	121.96	118.90
47	2	1074	G	C4-N9-C1'	5.10	133.13	126.50
47	2	1185	U	N1-C2-O2	5.10	126.37	122.80
1	1	427	C	N1-C2-O2	5.09	121.96	118.90
47	2	1214	U	N3-C2-O2	-5.09	118.63	122.20
1	1	142	C	C2-N1-C1'	5.09	124.40	118.80
1	1	1137	C	C5-C6-N1	5.09	123.55	121.00
1	1	1640	G	C4-N9-C1'	5.09	133.12	126.50
47	2	924	A	N7-C8-N9	5.09	116.35	113.80
1	1	292	U	C6-N1-C1'	-5.09	114.08	121.20
47	2	320	U	C5-C6-N1	5.09	125.24	122.70
47	2	1700	C	C6-N1-C2	-5.09	118.27	120.30
83	AZ	380	LEU	CA-CB-CG	5.09	127.00	115.30
37	g	57	LEU	CA-CB-CG	5.08	127.00	115.30
1	1	1037	C	C6-N1-C2	-5.08	118.27	120.30
1	1	2863	G	N3-C4-C5	-5.08	126.06	128.60
1	1	3385	U	C2-N1-C1'	5.08	123.80	117.70
3	4	76	C	C6-N1-C2	-5.08	118.27	120.30
1	1	2526	C	C6-N1-C2	-5.08	118.27	120.30
47	2	1128	C	C2-N1-C1'	5.08	124.38	118.80
47	2	566	C	N1-C2-O2	5.07	121.94	118.90
2	3	28	C	C2-N1-C1'	5.07	124.38	118.80
47	2	1393	C	C2-N1-C1'	5.07	124.38	118.80
1	1	2638	C	N3-C2-O2	-5.07	118.35	121.90
47	2	111	U	N1-C2-O2	5.07	126.35	122.80
47	2	189	C	N1-C2-O2	5.07	121.94	118.90
47	2	1209	C	C5-C6-N1	5.07	123.53	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	2	1405	G	N7-C8-N9	5.07	115.63	113.10
1	1	2950	G	C8-N9-C1'	-5.07	120.41	127.00
1	1	270	U	N3-C2-O2	-5.06	118.66	122.20
1	1	729	C	N1-C2-O2	5.06	121.94	118.90
1	1	1889	G	N3-C4-N9	5.06	129.04	126.00
1	1	2503	G	C4-C5-N7	5.06	112.83	110.80
47	2	1439	C	C2-N1-C1'	5.06	124.37	118.80
1	1	2270	A	P-O3'-C3'	5.06	125.77	119.70
1	1	2416	U	N3-C2-O2	-5.06	118.66	122.20
1	1	1254	C	C6-N1-C1'	5.06	126.87	120.80
1	1	2295	A	P-O3'-C3'	5.05	125.76	119.70
1	1	489	U	N1-C2-O2	5.05	126.34	122.80
1	1	19	U	C5-C6-N1	5.05	125.23	122.70
47	2	1241	G	O4'-C1'-N9	5.05	112.24	108.20
1	1	278	U	C2-N1-C1'	5.05	123.76	117.70
47	2	1365	C	C6-N1-C2	-5.05	118.28	120.30
1	1	178	U	C2-N1-C1'	5.05	123.76	117.70
1	1	1781	C	N1-C2-O2	5.05	121.93	118.90
47	2	1715	G	N3-C4-C5	-5.05	126.08	128.60
1	1	2116	G	N3-C4-N9	5.04	129.03	126.00
57	z	118	LEU	CA-CB-CG	5.04	126.90	115.30
1	1	1505	C	C2-N1-C1'	5.04	124.35	118.80
1	1	2464	U	C5-C6-N1	5.04	125.22	122.70
47	2	886	U	N1-C2-O2	5.04	126.33	122.80
47	2	1792	G	N3-C4-N9	5.04	129.03	126.00
52	u	246	LEU	CA-CB-CG	5.04	126.89	115.30
1	1	1555	U	C2-N1-C1'	5.04	123.75	117.70
1	1	1701	C	C2-N1-C1'	5.04	124.34	118.80
1	1	2516	U	N1-C2-O2	5.04	126.33	122.80
1	1	1872	C	N1-C2-O2	5.04	121.92	118.90
60	AC	45	LEU	CA-CB-CG	5.04	126.89	115.30
1	1	1146	C	C6-N1-C2	-5.04	118.28	120.30
2	3	39	C	C6-N1-C2	-5.04	118.28	120.30
47	2	691	C	C2-N1-C1'	5.04	124.34	118.80
1	1	970	A	C6-C5-N7	-5.04	128.78	132.30
1	1	861	C	C6-N1-C1'	-5.03	114.76	120.80
1	1	1496	C	N3-C2-O2	-5.03	118.38	121.90
1	1	2305	G	C2-N3-C4	5.03	114.42	111.90
1	1	1146	C	C2-N1-C1'	5.03	124.33	118.80
1	1	1254	C	C5-C4-N4	5.02	123.72	120.20
47	2	329	G	C4-N9-C1'	5.02	133.03	126.50
1	1	1149	G	C8-N9-C1'	5.02	133.53	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	1837	U	C5-C4-O4	-5.02	122.89	125.90
33	c	16	LEU	CA-CB-CG	5.02	126.85	115.30
2	3	90	U	C6-N1-C1'	5.02	128.22	121.20
1	1	1562	C	C6-N1-C2	-5.01	118.29	120.30
47	2	1217	A	N3-C4-N9	5.01	131.41	127.40
17	M	65	LEU	C-N-CA	5.01	134.22	121.70
47	2	1681	A	N7-C8-N9	5.01	116.31	113.80
8	C	318	LEU	CB-CG-CD2	-5.01	102.49	111.00
47	2	1529	C	C2-N1-C1'	5.01	124.31	118.80
1	1	3139	A	N9-C4-C5	-5.00	103.80	105.80
47	2	1357	A	N9-C4-C5	-5.00	103.80	105.80
47	2	283	U	N3-C2-O2	-5.00	118.70	122.20
1	1	2899	C	N1-C2-O2	5.00	121.90	118.90
47	2	1518	C	C6-N1-C1'	-5.00	114.80	120.80

There are no chirality outliers.

All (123) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	A	143	GLU	Peptide
59	AB	27	THR	Peptide
60	AC	110	GLY	Peptide
61	AD	104	ARG	Peptide
61	AD	138	ASN	Peptide
61	AD	25	TRP	Peptide
63	AF	100	LYS	Peptide
63	AF	89	MET	Peptide
64	AG	112	TYR	Peptide
64	AG	58	ASP	Peptide
64	AG	68	ARG	Peptide
65	AH	78	ARG	Peptide
65	AH	83	GLN	Peptide
66	AI	91	ASP	Peptide
69	AL	49	GLU	Peptide
69	AL	52	THR	Peptide
71	AN	113	ALA	Peptide
72	AO	37	LYS	Peptide
73	AP	54	VAL	Peptide
74	AQ	34	LYS	Peptide
74	AQ	43	ASN	Peptide
74	AQ	46	GLU	Peptide
74	AQ	47	ALA	Peptide

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Mol	Chain	Res	Type	Group
74	AQ	59	TYR	Peptide
74	AQ	63	ALA	Peptide
74	AQ	7	SER	Peptide
75	AR	55	THR	Peptide
75	AR	75	GLU	Peptide
79	AV	275	ARG	Peptide
83	AZ	111	PHE	Peptide
83	AZ	244	LEU	Peptide
83	AZ	246	GLY	Peptide
83	AZ	251	ASN	Peptide
83	AZ	276	PHE	Peptide
83	AZ	485	VAL	Peptide
83	AZ	487	PRO	Peptide
83	AZ	544	ASP	Peptide
83	AZ	645	LEU	Peptide
83	AZ	656	LEU	Peptide
83	AZ	668	GLN	Peptide
83	AZ	707	PRO	Peptide
83	AZ	721	ASP	Peptide
83	AZ	790	GLY	Peptide
7	B	25	ILE	Peptide
9	D	177	GLU	Peptide
9	D	20	PHE	Peptide
9	D	260	PHE	Peptide
9	D	43	LYS	Peptide
9	D	81	HIS	Peptide
10	E	58	LEU	Peptide
11	F	110	ARG	Peptide
11	F	157	ASN	Peptide
11	F	214	TRP	Peptide
12	G	156	ASP	Peptide
12	G	30	THR	Peptide
12	G	76	ALA	Peptide
13	H	20	ILE	Peptide
13	H	21	LYS	Peptide
14	I	217	PHE	Peptide
14	I	58	GLU	Peptide
15	J	167	TYR	Peptide
16	L	47	ALA	Peptide
19	O	110	PRO	Peptide
19	O	36	VAL	Peptide
4	P0	39	HIS	Peptide

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Mol	Chain	Res	Type	Group
4	P0	41	VAL	Peptide
5	P2	117	ARG	Peptide
21	Q	59	ARG	Peptide
24	T	103	GLN	Peptide
24	T	17	ARG	Peptide
26	V	104	ASN	Peptide
26	V	93	LEU	Peptide
27	W	14	TYR	Peptide
31	a	23	GLY	Peptide
34	d	56	ASN	Peptide
34	d	87	ASN	Peptide
35	e	20	HIS	Peptide
35	e	39	ASP	Peptide
36	f	58	GLU	Peptide
37	g	66	SER	Peptide
37	g	80	ARG	Peptide
37	g	82	ALA	Peptide
38	h	90	ARG	Peptide
39	i	12	ASN	Peptide
39	i	63	ASN	Peptide
39	i	97	SER	Peptide
40	j	5	THR	Peptide
42	l	29	LEU	Peptide
45	o	28	TYR	Peptide
45	o	34	SER	Peptide
45	o	7	THR	Peptide
48	q	107	PHE	Peptide
48	q	111	ILE	Peptide
48	q	112	THR	Peptide
48	q	192	THR	Peptide
49	r	147	ALA	Peptide
49	r	205	PHE	Peptide
49	r	206	PRO	Peptide
49	r	40	ASN	Peptide
51	t	219	ALA	Peptide
52	u	154	ILE	Peptide
52	u	194	THR	Peptide
52	u	195	ILE	Peptide
52	u	233	LYS	Peptide
52	u	94	ALA	Peptide
53	v	127	GLN	Peptide
53	v	57	SER	Peptide

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Mol	Chain	Res	Type	Group
54	w	100	ALA	Peptide
54	w	119	GLN	Peptide
54	w	13	GLN	Peptide
54	w	148	SER	Peptide
54	w	153	VAL	Peptide
54	w	67	VAL	Peptide
54	w	88	ARG	Peptide
54	w	9	VAL	Peptide
54	w	91	GLU	Peptide
54	w	92	ARG	Peptide
54	w	93	LYS	Peptide
55	x	110	GLN	Peptide
55	x	36	ALA	Peptide
56	y	20	GLN	Peptide
57	z	133	HIS	Peptide
57	z	163	PRO	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	P0	187/189 (99%)	151 (81%)	36 (19%)	0	100	100
5	P2	92/94 (98%)	71 (77%)	21 (23%)	0	100	100
6	A	250/252 (99%)	212 (85%)	38 (15%)	0	100	100
7	B	384/386 (100%)	337 (88%)	47 (12%)	0	100	100
8	C	359/361 (99%)	307 (86%)	52 (14%)	0	100	100
9	D	294/296 (99%)	257 (87%)	35 (12%)	2 (1%)	22	62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	E	152/175 (87%)	135 (89%)	17 (11%)	0	100	100
11	F	220/222 (99%)	184 (84%)	34 (16%)	2 (1%)	17	56
12	G	231/233 (99%)	199 (86%)	31 (13%)	1 (0%)	34	72
13	H	189/191 (99%)	159 (84%)	30 (16%)	0	100	100
14	I	207/220 (94%)	182 (88%)	24 (12%)	1 (0%)	29	68
15	J	167/169 (99%)	135 (81%)	31 (19%)	1 (1%)	25	65
16	L	191/193 (99%)	155 (81%)	34 (18%)	2 (1%)	15	54
17	M	134/136 (98%)	119 (89%)	15 (11%)	0	100	100
18	N	201/203 (99%)	171 (85%)	30 (15%)	0	100	100
19	O	195/197 (99%)	170 (87%)	22 (11%)	3 (2%)	10	46
20	P	181/183 (99%)	161 (89%)	20 (11%)	0	100	100
21	Q	183/185 (99%)	162 (88%)	21 (12%)	0	100	100
22	R	186/188 (99%)	173 (93%)	13 (7%)	0	100	100
23	S	170/172 (99%)	147 (86%)	23 (14%)	0	100	100
24	T	157/159 (99%)	137 (87%)	19 (12%)	1 (1%)	25	65
25	U	98/100 (98%)	85 (87%)	13 (13%)	0	100	100
26	V	134/136 (98%)	114 (85%)	19 (14%)	1 (1%)	22	62
27	W	61/63 (97%)	55 (90%)	6 (10%)	0	100	100
28	X	119/121 (98%)	103 (87%)	16 (13%)	0	100	100
29	Y	124/126 (98%)	112 (90%)	12 (10%)	0	100	100
30	Z	133/135 (98%)	111 (84%)	22 (16%)	0	100	100
31	a	146/148 (99%)	117 (80%)	28 (19%)	1 (1%)	22	62
32	b	56/58 (97%)	48 (86%)	8 (14%)	0	100	100
33	c	95/97 (98%)	84 (88%)	11 (12%)	0	100	100
34	d	107/109 (98%)	91 (85%)	16 (15%)	0	100	100
35	e	125/127 (98%)	111 (89%)	12 (10%)	2 (2%)	9	45
36	f	104/106 (98%)	82 (79%)	20 (19%)	2 (2%)	8	41
37	g	110/112 (98%)	99 (90%)	9 (8%)	2 (2%)	8	42
38	h	117/119 (98%)	103 (88%)	14 (12%)	0	100	100
39	i	97/99 (98%)	78 (80%)	19 (20%)	0	100	100
40	j	85/87 (98%)	65 (76%)	19 (22%)	1 (1%)	13	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	k	75/77 (97%)	67 (89%)	8 (11%)	0	100	100
42	l	48/50 (96%)	36 (75%)	11 (23%)	1 (2%)	7	39
43	m	50/52 (96%)	45 (90%)	5 (10%)	0	100	100
44	n	23/25 (92%)	23 (100%)	0	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%)	169 (83%)	33 (16%)	2 (1%)	15	54
49	r	212/214 (99%)	161 (76%)	49 (23%)	2 (1%)	17	56
50	s	215/217 (99%)	183 (85%)	32 (15%)	0	100	100
51	t	221/223 (99%)	182 (82%)	39 (18%)	0	100	100
52	u	258/260 (99%)	200 (78%)	56 (22%)	2 (1%)	19	60
53	v	204/206 (99%)	164 (80%)	40 (20%)	0	100	100
54	w	221/223 (99%)	157 (71%)	61 (28%)	3 (1%)	11	47
55	x	182/184 (99%)	150 (82%)	31 (17%)	1 (0%)	29	68
56	y	184/199 (92%)	141 (77%)	43 (23%)	0	100	100
57	z	183/185 (99%)	153 (84%)	30 (16%)	0	100	100
58	AA	94/105 (90%)	77 (82%)	16 (17%)	1 (1%)	14	52
59	AB	151/153 (99%)	125 (83%)	26 (17%)	0	100	100
60	AC	122/124 (98%)	98 (80%)	23 (19%)	1 (1%)	19	60
61	AD	148/150 (99%)	129 (87%)	15 (10%)	4 (3%)	5	34
62	AE	125/127 (98%)	105 (84%)	20 (16%)	0	100	100
63	AF	122/124 (98%)	85 (70%)	33 (27%)	4 (3%)	4	30
64	AG	139/141 (99%)	111 (80%)	26 (19%)	2 (1%)	11	47
65	AH	116/125 (93%)	97 (84%)	19 (16%)	0	100	100
66	AI	143/145 (99%)	122 (85%)	19 (13%)	2 (1%)	11	47
67	AJ	141/143 (99%)	124 (88%)	17 (12%)	0	100	100
68	AK	105/107 (98%)	91 (87%)	14 (13%)	0	100	100
69	AL	85/87 (98%)	64 (75%)	20 (24%)	1 (1%)	13	50
70	AM	127/129 (98%)	114 (90%)	12 (9%)	1 (1%)	19	60
71	AN	142/144 (99%)	114 (80%)	26 (18%)	2 (1%)	11	47
72	AO	132/134 (98%)	112 (85%)	20 (15%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
73	AP	68/70 (97%)	46 (68%)	21 (31%)	1 (2%)	10	46
74	AQ	95/97 (98%)	65 (68%)	30 (32%)	0	100	100
75	AR	79/81 (98%)	57 (72%)	21 (27%)	1 (1%)	12	48
76	AS	61/63 (97%)	54 (88%)	7 (12%)	0	100	100
77	AT	51/53 (96%)	46 (90%)	5 (10%)	0	100	100
78	AU	58/60 (97%)	49 (84%)	9 (16%)	0	100	100
79	AV	316/318 (99%)	254 (80%)	61 (19%)	1 (0%)	41	76
80	AW	35/37 (95%)	26 (74%)	9 (26%)	0	100	100
83	AZ	837/840 (100%)	676 (81%)	157 (19%)	4 (0%)	29	68
All	All	12005/12221 (98%)	10010 (83%)	1937 (16%)	58 (0%)	32	68

All (58) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	O	111	PRO
48	q	113	ARG
49	r	207	LEU
54	w	10	ASN
54	w	68	LEU
58	AA	88	PRO
61	AD	105	ASN
64	AG	59	LYS
16	L	48	PRO
16	L	77	LEU
26	V	105	PRO
35	e	79	VAL
36	f	58	GLU
36	f	59	VAL
42	l	30	ARG
49	r	206	PRO
52	u	195	ILE
54	w	93	LYS
71	AN	114	LYS
75	AR	76	GLY
11	F	159	GLN
24	T	159	PHE
48	q	112	THR
55	x	111	LYS
61	AD	85	PRO

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Mol	Chain	Res	Type
63	AF	30	THR
63	AF	53	PRO
73	AP	55	PRO
83	AZ	252	PRO
83	AZ	708	THR
83	AZ	722	PRO
11	F	158	LYS
14	I	24	ARG
19	O	37	ARG
31	a	78	LEU
37	g	66	SER
40	j	64	MET
52	u	155	LYS
61	AD	139	TRP
69	AL	81	ASN
79	AV	165	ASP
9	D	259	LYS
19	O	110	PRO
35	e	78	ASN
37	g	67	LYS
60	AC	131	ASP
61	AD	104	ARG
63	AF	125	PRO
83	AZ	639	ASP
9	D	20	PHE
15	J	165	GLN
63	AF	70	ASN
66	AI	9	GLY
12	G	157	VAL
71	AN	64	PRO
64	AG	33	GLY
66	AI	92	ILE
70	AM	67	GLY

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%)	158 (99%)	2 (1%)	69	82
5	P2	81/81 (100%)	77 (95%)	4 (5%)	25	51
6	A	193/194 (100%)	190 (98%)	3 (2%)	62	79
7	B	321/322 (100%)	315 (98%)	6 (2%)	57	75
8	C	288/288 (100%)	283 (98%)	5 (2%)	60	78
9	D	244/244 (100%)	241 (99%)	3 (1%)	71	84
10	E	134/152 (88%)	130 (97%)	4 (3%)	41	63
11	F	186/186 (100%)	181 (97%)	5 (3%)	44	66
12	G	187/191 (98%)	180 (96%)	7 (4%)	34	59
13	H	171/171 (100%)	164 (96%)	7 (4%)	30	56
14	I	177/186 (95%)	168 (95%)	9 (5%)	24	50
15	J	147/147 (100%)	143 (97%)	4 (3%)	44	66
16	L	154/154 (100%)	150 (97%)	4 (3%)	46	67
17	M	107/107 (100%)	104 (97%)	3 (3%)	43	65
18	N	175/175 (100%)	168 (96%)	7 (4%)	31	56
19	O	160/160 (100%)	156 (98%)	4 (2%)	47	68
20	P	140/145 (97%)	135 (96%)	5 (4%)	35	60
21	Q	150/150 (100%)	145 (97%)	5 (3%)	38	61
22	R	153/153 (100%)	148 (97%)	5 (3%)	38	61
23	S	156/156 (100%)	152 (97%)	4 (3%)	46	67
24	T	136/136 (100%)	130 (96%)	6 (4%)	28	54
25	U	87/87 (100%)	86 (99%)	1 (1%)	73	85
26	V	104/104 (100%)	103 (99%)	1 (1%)	76	86
27	W	55/55 (100%)	54 (98%)	1 (2%)	59	77
28	X	104/105 (99%)	104 (100%)	0	100	100
29	Y	109/109 (100%)	109 (100%)	0	100	100
30	Z	115/115 (100%)	112 (97%)	3 (3%)	46	67
31	a	118/118 (100%)	118 (100%)	0	100	100
32	b	46/46 (100%)	43 (94%)	3 (6%)	17	44
33	c	81/81 (100%)	79 (98%)	2 (2%)	47	68
34	d	94/96 (98%)	93 (99%)	1 (1%)	73	85
35	e	109/109 (100%)	106 (97%)	3 (3%)	43	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	f	90/90 (100%)	86 (96%)	4 (4%)	28	54
37	g	95/95 (100%)	91 (96%)	4 (4%)	30	55
38	h	104/104 (100%)	101 (97%)	3 (3%)	42	64
39	i	81/81 (100%)	79 (98%)	2 (2%)	47	68
40	j	70/70 (100%)	68 (97%)	2 (3%)	42	64
41	k	68/68 (100%)	66 (97%)	2 (3%)	42	64
42	l	45/45 (100%)	43 (96%)	2 (4%)	28	54
43	m	47/47 (100%)	46 (98%)	1 (2%)	53	72
44	n	22/23 (96%)	21 (96%)	1 (4%)	27	54
45	o	90/90 (100%)	89 (99%)	1 (1%)	73	85
46	p	71/71 (100%)	71 (100%)	0	100	100
48	q	164/173 (95%)	162 (99%)	2 (1%)	71	84
49	r	191/191 (100%)	184 (96%)	7 (4%)	34	59
50	s	176/176 (100%)	172 (98%)	4 (2%)	50	70
51	t	182/182 (100%)	172 (94%)	10 (6%)	21	49
52	u	221/221 (100%)	212 (96%)	9 (4%)	30	56
53	v	173/173 (100%)	171 (99%)	2 (1%)	71	84
54	w	189/191 (99%)	186 (98%)	3 (2%)	62	79
55	x	165/165 (100%)	163 (99%)	2 (1%)	71	84
56	y	150/160 (94%)	147 (98%)	3 (2%)	55	73
57	z	158/158 (100%)	155 (98%)	3 (2%)	57	75
58	AA	77/98 (79%)	75 (97%)	2 (3%)	46	67
59	AB	133/134 (99%)	130 (98%)	3 (2%)	50	70
60	AC	88/100 (88%)	87 (99%)	1 (1%)	73	85
61	AD	127/127 (100%)	125 (98%)	2 (2%)	62	79
62	AE	81/96 (84%)	79 (98%)	2 (2%)	47	68
63	AF	101/104 (97%)	97 (96%)	4 (4%)	31	56
64	AG	117/117 (100%)	117 (100%)	0	100	100
65	AH	94/113 (83%)	93 (99%)	1 (1%)	73	85
66	AI	128/128 (100%)	125 (98%)	3 (2%)	50	70
67	AJ	115/115 (100%)	112 (97%)	3 (3%)	46	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
68	AK	100/100 (100%)	97 (97%)	3 (3%)	41	63
69	AL	74/74 (100%)	74 (100%)	0	100	100
70	AM	110/110 (100%)	108 (98%)	2 (2%)	59	77
71	AN	119/119 (100%)	114 (96%)	5 (4%)	30	55
72	AO	112/112 (100%)	108 (96%)	4 (4%)	35	60
73	AP	61/61 (100%)	60 (98%)	1 (2%)	62	79
74	AQ	83/83 (100%)	78 (94%)	5 (6%)	19	46
75	AR	70/70 (100%)	68 (97%)	2 (3%)	42	64
76	AS	56/56 (100%)	56 (100%)	0	100	100
77	AT	47/47 (100%)	46 (98%)	1 (2%)	53	72
78	AU	51/51 (100%)	48 (94%)	3 (6%)	19	47
79	AV	259/261 (99%)	256 (99%)	3 (1%)	71	84
80	AW	31/31 (100%)	29 (94%)	2 (6%)	17	44
83	AZ	711/712 (100%)	693 (98%)	18 (2%)	47	68
All	All	10139/10276 (99%)	9885 (98%)	254 (2%)	50	68

All (254) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	P0	38	MET
4	P0	147	ARG
5	P2	57	LYS
5	P2	66	ASN
5	P2	119	LYS
5	P2	123	ARG
6	A	21	ARG
6	A	72	ARG
6	A	147	ARG
7	B	47	LEU
7	B	89	VAL
7	B	104	THR
7	B	270	ARG
7	B	284	ARG
7	B	345	ASN
8	C	43	ASN
8	C	99	MET
8	C	154	THR

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Mol	Chain	Res	Type
8	C	197	ARG
8	C	221	ASN
9	D	41	LYS
9	D	158	ARG
9	D	179	ARG
10	E	4	GLN
10	E	48	ARG
10	E	51	ARG
10	E	78	ARG
11	F	93	ASN
11	F	145	ARG
11	F	160	ARG
11	F	199	ASN
11	F	232	ARG
12	G	48	ARG
12	G	51	LYS
12	G	63	LYS
12	G	173	MET
12	G	204	ARG
12	G	213	LYS
12	G	249	ARG
13	H	23	ARG
13	H	37	ASN
13	H	62	ARG
13	H	78	MET
13	H	106	LYS
13	H	157	ASN
13	H	163	GLN
14	I	3	ARG
14	I	24	ARG
14	I	32	ARG
14	I	82	ARG
14	I	97	LEU
14	I	98	ARG
14	I	115	MET
14	I	183	LYS
14	I	211	ARG
15	J	35	LYS
15	J	51	ARG
15	J	60	ARG
15	J	165	GLN
16	L	42	ARG

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Mol	Chain	Res	Type
16	L	66	ASN
16	L	100	ARG
16	L	186	ARG
17	M	109	ARG
17	M	112	LEU
17	M	128	ARG
18	N	7	LEU
18	N	68	ARG
18	N	71	ARG
18	N	99	ARG
18	N	109	ARG
18	N	115	VAL
18	N	121	VAL
19	O	12	LYS
19	O	16	VAL
19	O	49	ARG
19	O	192	LYS
20	P	23	ARG
20	P	97	ASN
20	P	128	ARG
20	P	171	ARG
20	P	175	ARG
21	Q	45	ASN
21	Q	98	LYS
21	Q	105	ARG
21	Q	130	ARG
21	Q	147	ARG
22	R	39	ASN
22	R	46	LYS
22	R	98	ARG
22	R	117	LYS
22	R	166	ASN
23	S	1	MET
23	S	26	ARG
23	S	53	LYS
23	S	121	ILE
24	T	40	VAL
24	T	102	ARG
24	T	108	ARG
24	T	127	GLN
24	T	136	ARG
24	T	146	ASN

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Mol	Chain	Res	Type
25	U	104	ARG
26	V	48	ARG
27	W	41	LYS
30	Z	34	LYS
30	Z	126	LYS
30	Z	127	ASN
32	b	19	ASN
32	b	42	ASN
32	b	58	LYS
33	c	34	LEU
33	c	86	ARG
34	d	87	ASN
35	e	28	VAL
35	e	47	ARG
35	e	87	MET
36	f	24	ASN
36	f	73	ARG
36	f	77	ASN
36	f	86	ARG
37	g	4	ARG
37	g	37	LYS
37	g	60	ARG
37	g	113	LYS
38	h	26	LYS
38	h	71	LYS
38	h	78	LYS
39	i	35	ASN
39	i	98	ARG
40	j	64	MET
40	j	85	LYS
41	k	30	LYS
41	k	66	ILE
42	l	4	GLN
42	l	42	ARG
43	m	126	LYS
44	n	23	ARG
45	o	41	ARG
48	q	39	ASN
48	q	41	ARG
49	r	103	MET
49	r	144	ARG
49	r	166	LYS

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Mol	Chain	Res	Type
49	r	172	LEU
49	r	201	THR
49	r	209	ASN
49	r	222	LYS
50	s	73	LEU
50	s	81	MET
50	s	140	ARG
50	s	235	LEU
51	t	67	ASN
51	t	76	ARG
51	t	90	ARG
51	t	94	ARG
51	t	108	LYS
51	t	116	ARG
51	t	117	ARG
51	t	146	ARG
51	t	148	LYS
51	t	178	ARG
52	u	49	ARG
52	u	108	ARG
52	u	113	ARG
52	u	157	ASN
52	u	187	ARG
52	u	205	PHE
52	u	223	ASN
52	u	252	ARG
52	u	256	ARG
53	v	219	ARG
53	v	225	ARG
54	w	65	GLN
54	w	87	ARG
54	w	116	LYS
55	x	76	LYS
55	x	107	ARG
56	y	72	ILE
56	y	88	ASN
56	y	199	LYS
57	z	3	ARG
57	z	69	ARG
57	z	78	ARG
58	AA	56	LYS
58	AA	82	LEU

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Mol	Chain	Res	Type
59	AB	26	LYS
59	AB	67	ARG
59	AB	129	ARG
60	AC	121	VAL
61	AD	91	LEU
61	AD	117	LEU
62	AE	84	ARG
62	AE	110	LEU
63	AF	25	LEU
63	AF	77	ARG
63	AF	108	ARG
63	AF	127	ARG
65	AH	72	LYS
66	AI	44	ASN
66	AI	143	ARG
66	AI	145	ARG
67	AJ	24	ARG
67	AJ	68	ARG
67	AJ	89	ARG
68	AK	32	LYS
68	AK	36	ASN
68	AK	121	ASN
70	AM	88	LYS
70	AM	97	ARG
71	AN	7	ARG
71	AN	62	LYS
71	AN	63	GLN
71	AN	81	LYS
71	AN	89	ASN
72	AO	32	ARG
72	AO	102	LYS
72	AO	113	ASN
72	AO	123	LYS
73	AP	52	LYS
74	AQ	10	ARG
74	AQ	15	ARG
74	AQ	43	ASN
74	AQ	51	ARG
74	AQ	85	ARG
75	AR	21	LEU
75	AR	36	LYS
77	AT	19	ARG

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Mol	Chain	Res	Type
78	AU	10	ARG
78	AU	46	ASN
78	AU	53	LYS
79	AV	59	ARG
79	AV	148	ASN
79	AV	229	LYS
80	AW	123	ASN
80	AW	139	LEU
83	AZ	13	MET
83	AZ	87	LYS
83	AZ	243	ARG
83	AZ	259	ASN
83	AZ	276	PHE
83	AZ	349	GLN
83	AZ	437	MET
83	AZ	469	LEU
83	AZ	479	LYS
83	AZ	555	LYS
83	AZ	593	ILE
83	AZ	615	ARG
83	AZ	633	ILE
83	AZ	645	LEU
83	AZ	651	LYS
83	AZ	700	ARG
83	AZ	710	ARG
83	AZ	825	ARG

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	36	GLN
5	P2	66	ASN
6	A	205	ASN
7	B	109	HIS
7	B	177	HIS
7	B	345	ASN
7	B	377	HIS
8	C	43	ASN
8	C	59	GLN
8	C	140	HIS
8	C	291	ASN
9	D	4	GLN

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Mol	Chain	Res	Type
9	D	39	GLN
9	D	40	HIS
9	D	63	GLN
9	D	90	HIS
9	D	178	ASN
9	D	264	GLN
9	D	297	GLN
10	E	172	HIS
11	F	93	ASN
11	F	199	ASN
12	G	221	ASN
12	G	252	ASN
13	H	37	ASN
14	I	14	ASN
14	I	133	GLN
15	J	101	ASN
18	N	37	HIS
19	O	29	ASN
19	O	182	ASN
19	O	193	GLN
20	P	97	ASN
20	P	145	HIS
21	Q	45	ASN
22	R	27	ASN
22	R	39	ASN
22	R	166	ASN
23	S	88	HIS
24	T	54	HIS
24	T	146	ASN
26	V	98	ASN
28	X	85	GLN
29	Y	42	GLN
30	Z	36	HIS
30	Z	57	HIS
30	Z	78	ASN
30	Z	127	ASN
31	a	14	HIS
31	a	38	GLN
31	a	64	GLN
31	a	74	ASN
32	b	19	ASN
32	b	42	ASN

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Mol	Chain	Res	Type
34	d	87	ASN
36	f	24	ASN
36	f	77	ASN
37	g	61	GLN
39	i	12	ASN
40	j	76	ASN
42	l	4	GLN
45	o	82	GLN
48	q	39	ASN
48	q	46	HIS
49	r	42	ASN
49	r	199	ASN
49	r	209	ASN
50	s	199	GLN
50	s	220	ASN
51	t	174	HIS
52	u	98	ASN
52	u	223	ASN
52	u	259	GLN
53	v	72	HIS
53	v	86	GLN
53	v	95	ASN
53	v	104	ASN
53	v	128	ASN
53	v	131	GLN
53	v	158	GLN
54	w	56	ASN
54	w	139	ASN
55	x	110	GLN
56	y	88	ASN
57	z	139	GLN
57	z	176	ASN
58	AA	28	ASN
59	AB	8	GLN
61	AD	78	ASN
63	AF	15	HIS
63	AF	98	ASN
63	AF	103	ASN
64	AG	77	GLN
65	AH	31	ASN
65	AH	48	ASN
66	AI	44	ASN

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Mol	Chain	Res	Type
66	AI	63	GLN
67	AJ	43	ASN
68	AK	36	ASN
68	AK	48	HIS
68	AK	87	HIS
68	AK	105	GLN
68	AK	121	ASN
69	AL	70	ASN
70	AM	15	ASN
70	AM	16	ASN
70	AM	24	GLN
70	AM	42	GLN
71	AN	79	ASN
72	AO	113	ASN
73	AP	98	GLN
76	AS	51	ASN
78	AU	17	GLN
78	AU	46	ASN
79	AV	66	HIS
80	AW	123	ASN
83	AZ	27	HIS
83	AZ	201	GLN
83	AZ	224	GLN
83	AZ	251	ASN
83	AZ	259	ASN
83	AZ	274	ASN
83	AZ	409	GLN
83	AZ	452	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	3220/3396 (94%)	1049 (32%)	18 (0%)
2	3	120/121 (99%)	31 (25%)	0
3	4	157/158 (99%)	50 (31%)	2 (1%)
47	2	1774/1797 (98%)	665 (37%)	23 (1%)
81	AX	75/76 (98%)	33 (44%)	1 (1%)
82	AY	7/8 (87%)	5 (71%)	0
All	All	5353/5556 (96%)	1833 (34%)	44 (0%)

All (1833) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	11	A
1	1	15	C
1	1	16	A
1	1	18	G
1	1	19	U
1	1	20	A
1	1	22	G
1	1	24	G
1	1	25	U
1	1	26	A
1	1	37	U
1	1	40	A
1	1	43	A
1	1	47	C
1	1	48	A
1	1	50	U
1	1	59	G
1	1	60	A
1	1	65	A
1	1	66	A
1	1	67	A
1	1	73	C
1	1	74	G
1	1	77	A
1	1	85	A
1	1	89	A
1	1	92	G
1	1	93	C
1	1	96	G
1	1	99	A
1	1	105	C
1	1	108	A
1	1	109	A
1	1	110	G
1	1	111	C
1	1	113	C
1	1	119	U
1	1	120	G
1	1	121	A
1	1	128	G
1	1	130	A
1	1	133	U
1	1	134	U

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Mol	Chain	Res	Type
1	1	135	C
1	1	136	G
1	1	145	G
1	1	146	U
1	1	148	G
1	1	153	U
1	1	154	U
1	1	155	G
1	1	156	G
1	1	157	A
1	1	161	G
1	1	165	A
1	1	170	G
1	1	172	G
1	1	173	G
1	1	182	U
1	1	183	G
1	1	187	A
1	1	188	U
1	1	189	G
1	1	190	U
1	1	191	U
1	1	198	A
1	1	199	A
1	1	200	C
1	1	211	A
1	1	212	G
1	1	217	U
1	1	218	G
1	1	219	A
1	1	221	A
1	1	223	U
1	1	228	U
1	1	231	G
1	1	240	U
1	1	241	G
1	1	242	C
1	1	243	G
1	1	244	G
1	1	245	U
1	1	248	U
1	1	250	U

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Mol	Chain	Res	Type
1	1	251	G
1	1	252	U
1	1	253	A
1	1	263	C
1	1	266	A
1	1	267	G
1	1	268	A
1	1	269	G
1	1	278	U
1	1	283	G
1	1	286	U
1	1	291	C
1	1	292	U
1	1	295	A
1	1	298	U
1	1	305	U
1	1	315	C
1	1	318	A
1	1	329	U
1	1	337	G
1	1	341	G
1	1	343	U
1	1	346	C
1	1	350	C
1	1	352	A
1	1	357	A
1	1	359	U
1	1	364	G
1	1	365	A
1	1	371	G
1	1	374	A
1	1	376	G
1	1	382	U
1	1	387	A
1	1	390	G
1	1	394	G
1	1	397	A
1	1	398	A
1	1	401	U
1	1	402	A
1	1	403	C
1	1	404	G

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Mol	Chain	Res	Type
1	1	421	G
1	1	422	A
1	1	438	A
1	1	440	A
1	1	442	G
1	1	444	U
1	1	446	U
1	1	449	U
1	1	450	G
1	1	451	U
1	1	487	U
1	1	488	U
1	1	491	A
1	1	493	U
1	1	494	G
1	1	495	G
1	1	498	A
1	1	503	C
1	1	510	G
1	1	515	C
1	1	520	U
1	1	521	A
1	1	523	A
1	1	533	A
1	1	534	U
1	1	540	U
1	1	545	U
1	1	547	G
1	1	549	U
1	1	550	A
1	1	551	A
1	1	554	A
1	1	555	U
1	1	556	U
1	1	557	A
1	1	558	U
1	1	559	A
1	1	560	G
1	1	582	G
1	1	591	G
1	1	592	A
1	1	597	G

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Mol	Chain	Res	Type
1	1	600	G
1	1	604	G
1	1	611	A
1	1	619	A
1	1	620	U
1	1	623	U
1	1	636	C
1	1	637	C
1	1	643	U
1	1	644	G
1	1	647	A
1	1	649	A
1	1	656	A
1	1	660	A
1	1	661	G
1	1	666	A
1	1	667	C
1	1	669	U
1	1	675	C
1	1	676	G
1	1	677	A
1	1	678	G
1	1	681	U
1	1	682	U
1	1	683	U
1	1	685	G
1	1	689	U
1	1	691	A
1	1	697	A
1	1	699	A
1	1	705	A
1	1	712	G
1	1	716	A
1	1	717	C
1	1	718	G
1	1	719	U
1	1	720	A
1	1	726	G
1	1	727	G
1	1	735	A
1	1	737	G
1	1	744	A

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Mol	Chain	Res	Type
1	1	750	G
1	1	751	A
1	1	758	C
1	1	761	A
1	1	763	G
1	1	766	U
1	1	767	U
1	1	770	G
1	1	774	G
1	1	776	U
1	1	777	U
1	1	780	A
1	1	781	G
1	1	785	G
1	1	786	A
1	1	792	G
1	1	800	G
1	1	801	A
1	1	802	C
1	1	803	C
1	1	806	A
1	1	807	A
1	1	808	A
1	1	816	A
1	1	817	A
1	1	826	G
1	1	827	A
1	1	830	A
1	1	833	G
1	1	836	A
1	1	838	G
1	1	849	C
1	1	854	G
1	1	855	U
1	1	857	G
1	1	859	G
1	1	860	G
1	1	861	C
1	1	864	G
1	1	871	U
1	1	874	U
1	1	875	G

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Mol	Chain	Res	Type
1	1	879	U
1	1	880	G
1	1	888	A
1	1	896	A
1	1	897	U
1	1	907	G
1	1	908	G
1	1	909	G
1	1	914	A
1	1	915	A
1	1	916	G
1	1	917	A
1	1	921	A
1	1	924	G
1	1	925	A
1	1	932	U
1	1	934	G
1	1	937	G
1	1	939	U
1	1	941	G
1	1	943	U
1	1	944	C
1	1	949	C
1	1	951	A
1	1	959	C
1	1	960	U
1	1	962	A
1	1	967	A
1	1	970	A
1	1	977	C
1	1	979	U
1	1	980	A
1	1	981	U
1	1	984	G
1	1	985	U
1	1	991	G
1	1	994	G
1	1	1000	C
1	1	1002	A
1	1	1004	U
1	1	1006	A
1	1	1010	G

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Mol	Chain	Res	Type
1	1	1013	G
1	1	1014	U
1	1	1016	C
1	1	1017	C
1	1	1018	G
1	1	1021	G
1	1	1024	G
1	1	1026	A
1	1	1027	A
1	1	1028	U
1	1	1029	G
1	1	1031	C
1	1	1033	U
1	1	1041	U
1	1	1046	A
1	1	1047	A
1	1	1054	A
1	1	1063	G
1	1	1064	A
1	1	1065	A
1	1	1066	G
1	1	1072	G
1	1	1076	C
1	1	1081	U
1	1	1083	G
1	1	1086	C
1	1	1087	G
1	1	1094	U
1	1	1095	U
1	1	1097	G
1	1	1098	A
1	1	1102	A
1	1	1103	A
1	1	1106	G
1	1	1110	U
1	1	1116	G
1	1	1117	G
1	1	1121	U
1	1	1127	G
1	1	1129	A
1	1	1131	G
1	1	1137	C

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Mol	Chain	Res	Type
1	1	1143	A
1	1	1144	U
1	1	1152	G
1	1	1153	A
1	1	1155	C
1	1	1158	A
1	1	1159	A
1	1	1161	G
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	1185	C
1	1	1191	U
1	1	1192	C
1	1	1193	A
1	1	1194	G
1	1	1196	C
1	1	1197	A
1	1	1201	C
1	1	1209	G
1	1	1210	U
1	1	1213	G
1	1	1214	U
1	1	1217	A
1	1	1219	C
1	1	1221	A
1	1	1222	G
1	1	1230	G
1	1	1232	C
1	1	1236	G
1	1	1237	G
1	1	1245	A
1	1	1246	G
1	1	1249	G
1	1	1252	A
1	1	1253	U
1	1	1254	C

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Mol	Chain	Res	Type
1	1	1255	C
1	1	1256	G
1	1	1258	U
1	1	1259	A
1	1	1262	G
1	1	1263	A
1	1	1264	G
1	1	1268	G
1	1	1269	U
1	1	1270	A
1	1	1272	C
1	1	1273	A
1	1	1276	U
1	1	1277	C
1	1	1281	G
1	1	1282	G
1	1	1284	C
1	1	1285	G
1	1	1286	A
1	1	1287	A
1	1	1290	A
1	1	1292	C
1	1	1295	G
1	1	1297	C
1	1	1302	A
1	1	1305	U
1	1	1307	G
1	1	1308	A
1	1	1309	U
1	1	1313	G
1	1	1316	C
1	1	1317	A
1	1	1321	G
1	1	1323	G
1	1	1324	U
1	1	1325	U
1	1	1330	A
1	1	1348	U
1	1	1349	G
1	1	1350	A
1	1	1351	U
1	1	1352	A

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Mol	Chain	Res	Type
1	1	1353	U
1	1	1355	A
1	1	1356	U
1	1	1357	G
1	1	1362	G
1	1	1368	U
1	1	1372	C
1	1	1382	G
1	1	1385	C
1	1	1386	A
1	1	1391	C
1	1	1392	G
1	1	1394	A
1	1	1399	A
1	1	1400	G
1	1	1408	G
1	1	1418	A
1	1	1419	A
1	1	1422	G
1	1	1424	C
1	1	1425	U
1	1	1430	U
1	1	1434	G
1	1	1436	U
1	1	1437	C
1	1	1443	G
1	1	1446	A
1	1	1448	U
1	1	1450	G
1	1	1451	C
1	1	1455	U
1	1	1456	A
1	1	1457	U
1	1	1458	U
1	1	1468	A
1	1	1470	U
1	1	1471	U
1	1	1473	G
1	1	1482	A
1	1	1483	G
1	1	1485	G
1	1	1488	G

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Mol	Chain	Res	Type
1	1	1489	A
1	1	1494	U
1	1	1500	G
1	1	1501	U
1	1	1503	A
1	1	1507	G
1	1	1508	C
1	1	1511	U
1	1	1522	U
1	1	1523	U
1	1	1524	A
1	1	1525	G
1	1	1526	U
1	1	1533	U
1	1	1535	A
1	1	1553	U
1	1	1554	U
1	1	1555	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	1563	C
1	1	1565	G
1	1	1566	A
1	1	1570	U
1	1	1573	G
1	1	1574	C
1	1	1577	G
1	1	1579	C
1	1	1580	A
1	1	1581	C
1	1	1582	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	1595	U

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Mol	Chain	Res	Type
1	1	1596	C
1	1	1605	A
1	1	1606	U
1	1	1607	U
1	1	1613	A
1	1	1620	U
1	1	1628	C
1	1	1630	U
1	1	1635	G
1	1	1636	U
1	1	1637	A
1	1	1638	A
1	1	1643	A
1	1	1645	U
1	1	1646	G
1	1	1657	C
1	1	1659	U
1	1	1662	G
1	1	1664	G
1	1	1683	A
1	1	1687	U
1	1	1706	C
1	1	1707	A
1	1	1712	G
1	1	1713	G
1	1	1714	A
1	1	1716	U
1	1	1717	U
1	1	1720	U
1	1	1724	U
1	1	1728	G
1	1	1729	A
1	1	1730	G
1	1	1736	G
1	1	1737	U
1	1	1740	U
1	1	1741	A
1	1	1742	U
1	1	1750	A
1	1	1751	G
1	1	1756	C
1	1	1760	A

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Mol	Chain	Res	Type
1	1	1761	C
1	1	1763	U
1	1	1764	U
1	1	1765	U
1	1	1769	G
1	1	1770	G
1	1	1773	C
1	1	1775	G
1	1	1780	G
1	1	1781	C
1	1	1788	C
1	1	1793	C
1	1	1794	G
1	1	1795	U
1	1	1797	A
1	1	1808	G
1	1	1812	G
1	1	1813	A
1	1	1814	A
1	1	1815	U
1	1	1818	U
1	1	1820	U
1	1	1821	U
1	1	1835	A
1	1	1838	G
1	1	1840	U
1	1	1841	A
1	1	1842	A
1	1	1843	C
1	1	1844	C
1	1	1846	C
1	1	1848	G
1	1	1850	A
1	1	1851	G
1	1	1855	U
1	1	1863	G
1	1	1865	A
1	1	1874	A
1	1	1878	G
1	1	1879	A
1	1	1880	U
1	1	1881	A

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Mol	Chain	Res	Type
1	1	1884	A
1	1	1886	A
1	1	1889	G
1	1	1893	A
1	1	1896	A
1	1	1900	A
1	1	1904	C
1	1	1905	G
1	1	1906	G
1	1	1908	A
1	1	1912	U
1	1	1915	A
1	1	1926	C
1	1	1927	G
1	1	1928	G
1	1	1930	A
1	1	1931	U
1	1	1932	A
1	1	1935	G
1	1	1948	G
1	1	1953	G
1	1	1954	G
1	1	2094	C
1	1	2101	C
1	1	2102	U
1	1	2107	A
1	1	2111	G
1	1	2114	C
1	1	2116	G
1	1	2117	A
1	1	2118	C
1	1	2119	A
1	1	2122	G
1	1	2131	A
1	1	2134	G
1	1	2136	C
1	1	2137	U
1	1	2138	A
1	1	2139	A
1	1	2143	A
1	1	2145	A
1	1	2148	U

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Mol	Chain	Res	Type
1	1	2157	G
1	1	2158	A
1	1	2160	G
1	1	2166	A
1	1	2167	A
1	1	2168	A
1	1	2169	G
1	1	2170	U
1	1	2172	A
1	1	2176	U
1	1	2177	G
1	1	2178	A
1	1	2180	G
1	1	2184	U
1	1	2185	G
1	1	2186	U
1	1	2187	G
1	1	2188	A
1	1	2189	U
1	1	2194	G
1	1	2205	U
1	1	2206	G
1	1	2207	A
1	1	2223	A
1	1	2231	C
1	1	2239	G
1	1	2255	A
1	1	2257	C
1	1	2263	C
1	1	2269	U
1	1	2270	A
1	1	2271	A
1	1	2273	G
1	1	2279	A
1	1	2281	A
1	1	2285	C
1	1	2286	U
1	1	2288	G
1	1	2295	A
1	1	2296	A
1	1	2303	A
1	1	2304	C

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Mol	Chain	Res	Type
1	1	2306	C
1	1	2307	G
1	1	2309	A
1	1	2310	U
1	1	2312	A
1	1	2313	A
1	1	2315	G
1	1	2327	U
1	1	2334	U
1	1	2335	G
1	1	2336	U
1	1	2339	C
1	1	2344	U
1	1	2345	A
1	1	2347	U
1	1	2357	A
1	1	2361	A
1	1	2363	A
1	1	2364	G
1	1	2365	C
1	1	2370	G
1	1	2372	A
1	1	2373	A
1	1	2374	C
1	1	2375	G
1	1	2376	G
1	1	2383	C
1	1	2385	G
1	1	2388	U
1	1	2393	G
1	1	2397	A
1	1	2400	G
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	2415	C
1	1	2417	U
1	1	2418	G
1	1	2419	A

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Mol	Chain	Res	Type
1	1	2422	C
1	1	2424	A
1	1	2429	G
1	1	2432	A
1	1	2434	U
1	1	2438	A
1	1	2439	A
1	1	2452	G
1	1	2455	U
1	1	2456	A
1	1	2459	A
1	1	2460	U
1	1	2461	A
1	1	2462	A
1	1	2468	A
1	1	2469	G
1	1	2471	U
1	1	2474	G
1	1	2476	C
1	1	2479	C
1	1	2480	A
1	1	2482	U
1	1	2483	G
1	1	2486	A
1	1	2487	U
1	1	2488	A
1	1	2490	C
1	1	2491	A
1	1	2492	C
1	1	2494	A
1	1	2495	C
1	1	2496	C
1	1	2497	U
1	1	2500	A
1	1	2501	U
1	1	2502	A
1	1	2505	U
1	1	2507	C
1	1	2510	U
1	1	2514	U
1	1	2515	A
1	1	2522	G

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Mol	Chain	Res	Type
1	1	2524	A
1	1	2525	G
1	1	2526	C
1	1	2532	U
1	1	2537	U
1	1	2538	U
1	1	2540	A
1	1	2541	U
1	1	2542	U
1	1	2543	U
1	1	2549	G
1	1	2550	U
1	1	2552	C
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	2569	A
1	1	2570	U
1	1	2573	G
1	1	2575	G
1	1	2583	C
1	1	2584	G
1	1	2585	G
1	1	2593	A
1	1	2595	A
1	1	2606	G
1	1	2614	G
1	1	2615	G
1	1	2617	U
1	1	2618	G
1	1	2619	G
1	1	2620	G
1	1	2625	C
1	1	2628	A
1	1	2635	A
1	1	2639	G
1	1	2648	G
1	1	2649	A
1	1	2652	U

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Mol	Chain	Res	Type
1	1	2655	U
1	1	2656	A
1	1	2658	G
1	1	2669	G
1	1	2672	G
1	1	2674	A
1	1	2676	A
1	1	2677	G
1	1	2678	A
1	1	2680	A
1	1	2681	U
1	1	2686	A
1	1	2688	U
1	1	2689	A
1	1	2690	G
1	1	2691	A
1	1	2692	A
1	1	2701	U
1	1	2703	A
1	1	2704	A
1	1	2705	A
1	1	2712	U
1	1	2714	G
1	1	2716	U
1	1	2717	U
1	1	2719	U
1	1	2725	U
1	1	2726	C
1	1	2728	G
1	1	2729	U
1	1	2741	C
1	1	2749	G
1	1	2753	G
1	1	2755	C
1	1	2759	U
1	1	2760	C
1	1	2762	A
1	1	2765	C
1	1	2769	A
1	1	2771	U
1	1	2772	C
1	1	2773	C

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Mol	Chain	Res	Type
1	1	2777	G
1	1	2780	A
1	1	2787	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	2804	A
1	1	2808	A
1	1	2809	C
1	1	2810	C
1	1	2816	G
1	1	2817	A
1	1	2818	U
1	1	2821	C
1	1	2827	U
1	1	2838	A
1	1	2843	U
1	1	2844	C
1	1	2845	A
1	1	2847	A
1	1	2852	C
1	1	2858	U
1	1	2859	U
1	1	2860	U
1	1	2861	U
1	1	2863	G
1	1	2869	U
1	1	2871	G
1	1	2872	A
1	1	2873	U
1	1	2875	U
1	1	2886	U
1	1	2887	A
1	1	2889	C
1	1	2899	C
1	1	2901	G
1	1	2904	U
1	1	2905	U

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Mol	Chain	Res	Type
1	1	2907	G
1	1	2911	A
1	1	2912	G
1	1	2914	G
1	1	2925	C
1	1	2932	U
1	1	2934	A
1	1	2935	U
1	1	2936	A
1	1	2941	A
1	1	2942	C
1	1	2945	G
1	1	2946	A
1	1	2947	G
1	1	2954	U
1	1	2955	U
1	1	2968	G
1	1	2971	A
1	1	2978	U
1	1	2979	U
1	1	2981	U
1	1	2983	C
1	1	2984	C
1	1	2988	C
1	1	2992	U
1	1	2996	U
1	1	2997	G
1	1	3001	C
1	1	3003	G
1	1	3005	A
1	1	3006	A
1	1	3007	U
1	1	3011	A
1	1	3012	A
1	1	3014	U
1	1	3021	A
1	1	3026	G
1	1	3028	G
1	1	3030	G
1	1	3034	C
1	1	3036	G
1	1	3055	U

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Mol	Chain	Res	Type
1	1	3056	U
1	1	3057	U
1	1	3058	U
1	1	3059	G
1	1	3069	G
1	1	3070	A
1	1	3074	G
1	1	3075	G
1	1	3077	A
1	1	3078	U
1	1	3079	U
1	1	3080	G
1	1	3090	U
1	1	3092	C
1	1	3093	C
1	1	3099	C
1	1	3100	U
1	1	3101	G
1	1	3117	C
1	1	3122	A
1	1	3125	U
1	1	3129	A
1	1	3130	A
1	1	3131	U
1	1	3139	A
1	1	3142	A
1	1	3143	C
1	1	3153	U
1	1	3154	C
1	1	3156	U
1	1	3157	U
1	1	3158	G
1	1	3160	U
1	1	3162	C
1	1	3168	A
1	1	3170	A
1	1	3173	G
1	1	3174	A
1	1	3176	G
1	1	3178	A
1	1	3179	U
1	1	3180	A

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Mol	Chain	Res	Type
1	1	3182	G
1	1	3183	A
1	1	3185	U
1	1	3186	A
1	1	3187	A
1	1	3193	C
1	1	3194	C
1	1	3195	U
1	1	3196	U
1	1	3197	G
1	1	3202	G
1	1	3206	C
1	1	3207	U
1	1	3210	A
1	1	3212	C
1	1	3214	U
1	1	3216	G
1	1	3217	C
1	1	3218	A
1	1	3219	G
1	1	3222	U
1	1	3226	A
1	1	3228	C
1	1	3229	G
1	1	3235	C
1	1	3238	G
1	1	3243	A
1	1	3244	A
1	1	3246	G
1	1	3247	G
1	1	3259	U
1	1	3260	G
1	1	3264	G
1	1	3268	A
1	1	3269	U
1	1	3271	G
1	1	3272	C
1	1	3273	A
1	1	3275	U
1	1	3276	G
1	1	3278	C
1	1	3279	A

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Mol	Chain	Res	Type
1	1	3281	U
1	1	3288	G
1	1	3289	G
1	1	3292	A
1	1	3294	A
1	1	3295	A
1	1	3304	U
1	1	3308	C
1	1	3310	A
1	1	3313	U
1	1	3316	A
1	1	3317	U
1	1	3318	G
1	1	3320	A
1	1	3329	U
1	1	3339	A
1	1	3341	U
1	1	3345	G
1	1	3346	U
1	1	3349	C
1	1	3350	C
1	1	3351	U
1	1	3352	U
1	1	3354	U
1	1	3355	U
1	1	3356	G
1	1	3357	U
1	1	3362	A
1	1	3363	U
1	1	3368	U
1	1	3369	G
1	1	3375	A
1	1	3377	G
1	1	3378	C
1	1	3382	U
1	1	3384	U
1	1	3386	G
1	1	3388	C
1	1	3389	U
1	1	3390	G
2	3	4	U
2	3	6	C

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Mol	Chain	Res	Type
2	3	7	G
2	3	10	C
2	3	11	A
2	3	13	A
2	3	16	U
2	3	19	C
2	3	28	C
2	3	33	U
2	3	41	G
2	3	42	A
2	3	44	C
2	3	49	G
2	3	50	U
2	3	54	U
2	3	56	A
2	3	57	G
2	3	63	A
2	3	64	A
2	3	65	G
2	3	74	C
2	3	76	A
2	3	87	G
2	3	90	U
2	3	91	G
2	3	92	A
2	3	94	C
2	3	110	G
2	3	112	G
2	3	121	U
3	4	12	A
3	4	13	A
3	4	15	G
3	4	16	G
3	4	22	U
3	4	23	U
3	4	34	U
3	4	35	C
3	4	37	A
3	4	39	G
3	4	43	A
3	4	44	A
3	4	49	G

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Mol	Chain	Res	Type
3	4	50	C
3	4	51	G
3	4	54	A
3	4	59	A
3	4	62	C
3	4	63	G
3	4	71	A
3	4	72	A
3	4	75	G
3	4	80	A
3	4	81	U
3	4	82	U
3	4	83	C
3	4	84	C
3	4	86	U
3	4	87	G
3	4	88	A
3	4	89	A
3	4	95	G
3	4	96	A
3	4	100	U
3	4	102	U
3	4	104	A
3	4	106	C
3	4	107	G
3	4	112	U
3	4	113	U
3	4	125	U
3	4	126	A
3	4	127	U
3	4	131	A
3	4	138	A
3	4	148	G
3	4	151	C
3	4	152	G
3	4	155	A
3	4	158	U
47	2	2	A
47	2	3	U
47	2	4	C
47	2	5	U
47	2	8	U

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Mol	Chain	Res	Type
47	2	9	U
47	2	10	G
47	2	11	A
47	2	25	C
47	2	26	A
47	2	27	U
47	2	34	G
47	2	40	A
47	2	43	A
47	2	45	U
47	2	47	A
47	2	48	G
47	2	50	C
47	2	55	A
47	2	59	C
47	2	60	U
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	74	U
47	2	75	U
47	2	76	A
47	2	77	U
47	2	78	A
47	2	81	G
47	2	93	A
47	2	94	U
47	2	100	A
47	2	102	U
47	2	103	A
47	2	104	A
47	2	114	C
47	2	115	G
47	2	116	U
47	2	121	U
47	2	123	G
47	2	125	U

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Mol	Chain	Res	Type
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	135	A
47	2	136	C
47	2	137	U
47	2	138	A
47	2	139	C
47	2	141	U
47	2	142	G
47	2	144	U
47	2	145	A
47	2	146	U
47	2	153	G
47	2	157	A
47	2	159	U
47	2	169	A
47	2	171	A
47	2	188	A
47	2	189	C
47	2	191	C
47	2	192	U
47	2	194	U
47	2	195	G
47	2	196	G
47	2	200	A
47	2	203	U
47	2	204	G
47	2	217	A
47	2	218	A
47	2	224	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

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Mol	Chain	Res	Type
47	2	241	U
47	2	246	G
47	2	249	U
47	2	252	U
47	2	259	U
47	2	261	U
47	2	262	U
47	2	265	A
47	2	268	C
47	2	270	C
47	2	271	A
47	2	272	U
47	2	274	G
47	2	276	C
47	2	277	U
47	2	278	U
47	2	280	U
47	2	287	G
47	2	288	A
47	2	302	U
47	2	306	U
47	2	313	U
47	2	314	C
47	2	316	A
47	2	317	C
47	2	320	U
47	2	322	G
47	2	329	G
47	2	330	G
47	2	333	A
47	2	337	G
47	2	338	C
47	2	345	U
47	2	346	G
47	2	347	G
47	2	351	C
47	2	352	A
47	2	361	C
47	2	363	G
47	2	373	G
47	2	374	U
47	2	378	A

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Mol	Chain	Res	Type
47	2	391	A
47	2	400	A
47	2	401	A
47	2	402	C
47	2	403	G
47	2	404	G
47	2	412	A
47	2	417	A
47	2	419	G
47	2	421	A
47	2	423	G
47	2	424	C
47	2	426	G
47	2	428	A
47	2	432	G
47	2	434	G
47	2	435	C
47	2	439	U
47	2	444	C
47	2	445	A
47	2	452	A
47	2	454	U
47	2	455	C
47	2	456	A
47	2	458	G
47	2	460	A
47	2	461	G
47	2	464	A
47	2	469	C
47	2	471	A
47	2	475	A
47	2	480	G
47	2	481	A
47	2	486	G
47	2	488	G
47	2	490	C
47	2	492	A
47	2	493	U
47	2	495	C
47	2	496	G
47	2	502	U
47	2	506	A

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Mol	Chain	Res	Type
47	2	507	U
47	2	508	U
47	2	509	G
47	2	515	A
47	2	519	C
47	2	520	A
47	2	523	G
47	2	525	A
47	2	532	U
47	2	536	C
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	544	A
47	2	545	A
47	2	551	G
47	2	554	C
47	2	555	A
47	2	557	G
47	2	558	U
47	2	559	C
47	2	565	C
47	2	566	C
47	2	567	A
47	2	568	G
47	2	574	G
47	2	575	C
47	2	579	A
47	2	580	A
47	2	582	U
47	2	594	A
47	2	597	G
47	2	600	U
47	2	606	A
47	2	607	G
47	2	608	U
47	2	610	G
47	2	611	U
47	2	612	U

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Mol	Chain	Res	Type
47	2	613	G
47	2	617	U
47	2	618	U
47	2	619	A
47	2	620	A
47	2	622	A
47	2	623	A
47	2	624	G
47	2	635	A
47	2	638	U
47	2	639	U
47	2	653	C
47	2	654	C
47	2	655	G
47	2	657	U
47	2	658	C
47	2	677	G
47	2	678	A
47	2	681	U
47	2	687	G
47	2	691	C
47	2	692	C
47	2	694	U
47	2	695	U
47	2	696	C
47	2	697	C
47	2	698	U
47	2	700	C
47	2	701	U
47	2	704	C
47	2	705	U
47	2	706	A
47	2	707	A
47	2	708	C
47	2	709	C
47	2	710	U
47	2	711	U
47	2	712	G
47	2	713	A
47	2	716	C
47	2	717	C
47	2	718	U

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Mol	Chain	Res	Type
47	2	720	G
47	2	721	U
47	2	722	G
47	2	725	U
47	2	727	U
47	2	728	U
47	2	729	G
47	2	730	G
47	2	731	C
47	2	733	A
47	2	735	C
47	2	736	C
47	2	738	G
47	2	739	G
47	2	741	C
47	2	742	U
47	2	743	U
47	2	745	U
47	2	746	A
47	2	754	A
47	2	755	A
47	2	765	G
47	2	766	U
47	2	767	U
47	2	771	A
47	2	772	G
47	2	775	G
47	2	778	G
47	2	779	U
47	2	780	A
47	2	781	U
47	2	783	G
47	2	784	C
47	2	787	G
47	2	789	A
47	2	791	A
47	2	794	U
47	2	795	U
47	2	803	A
47	2	812	A
47	2	813	U
47	2	814	A

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Mol	Chain	Res	Type
47	2	815	G
47	2	820	U
47	2	821	U
47	2	823	G
47	2	824	G
47	2	829	A
47	2	830	U
47	2	833	U
47	2	837	G
47	2	841	U
47	2	845	G
47	2	846	G
47	2	848	C
47	2	849	C
47	2	850	A
47	2	852	C
47	2	854	U
47	2	859	A
47	2	860	U
47	2	862	A
47	2	863	A
47	2	865	A
47	2	866	G
47	2	880	C
47	2	886	U
47	2	888	U
47	2	898	A
47	2	900	A
47	2	903	U
47	2	913	G
47	2	914	G
47	2	915	A
47	2	916	U
47	2	921	U
47	2	928	U
47	2	929	A
47	2	933	A
47	2	935	U
47	2	938	G
47	2	939	A
47	2	942	G
47	2	944	A

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Mol	Chain	Res	Type
47	2	945	U
47	2	946	U
47	2	951	A
47	2	960	U
47	2	964	U
47	2	966	A
47	2	967	A
47	2	987	G
47	2	988	A
47	2	992	A
47	2	993	A
47	2	1007	C
47	2	1020	A
47	2	1021	C
47	2	1022	C
47	2	1025	A
47	2	1026	A
47	2	1027	A
47	2	1028	C
47	2	1031	U
47	2	1039	A
47	2	1052	U
47	2	1053	G
47	2	1054	U
47	2	1067	C
47	2	1074	G
47	2	1081	A
47	2	1082	C
47	2	1085	G
47	2	1092	A
47	2	1093	A
47	2	1097	U
47	2	1098	U
47	2	1099	U
47	2	1100	G
47	2	1109	G
47	2	1113	A
47	2	1122	G
47	2	1125	A
47	2	1126	G
47	2	1137	A
47	2	1138	A

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Mol	Chain	Res	Type
47	2	1139	A
47	2	1150	G
47	2	1151	A
47	2	1158	C
47	2	1159	C
47	2	1162	C
47	2	1163	A
47	2	1164	G
47	2	1166	A
47	2	1167	G
47	2	1170	G
47	2	1173	C
47	2	1180	C
47	2	1181	U
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	1191	U
47	2	1193	A
47	2	1194	A
47	2	1196	A
47	2	1199	G
47	2	1200	G
47	2	1202	A
47	2	1206	U
47	2	1207	C
47	2	1209	C
47	2	1212	G
47	2	1217	A
47	2	1218	G
47	2	1219	A
47	2	1221	A
47	2	1223	A
47	2	1225	U
47	2	1227	A
47	2	1228	G
47	2	1229	G
47	2	1230	A

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Mol	Chain	Res	Type
47	2	1232	U
47	2	1235	C
47	2	1238	A
47	2	1239	U
47	2	1241	G
47	2	1242	A
47	2	1244	A
47	2	1245	G
47	2	1246	C
47	2	1250	U
47	2	1251	U
47	2	1252	C
47	2	1255	G
47	2	1256	A
47	2	1257	U
47	2	1258	U
47	2	1260	U
47	2	1263	G
47	2	1264	G
47	2	1266	U
47	2	1267	G
47	2	1268	G
47	2	1269	U
47	2	1270	G
47	2	1273	G
47	2	1274	C
47	2	1275	A
47	2	1278	G
47	2	1284	C
47	2	1286	U
47	2	1287	A
47	2	1291	G
47	2	1297	G
47	2	1298	U
47	2	1299	G
47	2	1300	A
47	2	1301	U
47	2	1302	U
47	2	1306	C
47	2	1307	U
47	2	1309	C
47	2	1312	A

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Mol	Chain	Res	Type
47	2	1314	U
47	2	1315	U
47	2	1318	G
47	2	1321	A
47	2	1328	G
47	2	1336	A
47	2	1337	A
47	2	1339	C
47	2	1340	U
47	2	1342	C
47	2	1343	U
47	2	1347	U
47	2	1349	G
47	2	1351	G
47	2	1353	U
47	2	1354	G
47	2	1358	G
47	2	1361	U
47	2	1363	U
47	2	1364	G
47	2	1368	G
47	2	1370	U
47	2	1372	U
47	2	1378	U
47	2	1380	U
47	2	1382	A
47	2	1383	G
47	2	1384	A
47	2	1385	G
47	2	1388	A
47	2	1390	U
47	2	1392	U
47	2	1394	G
47	2	1397	U
47	2	1398	U
47	2	1399	C
47	2	1400	A
47	2	1402	G
47	2	1403	C
47	2	1404	C
47	2	1405	G
47	2	1409	G

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Mol	Chain	Res	Type
47	2	1410	A
47	2	1411	A
47	2	1412	G
47	2	1414	U
47	2	1415	U
47	2	1416	G
47	2	1418	G
47	2	1419	G
47	2	1427	A
47	2	1428	G
47	2	1429	G
47	2	1430	U
47	2	1432	U
47	2	1433	G
47	2	1434	U
47	2	1436	A
47	2	1444	A
47	2	1445	G
47	2	1446	A
47	2	1447	C
47	2	1451	C
47	2	1453	G
47	2	1457	C
47	2	1458	G
47	2	1459	C
47	2	1461	C
47	2	1469	A
47	2	1471	A
47	2	1472	C
47	2	1473	U
47	2	1474	G
47	2	1478	G
47	2	1479	A
47	2	1481	C
47	2	1482	C
47	2	1489	U
47	2	1490	C
47	2	1491	U
47	2	1492	A
47	2	1493	A
47	2	1496	U
47	2	1506	G

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Mol	Chain	Res	Type
47	2	1512	G
47	2	1514	U
47	2	1516	A
47	2	1517	U
47	2	1518	C
47	2	1520	U
47	2	1521	G
47	2	1522	U
47	2	1523	G
47	2	1524	A
47	2	1531	G
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	1541	G
47	2	1542	G
47	2	1543	A
47	2	1557	U
47	2	1559	A
47	2	1567	U
47	2	1568	C
47	2	1570	A
47	2	1571	C
47	2	1572	G
47	2	1583	A
47	2	1584	G
47	2	1586	A
47	2	1587	A
47	2	1589	C
47	2	1591	C
47	2	1596	C
47	2	1597	A
47	2	1601	G
47	2	1604	U
47	2	1605	G
47	2	1612	U
47	2	1613	U
47	2	1615	C
47	2	1616	G

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Mol	Chain	Res	Type
47	2	1617	U
47	2	1619	C
47	2	1625	C
47	2	1631	A
47	2	1634	C
47	2	1635	A
47	2	1636	C
47	2	1637	C
47	2	1638	G
47	2	1639	C
47	2	1647	U
47	2	1651	A
47	2	1653	C
47	2	1657	U
47	2	1658	G
47	2	1664	C
47	2	1670	G
47	2	1678	A
47	2	1679	G
47	2	1680	G
47	2	1681	A
47	2	1682	U
47	2	1683	C
47	2	1684	U
47	2	1685	G
47	2	1686	C
47	2	1689	A
47	2	1694	A
47	2	1696	G
47	2	1698	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	1705	C
47	2	1707	A
47	2	1708	U
47	2	1709	C
47	2	1710	U
47	2	1712	A

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Mol	Chain	Res	Type
47	2	1713	G
47	2	1715	G
47	2	1716	C
47	2	1717	G
47	2	1718	G
47	2	1720	G
47	2	1730	A
47	2	1736	G
47	2	1747	G
47	2	1749	A
47	2	1750	A
47	2	1755	A
47	2	1756	A
47	2	1757	G
47	2	1758	U
47	2	1761	U
47	2	1762	A
47	2	1766	A
47	2	1767	G
47	2	1769	U
47	2	1780	G
47	2	1782	A
47	2	1783	C
47	2	1791	A
47	2	1792	G
47	2	1793	G
47	2	1794	A
47	2	1795	U
47	2	1796	C
47	2	1798	U
81	AX	4	G
81	AX	9	A
81	AX	10	G
81	AX	11	C
81	AX	14	A
81	AX	16	U
81	AX	17	U
81	AX	18	G
81	AX	19	G
81	AX	20	G
81	AX	21	A
81	AX	22	G

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Mol	Chain	Res	Type
81	AX	24	G
81	AX	26	G
81	AX	27	C
81	AX	30	G
81	AX	34	G
81	AX	37	G
81	AX	38	A
81	AX	40	C
81	AX	42	G
81	AX	46	G
81	AX	47	U
81	AX	48	C
81	AX	49	C
81	AX	55	U
81	AX	59	U
81	AX	60	C
81	AX	61	C
81	AX	69	U
81	AX	74	C
81	AX	75	C
81	AX	76	A
82	AY	44	A
82	AY	45	A
82	AY	48	U
82	AY	49	U
82	AY	50	U

All (44) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	980	A
1	1	1053	A
1	1	1283	C
1	1	1285	G
1	1	1506	A
1	1	1562	C
1	1	1594	A
1	1	1629	U
1	1	2270	A
1	1	2295	A
1	1	2306	C
1	1	2461	A

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Mol	Chain	Res	Type
1	1	2541	U
1	1	2549	G
1	1	2874	G
1	1	3004	C
1	1	3078	U
1	1	3121	U
3	4	22	U
3	4	88	A
47	2	1	U
47	2	74	U
47	2	315	A
47	2	507	U
47	2	611	U
47	2	706	A
47	2	779	U
47	2	780	A
47	2	865	A
47	2	941	A
47	2	1138	A
47	2	1244	A
47	2	1273	G
47	2	1274	C
47	2	1298	U
47	2	1338	C
47	2	1399	C
47	2	1491	U
47	2	1536	G
47	2	1611	A
47	2	1637	C
47	2	1684	U
47	2	1756	A
81	AX	19	G

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	$\#\|Z\|>2$
83	DDE	AZ	699	83	14,20,21	1.97	3 (21%)	14,28,30	2.18	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
83	DDE	AZ	699	83	-	7/20/21/23	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	AZ	699	DDE	CBI-NAD	5.69	1.47	1.32
83	AZ	699	DDE	CAT-CE1	3.25	1.54	1.50
83	AZ	699	DDE	OAG-CBI	-2.11	1.19	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
83	AZ	699	DDE	CBW-CBI-NAD	5.22	121.94	115.28
83	AZ	699	DDE	CAC-NCB-CAB	3.55	117.80	108.10
83	AZ	699	DDE	OAG-CBI-NAD	-2.80	118.14	123.00
83	AZ	699	DDE	CAU-CBW-CBI	-2.27	106.70	111.20
83	AZ	699	DDE	CG-ND1-CE1	2.01	108.99	103.05

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
83	AZ	699	DDE	N-CA-CB-CG
83	AZ	699	DDE	C-CA-CB-CG
83	AZ	699	DDE	CAT-CAU-CBW-CBI
83	AZ	699	DDE	CAT-CAU-CBW-NCB
83	AZ	699	DDE	CE1-CAT-CAU-CBW
83	AZ	699	DDE	NAD-CBI-CBW-NCB
83	AZ	699	DDE	OAG-CBI-CBW-NCB

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 10 ligands modelled in this entry, 8 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
85	SO1	AZ	901	-	35,39,39	0.20	0	39,64,64	0.85	2 (5%)
86	GCP	AZ	902	-	27,34,34	1.18	4 (14%)	34,54,54	2.22	10 (29%)

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
85	SO1	AZ	901	-	-	9/21/104/104	0/7/5/5
86	GCP	AZ	902	-	-	6/15/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	AZ	902	GCP	C6-N1	3.06	1.38	1.33
86	AZ	902	GCP	PB-O2B	-2.73	1.50	1.56
86	AZ	902	GCP	PG-O1G	2.17	1.54	1.50
86	AZ	902	GCP	PG-O3G	-2.15	1.50	1.54

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
86	AZ	902	GCP	C5-C6-N1	-8.16	112.27	123.43
86	AZ	902	GCP	C2-N1-C6	5.76	125.08	115.93
85	AZ	901	SO1	C18-C9-C16	-4.13	97.73	103.64
86	AZ	902	GCP	O2B-PB-C3B	3.94	122.68	106.58
86	AZ	902	GCP	N3-C2-N1	-2.94	123.30	127.22
86	AZ	902	GCP	O3G-PG-C3B	2.58	112.66	106.40
86	AZ	902	GCP	O1G-PG-C3B	-2.41	106.06	111.24
86	AZ	902	GCP	C2-N3-C4	-2.37	112.66	115.36
86	AZ	902	GCP	C4-C5-C6	-2.28	118.62	120.80
85	AZ	901	SO1	C7-C2-C6	2.27	116.47	112.17
86	AZ	902	GCP	PB-O3A-PA	-2.25	125.41	132.56
86	AZ	902	GCP	O2G-PG-O1G	-2.06	106.95	112.39

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
86	AZ	902	GCP	PG-C3B-PB-O1B
86	AZ	902	GCP	PG-C3B-PB-O3A
85	AZ	901	SO1	C56-C55-O64-C65
85	AZ	901	SO1	C2-C1-C5-O14
85	AZ	901	SO1	C2-C1-C5-O15
86	AZ	902	GCP	C4'-C5'-O5'-PA
85	AZ	901	SO1	C3-C1-C5-O15
85	AZ	901	SO1	C3-C1-C5-O14
85	AZ	901	SO1	O19-C11-C3-C1
86	AZ	902	GCP	PB-C3B-PG-O1G
86	AZ	902	GCP	C5'-O5'-PA-O3A
86	AZ	902	GCP	C5'-O5'-PA-O2A
85	AZ	901	SO1	C20-C13-C4-C1
85	AZ	901	SO1	C1-C2-C8-O17
85	AZ	901	SO1	C54-C55-O64-C65

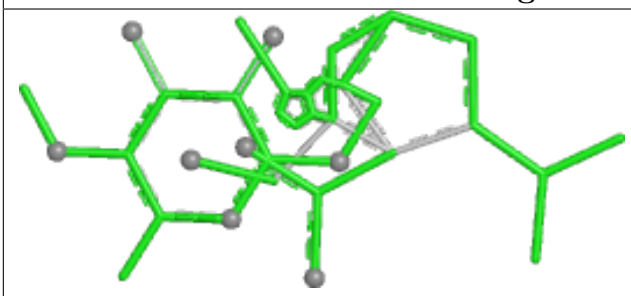
There are no ring outliers.

No monomer is involved in short contacts.

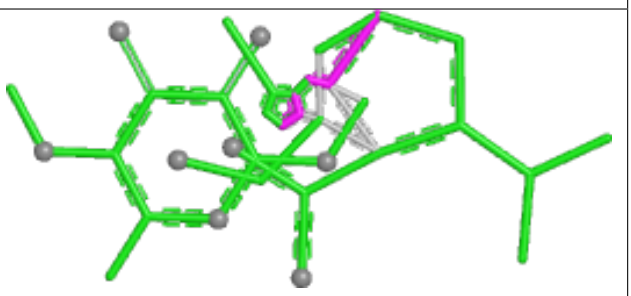
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

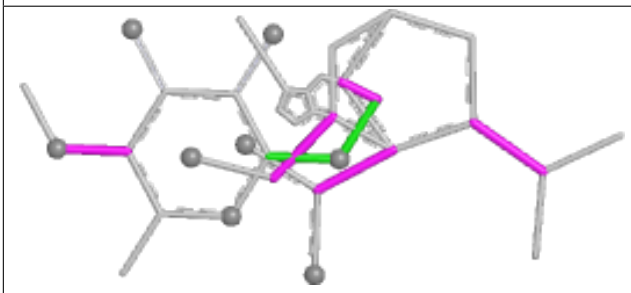
Ligand SO1 AZ 901



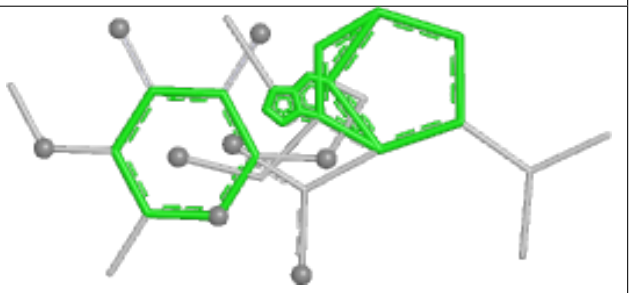
Bond lengths



Bond angles

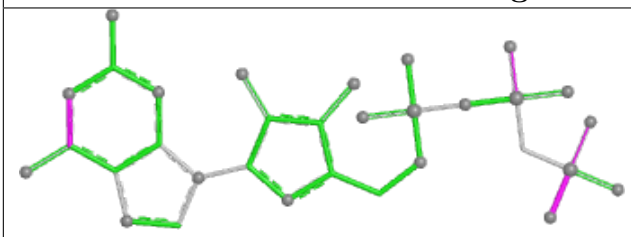


Torsions

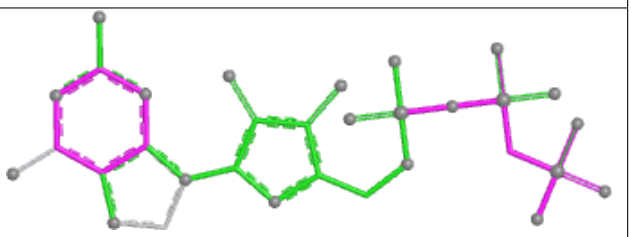


Rings

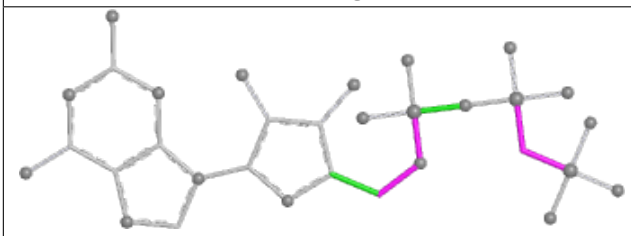
Ligand GCP AZ 902



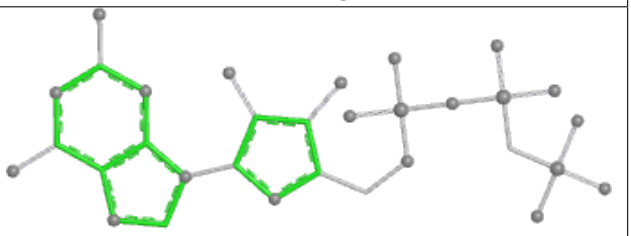
Bond lengths



Bond angles



Torsions



Rings

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.

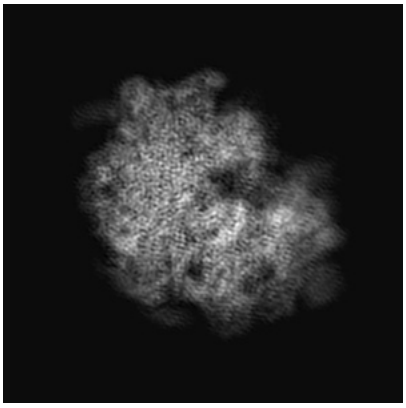
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-0047. These allow visual inspection of the internal detail of the map and identification of artifacts.

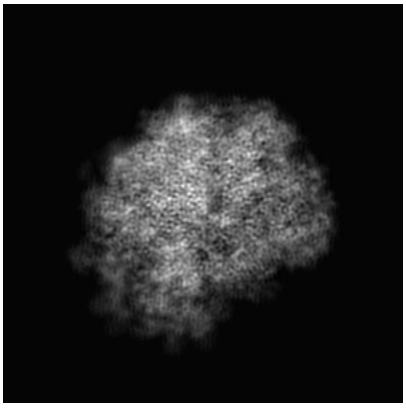
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

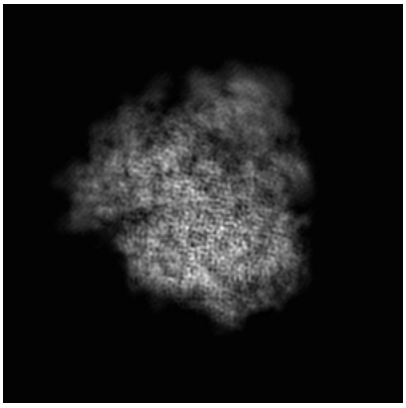
6.1.1 Primary map



X



Y

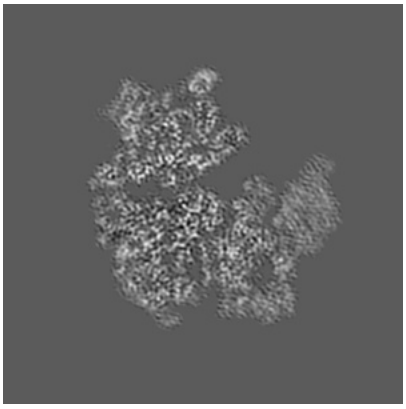


Z

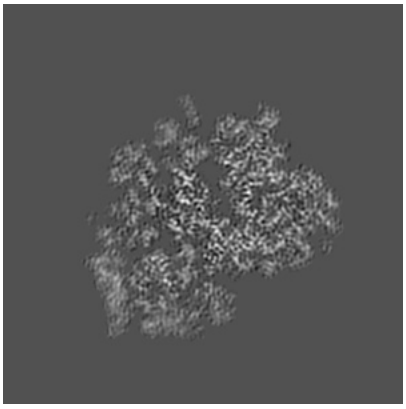
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

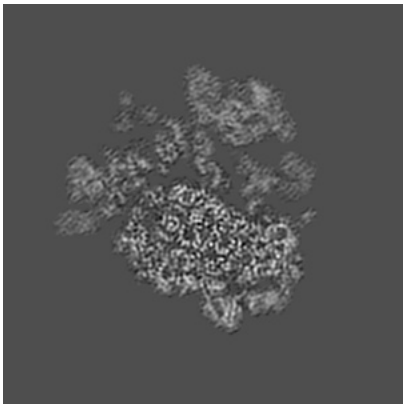
6.2.1 Primary map



X Index: 180



Y Index: 180

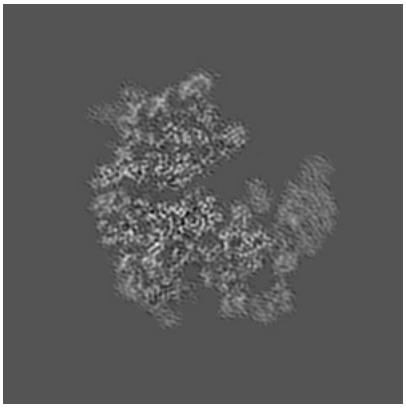


Z Index: 180

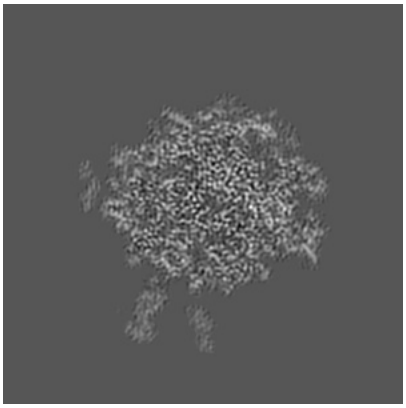
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

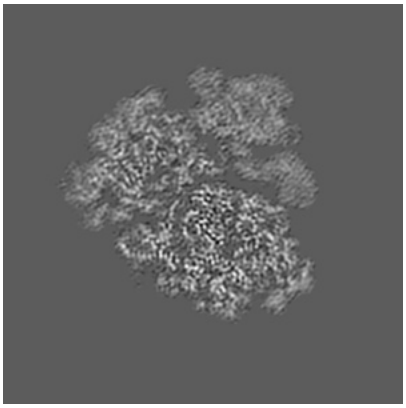
6.3.1 Primary map



X Index: 183



Y Index: 156



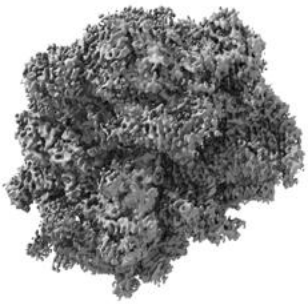
Z Index: 166

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

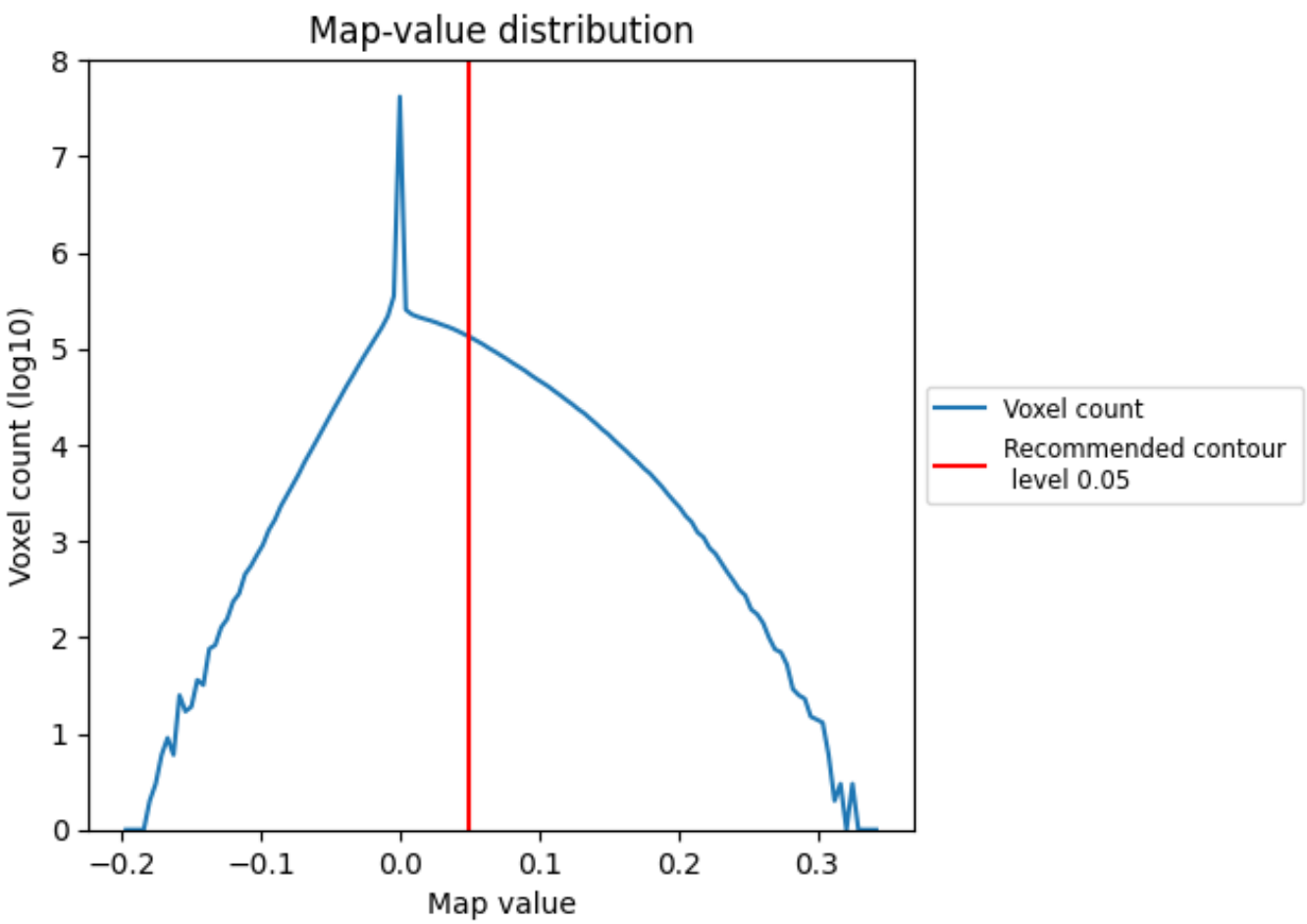
6.5 Mask visualisation (i)

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

7 Map analysis (i)

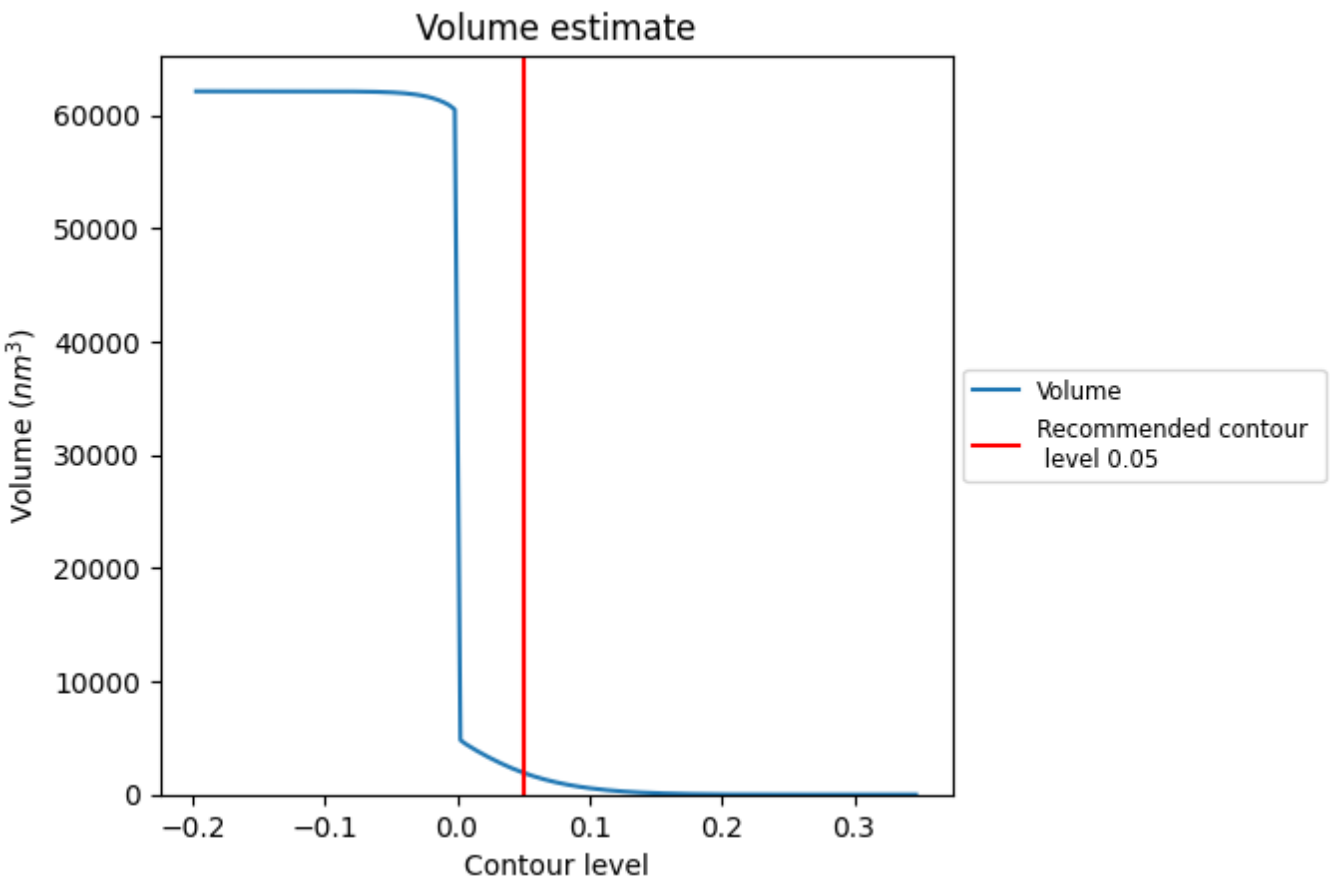
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

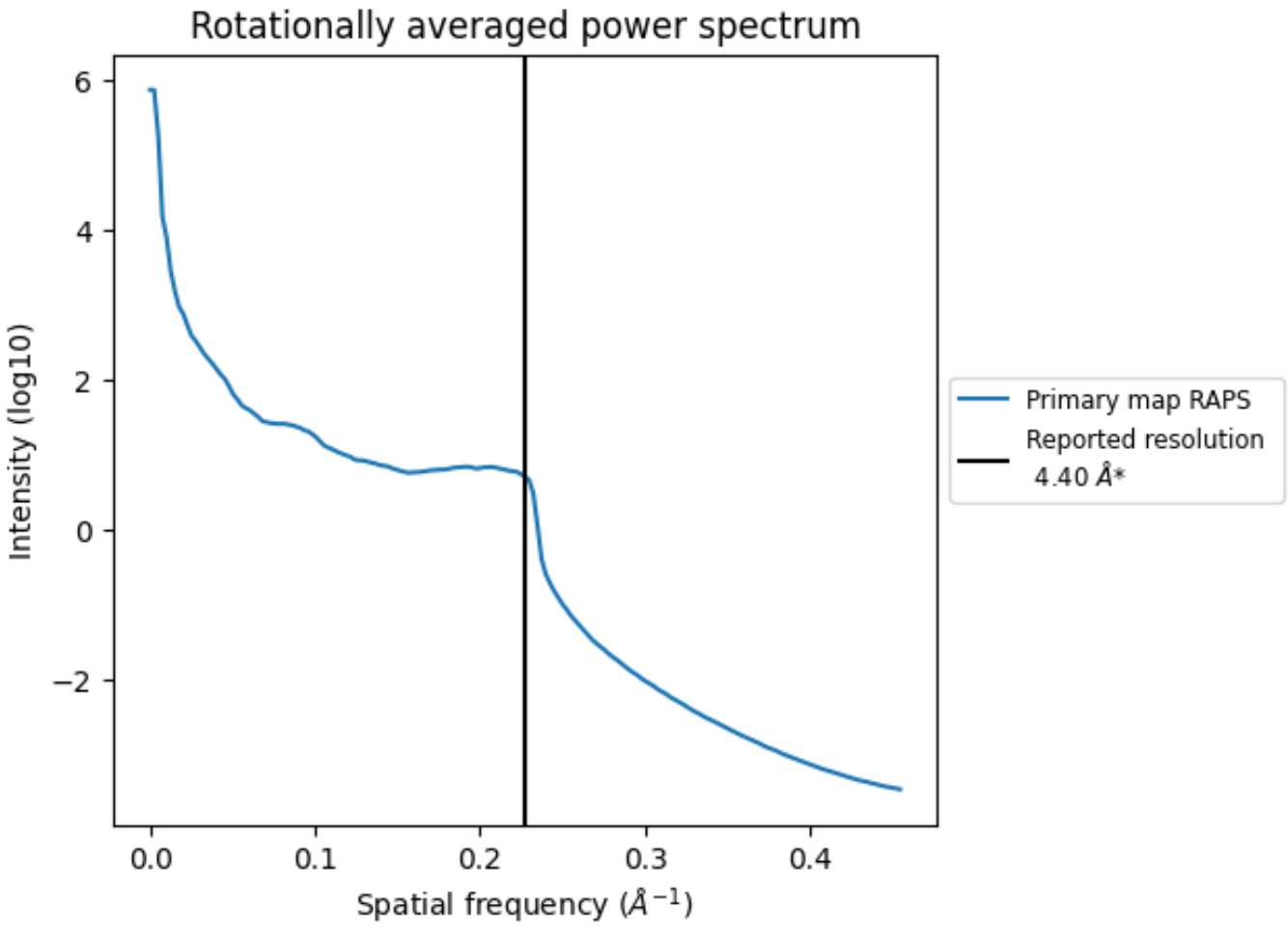
7.2 Volume estimate (i)



The volume at the recommended contour level is 1936 nm^3; this corresponds to an approximate mass of 1749 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 0.227 Å^{-1}

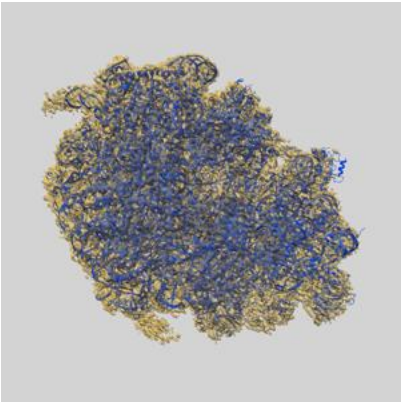
8 Fourier-Shell correlation (i)

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

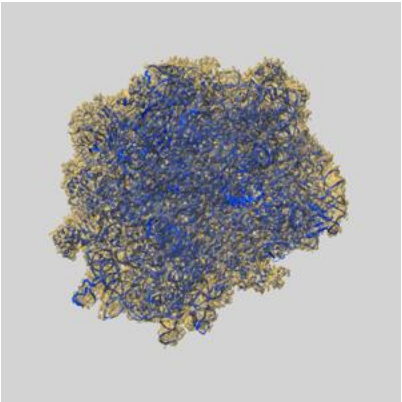
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-0047 and PDB model 6GQ1. Per-residue inclusion information can be found in section 3 on page 20.

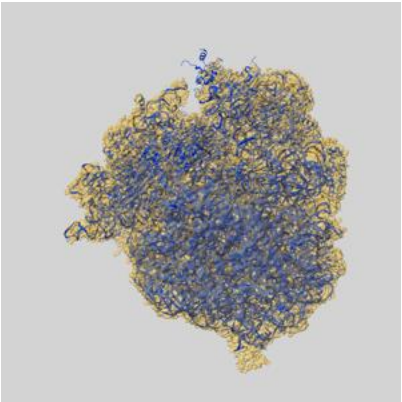
9.1 Map-model overlay (i)



X



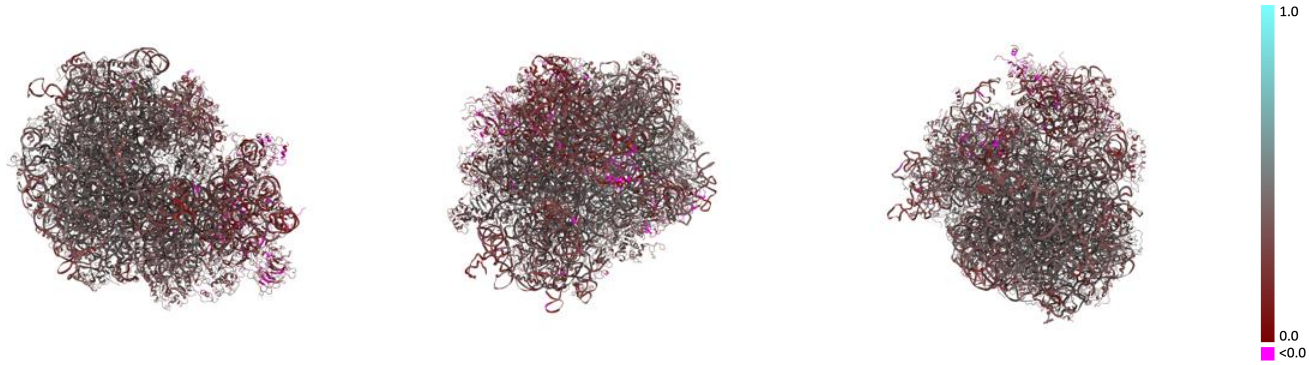
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

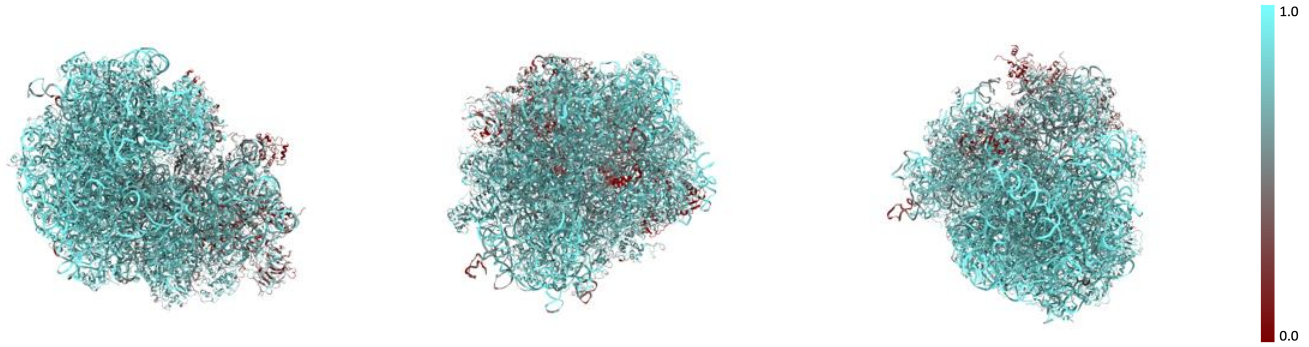
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

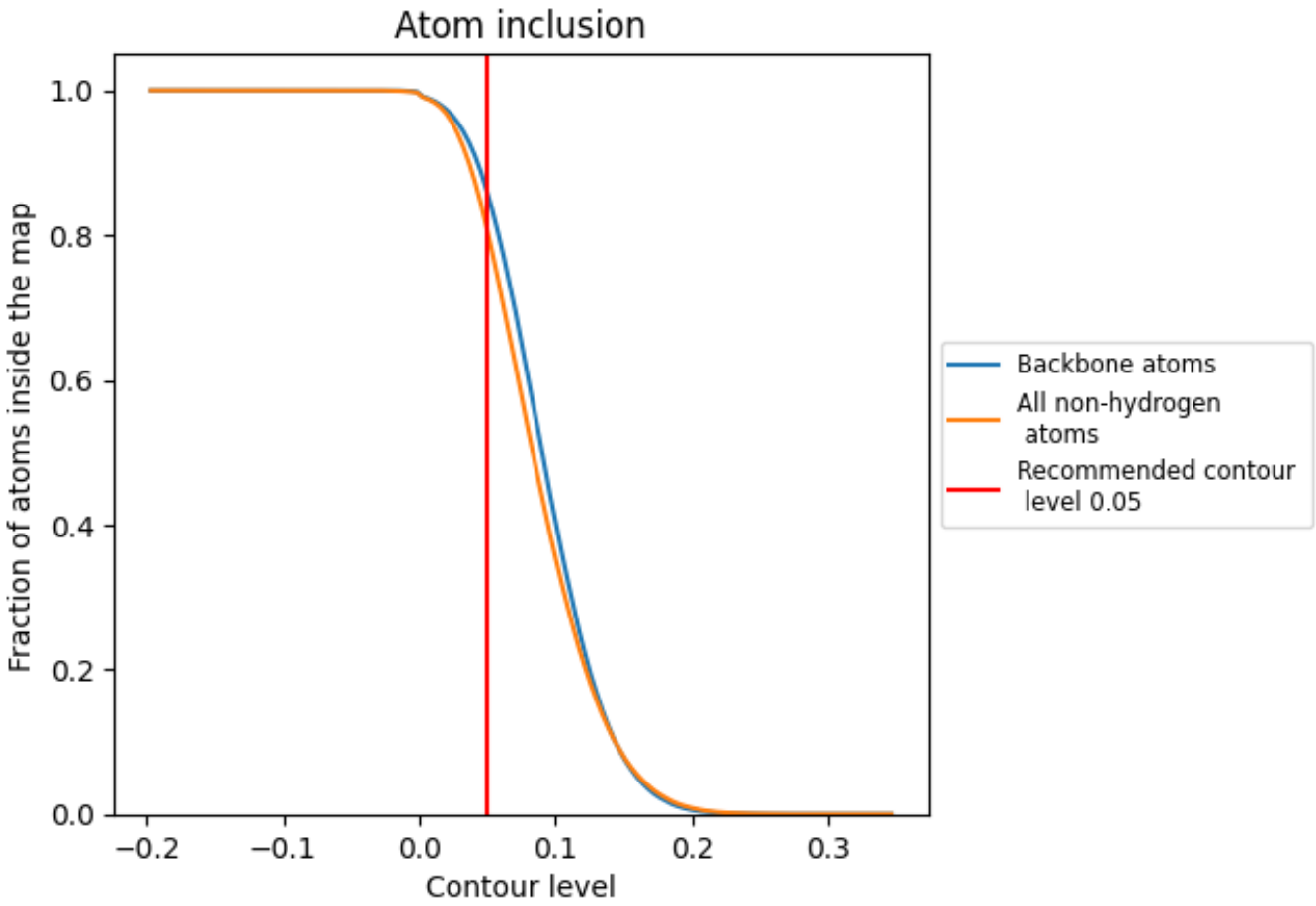
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8060	0.3570
1	0.9111	0.3810
2	0.8438	0.3240
3	0.9356	0.3530
4	0.9344	0.3930
A	0.7740	0.4380
AA	0.6570	0.2610
AB	0.6779	0.3880
AC	0.1068	0.1250
AD	0.7697	0.3720
AE	0.7993	0.3800
AF	0.5996	0.2770
AG	0.5533	0.2570
AH	0.5300	0.2530
AI	0.5572	0.2540
AJ	0.5782	0.2420
AK	0.3583	0.2170
AL	0.7108	0.3380
AM	0.7655	0.3910
AN	0.6984	0.3920
AO	0.7464	0.3370
AP	0.3711	0.1990
AQ	0.7459	0.3600
AR	0.7475	0.3620
AS	0.4109	0.2240
AT	0.7028	0.2720
AU	0.6253	0.3360
AV	0.4710	0.2100
AW	0.3214	0.1830
AX	0.6667	0.2570
AY	0.2988	0.3080
AZ	0.6606	0.3520
B	0.8064	0.4140
C	0.8276	0.4080
D	0.7764	0.3260

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Chain	Atom inclusion	Q-score
E	0.8087	0.3660
F	0.8175	0.3970
G	0.7980	0.3630
H	0.7725	0.3940
I	0.7785	0.4000
J	0.7445	0.3430
L	0.8117	0.3950
M	0.8109	0.3730
N	0.8332	0.4160
O	0.8137	0.3990
P	0.8198	0.4120
P0	0.1918	0.1770
P2	0.1749	0.1810
Q	0.8151	0.4190
R	0.7978	0.3970
S	0.8031	0.4050
T	0.7976	0.4070
U	0.7558	0.3640
V	0.7365	0.4370
W	0.7861	0.4210
X	0.7834	0.4060
Y	0.8323	0.4070
Z	0.8170	0.3910
a	0.8345	0.4160
b	0.7633	0.4150
c	0.7975	0.3830
d	0.7526	0.4080
e	0.8159	0.4230
f	0.8027	0.4150
g	0.7861	0.4240
h	0.7837	0.3870
i	0.7946	0.3630
j	0.8552	0.4370
k	0.7462	0.3910
l	0.7904	0.4110
m	0.7772	0.4180
n	0.6298	0.4360
o	0.7720	0.4100
p	0.7627	0.4320
q	0.7252	0.3320
r	0.7528	0.3650
s	0.7289	0.3740

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Chain	Atom inclusion	Q-score
t	0.5027	0.2530
u	0.7383	0.3500
v	0.4736	0.2470
w	0.7182	0.3120
x	0.7032	0.3170
y	0.7326	0.3570
z	0.7559	0.3450