Full wwPDB EM Validation Report (i)

Nov 20, 2022 – 04:36 am GMT

PDB ID	:	6GQB
EMDB ID	:	EMD-0048
Title	:	Cryo-EM reconstruction of yeast 80S ribosome in complex with mRNA, tRNA and eEF2 (GDP+AlF4/sordarin)
Authors	:	Pellegrino, S.; Yusupov, M.; Yusupova, G.; Hashem, Y.
Deposited on	:	2018-06-07
Resolution	:	3.90 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:

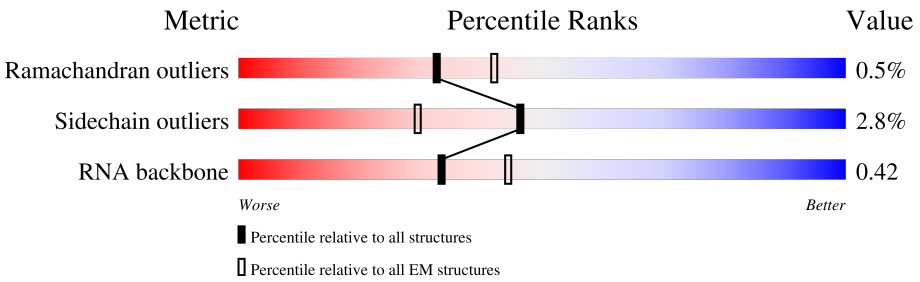
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.90 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	61% 31% • 5%
2	3	121	73% 26% •
3	4	158	66% 33% •
4	P0	189	80% 97% • •
5	P2	94	79% 94% 6%
6	A	252	94% 6%
7	B	386	97% •
8	C	361	97% •

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Mol	Chain	Length	Quality of chain
9	D	296	7% 96%
10	E	175	84% 5% 11%
11	F	222	97%
12	G	233	97%
13	H	191	92% 8%
14	I	220	5% 92%
15	J	169	5% 95%
16	L	193	95% 5%
17	M	136	99%
18	N	203	95% 5%
19	O	197	91% 9%
20	P	183	7% 97%
21	Q	185	98%
22	R	188	6% 96%
23	S	172	94% 5%
24	T	159	99%
25	U	100	98%
26	V	136	13% 96%
27	W	64	14% 97%
28	X	121	5% 98%
29	Y	126	98%
30	Z	135	96%
31	a	148	95% 5%
32	b	58	7% 98%
33	c	97	96%

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Mol	Chain	Length	Quality of chain
34	d	109	8% 96%
35	e	127	5% 98%
36	f	106	93% 6%
37	g	112	94% 6%
38	h	119	93% 7%
39	i	99	94% 6%
40	j	87	91% 9%
41	k	77	92% 6%
42	l	50	92% 8%
43	m	52	6% 98%
44	n	25	12% 92% 8%
45	o	105	5% 95% 5%
46	p	91	5% 98%
47	2	1797	5% 55% 39% 5%
48	q	206	8% 96%
49	r	214	7% 93% 7%
50	s	217	7% 98%
51	t	223	35% 95% 5%
52	u	260	7% 94% 5%
53	v	206	45% 92% 7%
54	w	223	15% 93% 6%
55	x	184	10% 95% 5%
56	y	199	8% 91% 6%
57	z	185	5% 94% 6%
58	AA	105	25% 88% 9%

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Mol	Chain	Length	Quality of chain
59	AB	153	19% 98%
60	AC	124	93% 98%
61	AD	150	91% 8%
62	AE	127	99%
63	AF	124	26% 94% 6%
64	AG	141	31% 93% 7%
65	AH	125	30% 89% 7%
66	AI	145	25% 94% 6%
67	AJ	143	24% 98%
68	AK	107	42% 96%
69	AL	87	13% 95% 5%
70	AM	129	95% 5%
71	AN	144	8% 94% 6%
72	AO	134	8% 98%
73	AP	70	69% 99%
74	AQ	97	8% 98%
75	AR	81	95% 5%
76	AS	63	59% 98%
77	AT	53	13% 96%
78	AU	60	25% 93% 7%
79	AV	318	45% 97%
80	AW	37	70% 100%
81	AX	76	54% 43%
82	AY	7	43% 43% 57%
83	BA	204	45% 97%

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Mol	Chain	Length	Quality of chain
84	AZ	840	64% 91% 8%

2 Entry composition (i)

There are 88 unique types of molecules in this entry. The entry contains 212143 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 5S ribosomal RNA.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			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	64	528	340	103	84	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	233	142	63	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	7	144	65	21	51	7	0	0

- Molecule 83 is a protein called 60S ribosomal protein L1-A.

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

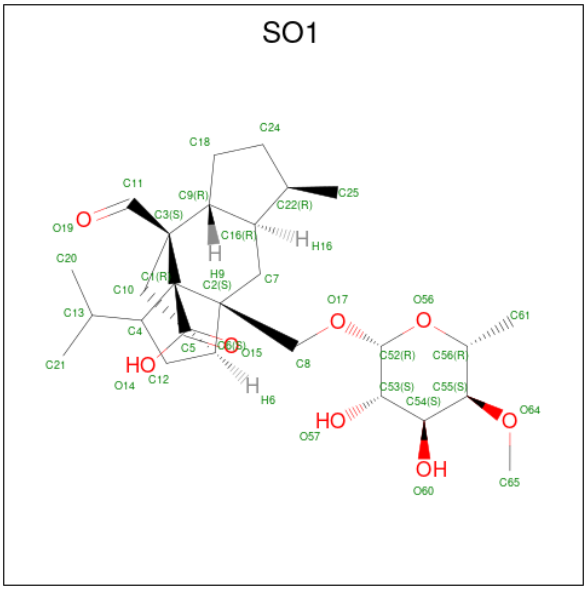
- Molecule 84 is a protein called Elongation factor 2.

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

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

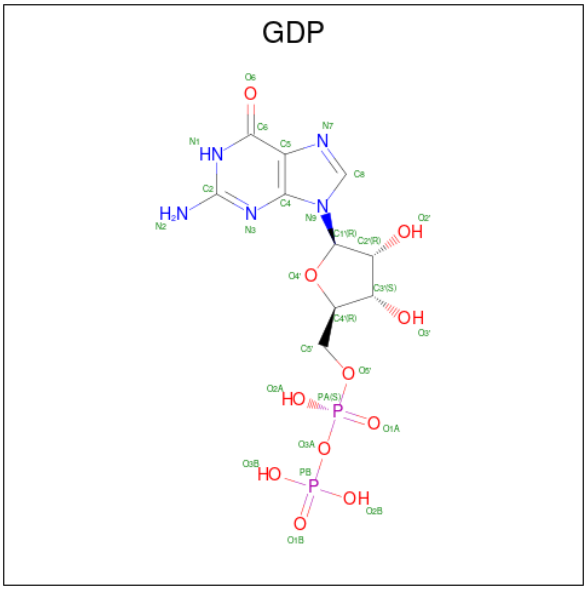
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
85	j	1	1	1	0
85	m	1	1	1	0
85	o	1	1	1	0
85	p	1	1	1	0
85	AQ	1	1	1	0
85	AR	1	1	1	0
85	AT	1	1	1	0
85	AW	1	1	1	0

- Molecule 86 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: $C_{27}H_{42}O_8$).



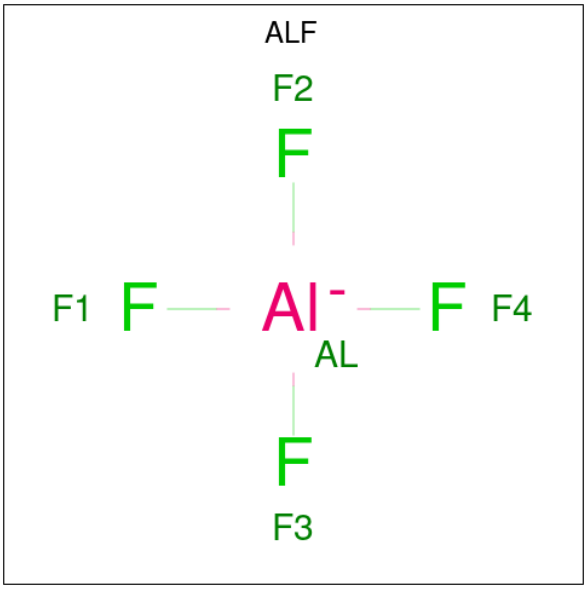
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
86	AZ	1	35	27	8	0

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



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

- Molecule 88 is TETRAFLUOROALUMINATE ION (three-letter code: ALF) (formula: AlF_4).



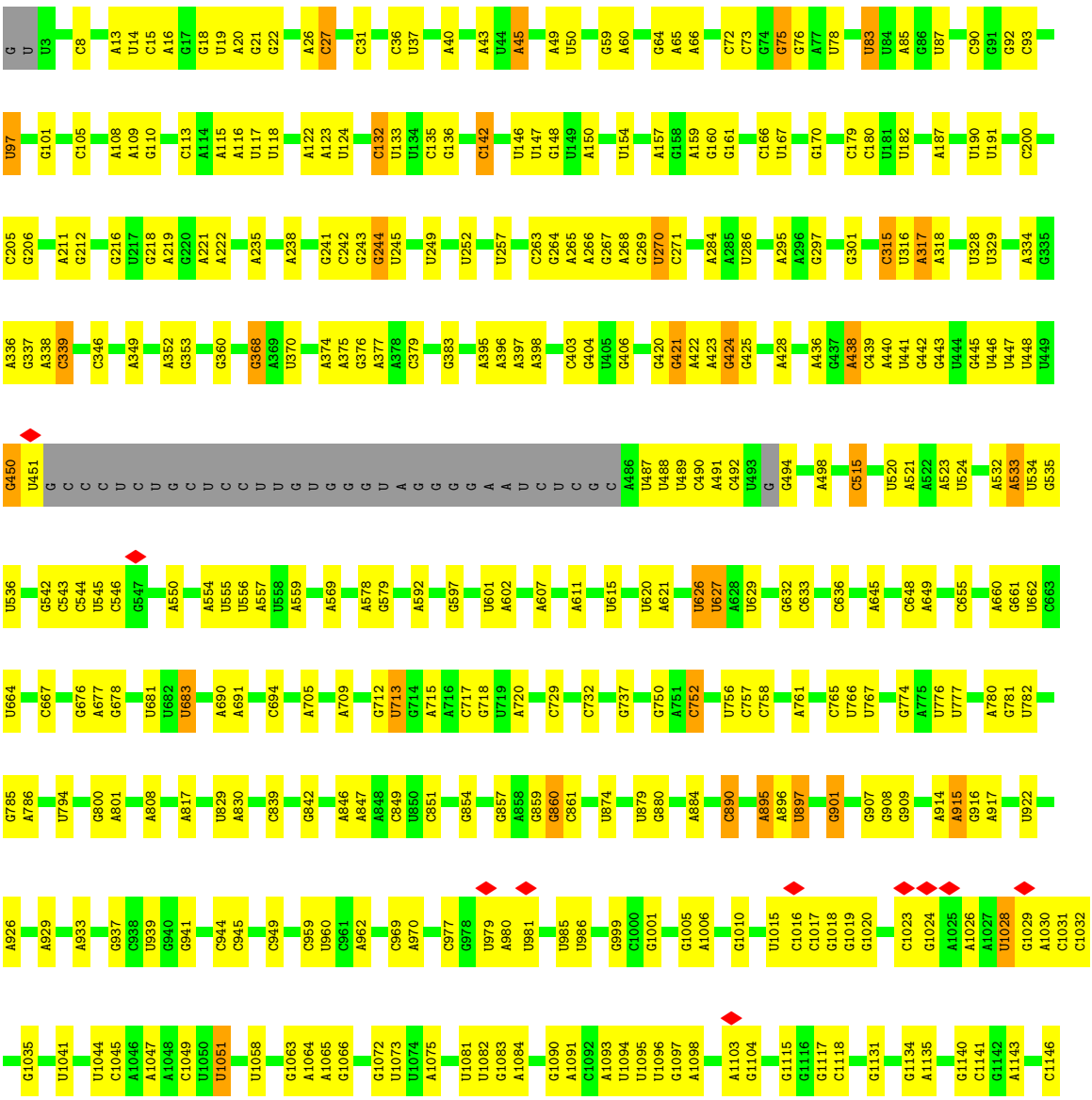
Mol	Chain	Residues	Atoms			AltConf
			Total	Al	F	
88	AZ	1	5	1	4	0

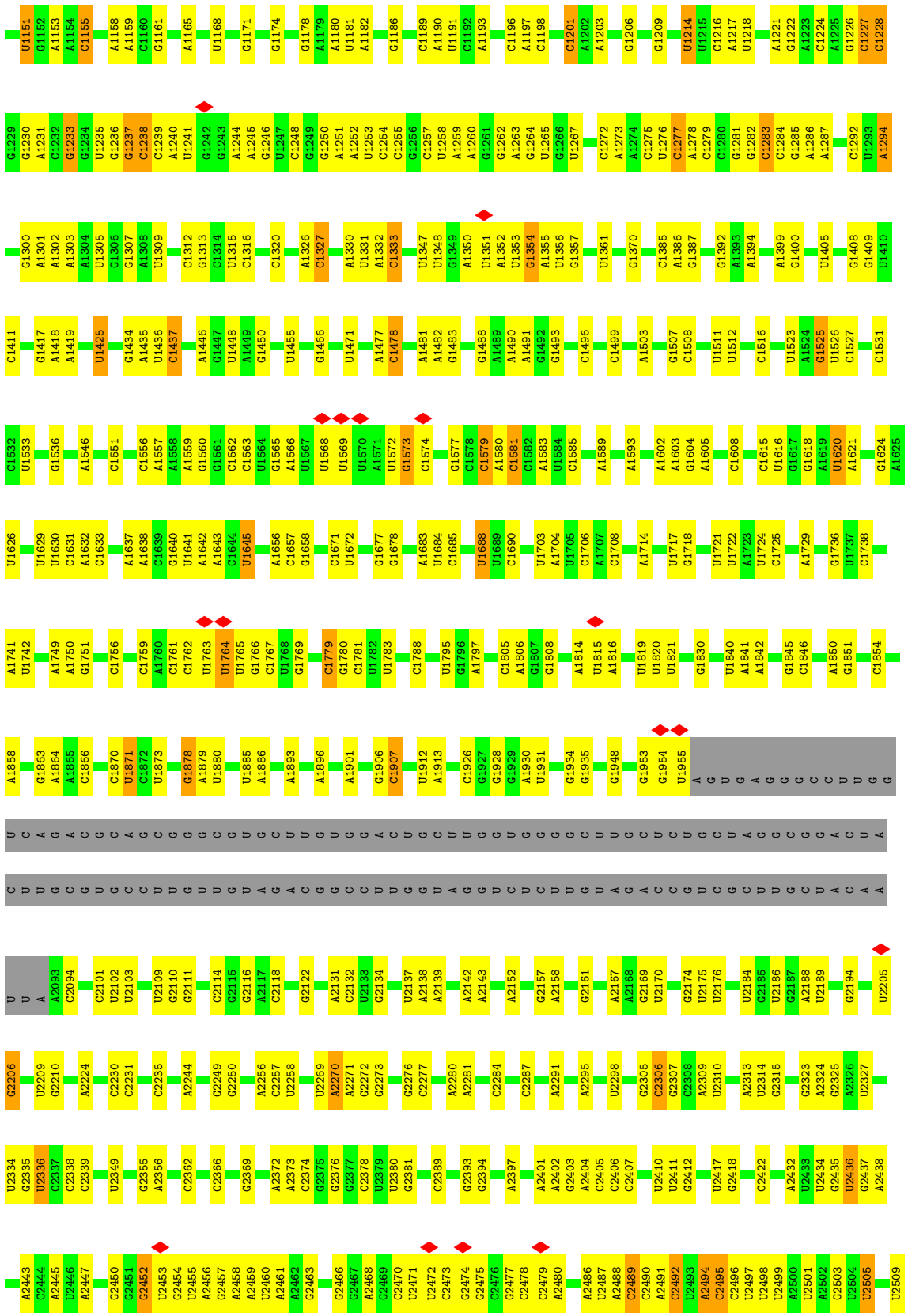
3 Residue-property plots (i)

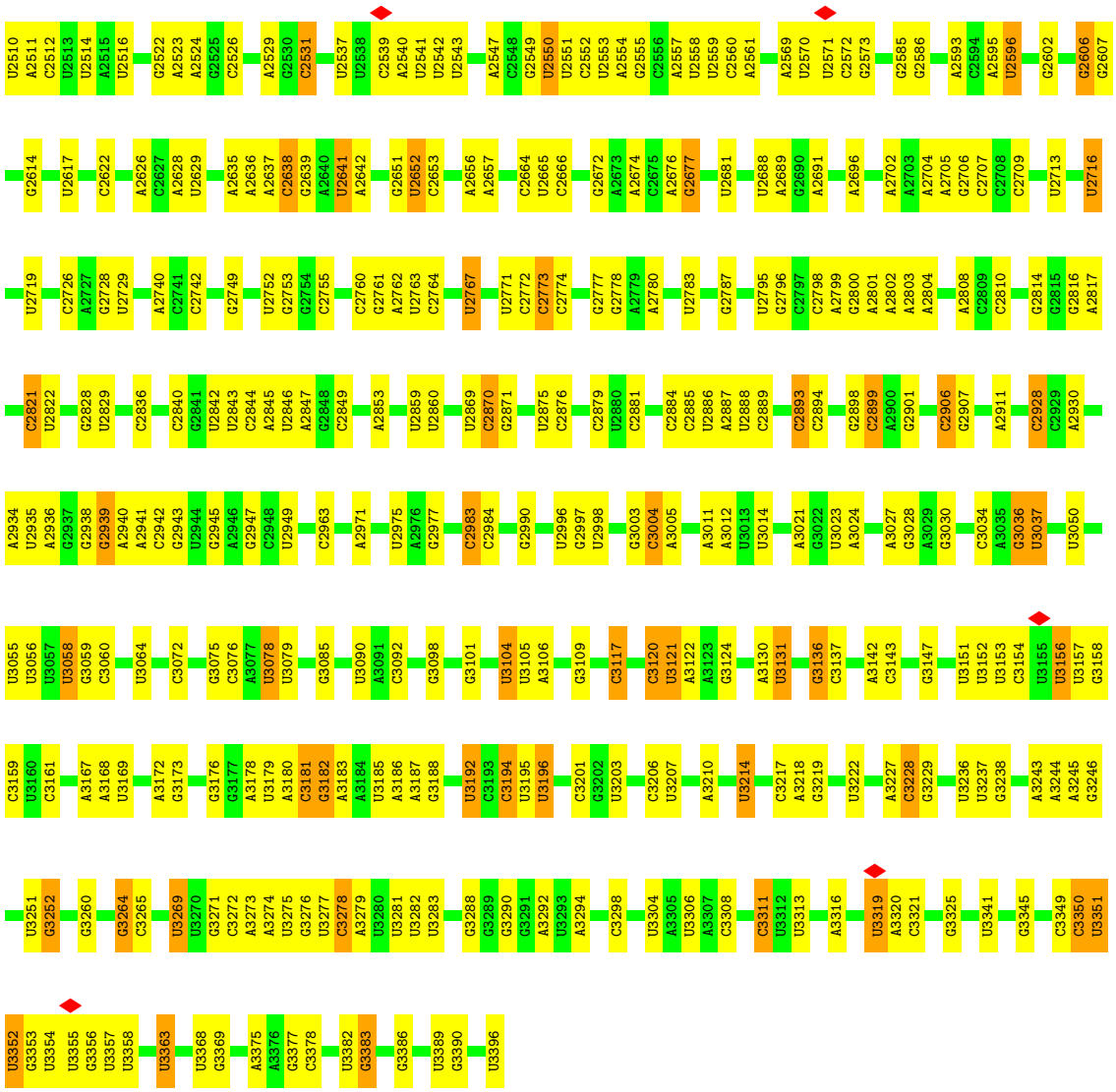
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 61% 31% 5%

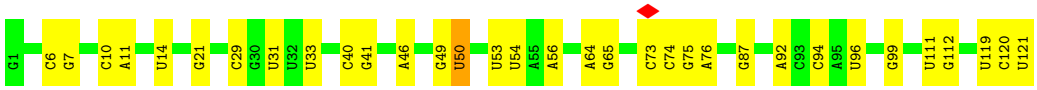



U1151 G1152 A1153 A1154 C1155 A1158 A1159 C1160 G1161 A1165 U1168 G1171 G1174 G1178 A1179 A1180 U1181 A1182 G1186 C1189 A1190 U1191 C1192 A1193 C1196 A1197 C1198 C1201 A1202 A1203 G1206 G1209 U1214 U1215 C1216 A1217 U1218 A1221 G1222 A1223 C1224 A1225 G1226 C1227 C1228
G1229 G1230 A1231 C1232 G1233 G1234 U1235 G1236 G1237 C1238 C1239 A1240 U1241 G1242 G1243 A1244 A1245 G1246 U1247 U1248 G1249 G1250 A1251 A1252 U1253 C1254 C1255 G1256 C1257 U1258 A1259 A1260 G1261 G1262 A1263 G1264 U1265 G1266 U1267 C1272 A1273 A1274 C1275 U1276 C1277 A1278 C1279 C1280 G1281 G1282 C1283 C1284 G1285 A1286 A1287 C1292 U1293 A1294
G1300 A1301 A1302 A1303 A1304 U1305 G1306 G1307 A1308 U1309 C1312 G1313 C1314 U1315 C1316 C1320 A1326 C1327 A1330 U1331 A1332 C1333 U1347 U1348 G1349 A1350 U1351 A1352 U1353 G1354 A1355 U1356 G1357 U1361 G1370 C1385 A1386 G1387 G1392 A1393 A1394 A1399 G1400 U1405 G1408 G1409 U1410
C1411 G1417 A1418 A1419 U1425 G1434 A1435 U1436 C1437 A1446 G1447 U1448 A1449 G1450 U1455 G1466 U1471 A1477 C1478 A1481 A1482 G1483 G1488 A1489 A1490 A1491 G1492 G1493 C1496 C1499 A1503 G1507 C1508 U1511 U1512 C1516 U1523 A1524 G1525 U1526 C1527 C1531
C1532 U1533 G1536 A1546 C1551 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 A1589 A1593 A1602 A1603 G1604 A1605 C1608 C1615 U1616 G1617 G1618 A1619 U1620 A1621 G1624 A1625
U1626 U1629 U1630 C1631 A1632 C1633 A1637 A1638 C1639 G1640 U1641 A1642 A1643 C1644 U1645 A1656 C1657 G1658 C1671 U1672 G1677 G1678 A1683 U1684 C1685 U1688 U1689 C1690 U1703 A1704 U1705 C1706 A1707 C1708 A1714 U1717 G1718 U1721 U1722 A1723 U1724 C1725 A1729 G1736 U1737 C1738
A1741 U1742 A1749 A1750 G1751 C1756 C1759 A1760 C1761 C1762 U1763 U1764 U1765 G1766 C1767 U1768 G1769 C1779 G1780 C1781 U1782 U1783 C1788 U1795 G1796 A1797 C1805 A1806 G1807 G1808 A1814 U1815 A1816 U1819 U1820 U1821 G1830 U1840 A1841 A1842 G1845 C1846 A1850 G1851 C1854
A1858 G1863 A1864 A1865 C1866 C1870 U1871 C1872 U1873 G1878 A1879 U1880 U1885 A1886 A1893 A1896 A1901 G1906 C1907 U1912 A1913 C1926 G1927 G1928 G1929 A1930 U1931 G1934 G1935 G1948 G1953 G1954 U1955 A G G U G A G G G C C U U G G
U C U A G A C G C A G C C U G G G C U U G C U U G G U G G G A C U G G C U U G G G U G G G C U U G A G C U C U G U C U G A G G C G G A C U A
C U U G C C G U G C C U U G U A G A C G G U U G U A G C U U G G U U G U A G C C U G C U U G G U G C U A G G G U C U C U G C U G C A C A A
U U A A2093 C2094 C2101 U2102 U2103 U2109 G2110 G2111 C2114 G2115 G2116 A2117 C2118 G2122 A2131 C2132 U2133 G2134 U2137 A2138 A2139 A2142 A2143 A2152 G2157 A2158 G2161 A2167 A2168 G2169 U2170 G2174 U2175 U2176 U2184 G2185 U2186 G2187 A2188 U2189 G2194 U2205
G2206 U2209 G2210 A2224 C2230 C2231 C2235 A2244 G2249 G2250 A2256 C2257 U2258 U2269 A2270 A2271 G2272 G2273 G2276 C2277 A2280 A2281 C2284 C2287 A2291 A2295 U2298 G2305 C2306 G2307 C2308 A2309 U2310 A2313 U2314 G2315 G2323 A2324 G2325 A2326 U2327
U2334 G2335 U2336 C2337 C2338 C2339 U2349 G2355 A2356 C2362 C2366 G2369 A2372 A2373 C2374 G2375 G2376 G2377 C2378 U2379 U2380 G2381 C2389 G2393 G2394 A2397 A2401 A2402 G2403 A2404 C2405 C2406 C2407 U2410 U2411 G2412 U2417 G2418 C2422 A2432 U2433 U2434 G2435 U2436 G2437 A2438
A2443 C2444 A2445 U2446 A2447 G2450 C2451 G2452 U2453 G2454 U2455 A2456 G2457 A2458 A2459 U2460 A2461 A2462 G2463 G2466 G2467 A2468 C2469 C2470 U2471 U2472 C2473 G2474 G2475 C2476 G2477 C2478 C2479 A2480 A2486 U2487 A2488 C2489 C2490 A2491 C2492 U2493 A2494 C2495 C2496 U2497 U2498 U2499 A2500 U2501 A2502 G2503 U2504 U2505 U2509



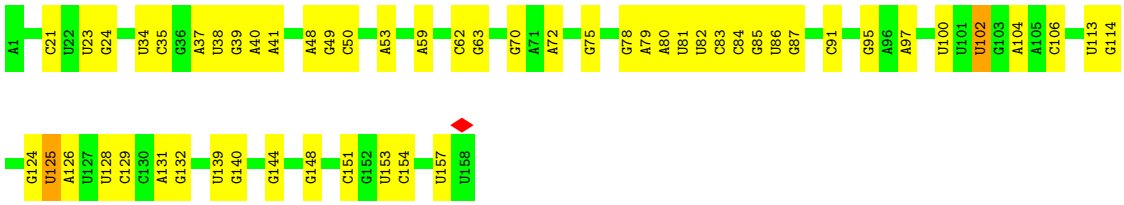
- Molecule 2: 5S ribosomal RNA

Chain 3:



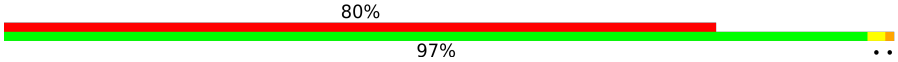
- Molecule 3: 5.8S ribosomal RNA

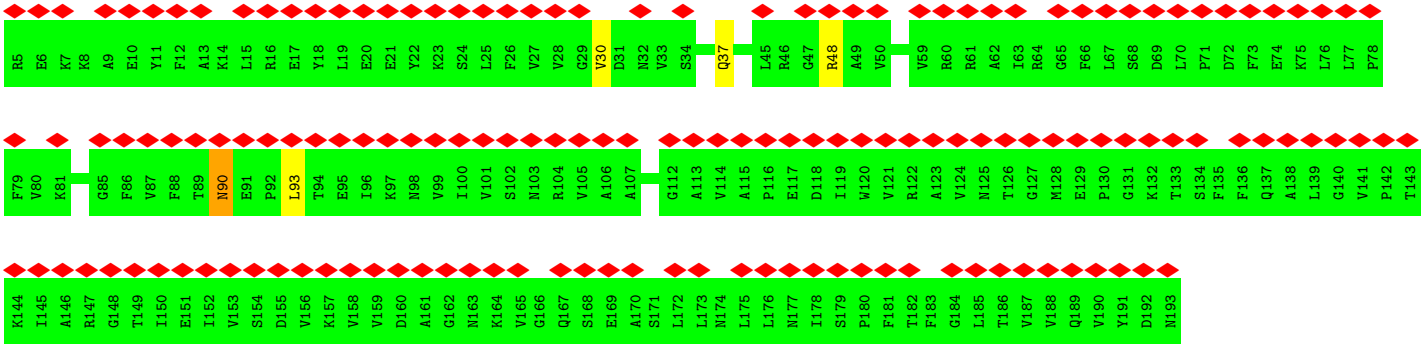
Chain 4:



- Molecule 4: 60S acidic ribosomal protein P0

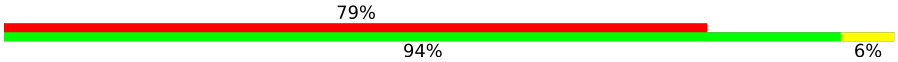
Chain P0:

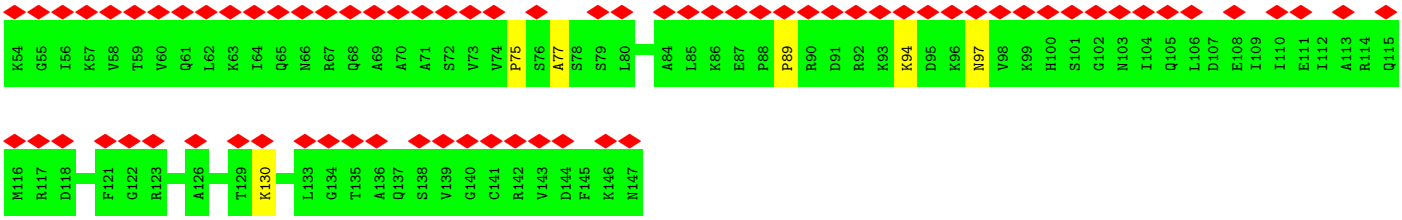




- Molecule 5: 60S ribosomal protein L12-A

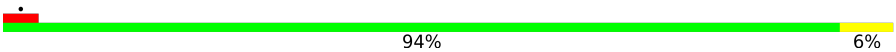
Chain P2:

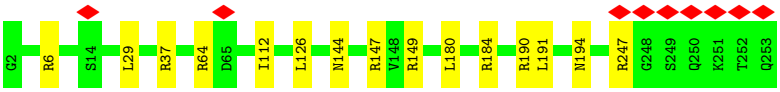




- Molecule 6: 60S ribosomal protein L2-A

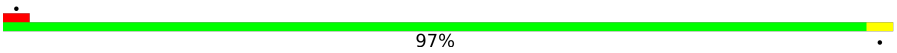
Chain A:

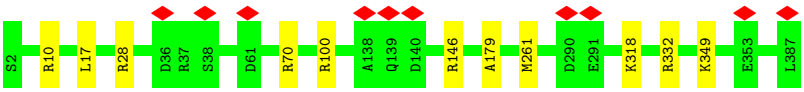




- Molecule 7: 60S ribosomal protein L3

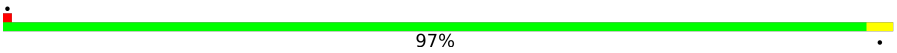
Chain B:

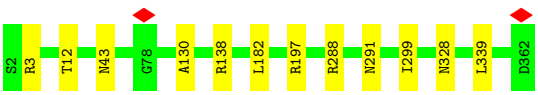




- Molecule 8: 60S ribosomal protein L4-A

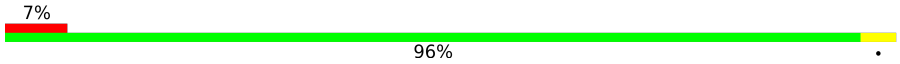
Chain C:

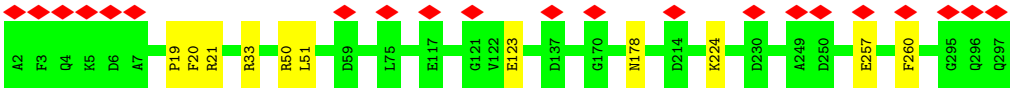




- Molecule 9: 60S ribosomal protein L5

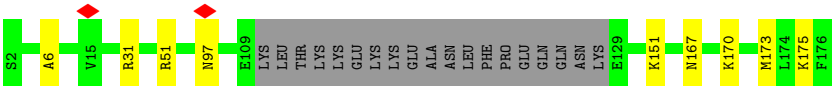
Chain D:





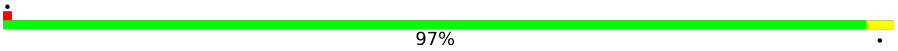
• Molecule 10: 60S ribosomal protein L6-A

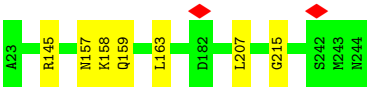
Chain E:



• Molecule 11: 60S ribosomal protein L7-A

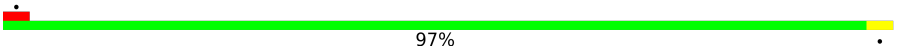
Chain F:

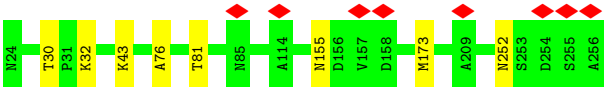




• Molecule 12: 60S ribosomal protein L8-A

Chain G:



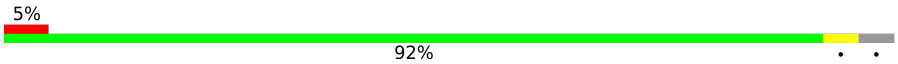


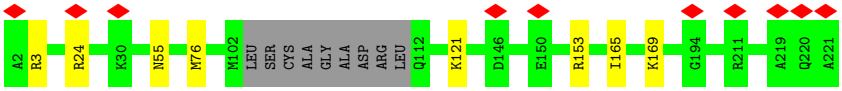
• Molecule 13: 60S ribosomal protein L9-A

Chain H:

• Molecule 14: 60S ribosomal protein L10

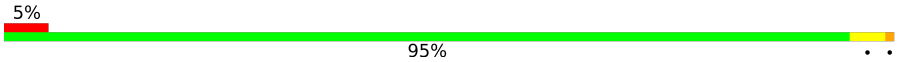
Chain I:

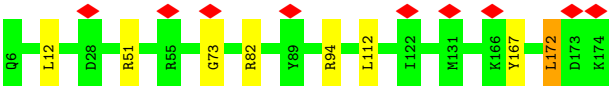




• Molecule 15: 60S ribosomal protein L11-B

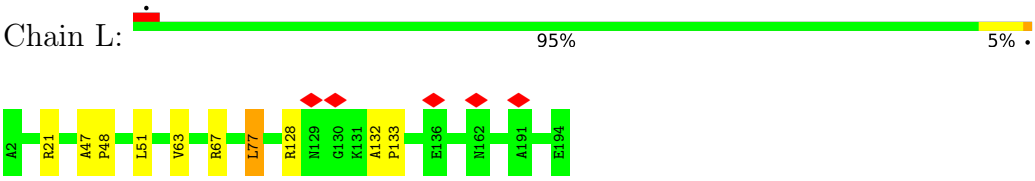
Chain J:





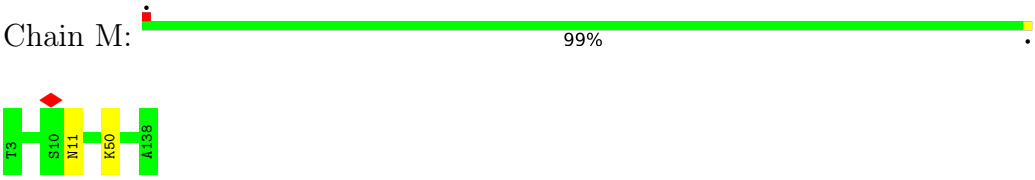
- Molecule 16: 60S ribosomal protein L13-A

Chain L:



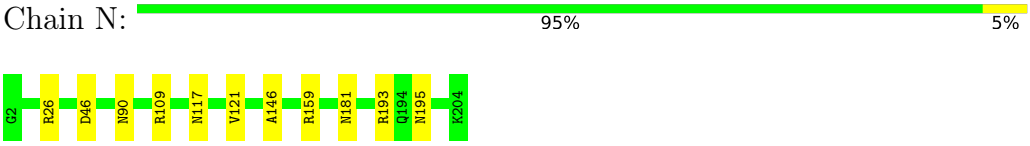
- Molecule 17: 60S ribosomal protein L14-A

Chain M:



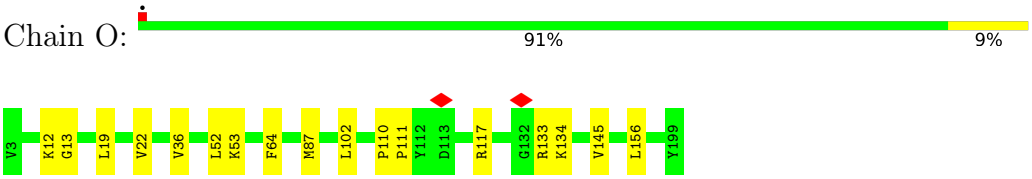
- Molecule 18: 60S ribosomal protein L15-A

Chain N:



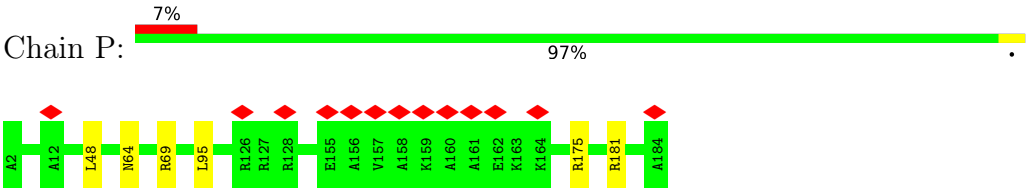
- Molecule 19: 60S ribosomal protein L16-A

Chain O:



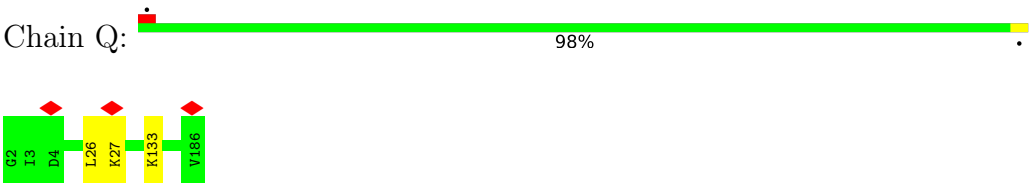
- Molecule 20: 60S ribosomal protein L17-A

Chain P:



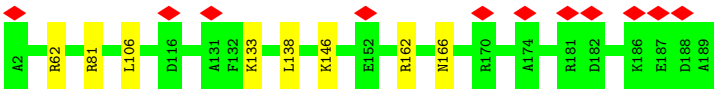
- Molecule 21: 60S ribosomal protein L18-A

Chain Q:



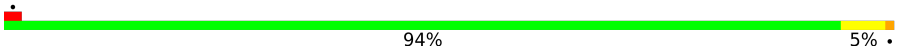
- Molecule 22: 60S ribosomal protein L19-A

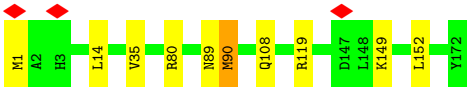
Chain R:



• Molecule 23: 60S ribosomal protein L20-A

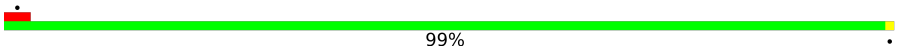
Chain S:

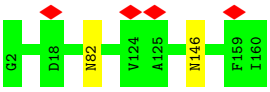




• Molecule 24: 60S ribosomal protein L21-A

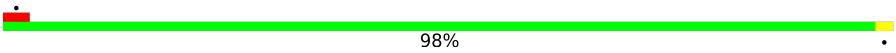
Chain T:

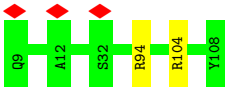




• Molecule 25: 60S ribosomal protein L22-A

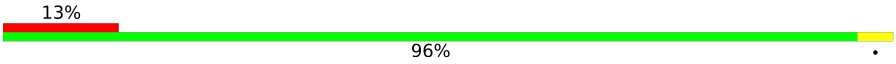
Chain U:

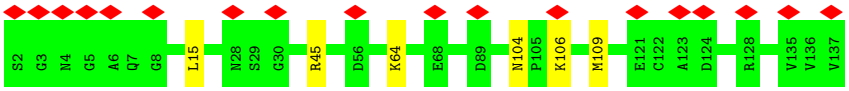




• Molecule 26: 60S ribosomal protein L23-A

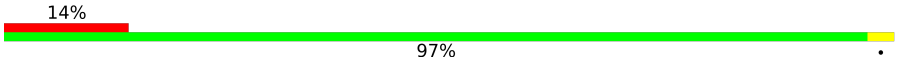
Chain V:

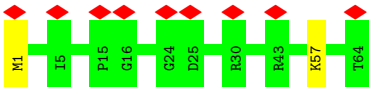




• Molecule 27: 60S ribosomal protein L24-A

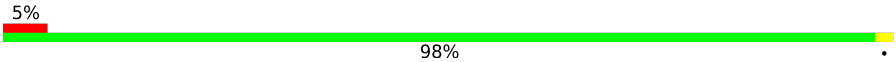
Chain W:

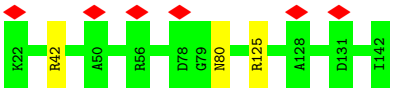




• Molecule 28: 60S ribosomal protein L25

Chain X:



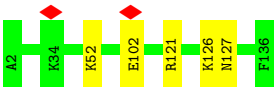


• Molecule 29: 60S ribosomal protein L26-A

Chain Y: 98%

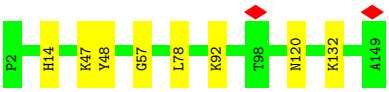
• Molecule 30: 60S ribosomal protein L27-A

Chain Z: 96%



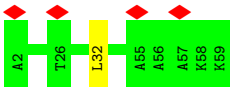
• Molecule 31: 60S ribosomal protein L28

Chain a: 95% 5%



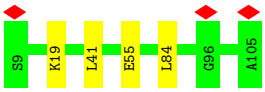
• Molecule 32: 60S ribosomal protein L29

Chain b: 7% 98%



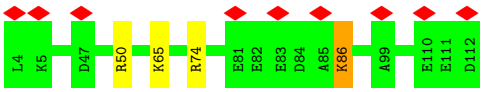
• Molecule 33: 60S ribosomal protein L30

Chain c: 96%



• Molecule 34: 60S ribosomal protein L31-A

Chain d: 8% 96%

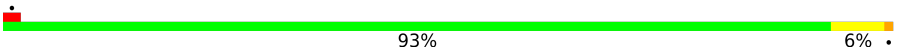


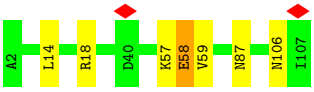
• Molecule 35: 60S ribosomal protein L32

Chain e: 5% 98%

- Molecule 36: 60S ribosomal protein L33-A

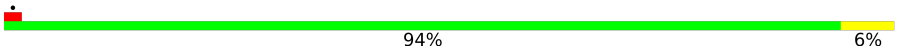
Chain f:

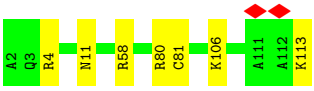




- Molecule 37: 60S ribosomal protein L34-A

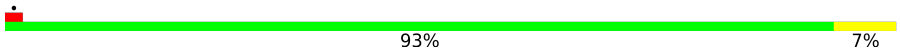
Chain g:

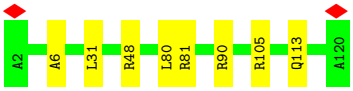




- Molecule 38: 60S ribosomal protein L35-A

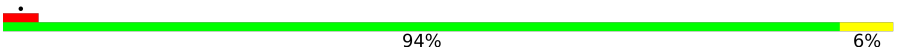
Chain h:

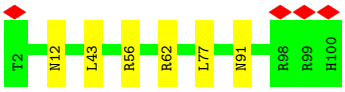




- Molecule 39: 60S ribosomal protein L36-A

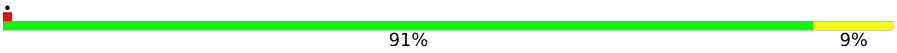
Chain i:

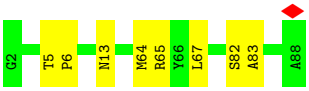




- Molecule 40: 60S ribosomal protein L37-A

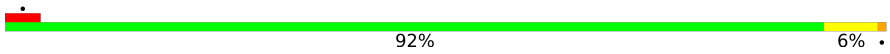
Chain j:

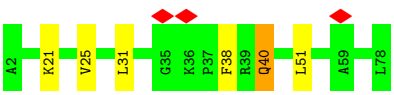




- Molecule 41: 60S ribosomal protein L38

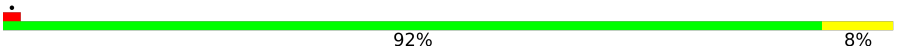
Chain k:

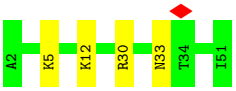




- Molecule 42: 60S ribosomal protein L39

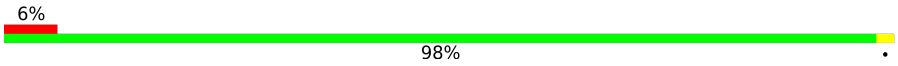
Chain l:

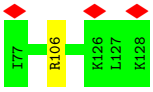




• Molecule 43: Ubiquitin-60S ribosomal protein L40

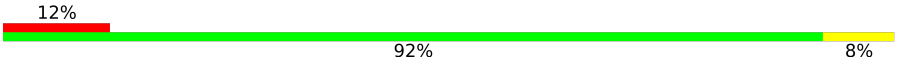
Chain m:

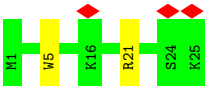




• Molecule 44: 60S ribosomal protein L41-B

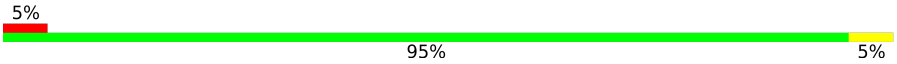
Chain n:





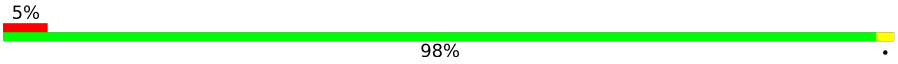
• Molecule 45: 60S ribosomal protein L42-A

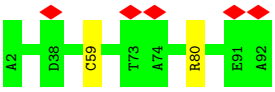
Chain o:



• Molecule 46: 60S ribosomal protein L43-A

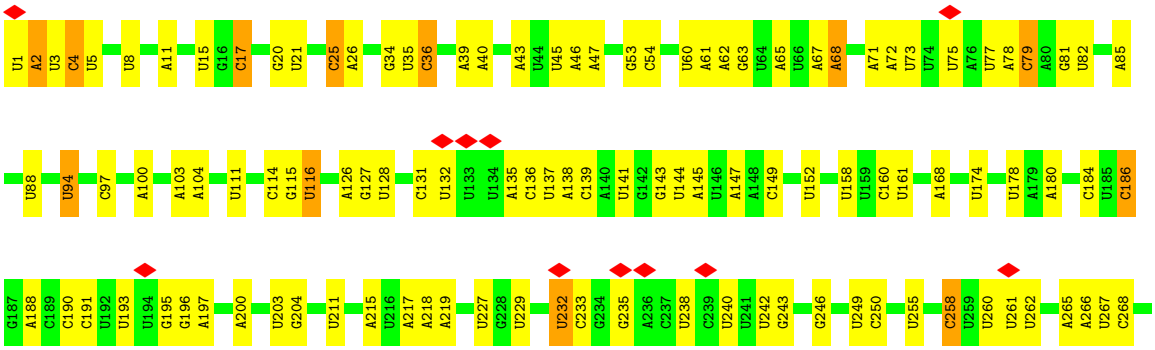
Chain p:

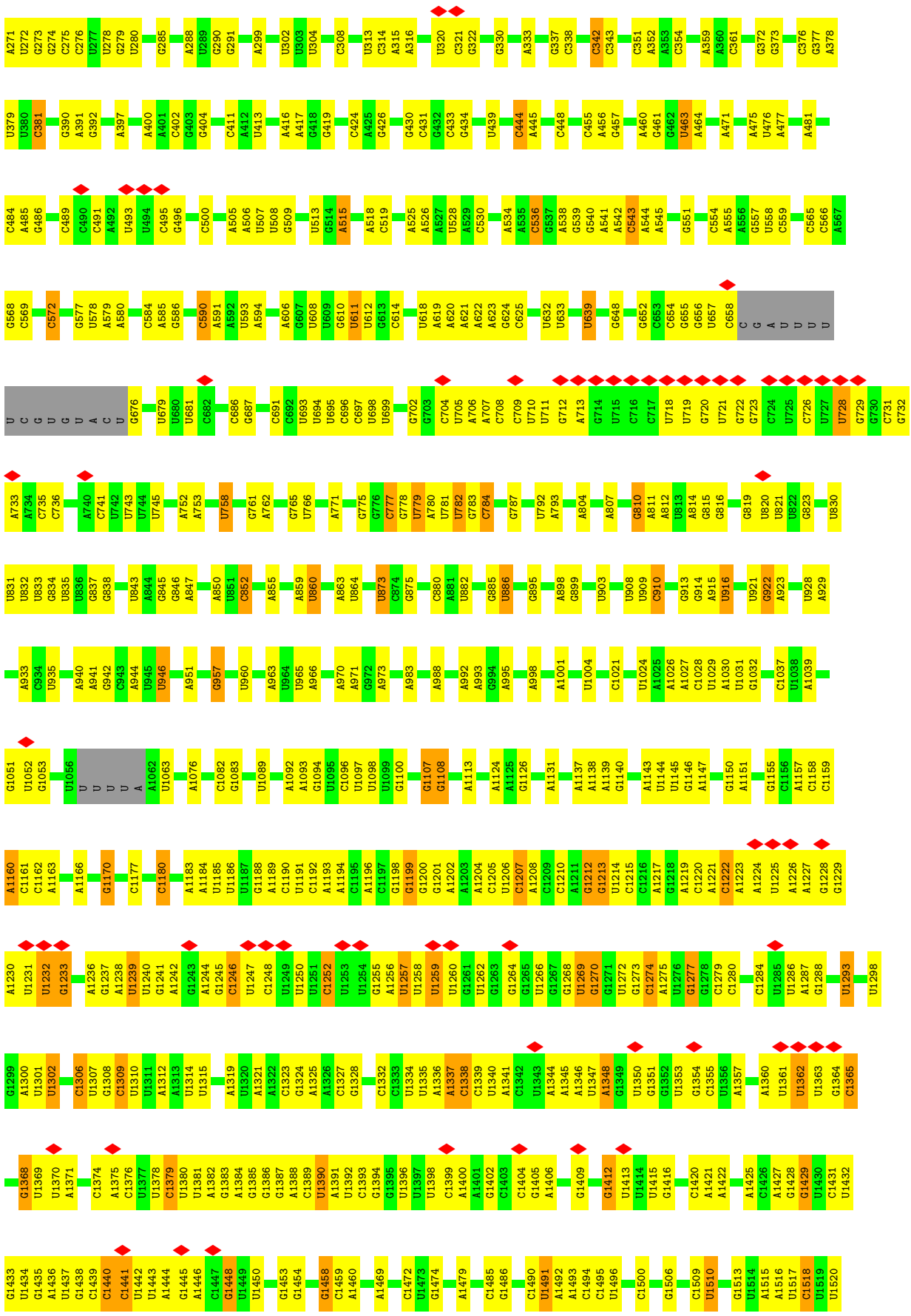




• Molecule 47: 18S ribosomal RNA

Chain 2:

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U379 U380 C381 G390 A391 G392 A397 A400 A401 C402 G403 G404 C411 A412 U413 A416 A417 G418 G419 C424 A425 G426 G430 C431 G432 C433 G434 U439 C444 A445 C448 C455 A456 G457 A460 G461 G462 U463 A464 A471 A475 U476 A477 A481
C484 A485 G486 C489 C490 C491 A492 U493 U494 C495 G496 C500 A505 A506 U507 U508 G509 U513 G514 A515 A518 C519 A525 A526 A527 U528 A529 C530 A534 A535 C536 G537 A538 G539 G540 A541 A542 C543 A544 A545 G551 C554 A555 A556 G557 U558 C559 C565 C566 A567
G568 C569 C572 G577 U578 A579 A580 C584 A585 G586 C590 A591 A592 U593 A594 A606 G607 U608 U609 G610 U611 U612 G613 C614 U618 A619 A620 A621 A622 A623 G624 C625 U632 U633 U639 G648 G652 C653 C654 G655 G656 U657 C658 C G A U U U U
U C G U G U A C U G676 U679 U680 U681 C682 C686 G687 C691 C692 U693 U694 U695 C696 C697 U698 U699 G702 G703 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 A740 C741 U742 U743 U744 U745 A752 A753 U758 G761 A762 G765 U766 A771 G775 G776 C777 G778 U779 A780 U781 U782 G783 C784 G787 U792 A793 A804 A807 G810 A811 A812 U813 A814 G815 G816 G819 U820 U821 U822 G823 U830
U831 U832 U833 G834 U835 U836 G837 G838 U843 A844 G845 G846 A847 A850 U851 C852 A855 A859 U860 A863 U864 U873 C874 G875 C880 A881 U882 G885 U886 G895 A898 G899 U903 U908 U909 C910 G913 G914 G915 U916 U921 G922 A923 U928 A929
A933 C934 U935 A940 A941 G942 C943 A944 U945 U946 A951 G957 U960 A963 U964 U965 A966 A970 A971 G972 A973 A983 A988 A992 A993 G994 A995 A998 A1001 U1004 C1021 U1024 A1025 A1026 A1027 C1028 U1029 A1030 U1031 G1032 C1037 U1038 A1039
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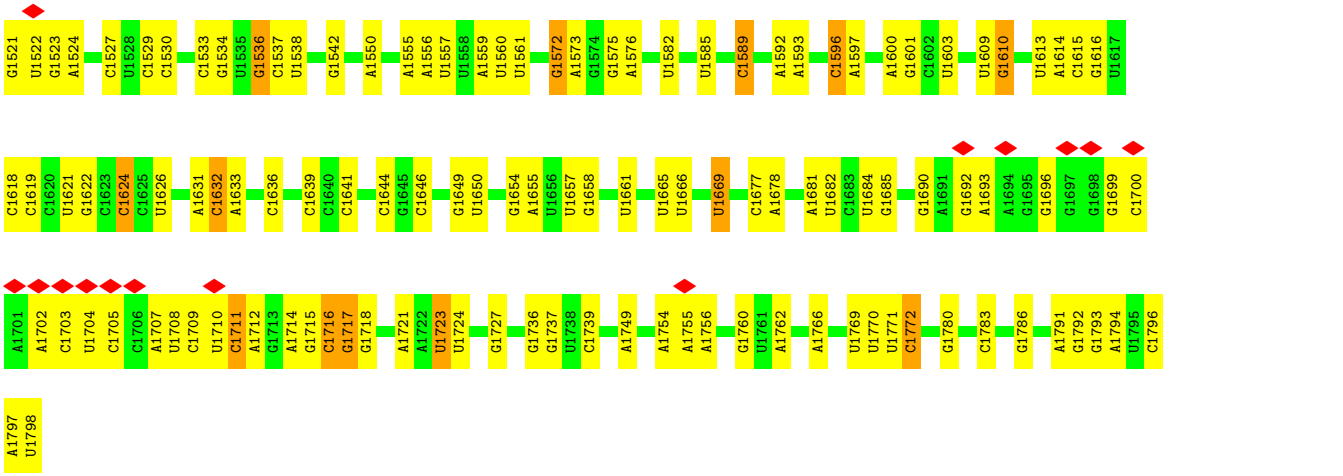
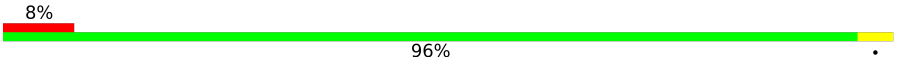
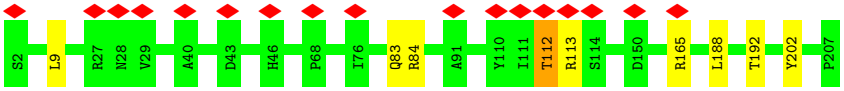
G1299 A1300 U1301 U1302 C1306 U1307 G1308 C1309 U1310 U1311 A1312 A1313 U1314 U1315 A1319 U1320 A1321 A1322 C1323 G1324 A1325 A1326 C1327 G1328 C1332 C1333 U1334 U1335 A1336 A1337 C1338 C1339 U1340 A1341 C1342 U1343 A1344 A1345 A1346 U1347 A1348 G1349 U1350 G1351 G1352 U1353 G1354 C1355 U1356 A1357 A1360 U1361 U1362 U1363 G1364 C1365
G1368 U1369 U1370 A1371 C1374 A1375 C1376 U1377 U1378 C1379 U1380 U1381 A1382 G1383 A1384 G1385 G1386 G1387 A1388 C1389 U1390 A1391 U1392 C1393 G1394 G1395 U1396 U1397 U1398 C1399 A1400 A1401 G1402 C1403 C1404 G1405 A1406 G1409 G1412 U1413 U1414 U1415 G1416 C1420 A1421 A1422 A1425 C1426 A1427 G1428 G1429 U1430 C1431 U1432
G1433 U1434 G1435 A1436 U1437 G1438 C1439 C1440 C1441 U1442 U1443 A1444 G1445 A1446 C1447 G1448 U1449 U1450 G1453 G1454 G1458 A1459 A1460 A1469 C1472 U1473 G1474 A1479 C1485 G1486 C1490 U1491 A1492 A1493 C1494 C1495 U1496 C1500 G1506 C1509 U1510 G1513 U1514 A1515 A1516 U1517 C1518 U1519 U1520



- Molecule 48: 40S ribosomal protein S0-A

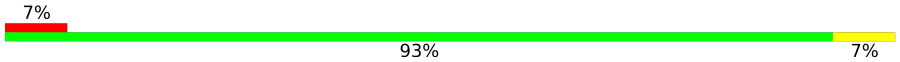
Chain q:





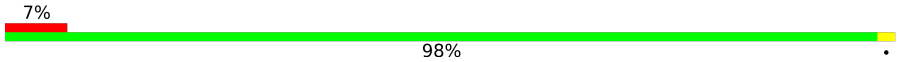
- Molecule 49: 40S ribosomal protein S1-A

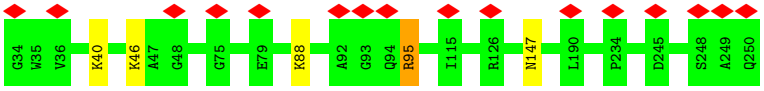
Chain r:



- Molecule 50: 40S ribosomal protein S2

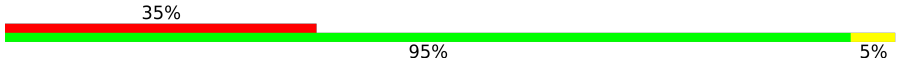
Chain s:

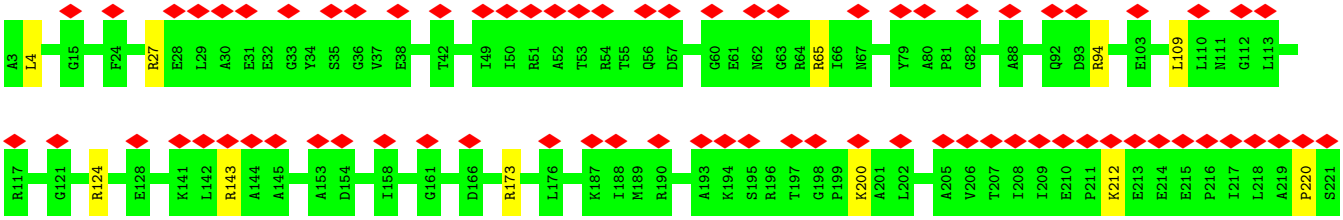


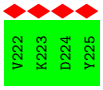


- Molecule 51: 40S ribosomal protein S3

Chain t:

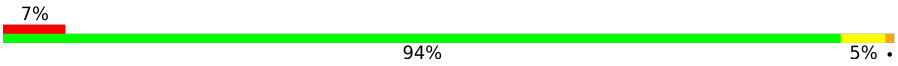


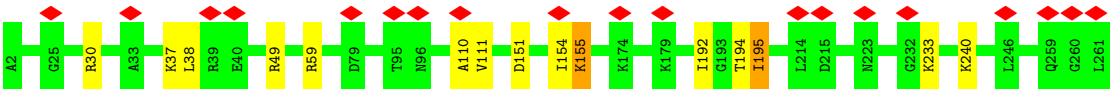




• Molecule 52: 40S ribosomal protein S4-A

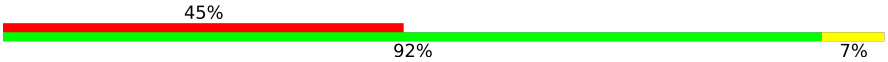
Chain u:

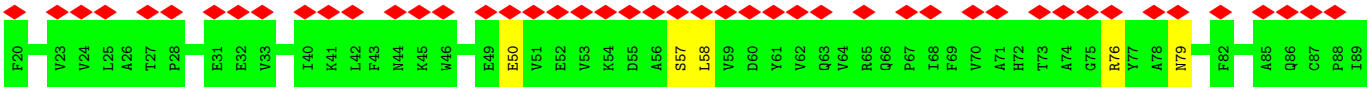


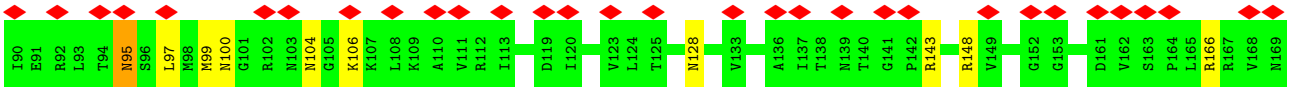


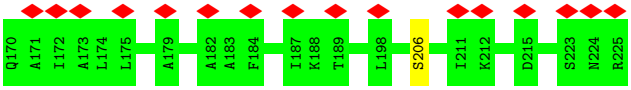
• Molecule 53: 40S ribosomal protein S5

Chain v:



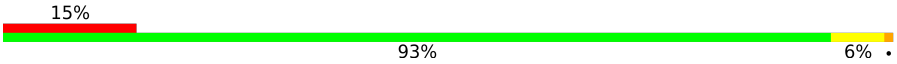


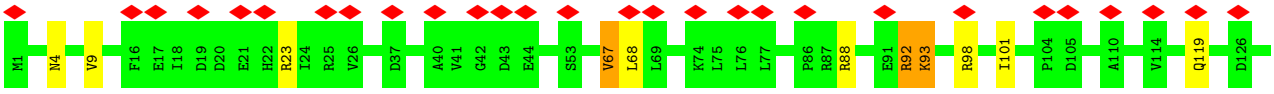


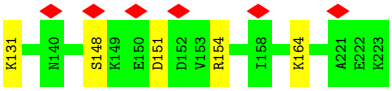


• Molecule 54: 40S ribosomal protein S6-A

Chain w:

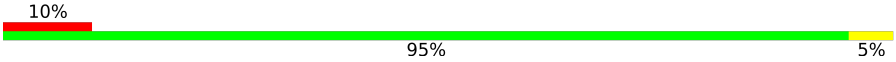


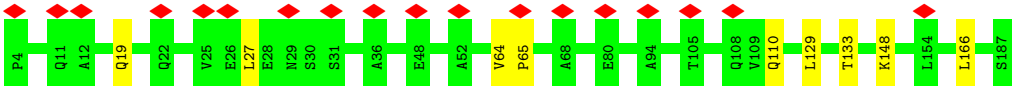




• Molecule 55: 40S ribosomal protein S7-A

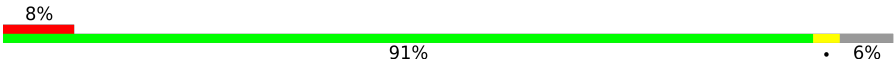
Chain x:

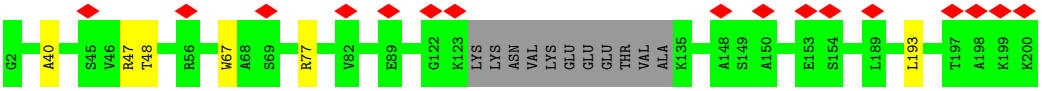




• Molecule 56: 40S ribosomal protein S8-A

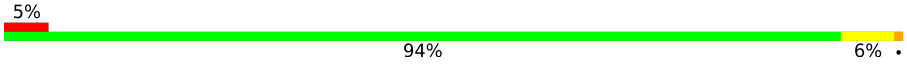
Chain y:

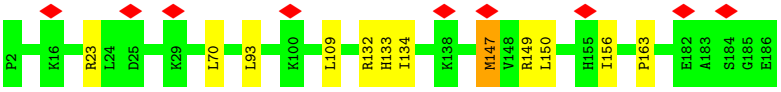




• Molecule 57: 40S ribosomal protein S9-A

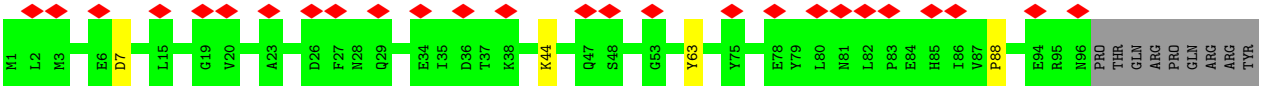
Chain z:





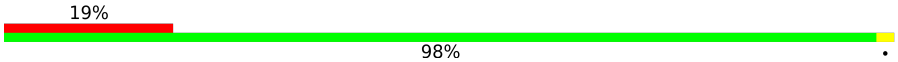
• Molecule 58: 40S ribosomal protein S10-A

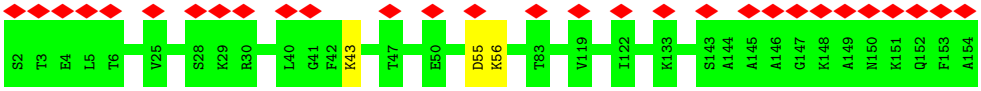
Chain AA:



• Molecule 59: 40S ribosomal protein S11-A

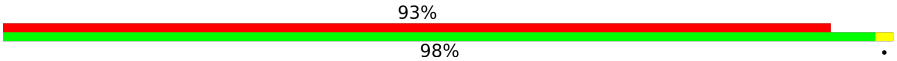
Chain AB:

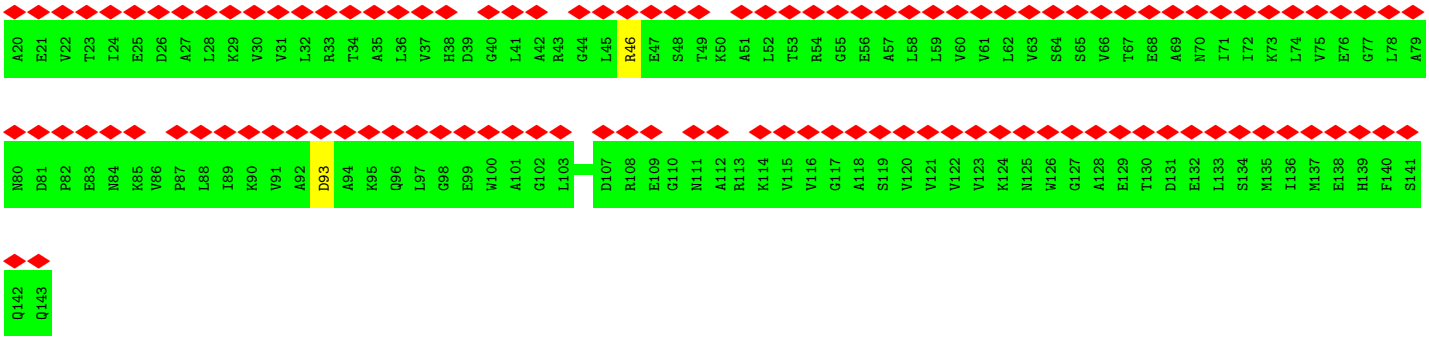




• Molecule 60: 40S ribosomal protein S12

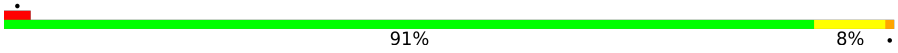
Chain AC:

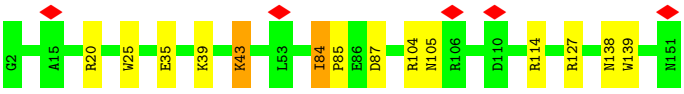




• Molecule 61: 40S ribosomal protein S13

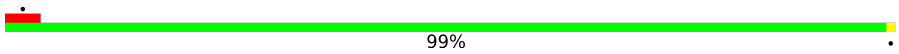
Chain AD:

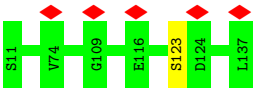




• Molecule 62: 40S ribosomal protein S14-B

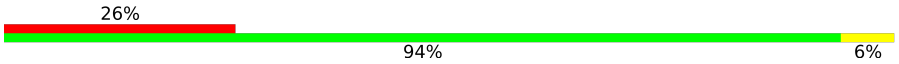
Chain AE:

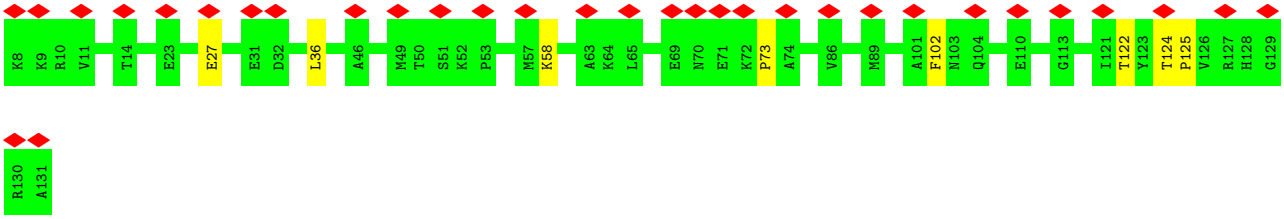




• Molecule 63: 40S ribosomal protein S15

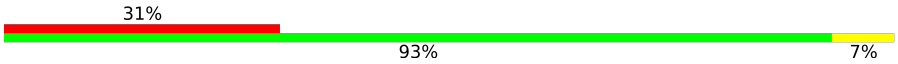
Chain AF:

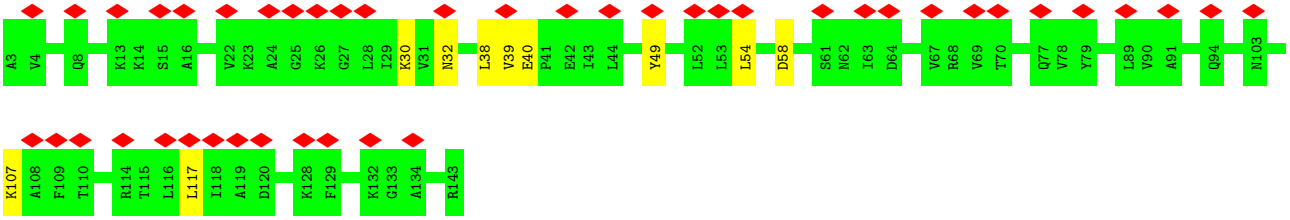




• Molecule 64: 40S ribosomal protein S16-A

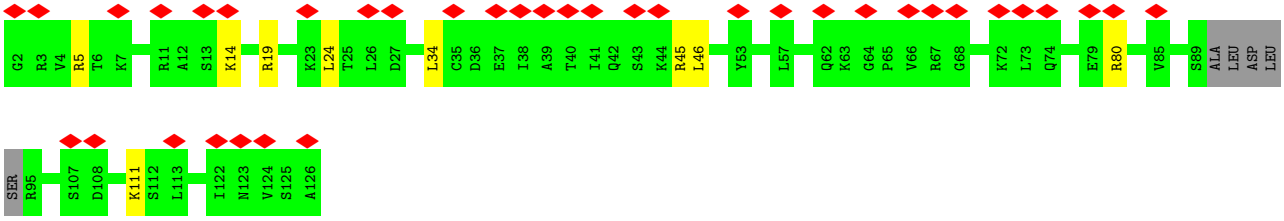
Chain AG:





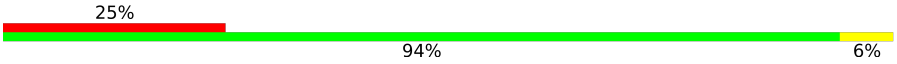
• Molecule 65: 40S ribosomal protein S17-B

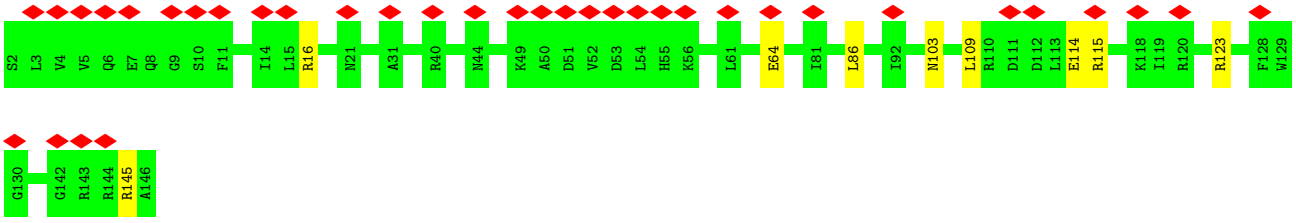
Chain AH:



• Molecule 66: 40S ribosomal protein S18-A

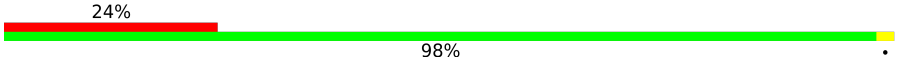
Chain AI:

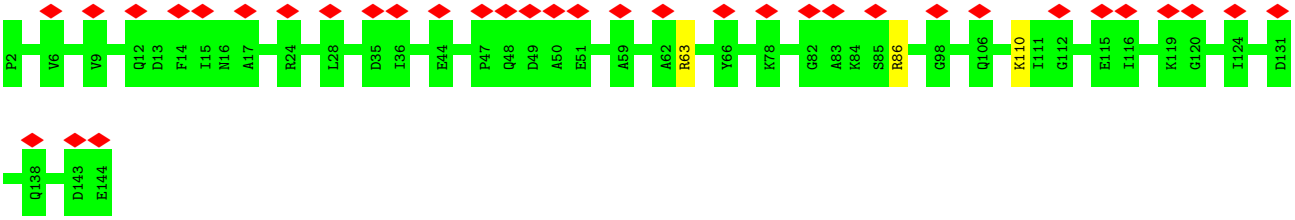




- Molecule 67: 40S ribosomal protein S19-A

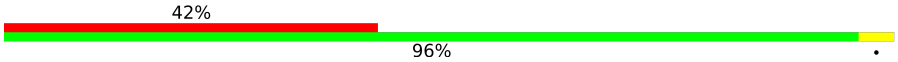
Chain AJ:

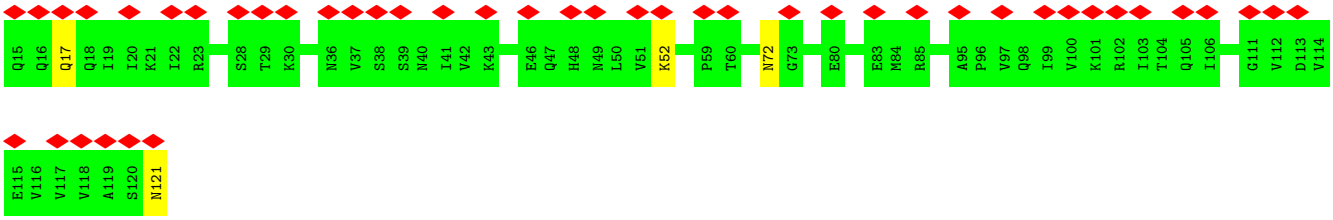




- Molecule 68: 40S ribosomal protein S20

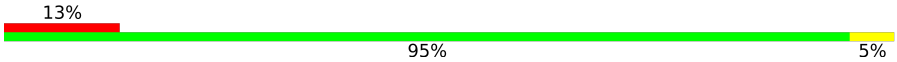
Chain AK:

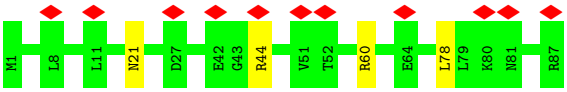




- Molecule 69: 40S ribosomal protein S21-A

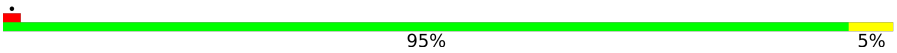
Chain AL:

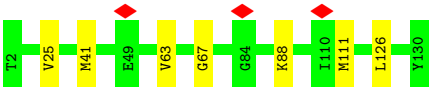




- Molecule 70: 40S ribosomal protein S22-A

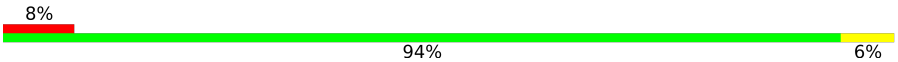
Chain AM:

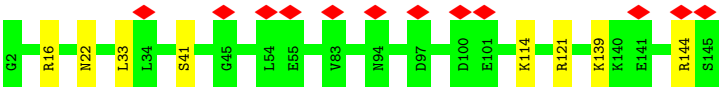




- Molecule 71: 40S ribosomal protein S23-A

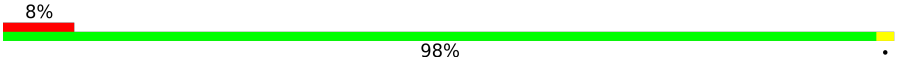
Chain AN:

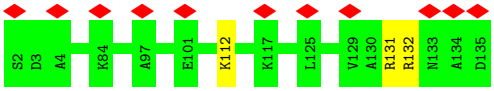




- Molecule 72: 40S ribosomal protein S24-A

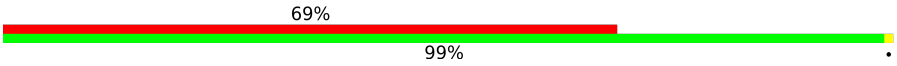
Chain AO:

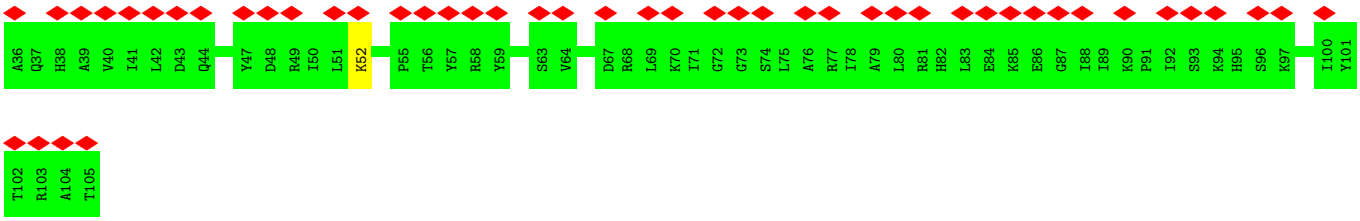




• Molecule 73: 40S ribosomal protein S25-A

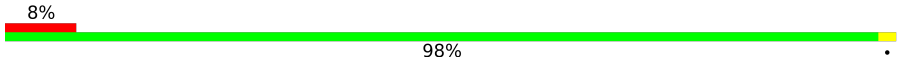
Chain AP:

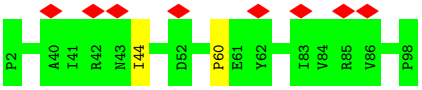




• Molecule 74: 40S ribosomal protein S26-B

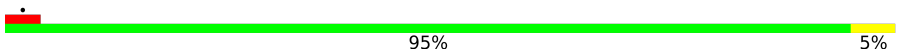
Chain AQ:

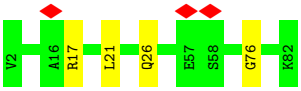




• Molecule 75: 40S ribosomal protein S27-A

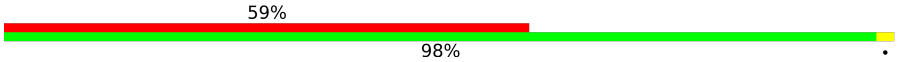
Chain AR:

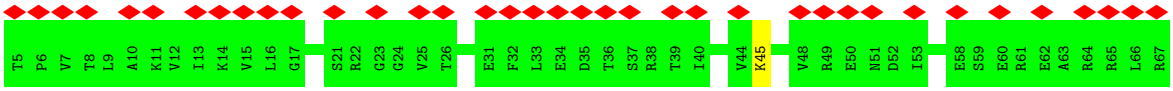




• Molecule 76: 40S ribosomal protein S28-A

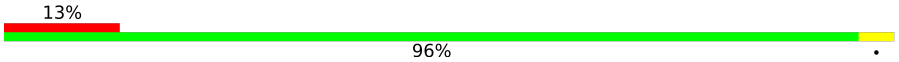
Chain AS:

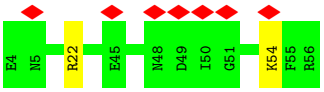




• Molecule 77: 40S ribosomal protein S29-A

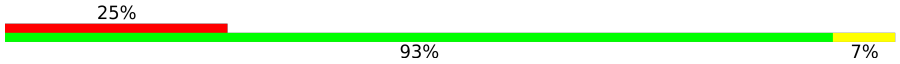
Chain AT:

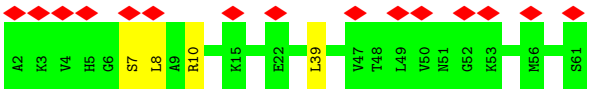




• Molecule 78: 40S ribosomal protein S30-A

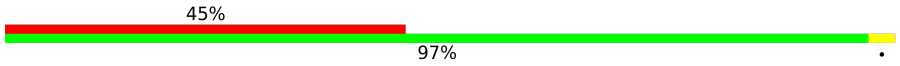
Chain AU:

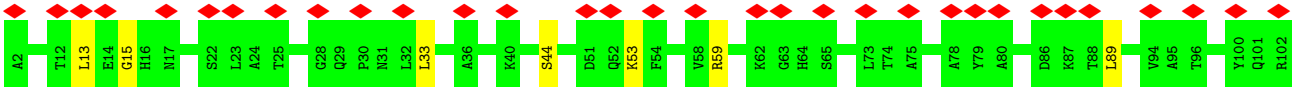


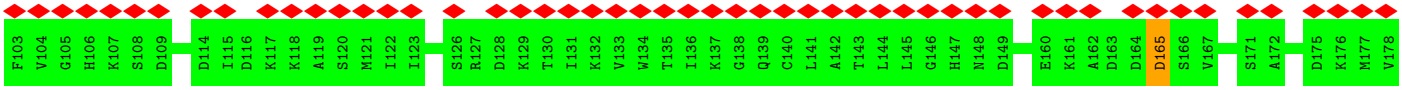


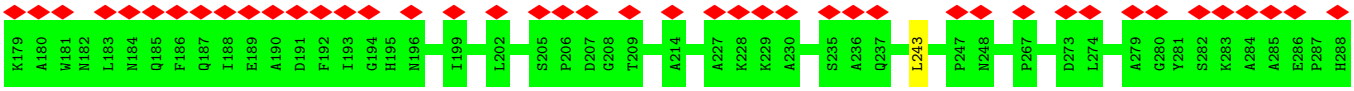
• Molecule 79: Guanine nucleotide-binding protein subunit beta-like protein

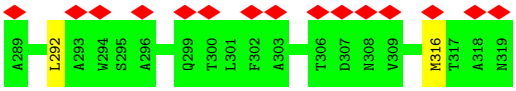
Chain AV:





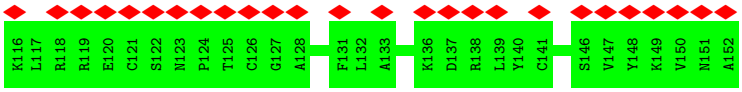






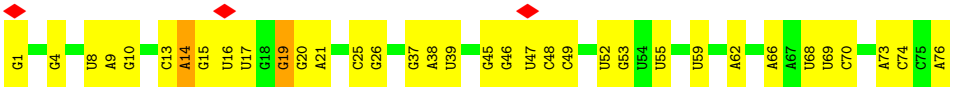
• Molecule 80: Ubiquitin-40S ribosomal protein S31

Chain AW:



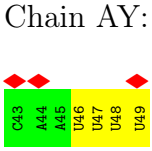
• Molecule 81: Transfer RNA - Phe

Chain AX:



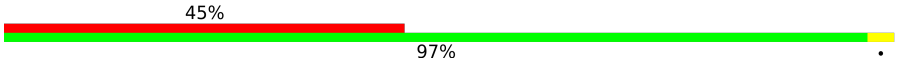
• Molecule 82: Messenger RNA

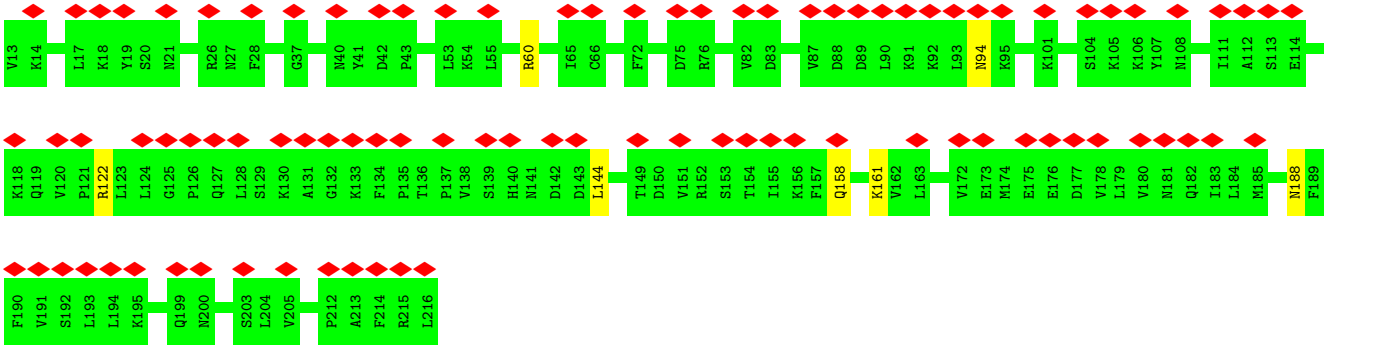
Chain AY:



• Molecule 83: 60S ribosomal protein L1-A

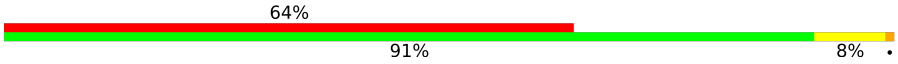
Chain BA:

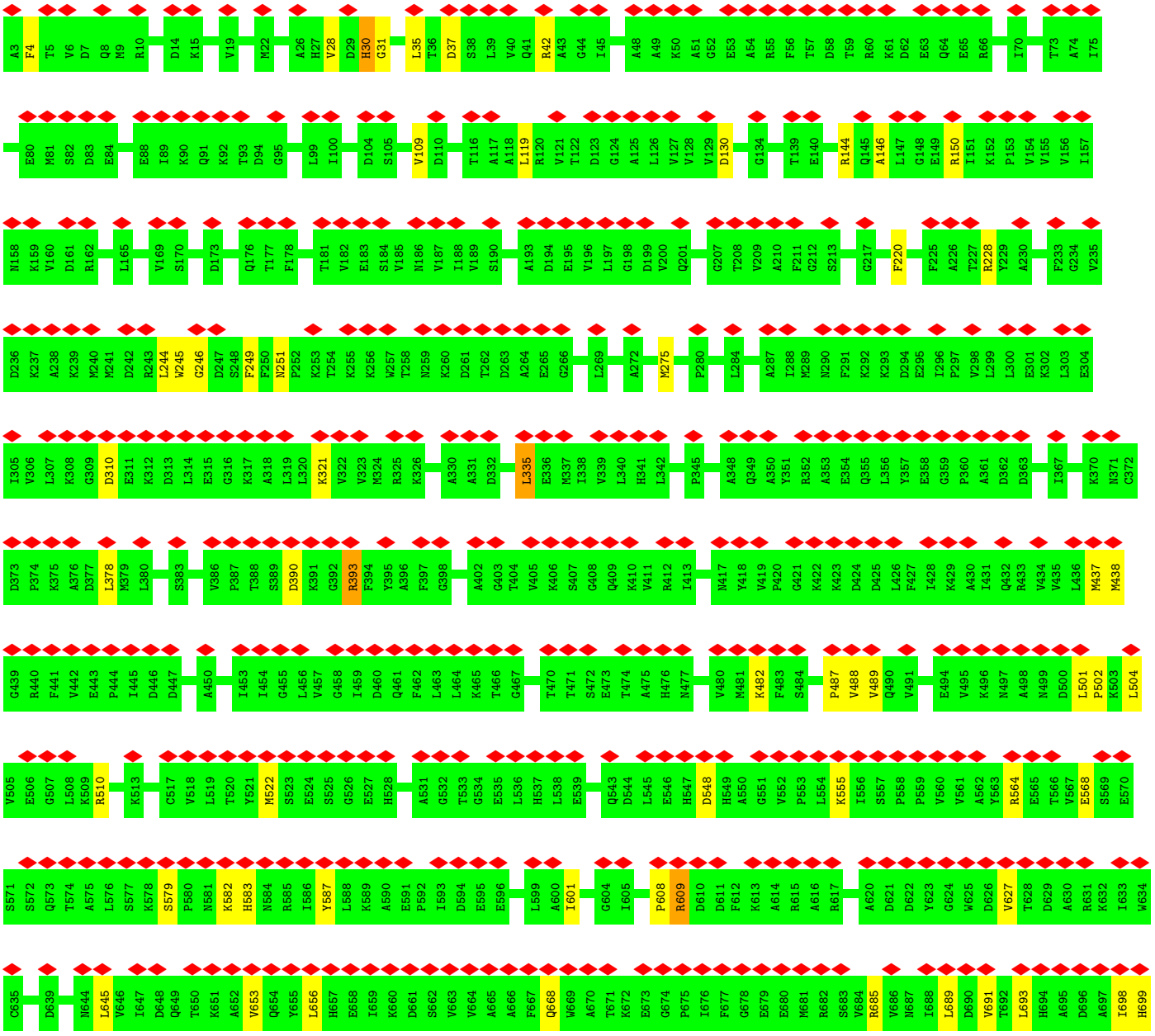


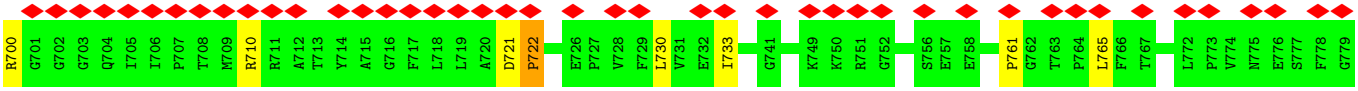


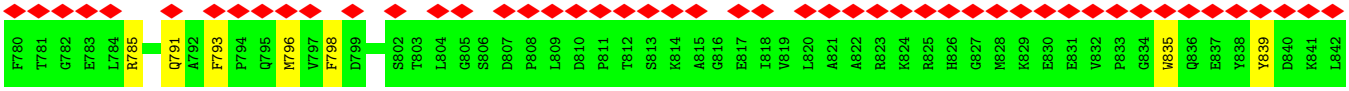
- Molecule 84: Elongation factor 2

Chain AZ:






R700
G701
G702
G703
Q704
I705
I706
P707
T708
M709
R710
R711
A712
T713
Y714
A715
G716
F717
L718
L719
A720
D721
P722
E726
P727
V728
F729
L730
V731
E732
I733
G741
K749
K750
R751
G752
S756
E757
E758
P761
G762
T763
P764
L765
F766
T767
L772
P773
V774
N775
E776
S777
F778
G779


F780
T781
G782
E783
L784
R785
Q791
A792
F793
P794
Q795
M796
V797
F798
D799
S802
T803
L804
G805
S806
D807
P808
L809
D810
P811
T812
S813
K814
A815
G816
E817
I818
V819
L820
A821
A822
R823
K824
R825
H826
G827
M828
K829
E830
E831
V832
P833
G834
W835
Q836
E837
Y838
Y839
D840
K841
L842

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	77200	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	0.358	Depositor
Minimum map value	-0.193	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: GDP, SO1, ALF, DDE, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	1	0.71	0/77157	1.22	611/120295 (0.5%)
2	3	0.58	0/2883	1.11	11/4491 (0.2%)
3	4	0.71	0/3746	1.18	19/5832 (0.3%)
4	P0	0.33	0/1498	0.72	2/2025 (0.1%)
5	P2	0.34	0/728	0.73	0/975
6	A	0.43	0/1948	0.69	3/2617 (0.1%)
7	B	0.41	0/3146	0.67	1/4228 (0.0%)
8	C	0.38	0/2800	0.69	1/3790 (0.0%)
9	D	0.38	0/2425	0.69	2/3271 (0.1%)
10	E	0.34	0/1260	0.62	0/1694
11	F	0.42	0/1821	0.72	2/2451 (0.1%)
12	G	0.37	0/1836	0.67	0/2481
13	H	0.39	0/1539	0.73	4/2073 (0.2%)
14	I	0.39	0/1741	0.64	0/2335
15	J	0.36	0/1374	0.78	2/1842 (0.1%)
16	L	0.39	0/1568	0.68	2/2106 (0.1%)
17	M	0.35	0/1068	0.62	0/1438
18	N	0.47	0/1757	0.72	0/2354
19	O	0.41	0/1585	0.76	3/2128 (0.1%)
20	P	0.42	0/1443	0.65	1/1944 (0.1%)
21	Q	0.37	0/1465	0.67	0/1965
22	R	0.35	0/1538	0.62	1/2050 (0.0%)
23	S	0.40	0/1481	0.68	2/1990 (0.1%)
24	T	0.39	0/1300	0.65	0/1743
25	U	0.37	0/812	0.66	0/1099
26	V	0.42	0/1018	0.72	1/1369 (0.1%)
27	W	0.39	0/540	0.58	0/717
28	X	0.42	0/979	0.65	0/1321
29	Y	0.37	0/1004	0.66	0/1341
30	Z	0.41	0/1118	0.66	0/1497
31	a	0.41	0/1204	0.74	1/1612 (0.1%)
32	b	0.32	0/473	0.60	1/629 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	c	0.39	0/751	0.71	1/1008 (0.1%)
34	d	0.42	0/897	0.72	1/1205 (0.1%)
35	e	0.39	0/1041	0.64	0/1394
36	f	0.44	0/868	0.69	1/1168 (0.1%)
37	g	0.46	0/890	0.68	0/1189
38	h	0.37	0/978	0.74	2/1301 (0.2%)
39	i	0.36	0/778	0.74	2/1034 (0.2%)
40	j	0.41	0/696	0.72	1/923 (0.1%)
41	k	0.35	0/618	0.81	2/826 (0.2%)
42	l	0.38	0/443	0.84	0/588
43	m	0.37	0/423	0.70	0/562
44	n	0.36	0/234	0.72	0/300
45	o	0.37	0/860	0.67	1/1136 (0.1%)
46	p	0.45	0/701	0.67	1/934 (0.1%)
47	2	0.58	2/42328 (0.0%)	1.25	408/65955 (0.6%)
48	q	0.35	0/1617	0.76	2/2215 (0.1%)
49	r	0.37	0/1735	0.77	4/2335 (0.2%)
50	s	0.35	0/1665	0.68	0/2263
51	t	0.32	0/1759	0.70	2/2368 (0.1%)
52	u	0.35	0/2109	0.79	1/2839 (0.0%)
53	v	0.32	0/1629	0.77	2/2202 (0.1%)
54	w	0.33	0/1814	0.77	0/2425
55	x	0.35	0/1506	0.75	3/2028 (0.1%)
56	y	0.35	0/1514	0.73	1/2021 (0.0%)
57	z	0.35	0/1519	0.75	4/2035 (0.2%)
58	AA	0.34	0/789	0.76	1/1067 (0.1%)
59	AB	0.39	0/1247	0.69	2/1681 (0.1%)
60	AC	0.30	0/898	0.71	1/1220 (0.1%)
61	AD	0.38	0/1215	0.76	0/1638
62	AE	0.33	0/901	0.61	0/1217
63	AF	0.34	0/998	0.70	1/1341 (0.1%)
64	AG	0.34	0/1125	0.74	2/1510 (0.1%)
65	AH	0.33	0/935	0.76	3/1254 (0.2%)
66	AI	0.32	0/1211	0.74	2/1628 (0.1%)
67	AJ	0.32	0/1130	0.68	0/1517
68	AK	0.32	0/865	0.69	0/1169
69	AL	0.40	0/693	0.84	1/935 (0.1%)
70	AM	0.38	0/1038	0.74	0/1395
71	AN	0.35	0/1139	0.72	0/1518
72	AO	0.33	0/1087	0.61	0/1449
73	AP	0.29	0/571	0.69	0/768
74	AQ	0.40	0/782	0.77	0/1047
75	AR	0.34	0/620	0.77	1/838 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
76	AS	0.34	0/499	0.76	0/670
77	AT	0.37	0/452	0.66	0/600
78	AU	0.32	0/483	0.67	1/643 (0.2%)
79	AV	0.33	0/2490	0.76	5/3389 (0.1%)
80	AW	0.34	0/292	0.67	0/390
81	AX	0.55	1/1818 (0.1%)	1.25	14/2831 (0.5%)
82	AY	0.44	0/159	1.01	1/244 (0.4%)
83	BA	0.31	0/1634	0.69	0/2195
84	AZ	0.43	0/6655	0.85	16/9009 (0.2%)
All	All	0.56	3/227354 (0.0%)	1.05	1160/333120 (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	1
5	P2	0	4
6	A	0	1
7	B	0	3
8	C	0	1
9	D	0	5
10	E	0	1
11	F	0	2
12	G	0	3
13	H	0	4
15	J	0	4
16	L	0	2
18	N	0	3
19	O	0	6
20	P	0	2
21	Q	0	1
23	S	0	4
26	V	0	1
30	Z	0	1
31	a	0	2
33	c	0	2
36	f	0	2
37	g	0	2
38	h	0	2
39	i	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
40	j	0	3
41	k	0	2
44	n	0	1
45	o	0	2
48	q	0	3
49	r	0	4
50	s	0	1
51	t	0	1
52	u	0	6
53	v	0	8
54	w	0	8
55	x	0	2
56	y	0	2
57	z	0	3
58	AA	0	2
61	AD	0	7
62	AE	0	1
63	AF	0	4
64	AG	0	6
66	AI	0	3
68	AK	0	1
70	AM	0	1
71	AN	0	2
72	AO	0	1
74	AQ	0	2
76	AS	0	1
78	AU	0	1
79	AV	0	2
83	BA	0	1
84	AZ	0	29
All	All	0	170

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	AX	1	G	OP3-P	-10.71	1.48	1.61
47	2	1221	A	N7-C5	-5.02	1.36	1.39
47	2	1221	A	C8-N7	-5.00	1.28	1.31

All (1160) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	2	94	U	C2-N3-C4	21.63	139.98	127.00
1	1	1581	C	N1-C2-O2	12.01	126.11	118.90
47	2	1362	U	C2-N1-C1'	11.91	131.99	117.70
47	2	258	C	C2-N1-C1'	11.68	131.65	118.80
47	2	1374	C	N1-C2-O2	11.52	125.81	118.90
47	2	639	U	C2-N1-C1'	11.18	131.12	117.70
47	2	94	U	N1-C2-N3	10.96	121.48	114.90
47	2	639	U	N1-C2-O2	10.94	130.46	122.80
1	1	3117	C	N1-C2-O2	10.85	125.41	118.90
47	2	258	C	N1-C2-O2	10.85	125.41	118.90
47	2	1362	U	N1-C2-O2	10.82	130.38	122.80
84	AZ	645	LEU	CA-CB-CG	10.76	140.05	115.30
1	1	3306	U	N3-C2-O2	-10.69	114.72	122.20
47	2	94	U	N3-C4-C5	10.69	121.01	114.60
1	1	3306	U	C2-N1-C1'	10.53	130.33	117.70
1	1	3306	U	N1-C2-O2	10.47	130.13	122.80
1	1	2638	C	N1-C2-O2	10.41	125.14	118.90
1	1	1581	C	C2-N1-C1'	10.20	130.01	118.80
3	4	21	C	C2-N1-C1'	10.09	129.90	118.80
47	2	618	U	C2-N1-C1'	10.07	129.78	117.70
1	1	3311	C	C2-N1-C1'	10.06	129.87	118.80
47	2	639	U	N3-C2-O2	-9.98	115.21	122.20
1	1	1146	C	C2-N1-C1'	9.96	129.76	118.80
1	1	1763	U	N1-C2-O2	9.88	129.72	122.80
1	1	1763	U	C2-N1-C1'	9.84	129.51	117.70
1	1	3058	U	N1-C2-O2	9.79	129.65	122.80
47	2	1389	C	N3-C2-O2	-9.73	115.09	121.90
47	2	1362	U	N3-C2-O2	-9.73	115.39	122.20
47	2	1389	C	N1-C2-O2	9.73	124.74	118.90
1	1	1763	U	N3-C2-O2	-9.72	115.39	122.20
1	1	3058	U	C2-N1-C1'	9.71	129.35	117.70
53	v	58	LEU	CA-CB-CG	9.69	137.58	115.30
47	2	94	U	N3-C2-O2	-9.61	115.47	122.20
47	2	1246	C	N1-C2-O2	9.51	124.61	118.90
1	1	1496	C	C2-N1-C1'	9.51	129.26	118.80
1	1	3117	C	N3-C2-O2	-9.40	115.32	121.90
1	1	922	U	C2-N1-C1'	9.32	128.89	117.70
47	2	1257	U	N3-C2-O2	-9.23	115.74	122.20
1	1	2716	U	C2-N1-C1'	9.17	128.70	117.70
47	2	1274	C	N1-C2-O2	9.15	124.39	118.90
1	1	1579	C	N3-C2-O2	-9.13	115.51	121.90
1	1	1353	U	N1-C2-O2	9.08	129.16	122.80
1	1	1437	C	C2-N1-C1'	9.06	128.76	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	4	125	U	N1-C2-O2	8.98	129.09	122.80
1	1	2531	C	N1-C2-O2	8.97	124.28	118.90
1	1	2638	C	C2-N1-C1'	8.95	128.65	118.80
47	2	784	C	N1-C2-O2	8.93	124.26	118.90
47	2	1246	C	C2-N1-C1'	8.88	128.57	118.80
1	1	545	U	C2-N1-C1'	8.87	128.34	117.70
47	2	258	C	C6-N1-C1'	-8.87	110.16	120.80
1	1	3117	C	C2-N1-C1'	8.82	128.50	118.80
1	1	3037	U	C2-N1-C1'	8.82	128.28	117.70
47	2	618	U	N1-C2-O2	8.79	128.95	122.80
1	1	1353	U	C2-N1-C1'	8.75	128.21	117.70
1	1	3058	U	N3-C2-O2	-8.74	116.08	122.20
1	1	1051	U	N3-C2-O2	-8.71	116.10	122.20
1	1	3214	U	N3-C2-O2	-8.71	116.10	122.20
1	1	2664	C	C2-N1-C1'	8.68	128.35	118.80
1	1	2716	U	N3-C2-O2	-8.68	116.12	122.20
1	1	1581	C	N3-C2-O2	-8.67	115.83	121.90
1	1	626	U	C2-N1-C1'	8.66	128.09	117.70
3	4	125	U	N3-C2-O2	-8.62	116.17	122.20
1	1	1155	C	N1-C2-O2	8.54	124.02	118.90
1	1	1051	U	N1-C2-O2	8.53	128.77	122.80
1	1	2846	U	N3-C2-O2	-8.51	116.25	122.20
47	2	572	C	C2-N1-C1'	8.50	128.15	118.80
47	2	1458	G	C4-N9-C1'	8.49	137.54	126.50
1	1	1604	G	C4-N9-C1'	8.48	137.53	126.50
47	2	1350	U	C5-C6-N1	8.41	126.90	122.70
1	1	1478	C	C2-N1-C1'	8.40	128.04	118.80
47	2	1362	U	C6-N1-C1'	-8.40	109.44	121.20
47	2	1440	C	N3-C2-O2	-8.40	116.02	121.90
47	2	1374	C	N3-C2-O2	-8.39	116.03	121.90
1	1	1525	G	C4-N9-C1'	8.38	137.39	126.50
81	AX	25	C	N3-C2-O2	-8.36	116.05	121.90
1	1	3214	U	N1-C2-O2	8.36	128.65	122.80
69	AL	78	LEU	CA-CB-CG	8.35	134.51	115.30
1	1	2846	U	N1-C2-O2	8.31	128.62	122.80
1	1	2492	C	C6-N1-C2	-8.30	116.98	120.30
47	2	1215	C	N1-C2-O2	8.30	123.88	118.90
1	1	1353	U	N3-C2-O2	-8.29	116.40	122.20
47	2	1212	G	N9-C4-C5	8.29	108.72	105.40
1	1	36	C	N1-C2-O2	8.27	123.86	118.90
1	1	545	U	N1-C2-O2	8.26	128.58	122.80
1	1	3181	C	N1-C2-O2	8.23	123.84	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	717	C	N1-C2-O2	8.22	123.83	118.90
47	2	648	G	N3-C4-N9	8.19	130.91	126.00
47	2	1440	C	N1-C2-O2	8.18	123.81	118.90
1	1	3311	C	N1-C2-O2	8.16	123.80	118.90
3	4	125	U	C2-N1-C1'	8.15	127.48	117.70
1	1	922	U	N1-C2-O2	8.14	128.50	122.80
1	1	2716	U	N1-C2-O2	8.12	128.49	122.80
79	AV	13	LEU	CA-CB-CG	8.07	133.85	115.30
1	1	3181	C	C2-N1-C1'	8.06	127.66	118.80
47	2	290	G	C8-N9-C4	-8.03	103.19	106.40
47	2	1389	C	C2-N1-C1'	8.02	127.62	118.80
1	1	8	C	C2-N1-C1'	8.01	127.61	118.80
1	1	2638	C	N3-C2-O2	-8.01	116.29	121.90
1	1	1437	C	C6-N1-C2	-7.99	117.11	120.30
1	1	2132	C	N1-C2-O2	7.96	123.68	118.90
84	AZ	335	LEU	CA-CB-CG	7.95	133.58	115.30
1	1	2726	C	C2-N1-C1'	7.94	127.54	118.80
1	1	1255	C	C5-C6-N1	7.94	124.97	121.00
1	1	1615	C	C2-N1-C1'	7.94	127.54	118.80
47	2	1438	G	C4-N9-C1'	7.94	136.82	126.50
47	2	1448	G	N3-C4-N9	-7.90	121.26	126.00
33	c	41	LEU	CA-CB-CG	7.90	133.46	115.30
48	q	188	LEU	CA-CB-CG	7.90	133.46	115.30
1	1	2094	C	N3-C2-O2	-7.89	116.37	121.90
1	1	1233	G	C6-C5-N7	-7.86	125.69	130.40
2	3	94	C	C2-N1-C1'	7.86	127.44	118.80
1	1	1277	C	C2-N1-C1'	7.85	127.44	118.80
1	1	2638	C	C6-N1-C2	-7.85	117.16	120.30
1	1	3117	C	C6-N1-C2	-7.84	117.16	120.30
47	2	728	U	N1-C2-O2	7.84	128.29	122.80
1	1	2836	C	C2-N1-C1'	7.84	127.42	118.80
1	1	1155	C	C2-N1-C1'	7.82	127.40	118.80
47	2	1374	C	C2-N1-C1'	7.81	127.39	118.80
1	1	27	C	C2-N1-C1'	7.80	127.38	118.80
47	2	258	C	N3-C2-O2	-7.80	116.44	121.90
47	2	618	U	N3-C2-O2	-7.80	116.74	122.20
47	2	728	U	C2-N1-C1'	7.79	127.04	117.70
1	1	545	U	N3-C2-O2	-7.78	116.75	122.20
47	2	1222	C	C5-C6-N1	7.76	124.88	121.00
47	2	572	C	C5-C6-N1	7.73	124.86	121.00
1	1	3034	C	N1-C2-O2	7.73	123.54	118.90
47	2	1396	U	N1-C2-O2	7.71	128.20	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	2132	C	C6-N1-C2	-7.70	117.22	120.30
47	2	1212	G	N3-C2-N2	-7.68	114.52	119.90
1	1	2405	C	C6-N1-C2	-7.68	117.23	120.30
1	1	492	C	N1-C2-O2	7.67	123.50	118.90
1	1	1146	C	C5-C6-N1	7.67	124.84	121.00
1	1	1233	G	C4-C5-N7	7.66	113.86	110.80
1	1	339	C	C6-N1-C2	-7.65	117.24	120.30
47	2	1458	G	N3-C4-N9	7.63	130.58	126.00
13	H	190	ASP	CB-CG-OD1	7.63	125.17	118.30
1	1	2306	C	OP2-P-O3'	7.62	121.97	105.20
47	2	1246	C	N3-C2-O2	-7.59	116.59	121.90
65	AH	46	LEU	CA-CB-CG	7.59	132.75	115.30
3	4	21	C	N1-C2-O2	7.59	123.45	118.90
1	1	339	C	C2-N1-C1'	7.58	127.14	118.80
47	2	572	C	N1-C2-O2	7.56	123.44	118.90
1	1	1478	C	C6-N1-C2	-7.55	117.28	120.30
1	1	1579	C	N1-C2-O2	7.54	123.43	118.90
47	2	864	U	N3-C2-O2	-7.53	116.93	122.20
1	1	922	U	N3-C2-O2	-7.53	116.93	122.20
47	2	35	U	N3-C2-O2	-7.53	116.93	122.20
1	1	2906	C	C2-N1-C1'	7.52	127.07	118.80
1	1	1051	U	C2-N1-C1'	7.51	126.72	117.70
1	1	1551	C	N3-C2-O2	-7.50	116.65	121.90
1	1	3181	C	C6-N1-C2	-7.50	117.30	120.30
47	2	2	A	O5'-P-OP1	-7.50	98.95	105.70
47	2	411	C	C2-N1-C1'	7.49	127.04	118.80
1	1	2846	U	C2-N1-C1'	7.49	126.69	117.70
47	2	1257	U	N1-C2-O2	7.48	128.03	122.80
3	4	21	C	C6-N1-C1'	-7.47	111.84	120.80
1	1	2836	C	N3-C2-O2	-7.45	116.68	121.90
47	2	1232	U	C2-N1-C1'	7.44	126.63	117.70
47	2	1396	U	N3-C2-O2	-7.44	116.99	122.20
1	1	1688	U	N1-C2-O2	7.43	128.00	122.80
47	2	1220	C	C6-N1-C2	-7.43	117.33	120.30
1	1	2943	G	N3-C4-N9	7.42	130.45	126.00
52	u	38	LEU	CA-CB-CG	7.42	132.37	115.30
47	2	160	C	C6-N1-C2	-7.41	117.33	120.30
15	J	112	LEU	CA-CB-CG	7.41	132.35	115.30
1	1	27	C	N1-C2-O2	7.41	123.34	118.90
6	A	126	LEU	CA-CB-CG	7.41	132.34	115.30
65	AH	24	LEU	CA-CB-CG	7.40	132.31	115.30
1	1	1525	G	C8-N9-C1'	-7.39	117.39	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	F	163	LEU	CA-CB-CG	7.38	132.28	115.30
1	1	2405	C	N1-C2-O2	7.38	123.33	118.90
47	2	1723	U	C2-N1-C1'	7.37	126.54	117.70
1	1	1146	C	C6-N1-C2	-7.36	117.36	120.30
79	AV	33	LEU	CA-CB-CG	7.34	132.19	115.30
23	S	14	LEU	CA-CB-CG	7.34	132.18	115.30
1	1	1238	C	C2-N1-C1'	7.34	126.87	118.80
1	1	2664	C	N1-C2-O2	7.33	123.30	118.90
47	2	1222	C	C2-N1-C1'	7.33	126.86	118.80
47	2	1458	G	C8-N9-C1'	-7.33	117.47	127.00
47	2	1215	C	N3-C2-O2	-7.33	116.77	121.90
47	2	1438	G	N3-C4-N9	7.31	130.39	126.00
47	2	1438	G	C8-N9-C1'	-7.31	117.50	127.00
1	1	969	C	N1-C2-O2	7.31	123.28	118.90
1	1	3311	C	C6-N1-C1'	-7.31	112.03	120.80
1	1	113	C	C2-N1-C1'	7.30	126.84	118.80
1	1	2132	C	N3-C2-O2	-7.30	116.79	121.90
1	1	752	C	C2-N1-C1'	7.26	126.78	118.80
41	k	51	LEU	CA-CB-CG	7.25	131.98	115.30
4	P0	93	LEU	CA-CB-CG	7.25	131.97	115.30
47	2	1232	U	N1-C2-O2	7.25	127.87	122.80
84	AZ	548	ASP	CB-CG-OD1	7.25	124.82	118.30
1	1	1581	C	C6-N1-C1'	-7.23	112.13	120.80
47	2	1527	C	N1-C2-O2	7.20	123.22	118.90
1	1	2836	C	N1-C2-O2	7.20	123.22	118.90
47	2	784	C	C2-N1-C1'	7.19	126.71	118.80
1	1	2235	C	C2-N1-C1'	7.18	126.70	118.80
47	2	639	U	C6-N1-C1'	-7.17	111.16	121.20
1	1	1604	G	C8-N9-C1'	-7.17	117.68	127.00
1	1	2836	C	O4'-C1'-N1	7.17	113.93	108.20
47	2	784	C	N3-C2-O2	-7.16	116.89	121.90
47	2	873	U	N3-C2-O2	-7.16	117.19	122.20
1	1	2405	C	C2-N1-C1'	7.16	126.67	118.80
1	1	515	C	C6-N1-C2	-7.15	117.44	120.30
47	2	1232	U	N3-C2-O2	-7.14	117.20	122.20
1	1	1633	C	N1-C2-O2	7.13	123.18	118.90
1	1	1255	C	N1-C2-O2	7.13	123.18	118.90
19	O	19	LEU	CA-CB-CG	7.13	131.69	115.30
1	1	1499	C	C6-N1-C2	-7.09	117.46	120.30
47	2	1222	C	N1-C2-O2	7.09	123.16	118.90
13	H	142	ASP	CB-CG-OD1	7.09	124.68	118.30
1	1	1579	C	C6-N1-C2	-7.07	117.47	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	2	1724	U	N1-C2-O2	7.06	127.74	122.80
47	2	779	U	OP1-P-O3'	7.05	120.72	105.20
1	1	1516	C	N1-C2-O2	7.03	123.12	118.90
1	1	3203	U	C2-N1-C1'	7.03	126.13	117.70
47	2	779	U	P-O3'-C3'	7.03	128.13	119.70
47	2	864	U	N1-C2-O2	7.02	127.71	122.80
47	2	1440	C	C6-N1-C2	-7.02	117.49	120.30
51	t	4	LEU	CA-CB-CG	7.01	131.43	115.30
1	1	97	U	C2-N1-C1'	7.01	126.11	117.70
1	1	2928	C	C6-N1-C2	-7.00	117.50	120.30
1	1	1499	C	C2-N1-C1'	7.00	126.50	118.80
1	1	1327	C	C2-N1-C1'	6.99	126.49	118.80
47	2	1491	U	P-O3'-C3'	6.98	128.08	119.70
1	1	1437	C	C5-C6-N1	6.98	124.49	121.00
47	2	1389	C	C6-N1-C2	-6.96	117.52	120.30
1	1	2470	C	N1-C2-O2	6.96	123.07	118.90
47	2	639	U	C5-C6-N1	6.96	126.18	122.70
1	1	1901	A	C2-N3-C4	6.94	114.07	110.60
1	1	3203	U	N1-C2-O2	6.94	127.66	122.80
47	2	1338	C	P-O3'-C3'	6.93	128.02	119.70
47	2	1221	A	N3-C4-N9	6.93	132.94	127.40
1	1	3350	C	N3-C2-O2	-6.92	117.05	121.90
1	1	78	U	N3-C2-O2	-6.92	117.36	122.20
1	1	1238	C	N1-C2-O2	6.92	123.05	118.90
1	1	2606	G	N3-C4-N9	6.91	130.15	126.00
47	2	860	U	N1-C2-O2	6.91	127.64	122.80
1	1	1551	C	N1-C2-O2	6.91	123.04	118.90
1	1	2306	C	P-O3'-C3'	6.90	127.97	119.70
47	2	1277	G	C4-N9-C1'	6.90	135.47	126.50
1	1	2638	C	C5-C6-N1	6.89	124.45	121.00
1	1	1233	G	N3-C4-N9	6.88	130.13	126.00
1	1	2984	C	C2-N1-C1'	6.88	126.37	118.80
55	x	129	LEU	CA-CB-CG	6.88	131.11	115.30
1	1	2821	C	N1-C2-O2	6.87	123.02	118.90
1	1	969	C	N3-C2-O2	-6.87	117.09	121.90
3	4	100	U	C2-N1-C1'	6.87	125.94	117.70
1	1	717	C	C2-N1-C1'	6.86	126.34	118.80
47	2	569	C	N1-C2-O2	6.86	123.01	118.90
47	2	1610	G	N3-C4-N9	-6.83	121.90	126.00
1	1	1146	C	N1-C2-O2	6.82	122.99	118.90
1	1	1233	G	N9-C4-C5	-6.80	102.68	105.40
1	1	1604	G	N3-C4-N9	6.80	130.08	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	36	C	N3-C2-O2	-6.80	117.14	121.90
1	1	2836	C	C6-N1-C2	-6.80	117.58	120.30
1	1	2906	C	N1-C2-O2	6.80	122.98	118.90
1	1	3325	G	O5'-P-OP1	-6.79	99.59	105.70
1	1	3181	C	N3-C2-O2	-6.79	117.15	121.90
1	1	2405	C	N3-C2-O2	-6.78	117.16	121.90
1	1	1049	C	C6-N1-C2	-6.77	117.59	120.30
84	AZ	730	LEU	CA-CB-CG	6.77	130.87	115.30
47	2	728	U	N3-C2-O2	-6.77	117.46	122.20
1	1	2726	C	N3-C2-O2	-6.76	117.17	121.90
47	2	1396	U	C2-N1-C1'	6.76	125.81	117.70
1	1	142	C	N1-C2-O2	6.75	122.95	118.90
1	1	1277	C	N1-C2-O2	6.75	122.95	118.90
47	2	85	A	N1-C6-N6	6.74	122.65	118.60
1	1	3214	U	C2-N1-C1'	6.73	125.78	117.70
1	1	3306	U	C6-N1-C1'	-6.73	111.78	121.20
1	1	717	C	N3-C2-O2	-6.72	117.19	121.90
47	2	1665	U	N1-C2-O2	6.72	127.51	122.80
47	2	88	U	N1-C2-O2	6.72	127.50	122.80
1	1	2189	U	N1-C2-O2	6.72	127.50	122.80
8	C	182	LEU	CA-CB-CG	6.71	130.73	115.30
47	2	1170	G	C4-N9-C1'	6.71	135.22	126.50
81	AX	25	C	N1-C2-O2	6.71	122.92	118.90
1	1	1146	C	C6-N1-C1'	-6.71	112.75	120.80
1	1	1228	C	C6-N1-C2	-6.69	117.62	120.30
57	z	93	LEU	CA-CB-CG	6.68	130.66	115.30
47	2	835	U	C5-C6-N1	6.68	126.04	122.70
1	1	8	C	C5-C6-N1	6.68	124.34	121.00
1	1	1761	C	C6-N1-C2	-6.67	117.63	120.30
1	1	1688	U	N3-C2-O2	-6.66	117.54	122.20
47	2	572	C	C6-N1-C2	-6.66	117.64	120.30
1	1	2531	C	N3-C2-O2	-6.66	117.24	121.90
1	1	1320	C	C6-N1-C2	-6.66	117.64	120.30
1	1	2726	C	C6-N1-C2	-6.65	117.64	120.30
1	1	2928	C	C2-N1-C1'	6.65	126.11	118.80
1	1	986	U	N1-C2-O2	6.64	127.45	122.80
47	2	1509	C	C5-C6-N1	6.63	124.32	121.00
1	1	901	G	C4-N9-C1'	6.63	135.12	126.50
1	1	1525	G	N3-C4-N9	6.63	129.98	126.00
1	1	1688	U	C2-N1-C1'	6.63	125.65	117.70
1	1	986	U	N3-C2-O2	-6.62	117.56	122.20
1	1	2184	U	C5-C6-N1	6.62	126.01	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	3104	U	N3-C2-O2	-6.61	117.57	122.20
1	1	2531	C	C6-N1-C2	-6.61	117.66	120.30
1	1	3058	U	C6-N1-C1'	-6.61	111.95	121.20
1	1	2899	C	C2-N1-C1'	6.60	126.06	118.80
47	2	431	C	C6-N1-C2	-6.60	117.66	120.30
47	2	1257	U	C2-N1-C1'	6.60	125.62	117.70
47	2	88	U	C2-N1-C1'	6.60	125.61	117.70
1	1	1708	C	C2-N1-C1'	6.59	126.05	118.80
47	2	1212	G	C8-N9-C4	-6.59	103.76	106.40
47	2	1274	C	N3-C2-O2	-6.59	117.29	121.90
47	2	1495	C	N3-C2-O2	-6.58	117.29	121.90
1	1	1496	C	C6-N1-C1'	-6.58	112.91	120.80
47	2	79	C	N1-C2-O2	6.58	122.85	118.90
63	AF	36	LEU	CA-CB-CG	6.58	130.42	115.30
1	1	1516	C	N3-C2-O2	-6.57	117.30	121.90
47	2	1603	U	N1-C2-O2	6.57	127.40	122.80
1	1	1781	C	C6-N1-C2	-6.56	117.68	120.30
47	2	618	U	C6-N1-C1'	-6.56	112.02	121.20
47	2	1274	C	C2-N1-C1'	6.55	126.01	118.80
1	1	2189	U	N3-C2-O2	-6.55	117.61	122.20
1	1	2496	C	N3-C2-O2	-6.55	117.32	121.90
1	1	2617	U	N3-C2-O2	-6.55	117.62	122.20
3	4	102	U	N3-C2-O2	-6.55	117.62	122.20
47	2	258	C	C5-C6-N1	6.55	124.27	121.00
1	1	3319	U	N1-C2-O2	6.54	127.38	122.80
1	1	3349	C	N1-C2-O2	6.54	122.83	118.90
1	1	2452	G	N3-C4-N9	-6.54	122.08	126.00
3	4	21	C	C5-C6-N1	6.53	124.27	121.00
47	2	1603	U	N3-C2-O2	-6.53	117.63	122.20
47	2	691	C	C2-N1-C1'	6.53	125.98	118.80
1	1	2531	C	C2-N1-C1'	6.53	125.98	118.80
1	1	1645	U	N3-C2-O2	-6.52	117.63	122.20
51	t	109	LEU	CA-CB-CG	6.52	130.29	115.30
34	d	86	LYS	C-N-CA	6.50	137.96	121.70
1	1	3264	G	N3-C4-N9	6.50	129.90	126.00
47	2	1207	C	P-O3'-C3'	6.50	127.50	119.70
1	1	3321	C	C5-C6-N1	6.50	124.25	121.00
47	2	1327	C	N1-C2-O2	6.50	122.80	118.90
1	1	3181	C	C5-C6-N1	6.49	124.24	121.00
1	1	1240	A	C8-N9-C4	-6.47	103.21	105.80
47	2	1213	G	C6-C5-N7	-6.47	126.52	130.40
1	1	2137	U	N1-C2-O2	6.47	127.33	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	2	1572	G	C4-N9-C1'	6.46	134.90	126.50
1	1	2184	U	C2-N1-C1'	6.46	125.45	117.70
2	3	94	C	C6-N1-C2	-6.46	117.72	120.30
47	2	88	U	N3-C2-O2	-6.46	117.68	122.20
1	1	1703	U	N1-C2-O2	6.45	127.32	122.80
47	2	1724	U	C2-N1-C1'	6.45	125.44	117.70
1	1	15	C	C6-N1-C2	-6.45	117.72	120.30
47	2	686	C	C2-N1-C1'	6.45	125.89	118.80
47	2	1665	U	N3-C2-O2	-6.45	117.69	122.20
84	AZ	378	LEU	CA-CB-CG	6.44	130.11	115.30
1	1	1496	C	C6-N1-C2	-6.43	117.73	120.30
1	1	1237	G	N3-C4-N9	6.43	129.86	126.00
47	2	810	G	N3-C4-C5	-6.43	125.39	128.60
47	2	860	U	C2-N1-C1'	6.42	125.41	117.70
47	2	530	C	N1-C2-O2	6.41	122.75	118.90
1	1	2407	C	C5-C6-N1	6.41	124.20	121.00
1	1	2235	C	C6-N1-C2	-6.40	117.74	120.30
1	1	1478	C	C5-C6-N1	6.40	124.20	121.00
1	1	713	U	N3-C2-O2	-6.39	117.72	122.20
1	1	1283	C	N1-C2-O2	6.39	122.73	118.90
1	1	1604	G	N3-C4-C5	-6.38	125.41	128.60
1	1	438	A	P-O3'-C3'	6.37	127.34	119.70
1	1	752	C	N1-C2-O2	6.36	122.72	118.90
9	D	33	ARG	NE-CZ-NH1	-6.36	117.12	120.30
47	2	1441	C	C5-C6-N1	6.36	124.18	121.00
1	1	2606	G	C4-N9-C1'	6.36	134.77	126.50
84	AZ	835	TRP	C-N-CA	6.36	137.59	121.70
1	1	1763	U	C6-N1-C1'	-6.35	112.31	121.20
47	2	21	U	N3-C2-O2	-6.34	117.76	122.20
47	2	1510	U	N1-C2-O2	6.34	127.24	122.80
1	1	113	C	N1-C2-O2	6.34	122.70	118.90
47	2	79	C	C2-N1-C1'	6.34	125.77	118.80
47	2	1429	G	O4'-C1'-N9	6.33	113.26	108.20
1	1	421	G	N3-C4-C5	-6.33	125.44	128.60
1	1	2132	C	C2-N1-C1'	6.32	125.76	118.80
1	1	3356	G	N1-C6-O6	-6.31	116.11	119.90
47	2	908	U	N3-C2-O2	-6.31	117.78	122.20
47	2	648	G	N9-C4-C5	-6.31	102.88	105.40
1	1	2531	C	C5-C6-N1	6.30	124.15	121.00
47	2	1307	U	C2-N1-C1'	6.30	125.26	117.70
47	2	1448	G	C8-N9-C1'	6.30	135.19	127.00
1	1	922	U	C6-N1-C1'	-6.29	112.39	121.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	2349	U	C2-N1-C1'	6.29	125.25	117.70
47	2	290	G	N7-C8-N9	6.28	116.24	113.10
47	2	17	C	C6-N1-C2	-6.28	117.79	120.30
3	4	157	U	N1-C2-O2	6.27	127.19	122.80
1	1	1581	C	C6-N1-C2	-6.27	117.79	120.30
1	1	2366	C	C5-C6-N1	6.27	124.14	121.00
1	1	3076	C	C6-N1-C2	-6.27	117.79	120.30
1	1	75	G	C4-N9-C1'	6.27	134.65	126.50
1	1	2652	U	N3-C2-O2	-6.27	117.81	122.20
1	1	1354	G	N3-C4-N9	6.26	129.76	126.00
47	2	810	G	C4-N9-C1'	6.26	134.64	126.50
47	2	186	C	C2-N1-C1'	6.26	125.69	118.80
1	1	2726	C	N1-C2-O2	6.26	122.66	118.90
47	2	908	U	N1-C2-O2	6.26	127.18	122.80
47	2	1221	A	C4-N9-C1'	6.26	137.56	126.30
47	2	648	G	C8-N9-C1'	-6.25	118.87	127.00
1	1	626	U	N1-C2-O2	6.25	127.17	122.80
47	2	1279	C	C6-N1-C2	-6.23	117.81	120.30
1	1	2664	C	C5-C6-N1	6.23	124.11	121.00
47	2	1458	G	N3-C4-C5	-6.23	125.49	128.60
1	1	1228	C	C5-C6-N1	6.22	124.11	121.00
3	4	102	U	N1-C2-O2	6.22	127.15	122.80
1	1	2664	C	C6-N1-C1'	-6.21	113.34	120.80
84	AZ	504	LEU	CA-CB-CG	6.21	129.58	115.30
47	2	1246	C	C6-N1-C1'	-6.21	113.35	120.80
47	2	1260	U	N3-C2-O2	-6.20	117.86	122.20
1	1	1044	U	C2-N1-C1'	6.20	125.14	117.70
1	1	1703	U	N3-C2-O2	-6.20	117.86	122.20
1	1	90	C	C6-N1-C2	-6.19	117.83	120.30
1	1	1907	C	N1-C2-O2	6.19	122.61	118.90
1	1	2258	U	N1-C2-O2	6.18	127.13	122.80
47	2	758	U	N1-C2-O2	6.18	127.13	122.80
47	2	1213	G	N7-C8-N9	6.18	116.19	113.10
47	2	1212	G	N1-C6-O6	-6.18	116.19	119.90
1	1	3050	U	N1-C2-O2	6.18	127.12	122.80
1	1	2436	U	N3-C2-O2	-6.17	117.88	122.20
1	1	1871	U	N3-C2-O2	-6.17	117.88	122.20
1	1	2641	U	C5-C6-N1	6.17	125.78	122.70
1	1	3037	U	C6-N1-C1'	-6.17	112.56	121.20
6	A	180	LEU	CA-CB-CG	6.17	129.49	115.30
1	1	1218	U	C2-N1-C1'	6.17	125.10	117.70
1	1	2928	C	C5-C6-N1	6.17	124.08	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	421	G	C4-N9-C1'	6.16	134.51	126.50
1	1	949	C	C6-N1-C2	-6.16	117.84	120.30
38	h	31	LEU	CA-CB-CG	6.16	129.47	115.30
84	AZ	689	LEU	CA-CB-CG	6.16	129.47	115.30
1	1	142	C	C6-N1-C2	-6.16	117.84	120.30
3	4	91	C	C2-N1-C1'	6.16	125.57	118.80
1	1	2606	G	C8-N9-C1'	-6.15	119.00	127.00
1	1	2641	U	N1-C2-O2	6.15	127.10	122.80
1	1	524	U	N1-C2-O2	6.13	127.09	122.80
47	2	97	C	C2-N1-C1'	6.13	125.54	118.80
47	2	1221	A	C6-C5-N7	-6.12	128.01	132.30
1	1	851	C	C2-N1-C1'	6.12	125.53	118.80
47	2	1510	U	N3-C2-O2	-6.12	117.92	122.20
1	1	945	C	C6-N1-C2	-6.11	117.85	120.30
47	2	1390	U	P-O3'-C3'	6.11	127.04	119.70
47	2	1260	U	C6-N1-C2	-6.11	117.33	121.00
47	2	1448	G	C4-N9-C1'	-6.11	118.55	126.50
1	1	2716	U	C6-N1-C1'	-6.11	112.65	121.20
1	1	1019	G	C4-N9-C1'	6.10	134.43	126.50
1	1	1354	G	N3-C4-C5	-6.10	125.55	128.60
1	1	3203	U	N3-C2-O2	-6.10	117.93	122.20
47	2	476	U	N3-C2-O2	-6.09	117.93	122.20
1	1	633	C	C5-C6-N1	6.09	124.05	121.00
66	AI	86	LEU	CA-CB-CG	6.09	129.31	115.30
47	2	1626	U	N1-C2-O2	6.09	127.06	122.80
49	r	22	ASP	CB-CG-OD1	6.09	123.78	118.30
1	1	1496	C	N1-C2-O2	6.08	122.55	118.90
1	1	97	U	N1-C2-O2	6.08	127.06	122.80
47	2	648	G	C6-C5-N7	-6.08	126.75	130.40
47	2	1626	U	C2-N1-C1'	6.08	124.99	117.70
47	2	882	U	C2-N1-C1'	6.07	124.99	117.70
47	2	354	C	N1-C2-O2	6.07	122.54	118.90
1	1	2492	C	C6-N1-C1'	6.07	128.08	120.80
84	AZ	35	LEU	CA-CB-CG	6.07	129.26	115.30
2	3	6	C	C6-N1-C2	-6.07	117.87	120.30
47	2	882	U	N1-C2-O2	6.06	127.04	122.80
47	2	784	C	C6-N1-C2	-6.06	117.88	120.30
1	1	3192	U	C2-N1-C1'	6.06	124.97	117.70
47	2	957	G	C4-N9-C1'	6.06	134.38	126.50
1	1	1907	C	N3-C2-O2	-6.05	117.66	121.90
1	1	3363	U	N3-C2-O2	-6.05	117.96	122.20
47	2	1527	C	C5-C6-N1	6.05	124.03	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	2137	U	C2-N1-C1'	6.05	124.96	117.70
2	3	94	C	C5-C6-N1	6.05	124.03	121.00
1	1	2963	C	C6-N1-C2	-6.05	117.88	120.30
47	2	1485	C	C6-N1-C2	-6.05	117.88	120.30
47	2	1096	C	N1-C2-O2	6.04	122.53	118.90
47	2	1596	C	C2-N1-C1'	6.04	125.45	118.80
81	AX	13	C	C5-C6-N1	6.04	124.02	121.00
47	2	354	C	C6-N1-C2	-6.03	117.89	120.30
47	2	860	U	N3-C2-O2	-6.03	117.98	122.20
47	2	35	U	N1-C2-O2	6.02	127.02	122.80
1	1	1551	C	C6-N1-C2	-6.02	117.89	120.30
47	2	268	C	C6-N1-C2	-6.02	117.89	120.30
1	1	1333	C	C6-N1-C2	-6.02	117.89	120.30
47	2	4	C	C2-N1-C1'	6.02	125.42	118.80
1	1	626	U	C6-N1-C1'	-6.02	112.78	121.20
1	1	2652	U	N1-C2-O2	6.01	127.01	122.80
47	2	699	U	C2-N1-C1'	6.01	124.91	117.70
47	2	1724	U	N3-C2-O2	-6.01	117.99	122.20
1	1	1781	C	C5-C6-N1	6.01	124.00	121.00
1	1	895	A	C6-C5-N7	-6.00	128.10	132.30
1	1	2641	U	C2-N1-C1'	6.00	124.90	117.70
47	2	686	C	N1-C2-O2	6.00	122.50	118.90
1	1	694	C	C6-N1-C2	-6.00	117.90	120.30
1	1	2470	C	N3-C2-O2	-6.00	117.70	121.90
3	4	21	C	C6-N1-C2	-6.00	117.90	120.30
3	4	100	U	N1-C2-O2	6.00	127.00	122.80
1	1	3251	U	N3-C2-O2	-6.00	118.00	122.20
1	1	901	G	C6-C5-N7	-6.00	126.80	130.40
1	1	1255	C	C6-N1-C2	-6.00	117.90	120.30
1	1	1581	C	C5-C6-N1	6.00	124.00	121.00
79	AV	165	ASP	CB-CG-OD1	6.00	123.70	118.30
1	1	179	C	C6-N1-C2	-6.00	117.90	120.30
1	1	2489	C	N1-C2-O2	5.99	122.50	118.90
47	2	1259	U	C5-C4-O4	-5.99	122.31	125.90
1	1	3120	C	N1-C2-O2	5.99	122.50	118.90
1	1	2235	C	C5-C6-N1	5.99	123.99	121.00
1	1	492	C	C2-N1-C1'	5.99	125.39	118.80
1	1	1028	U	P-O3'-C3'	5.99	126.88	119.70
47	2	1222	C	C6-N1-C2	-5.99	117.91	120.30
1	1	901	G	C8-N9-C1'	-5.98	119.22	127.00
47	2	648	G	C4-N9-C1'	5.98	134.28	126.50
1	1	897	U	C2-N1-C1'	5.98	124.88	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	1608	C	C2-N1-C1'	5.98	125.38	118.80
1	1	3349	C	N3-C2-O2	-5.97	117.72	121.90
47	2	1390	U	N1-C2-O2	5.97	126.98	122.80
1	1	1333	C	C5-C6-N1	5.96	123.98	121.00
47	2	699	U	N3-C2-O2	-5.96	118.03	122.20
47	2	1170	G	C8-N9-C1'	-5.96	119.25	127.00
57	z	147	MET	CA-CB-CG	5.96	123.43	113.30
1	1	2763	U	N1-C2-O2	5.95	126.97	122.80
47	2	610	G	C4-N9-C1'	5.95	134.24	126.50
47	2	946	U	N1-C2-O2	5.95	126.96	122.80
47	2	536	C	C6-N1-C2	-5.94	117.92	120.30
47	2	1223	A	N1-C6-N6	-5.94	115.03	118.60
1	1	515	C	C5-C6-N1	5.93	123.97	121.00
1	1	3319	U	C2-N1-C1'	5.93	124.82	117.70
47	2	54	C	C6-N1-C2	-5.93	117.93	120.30
1	1	895	A	C4-C5-N7	5.93	113.67	110.70
1	1	1353	U	C5-C6-N1	5.93	125.67	122.70
1	1	1174	G	C4-N9-C1'	5.93	134.21	126.50
1	1	2666	C	C6-N1-C2	-5.93	117.93	120.30
47	2	611	U	P-O3'-C3'	5.93	126.81	119.70
39	i	77	LEU	CA-CB-CG	5.92	128.93	115.30
47	2	1365	C	N1-C2-O2	5.92	122.45	118.90
1	1	829	U	C5-C4-O4	-5.92	122.35	125.90
1	1	1250	G	C6-C5-N7	-5.92	126.85	130.40
1	1	839	C	C2-N1-C1'	5.91	125.31	118.80
47	2	1624	C	N1-C2-O2	5.91	122.45	118.90
1	1	2436	U	N1-C2-O2	5.91	126.94	122.80
1	1	2706	G	N3-C4-N9	5.91	129.54	126.00
47	2	484	C	C5-C6-N1	5.90	123.95	121.00
47	2	211	U	N3-C2-O2	-5.90	118.07	122.20
1	1	1615	C	C6-N1-C1'	-5.90	113.72	120.80
47	2	1404	C	N1-C2-O2	5.90	122.44	118.90
47	2	1644	C	C6-N1-C2	-5.89	117.94	120.30
1	1	2378	C	C2-N1-C1'	5.89	125.28	118.80
47	2	528	U	N1-C2-O2	5.89	126.92	122.80
1	1	3352	U	P-O3'-C3'	5.88	126.76	119.70
2	3	53	U	N1-C2-O2	5.88	126.92	122.80
81	AX	13	C	N1-C2-O2	5.88	122.42	118.90
84	AZ	609	ARG	CA-CB-CG	5.87	126.32	113.40
1	1	8	C	C6-N1-C2	-5.87	117.95	120.30
47	2	302	U	N3-C2-O2	-5.87	118.09	122.20
1	1	2984	C	C6-N1-C2	-5.87	117.95	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	J	172	LEU	CB-CG-CD1	5.87	120.97	111.00
47	2	1350	U	C2-N1-C1'	5.87	124.74	117.70
47	2	1293	U	N3-C2-O2	-5.86	118.10	122.20
1	1	2949	U	N1-C2-O2	5.86	126.90	122.80
47	2	1221	A	C4-C5-C6	5.86	119.93	117.00
1	1	1788	C	C2-N1-C1'	5.86	125.24	118.80
1	1	2906	C	C6-N1-C2	-5.86	117.96	120.30
79	AV	243	LEU	CA-CB-CG	5.86	128.77	115.30
1	1	492	C	C5-C6-N1	5.86	123.93	121.00
1	1	3311	C	C5-C6-N1	5.86	123.93	121.00
1	1	3349	C	C2-N1-C1'	5.86	125.24	118.80
47	2	25	C	P-O3'-C3'	5.86	126.73	119.70
1	1	2596	U	C2-N1-C1'	5.85	124.72	117.70
1	1	1633	C	N3-C2-O2	-5.84	117.81	121.90
47	2	1374	C	C6-N1-C1'	-5.84	113.79	120.80
1	1	2452	G	N9-C4-C5	5.84	107.74	105.40
58	AA	88	PRO	N-CA-CB	5.84	110.31	103.30
47	2	330	G	C8-N9-C4	-5.84	104.06	106.40
47	2	1365	C	N3-C2-O2	-5.84	117.81	121.90
3	4	157	U	N3-C2-O2	-5.84	118.11	122.20
47	2	1260	U	C5-C4-O4	5.83	129.40	125.90
1	1	339	C	C5-C6-N1	5.83	123.92	121.00
45	o	93	LEU	CA-CB-CG	5.83	128.71	115.30
84	AZ	765	LEU	CA-CB-CG	5.83	128.70	115.30
81	AX	70	C	C6-N1-C2	-5.83	117.97	120.30
1	1	3034	C	N3-C2-O2	-5.82	117.83	121.90
1	1	2821	C	N3-C2-O2	-5.82	117.83	121.90
1	1	1155	C	N3-C2-O2	-5.82	117.83	121.90
47	2	271	A	C8-N9-C4	-5.82	103.47	105.80
47	2	1379	C	C6-N1-C2	-5.82	117.97	120.30
1	1	1425	U	C2-N1-C1'	5.81	124.68	117.70
47	2	1536	G	N3-C4-C5	-5.81	125.69	128.60
47	2	632	U	N3-C2-O2	-5.81	118.13	122.20
47	2	908	U	C2-N1-C1'	5.81	124.67	117.70
47	2	584	C	C5-C6-N1	5.80	123.90	121.00
81	AX	70	C	C5-C6-N1	5.80	123.90	121.00
1	1	2943	G	C6-C5-N7	-5.80	126.92	130.40
1	1	3104	U	N1-C2-O2	5.80	126.86	122.80
1	1	75	G	C8-N9-C1'	-5.79	119.47	127.00
1	1	2494	A	C4-N9-C1'	5.79	136.72	126.30
1	1	3311	C	C6-N1-C2	-5.79	117.98	120.30
1	1	1023	C	N1-C2-O2	5.79	122.37	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	2	1252	C	C2-N1-C1'	-5.79	112.43	118.80
47	2	1338	C	OP1-P-O3'	5.79	117.94	105.20
64	AG	117	LEU	CA-CB-CG	5.79	128.62	115.30
1	1	1615	C	N1-C2-O2	5.79	122.37	118.90
1	1	3105	U	N3-C2-O2	-5.79	118.15	122.20
1	1	2406	C	C6-N1-C2	-5.78	117.99	120.30
47	2	229	U	C5-C6-N1	5.78	125.59	122.70
1	1	3201	C	C6-N1-C2	-5.78	117.99	120.30
1	1	2870	C	C6-N1-C2	-5.78	117.99	120.30
47	2	1223	A	N9-C4-C5	5.77	108.11	105.80
84	AZ	501	LEU	CA-CB-CG	5.77	128.58	115.30
1	1	244	G	C4-N9-C1'	5.77	134.00	126.50
47	2	1458	G	C6-C5-N7	-5.77	126.94	130.40
47	2	1485	C	C5-C6-N1	5.77	123.88	121.00
1	1	3351	U	N1-C2-O2	5.76	126.83	122.80
1	1	2471	U	C5-C6-N1	5.76	125.58	122.70
1	1	3037	U	N1-C2-O2	5.76	126.83	122.80
1	1	2906	C	N3-C2-O2	-5.75	117.87	121.90
1	1	860	G	C2-N3-C4	5.75	114.78	111.90
1	1	1620	U	N3-C2-O2	-5.75	118.17	122.20
1	1	839	C	N1-C2-O2	5.75	122.35	118.90
81	AX	69	U	N3-C2-O2	-5.75	118.17	122.20
1	1	1049	C	C2-N1-C1'	5.75	125.12	118.80
47	2	17	C	C2-N1-C1'	5.75	125.12	118.80
1	1	379	C	C2-N1-C1'	5.75	125.12	118.80
1	1	986	U	C2-N1-C1'	5.75	124.60	117.70
13	H	189	GLU	C-N-CA	5.75	136.06	121.70
47	2	1368	G	C2'-C3'-O3'	5.75	122.89	113.70
47	2	1221	A	N9-C4-C5	-5.75	103.50	105.80
47	2	15	U	C2-N1-C1'	5.74	124.59	117.70
1	1	2338	C	N1-C2-O2	5.74	122.34	118.90
1	1	2103	U	C2-N1-C1'	5.74	124.58	117.70
47	2	431	C	C2-N1-C1'	5.74	125.11	118.80
47	2	569	C	C2-N1-C1'	5.74	125.11	118.80
47	2	1348	A	C5-C6-N6	-5.74	119.11	123.70
1	1	83	U	N1-C2-O2	5.73	126.81	122.80
1	1	1531	C	C6-N1-C2	-5.73	118.01	120.30
1	1	1437	C	C6-N1-C1'	-5.73	113.93	120.80
47	2	258	C	C6-N1-C2	-5.73	118.01	120.30
47	2	745	U	N3-C2-O2	-5.73	118.19	122.20
78	AU	8	LEU	CA-CB-CG	5.72	128.46	115.30
47	2	444	C	N1-C2-O2	5.72	122.33	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	2	676	G	N3-C4-C5	-5.72	125.74	128.60
47	2	1641	C	C6-N1-C2	-5.72	118.01	120.30
47	2	704	C	N1-C2-O2	5.71	122.32	118.90
47	2	1572	G	C8-N9-C1'	-5.71	119.58	127.00
1	1	1283	C	C6-N1-C2	-5.70	118.02	120.30
47	2	1221	A	C8-N9-C1'	-5.70	117.44	127.70
47	2	1170	G	N3-C4-N9	5.70	129.42	126.00
1	1	3356	G	C5-C6-O6	5.70	132.02	128.60
1	1	2235	C	N1-C2-O2	5.69	122.32	118.90
1	1	3192	U	N1-C2-O2	5.69	126.78	122.80
1	1	1573	G	N3-C4-C5	-5.69	125.76	128.60
1	1	1738	C	C6-N1-C1'	5.68	127.62	120.80
1	1	2284	C	C2-N1-C1'	5.68	125.05	118.80
1	1	317	A	P-O3'-C3'	5.68	126.52	119.70
47	2	782	U	C2-N1-C1'	5.68	124.52	117.70
47	2	873	U	N1-C2-O2	5.68	126.78	122.80
1	1	2884	C	C6-N1-C2	-5.68	118.03	120.30
1	1	542	G	N3-C4-N9	5.67	129.41	126.00
1	1	545	U	C6-N1-C1'	-5.67	113.25	121.20
47	2	810	G	C8-N9-C4	-5.67	104.13	106.40
1	1	3156	U	O4'-C1'-N1	5.67	112.74	108.20
47	2	1212	G	C4-C5-N7	-5.67	108.53	110.80
1	1	2362	C	C6-N1-C2	-5.67	118.03	120.30
1	1	3117	C	C6-N1-C1'	-5.67	114.00	120.80
1	1	1525	G	N3-C4-C5	-5.66	125.77	128.60
47	2	1621	U	C2-N1-C1'	5.66	124.49	117.70
1	1	915	A	C2-N3-C4	5.66	113.43	110.60
47	2	886	U	N3-C2-O2	-5.66	118.24	122.20
47	2	515	A	C8-N9-C4	-5.66	103.54	105.80
47	2	1536	G	N3-C4-N9	5.65	129.39	126.00
47	2	85	A	N7-C8-N9	5.65	116.62	113.80
47	2	880	C	C6-N1-C2	-5.65	118.04	120.30
19	O	156	LEU	CA-CB-CG	5.65	128.29	115.30
1	1	3319	U	N3-C2-O2	-5.64	118.25	122.20
47	2	610	G	C8-N9-C1'	-5.64	119.66	127.00
47	2	618	U	C5-C6-N1	5.64	125.52	122.70
1	1	1333	C	N1-C2-O2	5.64	122.28	118.90
1	1	97	U	C5-C6-N1	5.64	125.52	122.70
1	1	2277	C	C6-N1-C2	-5.64	118.05	120.30
1	1	2881	C	C6-N1-C2	-5.63	118.05	120.30
47	2	68	A	C2-N3-C4	5.63	113.42	110.60
47	2	1207	C	OP2-P-O3'	5.63	117.59	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	756	U	N3-C2-O2	-5.63	118.26	122.20
47	2	704	C	C2-N1-C1'	5.63	124.99	118.80
47	2	880	C	C5-C6-N1	5.63	123.81	121.00
47	2	1277	G	C8-N9-C1'	-5.63	119.68	127.00
1	1	1155	C	C6-N1-C1'	-5.62	114.05	120.80
1	1	2622	C	N1-C2-O2	5.62	122.27	118.90
1	1	113	C	C6-N1-C2	-5.61	118.06	120.30
1	1	3311	C	N3-C2-O2	-5.61	117.97	121.90
47	2	676	G	C4-N9-C1'	5.61	133.79	126.50
1	1	2407	C	C6-N1-C2	-5.61	118.06	120.30
1	1	2943	G	N3-C4-C5	-5.61	125.80	128.60
1	1	450	G	O4'-C1'-N9	5.60	112.68	108.20
1	1	2495	C	N3-C2-O2	-5.60	117.98	121.90
1	1	3050	U	N3-C2-O2	-5.60	118.28	122.20
57	z	109	LEU	CA-CB-CG	5.60	128.18	115.30
1	1	2366	C	C2-N1-C1'	5.60	124.96	118.80
1	1	1277	C	C6-N1-C1'	-5.60	114.08	120.80
47	2	411	C	N1-C2-O2	5.59	122.26	118.90
2	3	53	U	C2-N1-C1'	5.59	124.41	117.70
1	1	3078	U	P-O3'-C3'	5.59	126.41	119.70
60	AC	93	ASP	CB-CG-OD1	5.59	123.33	118.30
47	2	633	U	N3-C2-O2	-5.58	118.29	122.20
47	2	572	C	C6-N1-C1'	-5.58	114.11	120.80
1	1	1292	C	N1-C2-O2	5.58	122.25	118.90
1	1	37	U	N1-C2-O2	5.57	126.70	122.80
47	2	515	A	N7-C8-N9	5.57	116.58	113.80
1	1	1237	G	N3-C4-C5	-5.57	125.82	128.60
1	1	2103	U	N3-C2-O2	-5.57	118.30	122.20
47	2	1246	C	C6-N1-C2	-5.57	118.07	120.30
64	AG	54	LEU	CB-CG-CD2	-5.57	101.54	111.00
47	2	1390	U	N3-C2-O2	-5.56	118.31	122.20
47	2	1398	U	N1-C2-O2	5.56	126.69	122.80
1	1	2822	U	N1-C2-O2	5.56	126.69	122.80
47	2	160	C	C6-N1-C1'	5.56	127.47	120.80
47	2	476	U	C2-N1-C1'	5.56	124.37	117.70
47	2	1351	G	C4-C5-N7	5.56	113.02	110.80
1	1	3264	G	C4-N9-C1'	5.56	133.73	126.50
47	2	1199	G	N3-C4-C5	-5.56	125.82	128.60
47	2	758	U	N3-C2-O2	-5.56	118.31	122.20
1	1	895	A	N9-C4-C5	-5.55	103.58	105.80
1	1	2284	C	N1-C2-O2	5.55	122.23	118.90
48	q	9	LEU	CA-CB-CG	5.55	128.06	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	421	G	C2-N3-C4	5.55	114.67	111.90
1	1	1870	C	C6-N1-C2	-5.55	118.08	120.30
1	1	2094	C	N1-C2-O2	5.55	122.23	118.90
32	b	32	LEU	CA-CB-CG	5.55	128.06	115.30
47	2	569	C	N3-C2-O2	-5.54	118.02	121.90
1	1	1239	C	N1-C2-O2	5.54	122.22	118.90
47	2	946	U	C5-C6-N1	5.54	125.47	122.70
1	1	1233	G	C5-C6-O6	-5.54	125.28	128.60
1	1	1764	U	OP1-P-O3'	5.54	117.38	105.20
75	AR	21	LEU	CA-CB-CG	5.54	128.04	115.30
1	1	3105	U	N1-C2-O2	5.54	126.68	122.80
1	1	1871	U	N1-C2-O2	5.54	126.67	122.80
47	2	430	G	N3-C4-N9	5.54	129.32	126.00
1	1	271	C	N1-C2-O2	5.53	122.22	118.90
1	1	2638	C	C6-N1-C1'	-5.53	114.16	120.80
1	1	2184	U	N1-C2-O2	5.53	126.67	122.80
56	y	193	LEU	CA-CB-CG	5.53	128.02	115.30
1	1	2206	G	N1-C6-O6	-5.53	116.58	119.90
1	1	2787	G	N1-C6-O6	-5.53	116.58	119.90
1	1	757	C	C6-N1-C2	-5.53	118.09	120.30
1	1	1762	C	C6-N1-C2	-5.52	118.09	120.30
31	a	47	LYS	C-N-CA	5.52	135.51	121.70
47	2	648	G	C5-C6-O6	-5.52	125.29	128.60
47	2	1398	U	C2-N1-C1'	5.52	124.32	117.70
9	D	51	LEU	CA-CB-CG	5.51	127.98	115.30
47	2	1624	C	N3-C2-O2	-5.51	118.04	121.90
2	3	94	C	N1-C2-O2	5.51	122.21	118.90
1	1	1294	A	O4'-C1'-N9	5.51	112.61	108.20
47	2	639	U	C6-N1-C2	-5.51	117.70	121.00
47	2	1160	A	P-O3'-C3'	5.51	126.31	119.70
47	2	1199	G	N3-C4-N9	5.51	129.30	126.00
1	1	2452	G	C5-C6-O6	5.50	131.90	128.60
1	1	2998	U	C2-N1-C1'	5.50	124.31	117.70
1	1	8	C	C6-N1-C1'	-5.50	114.20	120.80
1	1	37	U	N3-C2-O2	-5.50	118.35	122.20
1	1	421	G	N3-C4-N9	5.50	129.30	126.00
47	2	381	C	C6-N1-C2	-5.50	118.10	120.30
1	1	3363	U	N1-C2-O2	5.50	126.65	122.80
2	3	53	U	N3-C2-O2	-5.50	118.35	122.20
1	1	1214	U	C2-N1-C1'	5.49	124.29	117.70
47	2	85	A	C5-C6-N6	-5.49	119.31	123.70
53	v	106	LYS	CA-CB-CG	5.49	125.49	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	2	1328	G	N3-C4-N9	5.49	129.29	126.00
47	2	184	C	C6-N1-C2	-5.49	118.11	120.30
47	2	1717	G	N3-C4-C5	-5.49	125.86	128.60
16	L	51	LEU	CA-CB-CG	5.48	127.91	115.30
1	1	2305	G	N3-C4-N9	5.48	129.29	126.00
47	2	1518	C	C2-N1-C1'	5.48	124.83	118.80
1	1	1237	G	C4-N9-C1'	5.48	133.62	126.50
1	1	2189	U	C2-N1-C1'	5.47	124.27	117.70
1	1	3004	C	P-O3'-C3'	5.47	126.27	119.70
1	1	2314	U	N3-C2-O2	-5.47	118.37	122.20
1	1	2707	C	C6-N1-C2	-5.47	118.11	120.30
1	1	142	C	N3-C2-O2	-5.47	118.07	121.90
1	1	244	G	N3-C4-N9	5.47	129.28	126.00
47	2	1527	C	C2-N1-C1'	5.47	124.81	118.80
47	2	758	U	C2-N1-C1'	5.46	124.25	117.70
47	2	1307	U	N3-C2-O2	-5.46	118.38	122.20
47	2	1327	C	C5-C6-N1	5.46	123.73	121.00
55	x	166	LEU	CA-CB-CG	5.46	127.85	115.30
1	1	3321	C	C6-N1-C2	-5.46	118.12	120.30
47	2	411	C	C6-N1-C2	-5.46	118.12	120.30
1	1	1551	C	C2-N1-C1'	5.46	124.80	118.80
1	1	1873	U	N3-C2-O2	-5.46	118.38	122.20
1	1	2338	C	C2-N1-C1'	5.45	124.80	118.80
47	2	268	C	C2-N1-C1'	5.45	124.80	118.80
16	L	77	LEU	CA-CB-CG	5.45	127.83	115.30
47	2	79	C	C6-N1-C2	-5.45	118.12	120.30
47	2	1213	G	C4-C5-N7	5.45	112.98	110.80
47	2	1596	C	N1-C2-O2	5.45	122.17	118.90
47	2	15	U	N1-C2-O2	5.44	126.61	122.80
1	1	732	C	C6-N1-C2	-5.44	118.12	120.30
1	1	1706	C	N1-C2-O2	5.44	122.16	118.90
47	2	1239	U	N3-C2-O2	-5.44	118.39	122.20
47	2	15	U	N3-C2-O2	-5.44	118.39	122.20
47	2	1711	C	C6-N1-C2	-5.44	118.12	120.30
1	1	2389	C	C6-N1-C2	-5.43	118.13	120.30
1	1	3136	G	C4-N9-C1'	5.43	133.57	126.50
47	2	15	U	C5-C6-N1	5.43	125.41	122.70
47	2	508	U	N1-C2-O2	5.43	126.60	122.80
47	2	1669	U	N3-C2-O2	-5.42	118.40	122.20
59	AB	43	LYS	C-N-CA	5.42	135.26	121.70
47	2	1037	C	C2-N1-C1'	5.42	124.77	118.80
47	2	160	C	C5-C6-N1	5.42	123.71	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	1690	C	N1-C2-O2	5.42	122.15	118.90
1	1	2822	U	N3-C2-O2	-5.42	118.41	122.20
47	2	342	C	P-O3'-C3'	5.41	126.19	119.70
81	AX	1	G	OP1-P-OP2	5.41	127.72	119.60
1	1	27	C	C6-N1-C1'	-5.41	114.31	120.80
1	1	45	A	C2-N3-C4	5.41	113.30	110.60
1	1	3064	U	N3-C2-O2	-5.41	118.42	122.20
26	V	15	LEU	CA-CB-CG	5.41	127.73	115.30
47	2	882	U	N3-C2-O2	-5.41	118.42	122.20
47	2	1727	G	C4-N9-C1'	5.41	133.53	126.50
1	1	1499	C	C5-C6-N1	5.40	123.70	121.00
47	2	149	C	N1-C2-O2	5.40	122.14	118.90
1	1	2516	U	N3-C2-O2	-5.40	118.42	122.20
47	2	4	C	C6-N1-C2	-5.40	118.14	120.30
84	AZ	568	GLU	CA-CB-CG	5.39	125.27	113.40
1	1	626	U	N3-C2-O2	-5.39	118.42	122.20
1	1	1425	U	N1-C2-O2	5.39	126.58	122.80
1	1	101	G	O4'-C1'-N9	5.39	112.51	108.20
1	1	1115	G	C4-N9-C1'	5.39	133.50	126.50
1	1	1283	C	C5-C6-N1	5.39	123.69	121.00
1	1	2362	C	C5-C6-N1	5.39	123.69	121.00
47	2	1404	C	C2-N1-C1'	5.39	124.73	118.80
1	1	1115	G	C8-N9-C1'	-5.39	120.00	127.00
47	2	1398	U	N3-C2-O2	-5.39	118.43	122.20
47	2	1518	C	C6-N1-C2	-5.39	118.14	120.30
1	1	729	C	C6-N1-C2	-5.38	118.15	120.30
66	AI	109	LEU	CA-CB-CG	5.38	127.68	115.30
47	2	232	U	N1-C2-O2	5.38	126.57	122.80
47	2	1454	G	N3-C4-N9	5.38	129.23	126.00
1	1	142	C	C5-C6-N1	5.38	123.69	121.00
47	2	463	U	N1-C2-O2	5.38	126.57	122.80
47	2	1302	U	N1-C2-O2	5.38	126.57	122.80
47	2	1362	U	C5-C6-N1	5.38	125.39	122.70
1	1	1224	C	N1-C2-O2	5.38	122.13	118.90
47	2	699	U	N1-C2-O2	5.37	126.56	122.80
3	4	125	U	C6-N1-C1'	-5.37	113.68	121.20
47	2	610	G	N3-C4-N9	5.37	129.22	126.00
1	1	1275	C	N1-C2-O2	5.37	122.12	118.90
1	1	1425	U	N3-C2-O2	-5.37	118.44	122.20
47	2	304	U	N1-C2-O2	5.37	126.56	122.80
47	2	1277	G	N3-C4-N9	5.37	129.22	126.00
23	S	152	LEU	CA-CB-CG	5.36	127.63	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	2	728	U	C6-N1-C1'	-5.36	113.69	121.20
47	2	1293	U	N1-C2-O2	5.36	126.56	122.80
47	2	1438	G	N3-C4-C5	-5.36	125.92	128.60
1	1	1058	U	N3-C2-O2	-5.36	118.45	122.20
47	2	1277	G	N3-C4-C5	-5.36	125.92	128.60
59	AB	55	ASP	CB-CG-OD1	5.36	123.13	118.30
1	1	450	G	C4-N9-C1'	5.36	133.47	126.50
1	1	1620	U	N1-C2-O2	5.36	126.55	122.80
4	P0	90	ASN	C-N-CA	5.36	135.09	121.70
47	2	484	C	C6-N1-C2	-5.36	118.16	120.30
1	1	1353	U	C6-N1-C1'	-5.36	113.70	121.20
1	1	2709	C	C2-N1-C1'	5.36	124.69	118.80
19	O	102	LEU	CA-CB-CG	5.36	127.62	115.30
47	2	782	U	N1-C2-O2	5.36	126.55	122.80
47	2	1716	C	O4'-C1'-N1	5.36	112.48	108.20
81	AX	25	C	C6-N1-C2	-5.36	118.16	120.30
1	1	1478	C	C6-N1-C1'	-5.35	114.38	120.80
1	1	524	U	N3-C2-O2	-5.35	118.46	122.20
47	2	1280	C	C6-N1-C2	-5.35	118.16	120.30
3	4	91	C	N1-C2-O2	5.35	122.11	118.90
1	1	1320	C	C5-C6-N1	5.34	123.67	121.00
1	1	1608	C	N1-C2-O2	5.34	122.11	118.90
1	1	1448	U	C2-N1-C1'	5.34	124.11	117.70
1	1	2763	U	C2-N1-C1'	5.34	124.11	117.70
1	1	3269	U	C2-N1-C1'	5.34	124.11	117.70
38	h	80	LEU	CA-CB-CG	5.34	127.58	115.30
1	1	1471	U	C5-C6-N1	5.33	125.37	122.70
1	1	2885	C	C2-N1-C1'	5.33	124.67	118.80
1	1	2783	U	N3-C2-O2	-5.33	118.47	122.20
47	2	726	C	N1-C2-O2	5.33	122.10	118.90
1	1	1585	C	C2-N1-C1'	5.33	124.66	118.80
47	2	1454	G	C4-N9-C1'	5.33	133.42	126.50
1	1	1708	C	N1-C2-O2	5.32	122.09	118.90
1	1	2706	G	C6-C5-N7	-5.32	127.21	130.40
47	2	1603	U	C2-N1-C1'	5.32	124.08	117.70
1	1	15	C	C5-C6-N1	5.32	123.66	121.00
1	1	75	G	N3-C4-N9	5.32	129.19	126.00
47	2	1300	A	OP1-P-O3'	5.32	116.89	105.20
1	1	83	U	N3-C2-O2	-5.31	118.48	122.20
1	1	1631	C	C6-N1-C1'	5.31	127.17	120.80
47	2	1323	C	C2-N1-C1'	5.31	124.64	118.80
1	1	1227	C	C6-N1-C2	-5.31	118.18	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	2	376	C	C2-N1-C1'	5.31	124.64	118.80
47	2	1448	G	N9-C4-C5	5.31	107.52	105.40
20	P	48	LEU	CA-CB-CG	5.30	127.49	115.30
47	2	864	U	C2-N1-C1'	5.30	124.06	117.70
1	1	633	C	C2-N1-C1'	5.29	124.62	118.80
1	1	1019	G	N3-C4-N9	5.29	129.18	126.00
1	1	2607	G	C4-N9-C1'	5.29	133.38	126.50
7	B	17	LEU	CA-CB-CG	5.29	127.47	115.30
1	1	627	U	O4'-C1'-N1	5.29	112.43	108.20
1	1	2606	G	N3-C4-C5	-5.29	125.95	128.60
1	1	2767	U	N3-C2-O2	-5.29	118.50	122.20
1	1	3264	G	N3-C4-C5	-5.29	125.95	128.60
47	2	255	U	N3-C2-O2	-5.29	118.50	122.20
1	1	1851	G	C4-N9-C1'	5.29	133.38	126.50
1	1	2983	C	N3-C2-O2	-5.29	118.20	121.90
1	1	2666	C	C2-N1-C1'	5.29	124.61	118.80
40	j	67	LEU	CA-CB-CG	5.29	127.46	115.30
1	1	2470	C	C2-N1-C1'	5.29	124.61	118.80
47	2	784	C	C5-C6-N1	5.29	123.64	121.00
47	2	1536	G	C4-N9-C1'	5.29	133.37	126.50
1	1	839	C	C5-C6-N1	5.28	123.64	121.00
47	2	1412	G	C5-C6-O6	5.28	131.77	128.60
47	2	536	C	C5-C6-N1	5.28	123.64	121.00
47	2	1180	C	N1-C2-O2	5.28	122.07	118.90
47	2	1223	A	C8-N9-C4	-5.28	103.69	105.80
47	2	4	C	N1-C2-O2	5.28	122.07	118.90
47	2	1108	G	C4-N9-C1'	5.28	133.37	126.50
3	4	100	U	N3-C2-O2	-5.28	118.50	122.20
1	1	101	G	C4-N9-C1'	5.28	133.36	126.50
1	1	1779	C	C5-C6-N1	5.28	123.64	121.00
41	k	31	LEU	CA-CB-CG	5.28	127.43	115.30
47	2	17	C	C5-C6-N1	5.28	123.64	121.00
1	1	2840	C	N1-C2-O2	5.27	122.06	118.90
47	2	810	G	N3-C4-N9	5.27	129.16	126.00
1	1	97	U	N3-C2-O2	-5.27	118.51	122.20
1	1	2879	C	C6-N1-C2	-5.27	118.19	120.30
1	1	2596	U	N1-C2-O2	5.27	126.49	122.80
47	2	832	U	N3-C2-O2	-5.27	118.51	122.20
1	1	2132	C	C5-C6-N1	5.26	123.63	121.00
81	AX	19	G	N1-C6-O6	-5.26	116.74	119.90
47	2	686	C	C6-N1-C1'	-5.26	114.49	120.80
47	2	330	G	N7-C8-N9	5.26	115.73	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	2	116	U	N3-C2-O2	-5.25	118.52	122.20
47	2	232	U	N3-C2-O2	-5.25	118.52	122.20
1	1	2369	G	C8-N9-C4	-5.25	104.30	106.40
47	2	648	G	C4-C5-N7	5.25	112.90	110.80
81	AX	13	C	C6-N1-C2	-5.25	118.20	120.30
1	1	1722	U	N1-C2-O2	5.24	126.47	122.80
1	1	3306	U	C6-N1-C2	-5.24	117.85	121.00
1	1	1741	A	O4'-C1'-N9	5.24	112.39	108.20
1	1	1255	C	N3-C2-O2	-5.24	118.23	121.90
1	1	2366	C	C6-N1-C2	-5.24	118.20	120.30
1	1	2706	G	C4-N9-C1'	5.24	133.31	126.50
47	2	1626	U	N3-C2-O2	-5.24	118.53	122.20
1	1	1761	C	C5-C6-N1	5.24	123.62	121.00
6	A	29	LEU	CA-CB-CG	5.24	127.35	115.30
47	2	381	C	N1-C2-O2	5.24	122.04	118.90
1	1	424	G	P-O3'-C3'	5.24	125.98	119.70
1	1	1525	G	C6-C5-N7	-5.24	127.26	130.40
47	2	632	U	N1-C2-O2	5.24	126.47	122.80
1	1	3037	U	N3-C2-O2	-5.24	118.53	122.20
47	2	411	C	C6-N1-C1'	-5.24	114.52	120.80
1	1	3386	G	C8-N9-C1'	-5.23	120.20	127.00
47	2	1448	G	N3-C4-C5	5.23	131.21	128.60
47	2	777	C	C6-N1-C2	-5.22	118.21	120.30
1	1	3036	G	C4-N9-C1'	5.22	133.29	126.50
47	2	922	G	C4-N9-C1'	5.22	133.29	126.50
47	2	1334	U	C2-N1-C1'	5.22	123.97	117.70
1	1	263	C	C6-N1-C2	-5.22	118.21	120.30
1	1	1493	G	N3-C4-N9	5.22	129.13	126.00
1	1	1721	U	N1-C2-O2	5.22	126.45	122.80
1	1	132	C	N1-C2-O2	5.22	122.03	118.90
47	2	584	C	C6-N1-C2	-5.22	118.21	120.30
47	2	946	U	C2-N1-C1'	5.22	123.96	117.70
47	2	1589	C	N1-C2-O2	5.22	122.03	118.90
1	1	2764	C	C6-N1-C2	-5.21	118.21	120.30
1	1	2885	C	C6-N1-C2	-5.21	118.22	120.30
47	2	36	C	N1-C2-O2	5.21	122.02	118.90
1	1	1437	C	N1-C2-O2	5.20	122.02	118.90
1	1	2928	C	N1-C2-O2	5.20	122.02	118.90
1	1	2378	C	C6-N1-C2	-5.20	118.22	120.30
1	1	3036	G	C8-N9-C1'	-5.20	120.25	127.00
1	1	2258	U	N3-C2-O2	-5.19	118.56	122.20
1	1	3228	C	P-O3'-C3'	5.19	125.93	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	3060	C	C6-N1-C2	-5.19	118.22	120.30
55	x	133	THR	C-N-CA	5.19	134.68	121.70
1	1	1044	U	N3-C2-O2	-5.19	118.57	122.20
1	1	922	U	C5-C6-N1	5.19	125.29	122.70
1	1	1174	G	C8-N9-C1'	-5.19	120.26	127.00
65	AH	34	LEU	CA-CB-CG	5.19	127.23	115.30
1	1	3252	G	N3-C2-N2	-5.19	116.27	119.90
1	1	2849	C	C6-N1-C2	-5.18	118.23	120.30
47	2	528	U	N3-C2-O2	-5.18	118.57	122.20
1	1	1901	A	N3-C4-C5	-5.18	123.17	126.80
1	1	3278	C	N1-C2-O2	5.18	122.01	118.90
1	1	270	U	N3-C2-O2	-5.18	118.58	122.20
1	1	655	C	C6-N1-C2	-5.18	118.23	120.30
1	1	3192	U	N3-C2-O2	-5.18	118.58	122.20
1	1	1250	G	N3-C4-N9	5.17	129.10	126.00
1	1	1763	U	C6-N1-C2	-5.17	117.89	121.00
1	1	3383	G	N3-C4-C5	-5.17	126.01	128.60
1	1	851	C	C5-C6-N1	5.17	123.59	121.00
81	AX	13	C	C2-N1-C1'	5.17	124.49	118.80
1	1	2494	A	N7-C8-N9	5.17	116.39	113.80
22	R	138	LEU	CA-CB-CG	5.17	127.19	115.30
84	AZ	310	ASP	CB-CG-OD2	5.17	122.95	118.30
47	2	1666	U	N1-C2-O2	5.17	126.42	122.80
1	1	2836	C	C6-N1-C1'	-5.17	114.60	120.80
1	1	3194	C	N1-C2-O2	5.17	122.00	118.90
47	2	1379	C	N1-C2-O2	5.17	122.00	118.90
1	1	626	U	C5-C6-N1	5.16	125.28	122.70
1	1	3131	U	C5-C6-N1	5.16	125.28	122.70
1	1	3251	U	N1-C2-O2	5.16	126.42	122.80
46	p	59	CYS	C-N-CA	5.16	134.61	121.70
1	1	729	C	C5-C6-N1	5.16	123.58	121.00
1	1	1671	C	N3-C2-O2	-5.16	118.29	121.90
47	2	85	A	C5-N7-C8	-5.16	101.32	103.90
1	1	945	C	C5-C6-N1	5.16	123.58	121.00
2	3	96	U	N3-C2-O2	-5.16	118.59	122.20
47	2	1220	C	N3-C2-O2	-5.16	118.29	121.90
1	1	2666	C	N1-C2-O2	5.16	121.99	118.90
47	2	1246	C	C5-C6-N1	5.16	123.58	121.00
47	2	54	C	C5-C6-N1	5.15	123.58	121.00
47	2	852	C	C5-C6-N1	5.15	123.58	121.00
1	1	1738	C	C2-N1-C1'	-5.15	113.13	118.80
1	1	2452	G	C8-N9-C1'	5.15	133.70	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	1722	U	N3-C2-O2	-5.15	118.59	122.20
47	2	1145	U	C5-C6-N1	5.15	125.28	122.70
81	AX	39	U	N3-C2-O2	-5.15	118.59	122.20
1	1	406	G	O4'-C1'-N9	5.15	112.32	108.20
1	1	1214	U	N3-C2-O2	-5.15	118.60	122.20
1	1	2664	C	C6-N1-C2	-5.15	118.24	120.30
47	2	1037	C	C6-N1-C2	-5.15	118.24	120.30
47	2	1724	U	C5-C6-N1	5.15	125.27	122.70
1	1	901	G	N3-C4-N9	5.15	129.09	126.00
47	2	957	G	C8-N9-C1'	-5.14	120.31	127.00
1	1	75	G	C6-C5-N7	-5.14	127.31	130.40
1	1	101	G	C8-N9-C1'	-5.14	120.31	127.00
1	1	1240	A	N7-C8-N9	5.14	116.37	113.80
1	1	1805	C	N3-C2-O2	-5.14	118.30	121.90
1	1	2963	C	C2-N1-C1'	5.14	124.46	118.80
13	H	76	ASP	CB-CG-OD1	5.14	122.93	118.30
47	2	530	C	C2-N1-C1'	5.14	124.46	118.80
47	2	1269	U	N3-C2-O2	-5.14	118.60	122.20
47	2	745	U	N1-C2-O2	5.14	126.40	122.80
49	r	22	ASP	CB-CG-OD2	-5.14	113.67	118.30
47	2	1727	G	C8-N9-C1'	-5.14	120.32	127.00
47	2	1327	C	N3-C2-O2	-5.14	118.30	121.90
47	2	411	C	C5-C6-N1	5.14	123.57	121.00
1	1	244	G	C8-N9-C1'	-5.13	120.33	127.00
47	2	1309	C	C6-N1-C2	-5.13	118.25	120.30
1	1	2452	G	C6-C5-N7	5.13	133.48	130.40
47	2	381	C	C2-N1-C1'	5.13	124.44	118.80
47	2	1213	G	C8-N9-C4	-5.13	104.35	106.40
47	2	1215	C	C2-N1-C1'	5.13	124.45	118.80
1	1	1684	U	N3-C2-O2	-5.13	118.61	122.20
1	1	1690	C	C2-N1-C1'	5.12	124.43	118.80
1	1	2550	U	C5-C6-N1	5.12	125.26	122.70
57	z	150	LEU	CA-CB-CG	5.12	127.08	115.30
1	1	3117	C	C5-C6-N1	5.12	123.56	121.00
1	1	1327	C	C5-C6-N1	5.12	123.56	121.00
47	2	590	C	P-O3'-C3'	5.12	125.84	119.70
1	1	683	U	N1-C2-O2	5.12	126.38	122.80
2	3	50	U	N3-C2-O2	-5.12	118.62	122.20
1	1	1764	U	P-O3'-C3'	5.12	125.84	119.70
1	1	2773	C	N3-C2-O2	-5.12	118.32	121.90
47	2	852	C	C2-N1-C1'	5.12	124.43	118.80
1	1	2943	G	C4-N9-C1'	5.11	133.15	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	732	C	C5-C6-N1	5.11	123.56	121.00
1	1	1721	U	N3-C2-O2	-5.11	118.62	122.20
1	1	3196	U	N3-C2-O2	-5.11	118.62	122.20
1	1	179	C	C2-N1-C1'	5.11	124.42	118.80
1	1	2436	U	C2-N1-C1'	5.11	123.83	117.70
1	1	142	C	C2-N1-C1'	5.10	124.41	118.80
1	1	1283	C	N3-C2-O2	-5.10	118.33	121.90
47	2	1307	U	N1-C2-O2	5.10	126.37	122.80
84	AZ	733	ILE	CG1-CB-CG2	-5.10	100.17	111.40
1	1	205	C	C5-C6-N1	5.10	123.55	121.00
1	1	1685	C	N3-C2-O2	-5.10	118.33	121.90
47	2	463	U	N3-C2-O2	-5.10	118.63	122.20
1	1	1312	C	N3-C2-O2	-5.10	118.33	121.90
47	2	1270	G	C5-C6-O6	5.10	131.66	128.60
1	1	27	C	N3-C2-O2	-5.10	118.33	121.90
1	1	3298	C	C6-N1-C2	-5.10	118.26	120.30
47	2	536	C	C2-N1-C1'	5.10	124.41	118.80
1	1	1201	C	N1-C2-O2	5.09	121.95	118.90
47	2	1632	C	P-O3'-C3'	5.09	125.81	119.70
1	1	368	G	C4-N9-C1'	5.09	133.11	126.50
49	r	82	ARG	CA-CB-CG	5.09	124.59	113.40
47	2	1144	U	N3-C2-O2	-5.08	118.64	122.20
1	1	2270	A	P-O3'-C3'	5.08	125.80	119.70
47	2	1666	U	N3-C2-O2	-5.08	118.64	122.20
1	1	2677	G	N3-C4-C5	-5.08	126.06	128.60
1	1	2706	G	C8-N9-C1'	-5.07	120.40	127.00
1	1	3078	U	OP2-P-O3'	5.07	116.36	105.20
1	1	1312	C	C6-N1-C2	-5.07	118.27	120.30
1	1	683	U	N3-C2-O2	-5.07	118.65	122.20
1	1	986	U	C5-C6-N1	5.07	125.23	122.70
1	1	1228	C	N1-C2-O2	5.07	121.94	118.90
47	2	1270	G	N1-C6-O6	-5.07	116.86	119.90
47	2	97	C	C6-N1-C2	-5.07	118.27	120.30
1	1	27	C	C6-N1-C2	-5.07	118.27	120.30
1	1	2103	U	N1-C2-O2	5.07	126.35	122.80
47	2	965	U	C2-N1-C1'	5.07	123.78	117.70
1	1	1233	G	N1-C6-O6	5.07	122.94	119.90
1	1	1725	C	C5-C6-N1	5.06	123.53	121.00
1	1	1292	C	N3-C2-O2	-5.06	118.36	121.90
47	2	782	U	N3-C2-O2	-5.06	118.66	122.20
1	1	1878	G	C4-N9-C1'	5.06	133.08	126.50
1	1	2893	C	P-O3'-C3'	5.06	125.77	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	1238	C	C6-N1-C2	-5.06	118.28	120.30
84	AZ	587	TYR	CA-CB-CG	5.06	123.01	113.40
1	1	1779	C	C6-N1-C2	-5.06	118.28	120.30
1	1	2939	G	P-O3'-C3'	5.06	125.77	119.70
47	2	354	C	C5-C6-N1	5.06	123.53	121.00
1	1	1830	G	N3-C4-N9	5.05	129.03	126.00
1	1	533	A	O4'-C1'-N9	5.05	112.24	108.20
1	1	3264	G	C8-N9-C1'	-5.05	120.43	127.00
1	1	2617	U	N1-C2-O2	5.05	126.33	122.80
47	2	1309	C	C5-C6-N1	5.05	123.52	121.00
1	1	1631	C	C2-N1-C1'	-5.04	113.25	118.80
1	1	1690	C	C5-C6-N1	5.04	123.52	121.00
1	1	1873	U	N1-C2-O2	5.04	126.33	122.80
1	1	370	U	N1-C2-O2	5.04	126.33	122.80
11	F	207	LEU	CA-CB-CG	5.04	126.90	115.30
1	1	3182	G	C5-C6-O6	-5.04	125.58	128.60
47	2	543	C	N1-C2-O2	5.04	121.92	118.90
47	2	508	U	N3-C2-O2	-5.04	118.67	122.20
47	2	1513	G	N3-C4-N9	-5.04	122.98	126.00
47	2	232	U	C2-N1-C1'	5.04	123.74	117.70
1	1	949	C	C5-C6-N1	5.04	123.52	121.00
1	1	3058	U	C5-C6-N1	5.04	125.22	122.70
1	1	890	C	C6-N1-C2	-5.03	118.29	120.30
47	2	1212	G	C5-C6-O6	5.03	131.62	128.60
82	AY	46	U	N3-C2-O2	-5.03	118.68	122.20
1	1	2949	U	N3-C2-O2	-5.03	118.68	122.20
1	1	629	U	C5-C6-N1	5.03	125.21	122.70
1	1	2452	G	N1-C6-O6	-5.03	116.88	119.90
1	1	3121	U	OP1-P-O3'	5.03	116.26	105.20
3	4	139	U	N3-C2-O2	-5.03	118.68	122.20
47	2	1448	G	C6-C5-N7	5.03	133.42	130.40
1	1	1284	C	N1-C2-O2	5.03	121.92	118.90
1	1	2949	U	C2-N1-C1'	5.03	123.73	117.70
1	1	2983	C	C2-N1-C1'	5.03	124.33	118.80
47	2	1306	C	C2-N1-C1'	5.02	124.33	118.80
2	3	94	C	C6-N1-C1'	-5.02	114.77	120.80
47	2	1262	U	C2-N1-C1'	5.02	123.73	117.70
47	2	1233	G	N3-C4-N9	-5.02	122.99	126.00
81	AX	14	A	N3-C4-N9	5.02	131.41	127.40
1	1	1224	C	C6-N1-C2	-5.02	118.29	120.30
47	2	1107	G	P-O3'-C3'	5.02	125.72	119.70
47	2	1337	A	C2-N3-C4	5.02	113.11	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	2	1454	G	C8-N9-C1'	-5.02	120.48	127.00
1	1	2336	U	N3-C2-O2	-5.01	118.69	122.20
47	2	1596	C	C6-N1-C1'	-5.01	114.78	120.80
47	2	1772	C	N1-C2-O2	5.01	121.91	118.90
47	2	910	C	C5-C6-N1	5.01	123.51	121.00
1	1	8	C	N1-C2-O2	5.01	121.91	118.90
49	r	61	LEU	CA-CB-CG	5.01	126.83	115.30
1	1	31	C	C6-N1-C2	-5.01	118.30	120.30
1	1	2505	U	N3-C2-O2	-5.01	118.69	122.20
79	AV	89	LEU	CA-CB-CG	5.01	126.82	115.30
1	1	315	C	P-O3'-C3'	5.01	125.71	119.70
47	2	463	U	C2-N1-C1'	5.01	123.71	117.70
47	2	1665	U	C5-C6-N1	5.01	125.20	122.70
1	1	1327	C	C6-N1-C2	-5.01	118.30	120.30
1	1	1645	U	N1-C2-O2	5.01	126.30	122.80
1	1	2906	C	C6-N1-C1'	-5.01	114.79	120.80
1	1	1708	C	C6-N1-C2	-5.00	118.30	120.30
47	2	1269	U	C2-N1-C1'	5.00	123.71	117.70
1	1	3351	U	C5-C6-N1	5.00	125.20	122.70
39	i	43	LEU	CA-CB-CG	5.00	126.81	115.30
47	2	227	U	N3-C2-O2	-5.00	118.70	122.20
1	1	1151	U	C2-N1-C1'	5.00	123.70	117.70
36	f	14	LEU	CA-CB-CG	5.00	126.81	115.30
47	2	94	U	N3-C4-O4	-5.00	115.90	119.40
47	2	916	U	N1-C2-O2	5.00	126.30	122.80

There are no chirality outliers.

All (170) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	A	247	ARG	Peptide
58	AA	63	TYR	Peptide
58	AA	7	ASP	Peptide
61	AD	114	ARG	Peptide
61	AD	138	ASN	Peptide
61	AD	25	TRP	Peptide
61	AD	35	GLU	Peptide
61	AD	43	LYS	Peptide
61	AD	84	ILE	Peptide
61	AD	87	ASP	Peptide
62	AE	123	SER	Peptide
63	AF	102	PHE	Peptide

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Mol	Chain	Res	Type	Group
63	AF	122	THR	Peptide
63	AF	124	THR	Peptide
63	AF	27	GLU	Peptide
64	AG	30	LYS	Peptide
64	AG	38	LEU	Peptide
64	AG	39	VAL	Peptide
64	AG	40	GLU	Peptide
64	AG	49	TYR	Peptide
64	AG	58	ASP	Peptide
66	AI	114	GLU	Peptide
66	AI	115	ARG	Peptide
66	AI	64	GLU	Peptide
68	AK	17	GLN	Peptide
70	AM	41	MET	Peptide
71	AN	33	LEU	Peptide
71	AN	41	SER	Peptide
72	AO	132	ARG	Peptide
74	AQ	44	ILE	Peptide
74	AQ	60	PRO	Peptide
76	AS	45	LYS	Peptide
78	AU	7	SER	Peptide
79	AV	15	GLY	Peptide
79	AV	44	SER	Peptide
84	AZ	144	ARG	Peptide
84	AZ	146	ALA	Peptide
84	AZ	220	PHE	Peptide
84	AZ	244	LEU	Peptide
84	AZ	246	GLY	Peptide
84	AZ	249	PHE	Peptide
84	AZ	251	ASN	Peptide
84	AZ	37	ASP	Peptide
84	AZ	390	ASP	Peptide
84	AZ	393	ARG	Peptide
84	AZ	4	PHE	Peptide
84	AZ	437	MET	Peptide
84	AZ	438	MET	Peptide
84	AZ	487	PRO	Peptide
84	AZ	502	PRO	Peptide
84	AZ	564	ARG	Peptide
84	AZ	579	SER	Peptide
84	AZ	582	LYS	Peptide
84	AZ	583	HIS	Peptide

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Mol	Chain	Res	Type	Group
84	AZ	601	ILE	Peptide
84	AZ	627	VAL	Peptide
84	AZ	653	VAL	Peptide
84	AZ	668	GLN	Peptide
84	AZ	691	VAL	Peptide
84	AZ	693	LEU	Peptide
84	AZ	721	ASP	Peptide
84	AZ	722	PRO	Peptide
84	AZ	761	PRO	Peptide
84	AZ	839	TYR	Peptide
7	B	179	ALA	Peptide
7	B	349	LYS	Peptide
7	B	70	ARG	Peptide
83	BA	158	GLN	Peptide
8	C	130	ALA	Peptide
9	D	123	GLU	Peptide
9	D	19	PRO	Peptide
9	D	20	PHE	Peptide
9	D	257	GLU	Peptide
9	D	260	PHE	Peptide
10	E	6	ALA	Peptide
11	F	157	ASN	Peptide
11	F	215	GLY	Peptide
12	G	155	ASN	Peptide
12	G	30	THR	Peptide
12	G	76	ALA	Peptide
13	H	140	VAL	Peptide
13	H	155	SER	Peptide
13	H	21	LYS	Peptide
13	H	71	VAL	Peptide
15	J	12	LEU	Peptide
15	J	167	TYR	Peptide
15	J	73	GLY	Peptide
15	J	94	ARG	Peptide
16	L	132	ALA	Peptide
16	L	47	ALA	Peptide
18	N	195	ASN	Peptide
18	N	26	ARG	Peptide
18	N	46	ASP	Peptide
19	O	110	PRO	Peptide
19	O	12	LYS	Peptide
19	O	133	ARG	Peptide

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Mol	Chain	Res	Type	Group
19	O	22	VAL	Peptide
19	O	36	VAL	Peptide
19	O	64	PHE	Peptide
20	P	64	ASN	Peptide
20	P	95	LEU	Peptide
4	P0	30	VAL	Peptide
5	P2	130	LYS	Peptide
5	P2	75	PRO	Peptide
5	P2	77	ALA	Peptide
5	P2	89	PRO	Peptide
21	Q	26	LEU	Peptide
23	S	108	GLN	Peptide
23	S	35	VAL	Peptide
23	S	89	ASN	Peptide
23	S	90	MET	Peptide
26	V	104	ASN	Peptide
30	Z	102	GLU	Peptide
31	a	14	HIS	Peptide
31	a	57	GLY	Peptide
33	c	55	GLU	Peptide
33	c	84	LEU	Peptide
36	f	57	LYS	Peptide
36	f	58	GLU	Peptide
37	g	58	ARG	Peptide
37	g	80	ARG	Peptide
38	h	6	ALA	Peptide
38	h	90	ARG	Peptide
39	i	12	ASN	Peptide
40	j	5	THR	Peptide
40	j	64	MET	Peptide
40	j	82	SER	Peptide
41	k	38	PHE	Peptide
41	k	40	GLN	Peptide
44	n	5	TRP	Peptide
45	o	37	ALA	Peptide
45	o	66	LYS	Peptide
48	q	112	THR	Peptide
48	q	192	THR	Peptide
48	q	202	TYR	Peptide
49	r	133	TYR	Peptide
49	r	147	ALA	Peptide
49	r	53	GLY	Peptide

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Mol	Chain	Res	Type	Group
49	r	61	LEU	Peptide
50	s	95	ARG	Peptide
51	t	173	ARG	Peptide
52	u	110	ALA	Peptide
52	u	151	ASP	Peptide
52	u	154	ILE	Peptide
52	u	155	LYS	Peptide
52	u	195	ILE	Peptide
52	u	233	LYS	Peptide
53	v	104	ASN	Peptide
53	v	128	ASN	Peptide
53	v	148	ARG	Peptide
53	v	166	ARG	Peptide
53	v	206	SER	Peptide
53	v	57	SER	Peptide
53	v	95	ASN	Peptide
53	v	97	LEU	Peptide
54	w	101	ILE	Peptide
54	w	119	GLN	Peptide
54	w	148	SER	Peptide
54	w	151	ASP	Peptide
54	w	67	VAL	Peptide
54	w	88	ARG	Peptide
54	w	9	VAL	Peptide
54	w	92	ARG	Peptide
55	x	110	GLN	Peptide
55	x	64	VAL	Peptide
56	y	40	ALA	Peptide
56	y	67	TRP	Peptide
57	z	133	HIS	Peptide
57	z	156	ILE	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%)	143 (76%)	44 (24%)	0	100	100
5	P2	92/94 (98%)	65 (71%)	27 (29%)	0	100	100
6	A	250/252 (99%)	216 (86%)	34 (14%)	0	100	100
7	B	384/386 (100%)	326 (85%)	58 (15%)	0	100	100
8	C	359/361 (99%)	298 (83%)	60 (17%)	1 (0%)	41	75
9	D	294/296 (99%)	256 (87%)	38 (13%)	0	100	100
10	E	152/175 (87%)	138 (91%)	14 (9%)	0	100	100
11	F	220/222 (99%)	196 (89%)	23 (10%)	1 (0%)	29	67
12	G	231/233 (99%)	202 (87%)	29 (13%)	0	100	100
13	H	189/191 (99%)	162 (86%)	27 (14%)	0	100	100
14	I	207/220 (94%)	178 (86%)	29 (14%)	0	100	100
15	J	167/169 (99%)	140 (84%)	27 (16%)	0	100	100
16	L	191/193 (99%)	158 (83%)	29 (15%)	4 (2%)	7	39
17	M	134/136 (98%)	120 (90%)	14 (10%)	0	100	100
18	N	201/203 (99%)	174 (87%)	26 (13%)	1 (0%)	29	67
19	O	195/197 (99%)	174 (89%)	19 (10%)	2 (1%)	15	52
20	P	181/183 (99%)	163 (90%)	18 (10%)	0	100	100
21	Q	183/185 (99%)	167 (91%)	16 (9%)	0	100	100
22	R	186/188 (99%)	169 (91%)	17 (9%)	0	100	100
23	S	170/172 (99%)	147 (86%)	22 (13%)	1 (1%)	25	63
24	T	157/159 (99%)	132 (84%)	25 (16%)	0	100	100
25	U	98/100 (98%)	85 (87%)	13 (13%)	0	100	100
26	V	134/136 (98%)	118 (88%)	16 (12%)	0	100	100
27	W	62/64 (97%)	57 (92%)	5 (8%)	0	100	100
28	X	119/121 (98%)	108 (91%)	11 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	Y	124/126 (98%)	114 (92%)	10 (8%)	0	100	100
30	Z	133/135 (98%)	115 (86%)	18 (14%)	0	100	100
31	a	146/148 (99%)	117 (80%)	27 (18%)	2 (1%)	11	46
32	b	56/58 (97%)	51 (91%)	5 (9%)	0	100	100
33	c	95/97 (98%)	88 (93%)	7 (7%)	0	100	100
34	d	107/109 (98%)	96 (90%)	11 (10%)	0	100	100
35	e	125/127 (98%)	110 (88%)	14 (11%)	1 (1%)	19	57
36	f	104/106 (98%)	88 (85%)	14 (14%)	2 (2%)	8	41
37	g	110/112 (98%)	96 (87%)	14 (13%)	0	100	100
38	h	117/119 (98%)	102 (87%)	15 (13%)	0	100	100
39	i	97/99 (98%)	75 (77%)	22 (23%)	0	100	100
40	j	85/87 (98%)	66 (78%)	16 (19%)	3 (4%)	3	30
41	k	75/77 (97%)	58 (77%)	16 (21%)	1 (1%)	12	48
42	l	48/50 (96%)	36 (75%)	10 (21%)	2 (4%)	3	26
43	m	50/52 (96%)	44 (88%)	6 (12%)	0	100	100
44	n	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
45	o	103/105 (98%)	81 (79%)	22 (21%)	0	100	100
46	p	89/91 (98%)	80 (90%)	9 (10%)	0	100	100
48	q	204/206 (99%)	157 (77%)	45 (22%)	2 (1%)	15	52
49	r	212/214 (99%)	171 (81%)	39 (18%)	2 (1%)	17	54
50	s	215/217 (99%)	184 (86%)	30 (14%)	1 (0%)	29	67
51	t	221/223 (99%)	189 (86%)	31 (14%)	1 (0%)	29	67
52	u	258/260 (99%)	209 (81%)	46 (18%)	3 (1%)	13	49
53	v	204/206 (99%)	163 (80%)	40 (20%)	1 (0%)	29	67
54	w	221/223 (99%)	176 (80%)	42 (19%)	3 (1%)	11	46
55	x	182/184 (99%)	142 (78%)	39 (21%)	1 (0%)	29	67
56	y	184/199 (92%)	134 (73%)	50 (27%)	0	100	100
57	z	183/185 (99%)	157 (86%)	25 (14%)	1 (0%)	29	67
58	AA	94/105 (90%)	71 (76%)	23 (24%)	0	100	100
59	AB	151/153 (99%)	125 (83%)	25 (17%)	1 (1%)	22	60
60	AC	122/124 (98%)	100 (82%)	22 (18%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
61	AD	148/150 (99%)	122 (82%)	22 (15%)	4 (3%)	5	35
62	AE	125/127 (98%)	110 (88%)	15 (12%)	0	100	100
63	AF	122/124 (98%)	88 (72%)	32 (26%)	2 (2%)	9	44
64	AG	139/141 (99%)	107 (77%)	31 (22%)	1 (1%)	22	60
65	AH	116/125 (93%)	98 (84%)	18 (16%)	0	100	100
66	AI	143/145 (99%)	109 (76%)	34 (24%)	0	100	100
67	AJ	141/143 (99%)	118 (84%)	23 (16%)	0	100	100
68	AK	105/107 (98%)	93 (89%)	12 (11%)	0	100	100
69	AL	85/87 (98%)	60 (71%)	24 (28%)	1 (1%)	13	49
70	AM	127/129 (98%)	109 (86%)	17 (13%)	1 (1%)	19	57
71	AN	142/144 (99%)	107 (75%)	34 (24%)	1 (1%)	22	60
72	AO	132/134 (98%)	116 (88%)	16 (12%)	0	100	100
73	AP	68/70 (97%)	53 (78%)	15 (22%)	0	100	100
74	AQ	95/97 (98%)	69 (73%)	26 (27%)	0	100	100
75	AR	79/81 (98%)	61 (77%)	17 (22%)	1 (1%)	12	48
76	AS	61/63 (97%)	48 (79%)	13 (21%)	0	100	100
77	AT	51/53 (96%)	42 (82%)	9 (18%)	0	100	100
78	AU	58/60 (97%)	47 (81%)	11 (19%)	0	100	100
79	AV	316/318 (99%)	256 (81%)	59 (19%)	1 (0%)	41	75
80	AW	35/37 (95%)	26 (74%)	9 (26%)	0	100	100
83	BA	202/204 (99%)	154 (76%)	48 (24%)	0	100	100
84	AZ	837/840 (100%)	626 (75%)	203 (24%)	8 (1%)	15	52
All	All	12208/12426 (98%)	10128 (83%)	2023 (17%)	57 (0%)	32	67

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
36	f	59	VAL
40	j	83	ALA
42	l	30	ARG
48	q	113	ARG
54	w	93	LYS
61	AD	105	ASN
16	L	63	VAL

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Mol	Chain	Res	Type
16	L	77	LEU
19	O	111	PRO
23	S	90	MET
31	a	78	LEU
36	f	58	GLU
40	j	65	ARG
52	u	195	ILE
54	w	68	LEU
59	AB	56	LYS
61	AD	139	TRP
75	AR	76	GLY
84	AZ	109	VAL
11	F	159	GLN
16	L	48	PRO
31	a	48	TYR
41	k	40	GLN
48	q	112	THR
53	v	50	GLU
54	w	92	ARG
55	x	65	PRO
64	AG	32	ASN
69	AL	21	ASN
84	AZ	31	GLY
18	N	146	ALA
40	j	6	PRO
50	s	40	LYS
61	AD	85	PRO
79	AV	165	ASP
84	AZ	30	HIS
84	AZ	608	PRO
84	AZ	698	ILE
84	AZ	700	ARG
8	C	339	LEU
35	e	79	VAL
42	l	33	ASN
52	u	194	THR
61	AD	104	ARG
70	AM	67	GLY
19	O	13	GLY
49	r	206	PRO
71	AN	114	LYS
84	AZ	245	TRP

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Mol	Chain	Res	Type
16	L	133	PRO
51	t	220	PRO
57	z	134	ILE
63	AF	125	PRO
52	u	192	ILE
63	AF	73	PRO
49	r	221	PRO
84	AZ	722	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	P0	160/160 (100%)	157 (98%)	3 (2%)	57	75
5	P2	81/81 (100%)	79 (98%)	2 (2%)	47	69
6	A	193/194 (100%)	182 (94%)	11 (6%)	20	50
7	B	320/322 (99%)	313 (98%)	7 (2%)	52	71
8	C	288/288 (100%)	279 (97%)	9 (3%)	40	64
9	D	244/244 (100%)	240 (98%)	4 (2%)	62	79
10	E	134/152 (88%)	126 (94%)	8 (6%)	19	49
11	F	186/186 (100%)	184 (99%)	2 (1%)	73	84
12	G	187/191 (98%)	182 (97%)	5 (3%)	44	67
13	H	171/171 (100%)	164 (96%)	7 (4%)	30	58
14	I	177/186 (95%)	169 (96%)	8 (4%)	27	56
15	J	147/147 (100%)	144 (98%)	3 (2%)	55	74
16	L	154/154 (100%)	151 (98%)	3 (2%)	57	75
17	M	107/107 (100%)	105 (98%)	2 (2%)	57	75
18	N	175/175 (100%)	168 (96%)	7 (4%)	31	58
19	O	160/160 (100%)	154 (96%)	6 (4%)	33	59
20	P	140/145 (97%)	137 (98%)	3 (2%)	53	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	Q	150/150 (100%)	148 (99%)	2 (1%)	69	82
22	R	153/153 (100%)	146 (95%)	7 (5%)	27	55
23	S	156/156 (100%)	152 (97%)	4 (3%)	46	68
24	T	136/136 (100%)	134 (98%)	2 (2%)	65	80
25	U	87/87 (100%)	85 (98%)	2 (2%)	50	71
26	V	104/104 (100%)	100 (96%)	4 (4%)	33	59
27	W	56/56 (100%)	54 (96%)	2 (4%)	35	61
28	X	104/105 (99%)	101 (97%)	3 (3%)	42	65
29	Y	109/109 (100%)	107 (98%)	2 (2%)	59	77
30	Z	115/115 (100%)	111 (96%)	4 (4%)	36	62
31	a	118/118 (100%)	115 (98%)	3 (2%)	47	69
32	b	46/46 (100%)	46 (100%)	0	100	100
33	c	81/81 (100%)	80 (99%)	1 (1%)	71	83
34	d	94/96 (98%)	90 (96%)	4 (4%)	29	57
35	e	109/109 (100%)	107 (98%)	2 (2%)	59	77
36	f	90/90 (100%)	87 (97%)	3 (3%)	38	63
37	g	95/95 (100%)	90 (95%)	5 (5%)	22	52
38	h	104/104 (100%)	100 (96%)	4 (4%)	33	59
39	i	81/81 (100%)	78 (96%)	3 (4%)	34	60
40	j	70/70 (100%)	69 (99%)	1 (1%)	67	81
41	k	68/68 (100%)	66 (97%)	2 (3%)	42	65
42	l	45/45 (100%)	43 (96%)	2 (4%)	28	56
43	m	47/47 (100%)	46 (98%)	1 (2%)	53	73
44	n	23/23 (100%)	22 (96%)	1 (4%)	29	57
45	o	90/90 (100%)	88 (98%)	2 (2%)	52	71
46	p	71/71 (100%)	70 (99%)	1 (1%)	67	81
48	q	164/173 (95%)	161 (98%)	3 (2%)	59	77
49	r	191/191 (100%)	183 (96%)	8 (4%)	30	57
50	s	176/176 (100%)	172 (98%)	4 (2%)	50	71
51	t	182/182 (100%)	175 (96%)	7 (4%)	33	59
52	u	221/221 (100%)	214 (97%)	7 (3%)	39	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	v	173/173 (100%)	167 (96%)	6 (4%)	36	62
54	w	189/191 (99%)	181 (96%)	8 (4%)	30	57
55	x	165/165 (100%)	162 (98%)	3 (2%)	59	77
56	y	150/160 (94%)	147 (98%)	3 (2%)	55	74
57	z	158/158 (100%)	153 (97%)	5 (3%)	39	63
58	AA	77/98 (79%)	76 (99%)	1 (1%)	69	82
59	AB	133/134 (99%)	133 (100%)	0	100	100
60	AC	88/100 (88%)	87 (99%)	1 (1%)	73	84
61	AD	127/127 (100%)	122 (96%)	5 (4%)	32	59
62	AE	81/96 (84%)	81 (100%)	0	100	100
63	AF	101/104 (97%)	100 (99%)	1 (1%)	76	86
64	AG	117/117 (100%)	116 (99%)	1 (1%)	78	87
65	AH	94/113 (83%)	88 (94%)	6 (6%)	17	47
66	AI	128/128 (100%)	124 (97%)	4 (3%)	40	64
67	AJ	115/115 (100%)	112 (97%)	3 (3%)	46	68
68	AK	100/100 (100%)	97 (97%)	3 (3%)	41	64
69	AL	74/74 (100%)	72 (97%)	2 (3%)	44	67
70	AM	110/110 (100%)	105 (96%)	5 (4%)	27	56
71	AN	119/119 (100%)	114 (96%)	5 (4%)	30	57
72	AO	112/112 (100%)	110 (98%)	2 (2%)	59	77
73	AP	61/61 (100%)	60 (98%)	1 (2%)	62	79
74	AQ	83/83 (100%)	83 (100%)	0	100	100
75	AR	70/70 (100%)	68 (97%)	2 (3%)	42	65
76	AS	56/56 (100%)	56 (100%)	0	100	100
77	AT	47/47 (100%)	45 (96%)	2 (4%)	29	57
78	AU	51/51 (100%)	49 (96%)	2 (4%)	32	59
79	AV	259/261 (99%)	255 (98%)	4 (2%)	65	80
80	AW	31/31 (100%)	31 (100%)	0	100	100
83	BA	185/185 (100%)	179 (97%)	6 (3%)	39	63
84	AZ	711/712 (100%)	685 (96%)	26 (4%)	34	60
All	All	10325/10462 (99%)	10032 (97%)	293 (3%)	46	66

All (293) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	P0	37	GLN
4	P0	48	ARG
4	P0	90	ASN
5	P2	94	LYS
5	P2	97	ASN
6	A	6	ARG
6	A	37	ARG
6	A	64	ARG
6	A	112	ILE
6	A	144	ASN
6	A	147	ARG
6	A	149	ARG
6	A	184	ARG
6	A	190	ARG
6	A	191	LEU
6	A	194	ASN
7	B	10	ARG
7	B	28	ARG
7	B	100	ARG
7	B	146	ARG
7	B	261	MET
7	B	318	LYS
7	B	332	ARG
8	C	3	ARG
8	C	12	THR
8	C	43	ASN
8	C	138	ARG
8	C	197	ARG
8	C	288	ARG
8	C	291	ASN
8	C	299	ILE
8	C	328	ASN
9	D	21	ARG
9	D	50	ARG
9	D	178	ASN
9	D	224	LYS
10	E	31	ARG
10	E	51	ARG
10	E	97	ASN
10	E	151	LYS
10	E	167	ASN
10	E	170	LYS

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Mol	Chain	Res	Type
10	E	173	MET
10	E	175	LYS
11	F	145	ARG
11	F	158	LYS
12	G	32	LYS
12	G	43	LYS
12	G	81	THR
12	G	173	MET
12	G	252	ASN
13	H	1	MET
13	H	23	ARG
13	H	62	ARG
13	H	129	ARG
13	H	141	LYS
13	H	157	ASN
13	H	184	LYS
14	I	3	ARG
14	I	24	ARG
14	I	55	ASN
14	I	76	MET
14	I	121	LYS
14	I	153	ARG
14	I	165	ILE
14	I	169	LYS
15	J	51	ARG
15	J	82	ARG
15	J	172	LEU
16	L	21	ARG
16	L	67	ARG
16	L	128	ARG
17	M	11	ASN
17	M	50	LYS
18	N	90	ASN
18	N	109	ARG
18	N	117	ASN
18	N	121	VAL
18	N	159	ARG
18	N	181	ASN
18	N	193	ARG
19	O	52	LEU
19	O	53	LYS
19	O	87	MET

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Mol	Chain	Res	Type
19	O	117	ARG
19	O	134	LYS
19	O	145	VAL
20	P	69	ARG
20	P	175	ARG
20	P	181	ARG
21	Q	27	LYS
21	Q	133	LYS
22	R	62	ARG
22	R	81	ARG
22	R	106	LEU
22	R	133	LYS
22	R	146	LYS
22	R	162	ARG
22	R	166	ASN
23	S	1	MET
23	S	80	ARG
23	S	119	ARG
23	S	149	LYS
24	T	82	ASN
24	T	146	ASN
25	U	94	ARG
25	U	104	ARG
26	V	45	ARG
26	V	64	LYS
26	V	106	LYS
26	V	109	MET
27	W	1	MET
27	W	57	LYS
28	X	42	ARG
28	X	80	ASN
28	X	125	ARG
29	Y	52	ARG
29	Y	77	LYS
30	Z	52	LYS
30	Z	121	ARG
30	Z	126	LYS
30	Z	127	ASN
31	a	92	LYS
31	a	120	ASN
31	a	132	LYS
33	c	19	LYS

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Mol	Chain	Res	Type
34	d	50	ARG
34	d	65	LYS
34	d	74	ARG
34	d	86	LYS
35	e	47	ARG
35	e	118	LYS
36	f	18	ARG
36	f	87	ASN
36	f	106	ASN
37	g	4	ARG
37	g	11	ASN
37	g	81	CYS
37	g	106	LYS
37	g	113	LYS
38	h	48	ARG
38	h	81	ARG
38	h	105	ARG
38	h	113	GLN
39	i	56	ARG
39	i	62	ARG
39	i	91	ASN
40	j	13	ASN
41	k	21	LYS
41	k	25	VAL
42	l	5	LYS
42	l	12	LYS
43	m	106	ARG
44	n	21	ARG
45	o	35	LEU
45	o	41	ARG
46	p	80	ARG
48	q	83	GLN
48	q	84	ARG
48	q	165	ARG
49	r	26	ARG
49	r	49	ASN
49	r	61	LEU
49	r	144	ARG
49	r	172	LEU
49	r	208	GLN
49	r	213	ARG
49	r	229	MET

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Mol	Chain	Res	Type
50	s	46	LYS
50	s	88	LYS
50	s	95	ARG
50	s	147	ASN
51	t	27	ARG
51	t	65	ARG
51	t	94	ARG
51	t	124	ARG
51	t	143	ARG
51	t	200	LYS
51	t	212	LYS
52	u	30	ARG
52	u	37	LYS
52	u	49	ARG
52	u	59	ARG
52	u	111	VAL
52	u	155	LYS
52	u	240	LYS
53	v	76	ARG
53	v	79	ASN
53	v	95	ASN
53	v	99	MET
53	v	100	ASN
53	v	143	ARG
54	w	4	ASN
54	w	23	ARG
54	w	67	VAL
54	w	93	LYS
54	w	98	ARG
54	w	131	LYS
54	w	154	ARG
54	w	164	LYS
55	x	19	GLN
55	x	27	LEU
55	x	148	LYS
56	y	47	ARG
56	y	48	THR
56	y	77	ARG
57	z	23	ARG
57	z	70	LEU
57	z	132	ARG
57	z	147	MET

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Mol	Chain	Res	Type
57	z	149	ARG
58	AA	44	LYS
60	AC	46	ARG
61	AD	20	ARG
61	AD	39	LYS
61	AD	43	LYS
61	AD	84	ILE
61	AD	127	ARG
63	AF	58	LYS
64	AG	107	LYS
65	AH	5	ARG
65	AH	14	LYS
65	AH	19	ARG
65	AH	45	ARG
65	AH	80	ARG
65	AH	111	LYS
66	AI	16	ARG
66	AI	103	ASN
66	AI	123	ARG
66	AI	145	ARG
67	AJ	63	ARG
67	AJ	86	ARG
67	AJ	110	LYS
68	AK	52	LYS
68	AK	72	ASN
68	AK	121	ASN
69	AL	44	ARG
69	AL	60	ARG
70	AM	25	VAL
70	AM	63	VAL
70	AM	88	LYS
70	AM	111	MET
70	AM	126	LEU
71	AN	16	ARG
71	AN	22	ASN
71	AN	121	ARG
71	AN	139	LYS
71	AN	144	ARG
72	AO	112	LYS
72	AO	131	ARG
73	AP	52	LYS
75	AR	17	ARG

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Mol	Chain	Res	Type
75	AR	26	GLN
77	AT	22	ARG
77	AT	54	LYS
78	AU	10	ARG
78	AU	39	LEU
79	AV	53	LYS
79	AV	59	ARG
79	AV	292	LEU
79	AV	316	MET
83	BA	60	ARG
83	BA	94	ASN
83	BA	122	ARG
83	BA	144	LEU
83	BA	161	LYS
83	BA	188	ASN
84	AZ	28	VAL
84	AZ	30	HIS
84	AZ	42	ARG
84	AZ	119	LEU
84	AZ	130	ASP
84	AZ	150	ARG
84	AZ	228	ARG
84	AZ	275	MET
84	AZ	321	LYS
84	AZ	335	LEU
84	AZ	393	ARG
84	AZ	482	LYS
84	AZ	488	VAL
84	AZ	489	VAL
84	AZ	510	ARG
84	AZ	522	MET
84	AZ	555	LYS
84	AZ	609	ARG
84	AZ	656	LEU
84	AZ	685	ARG
84	AZ	710	ARG
84	AZ	785	ARG
84	AZ	791	GLN
84	AZ	793	PHE
84	AZ	796	MET
84	AZ	798	PHE

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	83	ASN
4	P0	90	ASN
4	P0	189	GLN
5	P2	97	ASN
6	A	50	HIS
6	A	132	ASN
6	A	144	ASN
6	A	194	ASN
6	A	209	HIS
7	B	280	HIS
8	C	43	ASN
8	C	48	GLN
8	C	114	ASN
8	C	116	ASN
8	C	221	ASN
8	C	291	ASN
8	C	311	HIS
8	C	320	ASN
8	C	328	ASN
9	D	178	ASN
9	D	203	HIS
10	E	97	ASN
10	E	167	ASN
11	F	104	GLN
11	F	112	ASN
12	G	33	ASN
12	G	240	ASN
12	G	252	ASN
14	I	23	ASN
14	I	55	ASN
14	I	95	HIS
15	J	62	ASN
16	L	12	ASN
17	M	11	ASN
18	N	90	ASN
18	N	123	GLN
18	N	139	HIS
18	N	181	ASN
18	N	182	ASN
19	O	14	HIS
19	O	42	ASN
20	P	172	GLN

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Mol	Chain	Res	Type
21	Q	73	GLN
22	R	68	GLN
22	R	134	HIS
22	R	150	GLN
22	R	166	ASN
23	S	62	ASN
23	S	63	GLN
23	S	74	ASN
23	S	89	ASN
23	S	142	GLN
24	T	82	ASN
24	T	146	ASN
27	W	58	HIS
28	X	80	ASN
30	Z	57	HIS
31	a	120	ASN
33	c	36	GLN
35	e	31	ASN
36	f	87	ASN
36	f	88	ASN
37	g	11	ASN
37	g	33	GLN
37	g	34	HIS
38	h	59	ASN
38	h	113	GLN
39	i	91	ASN
40	j	13	ASN
40	j	76	ASN
42	l	33	ASN
45	o	82	GLN
45	o	102	GLN
48	q	49	ASN
48	q	140	ASN
49	r	49	ASN
49	r	124	ASN
49	r	149	GLN
50	s	82	ASN
51	t	22	ASN
51	t	74	GLN
52	u	142	HIS
52	u	153	ASN
52	u	209	HIS

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Mol	Chain	Res	Type
53	v	79	ASN
53	v	100	ASN
54	w	4	ASN
54	w	201	GLN
55	x	5	GLN
56	y	35	ASN
56	y	84	HIS
57	z	110	GLN
58	AA	81	ASN
61	AD	5	HIS
63	AF	128	HIS
64	AG	21	HIS
64	AG	100	GLN
65	AH	29	GLN
65	AH	31	ASN
66	AI	89	GLN
66	AI	103	ASN
67	AJ	43	ASN
68	AK	72	ASN
68	AK	121	ASN
69	AL	7	GLN
70	AM	42	GLN
70	AM	64	GLN
70	AM	70	ASN
71	AN	22	ASN
71	AN	63	GLN
72	AO	113	ASN
73	AP	98	GLN
79	AV	64	HIS
79	AV	224	ASN
83	BA	94	ASN
83	BA	188	ASN
84	AZ	27	HIS
84	AZ	64	GLN
84	AZ	365	ASN
84	AZ	371	ASN
84	AZ	581	ASN
84	AZ	654	GLN
84	AZ	657	HIS
84	AZ	748	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	3220/3396 (94%)	983 (30%)	24 (0%)
2	3	120/121 (99%)	29 (24%)	0
3	4	157/158 (99%)	49 (31%)	0
47	2	1774/1797 (98%)	695 (39%)	22 (1%)
81	AX	75/76 (98%)	29 (38%)	0
82	AY	6/7 (85%)	3 (50%)	1 (16%)
All	All	5352/5555 (96%)	1788 (33%)	47 (0%)

All (1788) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	14	U
1	1	16	A
1	1	18	G
1	1	19	U
1	1	20	A
1	1	21	G
1	1	22	G
1	1	26	A
1	1	27	C
1	1	40	A
1	1	43	A
1	1	45	A
1	1	49	A
1	1	50	U
1	1	59	G
1	1	60	A
1	1	64	G
1	1	65	A
1	1	66	A
1	1	72	C
1	1	73	C
1	1	75	G
1	1	76	G
1	1	83	U
1	1	85	A
1	1	87	U
1	1	92	G
1	1	93	C
1	1	97	U
1	1	105	C
1	1	108	A
1	1	109	A

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Mol	Chain	Res	Type
1	1	110	G
1	1	115	A
1	1	116	A
1	1	117	U
1	1	118	U
1	1	122	A
1	1	123	A
1	1	124	U
1	1	132	C
1	1	133	U
1	1	135	C
1	1	136	G
1	1	142	C
1	1	146	U
1	1	147	U
1	1	148	G
1	1	150	A
1	1	154	U
1	1	157	A
1	1	159	A
1	1	160	G
1	1	161	G
1	1	166	C
1	1	167	U
1	1	170	G
1	1	180	C
1	1	182	U
1	1	187	A
1	1	190	U
1	1	191	U
1	1	200	C
1	1	206	G
1	1	211	A
1	1	212	G
1	1	216	G
1	1	219	A
1	1	221	A
1	1	222	A
1	1	235	A
1	1	238	A
1	1	241	G
1	1	242	C

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Mol	Chain	Res	Type
1	1	243	G
1	1	244	G
1	1	245	U
1	1	249	U
1	1	252	U
1	1	257	U
1	1	264	G
1	1	265	A
1	1	266	A
1	1	267	G
1	1	268	A
1	1	269	G
1	1	270	U
1	1	284	A
1	1	286	U
1	1	295	A
1	1	297	G
1	1	301	G
1	1	316	U
1	1	317	A
1	1	318	A
1	1	328	U
1	1	329	U
1	1	334	A
1	1	336	A
1	1	337	G
1	1	338	A
1	1	339	C
1	1	346	C
1	1	349	A
1	1	352	A
1	1	353	G
1	1	360	G
1	1	368	G
1	1	374	A
1	1	375	A
1	1	376	G
1	1	377	A
1	1	383	G
1	1	395	A
1	1	396	A
1	1	397	A

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Mol	Chain	Res	Type
1	1	398	A
1	1	403	C
1	1	404	G
1	1	420	G
1	1	421	G
1	1	422	A
1	1	423	A
1	1	424	G
1	1	425	G
1	1	428	A
1	1	436	A
1	1	439	C
1	1	440	A
1	1	441	U
1	1	442	G
1	1	443	G
1	1	445	G
1	1	446	U
1	1	447	U
1	1	448	U
1	1	450	G
1	1	451	U
1	1	487	U
1	1	488	U
1	1	489	U
1	1	490	C
1	1	491	A
1	1	494	G
1	1	498	A
1	1	515	C
1	1	520	U
1	1	521	A
1	1	523	A
1	1	532	A
1	1	533	A
1	1	534	U
1	1	535	G
1	1	536	U
1	1	543	C
1	1	544	C
1	1	546	C
1	1	550	A

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Mol	Chain	Res	Type
1	1	554	A
1	1	555	U
1	1	556	U
1	1	557	A
1	1	559	A
1	1	569	A
1	1	578	A
1	1	579	G
1	1	592	A
1	1	597	G
1	1	601	U
1	1	602	A
1	1	607	A
1	1	611	A
1	1	615	U
1	1	620	U
1	1	621	A
1	1	626	U
1	1	627	U
1	1	632	G
1	1	636	C
1	1	645	A
1	1	648	C
1	1	649	A
1	1	660	A
1	1	661	G
1	1	662	U
1	1	664	U
1	1	667	C
1	1	676	G
1	1	677	A
1	1	678	G
1	1	681	U
1	1	683	U
1	1	690	A
1	1	691	A
1	1	705	A
1	1	709	A
1	1	712	G
1	1	713	U
1	1	715	A
1	1	718	G

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Mol	Chain	Res	Type
1	1	720	A
1	1	737	G
1	1	750	G
1	1	752	C
1	1	758	C
1	1	761	A
1	1	765	C
1	1	766	U
1	1	767	U
1	1	774	G
1	1	776	U
1	1	777	U
1	1	780	A
1	1	781	G
1	1	782	U
1	1	785	G
1	1	786	A
1	1	794	U
1	1	800	G
1	1	801	A
1	1	808	A
1	1	817	A
1	1	830	A
1	1	842	G
1	1	846	A
1	1	847	A
1	1	849	C
1	1	854	G
1	1	857	G
1	1	859	G
1	1	860	G
1	1	861	C
1	1	874	U
1	1	879	U
1	1	880	G
1	1	884	A
1	1	890	C
1	1	895	A
1	1	896	A
1	1	897	U
1	1	901	G
1	1	907	G

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Mol	Chain	Res	Type
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	926	A
1	1	929	A
1	1	933	A
1	1	937	G
1	1	939	U
1	1	941	G
1	1	944	C
1	1	959	C
1	1	960	U
1	1	962	A
1	1	970	A
1	1	977	C
1	1	979	U
1	1	980	A
1	1	981	U
1	1	985	U
1	1	999	G
1	1	1001	G
1	1	1005	G
1	1	1006	A
1	1	1010	G
1	1	1015	U
1	1	1016	C
1	1	1017	C
1	1	1018	G
1	1	1020	G
1	1	1024	G
1	1	1026	A
1	1	1028	U
1	1	1029	G
1	1	1030	A
1	1	1031	C
1	1	1032	C
1	1	1035	G
1	1	1041	U
1	1	1045	C

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Mol	Chain	Res	Type
1	1	1047	A
1	1	1051	U
1	1	1063	G
1	1	1064	A
1	1	1065	A
1	1	1066	G
1	1	1072	G
1	1	1073	U
1	1	1075	A
1	1	1081	U
1	1	1082	U
1	1	1083	G
1	1	1084	A
1	1	1090	G
1	1	1091	A
1	1	1093	A
1	1	1094	U
1	1	1095	U
1	1	1096	U
1	1	1097	G
1	1	1098	A
1	1	1103	A
1	1	1104	G
1	1	1117	G
1	1	1118	C
1	1	1131	G
1	1	1134	G
1	1	1135	A
1	1	1140	G
1	1	1141	C
1	1	1143	A
1	1	1151	U
1	1	1153	A
1	1	1155	C
1	1	1158	A
1	1	1159	A
1	1	1161	G
1	1	1165	A
1	1	1168	U
1	1	1171	G
1	1	1178	G
1	1	1180	A

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Mol	Chain	Res	Type
1	1	1181	U
1	1	1182	A
1	1	1186	G
1	1	1189	C
1	1	1190	A
1	1	1191	U
1	1	1193	A
1	1	1196	C
1	1	1197	A
1	1	1198	C
1	1	1201	C
1	1	1203	A
1	1	1206	G
1	1	1209	G
1	1	1214	U
1	1	1216	C
1	1	1217	A
1	1	1221	A
1	1	1222	G
1	1	1226	G
1	1	1227	C
1	1	1228	C
1	1	1230	G
1	1	1231	A
1	1	1233	G
1	1	1235	U
1	1	1236	G
1	1	1237	G
1	1	1238	C
1	1	1241	U
1	1	1244	A
1	1	1245	A
1	1	1246	G
1	1	1248	C
1	1	1251	A
1	1	1252	A
1	1	1253	U
1	1	1254	C
1	1	1257	C
1	1	1258	U
1	1	1259	A
1	1	1260	A

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Mol	Chain	Res	Type
1	1	1262	G
1	1	1263	A
1	1	1264	G
1	1	1265	U
1	1	1267	U
1	1	1272	C
1	1	1273	A
1	1	1276	U
1	1	1277	C
1	1	1278	A
1	1	1279	C
1	1	1281	G
1	1	1282	G
1	1	1283	C
1	1	1285	G
1	1	1286	A
1	1	1287	A
1	1	1294	A
1	1	1300	G
1	1	1301	A
1	1	1302	A
1	1	1303	A
1	1	1305	U
1	1	1307	G
1	1	1309	U
1	1	1313	G
1	1	1315	U
1	1	1316	C
1	1	1326	A
1	1	1327	C
1	1	1330	A
1	1	1331	U
1	1	1332	A
1	1	1333	C
1	1	1347	U
1	1	1348	U
1	1	1350	A
1	1	1351	U
1	1	1352	A
1	1	1354	G
1	1	1355	A
1	1	1356	U

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Mol	Chain	Res	Type
1	1	1357	G
1	1	1361	U
1	1	1370	G
1	1	1385	C
1	1	1386	A
1	1	1387	G
1	1	1392	G
1	1	1394	A
1	1	1399	A
1	1	1400	G
1	1	1408	G
1	1	1409	G
1	1	1411	C
1	1	1417	G
1	1	1418	A
1	1	1419	A
1	1	1425	U
1	1	1434	G
1	1	1435	A
1	1	1436	U
1	1	1437	C
1	1	1446	A
1	1	1450	G
1	1	1455	U
1	1	1466	G
1	1	1477	A
1	1	1478	C
1	1	1481	A
1	1	1482	A
1	1	1483	G
1	1	1488	G
1	1	1490	A
1	1	1491	A
1	1	1503	A
1	1	1507	G
1	1	1508	C
1	1	1511	U
1	1	1512	U
1	1	1523	U
1	1	1525	G
1	1	1526	U
1	1	1527	C

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Mol	Chain	Res	Type
1	1	1533	U
1	1	1536	G
1	1	1546	A
1	1	1556	C
1	1	1557	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	1568	U
1	1	1569	U
1	1	1572	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	1583	A
1	1	1589	A
1	1	1593	A
1	1	1602	A
1	1	1603	A
1	1	1605	A
1	1	1616	U
1	1	1618	G
1	1	1620	U
1	1	1621	A
1	1	1624	G
1	1	1626	U
1	1	1629	U
1	1	1630	U
1	1	1632	A
1	1	1637	A
1	1	1638	A
1	1	1640	G
1	1	1641	U
1	1	1642	A
1	1	1643	A
1	1	1645	U

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Mol	Chain	Res	Type
1	1	1656	A
1	1	1657	C
1	1	1658	G
1	1	1672	U
1	1	1677	G
1	1	1678	G
1	1	1683	A
1	1	1688	U
1	1	1704	A
1	1	1714	A
1	1	1717	U
1	1	1718	G
1	1	1724	U
1	1	1729	A
1	1	1736	G
1	1	1742	U
1	1	1749	A
1	1	1750	A
1	1	1751	G
1	1	1756	C
1	1	1759	C
1	1	1764	U
1	1	1765	U
1	1	1766	G
1	1	1767	C
1	1	1769	G
1	1	1779	C
1	1	1780	G
1	1	1783	U
1	1	1795	U
1	1	1797	A
1	1	1806	A
1	1	1808	G
1	1	1814	A
1	1	1815	U
1	1	1816	A
1	1	1819	U
1	1	1820	U
1	1	1821	U
1	1	1840	U
1	1	1841	A
1	1	1842	A

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Mol	Chain	Res	Type
1	1	1845	G
1	1	1846	C
1	1	1850	A
1	1	1854	C
1	1	1858	A
1	1	1863	G
1	1	1864	A
1	1	1866	C
1	1	1871	U
1	1	1878	G
1	1	1879	A
1	1	1880	U
1	1	1885	U
1	1	1886	A
1	1	1893	A
1	1	1896	A
1	1	1906	G
1	1	1907	C
1	1	1913	A
1	1	1926	C
1	1	1928	G
1	1	1930	A
1	1	1931	U
1	1	1934	G
1	1	1935	G
1	1	1948	G
1	1	1953	G
1	1	1954	G
1	1	1955	U
1	1	2101	C
1	1	2102	U
1	1	2109	U
1	1	2110	G
1	1	2111	G
1	1	2114	C
1	1	2116	G
1	1	2118	C
1	1	2122	G
1	1	2131	A
1	1	2134	G
1	1	2138	A
1	1	2139	A

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Mol	Chain	Res	Type
1	1	2142	A
1	1	2143	A
1	1	2152	A
1	1	2157	G
1	1	2158	A
1	1	2161	G
1	1	2167	A
1	1	2169	G
1	1	2170	U
1	1	2174	G
1	1	2175	U
1	1	2176	U
1	1	2186	U
1	1	2188	A
1	1	2194	G
1	1	2205	U
1	1	2206	G
1	1	2209	U
1	1	2210	G
1	1	2224	A
1	1	2230	C
1	1	2231	C
1	1	2244	A
1	1	2249	G
1	1	2250	G
1	1	2256	A
1	1	2257	C
1	1	2269	U
1	1	2270	A
1	1	2271	A
1	1	2272	G
1	1	2273	G
1	1	2276	G
1	1	2280	A
1	1	2281	A
1	1	2287	C
1	1	2291	A
1	1	2295	A
1	1	2298	U
1	1	2307	G
1	1	2309	A
1	1	2310	U

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Mol	Chain	Res	Type
1	1	2313	A
1	1	2315	G
1	1	2323	G
1	1	2324	A
1	1	2325	G
1	1	2327	U
1	1	2334	U
1	1	2335	G
1	1	2336	U
1	1	2339	C
1	1	2355	G
1	1	2356	A
1	1	2372	A
1	1	2373	A
1	1	2374	C
1	1	2376	G
1	1	2380	U
1	1	2381	G
1	1	2393	G
1	1	2394	G
1	1	2397	A
1	1	2401	A
1	1	2402	A
1	1	2403	G
1	1	2404	A
1	1	2410	U
1	1	2411	U
1	1	2412	G
1	1	2417	U
1	1	2418	G
1	1	2422	C
1	1	2432	A
1	1	2434	U
1	1	2435	G
1	1	2436	U
1	1	2437	G
1	1	2438	A
1	1	2443	A
1	1	2445	A
1	1	2447	A
1	1	2450	G
1	1	2452	G

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Mol	Chain	Res	Type
1	1	2453	U
1	1	2454	G
1	1	2455	U
1	1	2456	A
1	1	2457	G
1	1	2458	A
1	1	2459	A
1	1	2460	U
1	1	2461	A
1	1	2463	G
1	1	2466	G
1	1	2468	A
1	1	2472	U
1	1	2473	C
1	1	2474	G
1	1	2475	G
1	1	2477	G
1	1	2478	C
1	1	2479	C
1	1	2480	A
1	1	2486	A
1	1	2487	U
1	1	2488	A
1	1	2489	C
1	1	2490	C
1	1	2491	A
1	1	2492	C
1	1	2494	A
1	1	2495	C
1	1	2497	U
1	1	2498	U
1	1	2499	U
1	1	2501	U
1	1	2503	G
1	1	2505	U
1	1	2509	U
1	1	2510	U
1	1	2511	A
1	1	2512	C
1	1	2514	U
1	1	2522	G
1	1	2523	A

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Mol	Chain	Res	Type
1	1	2524	A
1	1	2526	C
1	1	2529	A
1	1	2531	C
1	1	2537	U
1	1	2539	C
1	1	2540	A
1	1	2541	U
1	1	2542	U
1	1	2543	U
1	1	2547	A
1	1	2549	G
1	1	2550	U
1	1	2551	U
1	1	2552	C
1	1	2553	U
1	1	2554	A
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	2571	U
1	1	2572	C
1	1	2573	G
1	1	2585	G
1	1	2586	G
1	1	2593	A
1	1	2595	A
1	1	2596	U
1	1	2602	G
1	1	2606	G
1	1	2614	G
1	1	2626	A
1	1	2628	A
1	1	2629	U
1	1	2635	A
1	1	2636	A
1	1	2637	A

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Mol	Chain	Res	Type
1	1	2638	C
1	1	2639	G
1	1	2641	U
1	1	2642	A
1	1	2651	G
1	1	2652	U
1	1	2653	C
1	1	2656	A
1	1	2657	A
1	1	2665	U
1	1	2672	G
1	1	2674	A
1	1	2676	A
1	1	2677	G
1	1	2681	U
1	1	2688	U
1	1	2689	A
1	1	2691	A
1	1	2696	A
1	1	2702	A
1	1	2704	A
1	1	2705	A
1	1	2713	U
1	1	2716	U
1	1	2719	U
1	1	2728	G
1	1	2729	U
1	1	2740	A
1	1	2742	C
1	1	2749	G
1	1	2752	U
1	1	2753	G
1	1	2755	C
1	1	2760	C
1	1	2761	G
1	1	2762	A
1	1	2767	U
1	1	2771	U
1	1	2772	C
1	1	2773	C
1	1	2774	C
1	1	2777	G

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Mol	Chain	Res	Type
1	1	2778	G
1	1	2780	A
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	2802	A
1	1	2803	A
1	1	2804	A
1	1	2808	A
1	1	2810	C
1	1	2814	G
1	1	2816	G
1	1	2817	A
1	1	2821	C
1	1	2828	G
1	1	2829	U
1	1	2842	U
1	1	2843	U
1	1	2844	C
1	1	2845	A
1	1	2847	A
1	1	2853	A
1	1	2859	U
1	1	2860	U
1	1	2869	U
1	1	2870	C
1	1	2871	G
1	1	2875	U
1	1	2876	C
1	1	2886	U
1	1	2887	A
1	1	2888	U
1	1	2889	C
1	1	2894	C
1	1	2898	G
1	1	2899	C
1	1	2901	G
1	1	2906	C
1	1	2907	G

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Mol	Chain	Res	Type
1	1	2911	A
1	1	2928	C
1	1	2930	A
1	1	2934	A
1	1	2935	U
1	1	2936	A
1	1	2938	G
1	1	2940	A
1	1	2941	A
1	1	2942	C
1	1	2945	G
1	1	2947	G
1	1	2971	A
1	1	2975	U
1	1	2977	G
1	1	2983	C
1	1	2990	G
1	1	2996	U
1	1	2997	G
1	1	3003	G
1	1	3005	A
1	1	3011	A
1	1	3012	A
1	1	3014	U
1	1	3021	A
1	1	3023	U
1	1	3024	A
1	1	3027	A
1	1	3028	G
1	1	3030	G
1	1	3036	G
1	1	3037	U
1	1	3055	U
1	1	3056	U
1	1	3058	U
1	1	3059	G
1	1	3072	C
1	1	3075	G
1	1	3078	U
1	1	3079	U
1	1	3085	G
1	1	3090	U

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Mol	Chain	Res	Type
1	1	3092	C
1	1	3098	G
1	1	3101	G
1	1	3104	U
1	1	3106	A
1	1	3109	G
1	1	3117	C
1	1	3120	C
1	1	3122	A
1	1	3124	G
1	1	3130	A
1	1	3131	U
1	1	3136	G
1	1	3137	C
1	1	3142	A
1	1	3143	C
1	1	3147	G
1	1	3151	U
1	1	3152	U
1	1	3153	U
1	1	3154	C
1	1	3156	U
1	1	3157	U
1	1	3158	G
1	1	3159	C
1	1	3161	C
1	1	3167	A
1	1	3168	A
1	1	3169	U
1	1	3172	A
1	1	3173	G
1	1	3176	G
1	1	3178	A
1	1	3179	U
1	1	3180	A
1	1	3181	C
1	1	3182	G
1	1	3183	A
1	1	3185	U
1	1	3186	A
1	1	3187	A
1	1	3188	G

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Mol	Chain	Res	Type
1	1	3192	U
1	1	3194	C
1	1	3195	U
1	1	3196	U
1	1	3206	C
1	1	3207	U
1	1	3210	A
1	1	3214	U
1	1	3217	C
1	1	3218	A
1	1	3219	G
1	1	3222	U
1	1	3227	A
1	1	3229	G
1	1	3236	U
1	1	3237	U
1	1	3238	G
1	1	3243	A
1	1	3244	A
1	1	3245	A
1	1	3246	G
1	1	3252	G
1	1	3260	G
1	1	3264	G
1	1	3265	C
1	1	3269	U
1	1	3271	G
1	1	3272	C
1	1	3273	A
1	1	3274	A
1	1	3275	U
1	1	3276	G
1	1	3277	U
1	1	3278	C
1	1	3279	A
1	1	3281	U
1	1	3282	U
1	1	3283	U
1	1	3288	G
1	1	3290	G
1	1	3292	A
1	1	3294	A

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Mol	Chain	Res	Type
1	1	3304	U
1	1	3308	C
1	1	3311	C
1	1	3313	U
1	1	3316	A
1	1	3319	U
1	1	3320	A
1	1	3341	U
1	1	3345	G
1	1	3350	C
1	1	3351	U
1	1	3353	G
1	1	3354	U
1	1	3355	U
1	1	3357	U
1	1	3358	U
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	3383	G
1	1	3389	U
1	1	3390	G
1	1	3396	U
2	3	7	G
2	3	10	C
2	3	11	A
2	3	14	U
2	3	21	G
2	3	29	C
2	3	31	U
2	3	33	U
2	3	40	C
2	3	41	G
2	3	46	A
2	3	49	G
2	3	50	U
2	3	54	U
2	3	56	A

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Mol	Chain	Res	Type
2	3	64	A
2	3	65	G
2	3	73	C
2	3	74	C
2	3	75	G
2	3	76	A
2	3	87	G
2	3	92	A
2	3	99	G
2	3	111	U
2	3	112	G
2	3	119	U
2	3	120	C
2	3	121	U
3	4	23	U
3	4	24	G
3	4	34	U
3	4	35	C
3	4	37	A
3	4	38	U
3	4	39	G
3	4	40	A
3	4	41	A
3	4	48	A
3	4	49	G
3	4	50	C
3	4	53	A
3	4	59	A
3	4	62	C
3	4	63	G
3	4	70	G
3	4	72	A
3	4	75	G
3	4	78	G
3	4	79	A
3	4	80	A
3	4	81	U
3	4	82	U
3	4	83	C
3	4	84	C
3	4	85	G
3	4	86	U

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Mol	Chain	Res	Type
3	4	87	G
3	4	95	G
3	4	97	A
3	4	102	U
3	4	104	A
3	4	106	C
3	4	113	U
3	4	114	G
3	4	124	G
3	4	125	U
3	4	126	A
3	4	128	U
3	4	129	C
3	4	131	A
3	4	132	G
3	4	140	G
3	4	144	G
3	4	148	G
3	4	151	C
3	4	153	U
3	4	154	C
47	2	2	A
47	2	3	U
47	2	4	C
47	2	5	U
47	2	8	U
47	2	11	A
47	2	17	C
47	2	20	G
47	2	25	C
47	2	26	A
47	2	34	G
47	2	36	C
47	2	39	A
47	2	40	A
47	2	43	A
47	2	45	U
47	2	46	A
47	2	47	A
47	2	53	G
47	2	60	U
47	2	61	A

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Mol	Chain	Res	Type
47	2	62	A
47	2	63	G
47	2	65	A
47	2	67	A
47	2	68	A
47	2	71	A
47	2	72	A
47	2	73	U
47	2	75	U
47	2	77	U
47	2	78	A
47	2	79	C
47	2	81	G
47	2	82	U
47	2	94	U
47	2	100	A
47	2	103	A
47	2	104	A
47	2	111	U
47	2	114	C
47	2	115	G
47	2	116	U
47	2	126	A
47	2	127	G
47	2	128	U
47	2	131	C
47	2	132	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	143	G
47	2	144	U
47	2	145	A
47	2	147	A
47	2	152	U
47	2	158	U
47	2	161	U
47	2	168	A
47	2	174	U

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Mol	Chain	Res	Type
47	2	178	U
47	2	180	A
47	2	186	C
47	2	188	A
47	2	190	C
47	2	191	C
47	2	193	U
47	2	195	G
47	2	196	G
47	2	197	A
47	2	200	A
47	2	203	U
47	2	204	G
47	2	215	A
47	2	217	A
47	2	218	A
47	2	219	A
47	2	232	U
47	2	233	C
47	2	235	G
47	2	238	U
47	2	240	U
47	2	242	U
47	2	243	G
47	2	246	G
47	2	249	U
47	2	250	C
47	2	258	C
47	2	260	U
47	2	261	U
47	2	262	U
47	2	265	A
47	2	266	A
47	2	267	U
47	2	272	U
47	2	273	G
47	2	274	G
47	2	275	C
47	2	276	C
47	2	278	U
47	2	279	G
47	2	280	U

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Mol	Chain	Res	Type
47	2	285	G
47	2	288	A
47	2	291	G
47	2	299	A
47	2	308	C
47	2	313	U
47	2	314	C
47	2	315	A
47	2	316	A
47	2	320	U
47	2	321	C
47	2	322	G
47	2	333	A
47	2	337	G
47	2	338	C
47	2	343	C
47	2	351	C
47	2	352	A
47	2	359	A
47	2	361	C
47	2	372	G
47	2	373	G
47	2	377	G
47	2	378	A
47	2	379	U
47	2	381	C
47	2	390	G
47	2	391	A
47	2	392	G
47	2	397	A
47	2	400	A
47	2	402	C
47	2	404	G
47	2	413	U
47	2	416	A
47	2	417	A
47	2	419	G
47	2	424	C
47	2	426	G
47	2	433	C
47	2	434	G
47	2	439	U

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Mol	Chain	Res	Type
47	2	444	C
47	2	445	A
47	2	448	C
47	2	455	C
47	2	456	A
47	2	457	G
47	2	460	A
47	2	461	G
47	2	463	U
47	2	464	A
47	2	471	A
47	2	475	A
47	2	477	A
47	2	481	A
47	2	485	A
47	2	486	G
47	2	489	C
47	2	491	C
47	2	493	U
47	2	495	C
47	2	496	G
47	2	500	C
47	2	505	A
47	2	506	A
47	2	507	U
47	2	509	G
47	2	513	U
47	2	515	A
47	2	518	A
47	2	519	C
47	2	525	A
47	2	526	A
47	2	534	A
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

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Mol	Chain	Res	Type
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	568	G
47	2	572	C
47	2	577	G
47	2	578	U
47	2	579	A
47	2	580	A
47	2	585	A
47	2	586	G
47	2	591	A
47	2	593	U
47	2	594	A
47	2	606	A
47	2	608	U
47	2	611	U
47	2	612	U
47	2	614	C
47	2	619	A
47	2	620	A
47	2	621	A
47	2	622	A
47	2	623	A
47	2	624	G
47	2	625	C
47	2	639	U
47	2	652	G
47	2	654	C
47	2	655	G
47	2	656	G
47	2	657	U
47	2	658	C
47	2	679	U
47	2	681	U
47	2	687	G
47	2	693	U

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Mol	Chain	Res	Type
47	2	694	U
47	2	695	U
47	2	696	C
47	2	697	C
47	2	698	U
47	2	702	G
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	718	U
47	2	719	U
47	2	720	G
47	2	721	U
47	2	722	G
47	2	723	G
47	2	728	U
47	2	729	G
47	2	731	C
47	2	732	G
47	2	733	A
47	2	735	C
47	2	736	C
47	2	741	C
47	2	743	U
47	2	752	A
47	2	753	A
47	2	758	U
47	2	761	G
47	2	762	A
47	2	765	G
47	2	766	U
47	2	771	A
47	2	775	G
47	2	777	C
47	2	778	G
47	2	779	U

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Mol	Chain	Res	Type
47	2	780	A
47	2	781	U
47	2	782	U
47	2	783	G
47	2	784	C
47	2	787	G
47	2	792	U
47	2	793	A
47	2	804	A
47	2	807	A
47	2	810	G
47	2	811	A
47	2	812	A
47	2	814	A
47	2	815	G
47	2	816	G
47	2	819	G
47	2	820	U
47	2	821	U
47	2	823	G
47	2	830	U
47	2	831	U
47	2	833	U
47	2	834	G
47	2	837	G
47	2	838	G
47	2	843	U
47	2	845	G
47	2	846	G
47	2	847	A
47	2	850	A
47	2	852	C
47	2	855	A
47	2	859	A
47	2	860	U
47	2	863	A
47	2	873	U
47	2	875	G
47	2	885	G
47	2	886	U
47	2	895	G
47	2	898	A

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Mol	Chain	Res	Type
47	2	899	G
47	2	903	U
47	2	909	U
47	2	910	C
47	2	913	G
47	2	914	G
47	2	915	A
47	2	916	U
47	2	921	U
47	2	922	G
47	2	923	A
47	2	928	U
47	2	929	A
47	2	933	A
47	2	935	U
47	2	940	A
47	2	941	A
47	2	942	G
47	2	944	A
47	2	946	U
47	2	951	A
47	2	957	G
47	2	960	U
47	2	963	A
47	2	966	A
47	2	970	A
47	2	971	A
47	2	973	A
47	2	983	A
47	2	988	A
47	2	992	A
47	2	993	A
47	2	995	A
47	2	998	A
47	2	1001	A
47	2	1004	U
47	2	1021	C
47	2	1024	U
47	2	1026	A
47	2	1027	A
47	2	1028	C
47	2	1029	U

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Mol	Chain	Res	Type
47	2	1030	A
47	2	1031	U
47	2	1032	G
47	2	1039	A
47	2	1051	G
47	2	1052	U
47	2	1053	G
47	2	1063	U
47	2	1076	A
47	2	1082	C
47	2	1083	G
47	2	1089	U
47	2	1092	A
47	2	1093	A
47	2	1094	G
47	2	1097	U
47	2	1098	U
47	2	1100	G
47	2	1108	G
47	2	1113	A
47	2	1124	A
47	2	1126	G
47	2	1131	A
47	2	1137	A
47	2	1138	A
47	2	1139	A
47	2	1140	G
47	2	1143	A
47	2	1146	G
47	2	1147	A
47	2	1150	G
47	2	1151	A
47	2	1155	G
47	2	1157	A
47	2	1158	C
47	2	1159	C
47	2	1160	A
47	2	1161	C
47	2	1162	C
47	2	1163	A
47	2	1166	A
47	2	1170	G

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Mol	Chain	Res	Type
47	2	1177	C
47	2	1180	C
47	2	1183	A
47	2	1184	A
47	2	1185	U
47	2	1186	U
47	2	1188	G
47	2	1189	A
47	2	1190	C
47	2	1191	U
47	2	1192	C
47	2	1193	A
47	2	1194	A
47	2	1196	A
47	2	1198	G
47	2	1199	G
47	2	1200	G
47	2	1201	G
47	2	1202	A
47	2	1204	A
47	2	1205	C
47	2	1206	U
47	2	1207	C
47	2	1208	A
47	2	1210	C
47	2	1212	G
47	2	1213	G
47	2	1214	U
47	2	1217	A
47	2	1219	A
47	2	1222	C
47	2	1224	A
47	2	1225	U
47	2	1226	A
47	2	1227	A
47	2	1228	G
47	2	1229	G
47	2	1230	A
47	2	1231	U
47	2	1232	U
47	2	1233	G
47	2	1236	A

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Mol	Chain	Res	Type
47	2	1237	G
47	2	1238	A
47	2	1239	U
47	2	1240	U
47	2	1241	G
47	2	1242	A
47	2	1244	A
47	2	1245	G
47	2	1246	C
47	2	1247	U
47	2	1248	C
47	2	1250	U
47	2	1252	C
47	2	1255	G
47	2	1256	A
47	2	1257	U
47	2	1258	U
47	2	1259	U
47	2	1264	G
47	2	1266	U
47	2	1268	G
47	2	1269	U
47	2	1270	G
47	2	1272	U
47	2	1273	G
47	2	1274	C
47	2	1275	A
47	2	1277	G
47	2	1284	C
47	2	1286	U
47	2	1287	A
47	2	1288	G
47	2	1293	U
47	2	1298	U
47	2	1301	U
47	2	1302	U
47	2	1306	C
47	2	1308	G
47	2	1309	C
47	2	1310	U
47	2	1312	A
47	2	1314	U

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Mol	Chain	Res	Type
47	2	1315	U
47	2	1319	A
47	2	1321	A
47	2	1324	G
47	2	1325	A
47	2	1332	C
47	2	1335	U
47	2	1336	A
47	2	1337	A
47	2	1338	C
47	2	1339	C
47	2	1340	U
47	2	1341	A
47	2	1344	A
47	2	1345	A
47	2	1346	A
47	2	1347	U
47	2	1348	A
47	2	1353	U
47	2	1354	G
47	2	1355	C
47	2	1357	A
47	2	1360	A
47	2	1361	U
47	2	1362	U
47	2	1363	U
47	2	1364	G
47	2	1365	C
47	2	1369	U
47	2	1370	U
47	2	1371	A
47	2	1375	A
47	2	1376	C
47	2	1378	U
47	2	1380	U
47	2	1381	U
47	2	1382	A
47	2	1383	G
47	2	1384	A
47	2	1385	G
47	2	1386	G
47	2	1387	G

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Mol	Chain	Res	Type
47	2	1388	A
47	2	1390	U
47	2	1391	A
47	2	1392	U
47	2	1393	C
47	2	1394	G
47	2	1399	C
47	2	1400	A
47	2	1402	G
47	2	1405	G
47	2	1406	A
47	2	1409	G
47	2	1412	G
47	2	1413	U
47	2	1415	U
47	2	1416	G
47	2	1420	C
47	2	1421	A
47	2	1422	A
47	2	1425	A
47	2	1427	A
47	2	1428	G
47	2	1429	G
47	2	1431	C
47	2	1432	U
47	2	1433	G
47	2	1434	U
47	2	1435	G
47	2	1436	A
47	2	1437	U
47	2	1439	C
47	2	1440	C
47	2	1441	C
47	2	1442	U
47	2	1443	U
47	2	1444	A
47	2	1445	G
47	2	1446	A
47	2	1448	G
47	2	1450	U
47	2	1453	G
47	2	1458	G

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Mol	Chain	Res	Type
47	2	1459	C
47	2	1460	A
47	2	1469	A
47	2	1472	C
47	2	1474	G
47	2	1479	A
47	2	1486	G
47	2	1490	C
47	2	1491	U
47	2	1492	A
47	2	1493	A
47	2	1494	C
47	2	1496	U
47	2	1500	C
47	2	1506	G
47	2	1510	U
47	2	1515	A
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	1529	C
47	2	1530	C
47	2	1533	C
47	2	1534	G
47	2	1536	G
47	2	1537	C
47	2	1538	U
47	2	1542	G
47	2	1550	A
47	2	1555	A
47	2	1556	A
47	2	1557	U
47	2	1559	A
47	2	1560	U
47	2	1561	U
47	2	1572	G
47	2	1573	A

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Mol	Chain	Res	Type
47	2	1575	G
47	2	1576	A
47	2	1582	U
47	2	1585	U
47	2	1589	C
47	2	1592	A
47	2	1593	A
47	2	1596	C
47	2	1597	A
47	2	1600	A
47	2	1601	G
47	2	1609	U
47	2	1610	G
47	2	1613	U
47	2	1614	A
47	2	1615	C
47	2	1616	G
47	2	1618	C
47	2	1619	C
47	2	1622	G
47	2	1624	C
47	2	1631	A
47	2	1632	C
47	2	1633	A
47	2	1636	C
47	2	1639	C
47	2	1646	C
47	2	1649	G
47	2	1650	U
47	2	1655	A
47	2	1657	U
47	2	1658	G
47	2	1661	U
47	2	1669	U
47	2	1677	C
47	2	1678	A
47	2	1681	A
47	2	1682	U
47	2	1684	U
47	2	1685	G
47	2	1690	G
47	2	1692	G

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Mol	Chain	Res	Type
47	2	1693	A
47	2	1696	G
47	2	1699	G
47	2	1700	C
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	1711	C
47	2	1712	A
47	2	1714	A
47	2	1715	G
47	2	1716	C
47	2	1717	G
47	2	1718	G
47	2	1721	A
47	2	1723	U
47	2	1736	G
47	2	1737	G
47	2	1739	C
47	2	1749	A
47	2	1754	A
47	2	1755	A
47	2	1756	A
47	2	1760	G
47	2	1762	A
47	2	1766	A
47	2	1769	U
47	2	1770	U
47	2	1772	C
47	2	1780	G
47	2	1783	C
47	2	1786	G
47	2	1791	A
47	2	1792	G
47	2	1793	G
47	2	1794	A
47	2	1796	C

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Mol	Chain	Res	Type
47	2	1797	A
47	2	1798	U
81	AX	4	G
81	AX	8	U
81	AX	9	A
81	AX	10	G
81	AX	14	A
81	AX	15	G
81	AX	16	U
81	AX	17	U
81	AX	19	G
81	AX	20	G
81	AX	21	A
81	AX	26	G
81	AX	37	G
81	AX	38	A
81	AX	45	G
81	AX	46	G
81	AX	47	U
81	AX	48	C
81	AX	49	C
81	AX	52	U
81	AX	53	G
81	AX	55	U
81	AX	59	U
81	AX	62	A
81	AX	66	A
81	AX	68	U
81	AX	73	A
81	AX	74	C
81	AX	76	A
82	AY	47	U
82	AY	48	U
82	AY	49	U

All (47) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	13	A
1	1	116	A
1	1	218	G
1	1	315	C

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Mol	Chain	Res	Type
1	1	317	A
1	1	424	G
1	1	438	A
1	1	1028	U
1	1	1196	C
1	1	1405	U
1	1	1912	U
1	1	2101	C
1	1	2270	A
1	1	2306	C
1	1	2828	G
1	1	2893	C
1	1	2939	G
1	1	3004	C
1	1	3027	A
1	1	3078	U
1	1	3121	U
1	1	3168	A
1	1	3228	C
1	1	3352	U
47	2	1	U
47	2	25	C
47	2	67	A
47	2	342	C
47	2	505	A
47	2	590	C
47	2	611	U
47	2	779	U
47	2	1107	G
47	2	1160	A
47	2	1162	C
47	2	1207	C
47	2	1338	C
47	2	1368	G
47	2	1379	C
47	2	1390	U
47	2	1428	G
47	2	1491	U
47	2	1522	U
47	2	1632	C
47	2	1654	G
47	2	1771	U

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Mol	Chain	Res	Type
82	AY	48	U

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
84	DDE	AZ	699	84	14,20,21	1.98	3 (21%)	14,28,30	3.40	7 (50%)

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
84	DDE	AZ	699	84	-	5/20/21/23	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	AZ	699	DDE	CBI-NAD	5.91	1.47	1.32
84	AZ	699	DDE	CAT-CE1	2.61	1.54	1.50
84	AZ	699	DDE	OAG-CBI	-2.59	1.18	1.23

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	AZ	699	DDE	CBW-CBI-NAD	9.82	127.80	115.28
84	AZ	699	DDE	OAG-CBI-NAD	-4.30	115.52	123.00
84	AZ	699	DDE	CAC-NCB-CAB	3.36	117.28	108.10
84	AZ	699	DDE	OAG-CBI-CBW	-3.02	116.67	120.49
84	AZ	699	DDE	CAU-CBW-CBI	-2.89	105.48	111.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	AZ	699	DDE	CAA-NCB-CAB	-2.81	100.41	108.10
84	AZ	699	DDE	CG-ND1-CE1	2.09	109.22	103.05

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
84	AZ	699	DDE	CA-CB-CG-ND1
84	AZ	699	DDE	CA-CB-CG-CD2
84	AZ	699	DDE	CAT-CAU-CBW-CBI
84	AZ	699	DDE	CAT-CAU-CBW-NCB
84	AZ	699	DDE	CE1-CAT-CAU-CBW

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 11 ligands modelled in this entry, 8 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
87	GDP	AZ	902	-	24,30,30	3.60	12 (50%)	30,47,47	1.62	6 (20%)
86	SO1	AZ	901	-	35,39,39	0.15	0	39,64,64	0.82	2 (5%)
88	ALF	AZ	903	-	0,4,4	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	GDP	AZ	902	-	-	0/12/32/32	0/3/3/3
86	SO1	AZ	901	-	-	16/21/104/104	0/7/5/5

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	AZ	902	GDP	C3'-C4'	-7.83	1.33	1.53
87	AZ	902	GDP	O4'-C4'	6.95	1.60	1.45
87	AZ	902	GDP	O4'-C1'	-6.23	1.32	1.41
87	AZ	902	GDP	C2-N2	5.69	1.47	1.34
87	AZ	902	GDP	C2-N3	5.42	1.46	1.33
87	AZ	902	GDP	C4-N3	5.26	1.50	1.37
87	AZ	902	GDP	C6-N1	4.54	1.44	1.37
87	AZ	902	GDP	C5-C6	3.76	1.55	1.47
87	AZ	902	GDP	C2-N1	2.91	1.44	1.37
87	AZ	902	GDP	C5-C4	-2.86	1.35	1.43
87	AZ	902	GDP	O2'-C2'	-2.55	1.37	1.43
87	AZ	902	GDP	PA-O5'	2.37	1.68	1.59

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	AZ	902	GDP	PA-O3A-PB	-4.83	116.24	132.83
86	AZ	901	SO1	C18-C9-C16	-3.92	98.02	103.64
87	AZ	902	GDP	C5-C6-N1	3.31	119.81	113.95
87	AZ	902	GDP	C8-N7-C5	2.96	108.63	102.99
87	AZ	902	GDP	C2-N1-C6	-2.75	120.03	125.10
87	AZ	902	GDP	C3'-C2'-C1'	2.24	104.35	100.98
86	AZ	901	SO1	C7-C2-C6	2.24	116.42	112.17
87	AZ	902	GDP	N1-C2-N3	-2.17	119.26	123.32

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
86	AZ	901	SO1	C4-C1-C5-O14
86	AZ	901	SO1	C2-C1-C5-O14
86	AZ	901	SO1	C2-C1-C5-O15
86	AZ	901	SO1	O19-C11-C3-C1

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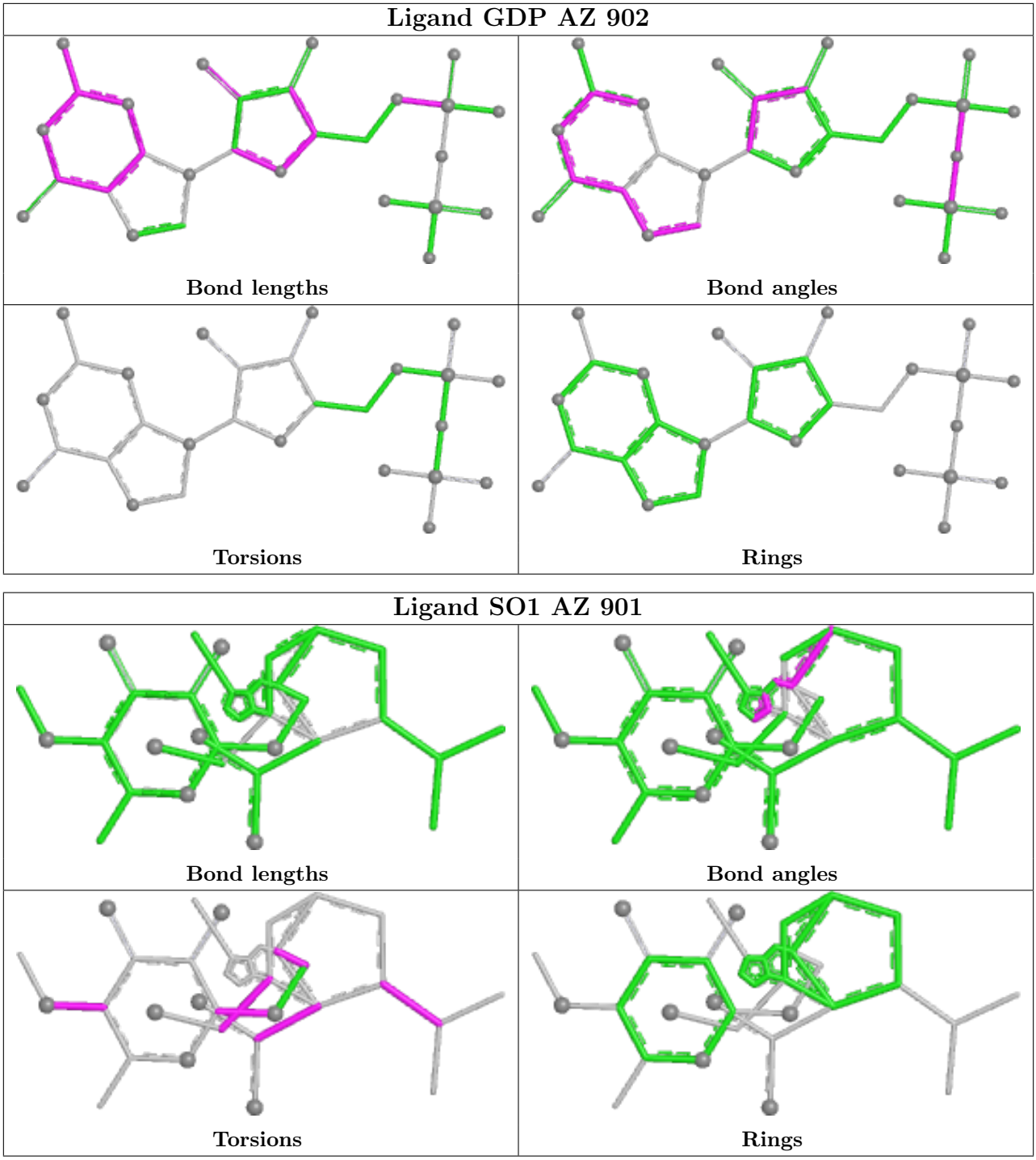
Mol	Chain	Res	Type	Atoms
86	AZ	901	SO1	C56-C55-O64-C65
86	AZ	901	SO1	O56-C52-O17-C8
86	AZ	901	SO1	C21-C13-C4-C12
86	AZ	901	SO1	C20-C13-C4-C12
86	AZ	901	SO1	C1-C2-C8-O17
86	AZ	901	SO1	C7-C2-C8-O17
86	AZ	901	SO1	C20-C13-C4-C1
86	AZ	901	SO1	C21-C13-C4-C1
86	AZ	901	SO1	O19-C11-C3-C10
86	AZ	901	SO1	C54-C55-O64-C65
86	AZ	901	SO1	C4-C1-C5-O15
86	AZ	901	SO1	C6-C2-C8-O17

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.



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.

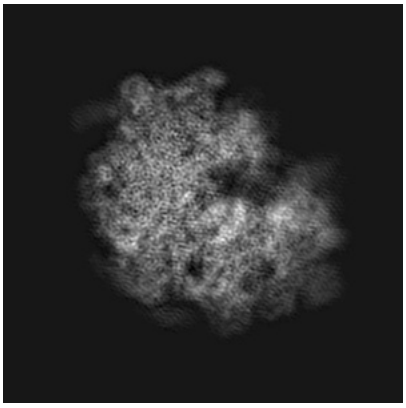
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-0048. These allow visual inspection of the internal detail of the map and identification of artifacts.

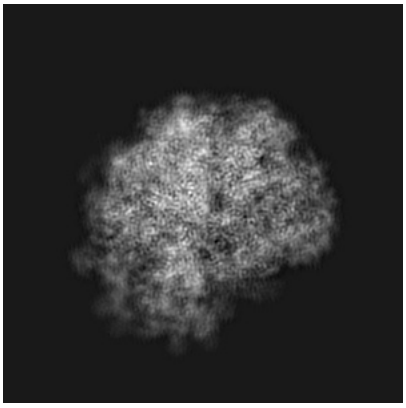
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

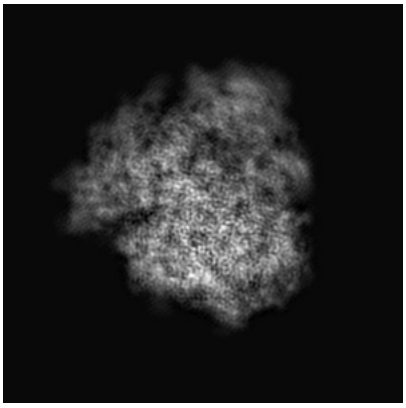
6.1.1 Primary map



X



Y

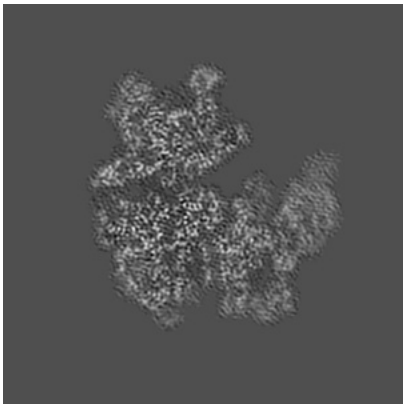


Z

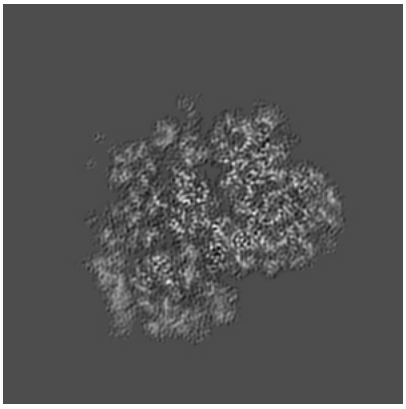
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

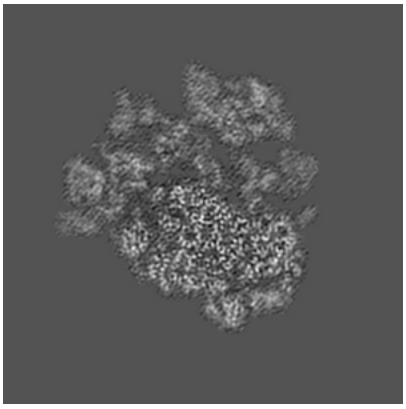
6.2.1 Primary map



X Index: 180



Y Index: 180

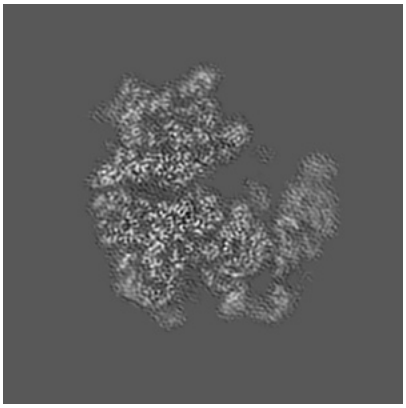


Z Index: 180

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

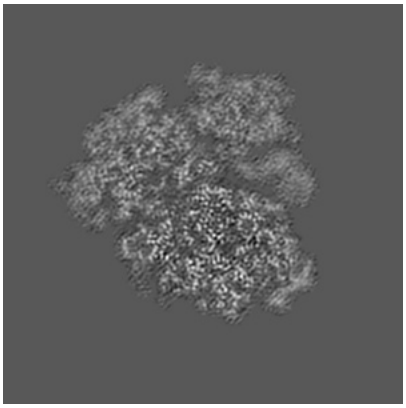
6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 184

Y Index: 157

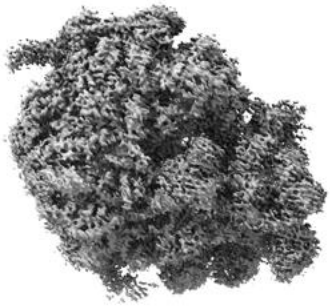


Z Index: 166

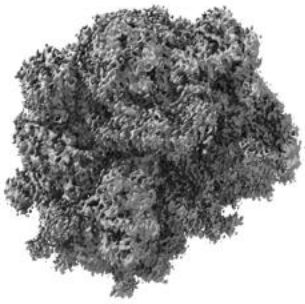
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

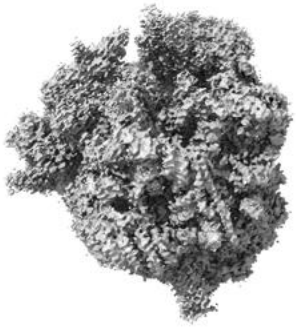
6.4.1 Primary map



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.

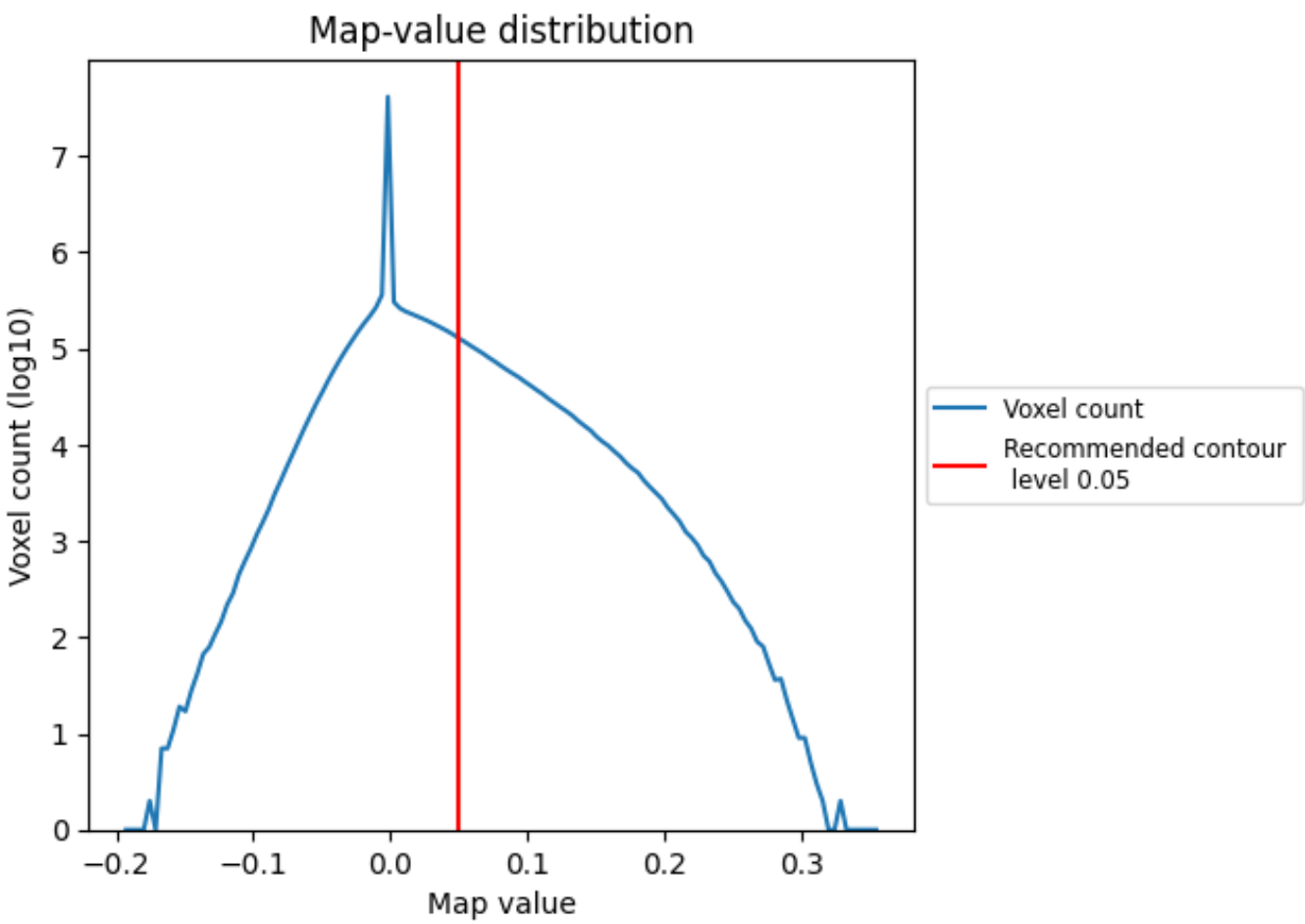
6.5 Mask visualisation (i)

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

7 Map analysis (i)

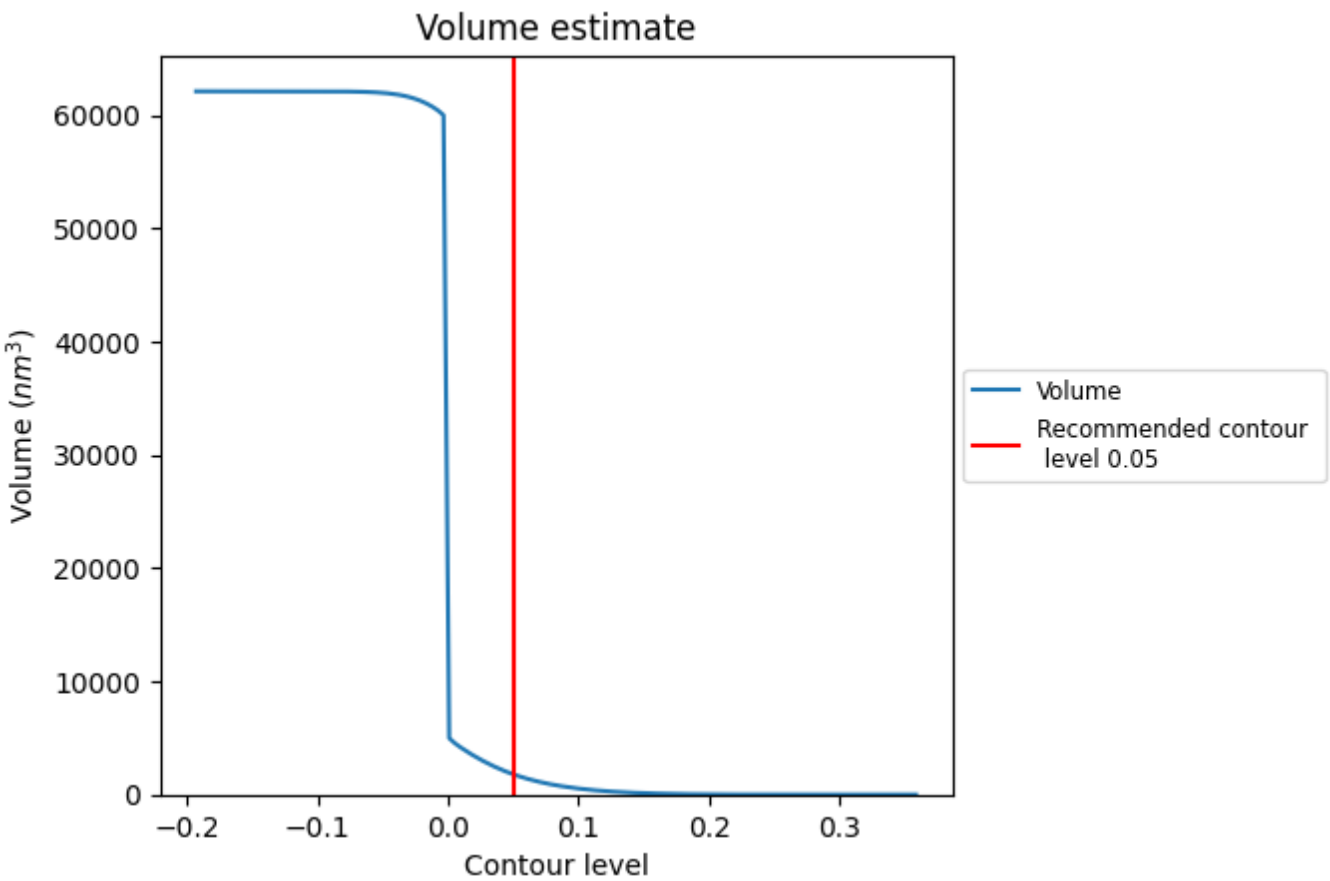
This section contains the results of statistical analysis of the map.

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.

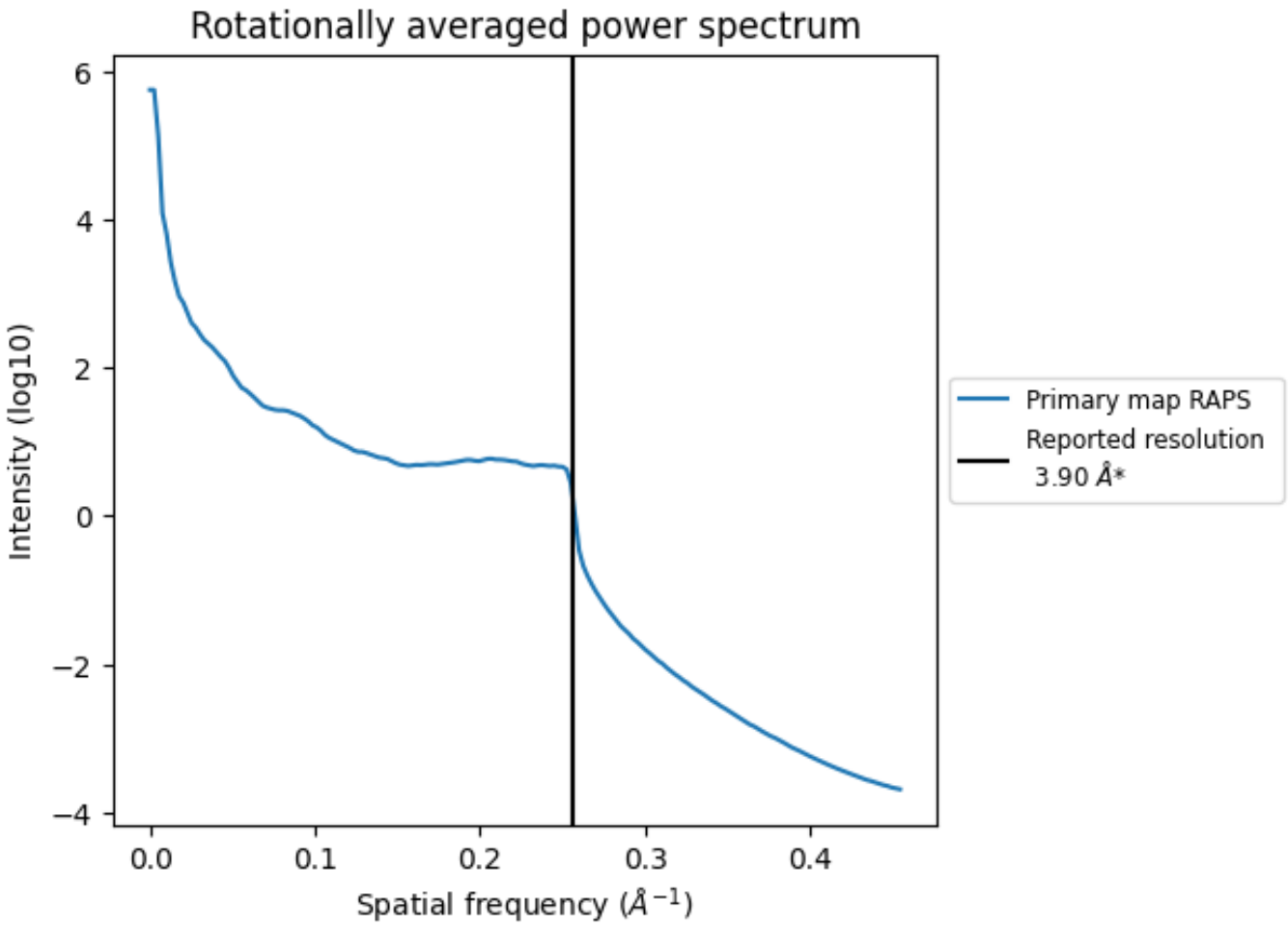
7.2 Volume estimate (i)



The volume at the recommended contour level is 1789 nm^3; this corresponds to an approximate mass of 1616 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 0.256 Å^{-1}

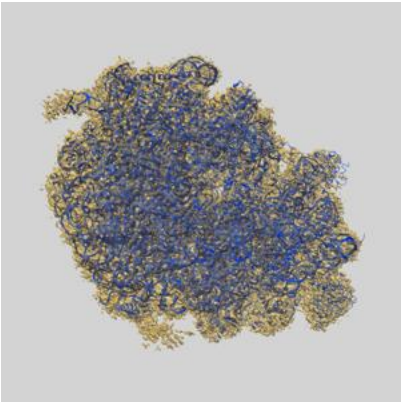
8 Fourier-Shell correlation (i)

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

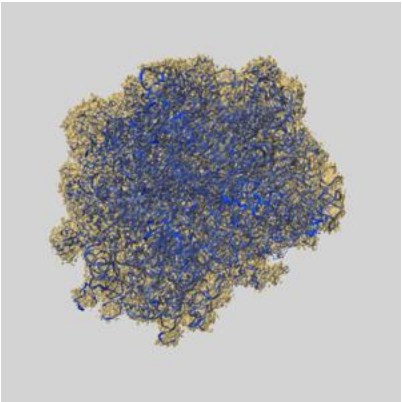
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-0048 and PDB model 6GQB. Per-residue inclusion information can be found in section 3 on page 22.

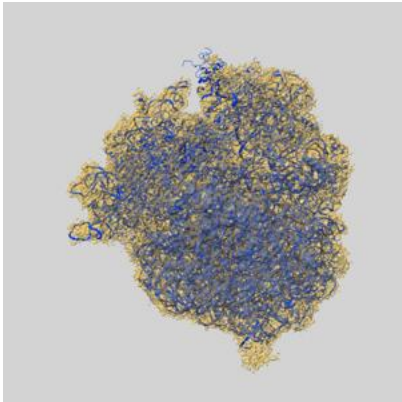
9.1 Map-model overlay (i)



X



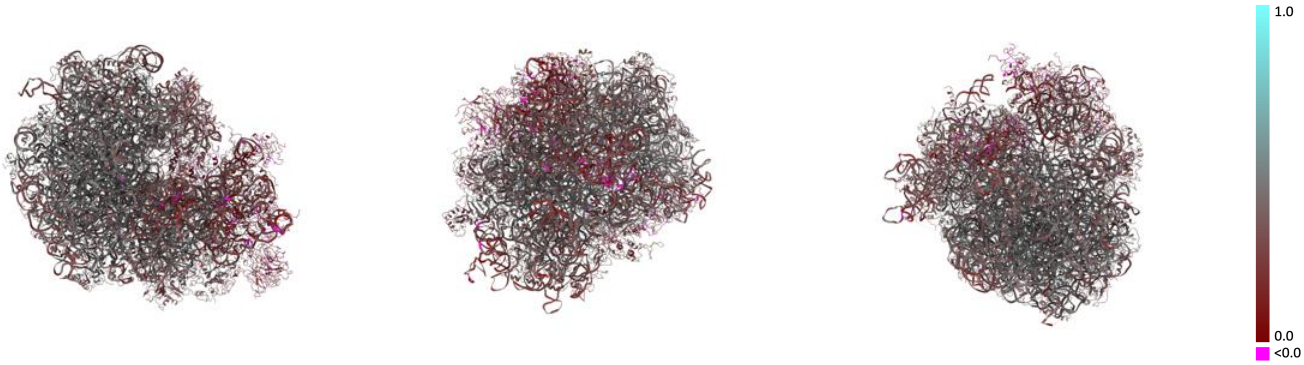
Y



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.

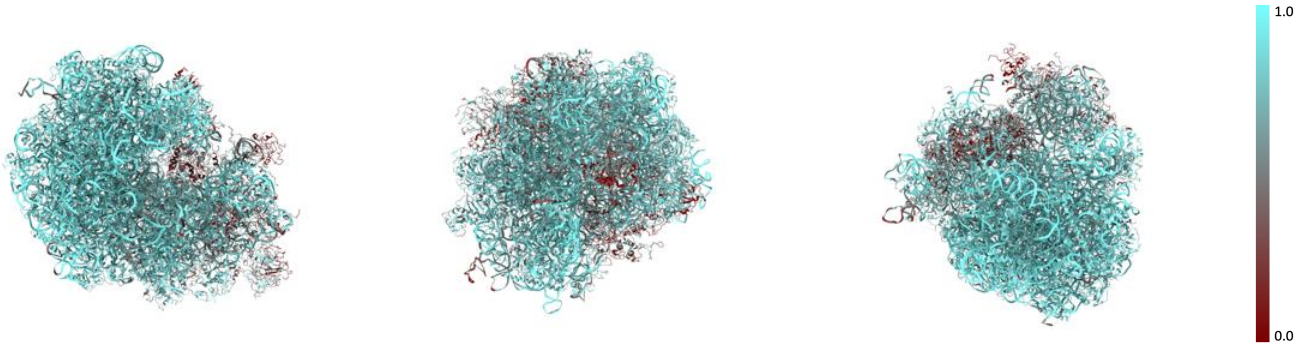
9.2 Q-score mapped to coordinate model (i)



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.

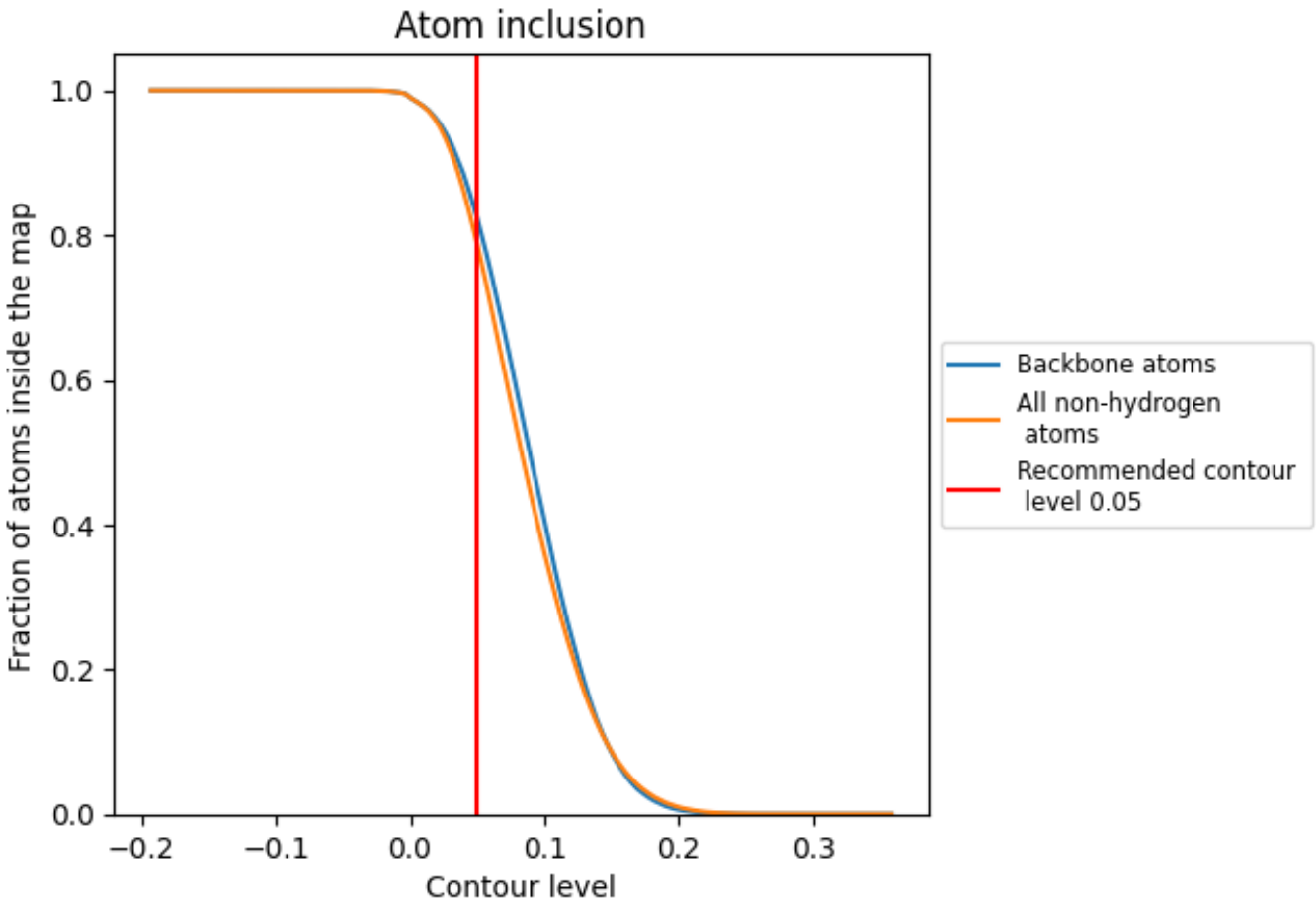
9.3 Atom inclusion mapped to coordinate model (i)



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, 82% of all backbone atoms, 79% 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	0.7871	0.3860
1	0.9088	0.4170
2	0.8326	0.3500
3	0.9372	0.4000
4	0.9275	0.4290
A	0.7648	0.4780
AA	0.6332	0.2540
AB	0.6341	0.4200
AC	0.0932	0.1320
AD	0.7524	0.4160
AE	0.7796	0.4120
AF	0.6207	0.2940
AG	0.5357	0.2490
AH	0.5533	0.2950
AI	0.6005	0.3030
AJ	0.5828	0.2620
AK	0.4631	0.2710
AL	0.7274	0.3860
AM	0.7315	0.4320
AN	0.6856	0.4300
AO	0.7233	0.3440
AP	0.3309	0.1820
AQ	0.7095	0.4060
AR	0.7342	0.3640
AS	0.3732	0.2350
AT	0.6792	0.3240
AU	0.6187	0.3780
AV	0.4669	0.2250
AW	0.3607	0.1930
AX	0.7153	0.2840
AY	0.4167	0.3360
AZ	0.3199	0.2650
B	0.8007	0.4530
BA	0.4440	0.2740
C	0.8246	0.4530

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Chain	Atom inclusion	Q-score
D	0.7686	0.3740
E	0.8219	0.4200
F	0.7997	0.4400
G	0.8030	0.4100
H	0.7638	0.4180
I	0.7730	0.4390
J	0.7186	0.3720
L	0.8319	0.4450
M	0.8129	0.4070
N	0.8332	0.4670
O	0.7853	0.4410
P	0.8045	0.4670
P0	0.1988	0.2200
P2	0.2059	0.2190
Q	0.8258	0.4670
R	0.7697	0.4340
S	0.7789	0.4420
T	0.7960	0.4520
U	0.7852	0.4150
V	0.6925	0.4590
W	0.7344	0.4460
X	0.7834	0.4410
Y	0.8447	0.4590
Z	0.8179	0.4320
a	0.8327	0.4580
b	0.7588	0.4310
c	0.8030	0.4260
d	0.7643	0.4500
e	0.7918	0.4720
f	0.8210	0.4850
g	0.7814	0.4600
h	0.8197	0.4320
i	0.7866	0.4100
j	0.8765	0.5050
k	0.7145	0.4030
l	0.8096	0.4560
m	0.7698	0.4340
n	0.6604	0.4620
o	0.7563	0.4480
p	0.7627	0.4760
q	0.6973	0.3590
r	0.7242	0.3790

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Chain	Atom inclusion	Q-score
s	0.6940	0.3960
t	0.5009	0.2560
u	0.7080	0.3760
v	0.4449	0.2560
w	0.6622	0.3180
x	0.7218	0.3530
y	0.7208	0.3890
z	0.7413	0.3760